



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:39 PM UTC

PDB ID : 6VP8 / pdb_00006vp8
EMDB ID : EMD-21250
Title : Cryo-EM structure of the C-terminal half of the Parkinson's Disease-linked protein Leucine Rich Repeat Kinase 2 (LRRK2)
Authors : Leschziner, A.; Deniston, C.; Lahiri, I.
Deposited on : 2020-02-01
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

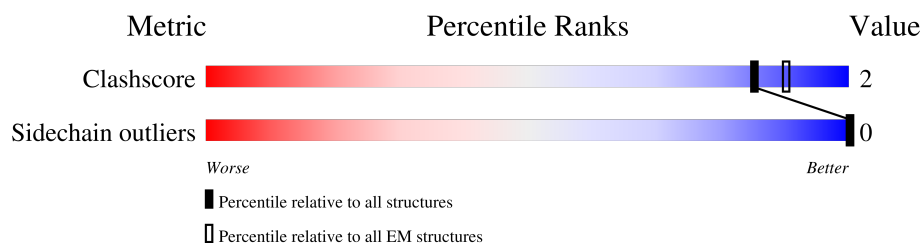
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	229148	23984
Sidechain outliers	223484	23102

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	1198	58% 81% 9% • 10%
2	B	281	59% 86% 8% 6%
3	C	359	49% 83% 6% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13158 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	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	265	Total	C	N	O	S	0	0
			2147	1387	360	386	14		

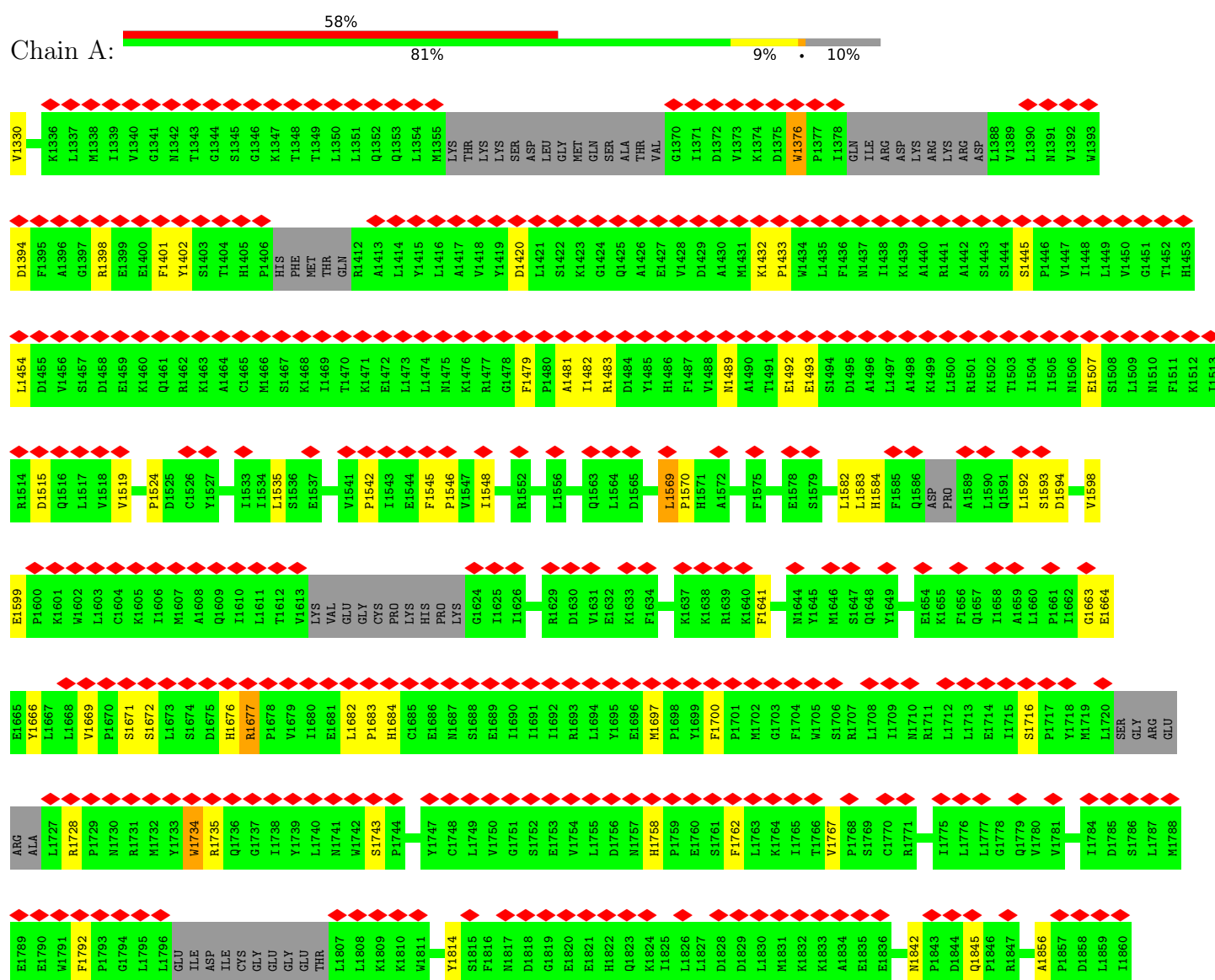
- Molecule 3 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

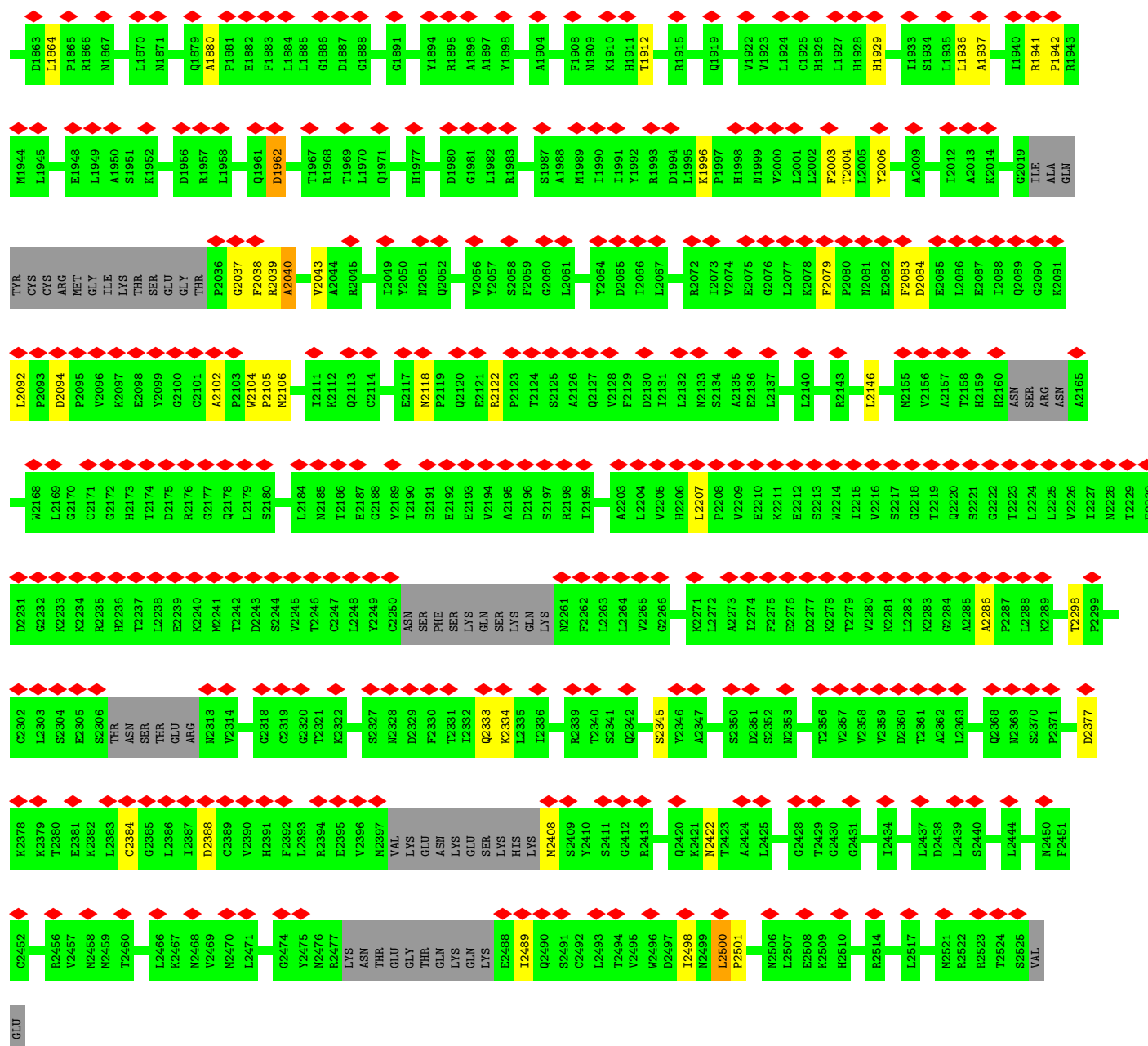
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	319	Total	C	N	O	S	0	0
			2480	1580	420	459	21		

