



Full wwPDB EM Validation Report ⓘ

Jul 13, 2026 – 01:33 PM EDT

PDB ID : 9MVE / pdb_00009mve
EMDB ID : EMD-48666
Title : Dengue virus serotype-3 (DENV3) complex with DC-SIGN CRD at 4C
Authors : Are, V.N.; Fokine, A.; Klose, T.; Kuhn, R.J.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on : 2025-01-15
Resolution : 3.40 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:

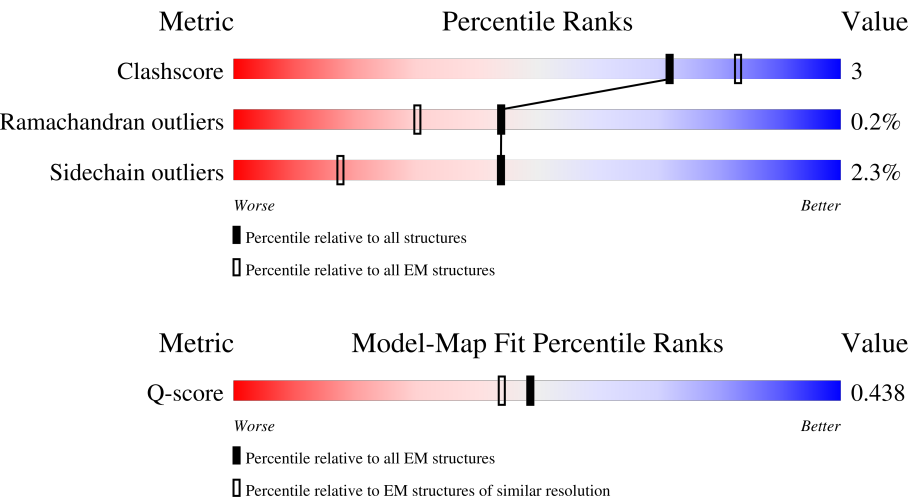
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	493	
1	C	493	
1	E	493	
2	B	75	

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Mol	Chain	Length	Quality of chain
2	D	75	95%5%
2	F	75	88%9%
3	J	192	68%61%7%32%
3	K	192	68%61%7%32%
3	L	192	68%63%5%32%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16317 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 Envelope protein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	493	Total	C	N	O	S	0	0
			3755	2379	641	708	27		
1	C	493	Total	C	N	O	S	0	0
			3755	2379	641	708	27		
1	E	493	Total	C	N	O	S	0	0
			3755	2379	641	708	27		

- Molecule 2 is a protein called M protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	75	Total	C	N	O	S	0	0
			589	387	98	100	4		
2	D	75	Total	C	N	O	S	0	0
			589	387	98	100	4		
2	F	75	Total	C	N	O	S	0	0
			589	387	98	100	4		

- Molecule 3 is a protein called DC-SIGN CRD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	131	Total	C	N	O	S	0	0
			1064	670	184	201	9		
3	J	131	Total	C	N	O	S	0	0
			1064	670	184	201	9		
3	L	131	Total	C	N	O	S	0	0
			1064	670	184	201	9		

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	213	MET	-	initiating methionine	UNP Q9NNX6
K	214	ALA	-	expression tag	UNP Q9NNX6
K	215	SER	-	expression tag	UNP Q9NNX6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	216	TRP	-	expression tag	UNP Q9NNX6
K	217	SER	-	expression tag	UNP Q9NNX6
K	218	HIS	-	expression tag	UNP Q9NNX6
K	219	PRO	-	expression tag	UNP Q9NNX6
K	220	GLN	-	expression tag	UNP Q9NNX6
K	221	PHE	-	expression tag	UNP Q9NNX6
K	222	GLU	-	expression tag	UNP Q9NNX6
K	223	LYS	-	expression tag	UNP Q9NNX6
K	224	GLY	-	expression tag	UNP Q9NNX6
K	225	SER	-	expression tag	UNP Q9NNX6
K	226	SER	-	expression tag	UNP Q9NNX6
K	227	HIS	-	expression tag	UNP Q9NNX6
K	228	HIS	-	expression tag	UNP Q9NNX6
K	229	HIS	-	expression tag	UNP Q9NNX6
K	230	HIS	-	expression tag	UNP Q9NNX6
K	231	HIS	-	expression tag	UNP Q9NNX6
K	232	HIS	-	expression tag	UNP Q9NNX6
K	233	SER	-	expression tag	UNP Q9NNX6
K	234	SER	-	expression tag	UNP Q9NNX6
K	235	GLY	-	expression tag	UNP Q9NNX6
K	236	SER	-	expression tag	UNP Q9NNX6
K	237	GLY	-	expression tag	UNP Q9NNX6
K	238	GLY	-	expression tag	UNP Q9NNX6
K	239	GLY	-	expression tag	UNP Q9NNX6
K	240	GLY	-	expression tag	UNP Q9NNX6
K	241	GLY	-	expression tag	UNP Q9NNX6
K	242	GLU	-	expression tag	UNP Q9NNX6
K	243	ASN	-	expression tag	UNP Q9NNX6
K	244	LEU	-	expression tag	UNP Q9NNX6
K	245	TYR	-	expression tag	UNP Q9NNX6
K	246	PHE	-	expression tag	UNP Q9NNX6
K	247	GLN	-	expression tag	UNP Q9NNX6
K	248	GLY	-	expression tag	UNP Q9NNX6
K	249	SER	-	expression tag	UNP Q9NNX6
J	213	MET	-	initiating methionine	UNP Q9NNX6
J	214	ALA	-	expression tag	UNP Q9NNX6
J	215	SER	-	expression tag	UNP Q9NNX6
J	216	TRP	-	expression tag	UNP Q9NNX6
J	217	SER	-	expression tag	UNP Q9NNX6
J	218	HIS	-	expression tag	UNP Q9NNX6
J	219	PRO	-	expression tag	UNP Q9NNX6
J	220	GLN	-	expression tag	UNP Q9NNX6

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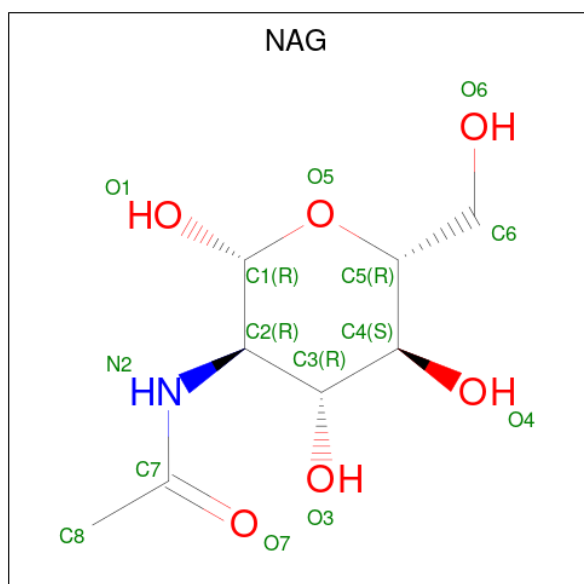
Chain	Residue	Modelled	Actual	Comment	Reference
J	221	PHE	-	expression tag	UNP Q9NNX6
J	222	GLU	-	expression tag	UNP Q9NNX6
J	223	LYS	-	expression tag	UNP Q9NNX6
J	224	GLY	-	expression tag	UNP Q9NNX6
J	225	SER	-	expression tag	UNP Q9NNX6
J	226	SER	-	expression tag	UNP Q9NNX6
J	227	HIS	-	expression tag	UNP Q9NNX6
J	228	HIS	-	expression tag	UNP Q9NNX6
J	229	HIS	-	expression tag	UNP Q9NNX6
J	230	HIS	-	expression tag	UNP Q9NNX6
J	231	HIS	-	expression tag	UNP Q9NNX6
J	232	HIS	-	expression tag	UNP Q9NNX6
J	233	SER	-	expression tag	UNP Q9NNX6
J	234	SER	-	expression tag	UNP Q9NNX6
J	235	GLY	-	expression tag	UNP Q9NNX6
J	236	SER	-	expression tag	UNP Q9NNX6
J	237	GLY	-	expression tag	UNP Q9NNX6
J	238	GLY	-	expression tag	UNP Q9NNX6
J	239	GLY	-	expression tag	UNP Q9NNX6
J	240	GLY	-	expression tag	UNP Q9NNX6
J	241	GLY	-	expression tag	UNP Q9NNX6
J	242	GLU	-	expression tag	UNP Q9NNX6
J	243	ASN	-	expression tag	UNP Q9NNX6
J	244	LEU	-	expression tag	UNP Q9NNX6
J	245	TYR	-	expression tag	UNP Q9NNX6
J	246	PHE	-	expression tag	UNP Q9NNX6
J	247	GLN	-	expression tag	UNP Q9NNX6
J	248	GLY	-	expression tag	UNP Q9NNX6
J	249	SER	-	expression tag	UNP Q9NNX6
L	213	MET	-	initiating methionine	UNP Q9NNX6
L	214	ALA	-	expression tag	UNP Q9NNX6
L	215	SER	-	expression tag	UNP Q9NNX6
L	216	TRP	-	expression tag	UNP Q9NNX6
L	217	SER	-	expression tag	UNP Q9NNX6
L	218	HIS	-	expression tag	UNP Q9NNX6
L	219	PRO	-	expression tag	UNP Q9NNX6
L	220	GLN	-	expression tag	UNP Q9NNX6
L	221	PHE	-	expression tag	UNP Q9NNX6
L	222	GLU	-	expression tag	UNP Q9NNX6
L	223	LYS	-	expression tag	UNP Q9NNX6
L	224	GLY	-	expression tag	UNP Q9NNX6
L	225	SER	-	expression tag	UNP Q9NNX6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	226	SER	-	expression tag	UNP Q9NNX6
L	227	HIS	-	expression tag	UNP Q9NNX6
L	228	HIS	-	expression tag	UNP Q9NNX6
L	229	HIS	-	expression tag	UNP Q9NNX6
L	230	HIS	-	expression tag	UNP Q9NNX6
L	231	HIS	-	expression tag	UNP Q9NNX6
L	232	HIS	-	expression tag	UNP Q9NNX6
L	233	SER	-	expression tag	UNP Q9NNX6
L	234	SER	-	expression tag	UNP Q9NNX6
L	235	GLY	-	expression tag	UNP Q9NNX6
L	236	SER	-	expression tag	UNP Q9NNX6
L	237	GLY	-	expression tag	UNP Q9NNX6
L	238	GLY	-	expression tag	UNP Q9NNX6
L	239	GLY	-	expression tag	UNP Q9NNX6
L	240	GLY	-	expression tag	UNP Q9NNX6
L	241	GLY	-	expression tag	UNP Q9NNX6
L	242	GLU	-	expression tag	UNP Q9NNX6
L	243	ASN	-	expression tag	UNP Q9NNX6
L	244	LEU	-	expression tag	UNP Q9NNX6
L	245	TYR	-	expression tag	UNP Q9NNX6
L	246	PHE	-	expression tag	UNP Q9NNX6
L	247	GLN	-	expression tag	UNP Q9NNX6
L	248	GLY	-	expression tag	UNP Q9NNX6
L	249	SER	-	expression tag	UNP Q9NNX6

