



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:01 AM UTC

PDB ID : 8IHN / pdb_00008ihn
EMDB ID : EMD-35450
Title : Cryo-EM structure of the Rpd3S core complex
Authors : Zhang, Y.; Gang, C.
Deposited on : 2023-02-23
Resolution : 3.37 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
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

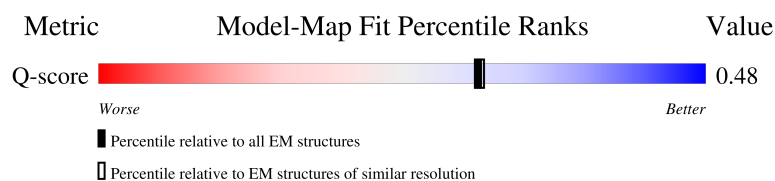
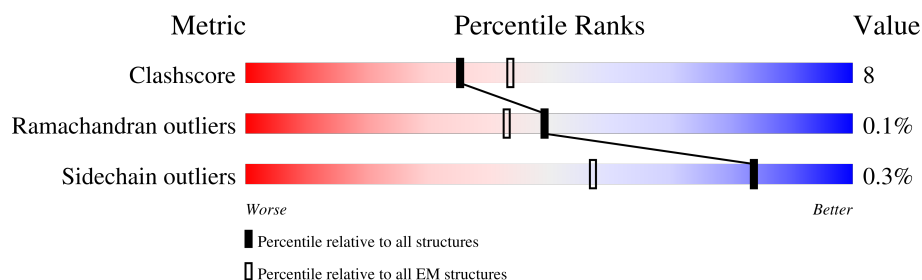
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14287 (2.87 - 3.87)

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	24	
2	K	1536	
3	L	433	
4	M	684	

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Mol	Chain	Length	Quality of chain
4	O	684	18%78%
5	N	401	39%6%54%
5	P	401	34%11%54%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14611 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 Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	24	Total	C	N	O	0	0
			169	101	37	31		

- Molecule 2 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	598	Total	C	N	O	S	0	0
			4716	3013	815	873	15		

- Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	410	Total	C	N	O	S	0	0
			3082	1949	527	584	22		

- Molecule 4 is a protein called RCO1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	357	Total	C	N	O	S	0	0
			2707	1708	469	519	11		
4	O	153	Total	C	N	O	S	0	0
			1133	722	195	211	5		

- Molecule 5 is a protein called Chromatin modification-related protein EAF3.

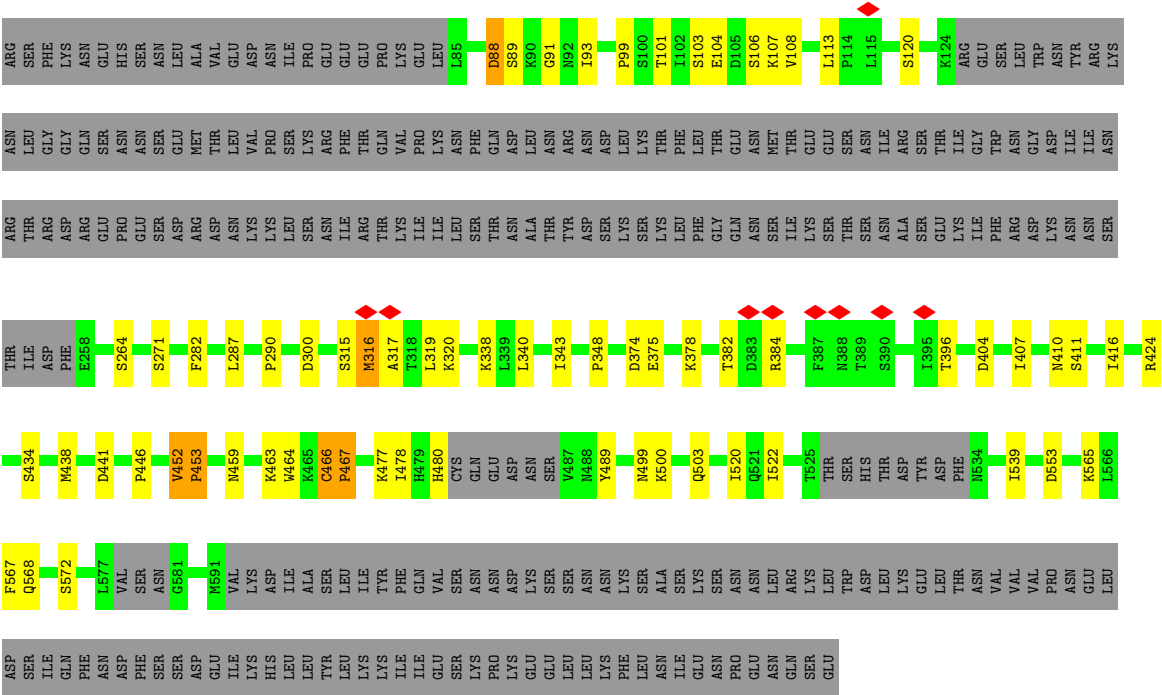
Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	183	Total	C	N	O	S	0	0
			1410	900	229	274	7		
5	P	184	Total	C	N	O	S	0	0
			1392	888	231	267	6		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	L	1	Total	Zn	0
			1	1	

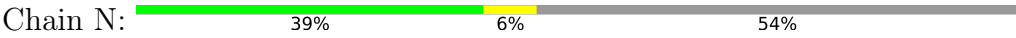
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	L	1	Total	Ca	0
			1	1	



THR	ASN	VAL	VAL	VAL	PRO	ASN	GLU	LEU	ASP	ASP	ILE	GLN	PHE	ASN	ASP	ASP	GLU	GLY	ILE	ASP	GLY	ASP	GLY	LEU	LEU	TYR	LEU	LYS	LYS	ILE	ILE	GLU	GLY	LEU	LYS	LEU	ASN	GLY	GLY	ASN	PRO	GLU	ASN	GLN	SER	GLU
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● Molecule 5: Chromatin modification-related protein EAF3



MET	VAL	ASP	LEU	GLU	GLN	GLY	PRO	PHE	ALA	GLY	GLY	ARG	CYS	LEU	ASN	PHE	HIS	GLY	PRO	GLY	LEU	TYR	GLN	GLY	TRP	GLU	ALA	LYS	ILE	LEU	ASP	PRO	SER	SER	LYS	PRO	LYS	ILE	MET	TYR	THR	SER	ILE	ASN	PRO	GLY	GLY	ASN	ALA	THR	LYS	GLU	ILE	LYS	PRO	GLN	LYS	LEU
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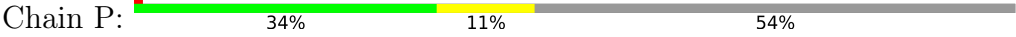
LEU	GLY	GLU	ASP	GLU	SER	ILE	PRO	GLY	GLU	ALA	ILE	ASN	GLY	LYS	LEU	ASP	ILE	GLN	HIS	TRP	LYS	SER	TRP	TRP	ASP	VAL	GLY	TYR	ASP	SER	SER	LYS	ARG	ILE	MET	ARG	ALA	TYR	SER	GLN	ASN	GLY	PRO	ASN	ILE	LYS	ASP	ASN	ALA	GLY	MET	LYS	LYS	ARG	LEU	ALA	ASN	GLY	ALA	GLU	LYS	ILE	LYS	GLU	ALA	PRO	LYS	GLN	LYS	LEU
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SER	LEU	GLY	GLU	GLN	LYS	LYS	LYS	LEU	SER	THR	SER	GLY	ASN	GLY	GLY	GLY	GLY	GLY	ASN	SER	ILE	GLY	GLY	ARG	ASN	ALA	SER	ILE	TYR	SER	LYS	LYS	THR	THR	SER	GLN	SER	PHE	ASN	GLY	LEU	THR	SER	VAL	SER	GLY	ARG	LYS	ARG	GLY	ASN	GLY	ALA	SER	ALA	PRO	SER	LEU
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HIS	PRO	GLY	SER	SER	LEU	ARG	SER	SER	SER	GLN	ASP	ASN	GLY	GLY	ASP	ASP	ARG	ARG	ARG	ARG	ARG	SER	SER	SER	LEU	LYS	SER	PRO	ASN	MET	SER	LEU	HIS	HIS	ILE	ALA	GLY	TYR	TYR	THR	P218	K227	V231	L232	Y238	D242	C246	V252	T253	V254	E255	M256	V257	L258	M259	L269
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Q275	S276	E280	L285	D307	S314	K315	L331	T346	L354	N380	L386	Y387	G400	MET
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● Molecule 5: Chromatin modification-related protein EAF3



