



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 08:18 am BST

PDB ID : 9TIF / pdb_00009tif
EMDB ID : EMD-55954
Title : Phage 812 baseplate in the pre-contraction state - lower arm
Authors : Binovsky, J.; Plevka, P.
Deposited on : 2025-12-05
Resolution : 5.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

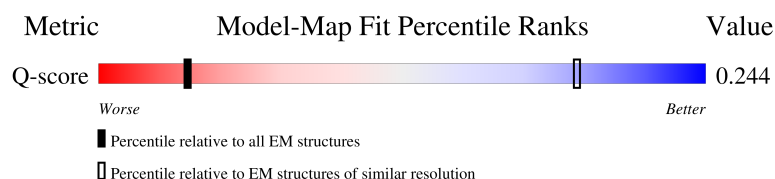
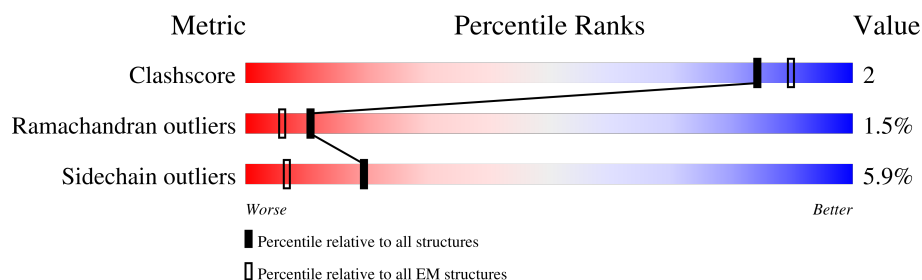
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.60 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.



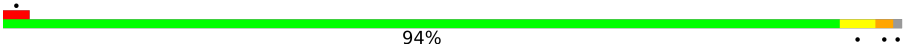
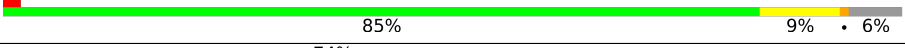
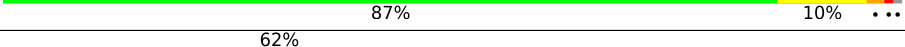
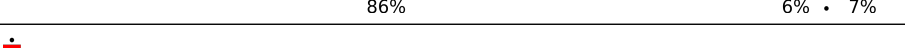
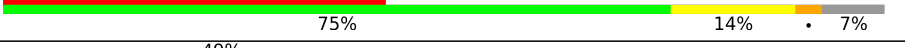
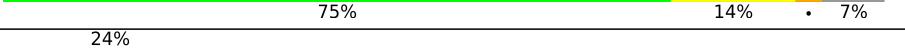
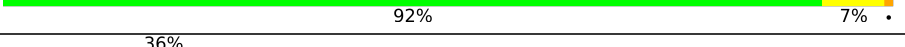
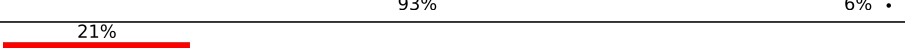
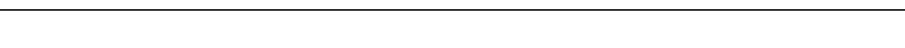
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	513 (5.10 - 6.10)

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	640	26% 91% 8% .
1	B	640	28% 90% 9% .
1	J	640	18% 89% 10% .
2	D	173	61% 82% 15% ..

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Mol	Chain	Length	Quality of chain
2	E	173	
2	I	173	
2	K	173	
2	L	173	
2	N	173	
2	O	173	
2	P	173	
2	Q	173	
2	R	173	
2	V	173	
2	c	173	
3	F	295	
4	G	124	
5	H	1152	
5	d	1152	
5	e	1152	
5	f	1152	
5	g	1152	
5	h	1152	
6	M	808	
7	S	458	
7	T	458	
7	U	458	
8	b	1019	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 100209 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 CBM-cenC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
1	B	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
1	J	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		

- Molecule 2 is a protein called ORF64.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	E	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	I	163	Total	C	N	O	S	0	0
			1277	817	208	251	1		
2	K	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	L	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	N	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	O	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	P	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	Q	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	R	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	V	161	Total	C	N	O	S	0	0
			1266	809	207	249	1		
2	c	162	Total	C	N	O	S	0	0
			1272	812	208	251	1		

- Molecule 3 is a protein called ORF57.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	139	Total	C	N	O	S	0	0
			1157	739	177	239	2		

- Molecule 4 is a protein called ORF67.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	71	Total	C	N	O	S	0	0
			597	390	94	113			

- Molecule 5 is a protein called ORF65.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	d	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	e	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	f	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	g	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	h	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		

- Molecule 6 is a protein called ORF56.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	136	Total	C	N	O	S	0	0
			1064	682	193	186	3		

- Molecule 7 is a protein called ORF68.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
7	T	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
7	U	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		

- Molecule 8 is a protein called ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	b	628	5070	3240	807	1013	10	0	0

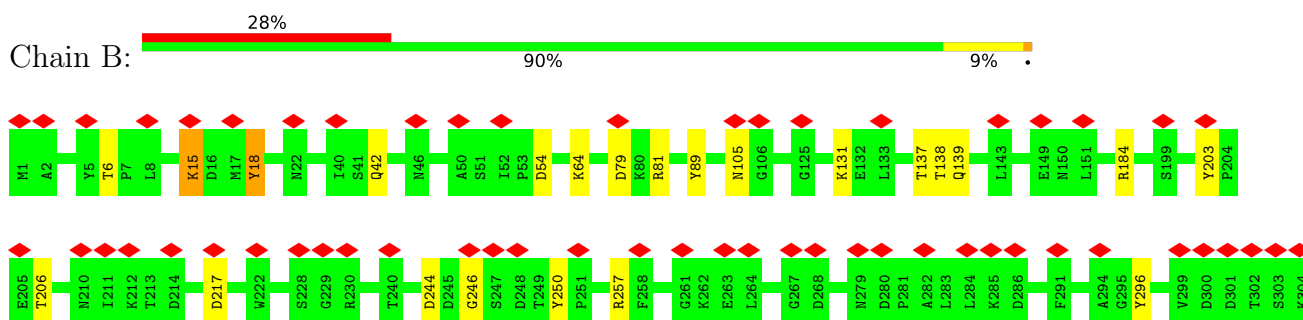
3 Residue-property plots

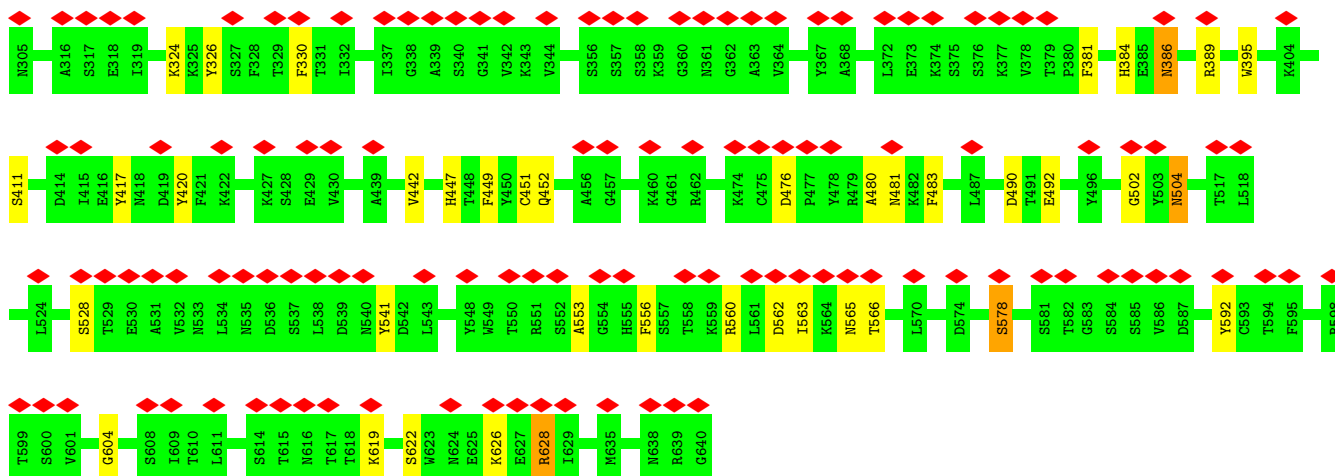
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CBM-cenC domain-containing protein

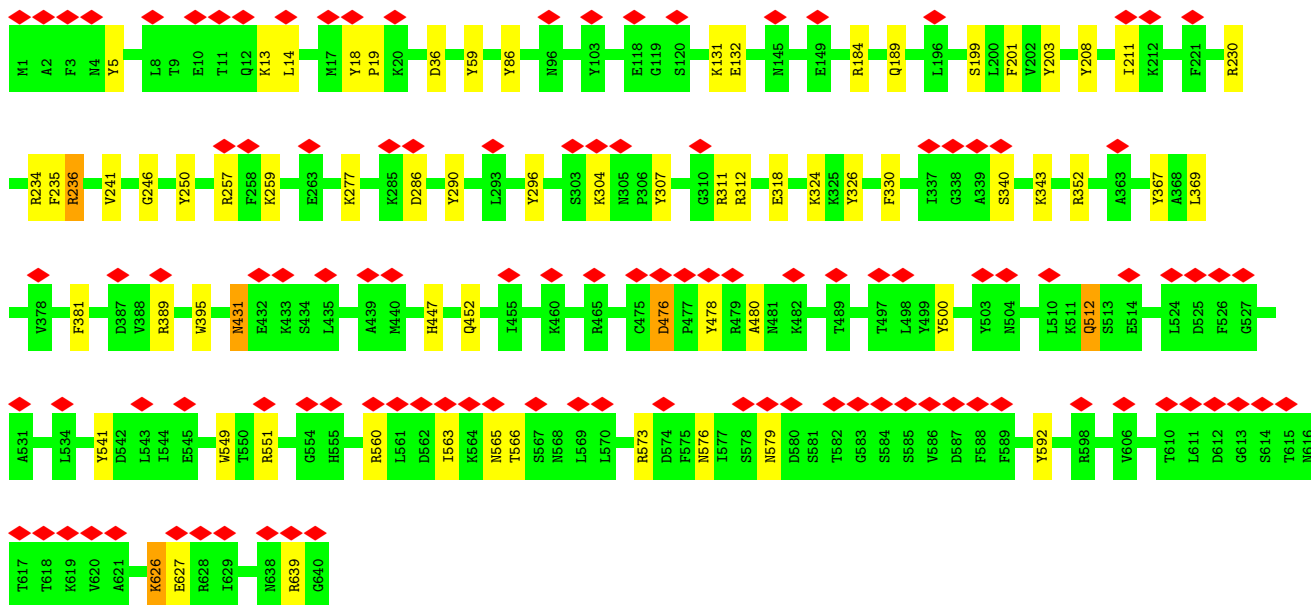
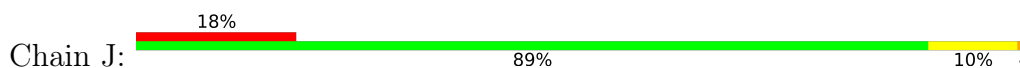


• Molecule 1: CBM-cenC domain-containing protein

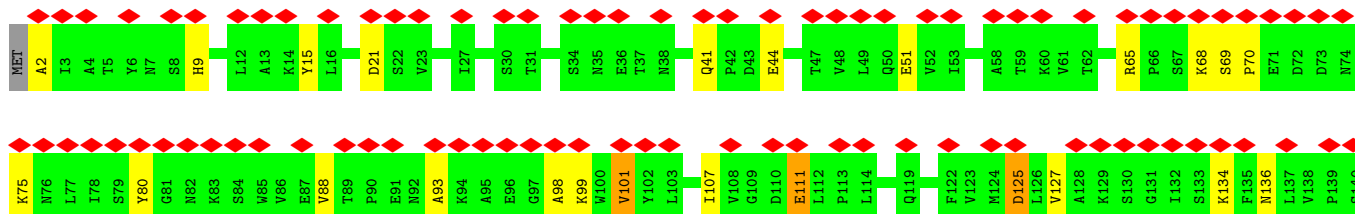
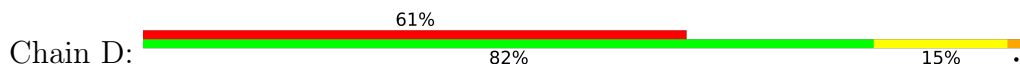


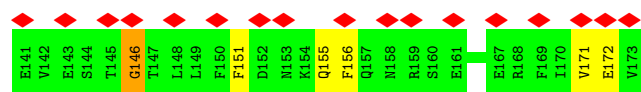


• Molecule 1: CBM-cenC domain-containing protein

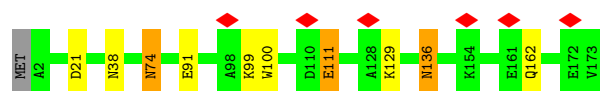


• Molecule 2: ORF64

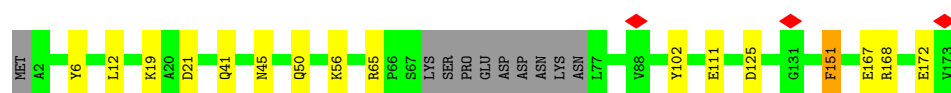
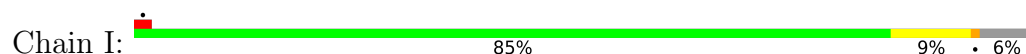




