wwPDB EM Validation Summary Report

Jan 30, 2024 – 01:48 PM EST

PDB ID	:	8FQC
EMDB ID	:	EMD-29383
Title	:	Structure of baseplate with receptor binding complex of Agrobacterium phage Milano
Authors	:	Sonani, R.R.; Leiman, P.G.; Wang, F.; Kreutzberger, M.A.B.; Sebastian, A.; Esteves, N.C.; Kelly, R.J.; Scharf, B.; Egelman, E.H.
Deposited on	:	2023-01-05
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

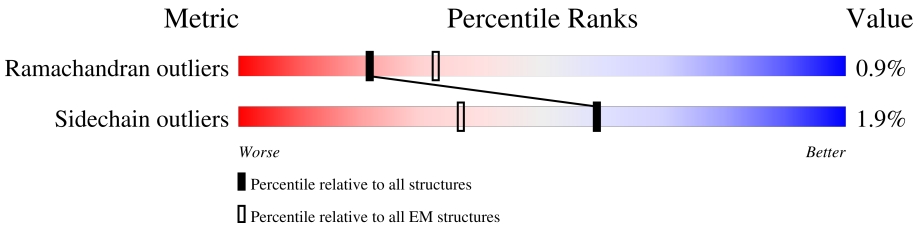
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	C1	457	68% 29%
2	E1	136	96%
2	a1	136	96%
2	f1	136	96%
2	g1	136	96%
3	F1	396	97%
3	G1	396	95%
3	h1	396	97%
3	i1	396	97%

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Mol	Chain	Length	Quality of chain
4	H1	178	98%
4	j1	178	98%
5	I1	503	98%
5	K1	503	95%
5	k1	503	96%
5	m1	503	96%
6	J1	286	93% 6%
6	l1	286	97%
7	P1	587	27% 72%
7	Q1	587	28% 71%
7	R1	587	29% 71%
7	r1	587	27% 72%
7	s1	587	29% 71%
7	t1	587	29% 71%
8	S1	300	39% 60%
8	T1	300	39% 60%
8	V1	300	39% 60%
8	W1	300	40% 60%
8	X1	300	40% 60%
8	Y1	300	40% 60%
8	u1	300	39% 60%
8	v1	300	39% 60%
8	w1	300	40% 60%
8	x1	300	39% 60%
8	y1	300	40% 60%

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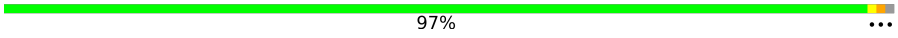
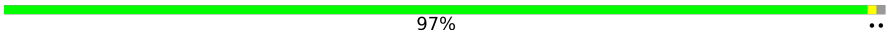
Mol	Chain	Length	Quality of chain
8	z1	300	
9	U1	398	
9	e1	398	
10	A	188	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 66089 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 Baseplate hub protein, gp26.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	326	Total	C	N	O	S	0	0
			2551	1610	434	500	7		

- Molecule 2 is a protein called Tail-tube, gp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	a1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	f1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	g1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		

- Molecule 3 is a protein called Baseplate Wedge 2 protein, gp29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	G1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	h1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	i1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		

- Molecule 4 is a protein called Baseplate wedge 1, gp28.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H1	176	Total	C	N	O	S	0	0
			1334	817	244	264	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	j1	176	Total	C	N	O	S	0	0
			1334	817	244	264	9		

- Molecule 5 is a protein called Tail sheath protein, gp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I1	498	Total	C	N	O	S	0	0
			3739	2342	633	742	22		
5	K1	494	Total	C	N	O	S	0	0
			3706	2322	628	735	21		
5	k1	498	Total	C	N	O	S	0	0
			3739	2342	633	742	22		
5	m1	494	Total	C	N	O	S	0	0
			3706	2322	628	735	21		

- Molecule 6 is a protein called Baseplate Wedge 3 protein, gp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J1	285	Total	C	N	O	S	0	0
			2185	1390	355	420	20		
6	l1	285	Total	C	N	O	S	0	0
			2185	1390	355	420	20		