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

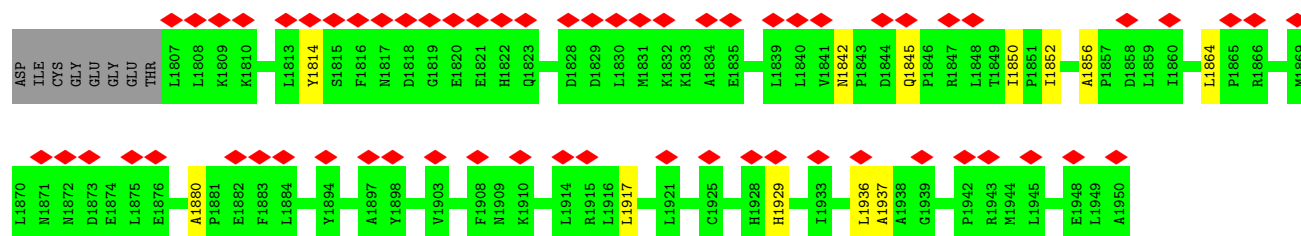




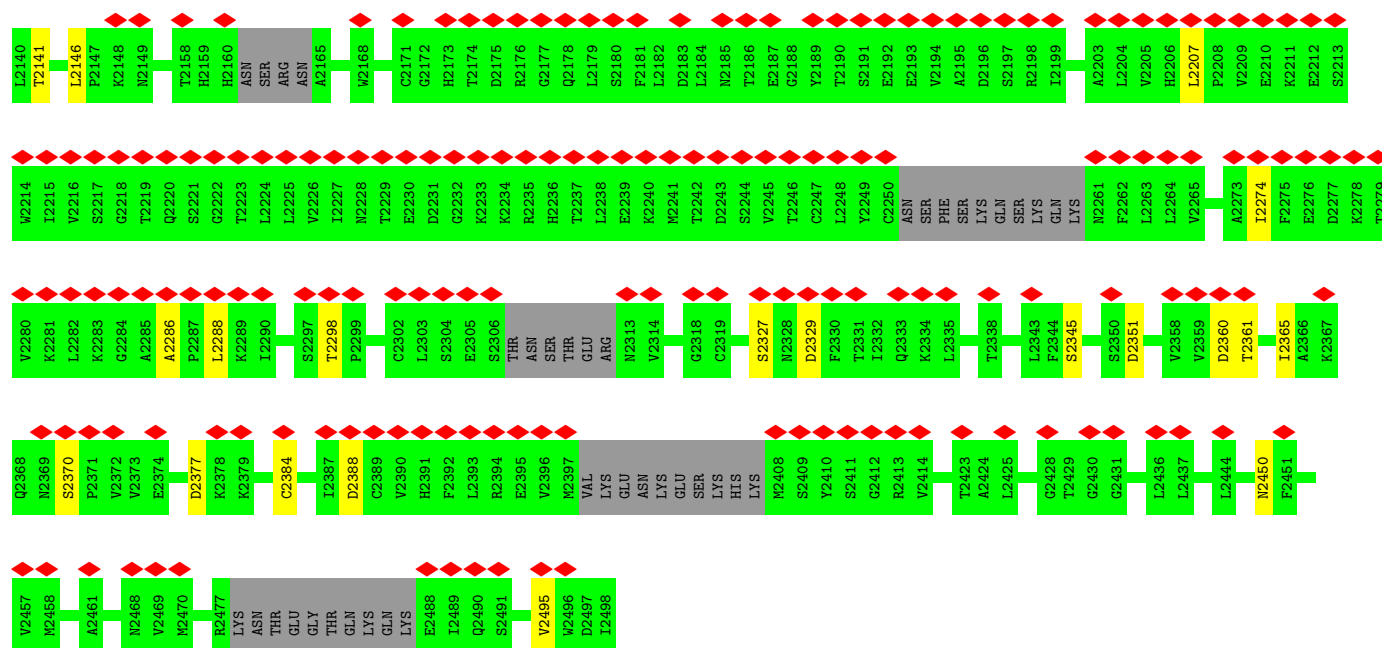
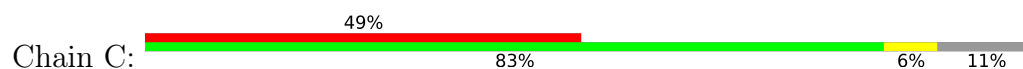
• Molecule 2: Leucine-rich repeat serine/threonine-protein kinase 2

Chain B:





• Molecule 3: Leucine-rich repeat serine/threonine-protein kinase 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	70953	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Per-particle CTF values	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	6.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0267	Depositor
Map size (Å)	380.92, 380.92, 380.92	wwPDB
Map dimensions	356, 356, 356	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: TPO

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	0.84	1/8682 (0.0%)	1.16	96/11746 (0.8%)
2	B	0.70	0/2200	1.24	35/2983 (1.2%)
3	C	0.71	0/2515	1.08	15/3397 (0.4%)
All	All	0.80	1/13397 (0.0%)	1.16	146/18126 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2040	ALA	C-N	9.10	1.45	1.33