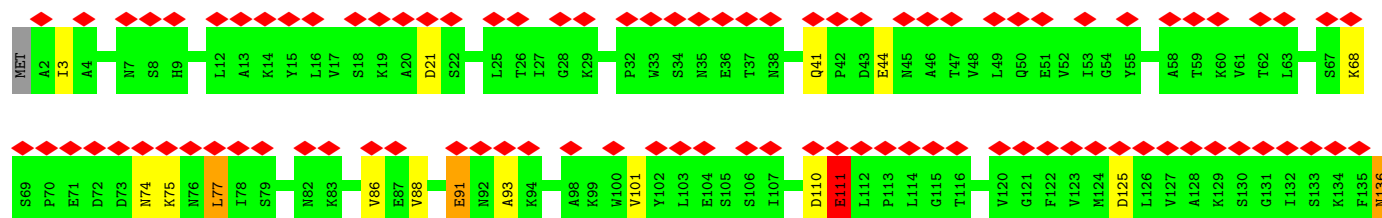
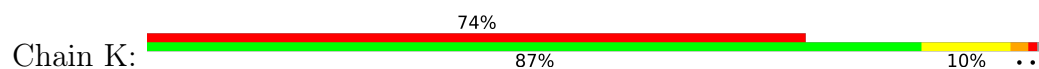
• Molecule 2: ORF64



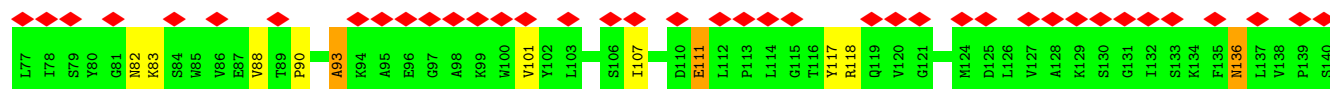
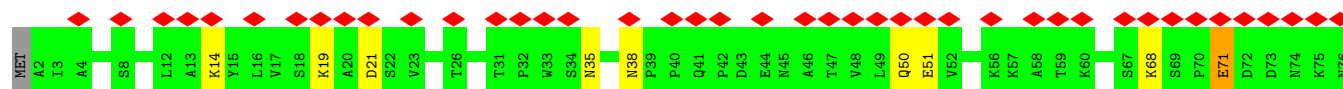
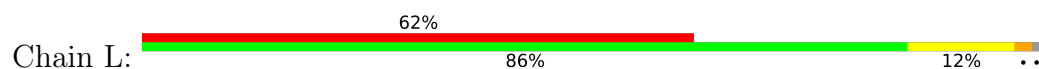
• Molecule 2: ORF64



• Molecule 2: ORF64

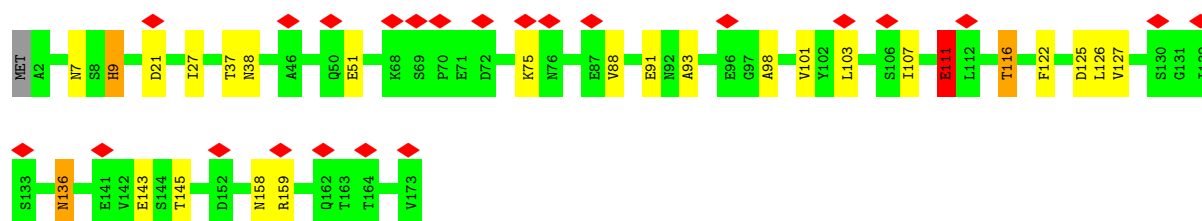


• Molecule 2: ORF64



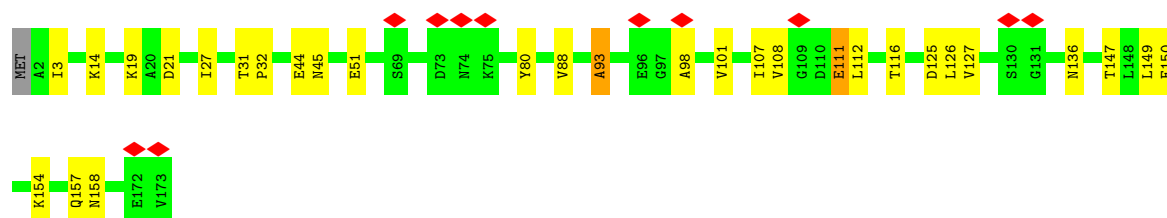
• Molecule 2: ORF64

Chain N: 



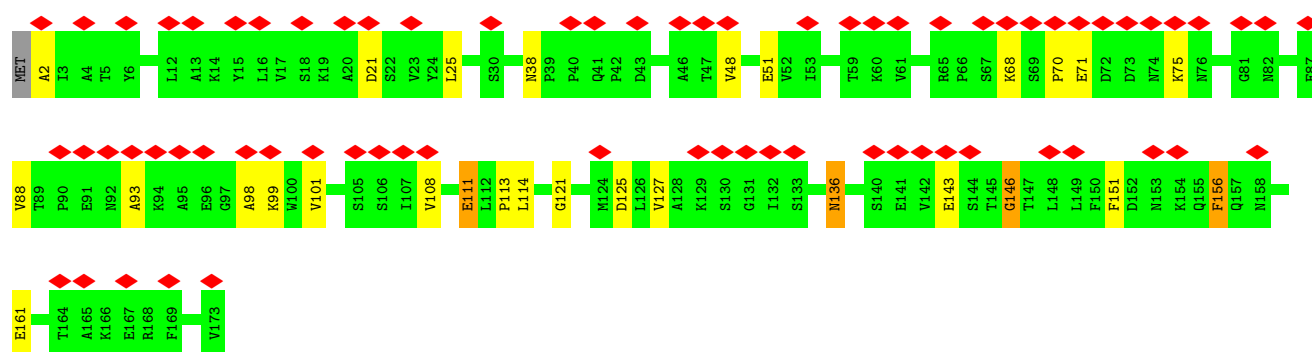
• Molecule 2: ORF64

Chain O: 



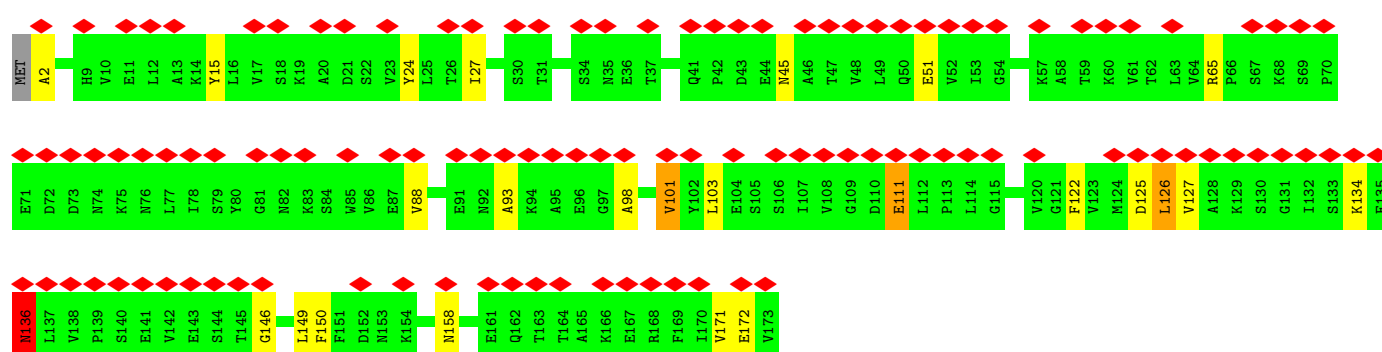
• Molecule 2: ORF64

Chain P: 

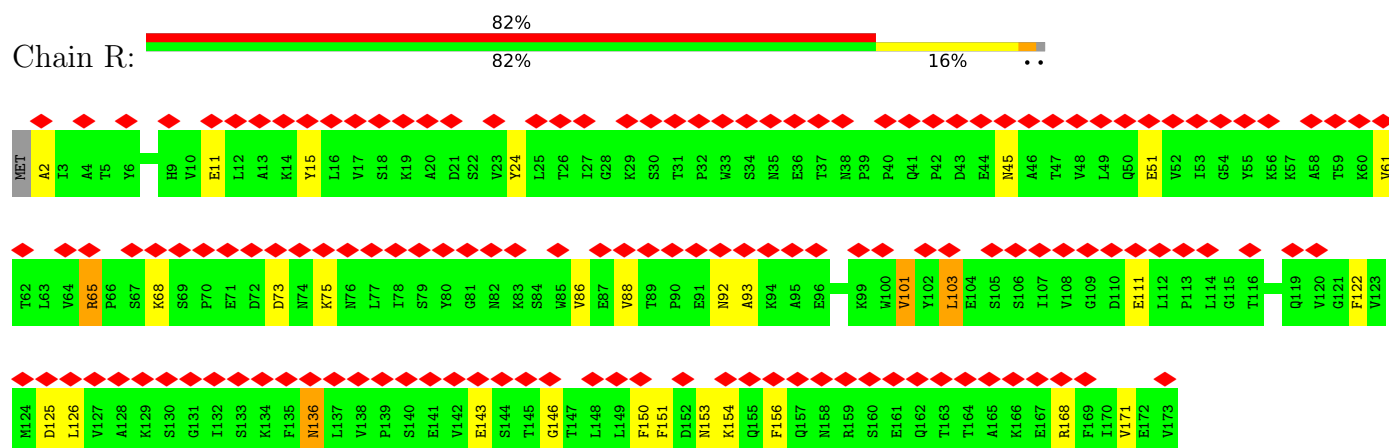


• Molecule 2: ORF64

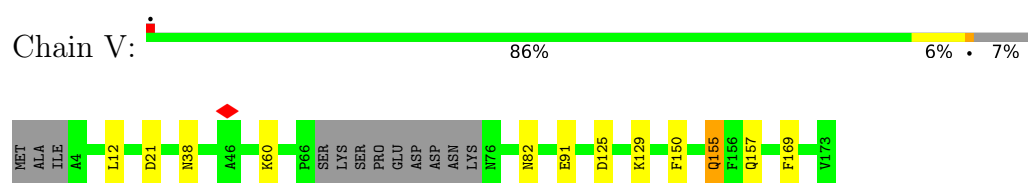
Chain Q: 