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	

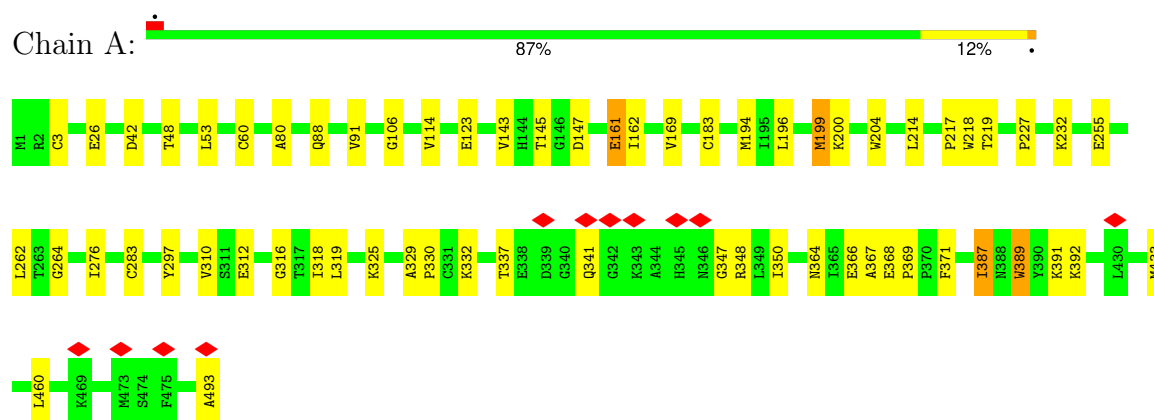
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	K	3	Total	Ca	0
			3	3	
5	J	3	Total	Ca	0
			3	3	
5	L	3	Total	Ca	0
			3	3	

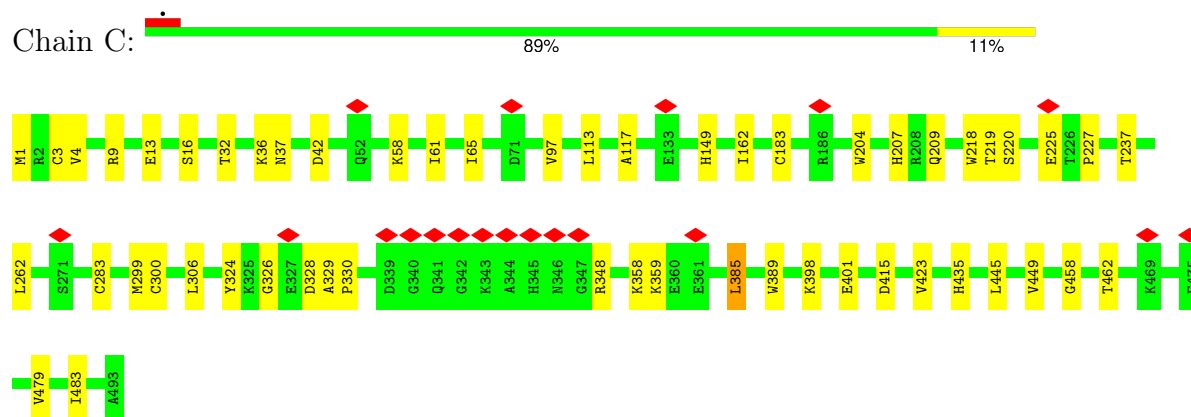
3 Residue-property plots

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

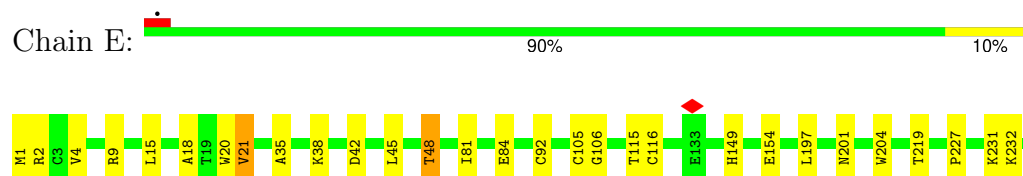
• Molecule 1: Envelope protein E

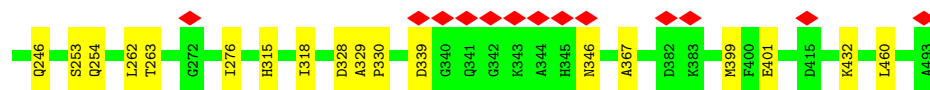


• Molecule 1: Envelope protein E

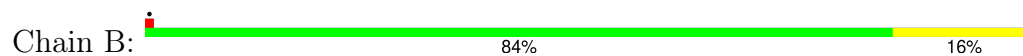


• Molecule 1: Envelope protein E





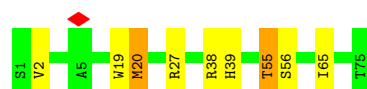
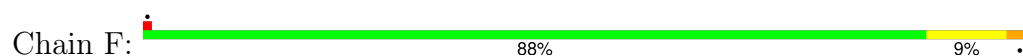
• Molecule 2: M protein



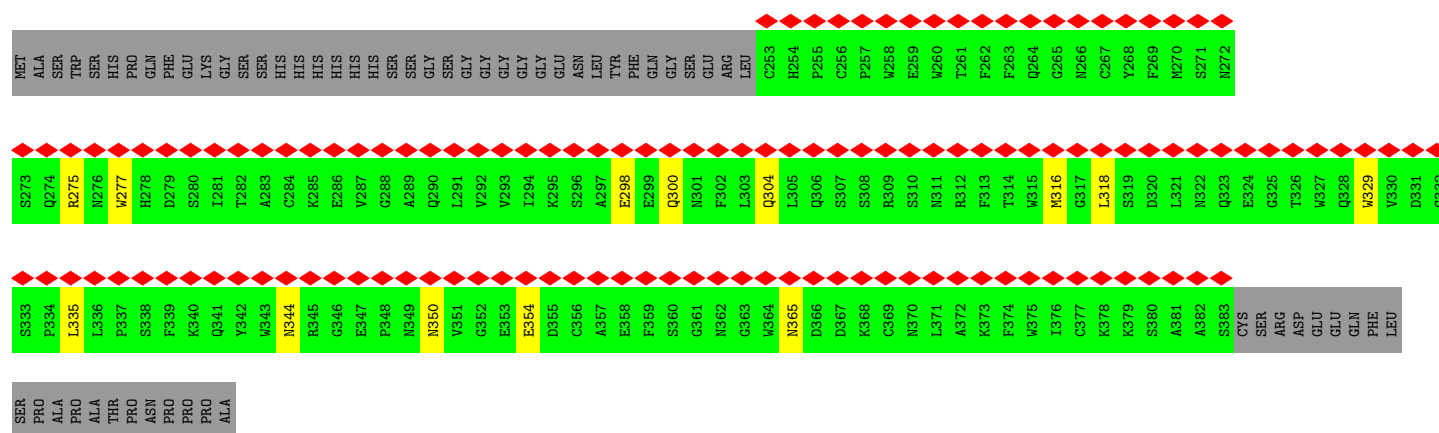
• Molecule 2: M protein



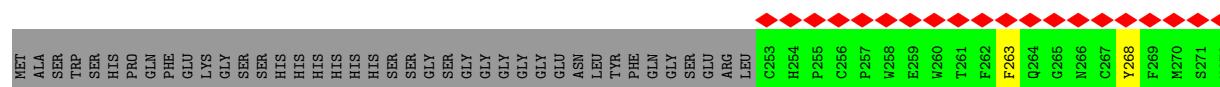
• Molecule 2: M protein



• Molecule 3: DC-SIGN CRD



• Molecule 3: DC-SIGN CRD



S273	Q274	R275	N276	W277	H278	D279	S280	I281	T282	A283	C284	K285	E286	V287	G288	A289	Q290	L291	V292	I294	K295	S296	A297	E298	E299	Q300	N301	F302	L303	Q304	L305	Q306	S307	S308	R309	S310	N311	R312	F313	T314	W315	M316	G317	L318	S319	D320	L321	N322	Q323	E324	G325	T326	W327	Q328	W329	D331	G332
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S333	P334	L335	L336	P337	S338	F339	K340	Q341	Y342	W343	N344	R345	G346	E347	P348	N349	N350	V351	G352	E353	E354	D355	C356	A357	E358	F359	S360	G361	N362	G363	W364	N365	D366	D367	K368	C369	N370	L371	A372	K373	F374	W375	I376	C377	K378	K379	S380	A381	A382	S383	CYS	SER	ARG	ASP	GLU	GLN	PHE	LEU
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SER	PRO	ALA	ALA	TRP	HIS	THR	PRO	ASN	PRO	PRO	PRO	ALA
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● Molecule 3: DC-SIGN CRD