- Molecule 7 is a protein called Tail Spike protein, gp124.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P1	162	Total	C	N	O	S	0	0
			1227	782	194	248	3		
7	Q1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	R1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	r1	162	Total	C	N	O	S	0	0
			1227	782	194	248	3		
7	s1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	t1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		

- Molecule 8 is a protein called Short Tail Fibers, gp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	T1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	V1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	W1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	X1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	Y1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	v1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	w1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	x1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	y1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	u1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	z1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		

- Molecule 9 is a protein called Baseplate Centerpiece, gp25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U1	394	Total	C	N	O	S	0	0
			3027	1910	522	590	5		
9	e1	394	Total	C	N	O	S	0	0
			3027	1910	522	590	5		

- Molecule 10 is a protein called Baseplate Central Spike, gp27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	168	Total	C	N	O	S	0	0
			1289	799	223	264	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

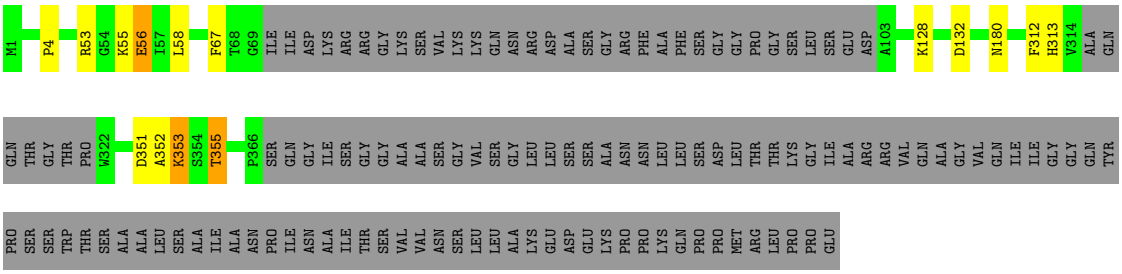
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
11	A	1	1	1	0

3 Residue-property plots (i)

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.

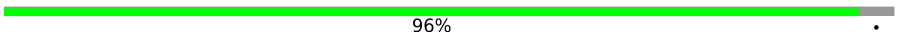
• Molecule 1: Baseplate hub protein, gp26

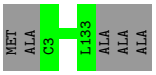
Chain C1:



• Molecule 2: Tail-tube, gp21

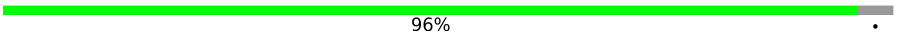
Chain E1:

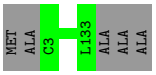




• Molecule 2: Tail-tube, gp21

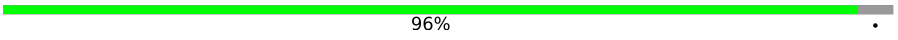
Chain a1:

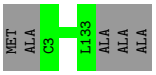




• Molecule 2: Tail-tube, gp21

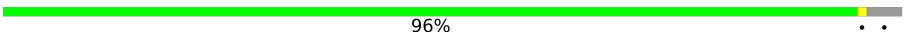
Chain f1:

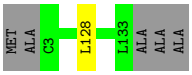




• Molecule 2: Tail-tube, gp21

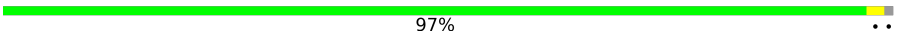
Chain g1:

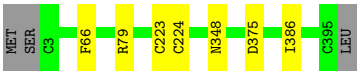




• Molecule 3: Baseplate Wedge 2 protein, gp29

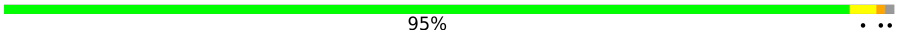
Chain F1:





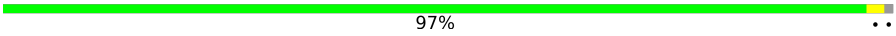
• Molecule 3: Baseplate Wedge 2 protein, gp29