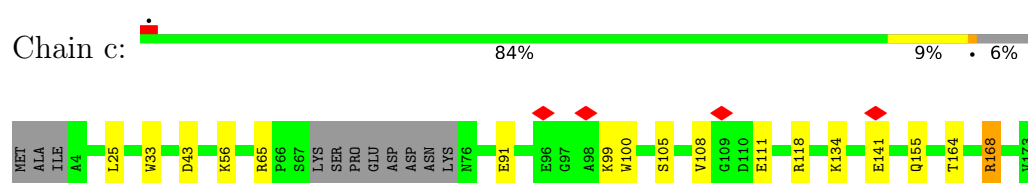
- Molecule 2: ORF64



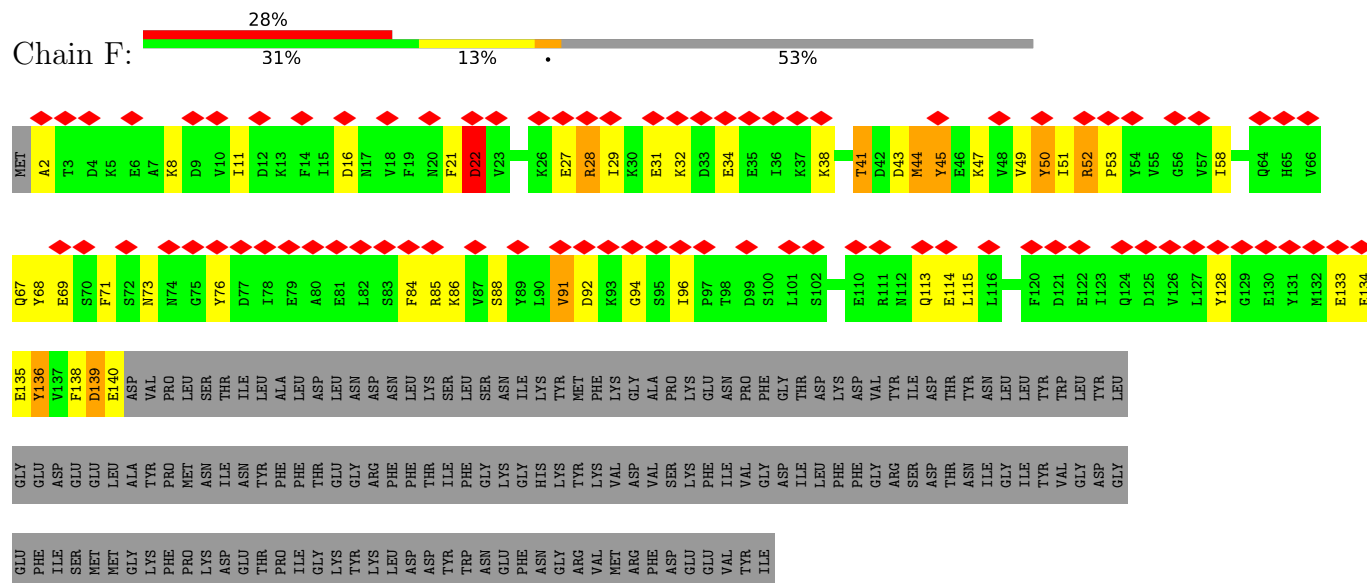
- Molecule 2: ORF64



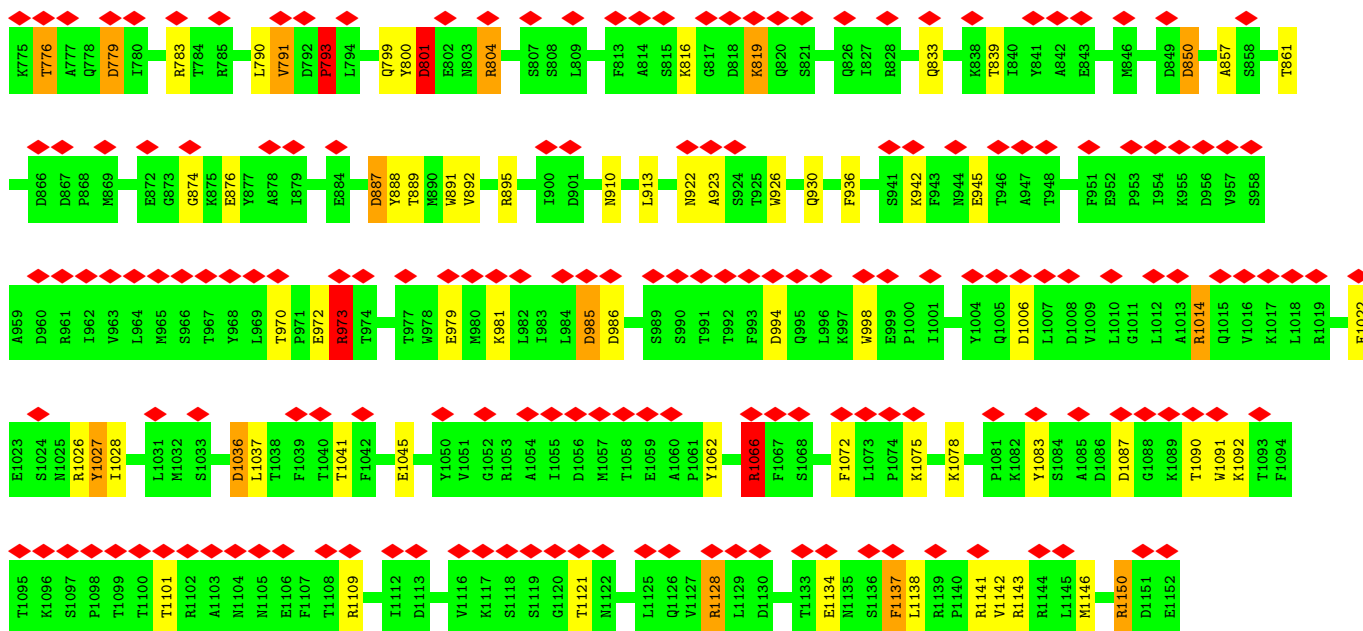
- Molecule 2: ORF64



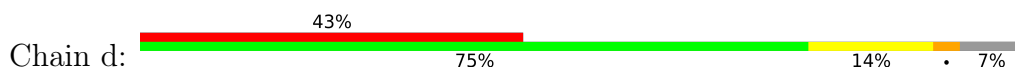
- Molecule 3: ORF57



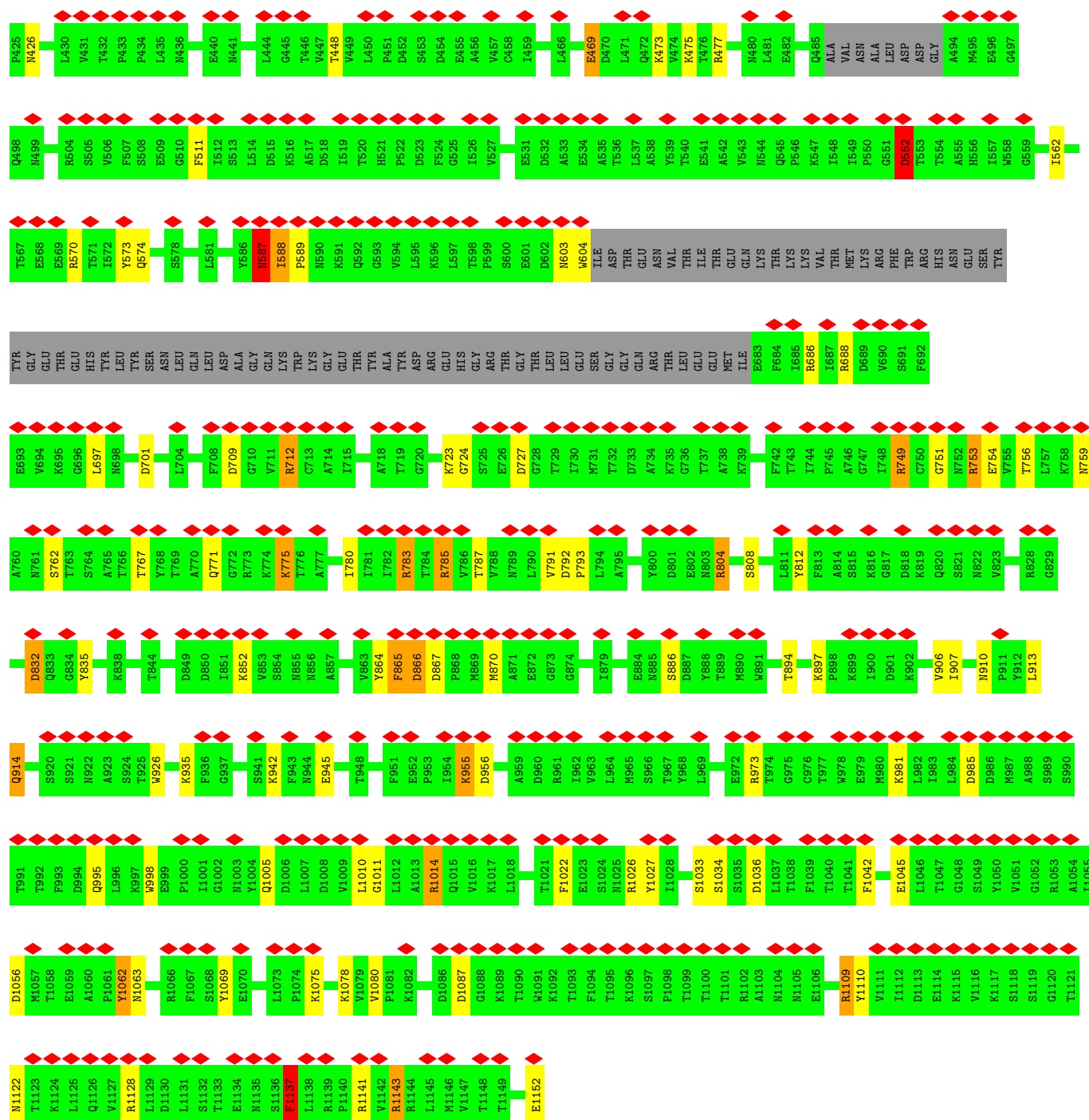
- Molecule 4: ORF67



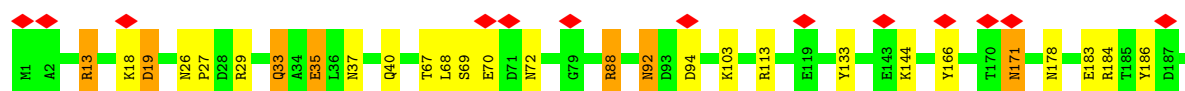
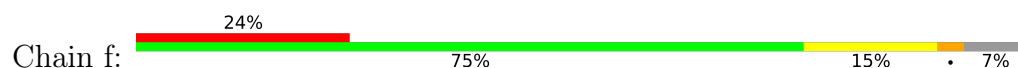
• Molecule 5: ORF65

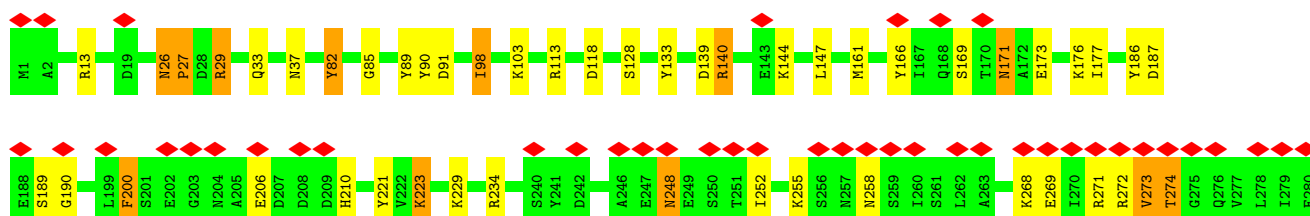
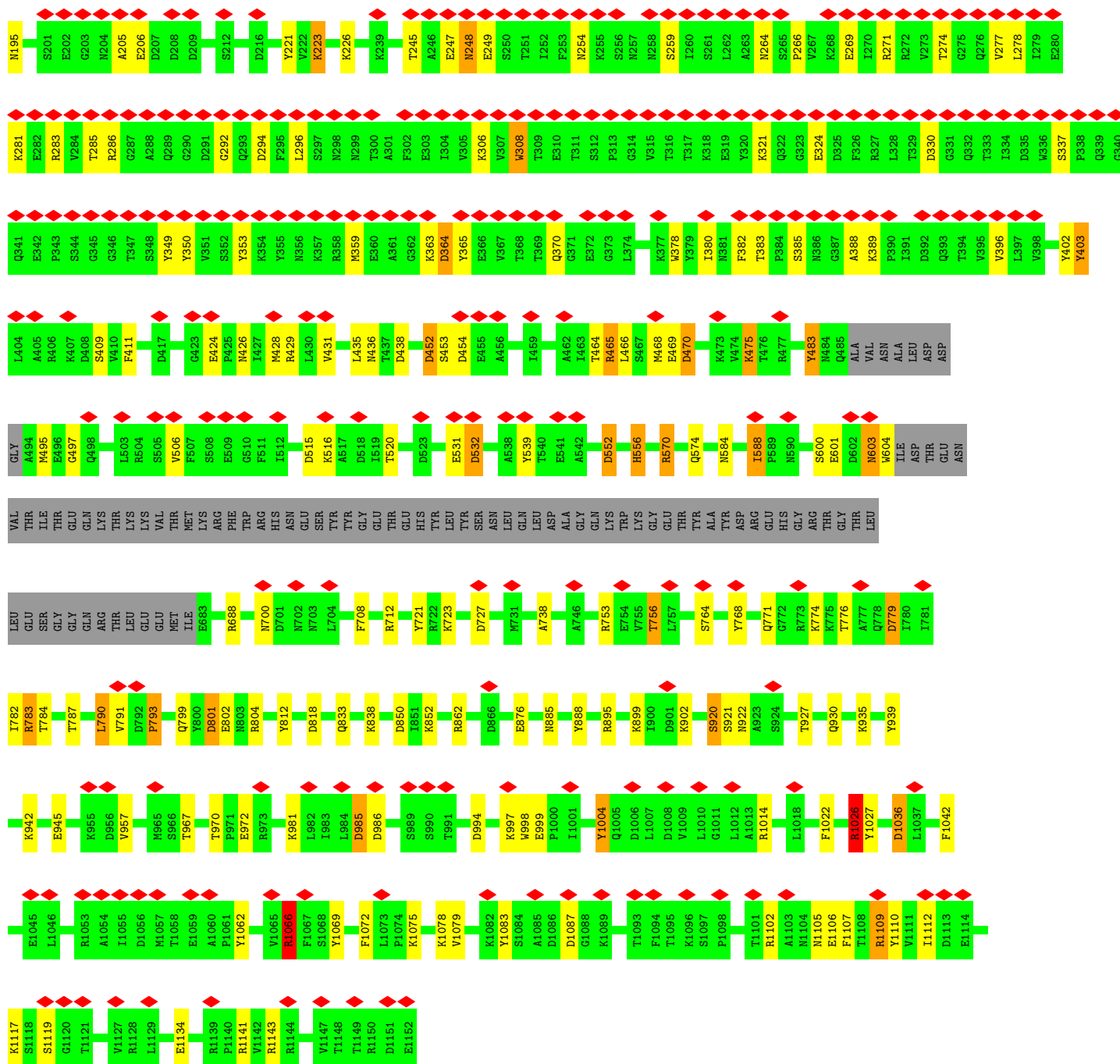