MET	ALA	SER	TRP	SER	HIS	PRO	GLN	PHE	LYS	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	SER	GLY	GLY	GLY	GLY	GLY	ASN	LEU	TYR	PHE	GLN	GLY	SER	ARG	LEU	C253	H254	P255	C256	P257	W258	E259	W260	T261	F262	P263	Q264	G265	N266	C267	Y268	F269	M270	S271	N272
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S273	Q274	R275	N276	W277	H278	D279	S280	I281	T282	A283	C284	K285	E286	V287	G288	A289	Q290	L291	V292	I294	K295	S296	A297	E298	E299	Q300	N301	F302	L303	Q304	L305	Q306	S307	S308	R309	S310	N311	R312	F313	T314	W315	M316	G317	L318	S319	D320	L321	N322	Q323	E324	G325	T326	W327	Q328	W329	D331	G332
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S333	P334	L335	L336	P337	S338	F339	K340	Q341	Y342	W343	N344	R345	G346	E347	P348	N349	N350	V351	G352	E353	E354	D355	C356	A357	E358	F359	S360	G361	N362	G363	W364	N365	D366	D367	K368	C369	N370	L371	A372	K373	F374	W375	I376	C377	K378	K379	S380	A381	A382	S383	CYS	SER	ARG	ASP	GLU	GLN	PHE	LEU
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SER	PRO	ALA	ALA	TRP	HIS	THR	PRO	ASN	PRO	PRO	PRO	ALA
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	39491	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 ($e^-/\text{\AA}^2$)	35.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.162	Depositor
Minimum map value	-1.248	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	860.54395, 860.54395, 860.54395	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.328, 1.328, 1.328	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: CA, NAG

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	0.13	0/3826	0.38	0/5177
1	C	0.11	0/3826	0.35	0/5177
1	E	0.12	0/3826	0.35	0/5177
2	B	0.10	0/605	0.34	0/825
2	D	0.10	0/605	0.33	0/825
2	F	0.11	0/605	0.32	0/825
3	J	0.09	0/1098	0.28	0/1490
3	K	0.10	0/1098	0.33	0/1490
3	L	0.08	0/1098	0.26	0/1490
All	All	0.11	0/16587	0.34	0/22476

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3755	0	3781	34	0
1	C	3755	0	3781	27	0
1	E	3755	0	3781	20	0
2	B	589	0	605	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	589	0	605	2	0
2	F	589	0	605	5	0
3	J	1064	0	961	8	0
3	K	1064	0	960	8	0
3	L	1064	0	960	5	0
4	A	28	0	26	0	0
4	C	28	0	26	0	0
4	E	28	0	26	0	0
5	J	3	0	0	0	0
5	K	3	0	0	0	0
5	L	3	0	0	0	0
All	All	16317	0	16117	109	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 3.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASP:OD1	1:C:435:HIS:ND1	2.11	0.82
1:A:48:THR:HG23	1:A:276:ILE:HB	1.62	0.80
1:A:371:PHE:HA	1:A:391:LYS:HD2	1.64	0.79
1:C:326:GLY:O	1:C:359:LYS:NZ	2.19	0.75
1:C:219:THR:HG21	1:C:227:PRO:HB3	1.75	0.69
3:J:304:GLN:NE2	3:J:361:GLY:O	2.28	0.67
3:K:350:ASN:HA	3:K:354:GLU:HB2	1.79	0.64
3:K:318:LEU:HD21	3:K:335:LEU:HD22	1.79	0.64
1:C:219:THR:HG22	1:C:220:SER:H	1.62	0.64
1:C:329:ALA:HB3	1:C:330:PRO:HD3	1.79	0.63
3:K:277:TRP:NE1	3:K:316:MET:O	2.35	0.59
1:E:1:MET:N	1:E:42:ASP:OD2	2.33	0.58
1:A:26:GLU:OE1	2:B:15:ARG:NH1	2.35	0.58
1:E:115:THR:OG1	1:E:246:GLN:NE2	2.37	0.58
1:E:2:ARG:NH2	1:E:154:GLU:O	2.40	0.55
1:A:341:GLN:N	1:A:341:GLN:OE1	2.39	0.55
2:B:20:MET:HG2	1:C:237:THR:HG21	1.87	0.55
1:A:199:MET:HE2	1:A:255:GLU:HG3	1.88	0.55
1:E:48:THR:HG23	1:E:276:ILE:HB	1.90	0.54
3:K:298:GLU:OE1	3:K:298:GLU:N	2.41	0.53
1:A:88:GLN:O	1:A:232:LYS:NZ	2.39	0.52
1:A:348:ARG:NH2	1:A:368:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:342:TYR:O	3:L:364:TRP:N	2.39	0.52
1:A:143:VAL:HG13	1:A:145:THR:HG23	1.91	0.52
1:C:162:ILE:HG21	1:C:183:CYS:HB2	1.92	0.51
3:L:304:GLN:NE2	3:L:361:GLY:O	2.41	0.51
1:A:3:CYS:SG	1:A:42:ASP:HB3	2.51	0.51
1:E:339:ASP:OD2	1:E:346:ASN:ND2	2.44	0.50
3:K:344:ASN:ND2	3:K:365:ASN:HB2	2.27	0.49
1:C:324:TYR:CZ	1:C:326:GLY:HA3	2.47	0.49
1:C:1:MET:N	1:C:42:ASP:OD2	2.36	0.49
1:A:183:CYS:HA	1:A:283:CYS:HA	1.94	0.49
1:C:16:SER:HB2	1:C:423:VAL:HG13	1.95	0.48
1:A:316:GLY:O	1:A:391:LYS:NZ	2.47	0.48
1:A:350:ILE:HD11	1:A:366:GLU:CD	2.38	0.48
1:E:239:LYS:HG2	1:E:241:ALA:H	1.78	0.48
1:C:65:ILE:HG23	1:C:117:ALA:HB1	1.95	0.47
2:F:19:TRP:CD1	2:F:20:MET:HG3	2.50	0.47
1:A:329:ALA:HB3	1:A:330:PRO:HD3	1.97	0.47
1:E:105:CYS:SG	1:E:106:GLY:N	2.88	0.47
1:C:1:MET:O	1:C:4:VAL:HG12	2.14	0.46
1:C:97:VAL:HG21	1:C:113:LEU:HD13	1.97	0.46
1:C:9:ARG:HE	1:C:32:THR:HG21	1.80	0.46
1:C:479:VAL:O	1:C:483:ILE:HG13	2.16	0.46
1:E:219:THR:HG21	1:E:227:PRO:HB3	1.98	0.46
1:A:219:THR:HG21	1:A:227:PRO:HB3	1.98	0.46
1:E:18:ALA:HB3	1:E:20:TRP:CD1	2.51	0.46
3:K:318:LEU:HD13	3:K:329:TRP:CE2	2.51	0.46
3:J:263:PHE:HB3	3:J:268:TYR:CE2	2.51	0.46
2:D:35:TRP:CD2	2:D:72:PRO:HB3	2.50	0.45
3:J:292:VAL:HG21	3:J:303:LEU:HD11	1.99	0.45
1:A:218:TRP:CH2	1:E:81:ILE:HB	2.50	0.45
2:B:73:SER:HB3	2:D:73:SER:HB3	1.98	0.45
1:C:183:CYS:HA	1:C:283:CYS:HA	1.99	0.45
1:E:15:LEU:HA	1:E:21:VAL:HG13	1.98	0.45
1:E:318:ILE:N	1:E:367:ALA:O	2.49	0.45
1:C:36:LYS:HG2	1:C:37:ASN:OD1	2.17	0.45
3:L:367:ASP:OD1	3:L:368:LYS:N	2.47	0.45
2:F:38:ARG:HD2	2:F:39:HIS:CE1	2.51	0.45
1:E:263:THR:HG21	2:F:27:ARG:NH2	2.32	0.45
1:E:35:ALA:HB3	1:E:38:LYS:HB2	2.00	0.44
1:C:207:HIS:CE1	1:C:209:GLN:HB2	2.53	0.44
1:A:123:GLU:OE2	1:A:200:LYS:NZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLU:OE2	1:C:348:ARG:NH2	2.50	0.43
1:E:328:ASP:OD1	1:E:328:ASP:N	2.50	0.43
3:K:300:GLN:NE2	3:K:304:GLN:HB2	2.33	0.43
1:A:204:TRP:CD2	1:A:262:LEU:HD13	2.53	0.43
1:A:297:TYR:O	1:A:332:LYS:HE2	2.19	0.43
3:J:281:ILE:HG12	3:J:291:LEU:HB2	2.00	0.43
1:A:161:GLU:O	1:A:169:VAL:HG21	2.19	0.43
1:A:337:THR:HG22	1:A:337:THR:O	2.19	0.43
2:B:35:TRP:CD2	2:B:72:PRO:HB3	2.53	0.43
1:A:369:PRO:HG2	1:A:391:LYS:HE2	2.00	0.43
1:E:1:MET:O	1:E:4:VAL:HG13	2.19	0.43
1:A:312:GLU:HB2	1:A:389:TRP:CZ2	2.55	0.42
1:C:328:ASP:OD1	1:C:328:ASP:N	2.48	0.42
1:E:204:TRP:CD2	1:E:262:LEU:HD13	2.54	0.42
3:L:350:ASN:OD1	3:L:354:GLU:N	2.52	0.42
1:C:398:LYS:O	1:C:401:GLU:HG3	2.19	0.42
1:A:194:MET:HE2	2:B:12:LEU:HD22	2.00	0.42
1:C:306:LEU:HG	1:C:385:LEU:HD11	2.02	0.42
2:B:49:LEU:O	2:B:53:ILE:HG12	2.18	0.42
1:C:458:GLY:O	1:C:462:THR:HG23	2.19	0.42
1:E:232:LYS:HB2	1:E:232:LYS:HE2	1.84	0.42
3:J:294:ILE:HD11	3:J:359:PHE:HZ	1.85	0.42
1:A:493:ALA:HB3	2:B:18:THR:H	1.85	0.42
1:A:60:CYS:HB3	1:A:217:PRO:HG2	2.02	0.42
1:E:329:ALA:HB3	1:E:330:PRO:HD3	2.00	0.42
1:A:391:LYS:HG2	1:A:392:LYS:N	2.35	0.42
1:A:80:ALA:HB3	1:A:114:VAL:HG23	2.01	0.42
1:A:310:VAL:HG21	1:A:387:ILE:HG23	2.01	0.42
2:F:55:THR:HG23	2:F:56:SER:H	1.85	0.41
3:L:307:SER:OG	3:L:312:ARG:O	2.37	0.41
3:J:298:GLU:OE1	3:J:298:GLU:N	2.50	0.41
2:F:38:ARG:HD2	2:F:39:HIS:HE1	1.86	0.41
1:A:318:ILE:N	1:A:367:ALA:O	2.52	0.41
1:C:3:CYS:SG	1:C:42:ASP:HB3	2.61	0.41
1:C:58:LYS:O	1:C:218:TRP:HA	2.21	0.41
1:A:162:ILE:HG21	1:A:183:CYS:HB2	2.03	0.41
1:A:337:THR:HG21	1:A:347:GLY:HA3	2.03	0.41
1:C:204:TRP:CD2	1:C:262:LEU:HD13	2.56	0.41
1:C:225:GLU:OE1	1:C:225:GLU:N	2.50	0.41
1:A:53:LEU:HD11	1:A:196:LEU:HD12	2.02	0.40
3:K:275:ARG:HH22	3:J:308:SER:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:ARG:HB3	1:E:315:HIS:NE2	2.36	0.40
3:J:340:LYS:HA	3:J:343:TRP:HD1	1.86	0.40
1:A:147:ASP:O	1:A:364:ASN:ND2	2.49	0.40
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.96	0.40
2:B:53:ILE:HD11	2:B:63:ILE:HG21	2.02	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	491/493 (100%)	451 (92%)	36 (7%)	4 (1%)	16	44
1	C	491/493 (100%)	456 (93%)	35 (7%)	0	100	100
1	E	491/493 (100%)	452 (92%)	39 (8%)	0	100	100
2	B	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
2	D	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
2	F	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
3	J	129/192 (67%)	124 (96%)	5 (4%)	0	100	100
3	K	129/192 (67%)	127 (98%)	2 (2%)	0	100	100
3	L	129/192 (67%)	125 (97%)	4 (3%)	0	100	100
All	All	2079/2280 (91%)	1944 (94%)	131 (6%)	4 (0%)	44	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	MET
1	A	264	GLY
1	A	106	GLY
1	A	387	ILE