MET	VAL	ASP	LEU	GLU	GLN	GLY	PRO	PHE	ALA	GLY	GLY	ARG	CYS	LEU	ASN	PHE	HIS	GLY	PRO	GLY	LEU	TYR	GLN	GLY	TRP	GLU	ALA	LYS	ILE	LEU	ASP	PRO	SER	SER	LYS	PRO	LYS	ILE	MET	TYR	THR	SER	ILE	ASN	PRO	GLY	GLY	ASN	ALA	THR	LYS	GLU	ILE	LYS	PRO	GLN	LYS	LEU
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LEU	GLY	GLU	ASP	GLU	SER	ILE	PRO	GLY	GLU	ALA	ILE	ASN	GLY	LYS	LEU	PHE	ILE	HIS	TRP	LYS	SER	SER	TRP	TRP	VAL	ASP	PRO	GLY	TYR	ASP	ARG	LYS	ILE	ARG	ALA	TYR	SER	GLN	ASN	GLY	PRO	ASN	ILE	LYS	ASP	ALA	MET	VAL	GLY	LYS	ARG	LEU	ALA	ASN	GLY	GLY	ARG	LYS	ILE	LYS	GLU	ALA	PRO	LYS	GLN	LYS	LEU
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SER	LEU	GLY	GLU	GLN	LYS	LYS	LYS	LEU	SER	THR	SER	GLY	ASN	GLY	LYS	GLY	GLY	GLY	ASN	PRO	ILE	GLY	GLY	ASP	PHE	ALA	SER	ILE	TYR	SER	LYS	ARG	LYS	THR	THR	SER	GLN	SER	PHE	LEU	THR	SER	VAL	SER	GLY	ARG	LYS	LEU	ALA	ASN	GLY	GLY	ARG	LYS	ILE	LYS	GLU	ALA	PRO	LYS	GLN	LYS	LEU
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HIS	PRO	GLY	SER	SER	LEU	ARG	SER	SER	SER	GLN	ASP	ASN	GLY	GLY	ASN	ASP	ARG	ARG	ARG	ARG	SER	TYR	SER	SER	LEU	LYS	SER	PRO	ASN	MET	SER	LEU	HIS	HIS	ILE	ALA	GLY	TYR	TYR	THR	P218	L222	Q223	I224	P225	I226	K229	C246	R247	L248	P249	V257	E262	H263	E264	V265	S266	Q267
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E268	L269	P272	G273	S274	D290	L297	L298	Y299	E302	I323	R324	I325	V326	G327	A328	I329	H330	L331	L332	R333	C352	Q353	L354	L355	Q358	T359	E360	D361	F362	L363	V364	L366	V370	D371	E372	F373	N375	D376	L248	K377	D378	P379	N380	R381	S382	D383	Y387	H401
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107252	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.810	Depositor
Minimum map value	-1.407	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.31	Depositor
Map size (Å)	359.52002, 359.52002, 359.52002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN

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	0.55	0/169	1.04	1/223 (0.4%)
2	K	0.27	0/4813	0.53	8/6510 (0.1%)
3	L	0.35	0/3153	0.61	6/4275 (0.1%)
4	M	0.42	1/2766 (0.0%)	0.79	15/3746 (0.4%)
4	O	0.27	0/1155	0.64	4/1556 (0.3%)
5	N	0.35	0/1436	0.55	1/1949 (0.1%)
5	P	0.23	0/1417	0.46	1/1923 (0.1%)
All	All	0.33	1/14909 (0.0%)	0.62	36/20182 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	452	VAL	CA-C	-8.65	1.46	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	452	VAL	N-CA-C	-15.70	90.18	107.77
4	O	289	PRO	N-CA-C	-10.09	98.40	110.70
1	A	21	ALA	N-CA-C	-9.29	99.54	112.45
4	M	452	VAL	CA-C-N	-9.11	110.38	119.76
4	M	452	VAL	C-N-CA	-9.11	110.38	119.76
4	M	107	LYS	N-CA-C	-8.97	98.69	110.53
4	M	108	VAL	N-CA-C	8.82	119.62	110.62
4	M	466	CYS	CA-C-N	-8.15	112.39	120.21
4	M	466	CYS	C-N-CA	-8.15	112.39	120.21
4	M	88	ASP	N-CA-C	-7.88	97.81	109.15
3	L	409	ALA	N-CA-C	7.62	121.67	112.38
4	O	289	PRO	CA-C-N	-7.20	112.35	119.76
4	O	289	PRO	C-N-CA	-7.20	112.35	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	872	ASP	N-CA-C	7.17	121.42	111.74
5	N	380	ASN	N-CA-C	-7.10	103.62	111.36
2	K	875	ARG	N-CA-C	-7.04	103.61	111.28
3	L	125	GLY	N-CA-C	-7.04	105.64	114.16
4	M	317	ALA	N-CA-C	6.96	118.87	111.28
4	M	453	PRO	N-CA-C	-6.79	100.55	111.14
5	P	355	LEU	N-CA-C	-6.74	103.94	111.28
4	M	452	VAL	CB-CA-C	-6.54	103.25	110.78
3	L	410	GLU	N-CA-C	6.49	118.35	111.28
4	M	467	PRO	N-CA-C	-6.47	102.16	111.22
4	M	106	SER	N-CA-C	-5.91	104.84	111.28
2	K	1081	ASN	CB-CA-C	5.76	121.04	110.10
4	M	108	VAL	CB-CA-C	-5.71	104.43	112.14
3	L	403	ASP	N-CA-C	-5.59	101.77	110.10
4	O	288	ASP	N-CA-C	-5.58	105.24	113.16
2	K	852	PRO	CA-C-N	-5.50	114.03	119.92
2	K	852	PRO	C-N-CA	-5.50	114.03	119.92
2	K	962	LYS	N-CA-C	-5.47	105.31	111.28
2	K	871	TYR	N-CA-C	5.15	117.84	110.68
3	L	365	THR	CA-C-N	-5.15	113.62	119.28
3	L	365	THR	C-N-CA	-5.15	113.62	119.28
4	M	316	MET	N-CA-C	-5.09	104.37	111.39
2	K	873	LYS	CB-CA-C	-5.05	110.36	117.23

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	169	0	184	17	0
2	K	4716	0	4466	76	0
3	L	3082	0	2838	49	0
4	M	2707	0	2455	40	0
4	O	1133	0	1026	21	0
5	N	1410	0	1361	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	1392	0	1320	33	0
6	L	1	0	0	0	0
7	L	1	0	0	0	0
All	All	14611	0	13650	222	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 8.