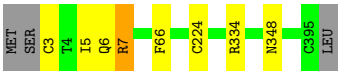
Chain G1:



• Molecule 3: Baseplate Wedge 2 protein, gp29

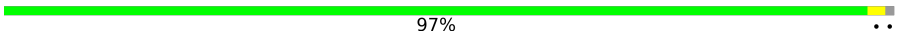
Chain h1:





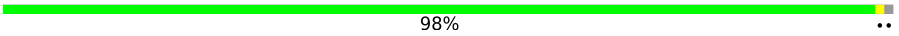
• Molecule 3: Baseplate Wedge 2 protein, gp29

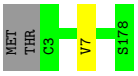
Chain i1:



• Molecule 4: Baseplate wedge 1, gp28

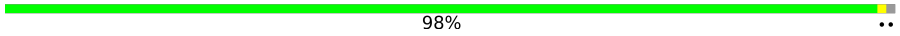
Chain H1:





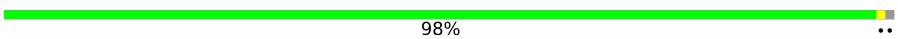
• Molecule 4: Baseplate wedge 1, gp28

Chain j1:



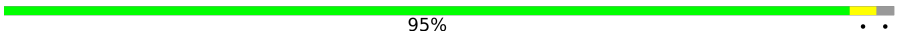
• Molecule 5: Tail sheath protein, gp20

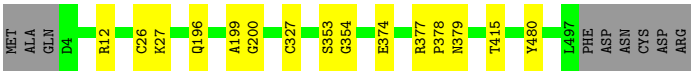
Chain I1:



• Molecule 5: Tail sheath protein, gp20

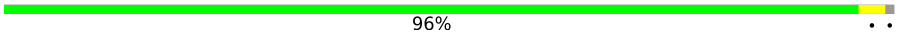
Chain K1:





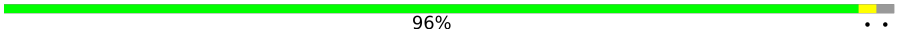
• Molecule 5: Tail sheath protein, gp20

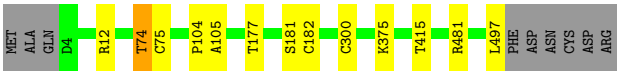
Chain k1:



• Molecule 5: Tail sheath protein, gp20

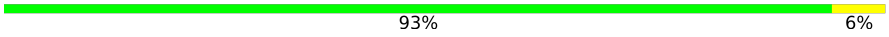
Chain m1:

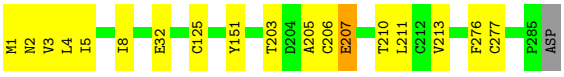




• Molecule 6: Baseplate Wedge 3 protein, gp30

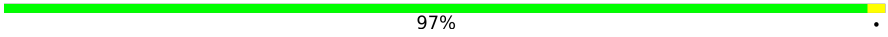
Chain J1:





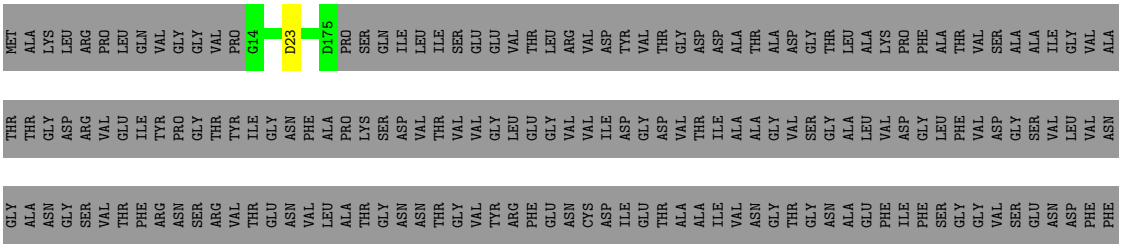
• Molecule 6: Baseplate Wedge 3 protein, gp30

