



Full wwPDB EM Validation Report ⓘ

Aug 21, 2025 – 09:32 pm BST

PDB ID : 9GS0 / pdb_00009gs0
EMDB ID : EMD-51530
Title : Capsid of full Haloferax tailed virus 1 without turret head protein gp31.
Authors : Zhang, D.; Daum, B.; Isupov, M.N.; McLaren, M.; Stuart, W.
Deposited on : 2024-09-13
Resolution : 2.37 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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.45.1

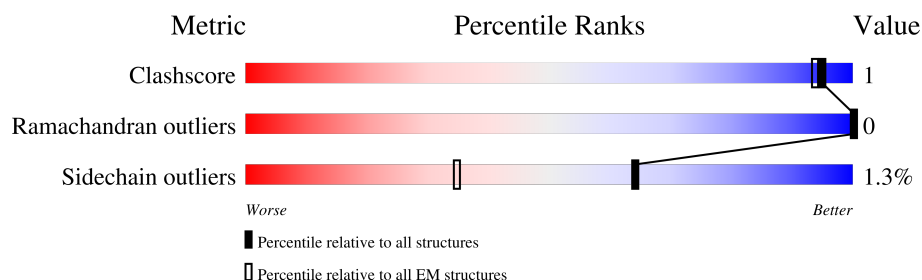
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.37 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.



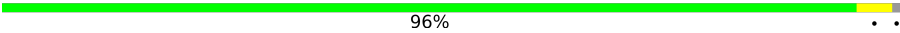
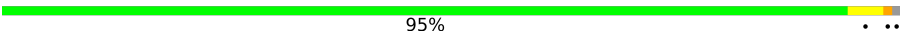
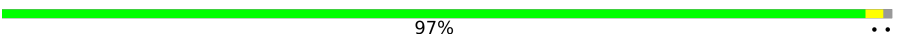
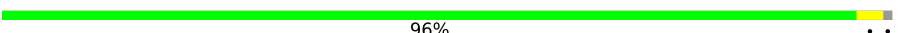
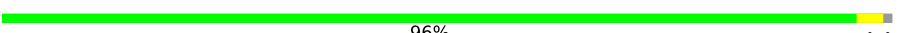
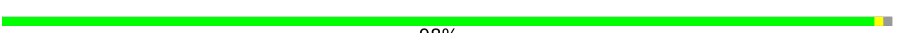






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	AA	396	69% 6% 25%
1	AB	396	70% 5% 25%
1	AC	396	70% . . 25%
1	AD	396	71% . 25%
1	AE	396	71% . . 25%
1	AF	396	68% 6% 25%
1	AG	396	71% . 25%
2	AI	137	95% . .

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Mol	Chain	Length	Quality of chain
2	AJ	137	 96% . .
2	AK	137	 95% . .
2	AL	137	 97% . .
2	AM	137	 96% . .
2	AN	137	 96% . .
2	AO	137	 98% . .
3	As	115	 94% 5% . .
3	At	115	 94% 5% . .
3	Au	115	 93% 6% . .
3	Av	115	 95% . .
3	Aw	115	 94% 5% . .
3	Ax	115	 93% 6% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27880 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 HK97 gp5-like major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	AB	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	AC	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	AD	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	AE	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	AF	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	AG	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		

- Molecule 2 is a protein called Capsid stabilization protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AI	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	AJ	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	AK	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	AL	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	AM	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	AN	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	AO	136	Total	C	N	O	S	0	0
			967	596	150	219	2		

- Molecule 3 is a protein called Gp30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	As	114	Total	C	N	O	0	0
			829	503	136	190		
3	At	114	Total	C	N	O	0	0
			829	503	136	190		
3	Au	114	Total	C	N	O	0	0
			829	503	136	190		
3	Av	114	Total	C	N	O	0	0
			829	503	136	190		
3	Aw	114	Total	C	N	O	0	0
			829	503	136	190		
3	Ax	114	Total	C	N	O	0	0
			829	503	136	190		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	AA	6	Total	Mg	0
			6	6	
4	AB	8	Total	Mg	0
			8	8	
4	AC	6	Total	Mg	0
			6	6	
4	AD	6	Total	Mg	0
			6	6	
4	AE	6	Total	Mg	0
			6	6	
4	AF	4	Total	Mg	0
			4	4	
4	As	1	Total	Mg	0
			1	1	
4	At	1	Total	Mg	0
			1	1	
4	Au	1	Total	Mg	0
			1	1	
4	Av	1	Total	Mg	0
			1	1	
4	Aw	1	Total	Mg	0
			1	1	
4	Ax	1	Total	Mg	0
			1	1	
4	AG	6	Total	Mg	0
			6	6	

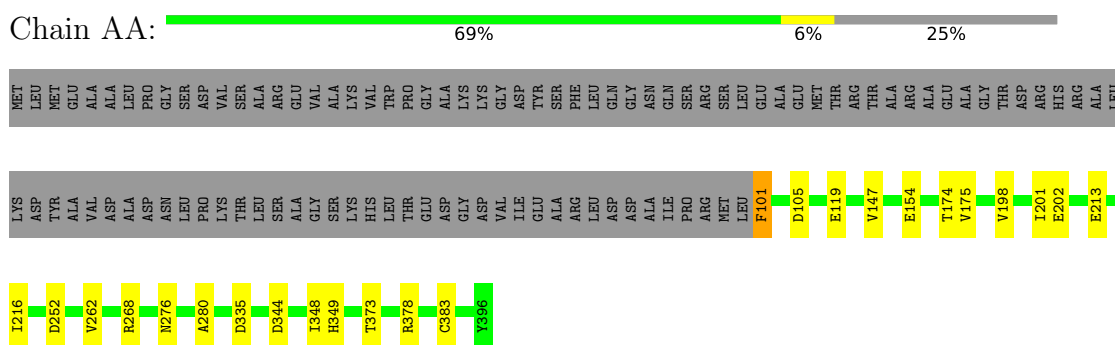
- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	AI	1	Total 1	K 1	0
5	AL	1	Total 1	K 1	0
5	AO	1	Total 1	K 1	0

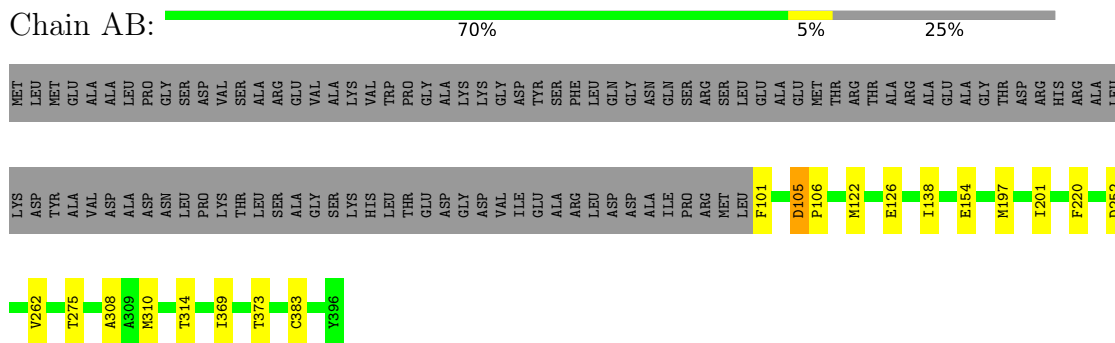
3 Residue-property plots

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

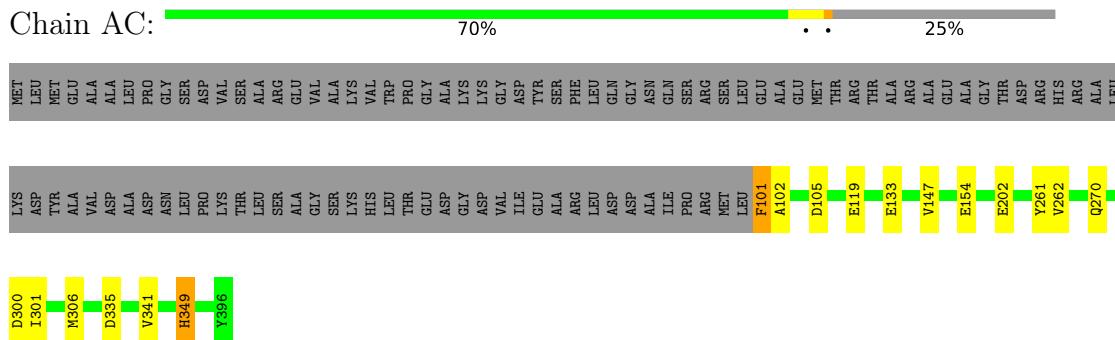
- Molecule 1: HK97 gp5-like major capsid protein