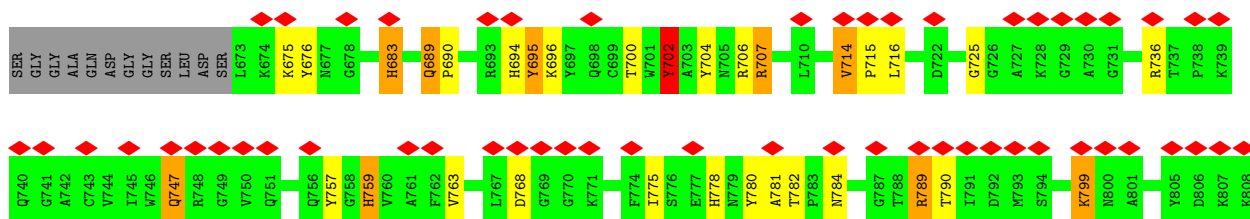


• Molecule 5: ORF65

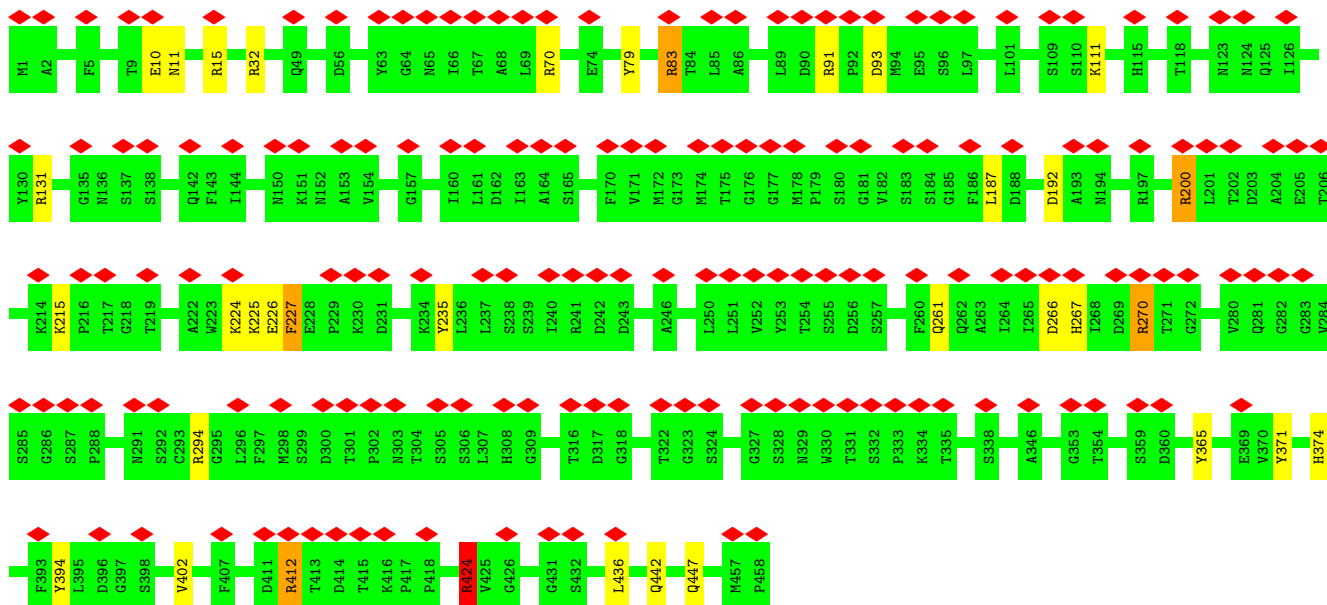




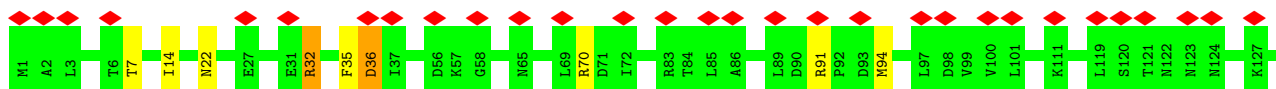
LYS	ASN	THR	HIS	ARG
ILE	LYS	THR	GLY	GLY
MET	VAL	ALA	ASN	THR
LYS	ASP	THR	PRO	LYS
ASP	GLY	THR	ASP	ASP
LEU	GLY	LEU	PHE	ALA
SER	LEU	LEU	TYR	ILE
ASN	THR	ASP	ALA	LEU
GLY	SER	GLY	GLY	LEU
ARG	ASP	TYR	ASP	ASP
ASN	GLY	ILE	ASP	GLY
ASP	ARG	LYS	ILE	LYS
ASN	PRO	TYR	VAL	GLY
ILE	LYS	LYS	LEU	SER
SER	LEU	GLY	GLY	PRO
LYS	THR	GLY	ASP	HIS
GLY	LYS	GLY	PRO	ARG
ILE	GLY	PRO	LYS	PHE
ASP	LYS	ASN	TYR	ALA
LYS	LEU	ASP	ASP	GLY
LYS	LEU	GLY	LEU	TRP
THR	ILE	ALA	GLY	TRP
SER	LYS	GLN	LYS	ASN
LEU	GLY	GLY	LEU	SER
SER	LEU	PHE	SER	SER
SER	SER	ILE	ASP	ASP
LYS	PHE	LYS	LEU	ASP
TYR	LYS	ALA	GLY	MET
LYS	GLY	ILE	ASP	GLY
LYS	THR	ILE	LYS	GLY
ILE	LYS	GLY	LEU	GLY
LYS	LYS	GLY	VAL	GLY
GLY	LYS	SER	ALA	ASP
LYS	ALA	ASP	ALA	LYS
PHE	VAL	THR	SER	GLY
VAL	LYS	VAL	LYS	VAL
THR	LYS	THR	GLY	VAL
LYS	GLY	THR	TYR	GLY
GLY	GLY	THR	ARG	ASP
LYS	LYS	TYR	LEU	ASP
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ILE	GLY	ASN	GLY	ASN
THR	LYS	THR	VAL	THR

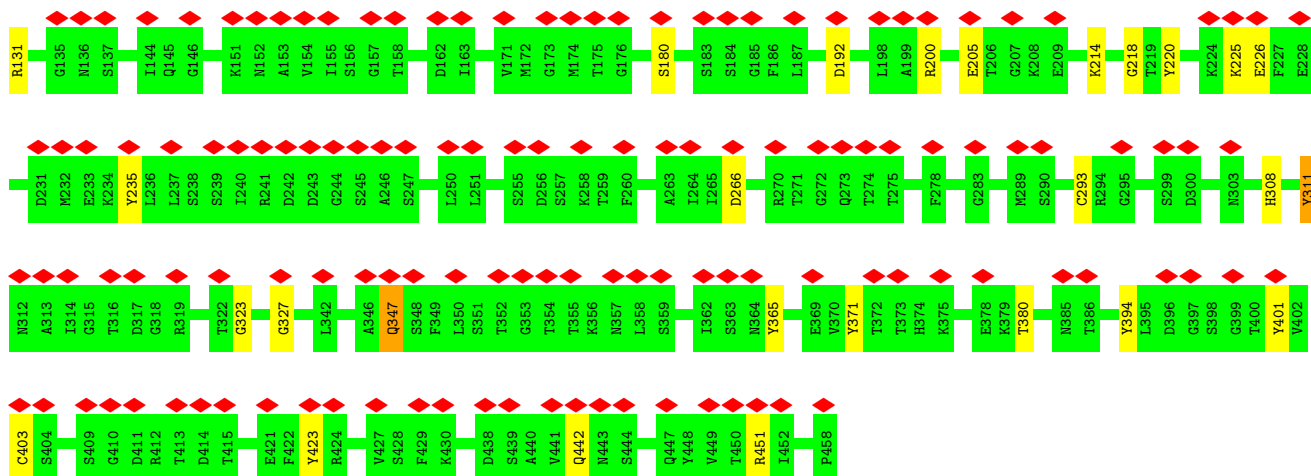


• Molecule 7: ORF68

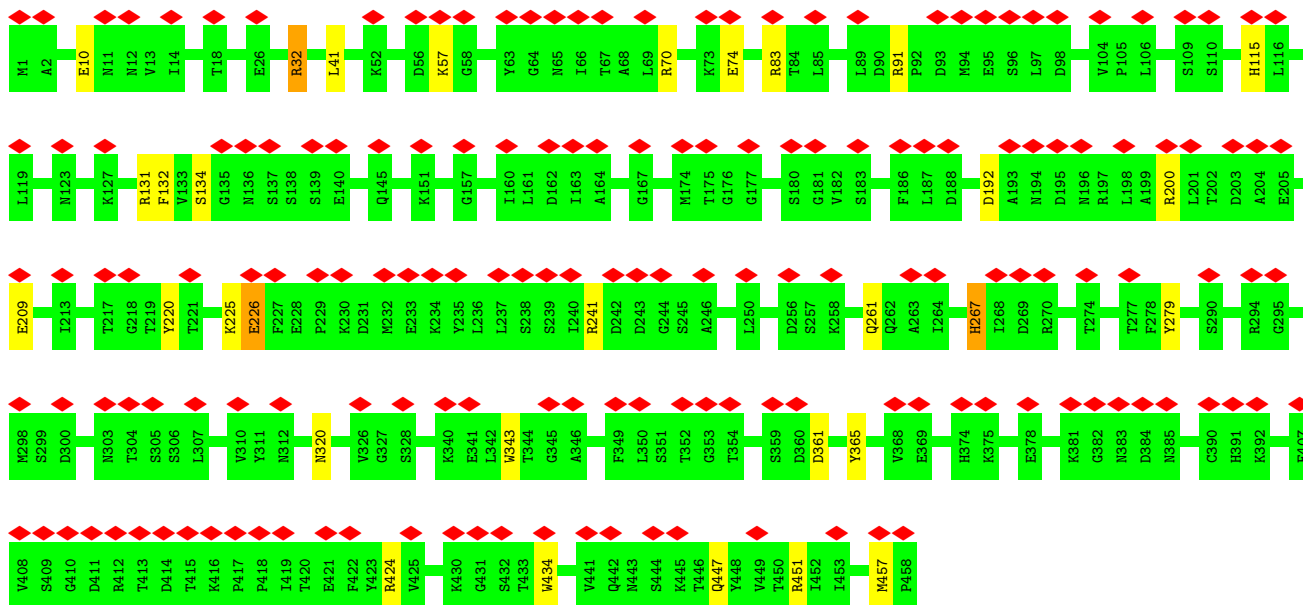
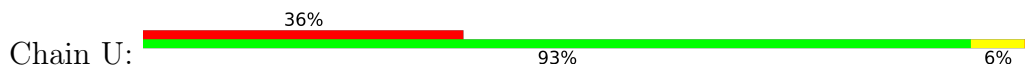