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	408/408 (100%)	401 (98%)	7 (2%)	53	67
1	C	408/408 (100%)	399 (98%)	9 (2%)	45	63
1	E	408/408 (100%)	391 (96%)	17 (4%)	26	52
2	B	63/63 (100%)	61 (97%)	2 (3%)	34	58
2	D	63/63 (100%)	62 (98%)	1 (2%)	55	68
2	F	63/63 (100%)	59 (94%)	4 (6%)	16	42
3	J	115/164 (70%)	115 (100%)	0	100	100
3	K	115/164 (70%)	115 (100%)	0	100	100
3	L	115/164 (70%)	115 (100%)	0	100	100
All	All	1758/1905 (92%)	1718 (98%)	40 (2%)	44	63

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	VAL
1	A	161	GLU
1	A	319	LEU
1	A	325	LYS
1	A	389	TRP
1	A	433	MET
1	A	460	LEU
2	B	43	THR
2	B	57	LEU
1	C	61	ILE
1	C	149	HIS
1	C	299	MET
1	C	300	CYS
1	C	358	LYS
1	C	385	LEU
1	C	389	TRP
1	C	445	LEU
1	C	449	VAL

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Mol	Chain	Res	Type
2	D	57	LEU
1	E	21	VAL
1	E	45	LEU
1	E	48	THR
1	E	84	GLU
1	E	92	CYS
1	E	116	CYS
1	E	149	HIS
1	E	197	LEU
1	E	201	ASN
1	E	231	LYS
1	E	235	LEU
1	E	253	SER
1	E	254	GLN
1	E	399	MET
1	E	401	GLU
1	E	432	LYS
1	E	460	LEU
2	F	2	VAL
2	F	20	MET
2	F	55	THR
2	F	65	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	52	GLN
1	A	134	ASN
1	A	230	ASN
1	A	246	GLN
1	A	346	ASN
2	B	59	GLN
1	C	46	GLN
1	C	77	GLN
1	C	132	HIS
1	C	150	GLN
1	E	86	GLN
1	E	94	HIS
1	E	246	GLN
1	E	280	HIS
1	E	388	ASN

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Mol	Chain	Res	Type
1	E	436	GLN
1	E	467	ASN
1	E	492	GLN
2	F	7	HIS
2	F	39	HIS
2	F	59	GLN
3	K	301	ASN
3	J	323	GLN
3	L	323	GLN

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 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	501	1	14,14,15	0.71	0	17,19,21	1.06	1 (5%)
4	NAG	A	502	1	14,14,15	0.70	0	17,19,21	1.54	3 (17%)
4	NAG	C	501	1	14,14,15	0.65	0	17,19,21	1.74	3 (17%)
4	NAG	C	502	1	14,14,15	0.73	0	17,19,21	1.72	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	501	1	14,14,15	0.67	0	17,19,21	1.68	3 (17%)
4	NAG	E	502	1	14,14,15	0.71	0	17,19,21	1.57	4 (23%)

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
4	NAG	A	501	1	-	1/6/23/26	0/1/1/1
4	NAG	A	502	1	-	3/6/23/26	0/1/1/1
4	NAG	C	501	1	-	1/6/23/26	0/1/1/1
4	NAG	C	502	1	-	2/6/23/26	0/1/1/1
4	NAG	E	501	1	-	2/6/23/26	0/1/1/1
4	NAG	E	502	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	NAG	C1-O5-C5	5.33	119.32	112.19
4	C	502	NAG	C1-O5-C5	4.24	117.86	112.19
4	A	502	NAG	C1-O5-C5	4.09	117.66	112.19
4	E	501	NAG	C2-N2-C7	3.68	127.83	122.90
4	E	501	NAG	C4-C3-C2	-3.53	105.84	111.02
4	A	501	NAG	C1-O5-C5	3.53	116.91	112.19
4	E	502	NAG	C1-O5-C5	3.32	116.63	112.19
4	E	502	NAG	C2-N2-C7	3.21	127.21	122.90
4	E	501	NAG	C1-O5-C5	3.21	116.49	112.19
4	C	502	NAG	C2-N2-C7	2.99	126.90	122.90
4	A	502	NAG	C2-N2-C7	2.82	126.68	122.90
4	C	501	NAG	C2-N2-C7	2.72	126.55	122.90
4	C	502	NAG	C4-C3-C2	-2.64	107.15	111.02
4	C	501	NAG	C1-C2-N2	2.16	113.83	110.43
4	E	502	NAG	C1-C2-N2	2.13	113.79	110.43
4	E	502	NAG	O4-C4-C3	-2.12	105.39	110.38
4	A	502	NAG	O4-C4-C3	-2.12	105.39	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	502	NAG	C1-C2-N2-C7
4	E	501	NAG	C1-C2-N2-C7
4	E	502	NAG	C1-C2-N2-C7
4	A	501	NAG	O5-C5-C6-O6
4	C	501	NAG	C3-C2-N2-C7
4	A	502	NAG	C3-C2-N2-C7
4	A	502	NAG	C1-C2-N2-C7
4	C	502	NAG	C3-C2-N2-C7
4	E	501	NAG	C3-C2-N2-C7
4	E	502	NAG	C3-C2-N2-C7
4	A	502	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

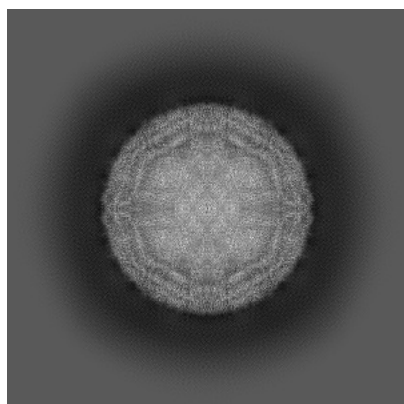
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48666. These allow visual inspection of the internal detail of the map and identification of artifacts.

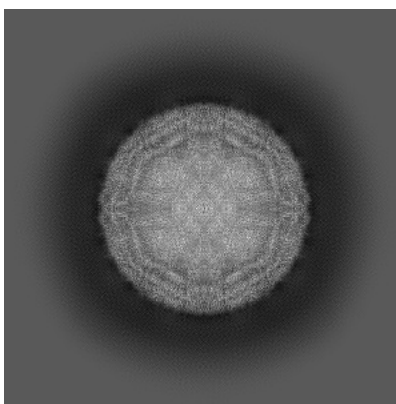
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

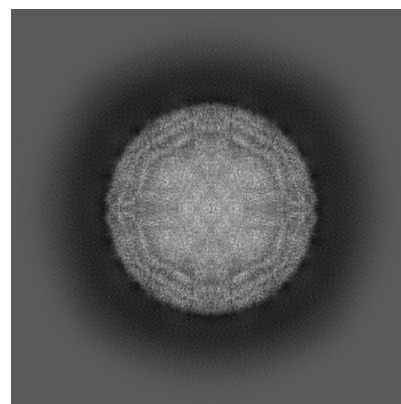
6.1.1 Primary map



X

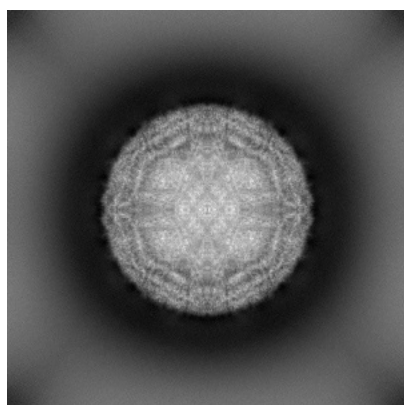


Y

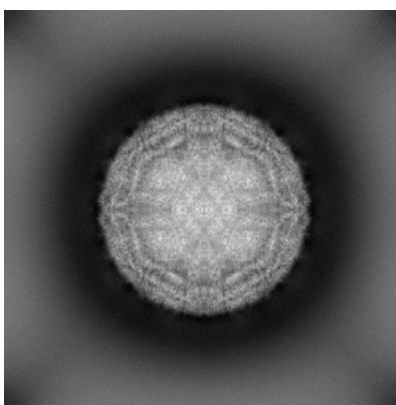


Z

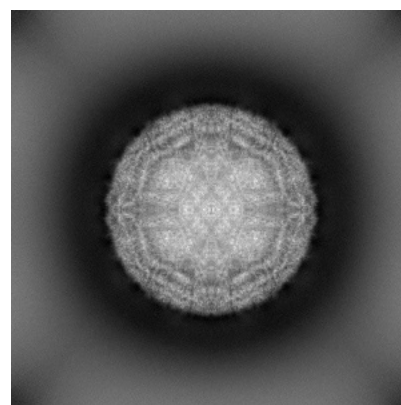
6.1.2 Raw map



X



Y

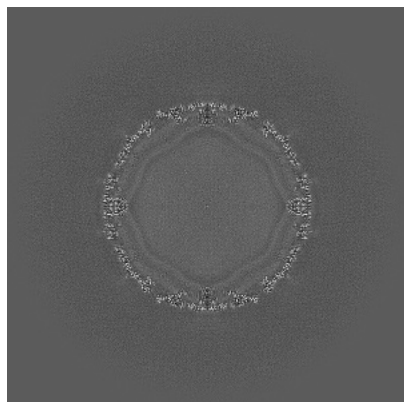


Z

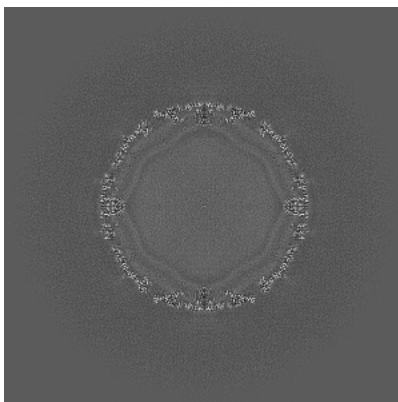
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