- Molecule 1: HK97 gp5-like major capsid protein

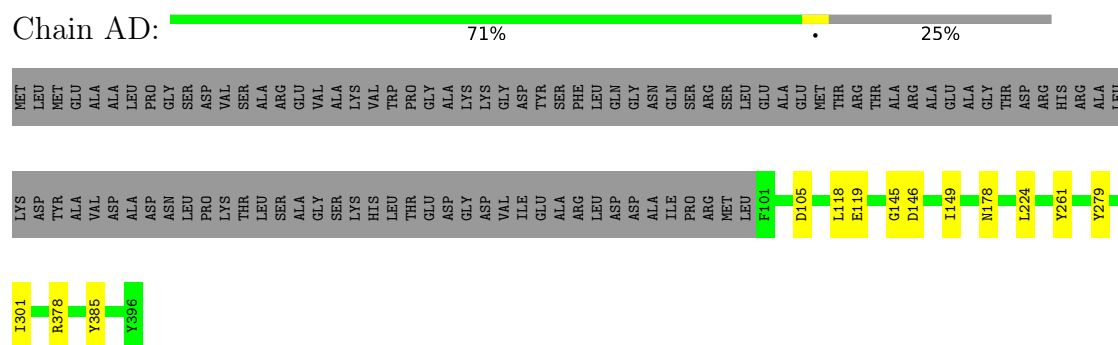


- Molecule 1: HK97 gp5-like major capsid protein



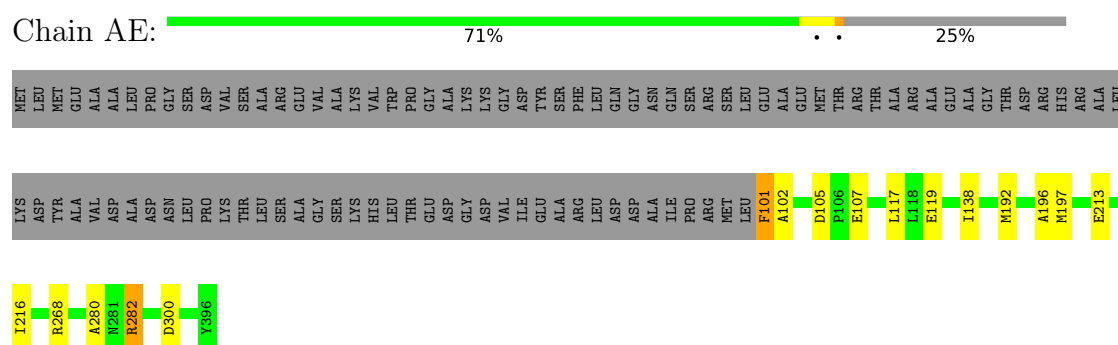
• Molecule 1: HK97 gp5-like major capsid protein

Chain AD:



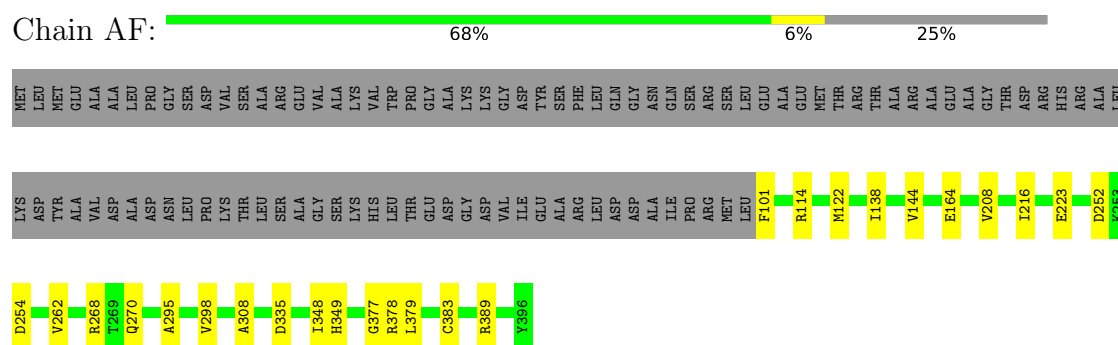
• Molecule 1: HK97 gp5-like major capsid protein

Chain AE:



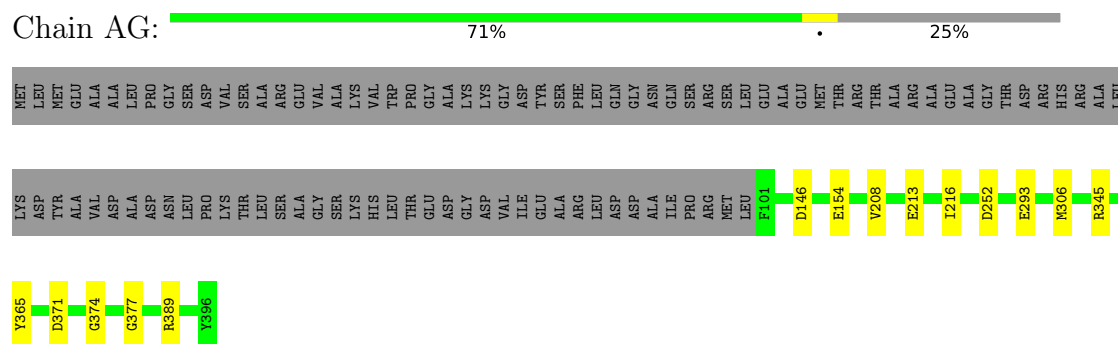
• Molecule 1: HK97 gp5-like major capsid protein

Chain AF:



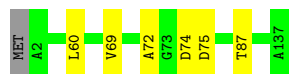
• Molecule 1: HK97 gp5-like major capsid protein

Chain AG:



- Molecule 2: Capsid stabilization protein

Chain AI:  95% ..



- Molecule 2: Capsid stabilization protein

Chain AJ:  96% ..



- Molecule 2: Capsid stabilization protein

Chain AK:  95% ..



- Molecule 2: Capsid stabilization protein

Chain AL:  97% ..



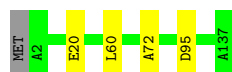
- Molecule 2: Capsid stabilization protein

Chain AM:  96% ..



- Molecule 2: Capsid stabilization protein

Chain AN:  96% ..



- Molecule 2: Capsid stabilization protein

Chain AO:  98% ..



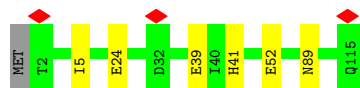
- Molecule 3: Gp30

Chain As:  94% 5% .



• Molecule 3: Gp30

Chain At:  94% 5% .



• Molecule 3: Gp30

Chain Au:  93% 6% .



• Molecule 3: Gp30

Chain Av:  95% 5% .



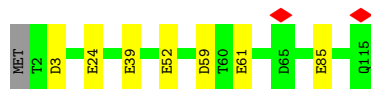
• Molecule 3: Gp30

Chain Aw:  94% 5% .



• Molecule 3: Gp30

Chain Ax:  93% 6% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2512500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.579	Depositor
Minimum map value	-1.129	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.137	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	1049.2161, 1049.2161, 1049.2161	wwPDB
Map dimensions	896, 896, 896	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1710001, 1.1710001, 1.1710001	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: K, 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	AA	0.78	6/2335 (0.3%)	1.18	5/3172 (0.2%)
1	AB	0.78	4/2335 (0.2%)	1.16	0/3172
1	AC	0.77	6/2335 (0.3%)	1.18	4/3172 (0.1%)
1	AD	0.73	2/2335 (0.1%)	1.16	1/3172 (0.0%)
1	AE	0.72	1/2335 (0.0%)	1.18	3/3172 (0.1%)
1	AF	0.78	2/2335 (0.1%)	1.18	3/3172 (0.1%)
1	AG	0.79	4/2335 (0.2%)	1.15	2/3172 (0.1%)
2	AI	0.74	0/980	1.00	0/1337
2	AJ	0.73	0/980	1.00	0/1337
2	AK	0.72	0/980	1.01	2/1337 (0.1%)
2	AL	0.78	3/980 (0.3%)	1.03	1/1337 (0.1%)
2	AM	0.77	1/980 (0.1%)	1.01	1/1337 (0.1%)
2	AN	0.79	1/980 (0.1%)	1.00	1/1337 (0.1%)
2	AO	0.76	0/980	1.01	0/1337
3	As	1.14	4/836 (0.5%)	1.03	0/1137
3	At	1.14	4/836 (0.5%)	1.06	0/1137
3	Au	1.18	9/836 (1.1%)	1.09	0/1137
3	Av	1.15	4/836 (0.5%)	1.05	0/1137
3	Aw	1.24	7/836 (0.8%)	1.03	1/1137 (0.1%)
3	Ax	1.18	8/836 (1.0%)	1.06	1/1137 (0.1%)
All	All	0.85	66/28221 (0.2%)	1.11	25/38385 (0.1%)

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	AB	0	1
1	AC	0	1
1	AE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	AF	0	1
All	All	0	4