• Molecule 7: ORF68

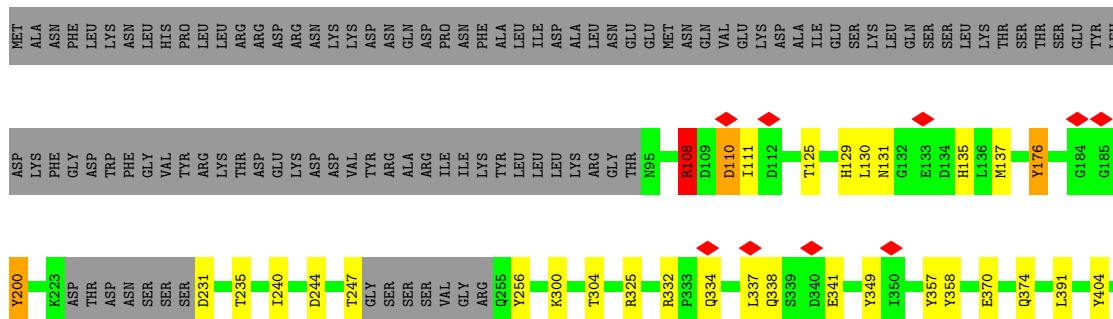


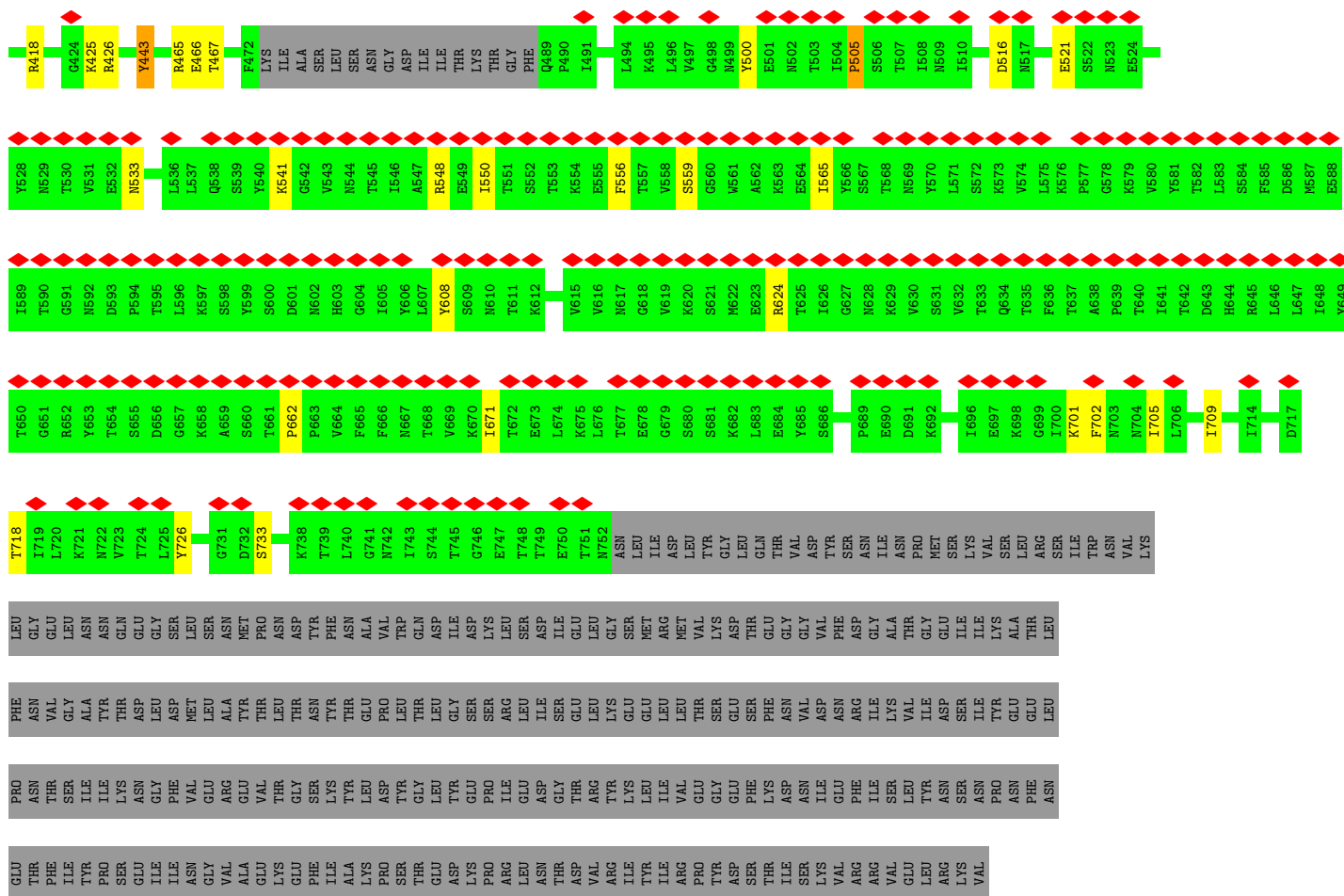


• Molecule 7: ORF68



• Molecule 8: ORF63





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	600.192, 600.192, 600.192	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.6672001, 1.6672001, 1.6672001	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.74	0/5253	1.30	17/7135 (0.2%)
1	B	0.75	0/5253	1.31	22/7135 (0.3%)
1	J	0.74	0/5253	1.31	19/7135 (0.3%)
2	D	0.75	0/1377	1.48	9/1872 (0.5%)
2	E	0.71	0/1377	1.29	5/1872 (0.3%)
2	I	0.71	0/1303	1.27	3/1771 (0.2%)
2	K	0.80	0/1377	1.51	9/1872 (0.5%)
2	L	0.78	0/1377	1.46	11/1872 (0.6%)
2	N	0.70	0/1377	1.42	8/1872 (0.4%)
2	O	0.73	0/1377	1.39	7/1872 (0.4%)
2	P	0.74	0/1377	1.43	8/1872 (0.4%)
2	Q	0.76	0/1377	1.46	7/1872 (0.4%)
2	R	0.80	0/1377	1.47	8/1872 (0.4%)
2	V	0.71	0/1292	1.29	1/1756 (0.1%)
2	c	0.73	0/1298	1.21	3/1764 (0.2%)
3	F	0.78	0/1178	1.59	11/1593 (0.7%)
4	G	0.77	0/613	1.32	0/830
5	H	0.81	0/8552	1.50	71/11599 (0.6%)
5	d	0.79	0/8552	1.46	63/11599 (0.5%)
5	e	0.77	0/8552	1.41	48/11599 (0.4%)
5	f	0.77	0/8552	1.41	61/11599 (0.5%)
5	g	0.77	0/8552	1.44	55/11599 (0.5%)
5	h	0.77	0/8552	1.46	71/11599 (0.6%)
6	M	0.80	0/1097	1.43	7/1482 (0.5%)
7	S	0.72	0/3619	1.26	14/4913 (0.3%)
7	T	0.75	0/3619	1.29	12/4913 (0.2%)
7	U	0.72	0/3619	1.27	11/4913 (0.2%)
8	b	0.76	0/5179	1.30	15/7040 (0.2%)
All	All	0.76	0/102281	1.39	576/138822 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	11
1	J	0	16
2	D	0	2
2	I	0	2
2	L	0	2
2	N	0	1
2	O	0	1
2	Q	0	1
2	R	0	3
2	V	0	1
2	c	0	1
3	F	0	5
4	G	0	6
5	H	0	17
5	d	0	25
5	e	0	23
5	f	0	21
5	g	0	19
5	h	0	30
6	M	0	8
7	S	0	10
7	T	0	9
7	U	0	7
8	b	0	14
All	All	0	247

There are no bond length outliers.

The worst 5 of 576 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	171	ASN	CA-CB-CG	11.87	124.47	112.60
5	e	552	ASP	CA-CB-CG	11.68	124.28	112.60
5	H	243	LEU	CA-C-N	10.48	129.68	121.61
5	H	243	LEU	C-N-CA	10.48	129.68	121.61
5	h	43	ASP	CA-CB-CG	-9.52	103.08	112.60

There are no chirality outliers.

5 of 247 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	18	TYR	Sidechain
1	A	208	TYR	Sidechain
1	A	5	TYR	Sidechain
1	A	93	TYR	Sidechain

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	5127	0	4969	16	0
1	B	5127	0	4969	16	0
1	J	5127	0	4969	17	0
2	D	1349	0	1339	8	0
2	E	1349	0	1339	5	0
2	I	1277	0	1274	6	0
2	K	1349	0	1339	7	0
2	L	1349	0	1339	6	0
2	N	1349	0	1339	6	0
2	O	1349	0	1339	8	0
2	P	1349	0	1339	5	0
2	Q	1349	0	1339	7	0
2	R	1349	0	1339	8	0
2	V	1266	0	1259	3	0
2	c	1272	0	1264	8	0
3	F	1157	0	1111	14	0
4	G	597	0	570	3	0
5	H	8390	0	8229	61	0
5	d	8390	0	8229	49	0
5	e	8390	0	8229	55	0
5	f	8390	0	8229	52	0
5	g	8390	0	8229	39	0
5	h	8390	0	8229	43	0
6	M	1064	0	1039	14	0
7	S	3548	0	3468	12	0
7	T	3548	0	3468	10	0
7	U	3548	0	3468	7	0
8	b	5070	0	4932	12	0
All	All	100209	0	98185	452	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 452 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)
7:S:424:ARG:NH1	7:T:380:THR:HG21	2.01	0.75
3:F:53:PRO:HB3	6:M:782:THR:HG23	1.70	0.71
5:d:33:GLN:HE21	5:e:27:PRO:HA	1.57	0.70
2:I:12:LEU:HD21	2:V:12:LEU:HD22	1.76	0.68
2:N:116:THR:HG22	2:N:158:ASN:HA	1.76	0.68

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	638/640 (100%)	607 (95%)	29 (4%)	2 (0%)	36	72
1	B	638/640 (100%)	604 (95%)	30 (5%)	4 (1%)	21	59
1	J	638/640 (100%)	607 (95%)	25 (4%)	6 (1%)	14	50
2	D	170/173 (98%)	149 (88%)	19 (11%)	2 (1%)	10	43
2	E	170/173 (98%)	155 (91%)	15 (9%)	0	100	100
2	I	159/173 (92%)	150 (94%)	9 (6%)	0	100	100
2	K	170/173 (98%)	150 (88%)	16 (9%)	4 (2%)	4	26
2	L	170/173 (98%)	154 (91%)	14 (8%)	2 (1%)	10	43
2	N	170/173 (98%)	153 (90%)	14 (8%)	3 (2%)	6	33
2	O	170/173 (98%)	155 (91%)	13 (8%)	2 (1%)	10	43
2	P	170/173 (98%)	148 (87%)	17 (10%)	5 (3%)	3	23
2	Q	170/173 (98%)	152 (89%)	16 (9%)	2 (1%)	10	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	170/173 (98%)	149 (88%)	18 (11%)	3 (2%)	6	33
2	V	157/173 (91%)	153 (98%)	4 (2%)	0	100	100
2	c	158/173 (91%)	151 (96%)	7 (4%)	0	100	100
3	F	137/295 (46%)	104 (76%)	25 (18%)	8 (6%)	1	13
4	G	69/124 (56%)	59 (86%)	8 (12%)	2 (3%)	3	23
5	H	1060/1152 (92%)	916 (86%)	120 (11%)	24 (2%)	5	27
5	d	1060/1152 (92%)	896 (84%)	134 (13%)	30 (3%)	4	24
5	e	1060/1152 (92%)	920 (87%)	117 (11%)	23 (2%)	5	28
5	f	1060/1152 (92%)	930 (88%)	113 (11%)	17 (2%)	7	36
5	g	1060/1152 (92%)	928 (88%)	118 (11%)	14 (1%)	9	41
5	h	1060/1152 (92%)	933 (88%)	98 (9%)	29 (3%)	4	24
6	M	134/808 (17%)	115 (86%)	18 (13%)	1 (1%)	18	55
7	S	456/458 (100%)	440 (96%)	15 (3%)	1 (0%)	43	77
7	T	456/458 (100%)	434 (95%)	21 (5%)	1 (0%)	43	77
7	U	456/458 (100%)	436 (96%)	19 (4%)	1 (0%)	43	77
8	b	620/1019 (61%)	568 (92%)	45 (7%)	7 (1%)	11	45
All	All	12606/14528 (87%)	11316 (90%)	1097 (9%)	193 (2%)	11	38

5 of 193 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
5	H	452	ASP
5	H	791	VAL
2	L	93	ALA
2	N	93	ALA

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	577/577 (100%)	566 (98%)	11 (2%)	50	66
1	B	577/577 (100%)	565 (98%)	12 (2%)	47	65
1	J	577/577 (100%)	563 (98%)	14 (2%)	43	63
2	D	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	E	152/153 (99%)	149 (98%)	3 (2%)	48	66
2	I	143/153 (94%)	139 (97%)	4 (3%)	38	59
2	K	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	L	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	N	152/153 (99%)	138 (91%)	14 (9%)	8	26
2	O	152/153 (99%)	138 (91%)	14 (9%)	8	26
2	P	152/153 (99%)	138 (91%)	14 (9%)	8	26
2	Q	152/153 (99%)	140 (92%)	12 (8%)	11	31
2	R	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	V	142/153 (93%)	134 (94%)	8 (6%)	19	40
2	c	143/153 (94%)	142 (99%)	1 (1%)	76	80
3	F	132/271 (49%)	109 (83%)	23 (17%)	2	10
4	G	63/112 (56%)	61 (97%)	2 (3%)	34	55
5	H	936/1010 (93%)	848 (91%)	88 (9%)	8	25
5	d	936/1010 (93%)	865 (92%)	71 (8%)	12	32
5	e	936/1010 (93%)	871 (93%)	65 (7%)	14	36
5	f	936/1010 (93%)	859 (92%)	77 (8%)	10	30
5	g	936/1010 (93%)	863 (92%)	73 (8%)	11	32
5	h	936/1010 (93%)	875 (94%)	61 (6%)	15	37
6	M	105/695 (15%)	95 (90%)	10 (10%)	8	25
7	S	405/405 (100%)	399 (98%)	6 (2%)	57	71
7	T	405/405 (100%)	398 (98%)	7 (2%)	53	68
7	U	405/405 (100%)	399 (98%)	6 (2%)	57	71
8	b	573/928 (62%)	553 (96%)	20 (4%)	32	53
All	All	11231/12848 (87%)	10571 (94%)	660 (6%)	19	39

5 of 660 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	f	254	ASN
5	g	729	THR
5	f	454	ASP
5	f	249	GLU
5	f	1075	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
7	U	262	GLN
5	g	484	ASN
8	b	710	GLN
5	g	443	GLN
5	h	356	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

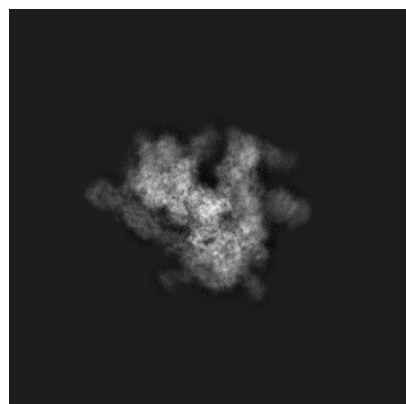
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55954. These allow visual inspection of the internal detail of the map and identification of artifacts.

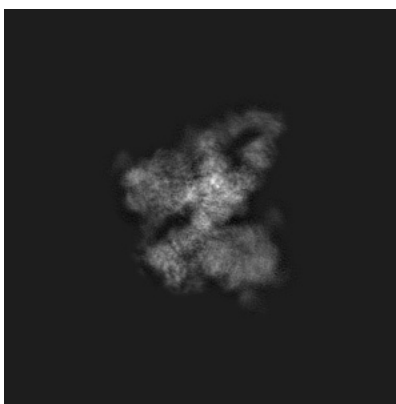
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