All (222) 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:20:LEU:CB	1:A:23:LYS:H	2.05	0.69
4:M:315:SER:O	4:M:316:MET:C	2.38	0.67
1:A:4:LYS:O	1:A:5:GLN:HG2	1.97	0.63
5:P:372:GLU:HA	5:P:377:LYS:HD2	1.82	0.62
5:N:314:SER:OG	5:N:315:LYS:NZ	2.32	0.61
1:A:8:ARG:HD3	1:A:14:LYS:NZ	2.15	0.61
1:A:16:PRO:HG2	2:K:787:VAL:HG12	1.82	0.61
5:P:329:ILE:HG23	5:P:330:HIS:HD2	1.66	0.60
1:A:8:ARG:CZ	1:A:22:THR:HG21	2.32	0.60
3:L:402:GLY:O	3:L:403:ASP:C	2.46	0.59
2:K:1021:PHE:O	2:K:1273:ARG:NH2	2.36	0.59
4:M:374:ASP:OD1	4:M:375:GLU:N	2.33	0.58
3:L:142:ALA:HB3	3:L:306:MET:HG3	1.86	0.58
4:O:351:PHE:CE1	5:P:333:ARG:HB3	2.39	0.57
2:K:1196:LEU:HD11	2:K:1219:LEU:HD11	1.86	0.57
4:O:326:PHE:O	4:O:330:ASN:ND2	2.30	0.57
5:N:253:THR:H	5:N:256:MET:HE3	1.69	0.57
4:O:564:ARG:HH22	4:O:565:LYS:HG3	1.70	0.57
1:A:14:LYS:HE2	1:A:22:THR:HG23	1.87	0.56
2:K:962:LYS:O	2:K:966:TRP:N	2.37	0.56
5:N:269:LEU:HD11	5:N:275:GLN:HG3	1.87	0.56
2:K:1234:ASN:O	3:L:359:ASN:ND2	2.37	0.56
3:L:109:ASP:OD1	3:L:110:CYS:N	2.37	0.56
1:A:14:LYS:HG2	1:A:21:ALA:H	1.70	0.56
4:O:336:PHE:HE1	5:P:355:LEU:HD21	1.71	0.56
2:K:853:PRO:HA	2:K:884:HIS:CE1	2.41	0.55
2:K:1186:LEU:HD23	3:L:351:TYR:CZ	2.42	0.55
5:P:222:LEU:HD11	5:P:359:THR:HG21	1.88	0.55
4:O:357:ILE:HD11	5:P:229:LYS:HA	1.88	0.55
2:K:690:ASN:ND2	4:M:520:ILE:HG13	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:376:ASP:HB3	5:P:379:PRO:HB3	1.88	0.55
2:K:960:THR:O	2:K:963:LYS:HB3	2.06	0.54
2:K:906:ARG:HB3	2:K:910:ARG:HH21	1.73	0.54
3:L:401:LEU:O	3:L:402:GLY:C	2.46	0.53
1:A:8:ARG:HD3	1:A:14:LYS:HZ1	1.73	0.53
5:P:226:ILE:HA	5:P:229:LYS:HD3	1.90	0.53
4:M:99:PRO:HB2	4:M:101:THR:HG23	1.89	0.53
5:N:256:MET:HA	5:N:259:ASN:HB2	1.90	0.53
3:L:89:VAL:HG22	3:L:112:VAL:HG11	1.90	0.53
2:K:796:ILE:HD13	4:M:396:THR:CB	2.38	0.52
3:L:74:MET:HE3	3:L:163:LEU:HD22	1.91	0.52
3:L:335:ASP:OD2	3:L:336:LYS:N	2.42	0.52
4:O:262:PHE:HA	4:O:269:SER:HA	1.91	0.52
4:O:344:ASP:OD1	4:O:345:SER:N	2.42	0.52
2:K:810:ILE:HD11	2:K:919:LEU:HD23	1.92	0.51
2:K:748:CYS:SG	2:K:749:GLU:N	2.83	0.51
2:K:962:LYS:O	2:K:965:HIS:N	2.44	0.51
2:K:1013:LEU:HD22	2:K:1257:MET:SD	2.51	0.51
2:K:962:LYS:O	2:K:963:LYS:C	2.51	0.51
4:M:452:VAL:O	4:M:453:PRO:C	2.50	0.51
3:L:184:ASP:HB3	3:L:207:SER:HA	1.92	0.51
2:K:1219:LEU:HD23	2:K:1224:PHE:HB2	1.93	0.50
3:L:279:ASP:HA	3:L:314:THR:OG1	2.12	0.50
4:M:103:SER:O	4:M:104:GLU:C	2.50	0.50
5:P:299:TYR:H	5:P:302:GLU:HB2	1.75	0.50
3:L:406:GLU:O	3:L:407:ASP:HB2	2.11	0.50
4:M:553:ASP:HA	5:P:272:PRO:HD2	1.92	0.50
2:K:1075:GLN:O	2:K:1079:ARG:N	2.37	0.50
2:K:853:PRO:HA	2:K:884:HIS:HE1	1.76	0.50
4:M:441:ASP:HB3	4:M:463:LYS:HD3	1.94	0.50
2:K:683:THR:HG23	4:M:522:ILE:HG13	1.92	0.49
5:P:366:LEU:HD12	5:P:374:PHE:CE1	2.47	0.49
4:M:410:ASN:OD1	4:M:411:SER:N	2.45	0.49
5:N:238:TYR:HA	5:N:242:ASP:HB2	1.95	0.49
4:M:424:ARG:O	4:M:434:SER:HA	2.12	0.49
5:N:254:VAL:HG13	5:N:331:LEU:HD22	1.94	0.49
4:O:351:PHE:HD1	5:P:297:LEU:HA	1.75	0.49
3:L:410:GLU:O	3:L:411:ALA:C	2.55	0.49
5:P:246:CYS:HB2	5:P:387:TYR:CE1	2.48	0.49
2:K:1303:ILE:HG13	2:K:1314:ILE:HG12	1.93	0.49
5:N:246:CYS:HA	5:N:387:TYR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:O	1:A:4:LYS:O	2.30	0.49
3:L:111:PRO:O	3:L:162:TYR:OH	2.23	0.49
2:K:778:LEU:HD21	3:L:171:ILE:HD11	1.95	0.49
3:L:163:LEU:HD11	3:L:168:LEU:HD11	1.95	0.49
5:P:223:GLN:NE2	5:P:224:ILE:O	2.46	0.49
5:P:264:GLU:HA	5:P:267:GLN:NE2	2.28	0.48
2:K:771:ASP:OD1	2:K:772:ASP:N	2.46	0.48
4:M:264:SER:HB2	4:M:282:PHE:CE1	2.48	0.48
5:P:269:LEU:HD22	5:P:274:SER:HB3	1.95	0.48
2:K:798:HIS:CG	3:L:283:CYS:HB3	2.49	0.48
1:A:20:LEU:CB	1:A:23:LYS:HB3	2.43	0.48
5:P:333:ARG:NH2	5:P:387:TYR:OH	2.46	0.48
5:P:358:GLN:O	5:P:362:PHE:N	2.41	0.48
2:K:666:VAL:HG11	4:O:552:PHE:HD1	1.78	0.48
2:K:961:ASN:O	2:K:964:ILE:HB	2.14	0.47
4:M:404:ASP:O	4:M:407:ILE:HG22	2.14	0.47
2:K:672:ALA:O	2:K:676:ILE:HG12	2.14	0.47
2:K:918:GLU:HB2	4:M:120:SER:O	2.15	0.47
4:M:416:ILE:O	4:M:446:PRO:HG2	2.14	0.47
5:P:360:GLU:O	5:P:364:VAL:HG23	2.15	0.47
2:K:1209:ARG:O	2:K:1213:ARG:HG3	2.15	0.47
2:K:1309:THR:O	2:K:1310:LEU:C	2.56	0.47
3:L:377:PHE:O	3:L:381:GLU:HG3	2.14	0.47
4:M:88:ASP:O	4:M:91:GLY:N	2.48	0.47
1:A:4:LYS:HB2	1:A:5:GLN:H	1.48	0.47
1:A:6:THR:OG1	4:M:271:SER:N	2.48	0.47
2:K:834:ILE:O	2:K:838:ILE:HD12	2.14	0.47
4:M:478:ILE:HG13	4:M:480:HIS:H	1.79	0.47
3:L:212:GLY:O	3:L:213:GLU:HG2	2.15	0.47
2:K:1138:LEU:HD12	2:K:1269:PHE:CZ	2.50	0.47
4:M:287:LEU:HA	4:M:348:PRO:HG2	1.96	0.47
4:O:323:GLU:O	4:O:327:ILE:HD12	2.15	0.47
2:K:1027:GLU:OE1	2:K:1027:GLU:N	2.32	0.46
2:K:963:LYS:HE3	2:K:970:LYS:HB3	1.97	0.46
2:K:1235:LYS:HA	2:K:1235:LYS:HD3	1.52	0.46
3:L:65:ARG:HB2	3:L:409:ALA:HB2	1.98	0.46
4:O:355:ASN:O	4:O:359:GLU:N	2.39	0.46
2:K:993:ASP:OD1	2:K:1011:LYS:HE3	2.15	0.46
4:M:438:MET:HE2	4:M:464:TRP:CE3	2.51	0.46
3:L:237:PRO:O	3:L:368:TYR:OH	2.30	0.46
4:O:327:ILE:HG13	4:O:337:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:567:PHE:HB3	4:O:569:PHE:CE2	2.51	0.46
5:N:276:SER:O	5:N:280:GLU:HG2	2.16	0.46
5:P:290:ASP:OD1	5:P:323:ILE:HG23	2.16	0.46
5:P:366:LEU:O	5:P:370:VAL:N	2.49	0.46
3:L:60:LYS:HE2	3:L:332:VAL:HG21	1.97	0.45
3:L:149:LEU:HB3	3:L:161:CYS:HB3	1.99	0.45
3:L:104:PHE:O	3:L:106:VAL:N	2.50	0.45
2:K:999:THR:HG22	2:K:1001:ALA:H	1.80	0.45
2:K:919:LEU:HD22	4:M:120:SER:OG	2.17	0.45
2:K:1013:LEU:HD23	2:K:1253:ALA:HB1	1.98	0.45
4:M:338:LYS:NZ	5:N:346:THR:O	2.47	0.45
2:K:1176:SER:O	3:L:352:LYS:NZ	2.46	0.45
3:L:19:ARG:NH2	3:L:299:LYS:O	2.50	0.45
2:K:714:LYS:HB2	2:K:714:LYS:NZ	2.32	0.45
2:K:1131:GLN:O	2:K:1277:THR:HG22	2.17	0.45
4:O:302:HIS:O	4:O:307:LYS:NZ	2.35	0.45
3:L:242:ILE:HG12	3:L:247:TYR:HD1	1.82	0.45
3:L:316:ARG:O	3:L:320:ARG:HG3	2.17	0.45
4:M:503:GLN:HE21	4:M:539:ILE:HG12	1.82	0.45
5:N:227:LYS:O	5:N:231:VAL:HG23	2.17	0.45
3:L:186:ASP:OD1	3:L:187:VAL:N	2.50	0.44
1:A:14:LYS:HE3	1:A:21:ALA:HB3	1.99	0.44
4:M:300:ASP:OD1	4:M:300:ASP:N	2.50	0.44
5:P:247:ARG:HH21	5:P:383:ASP:HB2	1.81	0.44
2:K:1300:MET:HE2	2:K:1319:LEU:HD21	1.98	0.44
3:L:81:GLU:HG3	3:L:104:PHE:HZ	1.82	0.44
4:M:319:LEU:O	4:M:320:LYS:C	2.59	0.44
5:N:231:VAL:O	5:N:232:LEU:C	2.57	0.44
5:P:354:LEU:O	5:P:355:LEU:C	2.58	0.44
3:L:198:TYR:CE2	3:L:225:GLY:HA2	2.52	0.44
4:M:382:THR:HG22	4:M:384:ARG:H	1.83	0.44
1:A:14:LYS:HD2	3:L:108:ASP:OD2	2.17	0.44
2:K:785:HIS:ND1	2:K:787:VAL:HG22	2.33	0.44
2:K:1027:GLU:O	2:K:1031:GLU:HG2	2.17	0.44
5:P:248:LEU:HA	5:P:249:PRO:C	2.43	0.44
2:K:809:LYS:O	2:K:813:GLU:HG3	2.18	0.44
2:K:911:GLU:HG3	4:M:113:LEU:HD22	2.00	0.44
3:L:236:VAL:HG22	3:L:376:ILE:HD13	2.00	0.44
4:M:477:LYS:NZ	4:M:489:TYR:HB3	2.33	0.44
2:K:890:THR:HA	4:M:93:ILE:HD13	1.99	0.43
3:L:259:MET:HE1	3:L:298:VAL:HG13	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:773:MET:HE1	3:L:171:ILE:HG23	2.00	0.43
2:K:1117:THR:HB	2:K:1120:LEU:HG	1.99	0.43
3:L:45:ILE:HG12	3:L:146:ALA:HA	2.00	0.43
5:P:248:LEU:HD13	5:P:326:TYR:CE2	2.52	0.43
5:P:262:GLU:O	5:P:266:SER:HB3	2.18	0.43
2:K:898:LEU:HD23	2:K:898:LEU:HA	1.89	0.43
2:K:987:ASP:OD2	2:K:1204:TYR:OH	2.29	0.43
2:K:1137:ASN:HA	2:K:1304:GLU:HA	2.00	0.43
3:L:198:TYR:CZ	3:L:225:GLY:HA2	2.53	0.43
4:M:568:GLN:O	4:M:572:SER:N	2.50	0.43
2:K:1134:SER:HB3	2:K:1307:LYS:HB3	2.00	0.43
3:L:84:ASP:OD2	3:L:88:ARG:NH2	2.52	0.43
4:O:265:ALA:O	4:O:350:GLN:HB2	2.18	0.43
5:P:257:VAL:HG21	5:P:328:ALA:HB2	2.01	0.43
4:M:290:PRO:HG2	5:N:307:ASP:HB2	2.01	0.43
4:M:499:ASN:OD1	4:M:500:LYS:N	2.52	0.43
4:O:293:PRO:O	4:O:296:LEU:HG	2.18	0.43
5:P:246:CYS:HB2	5:P:387:TYR:CD1	2.54	0.43
2:K:676:ILE:HD12	2:K:709:TYR:HD1	1.82	0.43
2:K:1111:ALA:O	2:K:1112:LYS:C	2.62	0.43
2:K:949:ILE:HD11	2:K:1142:THR:HG23	1.99	0.43
2:K:1036:HIS:CB	2:K:1212:ARG:HH22	2.32	0.43
3:L:220:GLU:OE1	3:L:221:LEU:N	2.51	0.43
4:M:396:THR:O	4:M:459:ASN:ND2	2.51	0.42
5:P:332:LEU:HD22	5:P:374:PHE:CE1	2.55	0.42
2:K:926:LYS:NZ	2:K:1226:GLU:OE2	2.52	0.42
2:K:1013:LEU:HD12	2:K:1065:LEU:HD11	2.00	0.42
4:O:289:PRO:O	4:O:290:PRO:C	2.60	0.42
3:L:280:ARG:HG3	3:L:281:LEU:HG	2.00	0.42
2:K:824:ASN:O	2:K:828:ILE:HG12	2.20	0.42
2:K:909:GLN:O	2:K:913:ASN:N	2.53	0.42
1:A:4:LYS:H	1:A:4:LYS:HG2	1.54	0.42
2:K:757:ARG:HG3	2:K:781:GLU:HG2	2.01	0.42
2:K:951:GLU:CD	2:K:1149:ARG:HH22	2.28	0.42
2:K:860:MET:O	2:K:864:LYS:HE2	2.20	0.41
2:K:879:ILE:O	2:K:883:LEU:N	2.46	0.41
4:M:565:LYS:HA	4:M:565:LYS:HD3	1.96	0.41
5:N:258:LEU:HD21	5:N:285:LEU:HD23	2.02	0.41
4:O:288:ASP:CB	4:O:289:PRO:HD3	2.51	0.41
4:M:378:LYS:HB2	4:M:378:LYS:HE2	1.90	0.41
4:O:336:PHE:CE1	5:P:355:LEU:HD21	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:248:LEU:HD22	5:P:326:TYR:CD2	2.55	0.41
2:K:1162:LYS:HD2	2:K:1204:TYR:CE2	2.56	0.41
4:M:340:LEU:O	4:M:343:ILE:HG22	2.20	0.41
2:K:782:TRP:CE2	3:L:226:VAL:HG21	2.55	0.41
5:P:352:CYS:O	5:P:353:GLN:C	2.61	0.41
2:K:1081:ASN:N	2:K:1081:ASN:OD1	2.53	0.41
3:L:39:PRO:HB3	3:L:280:ARG:HD3	2.03	0.41
3:L:186:ASP:OD1	3:L:274:ASP:HB2	2.20	0.41
1:A:8:ARG:HD3	1:A:14:LYS:HZ3	1.86	0.41
2:K:1266:MET:HA	2:K:1269:PHE:HB3	2.02	0.41
3:L:131:ALA:HB1	3:L:173:LEU:HG	2.02	0.41
4:M:466:CYS:C	4:M:467:PRO:O	2.61	0.41
4:O:305:GLU:HG2	4:O:309:LYS:NZ	2.35	0.41
5:P:325:ILE:HG13	5:P:326:TYR:N	2.36	0.41
2:K:1018:ILE:HD13	2:K:1018:ILE:HA	1.92	0.41
3:L:340:TYR:HE2	3:L:421:ALA:HB3	1.86	0.41
2:K:666:VAL:HG11	4:O:552:PHE:CD1	2.56	0.40
3:L:19:ARG:HH21	3:L:302:GLY:CA	2.35	0.40
5:N:354:LEU:HD12	5:N:354:LEU:HA	1.88	0.40
5:N:386:LEU:H	5:N:386:LEU:HG	1.66	0.40
2:K:835:VAL:HA	2:K:838:ILE:HD13	2.03	0.40
2:K:1148:PHE:CZ	2:K:1312:VAL:HG11	2.57	0.40
2:K:1180:PHE:CD2	3:L:340:TYR:HB2	2.56	0.40
1:A:23:LYS:HB3	1:A:23:LYS:HE2	1.61	0.40
2:K:1196:LEU:HB3	2:K:1227:SER:HB2	2.04	0.40
3:L:94:LEU:HD23	3:L:94:LEU:HA	1.80	0.40
3:L:150:HIS:NE2	3:L:186:ASP:OD2	2.50	0.40
4:M:88:ASP:O	4:M:89:SER:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2	12
2	K	590/1536 (38%)	568 (96%)	22 (4%)	0	100	100
3	L	406/433 (94%)	392 (97%)	14 (3%)	0	100	100
4	M	347/684 (51%)	327 (94%)	20 (6%)	0	100	100
4	O	149/684 (22%)	143 (96%)	5 (3%)	1 (1%)	18	46
5	N	181/401 (45%)	175 (97%)	6 (3%)	0	100	100
5	P	182/401 (45%)	178 (98%)	4 (2%)	0	100	100
All	All	1877/4163 (45%)	1801 (96%)	74 (4%)	2 (0%)	49	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
4	O	289	PRO