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Aw	59	ASP	CG-OD2	-11.13	1.04	1.25
1	AG	154	GLU	CD-OE2	-10.93	1.04	1.25
1	AF	164	GLU	CD-OE1	-10.80	1.04	1.25
3	Aw	59	ASP	CG-OD1	-10.59	1.05	1.25
1	AG	154	GLU	CD-OE1	-10.48	1.05	1.25
1	AB	154	GLU	CD-OE2	-9.65	1.07	1.25
1	AF	164	GLU	CD-OE2	-9.59	1.07	1.25
1	AA	154	GLU	CD-OE2	-8.99	1.08	1.25
1	AB	154	GLU	CD-OE1	-8.87	1.08	1.25
1	AA	154	GLU	CD-OE1	-8.75	1.08	1.25
3	Au	52	GLU	CD-OE1	-6.98	1.12	1.25
3	Aw	52	GLU	CD-OE1	-6.86	1.12	1.25
2	AN	20	GLU	CD-OE2	-6.76	1.12	1.25
1	AB	197	MET	CG-SD	-6.74	1.63	1.80
1	AA	335	ASP	CG-OD2	-6.48	1.13	1.25
3	Ax	59	ASP	CG-OD2	-6.38	1.13	1.25
3	Aw	52	GLU	CD-OE2	-6.19	1.13	1.25
3	Au	59	ASP	CG-OD2	-6.18	1.13	1.25
3	Ax	52	GLU	CD-OE1	-6.13	1.13	1.25
1	AA	335	ASP	CG-OD1	-6.01	1.14	1.25
3	As	52	GLU	CD-OE2	-5.98	1.14	1.25
3	Ax	52	GLU	CD-OE2	-5.94	1.14	1.25
1	AA	119	GLU	CD-OE1	-5.83	1.14	1.25
3	At	24	GLU	CD-OE1	-5.83	1.14	1.25
3	Av	39	GLU	CD-OE2	-5.82	1.14	1.25
1	AD	119	GLU	CD-OE1	-5.75	1.14	1.25
3	As	52	GLU	CD-OE1	-5.74	1.14	1.25
3	Aw	85	GLU	CD-OE2	-5.66	1.14	1.25
3	Au	52	GLU	CD-OE2	-5.63	1.14	1.25
3	Ax	39	GLU	CD-OE2	-5.62	1.14	1.25
3	Ax	24	GLU	CD-OE1	-5.61	1.14	1.25
1	AC	119	GLU	CD-OE1	-5.60	1.14	1.25
3	Au	61	GLU	CD-OE2	-5.58	1.14	1.25
1	AC	300	ASP	CG-OD1	-5.54	1.14	1.25
3	Ax	61	GLU	CD-OE1	-5.51	1.14	1.25
1	AG	293	GLU	CD-OE2	-5.49	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AG	293	GLU	CD-OE1	-5.45	1.15	1.25
3	Av	61	GLU	CD-OE1	-5.42	1.15	1.25
3	Av	39	GLU	CD-OE1	-5.41	1.15	1.25
2	AL	123	GLU	CD-OE2	-5.37	1.15	1.25
3	Av	52	GLU	CD-OE1	-5.36	1.15	1.25
3	Ax	85	GLU	CD-OE2	-5.36	1.15	1.25
1	AC	154	GLU	CD-OE1	-5.27	1.15	1.25
2	AL	123	GLU	CD-OE1	-5.26	1.15	1.25
3	At	39	GLU	CD-OE2	-5.23	1.15	1.25
3	At	41	HIS	CE1-NE2	-5.22	1.27	1.32
3	Au	76	GLU	CD-OE2	-5.19	1.15	1.25
3	As	39	GLU	CD-OE1	-5.17	1.15	1.25
3	Au	24	GLU	CD-OE1	-5.17	1.15	1.25
3	Aw	61	GLU	CD-OE2	-5.16	1.15	1.25
2	AL	20	GLU	CD-OE2	-5.16	1.15	1.25
1	AC	202	GLU	CD-OE2	-5.15	1.15	1.25
3	Ax	59	ASP	CG-OD1	-5.15	1.15	1.25
1	AC	300	ASP	CG-OD2	-5.14	1.15	1.25
3	Au	59	ASP	CG-OD1	-5.13	1.15	1.25
1	AC	119	GLU	CD-OE2	-5.09	1.15	1.25
1	AE	119	GLU	CD-OE1	-5.08	1.15	1.25
1	AD	119	GLU	CD-OE2	-5.08	1.15	1.25
3	Au	61	GLU	CD-OE1	-5.08	1.15	1.25
3	At	52	GLU	CD-OE1	-5.07	1.15	1.25
2	AM	123	GLU	CD-OE2	-5.06	1.15	1.25
3	As	22	ASP	CG-OD1	-5.06	1.15	1.25
1	AA	202	GLU	CD-OE2	-5.05	1.15	1.25
3	Aw	39	GLU	CD-OE2	-5.04	1.15	1.25
3	Au	24	GLU	CD-OE2	-5.03	1.15	1.25
1	AB	126	GLU	CD-OE2	-5.01	1.15	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AC	335	ASP	CA-CB-CG	8.49	121.09	112.60
1	AF	335	ASP	CA-CB-CG	6.55	119.15	112.60
1	AE	280	ALA	CA-C-N	6.18	128.81	120.65
1	AE	280	ALA	C-N-CA	6.18	128.81	120.65
2	AK	95	ASP	CA-CB-CG	6.14	118.74	112.60
2	AL	95	ASP	CA-CB-CG	5.95	118.55	112.60
2	AN	95	ASP	CA-CB-CG	5.71	118.31	112.60
1	AA	280	ALA	CA-C-N	5.60	128.09	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	280	ALA	C-N-CA	5.60	128.09	120.54
1	AG	252	ASP	CA-C-N	5.59	127.77	120.28
1	AG	252	ASP	C-N-CA	5.59	127.77	120.28
1	AC	105	ASP	CB-CA-C	-5.52	102.48	112.76
3	Ax	3	ASP	CA-CB-CG	5.46	118.06	112.60
1	AF	254	ASP	CA-CB-CG	5.43	118.03	112.60
2	AM	95	ASP	CA-CB-CG	5.42	118.02	112.60
1	AF	389	ARG	CG-CD-NE	-5.41	100.09	112.00
2	AK	75	ASP	CA-CB-CG	5.37	117.97	112.60
1	AA	344	ASP	CA-C-N	5.36	128.00	120.28
1	AA	344	ASP	C-N-CA	5.36	128.00	120.28
1	AE	300	ASP	CA-CB-CG	5.22	117.82	112.60
1	AA	101	PHE	CA-CB-CG	5.08	118.88	113.80
1	AD	178	ASN	CB-CA-C	5.07	117.94	110.14
1	AC	300	ASP	CA-CB-CG	5.07	117.67	112.60
1	AC	349	HIS	CA-CB-CG	-5.04	108.75	113.80
3	Aw	3	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	101	PHE	Peptide
1	AC	101	PHE	Peptide
1	AE	101	PHE	Peptide
1	AF	101	PHE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2298	0	2139	7	0
1	AB	2298	0	2139	11	0
1	AC	2298	0	2139	6	0
1	AD	2298	0	2139	6	0
1	AE	2298	0	2139	10	0
1	AF	2298	0	2139	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AG	2298	0	2139	5	0
2	AI	967	0	894	2	0
2	AJ	967	0	894	2	0
2	AK	967	0	894	2	0
2	AL	967	0	894	0	0
2	AM	967	0	894	1	0
2	AN	967	0	894	1	0
2	AO	967	0	894	1	0
3	As	829	0	779	0	0
3	At	829	0	779	0	0
3	Au	829	0	779	0	0
3	Av	829	0	779	0	0
3	Aw	829	0	779	0	0
3	Ax	829	0	779	0	0
4	AA	6	0	0	0	0
4	AB	8	0	0	0	0
4	AC	6	0	0	0	0
4	AD	6	0	0	0	0
4	AE	6	0	0	0	0
4	AF	4	0	0	0	0
4	AG	6	0	0	0	0
4	As	1	0	0	0	0
4	At	1	0	0	0	0
4	Au	1	0	0	0	0
4	Av	1	0	0	0	0
4	Aw	1	0	0	0	0
4	Ax	1	0	0	0	0
5	AI	1	0	0	0	0
5	AL	1	0	0	0	0
5	AO	1	0	0	0	0
All	All	27880	0	25905	54	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 1.

All (54) 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:AB:122:MET:HE2	1:AC:147:VAL:HG21	1.57	0.86
1:AB:122:MET:HE1	1:AC:349:HIS:CE1	2.16	0.79
1:AE:117:LEU:HD13	1:AE:197:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:213:GLU:HA	1:AE:216:ILE:HD12	1.76	0.67
2:AK:73:GLY:O	2:AK:76:CYS:SG	2.62	0.58
2:AO:60:LEU:HD21	2:AO:72:ALA:HB2	1.85	0.58
2:AN:60:LEU:HD21	2:AN:72:ALA:HB2	1.87	0.56
1:AG:213:GLU:HA	1:AG:216:ILE:HD12	1.90	0.53
1:AF:262:VAL:HG12	1:AF:308:ALA:HB3	1.90	0.53
2:AI:60:LEU:HD21	2:AI:72:ALA:HB2	1.93	0.51
1:AE:117:LEU:HB3	1:AE:197:MET:HE1	1.93	0.51
1:AD:261:TYR:CE1	1:AD:301:ILE:HD11	2.46	0.51
2:AJ:60:LEU:HD21	2:AJ:72:ALA:HB2	1.94	0.50
1:AB:201:ILE:HD11	1:AB:373:THR:HG21	1.92	0.50
1:AF:216:ILE:HD11	1:AF:379:LEU:CD2	2.43	0.49
1:AB:122:MET:HE1	1:AC:349:HIS:NE2	2.27	0.48
1:AF:348:ILE:HD11	1:AF:383:CYS:SG	2.55	0.47
1:AG:208:VAL:CG1	1:AG:377:GLY:HA3	2.45	0.47
1:AA:252:ASP:CG	1:AF:268:ARG:HH11	2.24	0.46
1:AA:378:ARG:HE	1:AG:371:ASP:CG	2.23	0.46
1:AD:261:TYR:CZ	1:AD:301:ILE:HD11	2.51	0.46
1:AE:268:ARG:HH11	1:AF:252:ASP:CG	2.24	0.46
1:AB:138:ILE:HD12	1:AB:138:ILE:N	2.31	0.45
1:AC:101:PHE:CG	1:AC:102:ALA:N	2.83	0.45
1:AC:133:GLU:C	1:AC:306:MET:HE1	2.41	0.45
1:AB:262:VAL:HG22	1:AB:308:ALA:HB3	1.98	0.45
1:AF:138:ILE:HD11	1:AF:349:HIS:CD2	2.52	0.45
1:AB:201:ILE:CD1	1:AB:373:THR:HG21	2.46	0.44
1:AG:365:TYR:CZ	1:AG:374:GLY:HA3	2.52	0.44
1:AA:213:GLU:HA	1:AA:216:ILE:HD12	1.99	0.44
2:AK:60:LEU:HD21	2:AK:72:ALA:HB2	1.99	0.44
1:AA:201:ILE:HD11	1:AA:373:THR:HG21	2.00	0.43
1:AB:105:ASP:N	1:AB:106:PRO:HD2	2.33	0.43
2:AM:25:TYR:CZ	2:AM:56:LEU:HD21	2.53	0.43
1:AD:145:GLY:O	1:AD:146:ASP:OD1	2.36	0.43
1:AE:117:LEU:HD13	1:AE:197:MET:CE	2.46	0.43
1:AF:208:VAL:CG1	1:AF:377:GLY:HA3	2.49	0.43
1:AB:310:MET:HE2	1:AB:314:THR:HG21	2.00	0.42
1:AF:223:GLU:HG2	1:AF:383:CYS:SG	2.59	0.42
1:AE:101:PHE:N	1:AE:107:GLU:OE2	2.52	0.42
1:AA:348:ILE:HD11	1:AA:383:CYS:SG	2.59	0.42
1:AD:279:TYR:CG	1:AE:282:ARG:HD2	2.55	0.42
2:AJ:21:GLU:HG3	2:AJ:23:ARG:HH21	1.85	0.42
1:AA:349:HIS:CE1	1:AF:122:MET:HE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:118:LEU:HD11	1:AE:138:ILE:HD13	2.01	0.42
1:AE:101:PHE:CG	1:AE:102:ALA:N	2.88	0.41
1:AG:306:MET:HB2	1:AG:345:ARG:NH1	2.35	0.41
1:AA:268:ARG:HH11	1:AB:252:ASP:CG	2.28	0.41
2:AI:74:ASP:O	2:AI:75:ASP:HB2	2.19	0.41
1:AC:261:TYR:OH	1:AC:301:ILE:HD12	2.21	0.41
1:AF:295:ALA:HB3	1:AF:298:VAL:HG23	2.02	0.41
1:AE:192:MET:HE3	1:AE:196:ALA:HB2	2.03	0.41
1:AB:220:PHE:HA	1:AB:383:CYS:SG	2.61	0.40
1:AD:224:LEU:HD12	1:AD:385:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	AA	294/396 (74%)	283 (96%)	11 (4%)	0	100	100
1	AB	294/396 (74%)	284 (97%)	10 (3%)	0	100	100
1	AC	294/396 (74%)	281 (96%)	13 (4%)	0	100	100
1	AD	294/396 (74%)	282 (96%)	12 (4%)	0	100	100
1	AE	294/396 (74%)	285 (97%)	9 (3%)	0	100	100
1	AF	294/396 (74%)	284 (97%)	10 (3%)	0	100	100
1	AG	294/396 (74%)	288 (98%)	6 (2%)	0	100	100
2	AI	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
2	AJ	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
2	AK	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
2	AL	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
2	AM	134/137 (98%)	131 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AN	134/137 (98%)	133 (99%)	1 (1%)	0	100	100
2	AO	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
3	As	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
3	At	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
3	Au	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
3	Av	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
3	Aw	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
3	Ax	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
All	All	3668/4421 (83%)	3559 (97%)	109 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	244/322 (76%)	236 (97%)	8 (3%)	33	50
1	AB	244/322 (76%)	241 (99%)	3 (1%)	67	82
1	AC	244/322 (76%)	241 (99%)	3 (1%)	67	82
1	AD	244/322 (76%)	241 (99%)	3 (1%)	67	82
1	AE	244/322 (76%)	242 (99%)	2 (1%)	79	89
1	AF	244/322 (76%)	240 (98%)	4 (2%)	58	75
1	AG	244/322 (76%)	242 (99%)	2 (1%)	79	89
2	AI	99/100 (99%)	97 (98%)	2 (2%)	50	68
2	AJ	99/100 (99%)	98 (99%)	1 (1%)	73	85
2	AK	99/100 (99%)	98 (99%)	1 (1%)	73	85
2	AL	99/100 (99%)	99 (100%)	0	100	100
2	AM	99/100 (99%)	99 (100%)	0	100	100
2	AN	99/100 (99%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AO	99/100 (99%)	99 (100%)	0	100	100
3	As	92/93 (99%)	89 (97%)	3 (3%)	33	50
3	At	92/93 (99%)	90 (98%)	2 (2%)	47	65
3	Au	92/93 (99%)	90 (98%)	2 (2%)	47	65
3	Av	92/93 (99%)	90 (98%)	2 (2%)	47	65
3	Aw	92/93 (99%)	92 (100%)	0	100	100
3	Ax	92/93 (99%)	92 (100%)	0	100	100
All	All	2953/3512 (84%)	2915 (99%)	38 (1%)	64	80