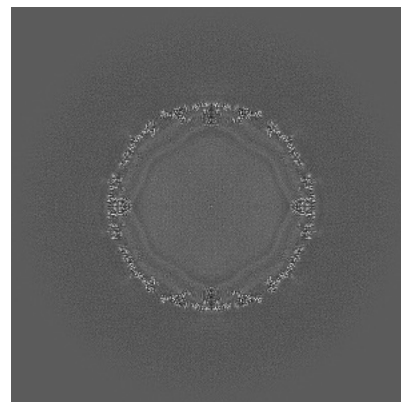
6.2.1 Primary map



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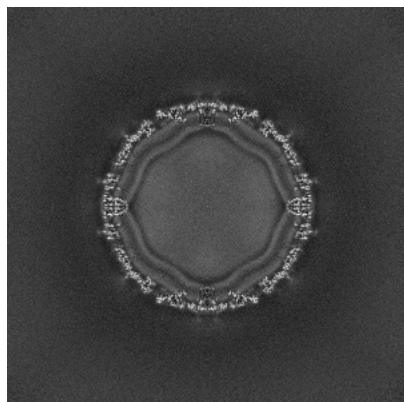


Y Index: 324

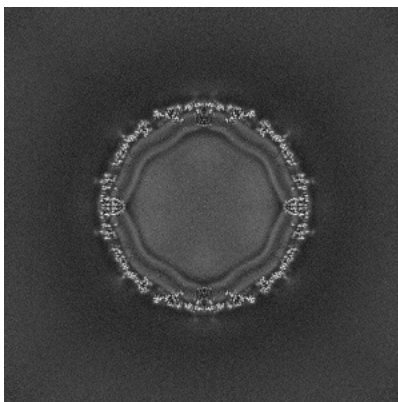


Z Index: 324

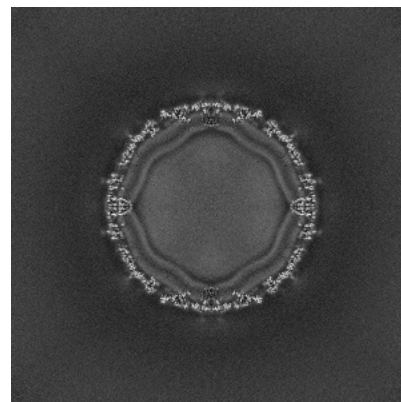
6.2.2 Raw map



X Index: 324



Y Index: 324

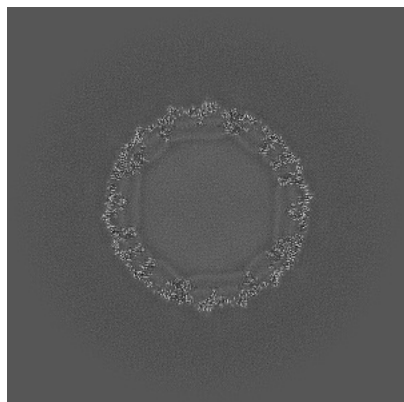


Z Index: 324

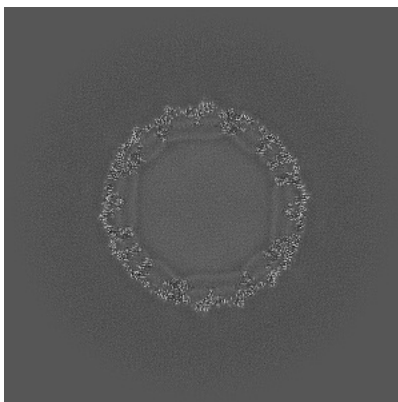
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

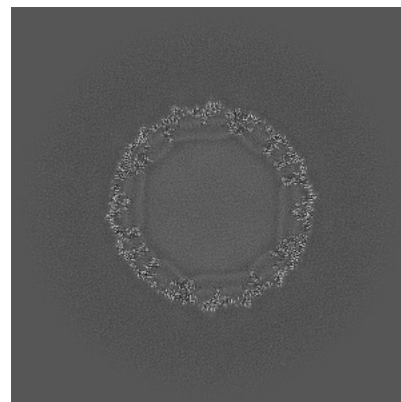
6.3.1 Primary map



X Index: 284

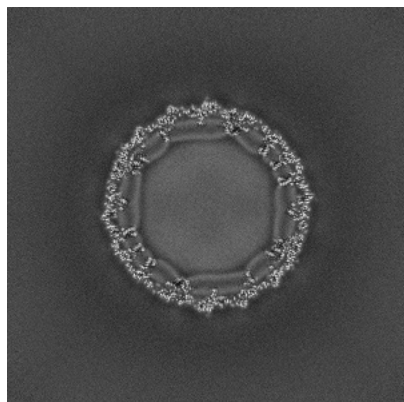


Y Index: 284

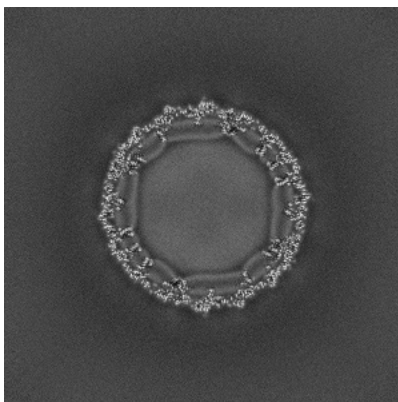


Z Index: 284

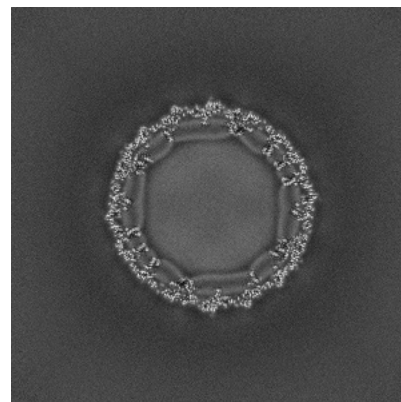
6.3.2 Raw map



X Index: 284



Y Index: 284

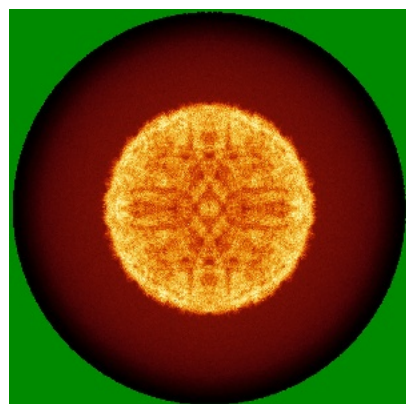


Z Index: 284

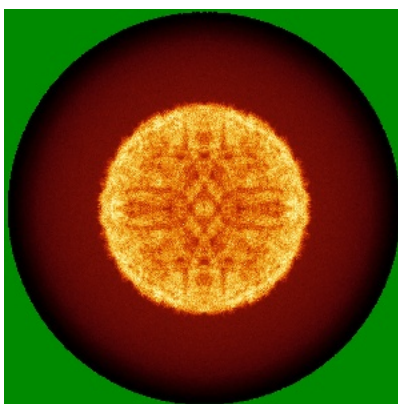
The images above show the largest variance slices of the map in three orthogonal directions.