5.3.2 Protein sidechains ⓘ

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	15/17 (88%)	12 (80%)	3 (20%)	1	4
2	K	479/1391 (34%)	479 (100%)	0	100	100
3	L	300/367 (82%)	299 (100%)	1 (0%)	86	84
4	M	275/653 (42%)	275 (100%)	0	100	100
4	O	111/653 (17%)	111 (100%)	0	100	100
5	N	152/359 (42%)	151 (99%)	1 (1%)	76	78
5	P	143/359 (40%)	143 (100%)	0	100	100
All	All	1475/3799 (39%)	1470 (100%)	5 (0%)	84	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	22	THR
1	A	23	LYS
3	L	122	ILE
5	N	252	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	690	ASN
2	K	727	GLN
2	K	1206	GLN
2	K	1221	HIS
3	L	341	ASN
4	M	325	ASN
4	M	342	ASN
4	M	346	HIS
4	M	444	GLN
4	M	495	GLN
4	M	545	ASN
5	N	317	GLN
5	N	358	GLN
4	O	583	GLN
5	P	263	HIS
5	P	277	GLN
5	P	330	HIS
5	P	389	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

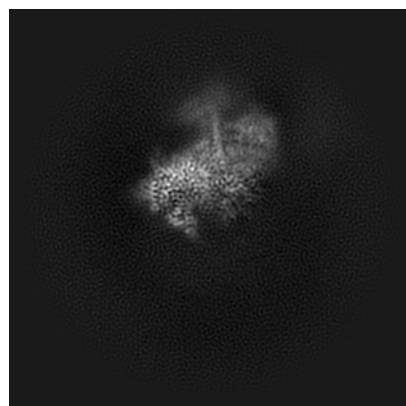
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35450. These allow visual inspection of the internal detail of the map and identification of artifacts.

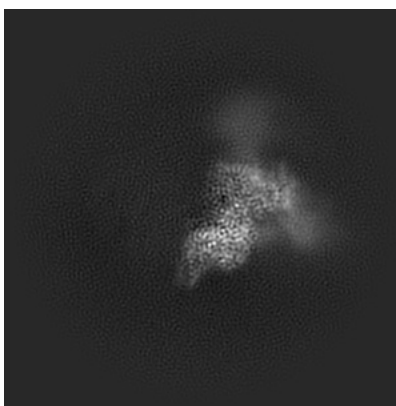
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