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	101	PHE
1	AA	105	ASP
1	AA	147	VAL
1	AA	174	THR
1	AA	175	VAL
1	AA	198	VAL
1	AA	262	VAL
1	AA	276	ASN
1	AB	105	ASP
1	AB	275	THR
1	AB	369	ILE
1	AC	262	VAL
1	AC	270	GLN
1	AC	341	VAL
1	AD	105	ASP
1	AD	149	ILE
1	AD	378	ARG
1	AE	105	ASP
1	AE	282	ARG
1	AF	114	ARG
1	AF	144	VAL
1	AF	270	GLN
1	AF	378	ARG
2	AI	69	VAL
2	AI	87	THR
2	AJ	132	VAL
2	AK	75	ASP
3	As	5	ILE

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Mol	Chain	Res	Type
3	As	78	ILE
3	As	114	SER
3	At	5	ILE
3	At	89	ASN
3	Au	5	ILE
3	Au	87	SER
3	Av	5	ILE
3	Av	114	SER
1	AG	146	ASP
1	AG	389	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	136	ASN
1	AA	231	ASN
1	AA	281	ASN
1	AA	347	ASN
1	AB	347	ASN
1	AB	349	HIS
1	AC	136	ASN
1	AC	161	GLN
1	AC	276	ASN
1	AC	347	ASN
1	AC	380	HIS
1	AD	136	ASN
1	AD	161	GLN
1	AD	349	HIS
1	AD	380	HIS
1	AE	136	ASN
1	AE	347	ASN
1	AF	276	ASN
1	AF	349	HIS
1	AF	376	ASN
2	AI	59	ASN
2	AI	116	GLN
2	AJ	9	HIS
2	AJ	59	ASN
2	AJ	116	GLN
2	AK	9	HIS
2	AK	59	ASN
2	AK	116	GLN

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Mol	Chain	Res	Type
2	AL	59	ASN
2	AM	9	HIS
2	AM	59	ASN
2	AM	89	ASN
2	AM	116	GLN
2	AN	59	ASN
2	AN	85	GLN
2	AN	116	GLN
2	AO	59	ASN
3	As	7	ASN
3	As	9	GLN
3	As	42	ASN
3	At	9	GLN
3	At	42	ASN
3	Au	7	ASN
3	Au	42	ASN
3	Av	7	ASN
3	Ax	9	GLN
1	AG	136	ASN
1	AG	349	HIS
1	AG	380	HIS

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 51 ligands modelled in this entry, 51 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.

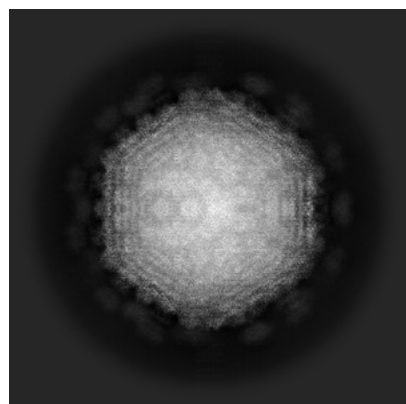
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51530. These allow visual inspection of the internal detail of the map and identification of artifacts.

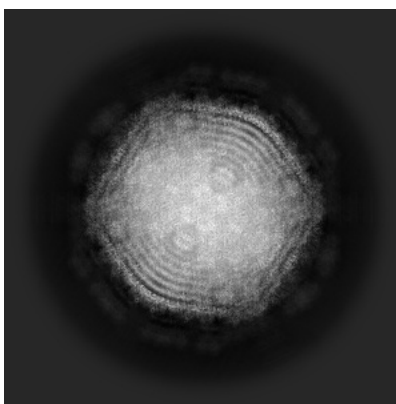
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

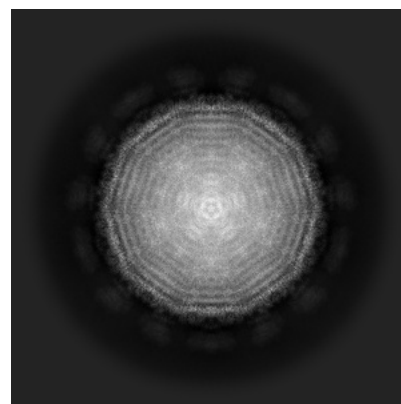
6.1.1 Primary map



X

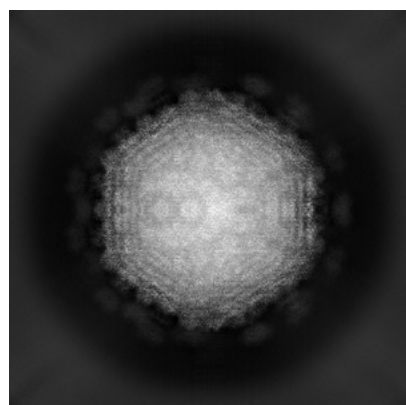


Y

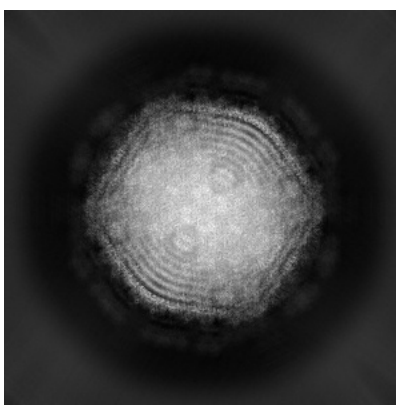


Z

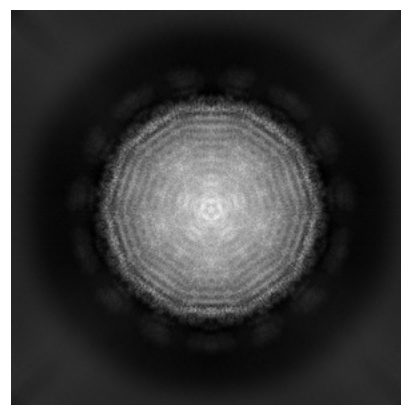
6.1.2 Raw map



X



Y

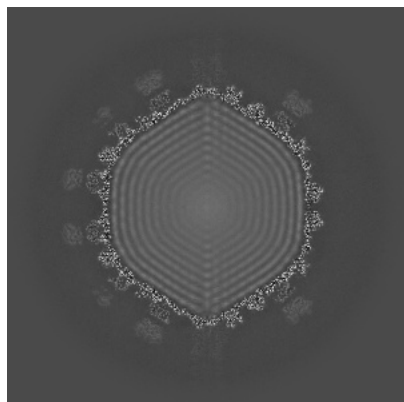


Z

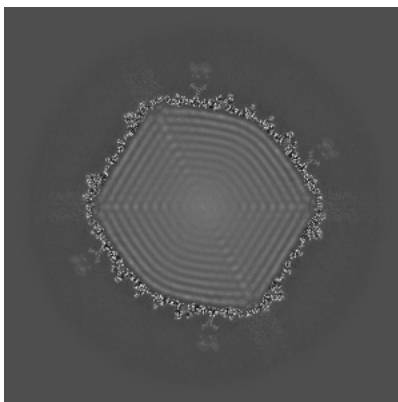
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