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1728	ARG	CA-C-N	9.45	129.28	120.21
2	B	1728	ARG	C-N-CA	9.45	129.28	120.21
2	B	1677	ARG	CA-C-N	8.91	128.99	119.90
2	B	1677	ARG	C-N-CA	8.91	128.99	119.90
1	A	2079	PHE	CA-C-N	8.73	128.47	119.56
1	A	2079	PHE	C-N-CA	8.73	128.47	119.56
2	B	1758	HIS	CA-C-N	8.66	128.39	119.56
2	B	1758	HIS	C-N-CA	8.66	128.39	119.56
1	A	2122	ARG	CA-C-N	8.64	128.68	119.78
1	A	2122	ARG	C-N-CA	8.64	128.68	119.78
3	C	2360	ASP	CA-CB-CG	8.50	121.10	112.60
1	A	2298	THR	CA-C-N	8.45	128.38	119.85
1	A	2298	THR	C-N-CA	8.45	128.38	119.85
1	A	1845	GLN	CA-C-N	8.31	129.11	119.47
1	A	1845	GLN	C-N-CA	8.31	129.11	119.47
1	A	1677	ARG	CA-C-N	8.13	128.18	119.89
1	A	1677	ARG	C-N-CA	8.13	128.18	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1845	GLN	CA-C-N	7.94	129.77	119.84
2	B	1845	GLN	C-N-CA	7.94	129.77	119.84
1	A	1880	ALA	CA-C-N	7.94	128.37	119.32
1	A	1880	ALA	C-N-CA	7.94	128.37	119.32
3	C	2298	THR	CA-C-N	7.93	127.86	119.85
3	C	2298	THR	C-N-CA	7.93	127.86	119.85
3	C	2207	LEU	CA-C-N	7.92	127.64	119.56
3	C	2207	LEU	C-N-CA	7.92	127.64	119.56
2	B	1880	ALA	CA-C-N	7.77	128.48	119.47
2	B	1880	ALA	C-N-CA	7.77	128.48	119.47
1	A	1599	GLU	CA-C-N	7.76	128.17	119.32
1	A	1599	GLU	C-N-CA	7.76	128.17	119.32
1	A	2102	ALA	CA-C-N	7.72	127.78	119.90
1	A	2102	ALA	C-N-CA	7.72	127.78	119.90
2	B	1842	ASN	CA-C-N	7.61	127.32	119.56
2	B	1842	ASN	C-N-CA	7.61	127.32	119.56
1	A	1734	TRP	CB-CA-C	-7.59	97.34	110.17
1	A	1728	ARG	CA-C-N	7.55	127.47	119.85
1	A	1728	ARG	C-N-CA	7.55	127.47	119.85
1	A	1758	HIS	CA-C-N	7.52	128.20	119.47
1	A	1758	HIS	C-N-CA	7.52	128.20	119.47
1	A	1524	PRO	N-CA-CB	7.52	111.15	103.25
1	A	1545	PHE	CA-C-N	7.52	129.24	119.84
1	A	1545	PHE	C-N-CA	7.52	129.24	119.84
2	B	1716	SER	CA-C-N	7.51	127.15	119.56
2	B	1716	SER	C-N-CA	7.51	127.15	119.56
2	B	1697	MET	CA-C-N	7.51	127.88	119.32
2	B	1697	MET	C-N-CA	7.51	127.88	119.32
1	A	1856	ALA	CA-C-N	7.47	128.41	120.12
1	A	1856	ALA	C-N-CA	7.47	128.41	120.12
1	A	1546	PRO	N-CA-CB	7.47	111.09	103.25
1	A	2118	ASN	CA-C-N	7.47	128.13	119.47
1	A	2118	ASN	C-N-CA	7.47	128.13	119.47
1	A	2006	TYR	CA-C-N	7.41	127.77	119.32
1	A	2006	TYR	C-N-CA	7.41	127.77	119.32
1	A	1716	SER	CA-C-N	7.36	127.52	119.87
1	A	1716	SER	C-N-CA	7.36	127.52	119.87
1	A	2092	LEU	CA-C-N	7.28	127.44	120.31
1	A	2092	LEU	C-N-CA	7.28	127.44	120.31
2	B	1929	HIS	CA-C-N	7.15	127.76	119.47
2	B	1929	HIS	C-N-CA	7.15	127.76	119.47
1	A	2286	ALA	CA-C-N	7.14	127.10	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2286	ALA	C-N-CA	7.14	127.10	120.03
1	A	1542	PRO	N-CA-CB	7.14	110.74	103.25
1	A	2207	LEU	CA-C-N	7.09	126.79	119.56
1	A	2207	LEU	C-N-CA	7.09	126.79	119.56
2	B	1743	SER	CA-C-N	7.08	127.07	119.28
2	B	1743	SER	C-N-CA	7.08	127.07	119.28
2	B	1856	ALA	CA-C-N	7.08	127.69	119.47
2	B	1856	ALA	C-N-CA	7.08	127.69	119.47
1	A	1842	ASN	CA-C-N	6.96	126.66	119.56
1	A	1842	ASN	C-N-CA	6.96	126.66	119.56
2	B	1682	LEU	CA-C-N	6.96	127.41	120.52
2	B	1682	LEU	C-N-CA	6.96	127.41	120.52
2	B	1703	GLY	N-CA-C	-6.92	106.17	113.58
1	A	1479	PHE	CA-C-N	6.92	128.49	119.84
1	A	1479	PHE	C-N-CA	6.92	128.49	119.84
1	A	1700	PHE	CA-C-N	6.83	126.81	119.78
1	A	1700	PHE	C-N-CA	6.83	126.81	119.78
1	A	1330	VAL	CA-C-N	6.78	128.31	119.84
1	A	1330	VAL	C-N-CA	6.78	128.31	119.84
1	A	2094	ASP	CA-C-N	6.77	126.47	119.56
1	A	2094	ASP	C-N-CA	6.77	126.47	119.56
1	A	1996	LYS	CA-C-N	6.75	128.27	119.84
1	A	1996	LYS	C-N-CA	6.75	128.27	119.84
1	A	2040	ALA	CA-C-N	6.68	126.63	119.28
1	A	2040	ALA	C-N-CA	6.68	126.63	119.28
1	A	1445	SER	CA-C-N	6.57	127.09	119.99
1	A	1445	SER	C-N-CA	6.57	127.09	119.99
1	A	1376	TRP	CA-C-N	6.56	126.92	119.83
1	A	1376	TRP	C-N-CA	6.56	126.92	119.83
1	A	1864	LEU	CA-C-N	6.51	126.48	119.78
1	A	1864	LEU	C-N-CA	6.51	126.48	119.78
3	C	2286	ALA	CA-C-N	6.45	126.98	120.14
3	C	2286	ALA	C-N-CA	6.45	126.98	120.14
1	A	1641	PHE	CA-C-N	6.38	126.33	119.76
1	A	1641	PHE	C-N-CA	6.38	126.33	119.76
1	A	1548	ILE	N-CA-C	6.38	117.10	108.17
3	C	2345	SER	CB-CA-C	-6.36	109.25	116.63
1	A	1792	PHE	CA-C-N	6.35	126.27	119.85
1	A	1792	PHE	C-N-CA	6.35	126.27	119.85
1	A	1697	MET	CA-C-N	6.34	126.05	119.64
1	A	1697	MET	C-N-CA	6.34	126.05	119.64
1	A	1669	VAL	CA-C-N	6.30	127.71	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1669	VAL	C-N-CA	6.30	127.71	119.84
3	C	2361	THR	N-CA-C	-6.30	105.91	113.97
1	A	1762	PHE	N-CA-C	6.24	118.03	108.42
1	A	2146	LEU	CA-C-N	6.23	126.20	119.78
1	A	2146	LEU	C-N-CA	6.23	126.20	119.78
1	A	1929	HIS	CA-C-N	6.23	126.69	119.47
1	A	1929	HIS	C-N-CA	6.23	126.69	119.47
3	C	2146	LEU	CA-C-N	6.16	126.12	119.78
3	C	2146	LEU	C-N-CA	6.16	126.12	119.78
1	A	2345	SER	CB-CA-C	-6.16	109.48	116.63
1	A	1767	VAL	CA-C-N	6.02	126.52	120.14
1	A	1767	VAL	C-N-CA	6.02	126.52	120.14
1	A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	A	1682	LEU	CA-C-N	5.94	126.44	120.14
1	A	1682	LEU	C-N-CA	5.94	126.44	120.14
1	A	1663	GLY	N-CA-C	-5.82	103.69	112.60
2	B	1850	ILE	CA-C-N	5.76	127.04	119.84
2	B	1850	ILE	C-N-CA	5.76	127.04	119.84
1	A	1743	SER	CA-C-N	5.72	126.10	119.47
1	A	1743	SER	C-N-CA	5.72	126.10	119.47
1	A	1583	LEU	N-CA-C	5.67	117.94	108.02
3	C	2370	SER	CA-C-N	5.58	127.80	121.04
3	C	2370	SER	C-N-CA	5.58	127.80	121.04
1	A	2500	LEU	CA-C-N	5.58	125.68	119.32
1	A	2500	LEU	C-N-CA	5.58	125.68	119.32
1	A	1962	ASP	N-CA-C	5.55	116.47	107.32
1	A	1598	VAL	N-CA-C	5.51	115.89	108.17
3	C	2450	ASN	CA-CB-CG	-5.43	107.17	112.60
2	B	1700	PHE	CA-C-N	5.37	126.55	119.84
2	B	1700	PHE	C-N-CA	5.37	126.55	119.84
2	B	1767	VAL	CA-C-N	5.29	125.19	119.85
2	B	1767	VAL	C-N-CA	5.29	125.19	119.85
1	A	1401	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	1569	LEU	CA-C-N	5.22	124.85	119.05
1	A	1569	LEU	C-N-CA	5.22	124.85	119.05
3	C	2365	ILE	N-CA-C	5.20	115.07	107.37
2	B	1864	LEU	CA-C-N	5.14	125.43	119.93
2	B	1864	LEU	C-N-CA	5.14	125.43	119.93
1	A	1666	TYR	N-CA-C	5.14	117.19	109.23
1	A	1762	PHE	CA-CB-CG	5.11	118.91	113.80
2	B	1683	PRO	N-CA-C	-5.06	103.59	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1852	ILE	N-CA-C	5.02	119.78	109.34
1	A	2104	TRP	CA-C-N	5.02	126.11	119.84
1	A	2104	TRP	C-N-CA	5.02	126.11	119.84

There are no chirality outliers.

There are no planarity outliers.

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	8531	0	8567	48	0
2	B	2147	0	2156	3	0
3	C	2480	0	2549	6	0
All	All	13158	0	13272	57	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 2.