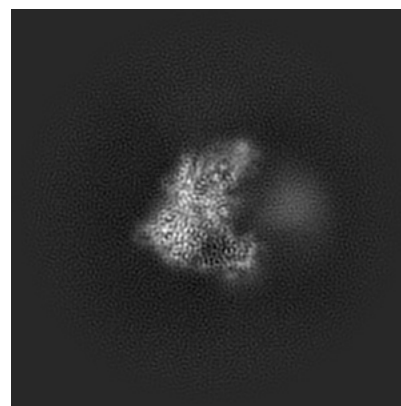
6.1.1 Primary map



X

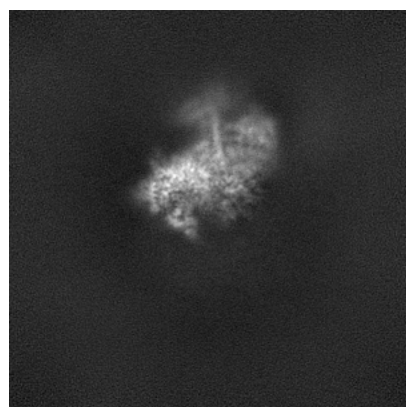


Y

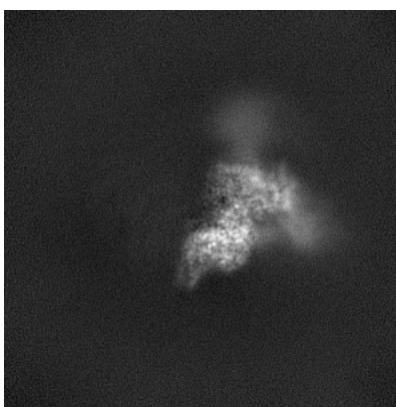


Z

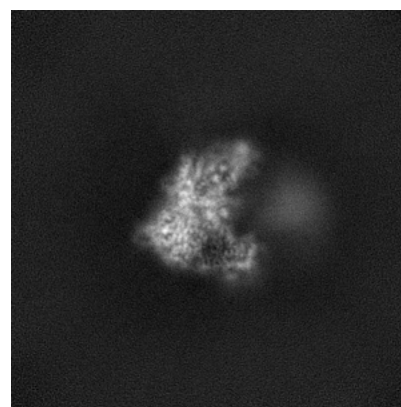
6.1.2 Raw map



X



Y

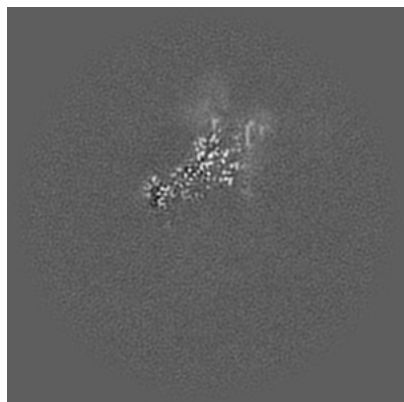


Z

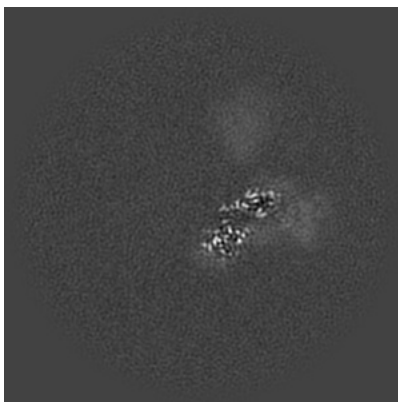
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

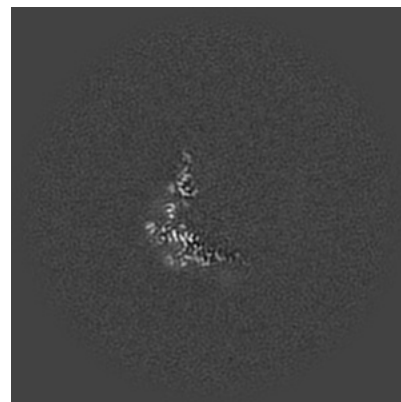
6.2.1 Primary map



X Index: 168

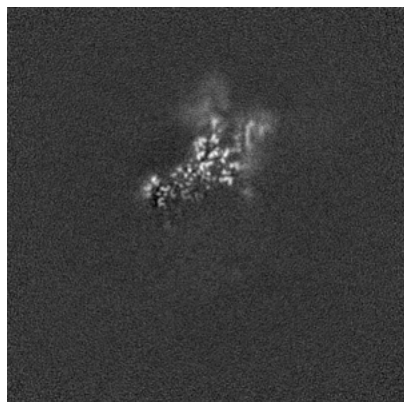


Y Index: 168

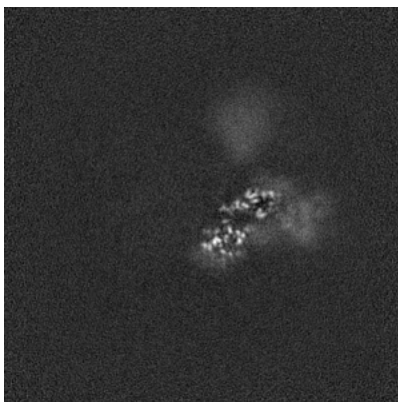


Z Index: 168

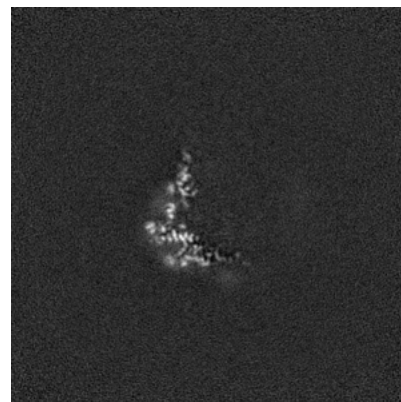
6.2.2 Raw map



X Index: 168



Y Index: 168

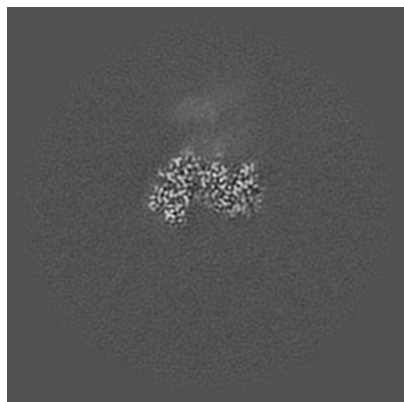


Z Index: 168

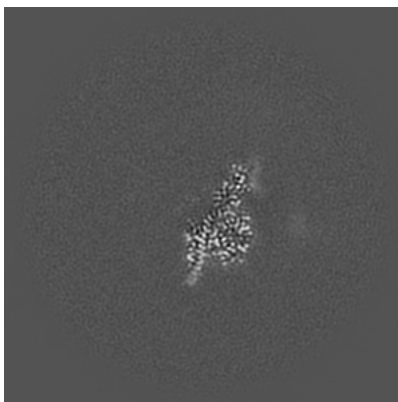
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

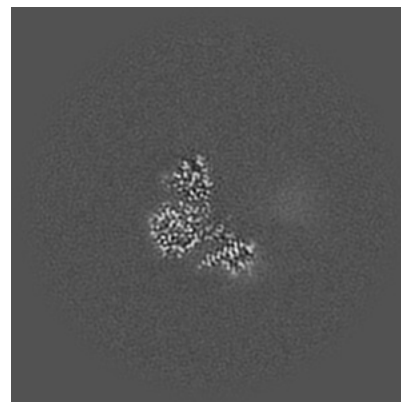
6.3.1 Primary map



X Index: 146

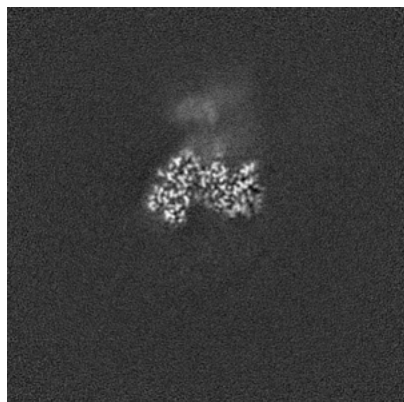


Y Index: 141

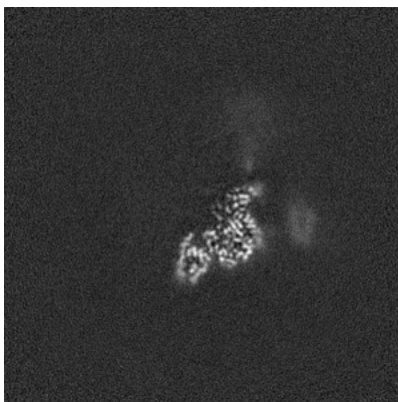


Z Index: 188

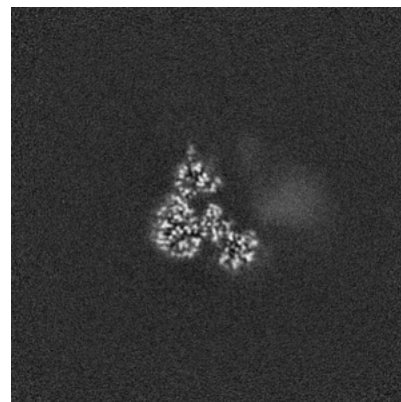
6.3.2 Raw map



X Index: 146



Y Index: 150

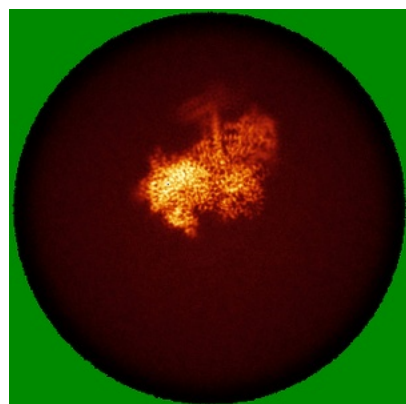


Z Index: 196

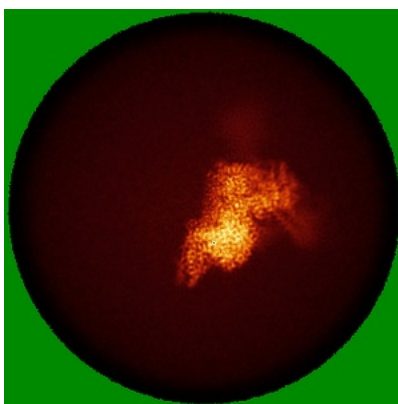
The images above show the largest variance slices of the map in three orthogonal directions.