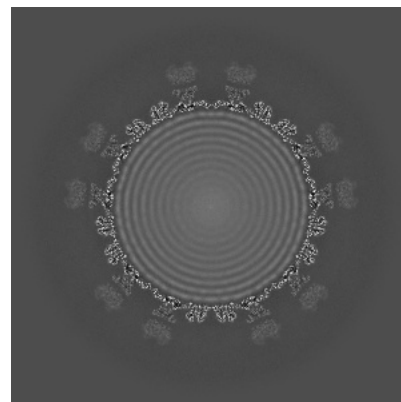
6.2.1 Primary map



X Index: 448

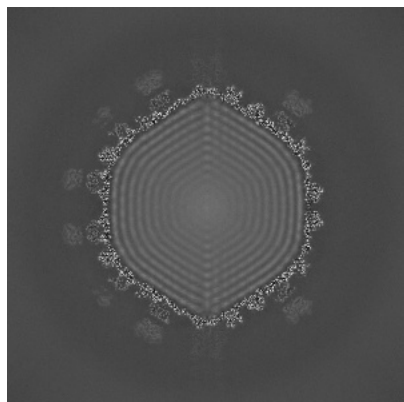


Y Index: 448

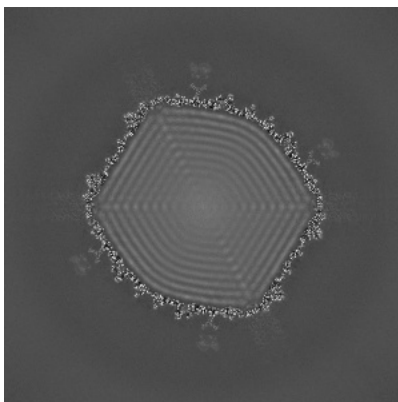


Z Index: 448

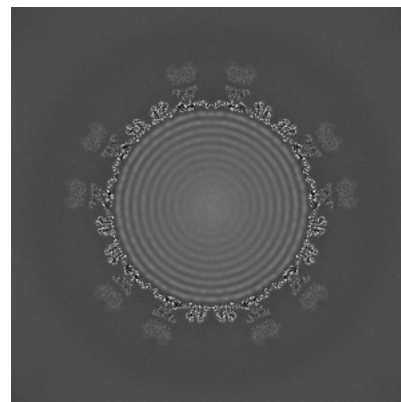
6.2.2 Raw map



X Index: 448



Y Index: 448

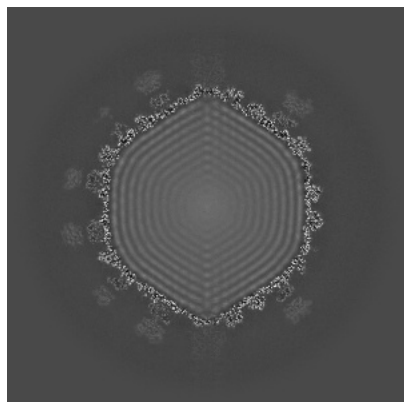


Z Index: 448

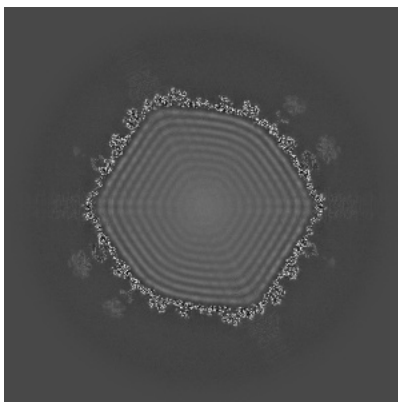
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

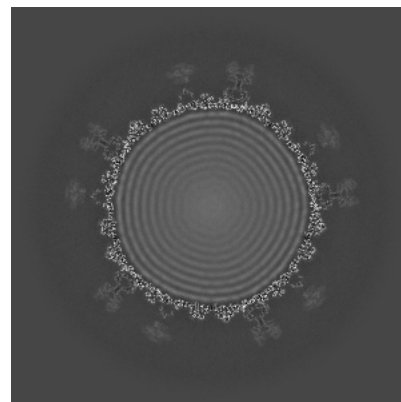
6.3.1 Primary map



X Index: 445

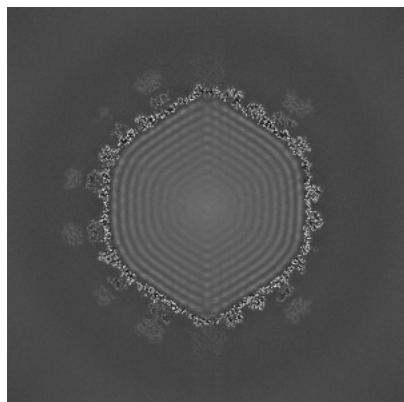


Y Index: 431

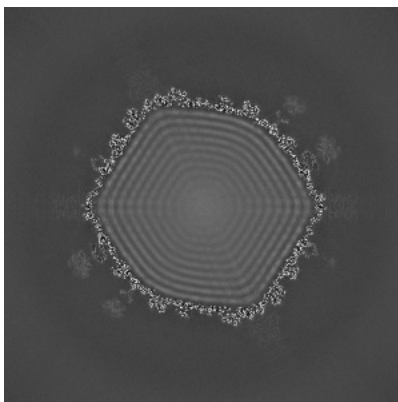


Z Index: 436

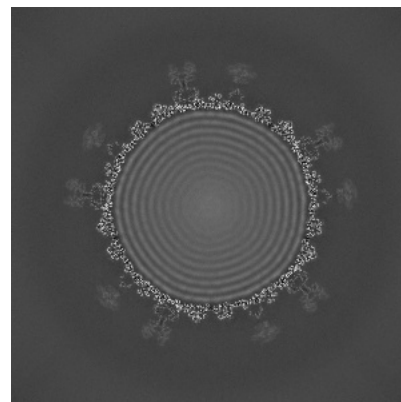
6.3.2 Raw map



X Index: 445



Y Index: 431

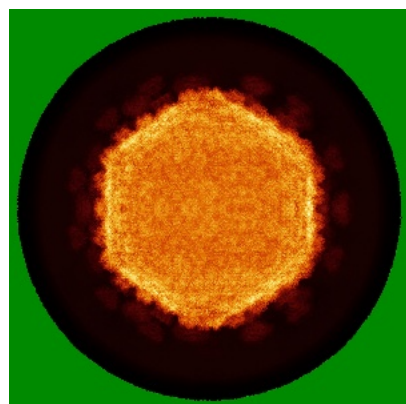


Z Index: 460

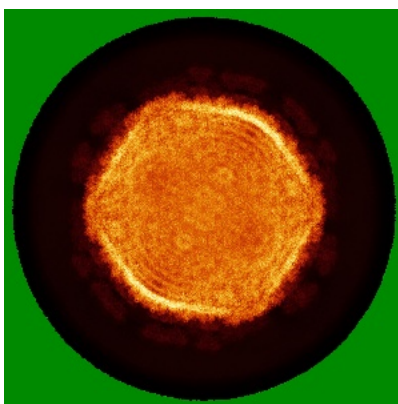
The images above show the largest variance slices of the map in three orthogonal directions.