All (57) 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:2037:GLY:O	1:A:2083:PHE:CE2	2.44	0.70
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.94	0.68
1:A:2037:GLY:O	1:A:2083:PHE:HE2	1.81	0.64
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.26	0.60
1:A:1398:ARG:O	1:A:1398:ARG:HG3	2.01	0.59
1:A:2408:MET:O	1:A:2408:MET:SD	2.62	0.58
1:A:1483:ARG:NE	1:A:1483:ARG:HA	2.22	0.55
1:A:1912:THR:HG22	1:A:1912:THR:O	2.07	0.54
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.53
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.08	0.53
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.10	0.52
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.92	0.50
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.36	0.50
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	1.94	0.49
3:C:2388:ASP:OD1	3:C:2388:ASP:C	2.56	0.48
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.63	0.46
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.73	0.46
3:C:2377:ASP:HB2	3:C:2384:CYS:SG	2.55	0.46
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.16	0.46
2:B:1814:TYR:CD2	2:B:1814:TYR:C	2.93	0.46
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.56	0.45
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	1.98	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.17	0.45
1:A:1394:ASP:OD1	1:A:1394:ASP:C	2.61	0.44
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.96	0.44
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.17	0.44
1:A:2039:ARG:NH2	1:A:2084:ASP:OD1	2.38	0.44
1:A:1402:TYR:CD1	1:A:1402:TYR:C	2.95	0.44
1:A:1676:HIS:O	1:A:1677:ARG:C	2.61	0.44
3:C:2141:THR:N	3:C:2495:VAL:O	2.51	0.44
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.59	0.44
3:C:2327:SER:OG	3:C:2329:ASP:OD1	2.35	0.43
1:A:1376:TRP:CD1	1:A:1376:TRP:C	2.97	0.43
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.18	0.43
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.57	0.42
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.19	0.42
1:A:1582:LEU:C	1:A:1582:LEU:CD1	2.92	0.42
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
3:C:2274:ILE:O	3:C:2288:LEU:N	2.52	0.42
1:A:1664:GLU:OE1	1:A:1664:GLU:N	2.40	0.42
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.44	0.42
1:A:1593:SER:OG	1:A:1594:ASP:N	2.51	0.42
1:A:1481:ALA:O	1:A:1482:ILE:C	2.62	0.42
1:A:2003:PHE:O	1:A:2004:THR:HB	2.19	0.41
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.41
2:B:1917:LEU:C	2:B:1917:LEU:HD23	2.45	0.41
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.20	0.41
1:A:2039:ARG:HH21	1:A:2084:ASP:CG	2.25	0.41
1:A:1432:LYS:HB2	1:A:1433:PRO:HD3	2.02	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2351:ASP:C	3:C:2351:ASP:OD1	2.63	0.40
2:B:1936:LEU:O	2:B:1937:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	909/1071 (85%)	909 (100%)	0	100	100
2	B	240/252 (95%)	240 (100%)	0	100	100
3	C	283/322 (88%)	283 (100%)	0	100	100
All	All	1432/1645 (87%)	1432 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1657	GLN
1	A	1676	HIS
1	A	2089	GLN
1	A	2333	GLN
1	A	2468	ASN
2	B	1676	HIS
2	B	1741	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	TPO	A	1343	1	8,10,11	0.93	0	10,14,16	0.76	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
1	TPO	A	1343	1	-	1/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1343	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

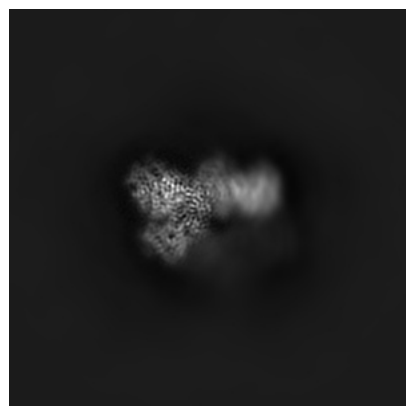
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21250. These allow visual inspection of the internal detail of the map and identification of artifacts.

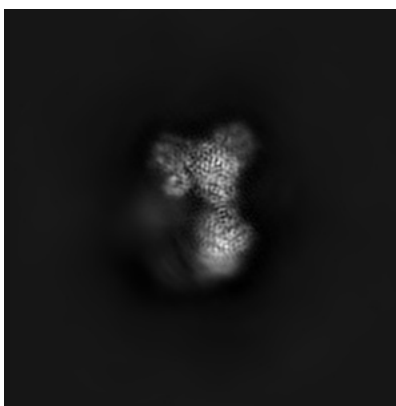
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

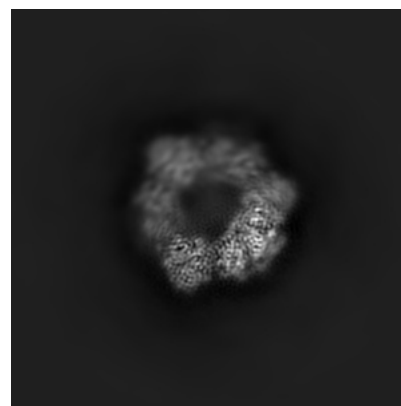
6.1.1 Primary map



X

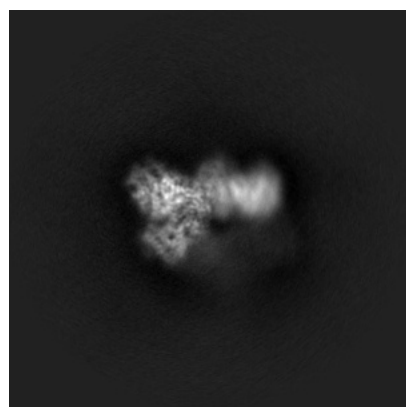


Y

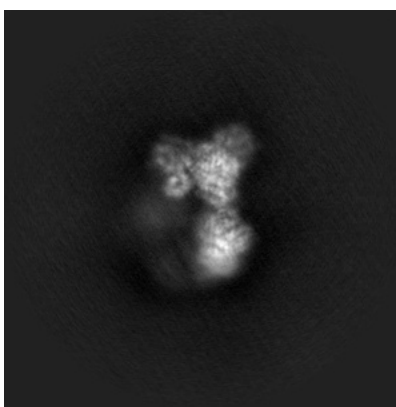


Z

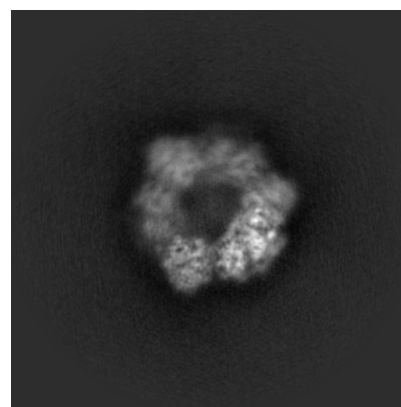
6.1.2 Raw map



X



Y

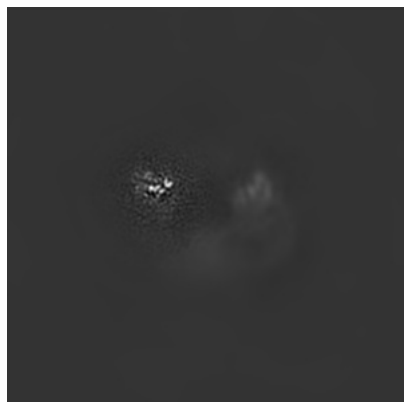


Z

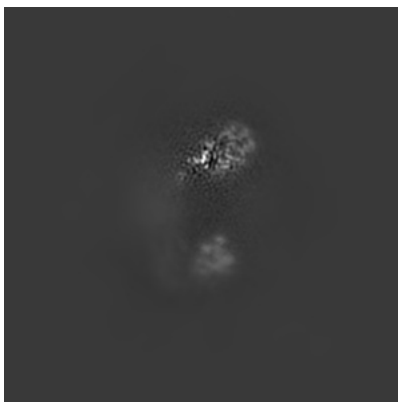
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