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

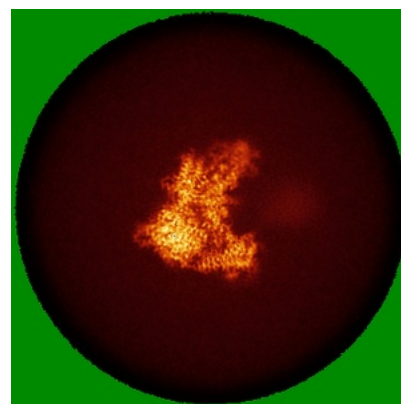
6.4.1 Primary map



X



Y

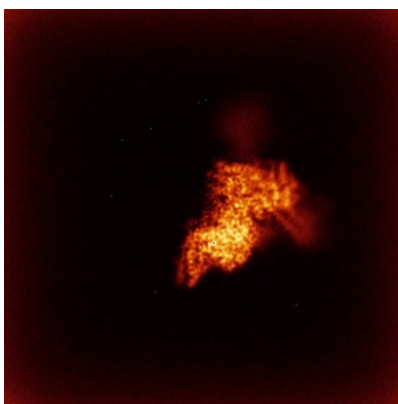


Z

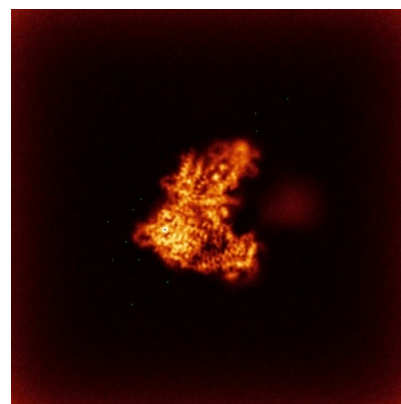
6.4.2 Raw map



X



Y

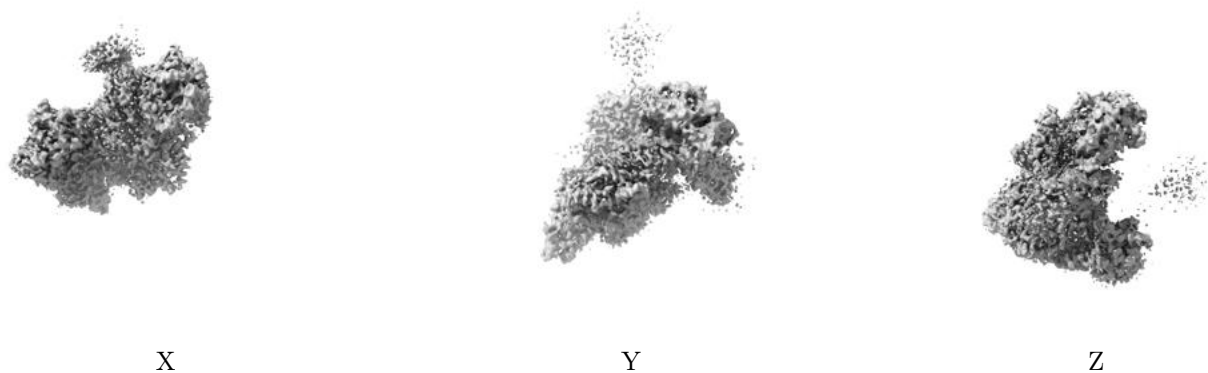


Z

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.

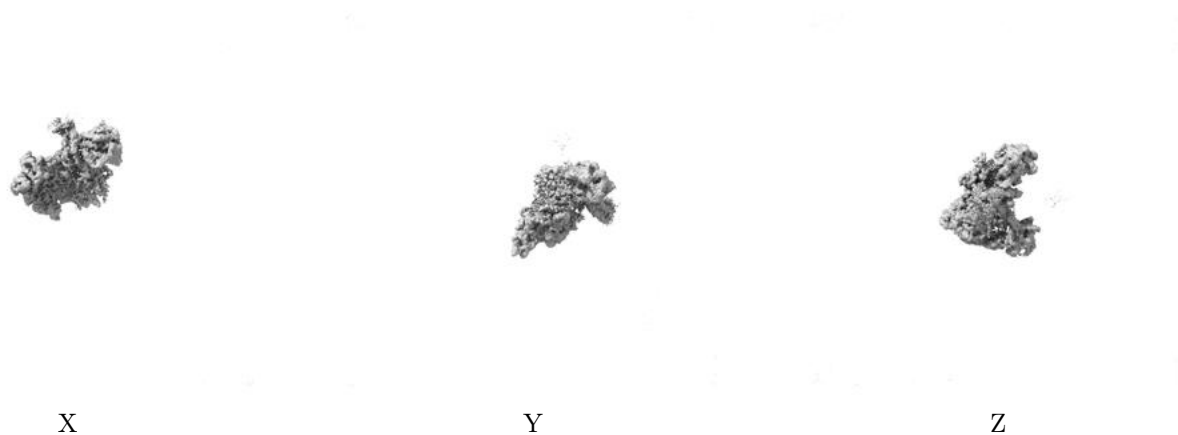
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.31. 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.

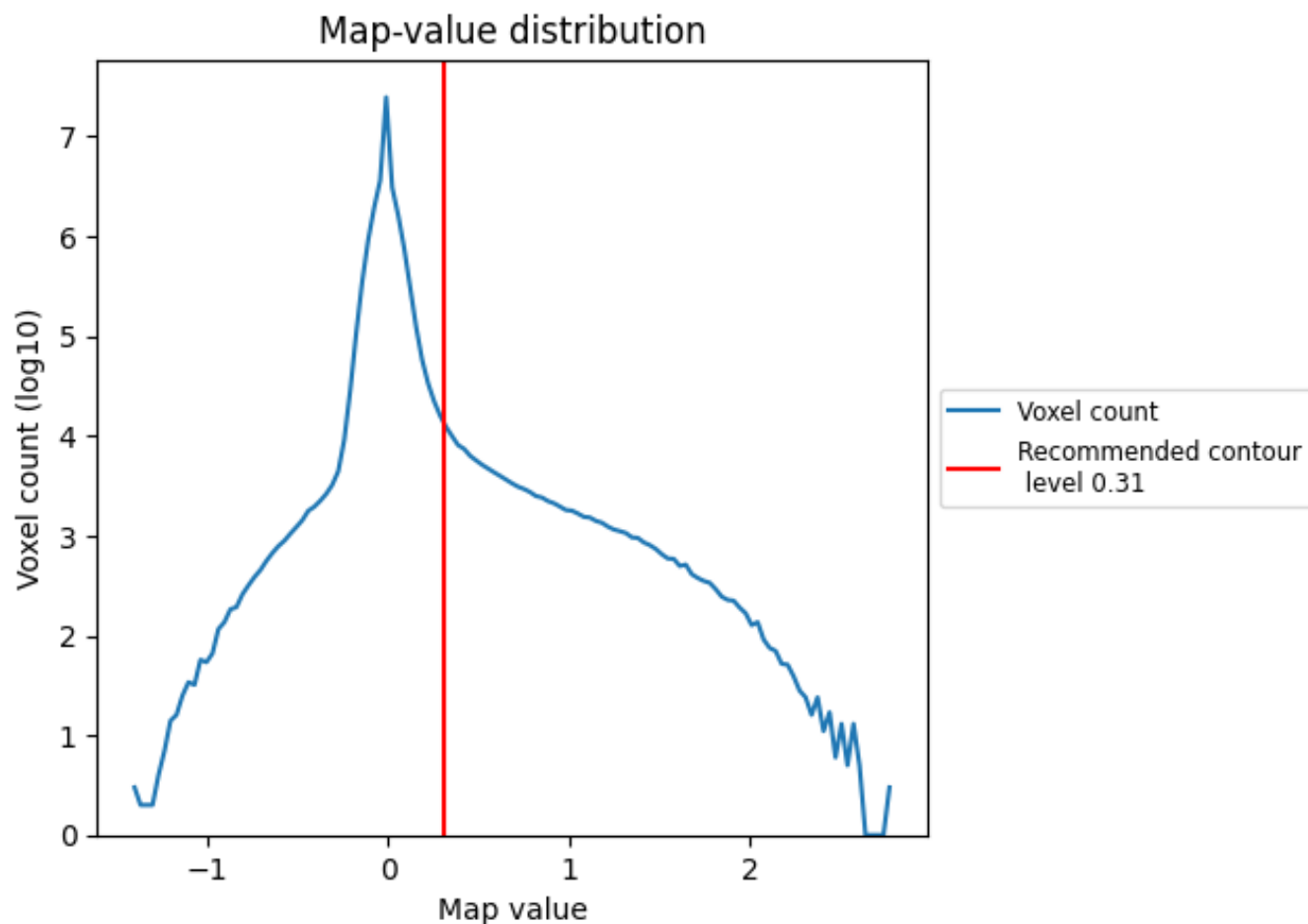
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