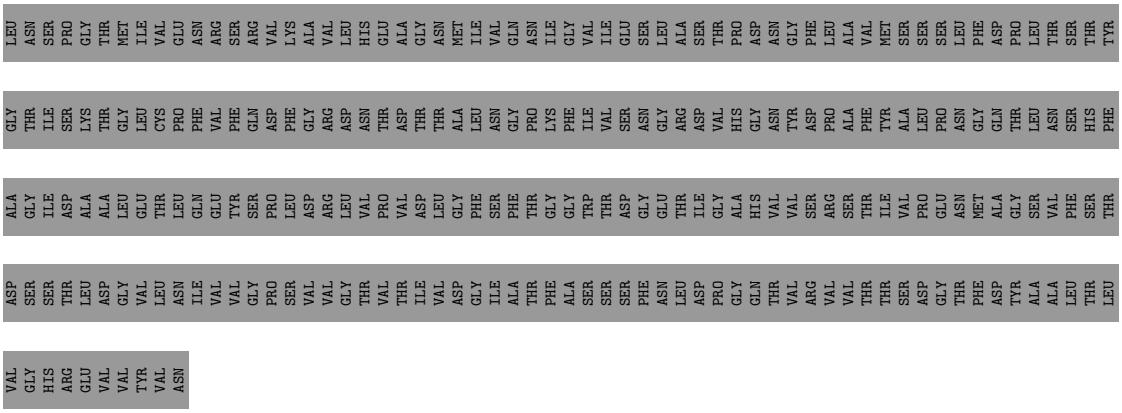
Chain l1:



• Molecule 7: Tail Spike protein, gp124

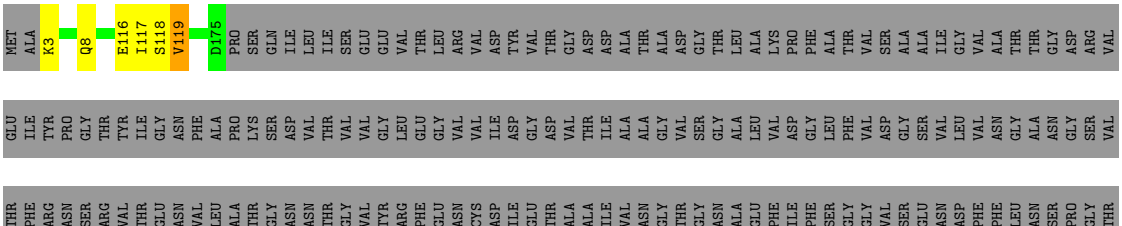
Chain P1:





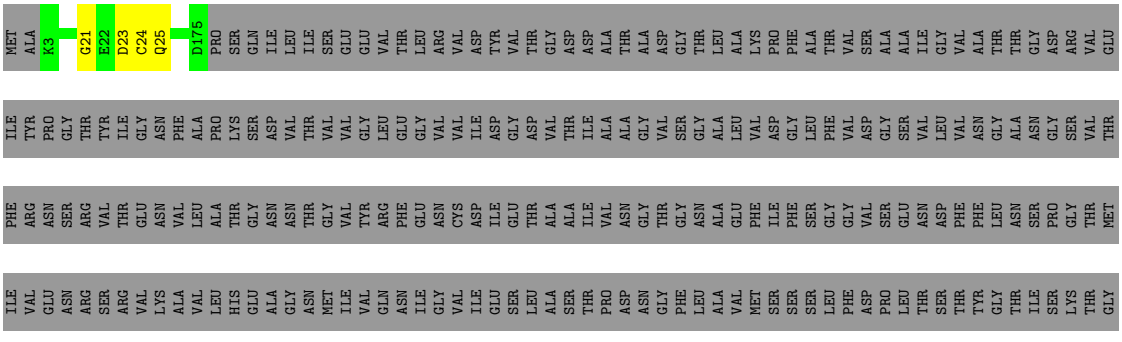
• Molecule 7: Tail Spike protein, gp124

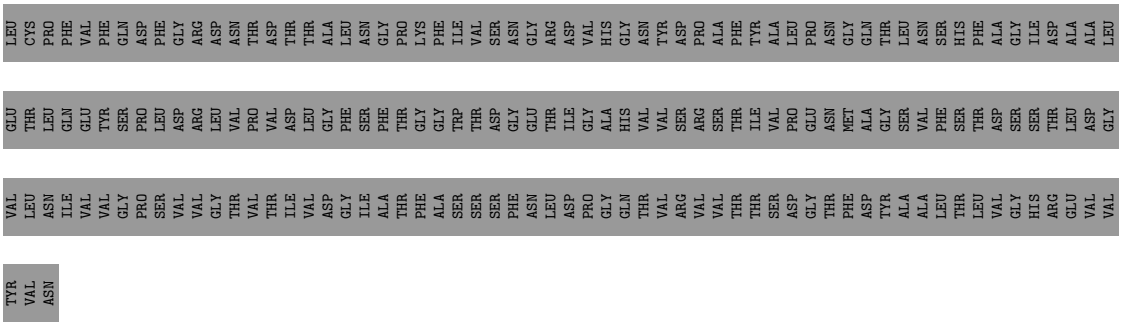
Chain Q1:



• Molecule 7: Tail Spike protein, gp124

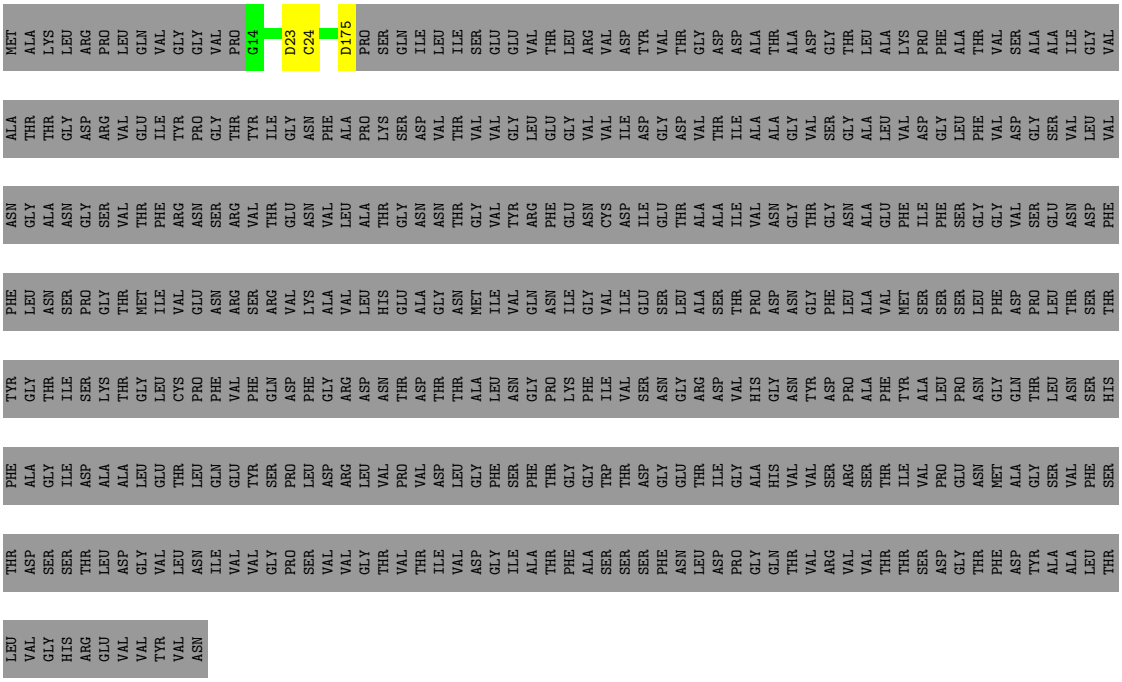
Chain R1:





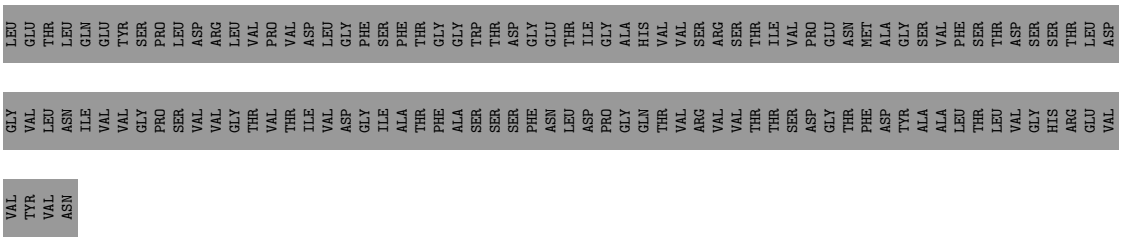
• Molecule 7: Tail Spike protein, gp124

Chain r1: 27% 72%



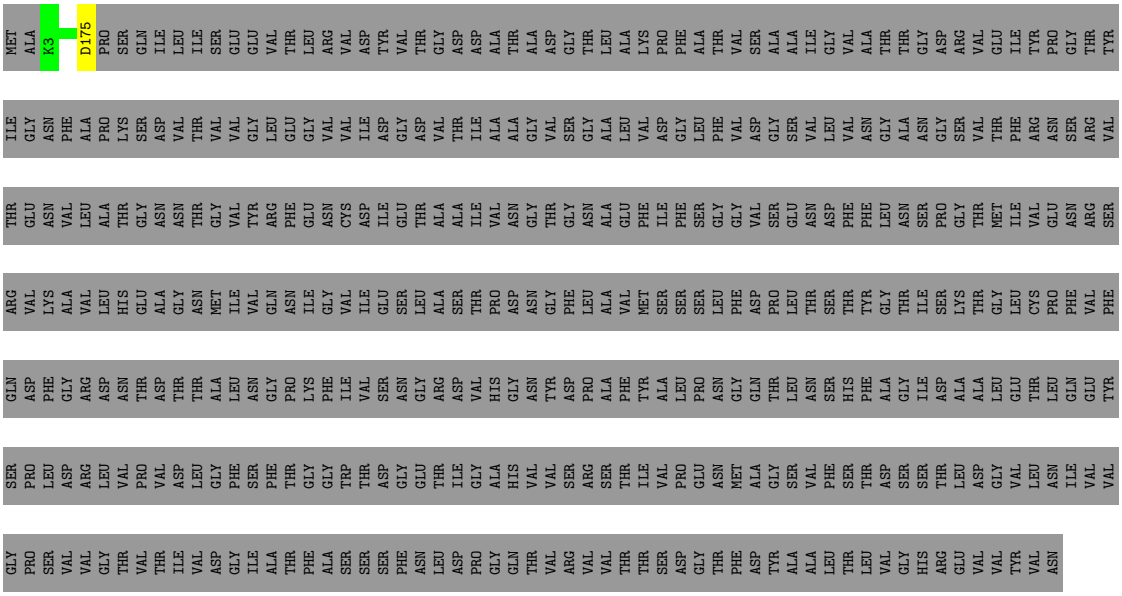
• Molecule 7: Tail Spike protein, gp124

Chain s1: 29% 71%



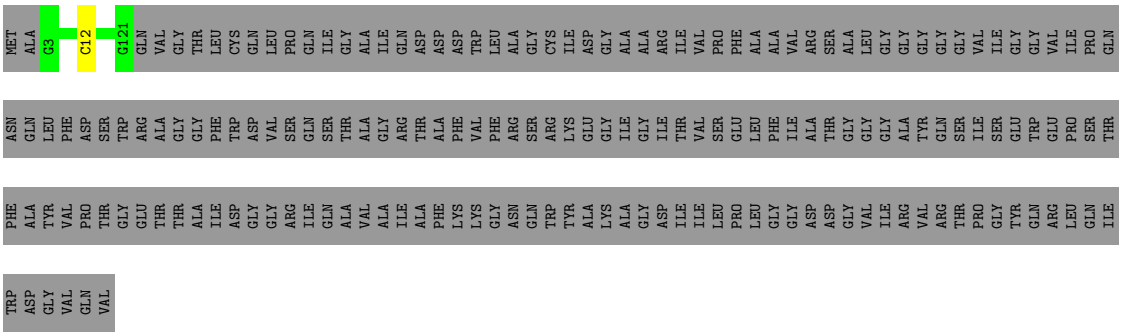
• Molecule 7: Tail Spike protein, gp124