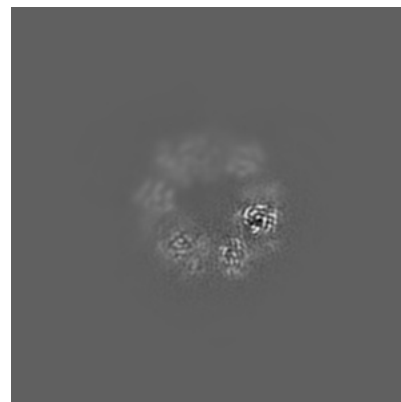
6.2.1 Primary map



X Index: 178

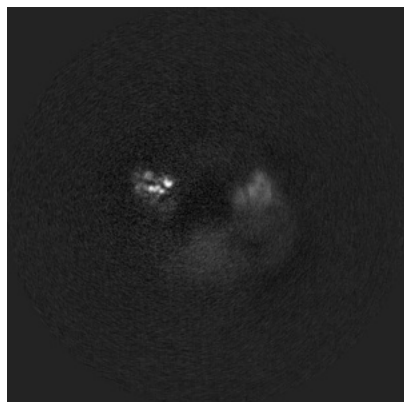


Y Index: 178

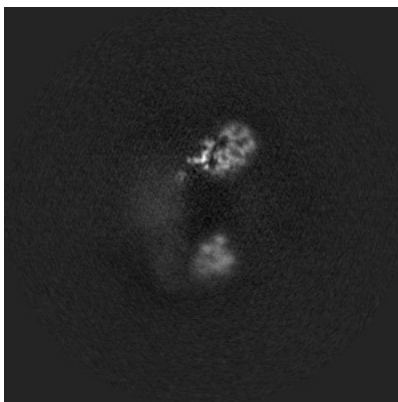


Z Index: 178

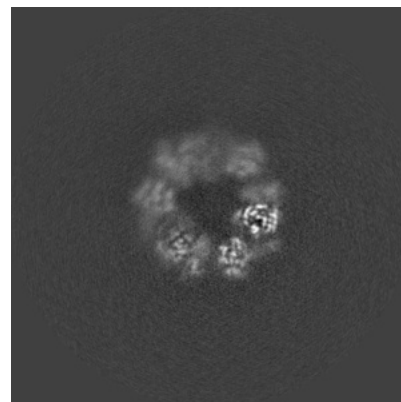
6.2.2 Raw map



X Index: 178



Y Index: 178

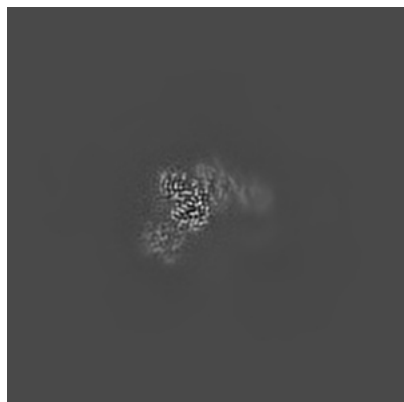


Z Index: 178

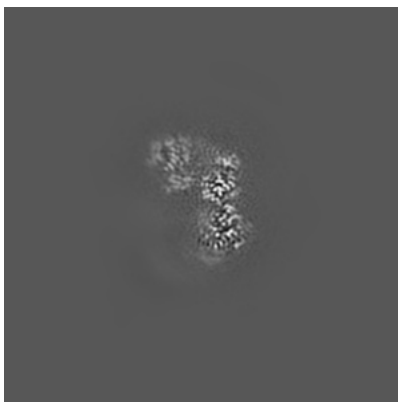
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

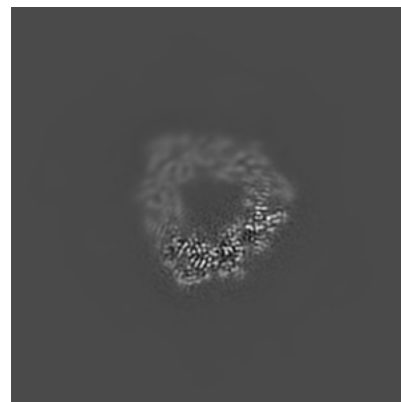
6.3.1 Primary map



X Index: 218

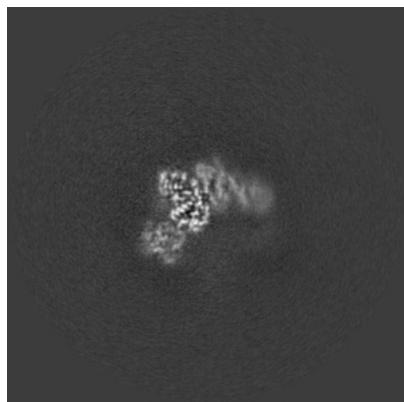


Y Index: 141

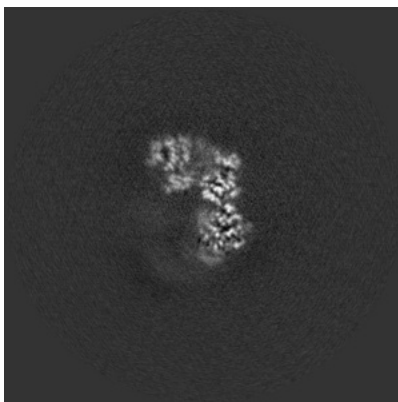


Z Index: 191

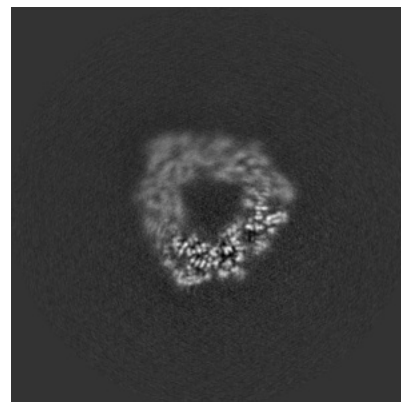
6.3.2 Raw map



X Index: 218



Y Index: 141

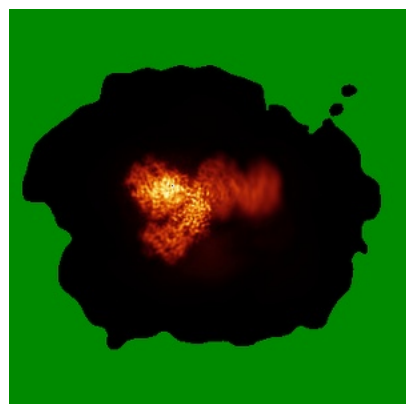


Z Index: 191

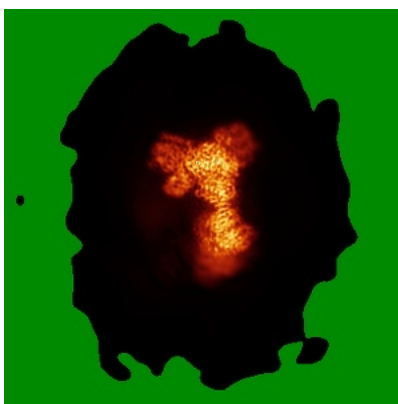
The images above show the largest variance slices of the map in three orthogonal directions.

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

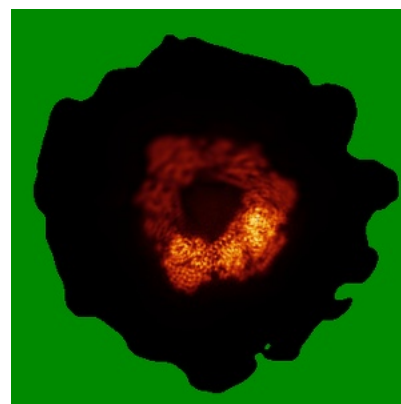
6.4.1 Primary map



X



Y

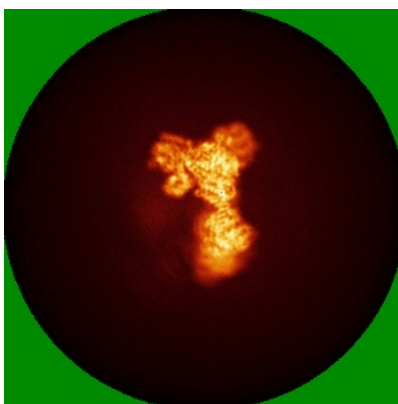


Z

6.4.2 Raw map



X



Y

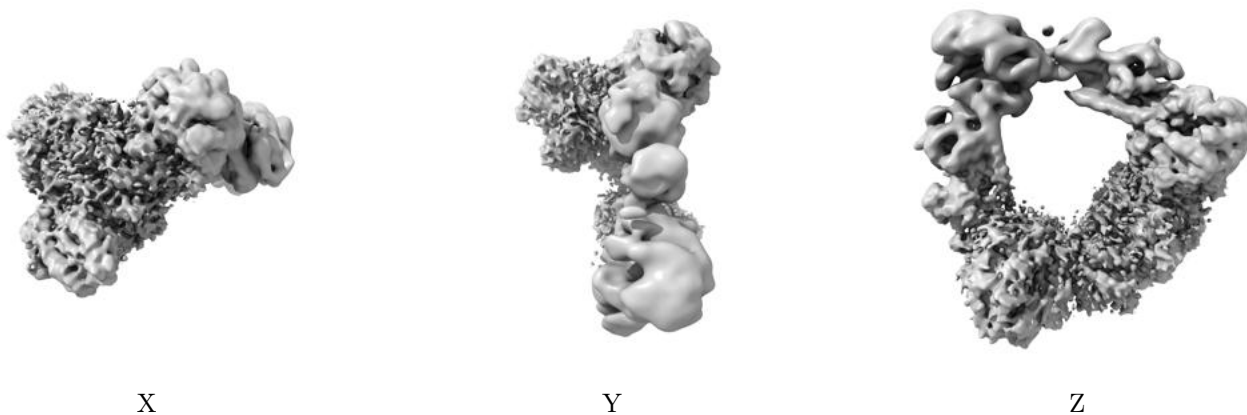


Z

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.