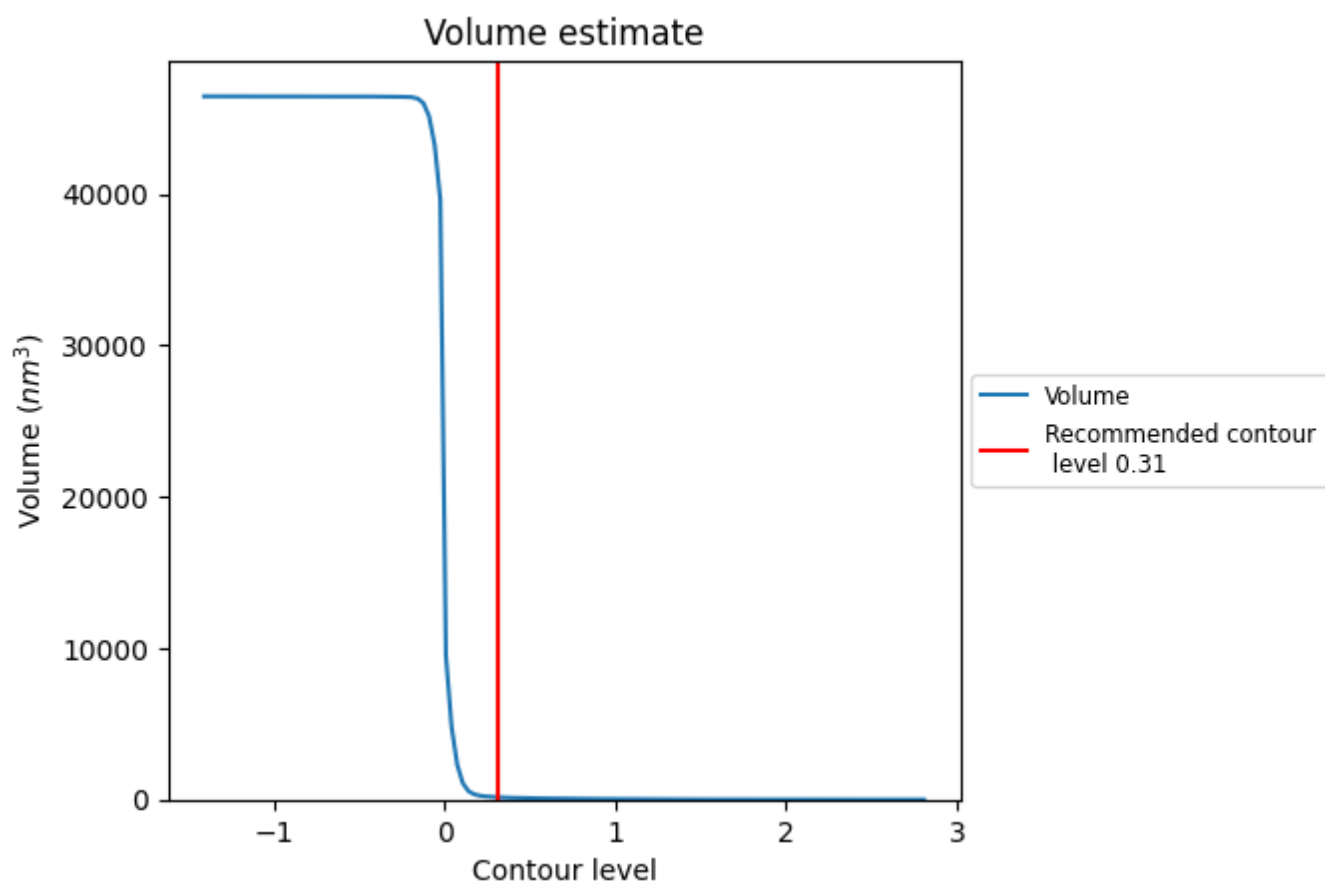
This section contains the results of statistical analysis of the map.

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.

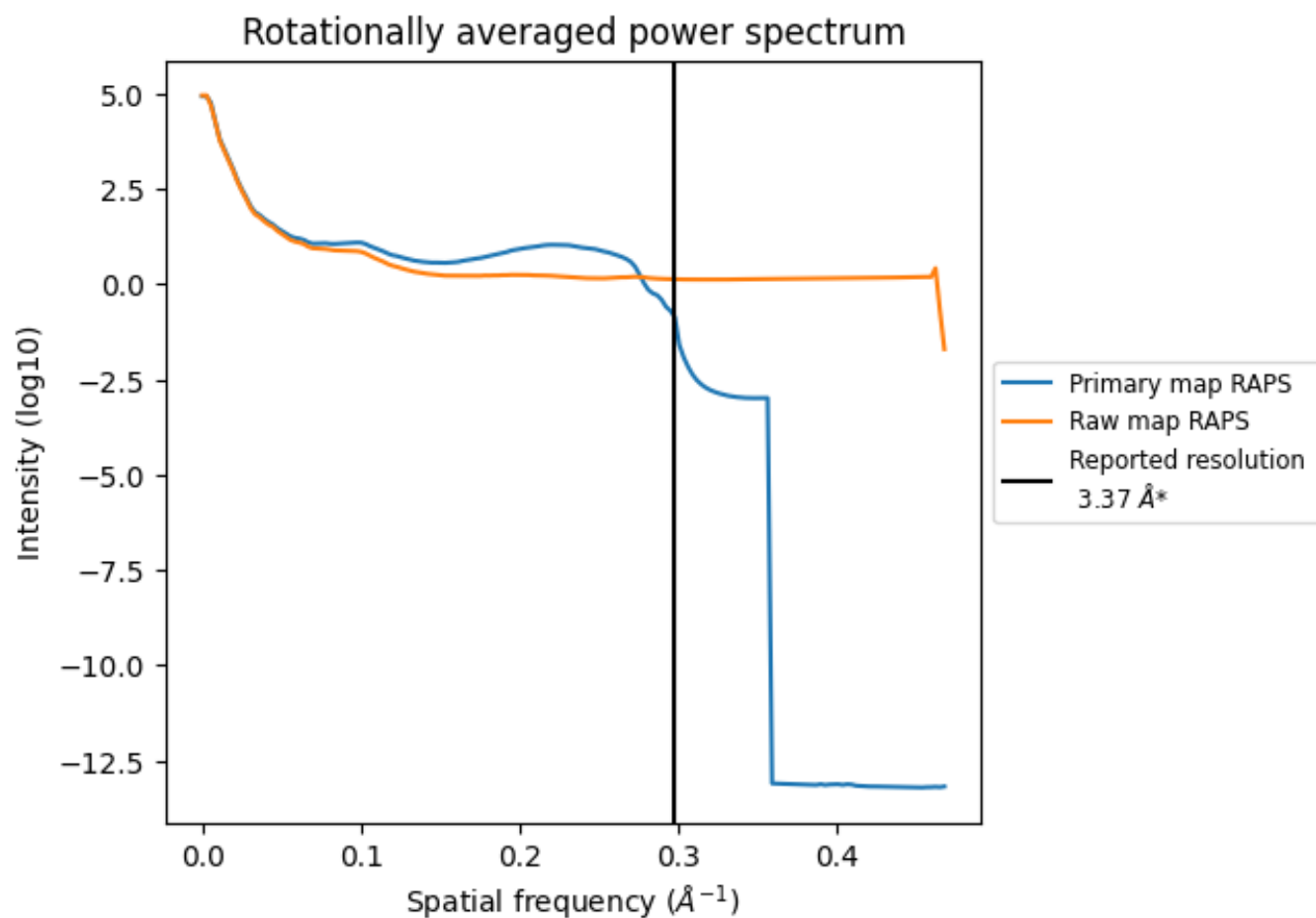
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

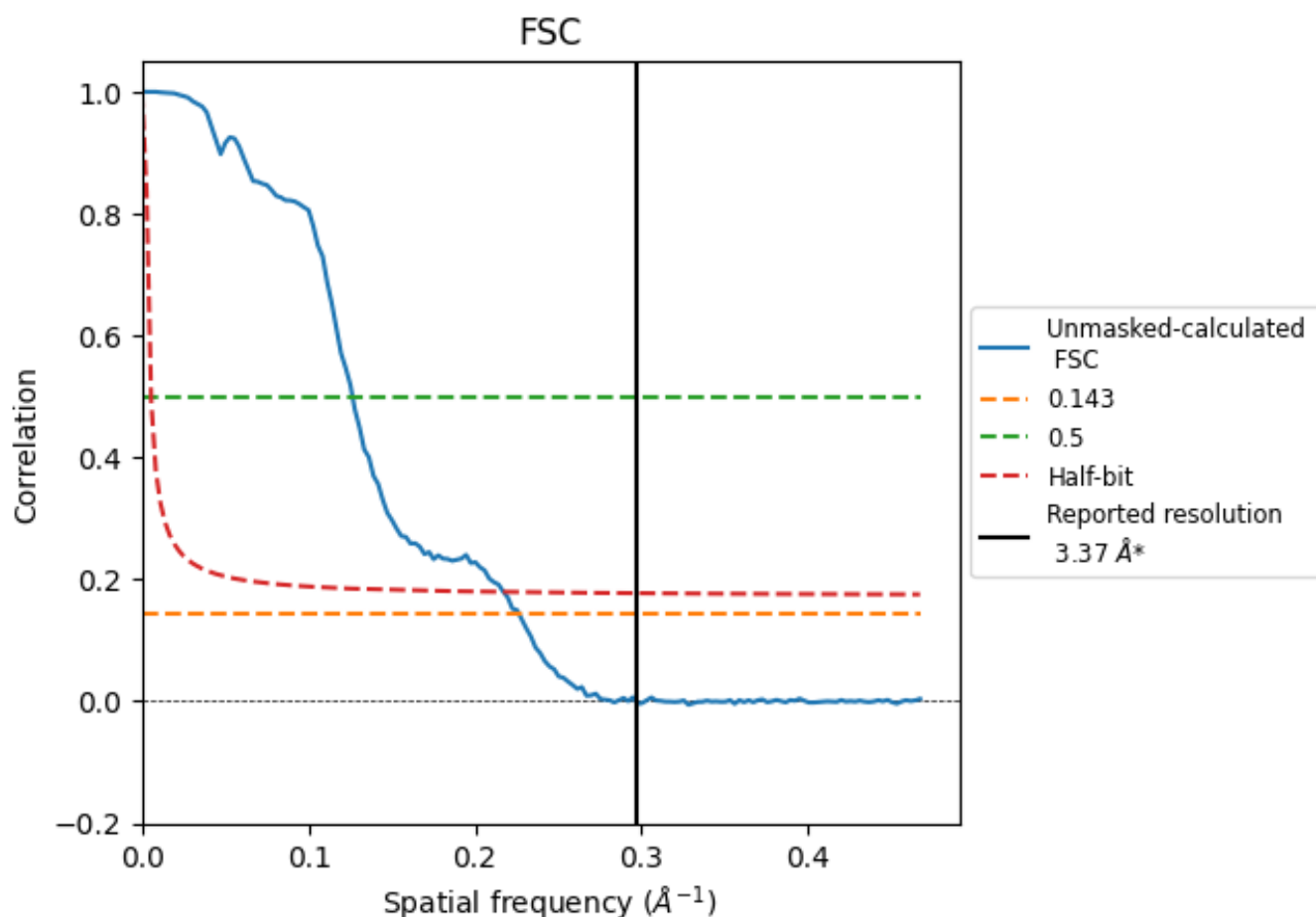


*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

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 $0.297 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