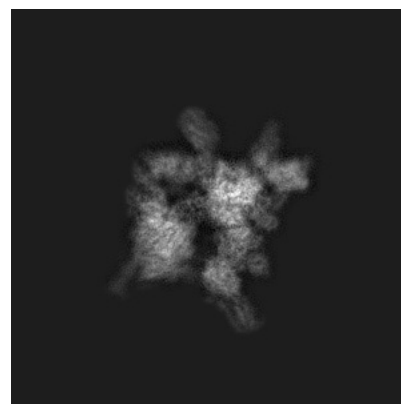
6.1.1 Primary map



X

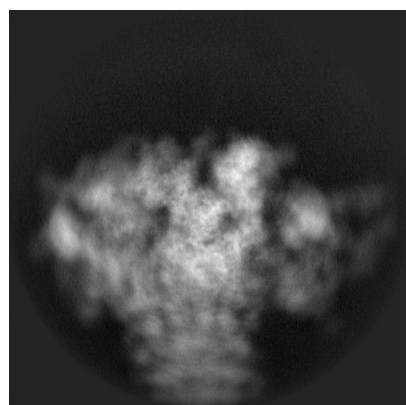


Y

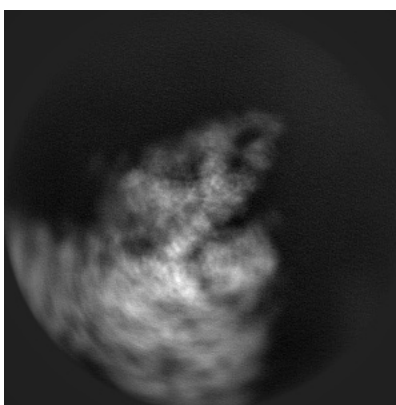


Z

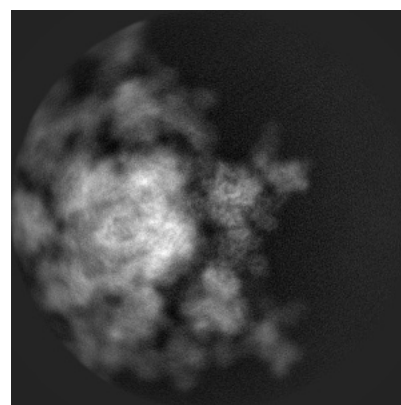
6.1.2 Raw map



X



Y

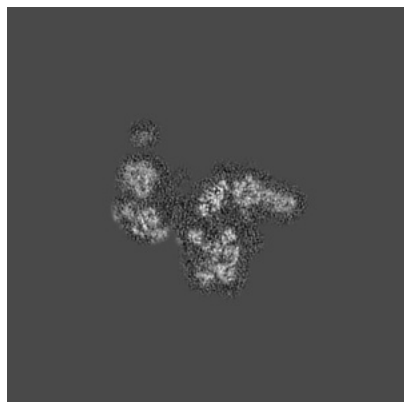


Z

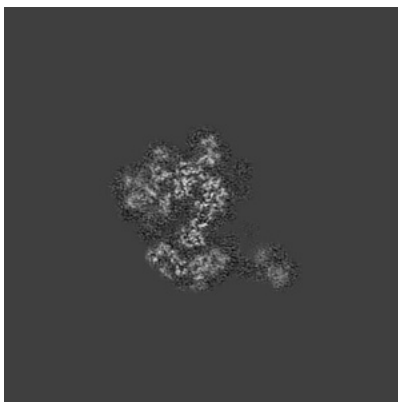
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

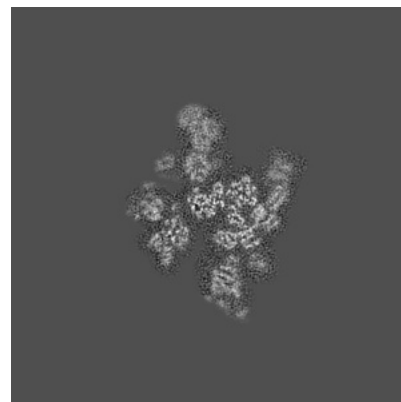
6.2.1 Primary map



X Index: 180

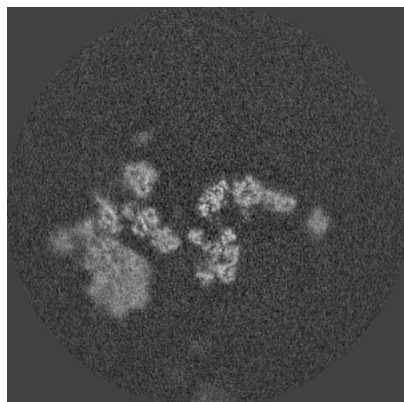


Y Index: 180

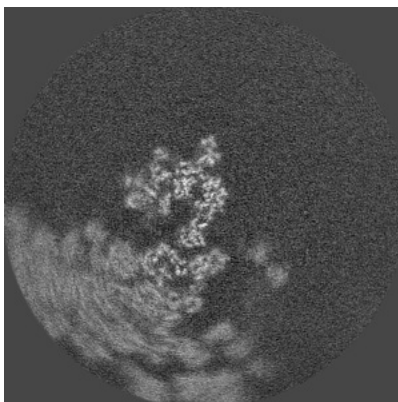


Z Index: 180

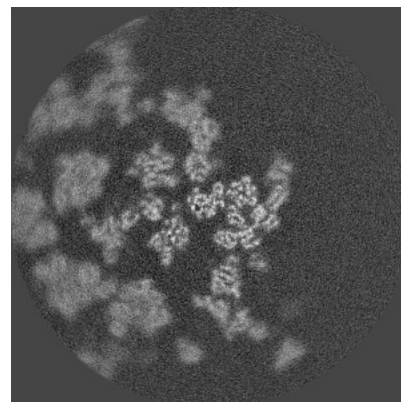
6.2.2 Raw map



X Index: 180



Y Index: 180

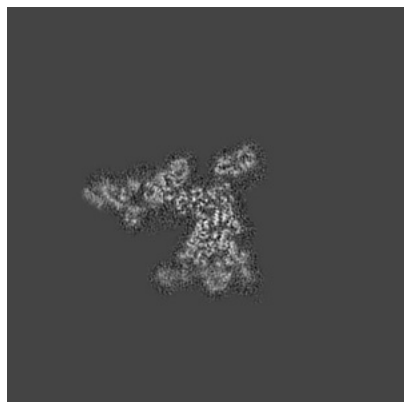


Z Index: 180

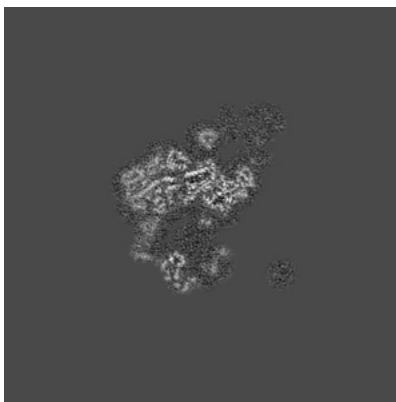
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

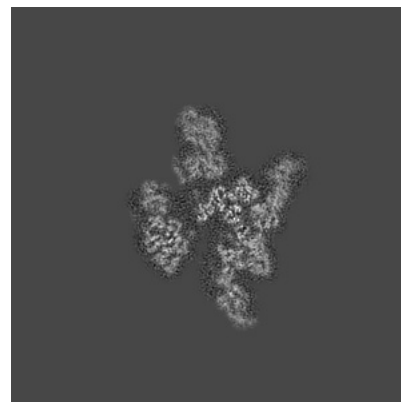
6.3.1 Primary map



X Index: 204

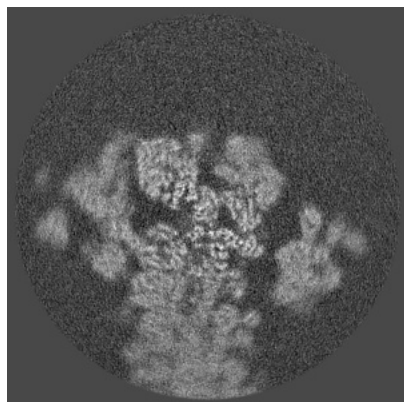


Y Index: 192

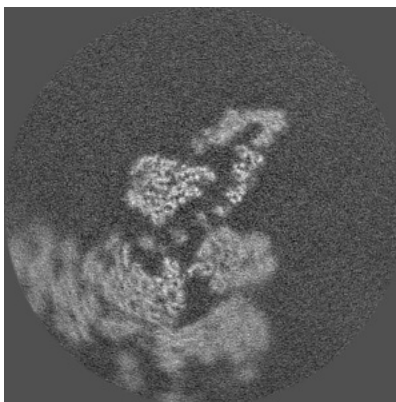


Z Index: 186

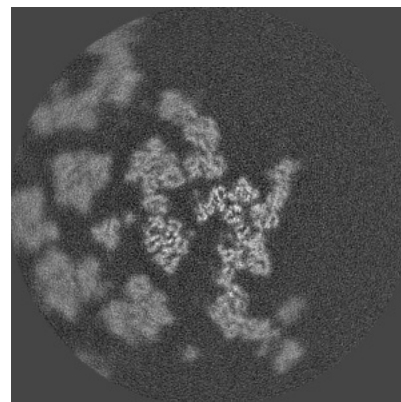
6.3.2 Raw map



X Index: 127



Y Index: 203

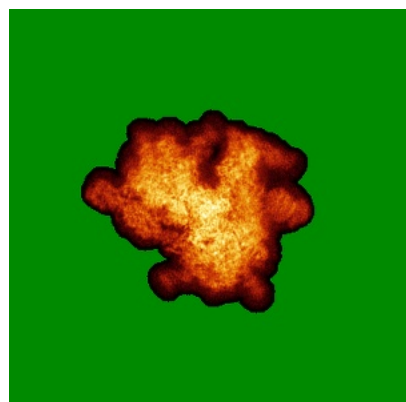


Z Index: 186

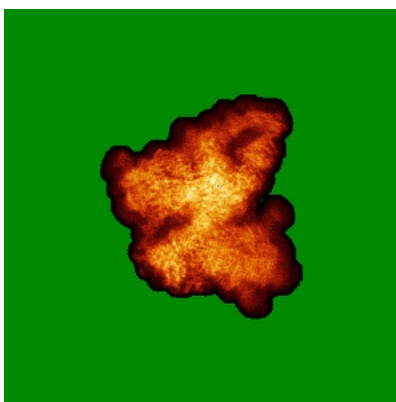
The images above show the largest variance slices of the map in three orthogonal directions.

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

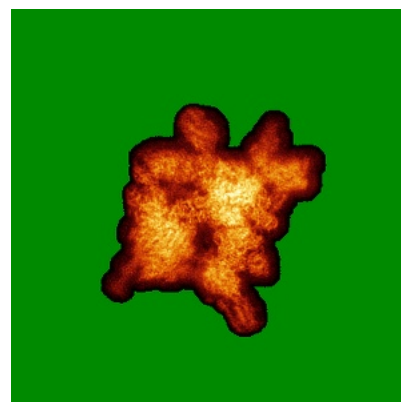
6.4.1 Primary map



X

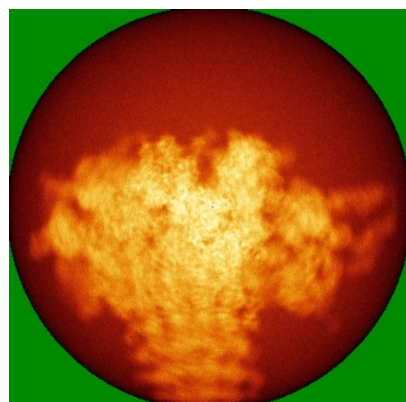


Y

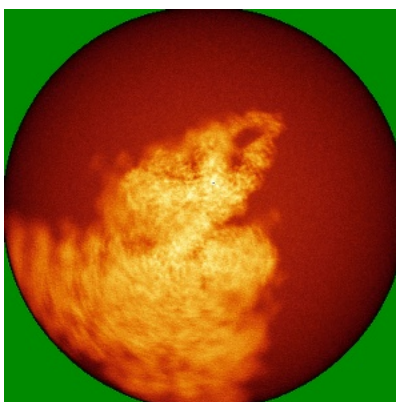


Z

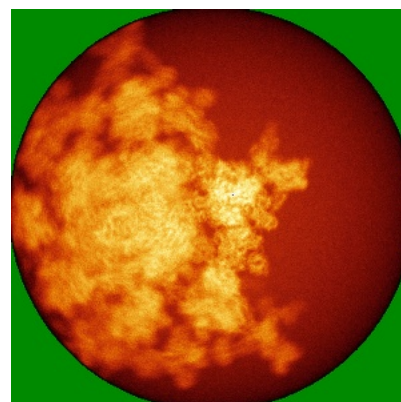
6.4.2 Raw map



X



Y

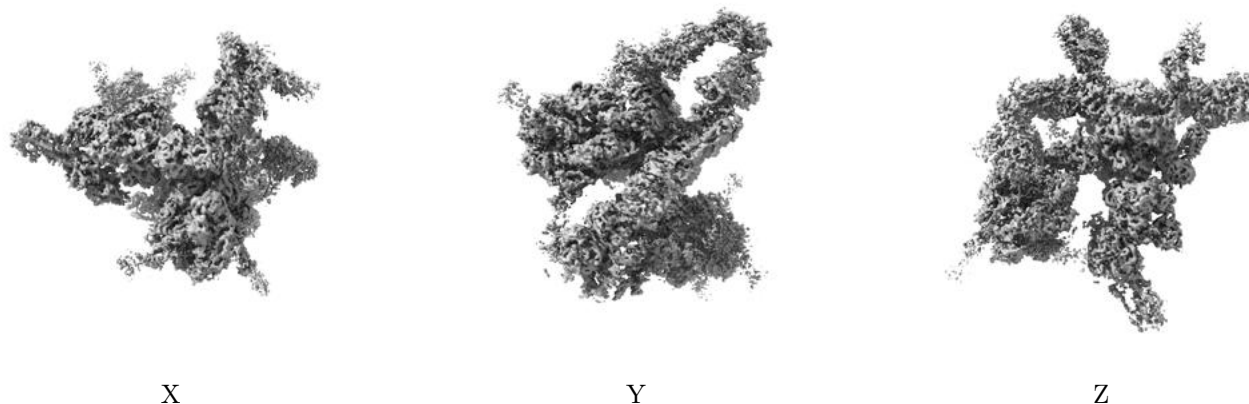


Z

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

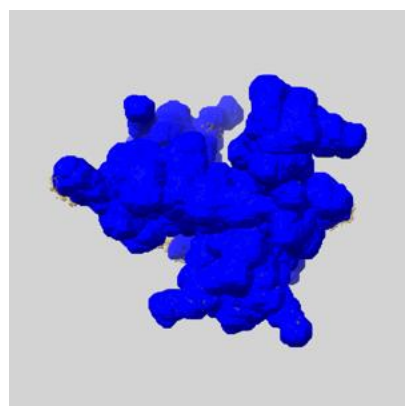
6.6 Mask visualisation [i](#)