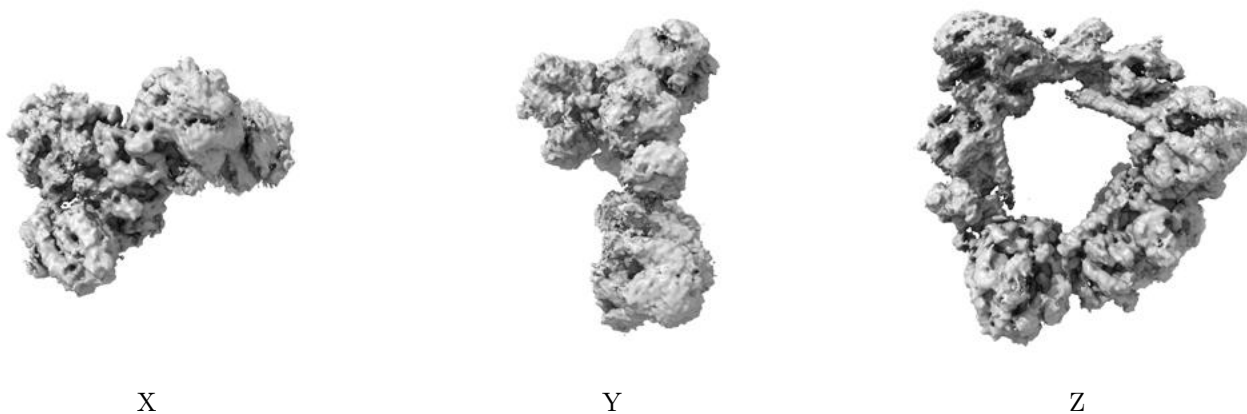
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0267. 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.

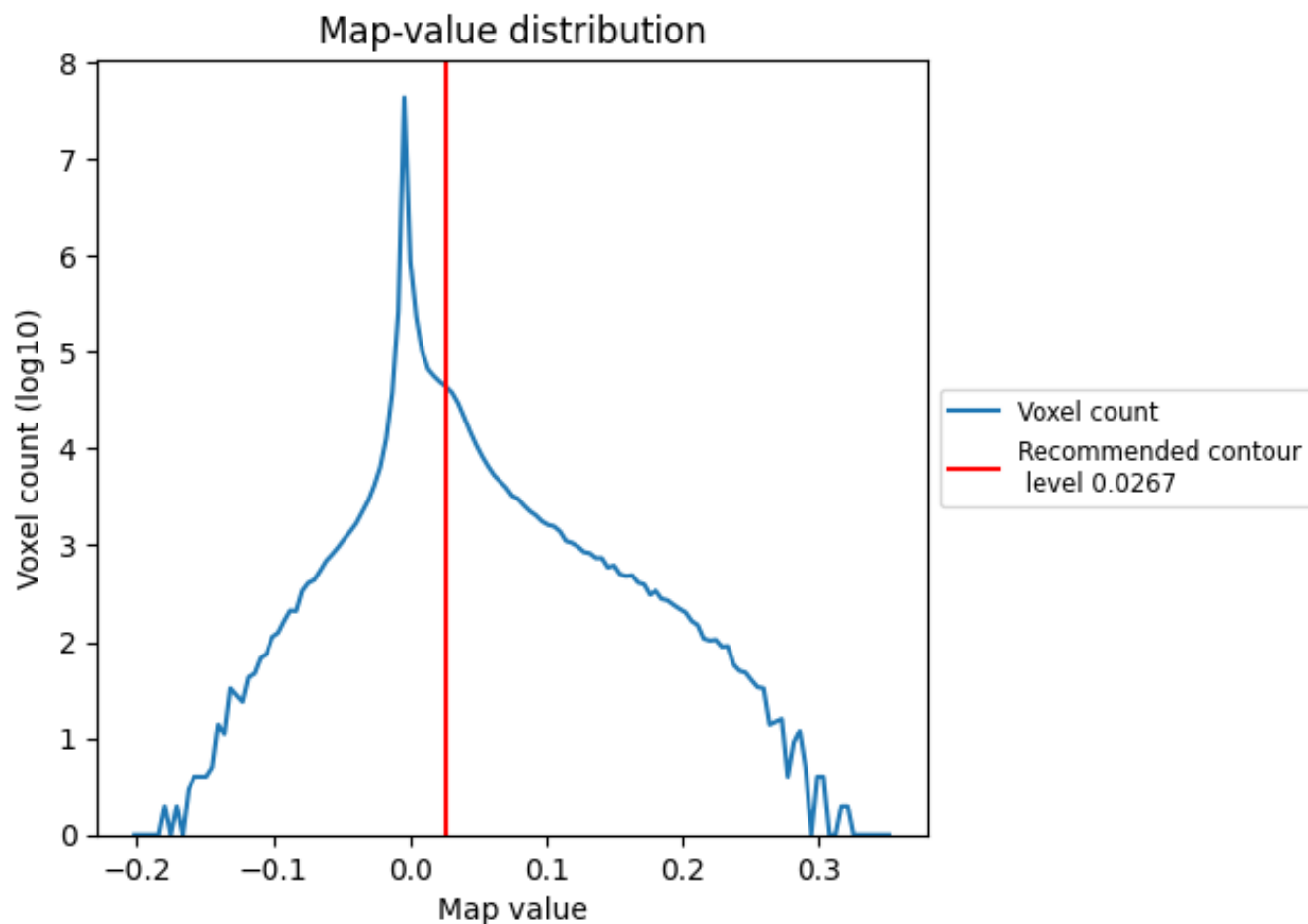
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

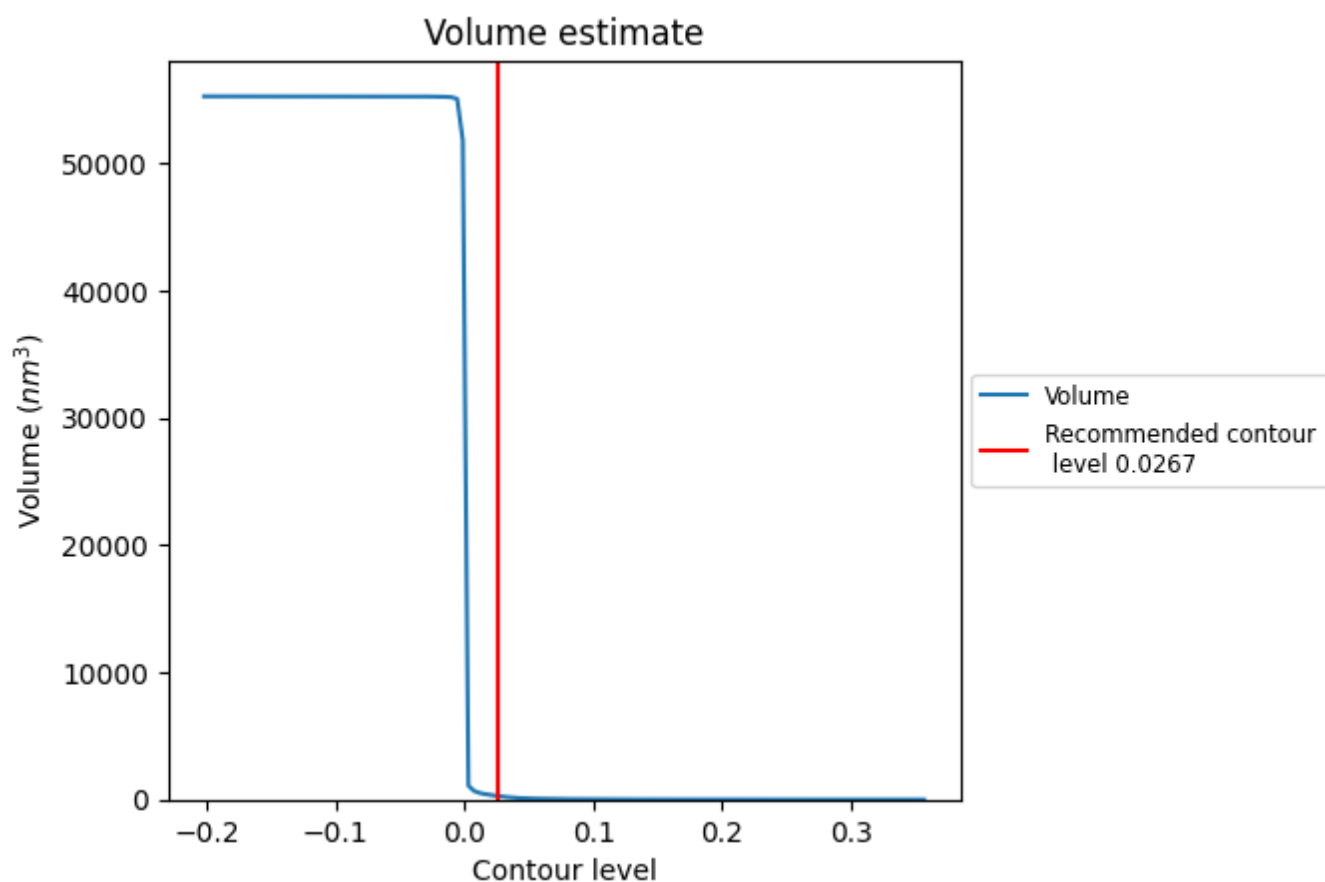
This section contains the results of statistical analysis of the map.