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

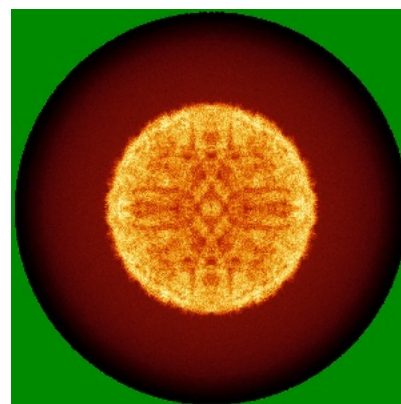
6.4.1 Primary map



X

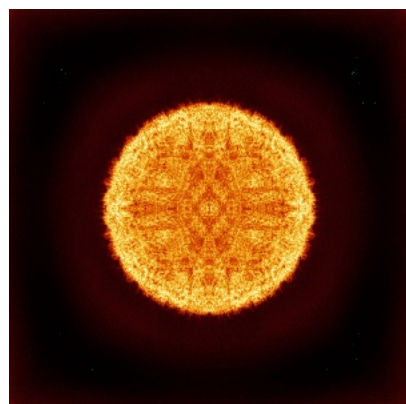


Y

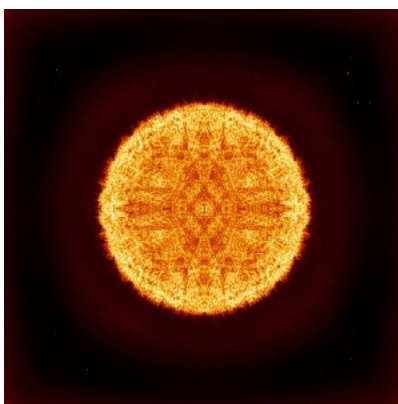


Z

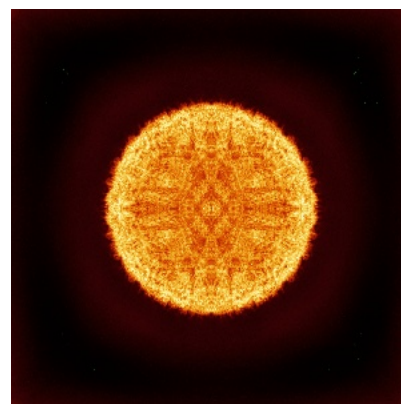
6.4.2 Raw map



X



Y

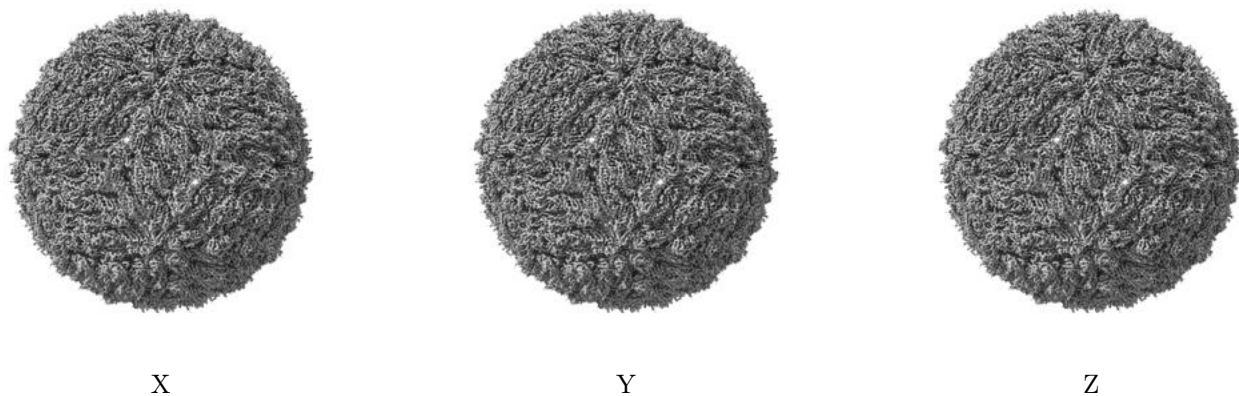


Z

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.

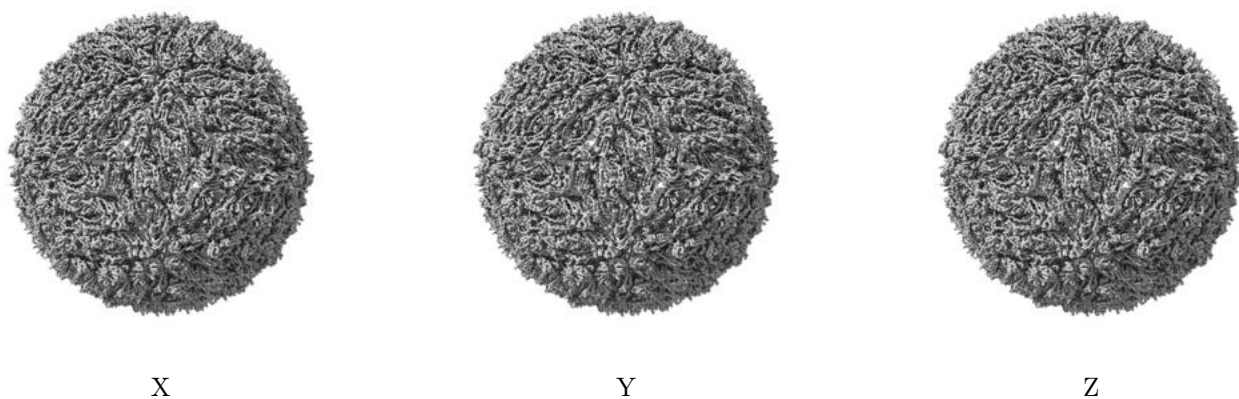
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

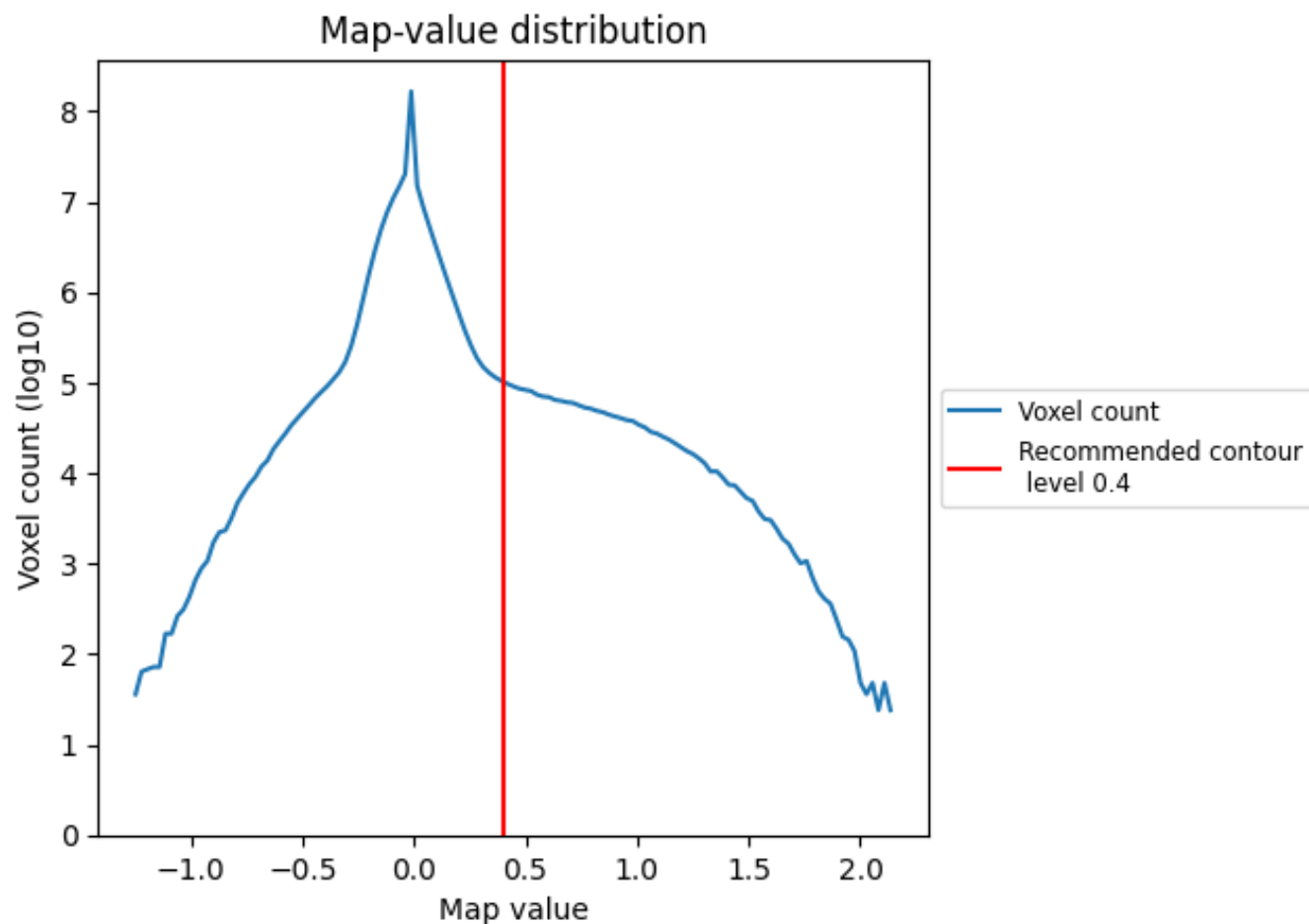
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

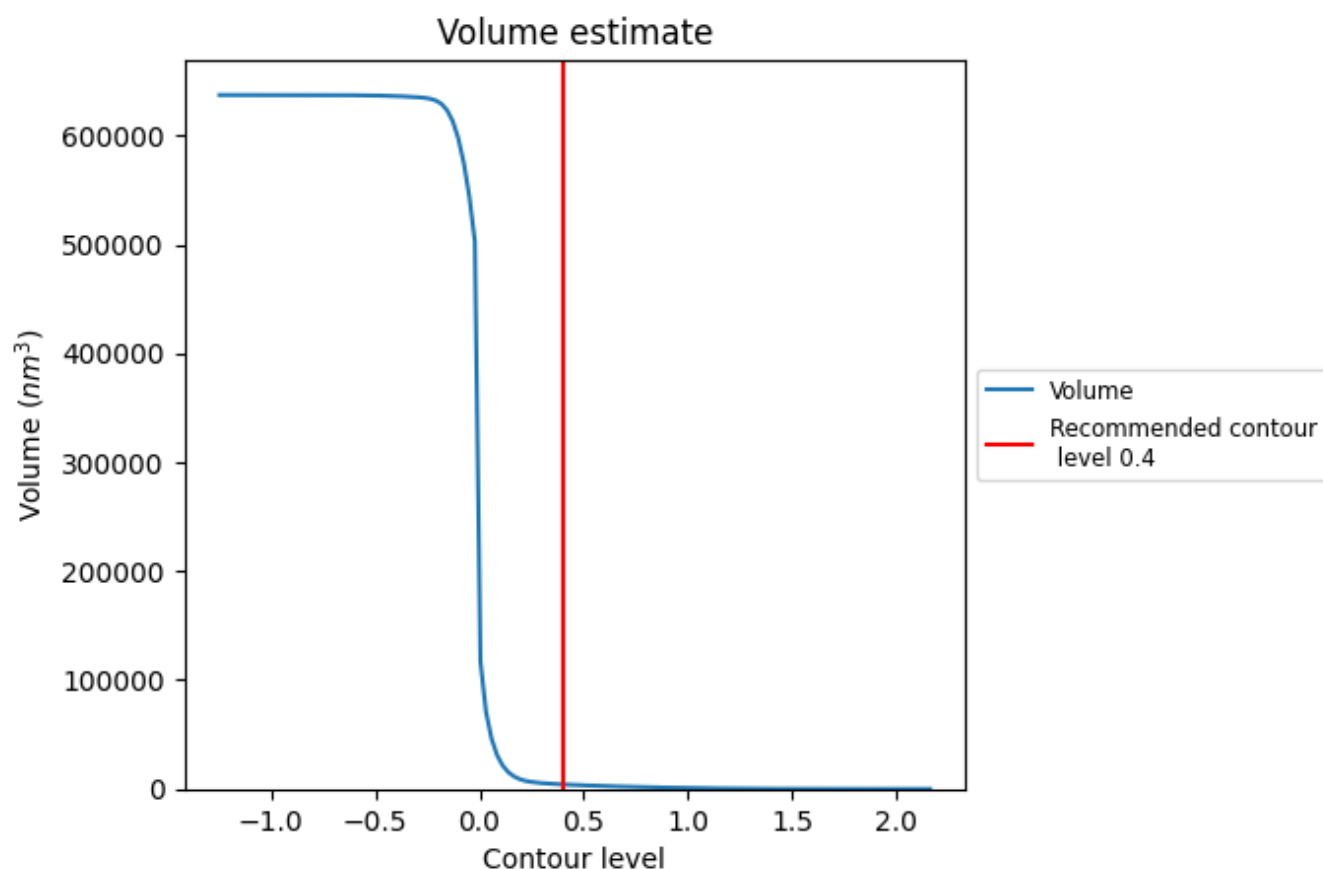
This section contains the results of statistical analysis of the map.