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

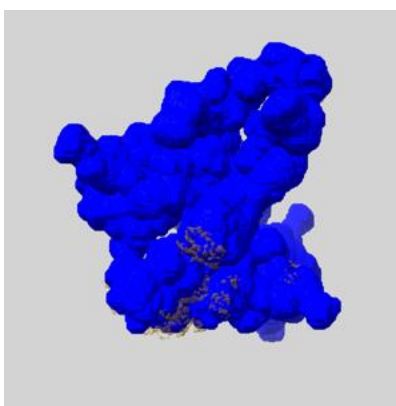
A mask typically either:

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

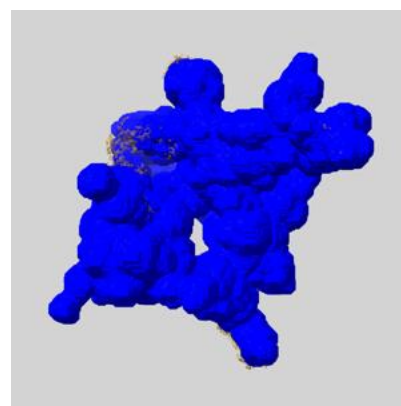
6.6.1 emd_55954_msk_1.map [i](#)



X



Y

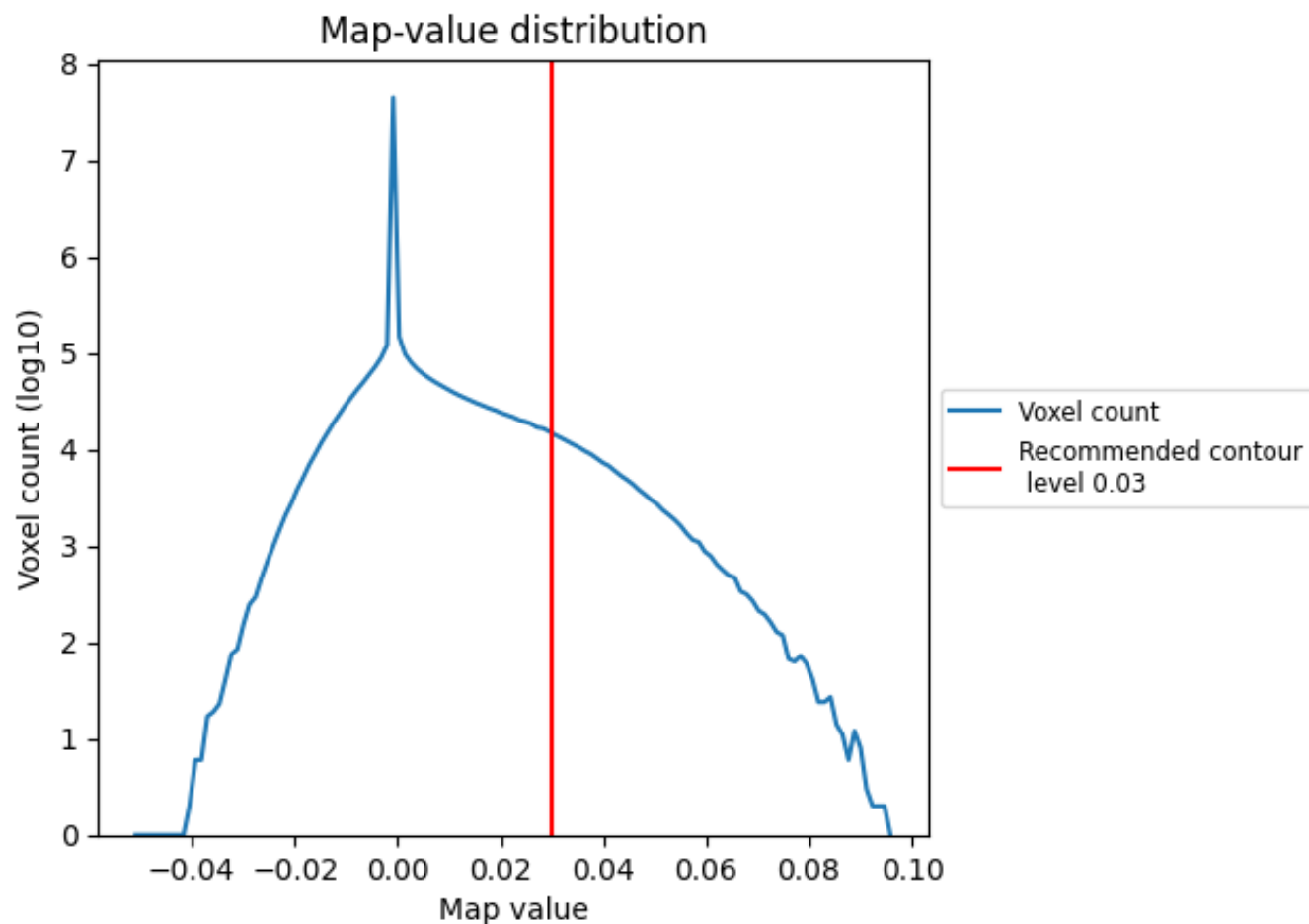


Z

7 Map analysis [i](#)

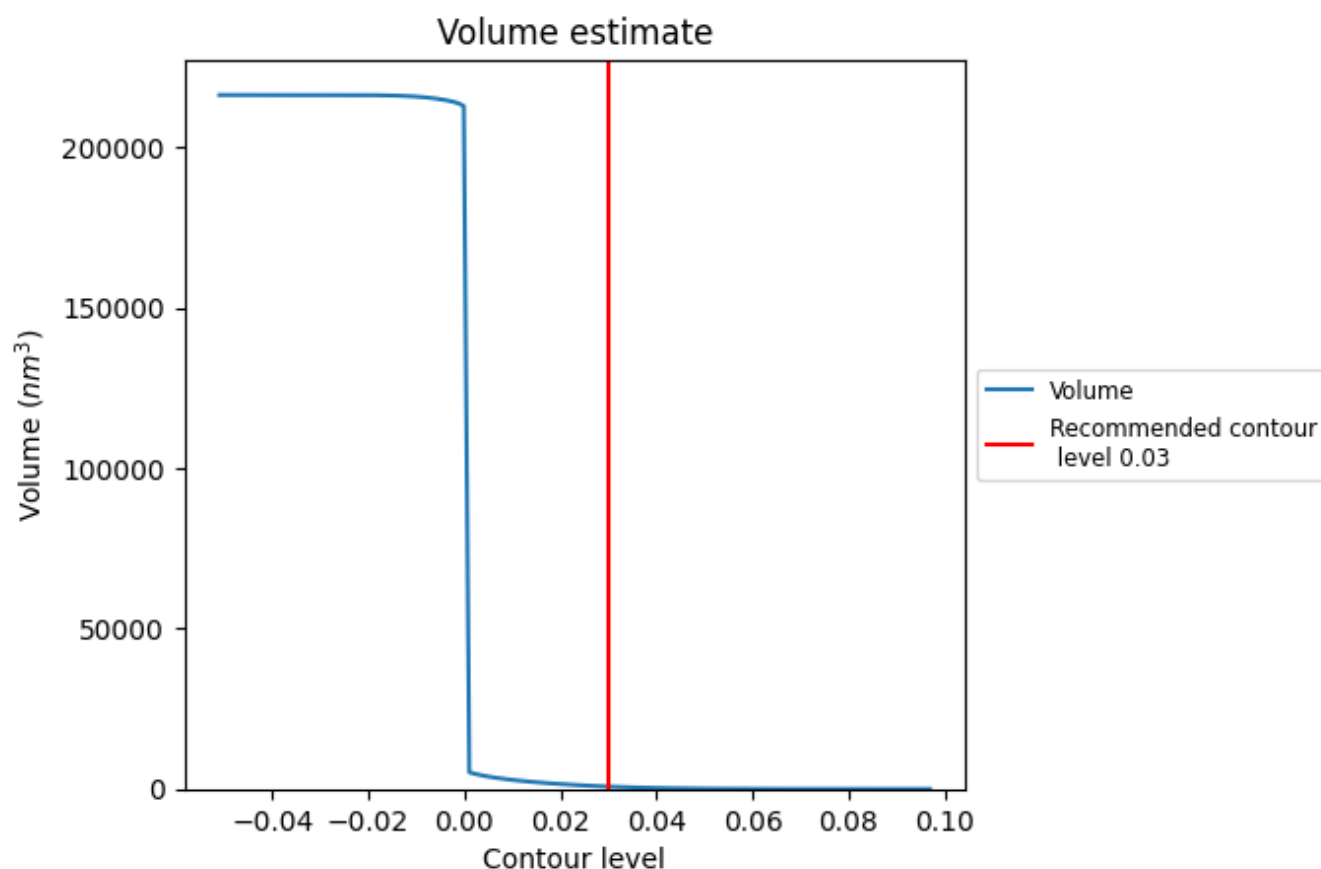
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

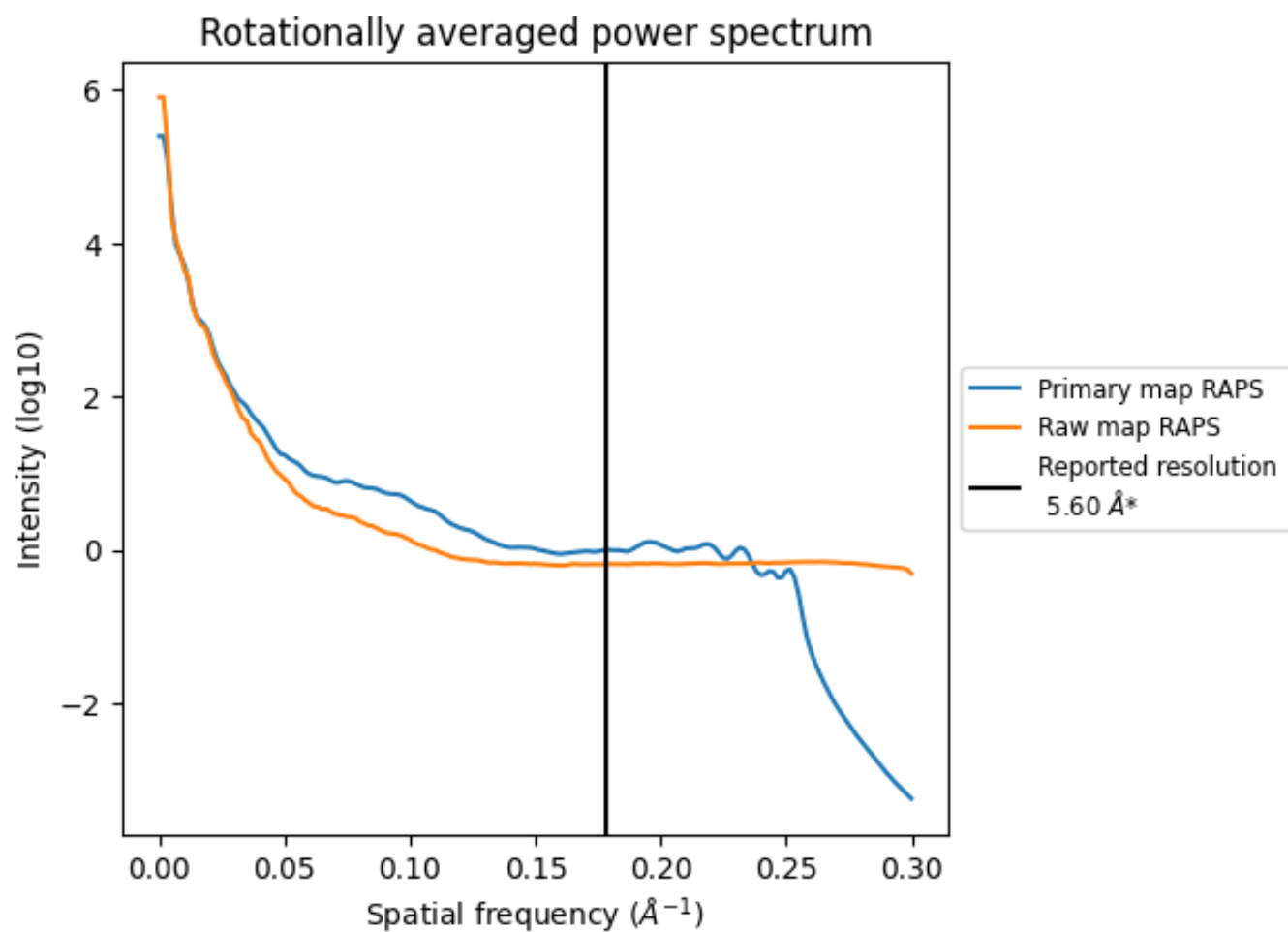
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 745 nm³; this corresponds to an approximate mass of 673 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 ⓘ