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.

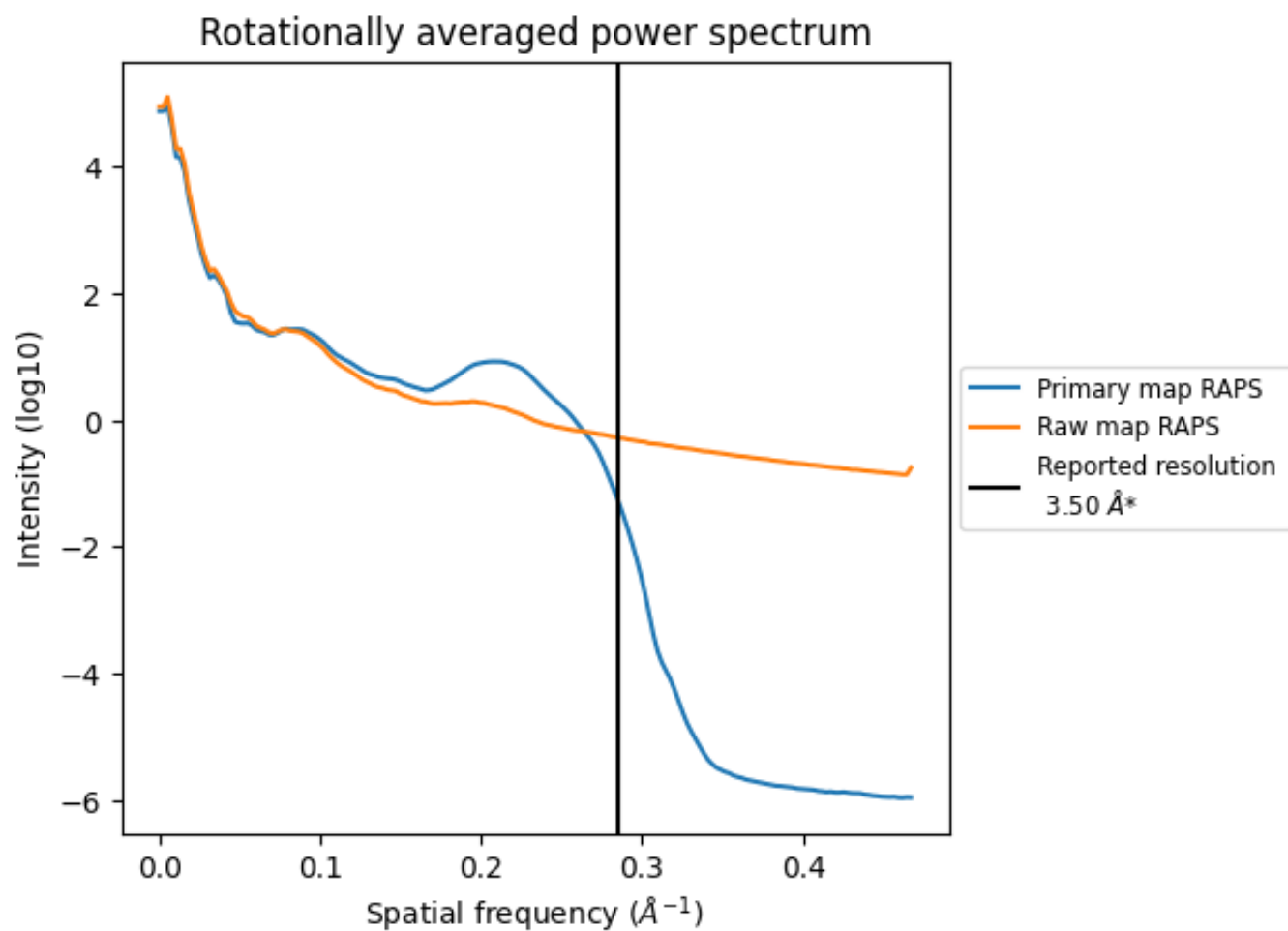
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm³; this corresponds to an approximate mass of 244 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 ⓘ