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

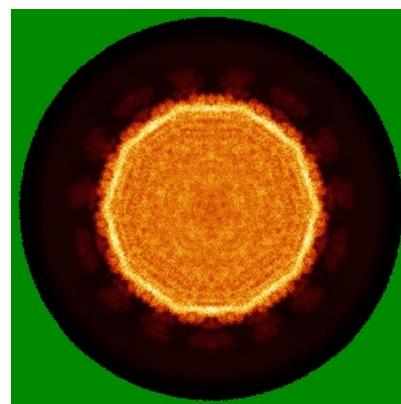
6.4.1 Primary map



X

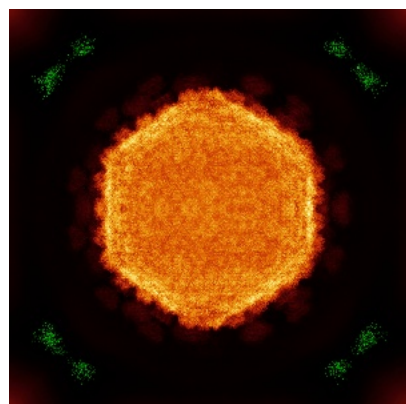


Y

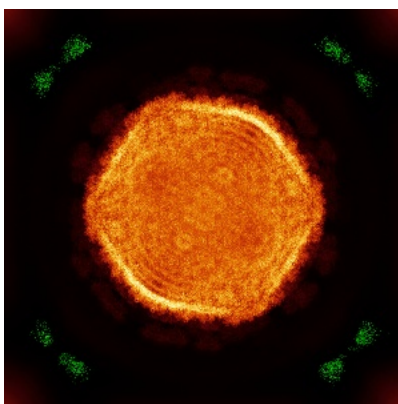


Z

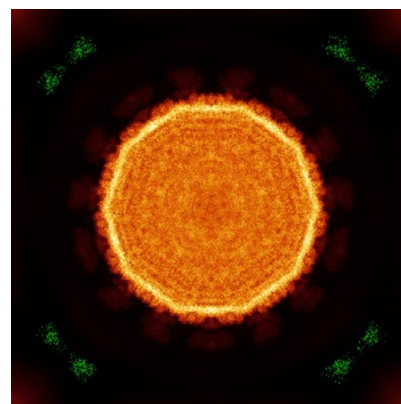
6.4.2 Raw map



X



Y

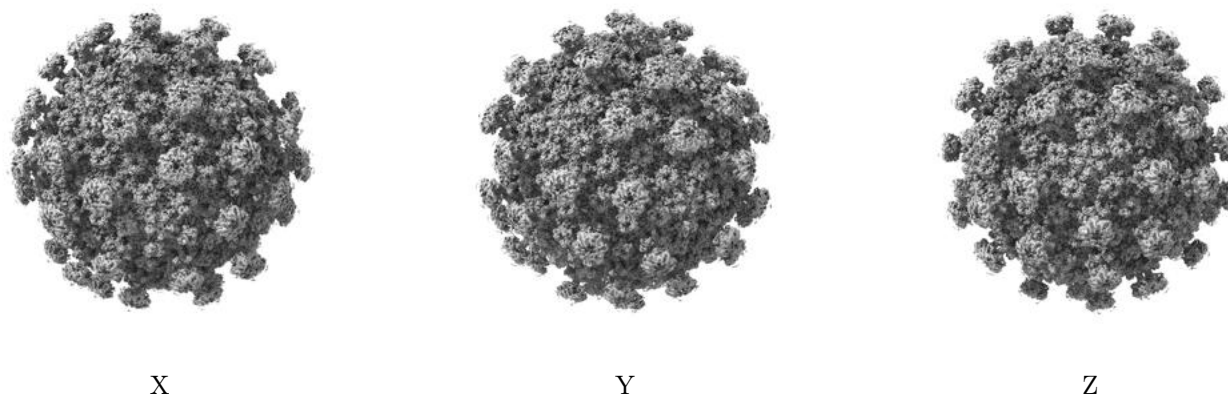


Z

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.

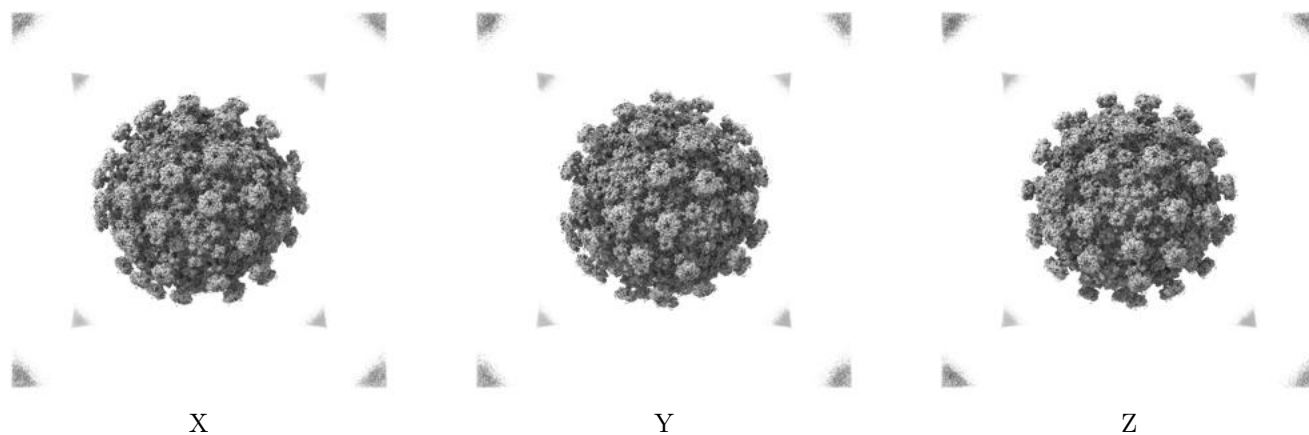
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

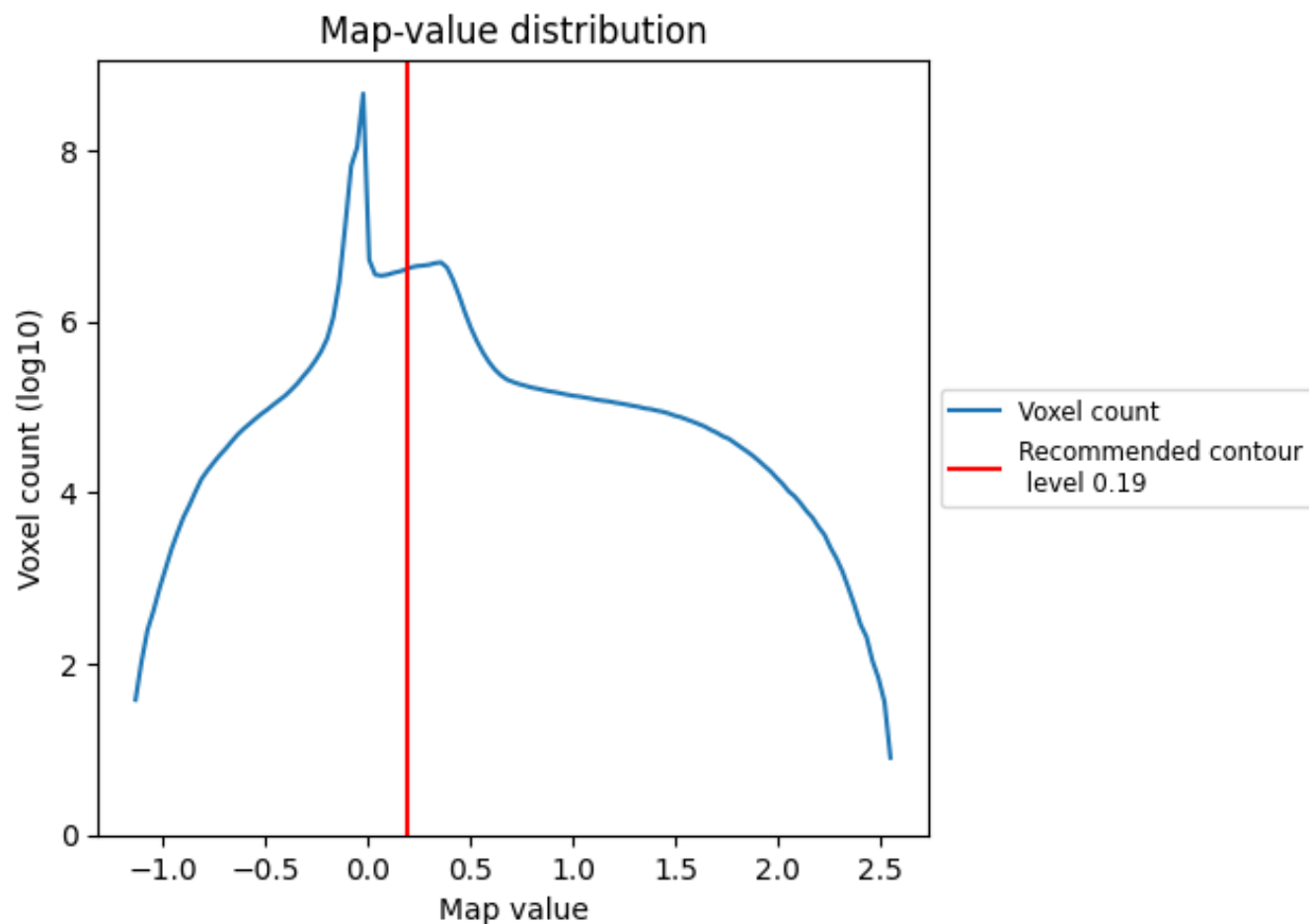
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

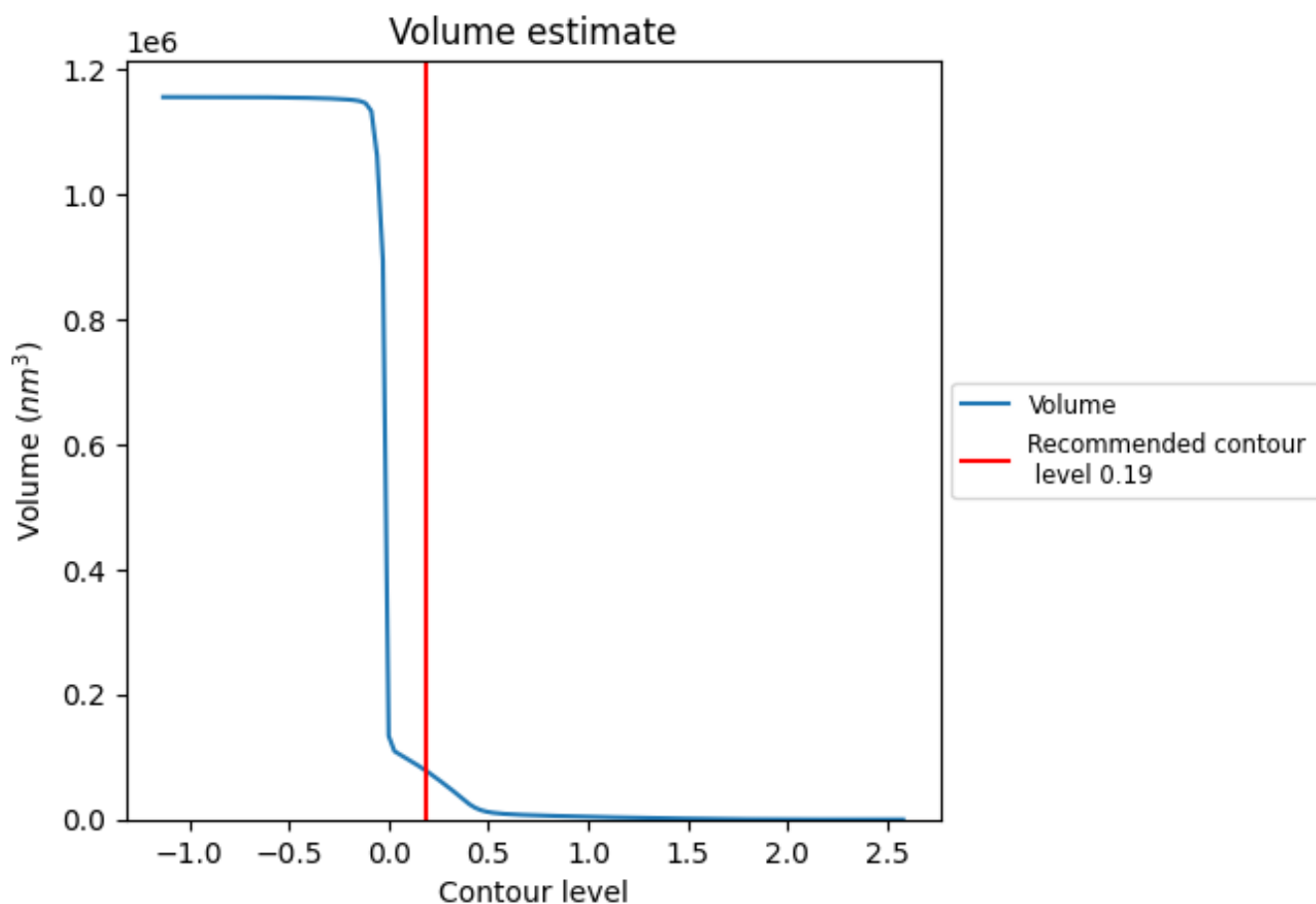
This section contains the results of statistical analysis of the map.