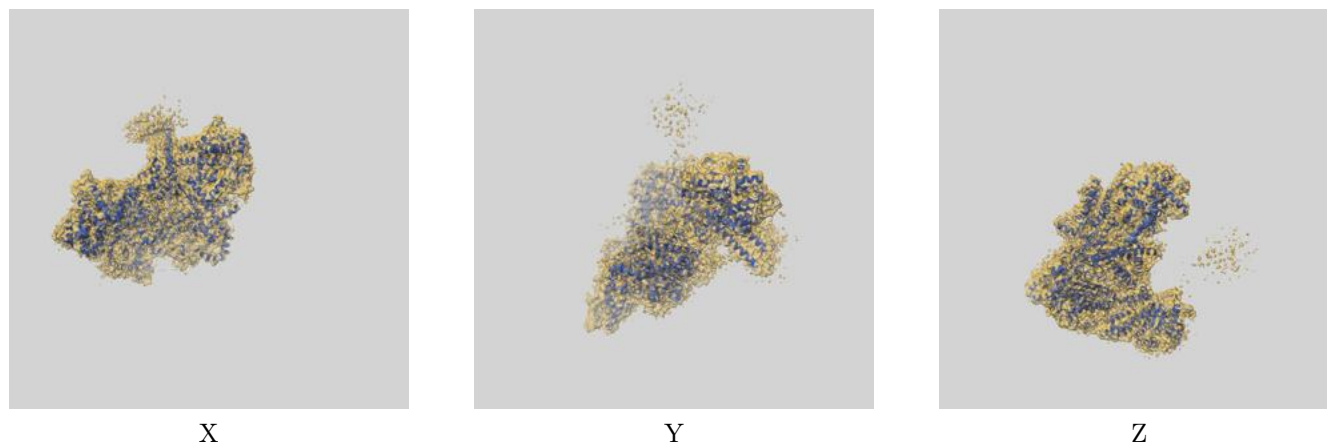
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.42	7.91	4.61

*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 4.42 differs from the reported value 3.37 by more than 10 %

9 Map-model fit [i](#)

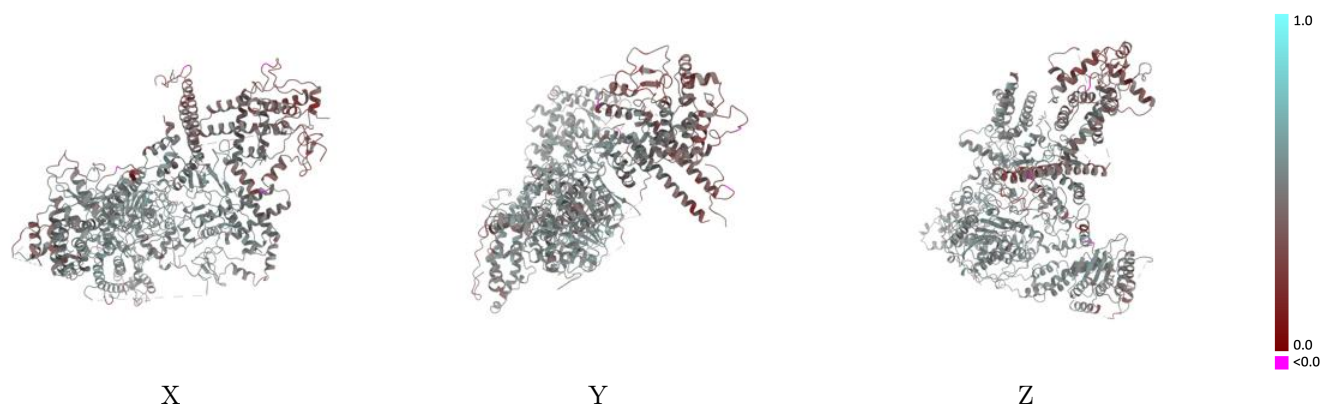
This section contains information regarding the fit between EMDB map EMD-35450 and PDB model 8IHN. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



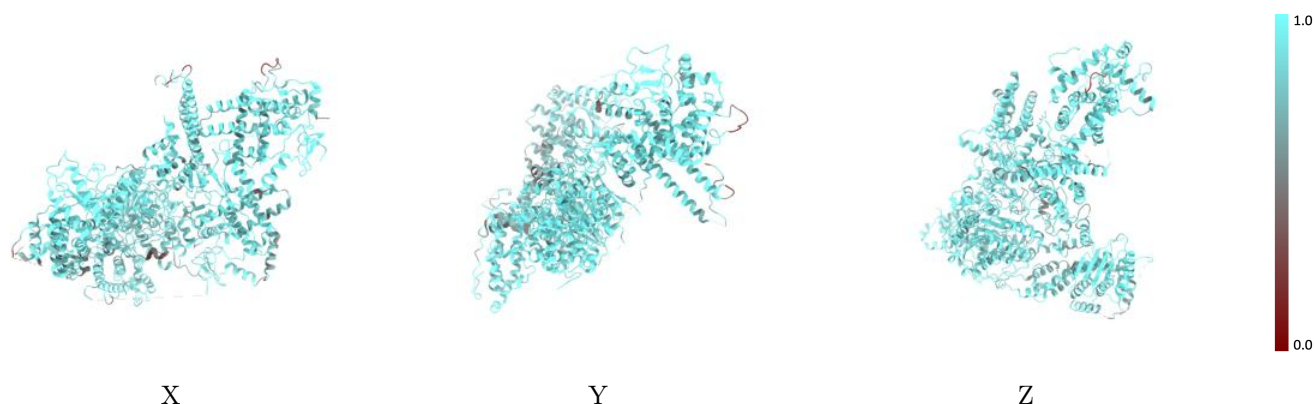
The images above show the 3D surface view of the map at the recommended contour level 0.31 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



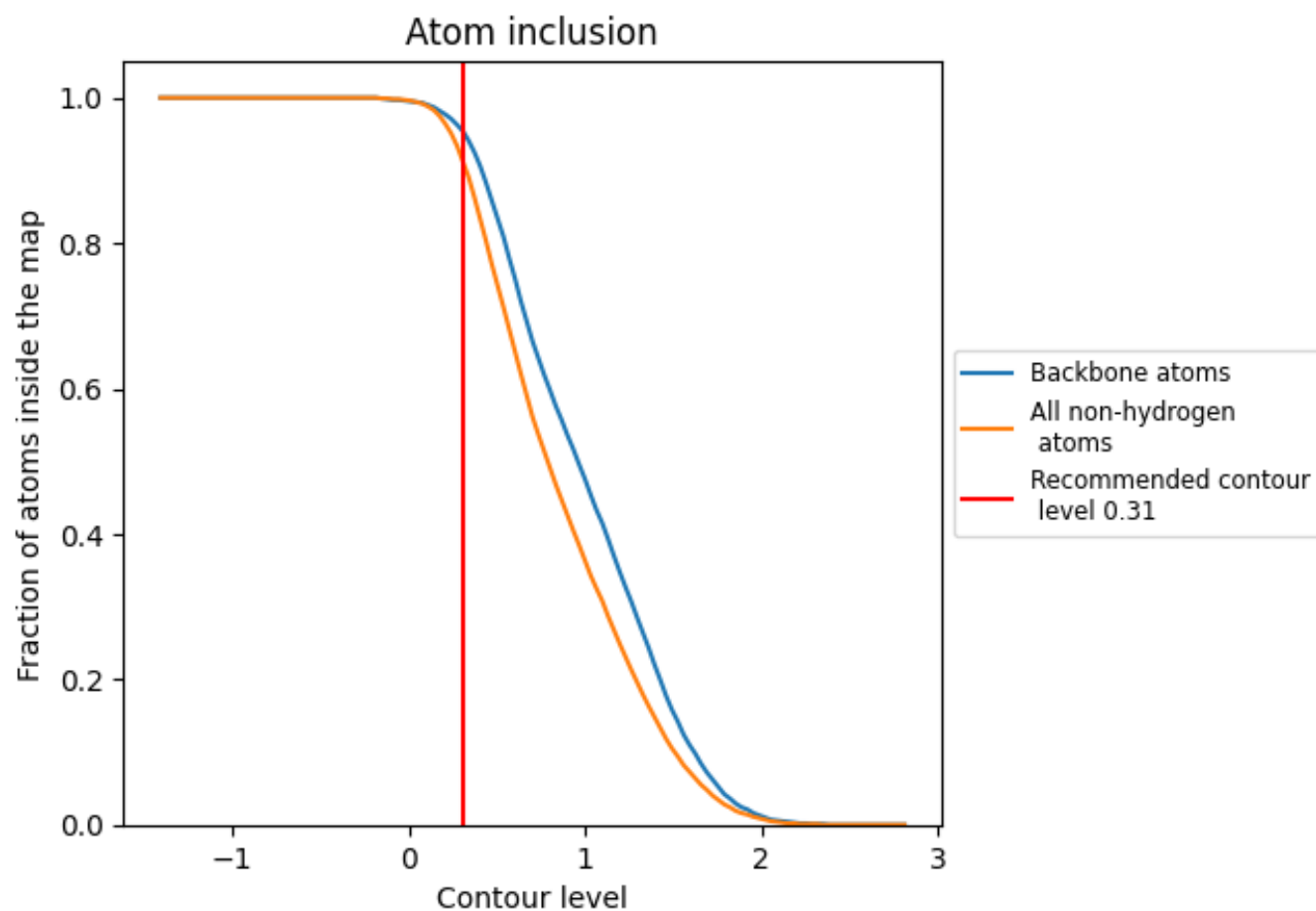
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.31).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.4800
A	0.7820	0.4460
K	0.9050	0.4920
L	0.9690	0.5240
M	0.8720	0.4860
N	0.9330	0.5090
O	0.8980	0.3740
P	0.8750	0.3950

1.0

0.0

<0.0