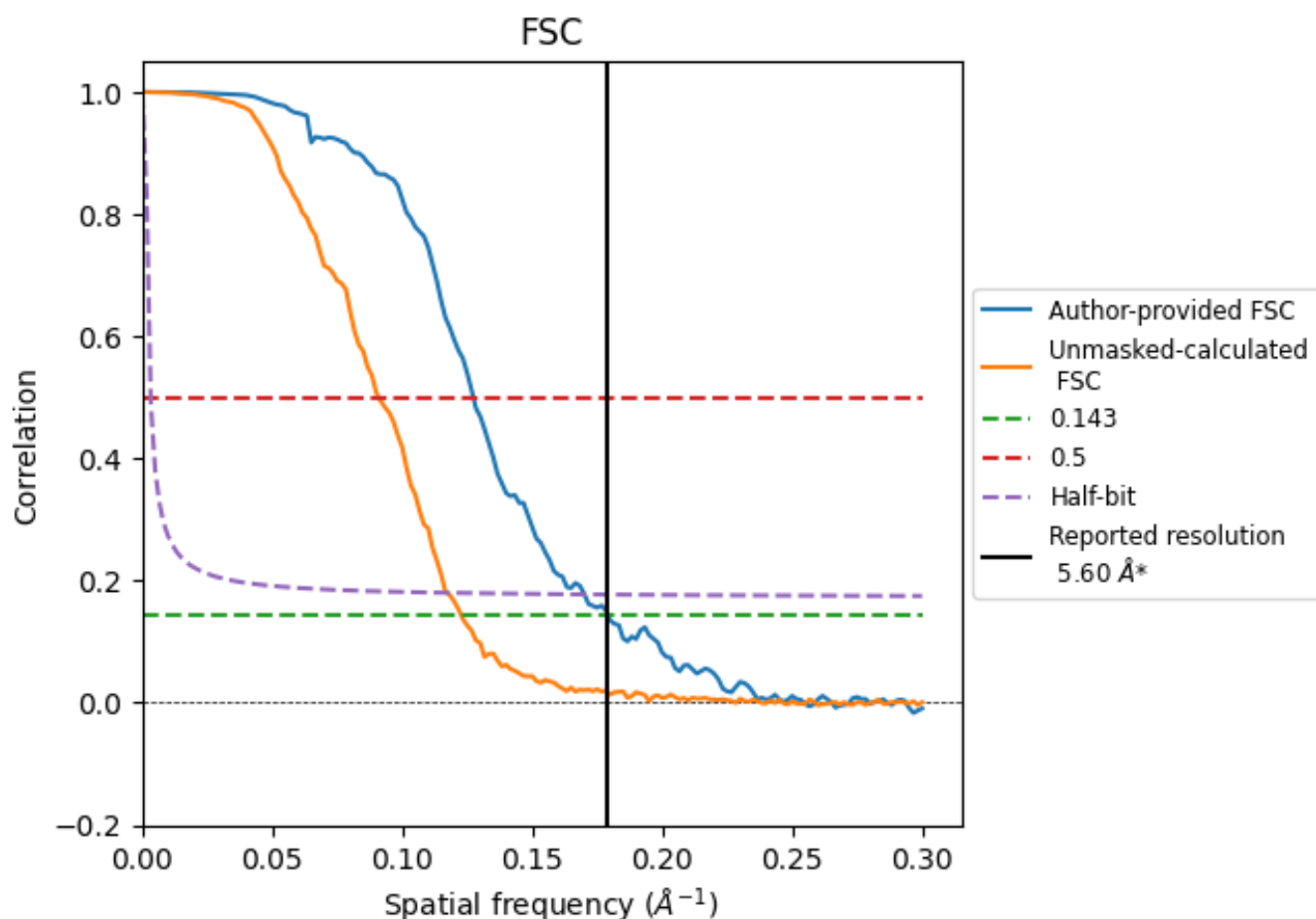


*Reported resolution corresponds to spatial frequency of $0.179 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.179 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

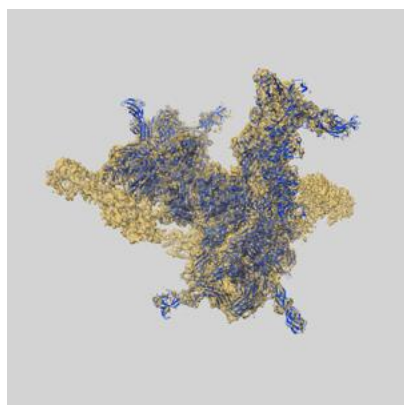
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.60	-	-
Author-provided FSC curve	5.58	7.86	5.88
Unmasked-calculated*	8.15	10.99	8.53

*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 8.15 differs from the reported value 5.6 by more than 10 %

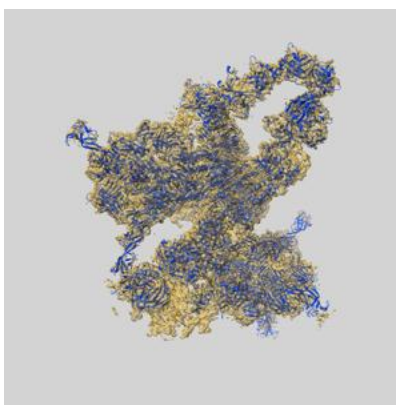
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55954 and PDB model 9TIF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

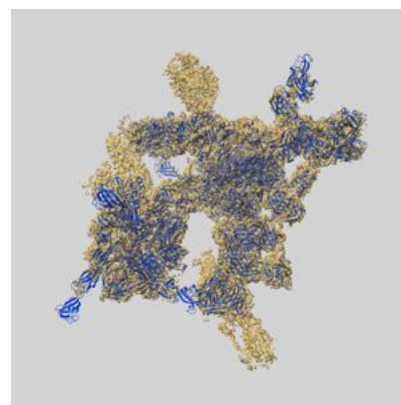
9.1 Map-model overlay [i](#)



X



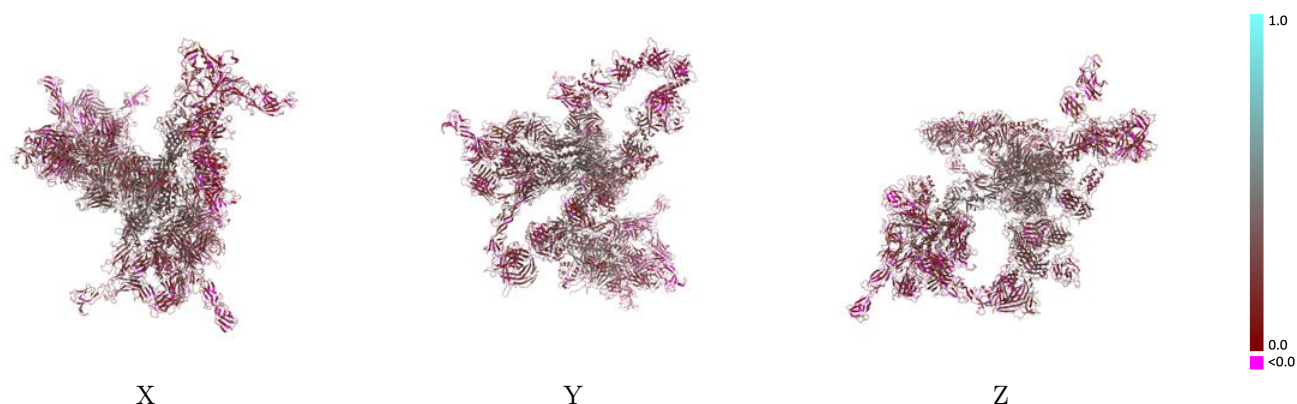
Y



Z

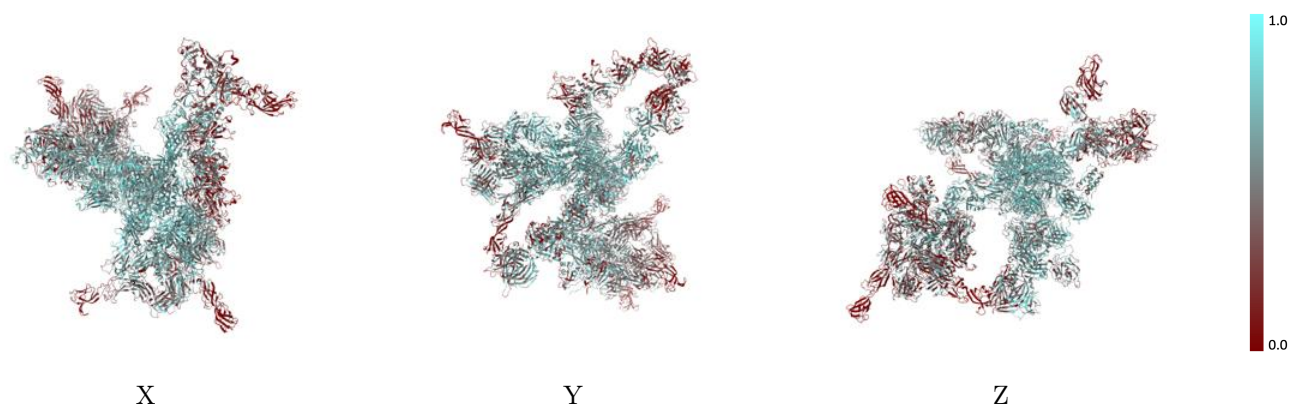
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



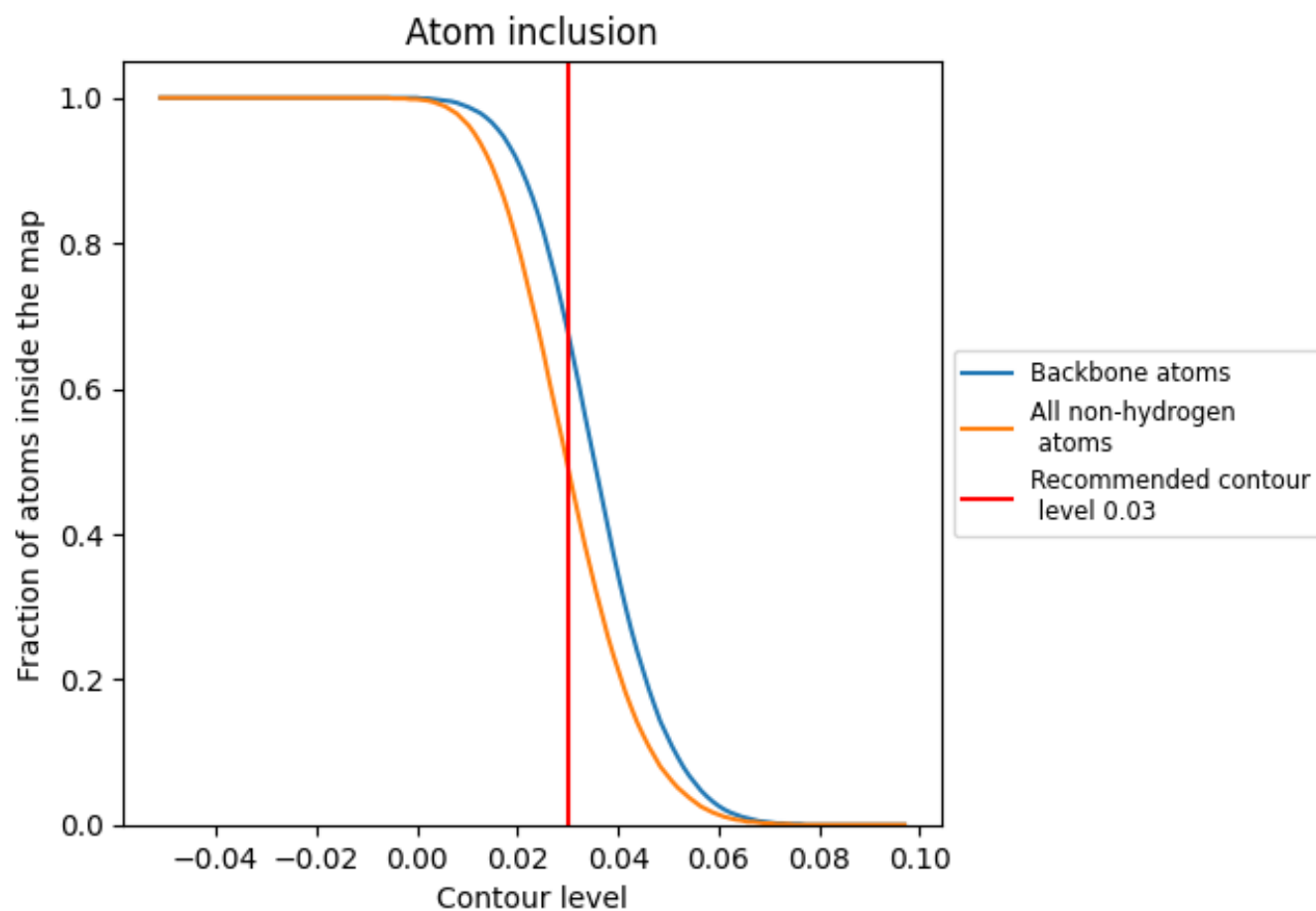
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 49% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4940	 0.2440
A	 0.5570	 0.2400
B	 0.5450	 0.2410
D	 0.3340	 0.1580
E	 0.6980	 0.3590
F	 0.3580	 0.2340
G	 0.5740	 0.2920
H	 0.4060	 0.2010
I	 0.7060	 0.3670
J	 0.6040	 0.2880
K	 0.2670	 0.1480
L	 0.3060	 0.1710
M	 0.4790	 0.1960
N	 0.5770	 0.2800
O	 0.6600	 0.3150
P	 0.4480	 0.2330
Q	 0.2940	 0.1620
R	 0.1980	 0.1520
S	 0.4730	 0.2210
T	 0.4910	 0.2260
U	 0.4940	 0.2360
V	 0.7080	 0.3820
b	 0.5210	 0.2880
c	 0.7310	 0.3880
d	 0.4200	 0.2280
e	 0.3790	 0.1950
f	 0.5520	 0.2650
g	 0.5460	 0.2640
h	 0.5420	 0.2550