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.

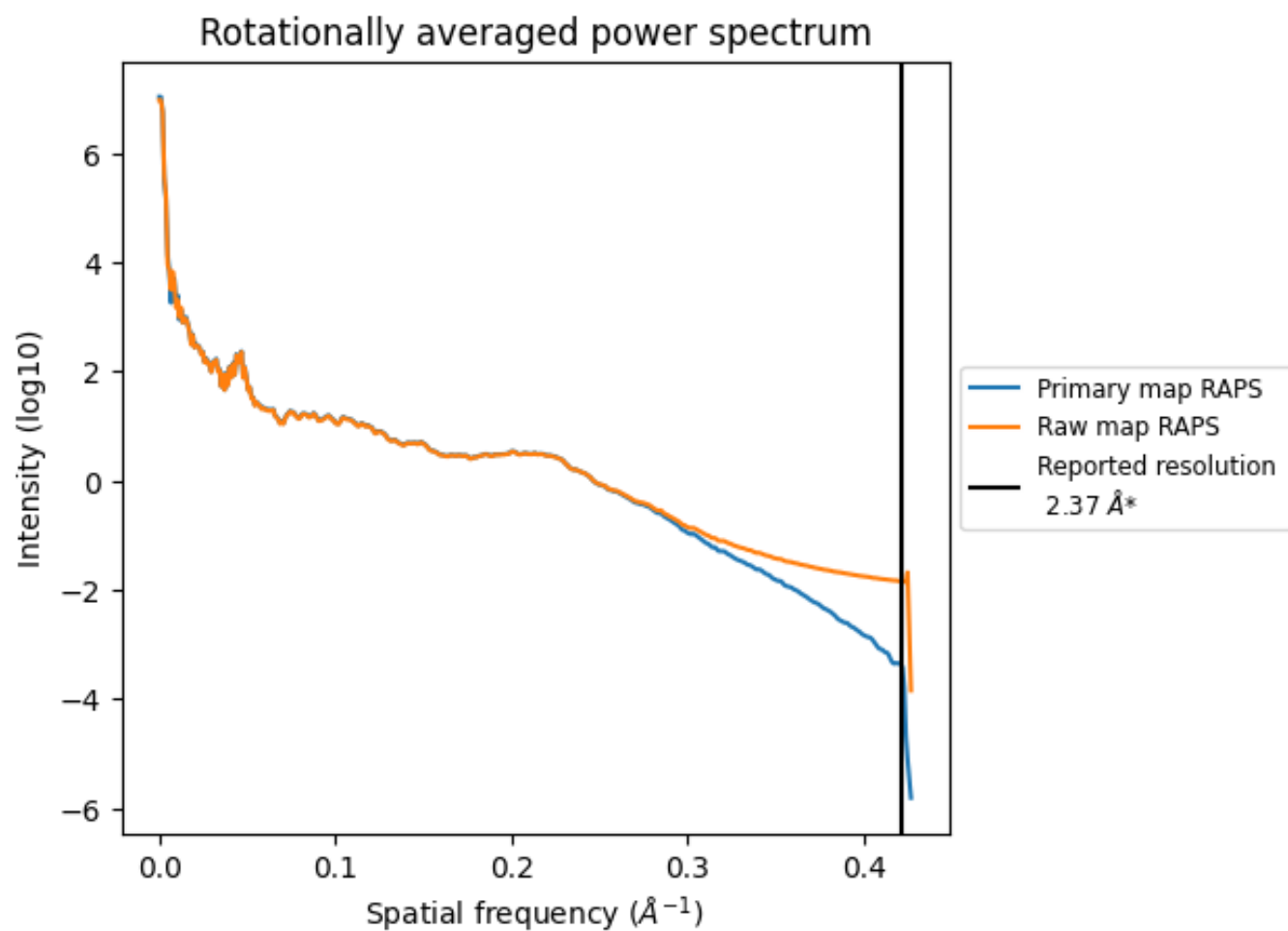
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77449 nm^3 ; this corresponds to an approximate mass of 69962 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 ⓘ

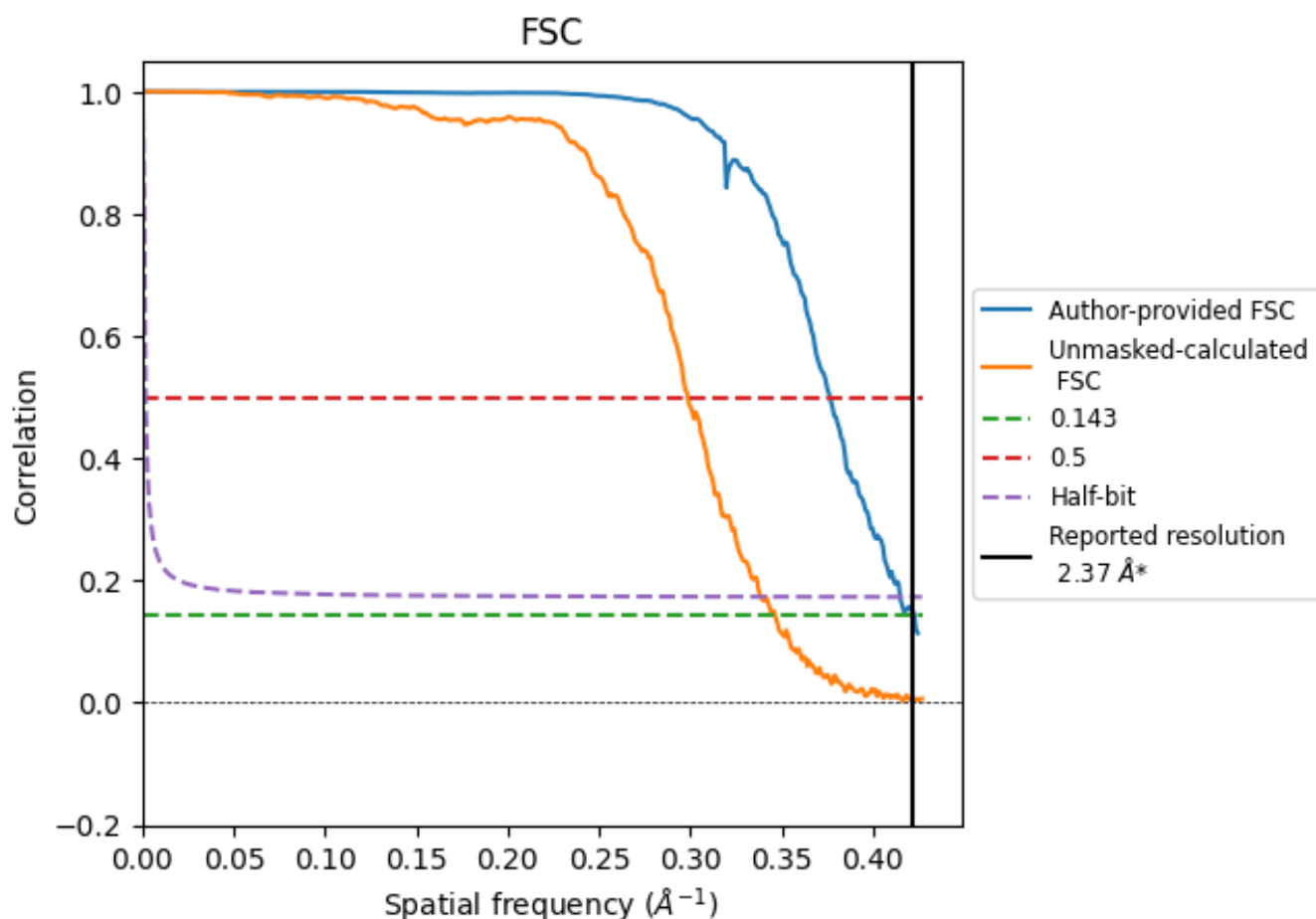


*Reported resolution corresponds to spatial frequency of 0.422 Å⁻¹

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 0.422 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.37	-	-
Author-provided FSC curve	2.37	2.66	2.41
Unmasked-calculated*	2.89	3.35	2.95