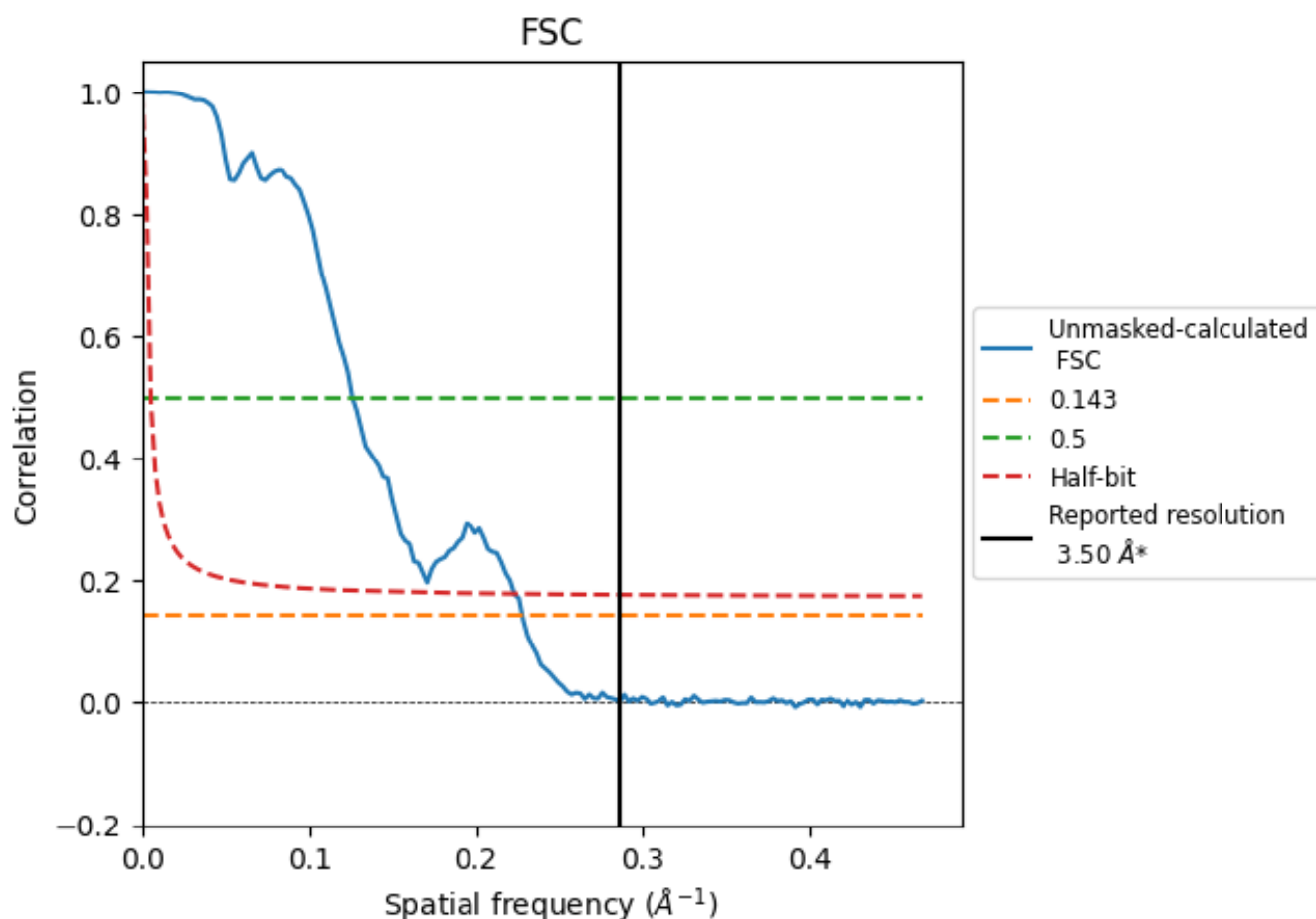


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

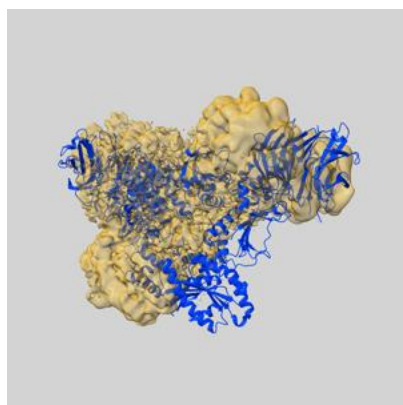
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.39	7.94	4.48

*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 4.39 differs from the reported value 3.5 by more than 10 %

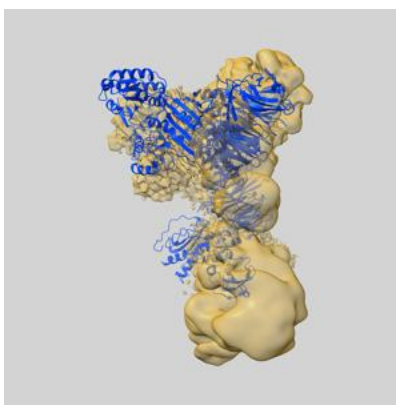
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21250 and PDB model 6VP8. Per-residue inclusion information can be found in section [3](#) on page [4](#).

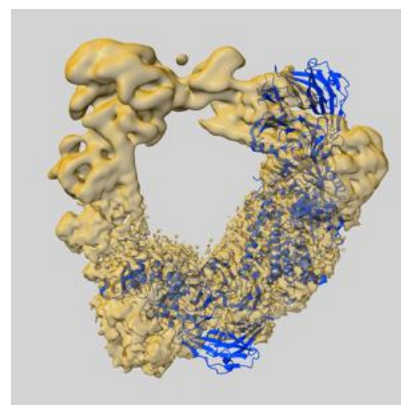
9.1 Map-model overlay [i](#)



X



Y



Z

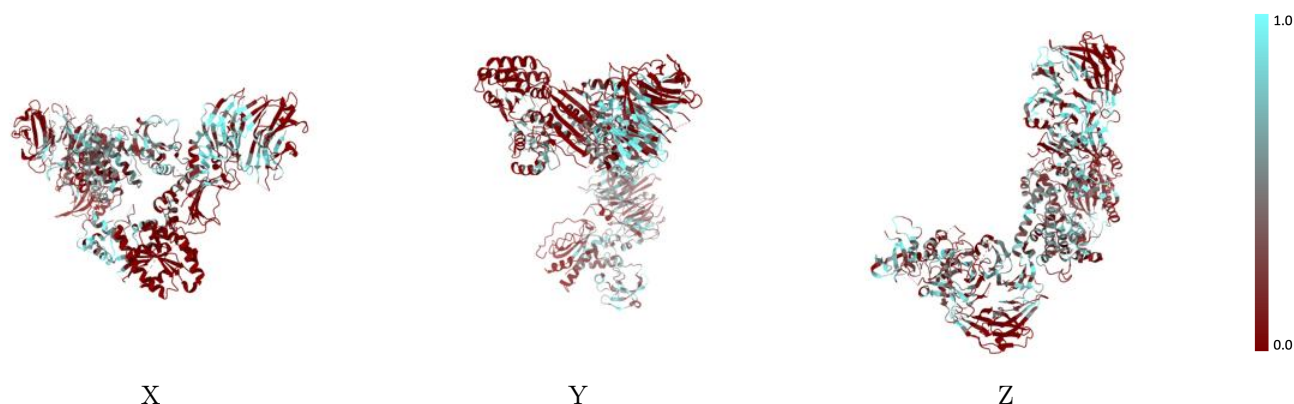
The images above show the 3D surface view of the map at the recommended contour level 0.0267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



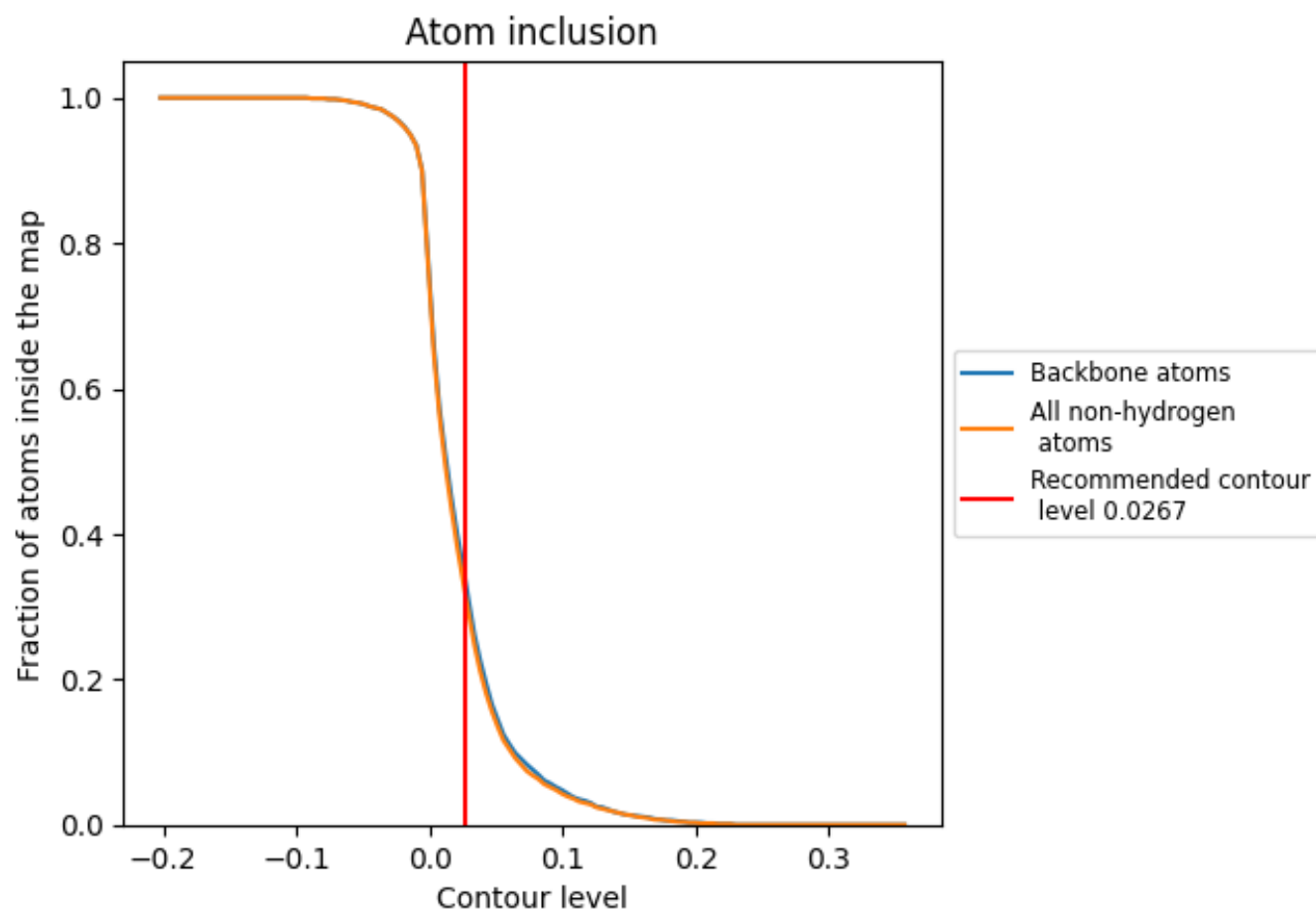
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0267).

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 32% 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 (0.0267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3180	0.0000
A	0.3010	-0.0030
B	0.3010	0.0130
C	0.3930	0.0010