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.

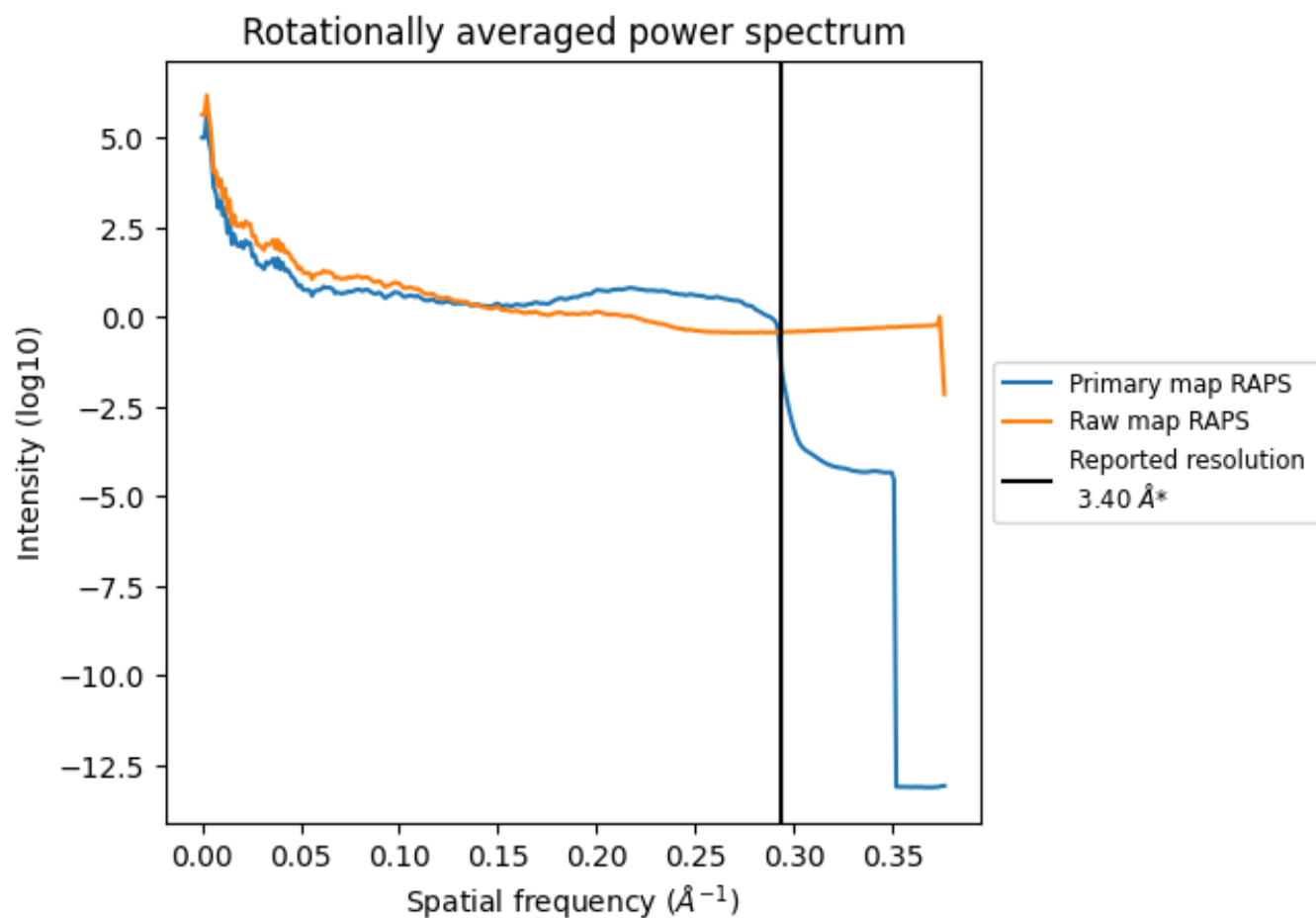
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4176 nm³; this corresponds to an approximate mass of 3772 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 ⓘ

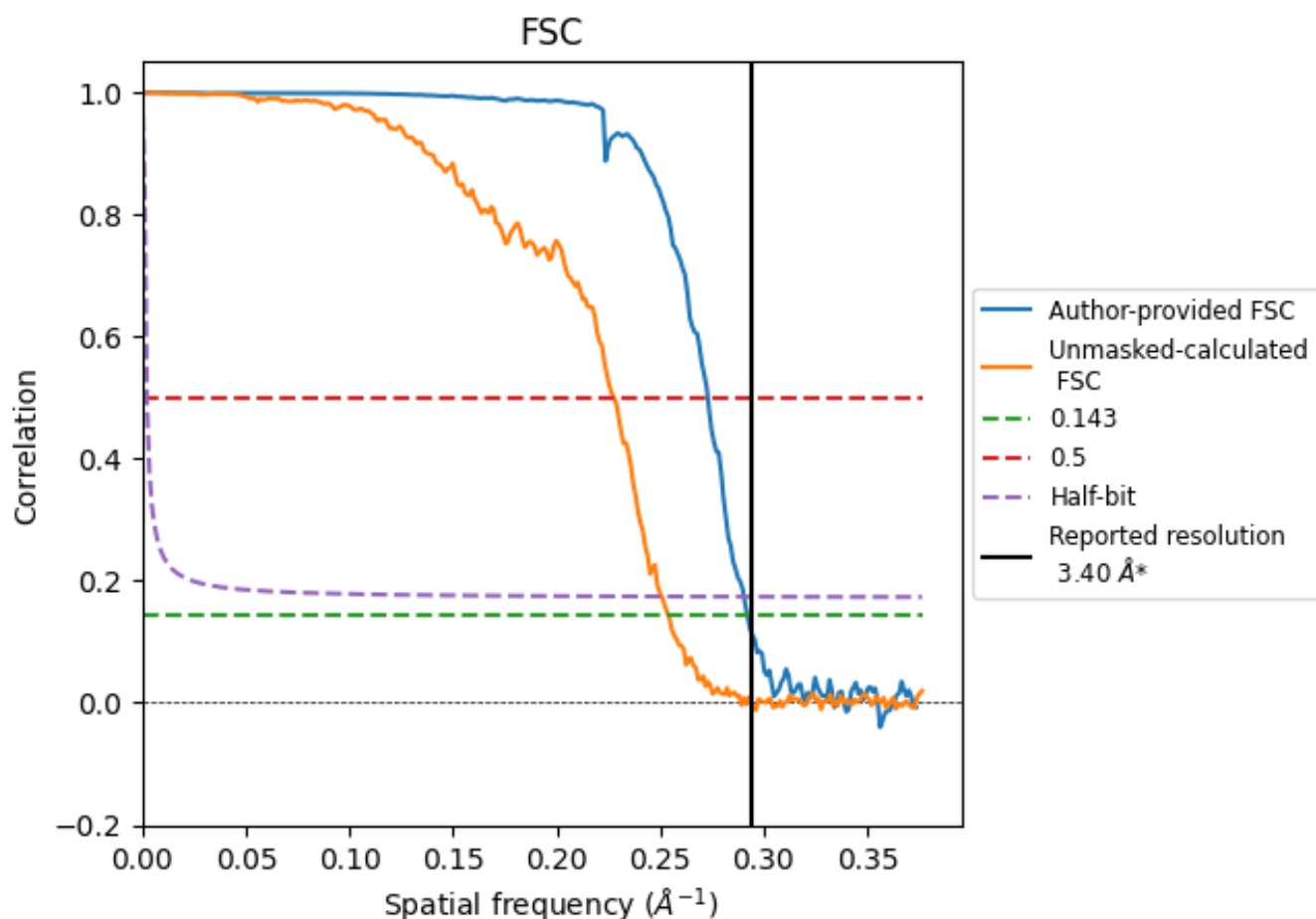


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	3.66	3.44
Unmasked-calculated*	3.94	4.39	3.99

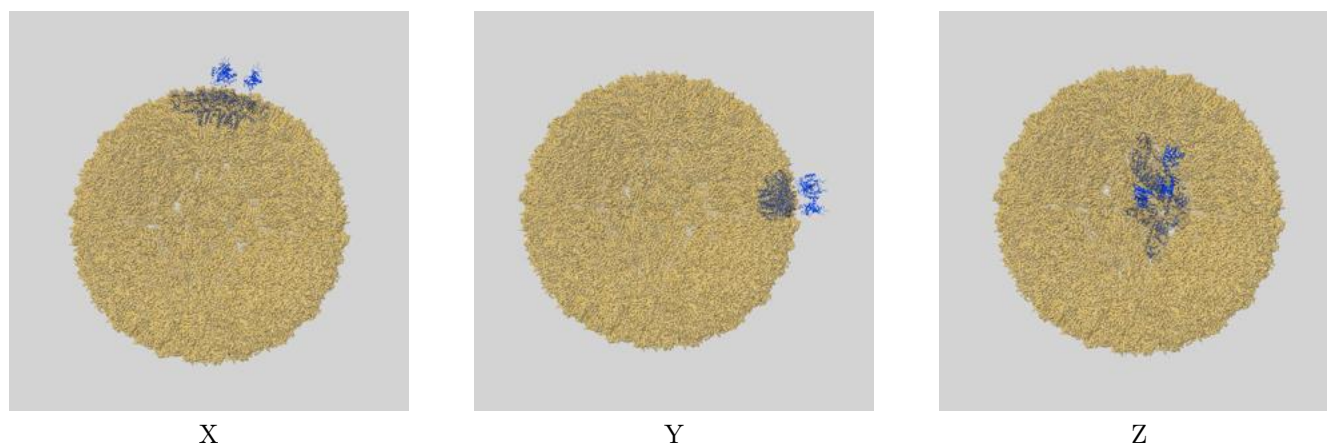
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