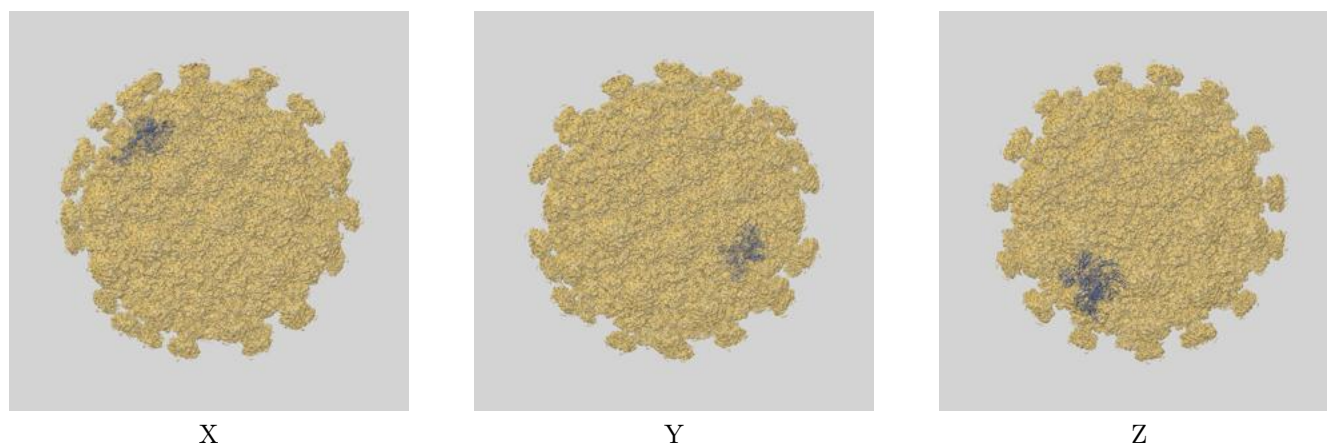
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.89 differs from the reported value 2.37 by more than 10 %

9 Map-model fit [i](#)

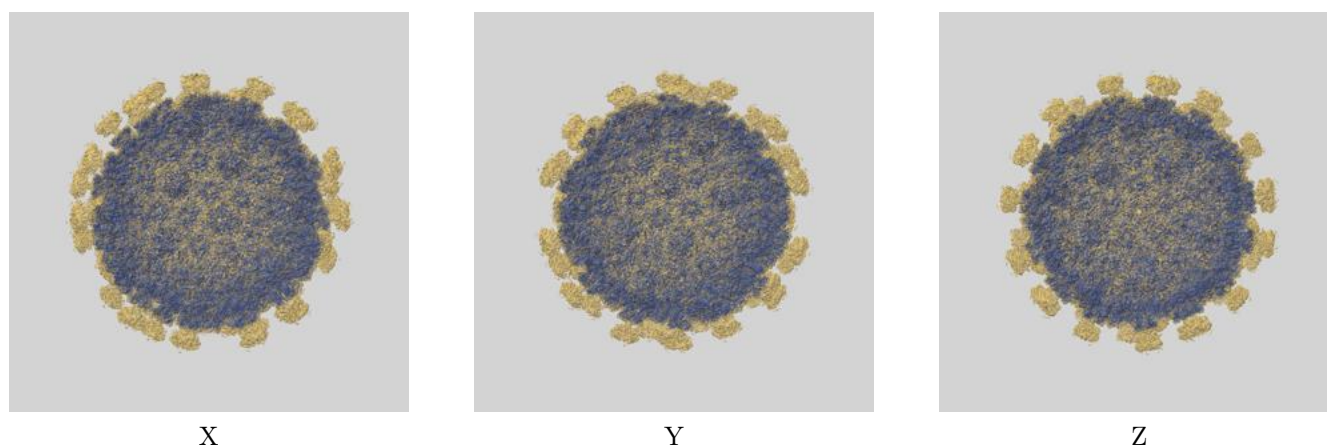
This section contains information regarding the fit between EMDB map EMD-51530 and PDB model 9GS0. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



9.1.2 Map-model assembly overlay [i](#)



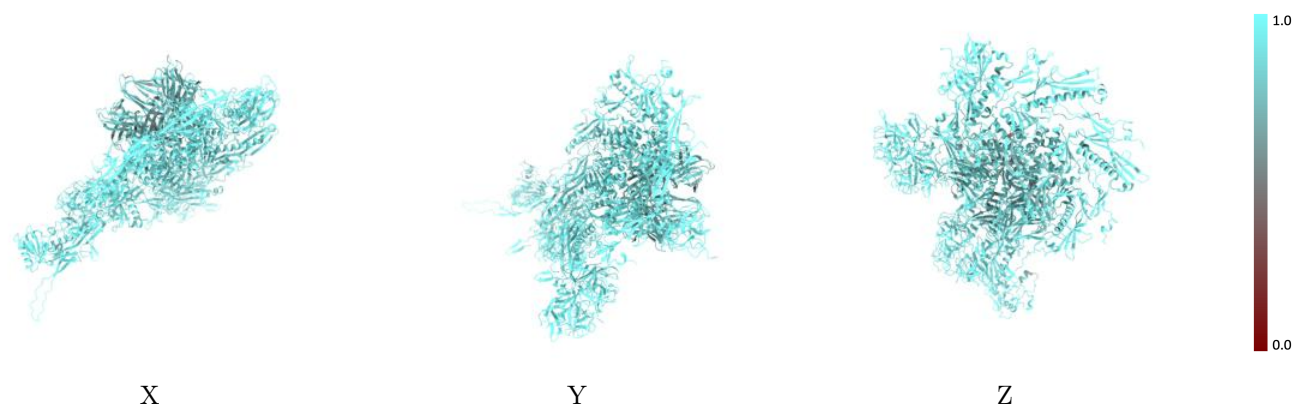
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



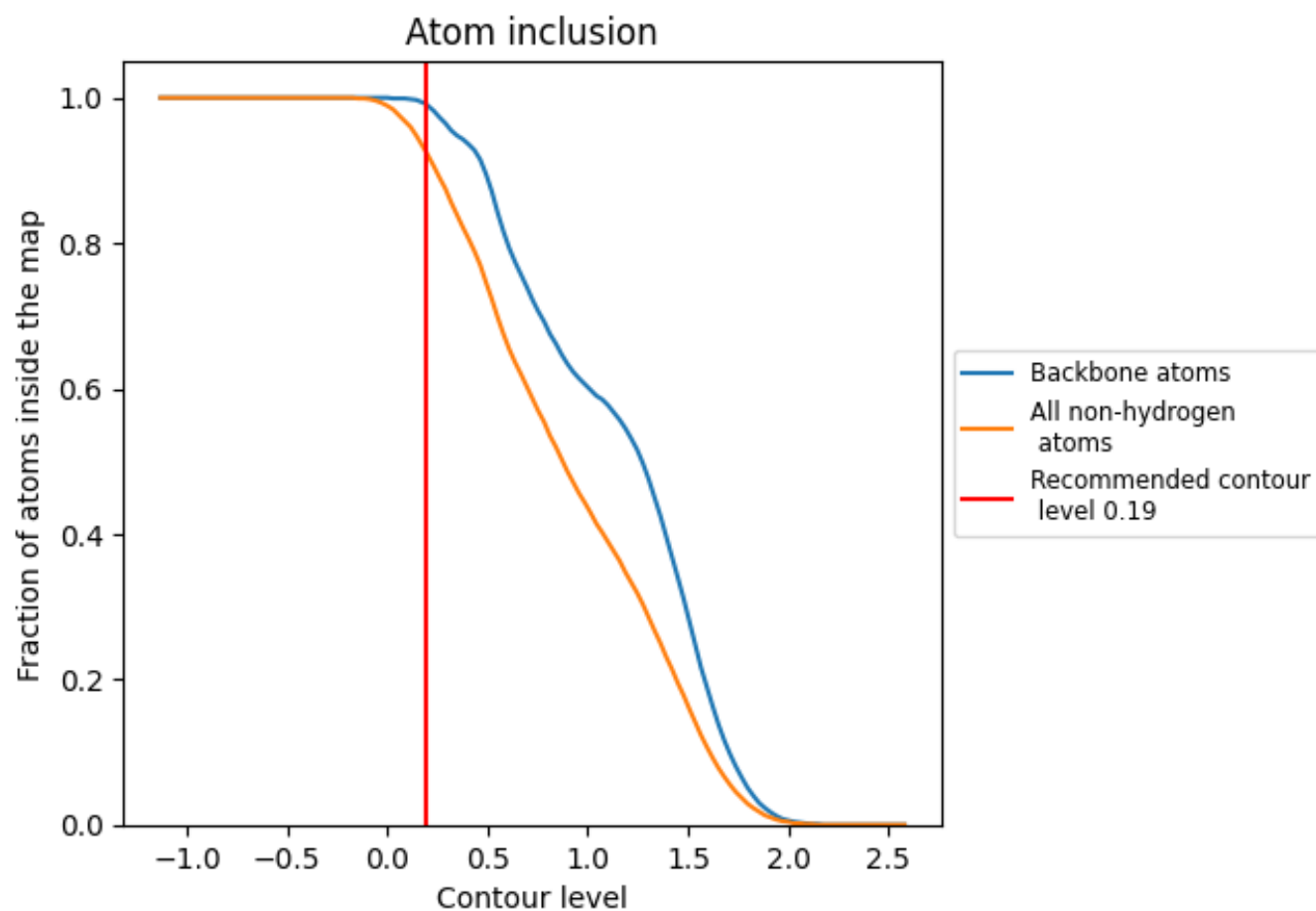
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).











































9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9270	 0.5330
AA	 0.9680	 0.5380
AB	 0.9610	 0.5350
AC	 0.9600	 0.5330
AD	 0.9580	 0.5330
AE	 0.9540	 0.5330
AF	 0.9620	 0.5370
AG	 0.9580	 0.5320
AI	 0.9650	 0.5430
AJ	 0.9700	 0.5390
AK	 0.9680	 0.5430
AL	 0.9660	 0.5350
AM	 0.9570	 0.5380
AN	 0.9670	 0.5340
AO	 0.9680	 0.5390
As	 0.7610	 0.5190
At	 0.7700	 0.5290
Au	 0.7810	 0.5170
Av	 0.7730	 0.5210
Aw	 0.7730	 0.5150
Ax	 0.7730	 0.5150