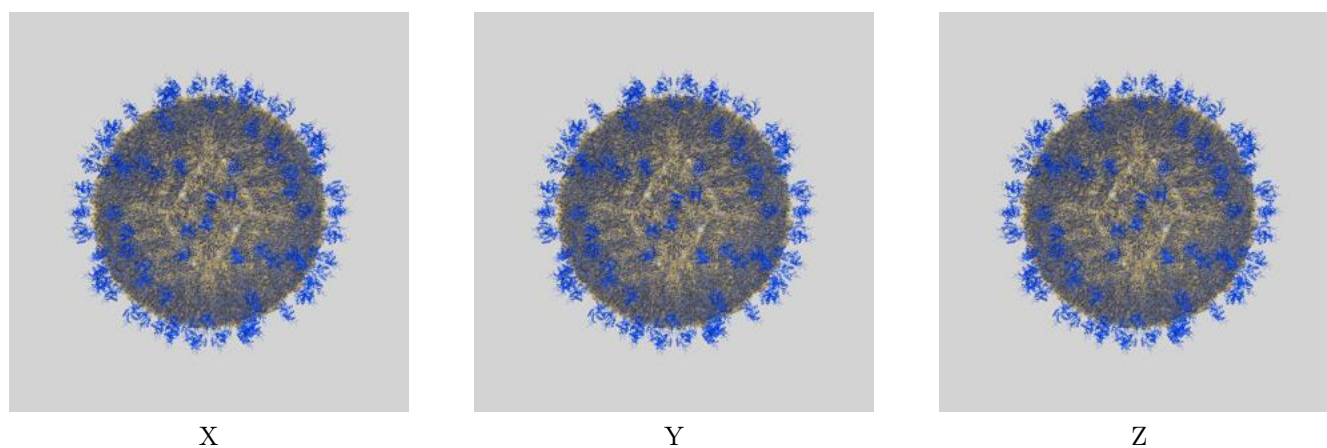
This section contains information regarding the fit between EMDB map EMD-48666 and PDB model 9MVE. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

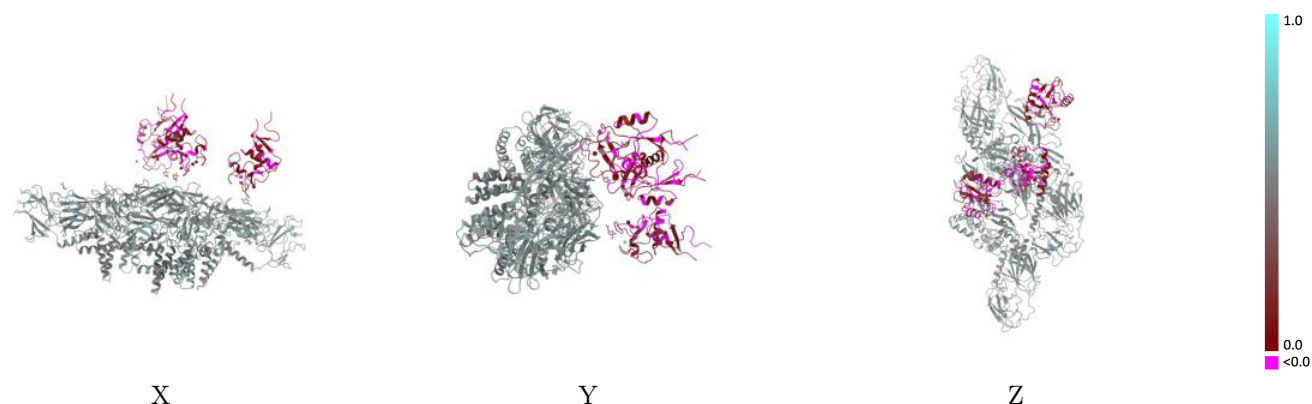


9.1.2 Map-model assembly overlay [i](#)



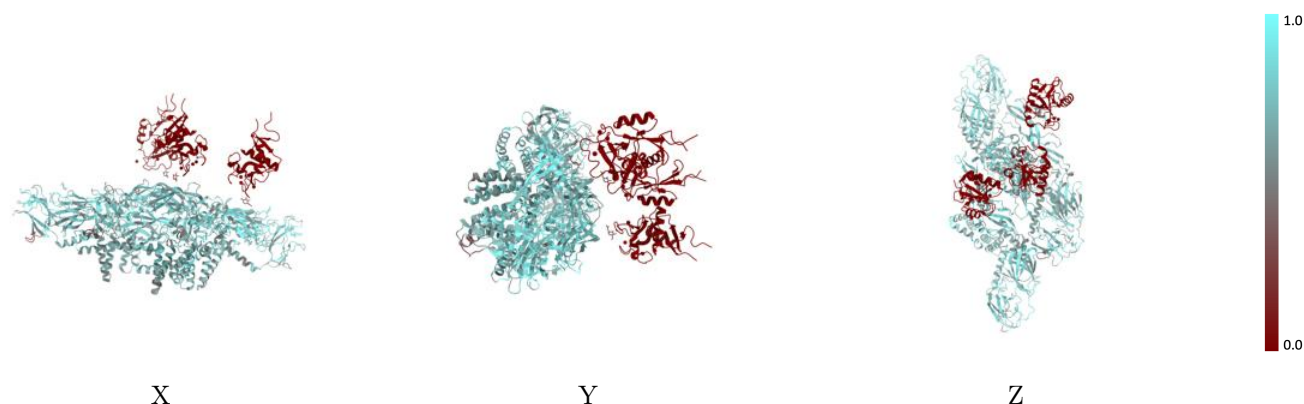
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



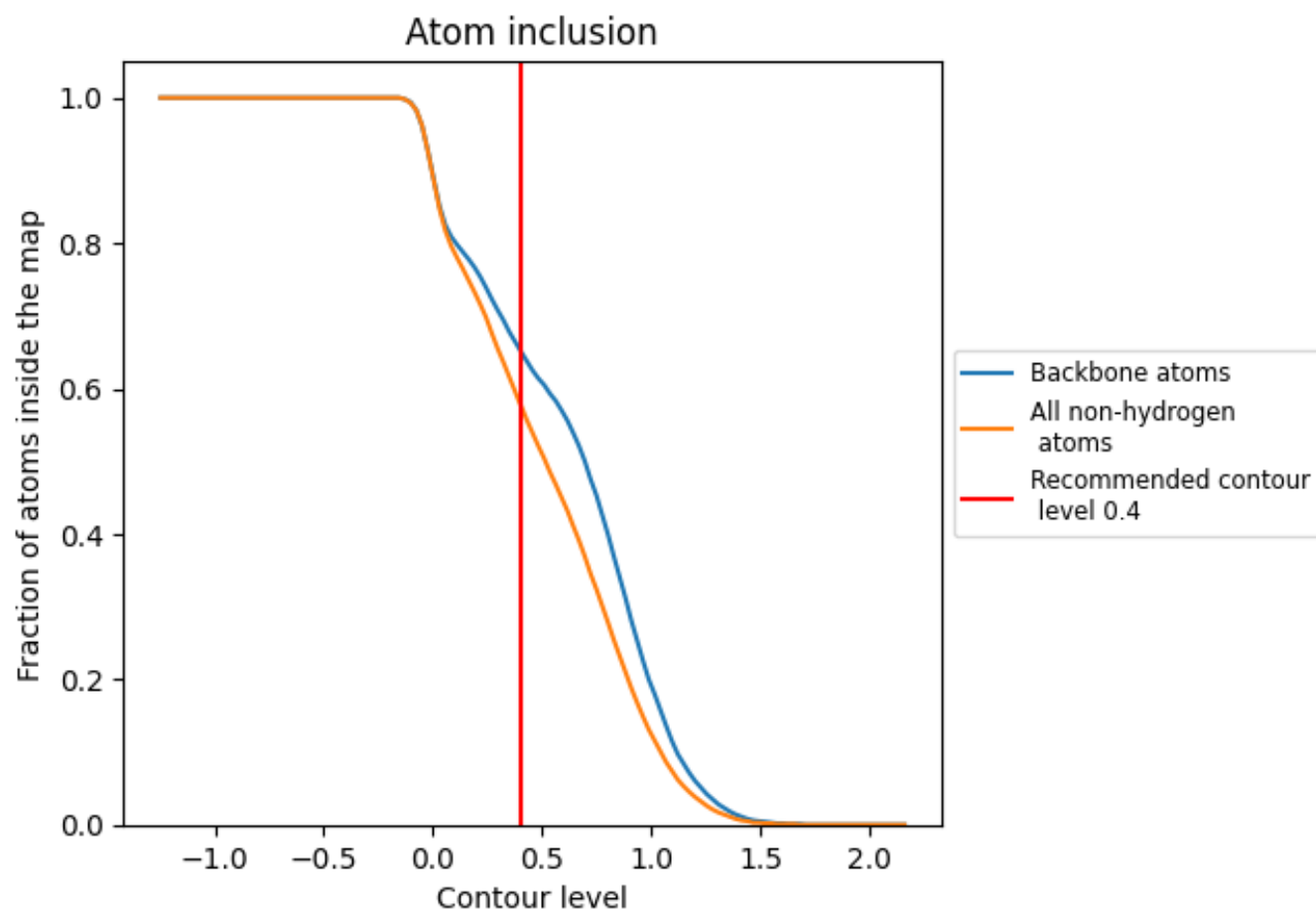
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 58% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5790	0.4380
A	0.7380	0.5300
B	0.7240	0.5400
C	0.6970	0.5170
D	0.6940	0.5330
E	0.7290	0.5240
F	0.7220	0.5430
J	0.0000	0.0970
K	0.0000	0.0390
L	0.0000	0.0970

1.0

0.0

<0.0