Chain t1:



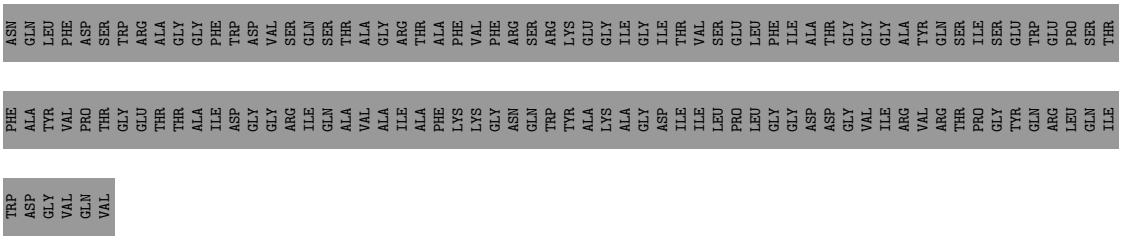
• Molecule 8: Short Tail Fibers, gp31

Chain S1:



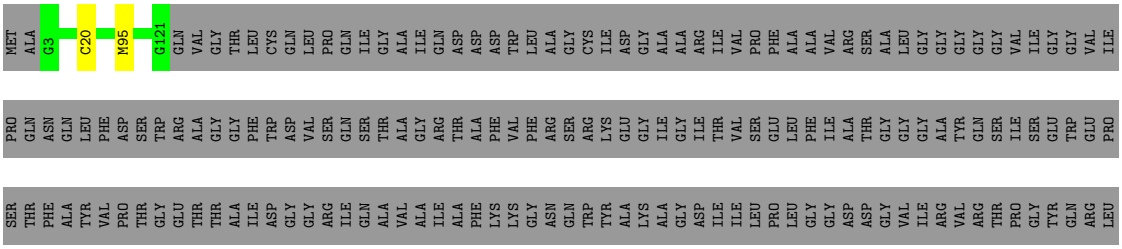
• Molecule 8: Short Tail Fibers, gp31

Chain T1:



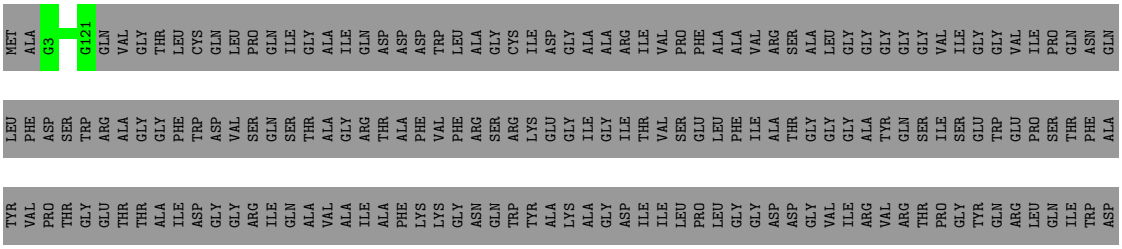
• Molecule 8: Short Tail Fibers, gp31

Chain V1:



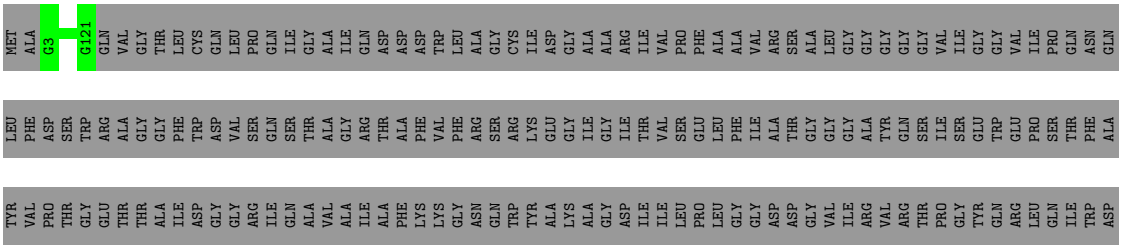
• Molecule 8: Short Tail Fibers, gp31

Chain W1:



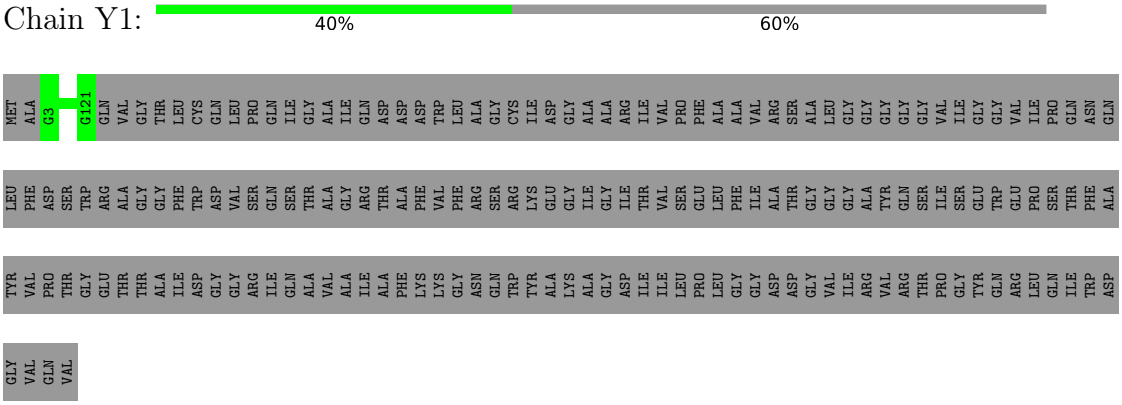
• Molecule 8: Short Tail Fibers, gp31

Chain X1:



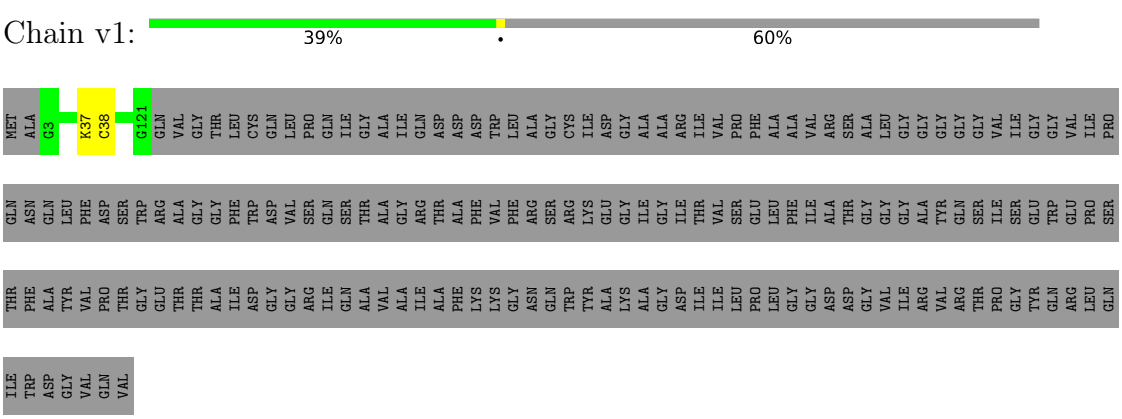
• Molecule 8: Short Tail Fibers, gp31

Chain Y1:



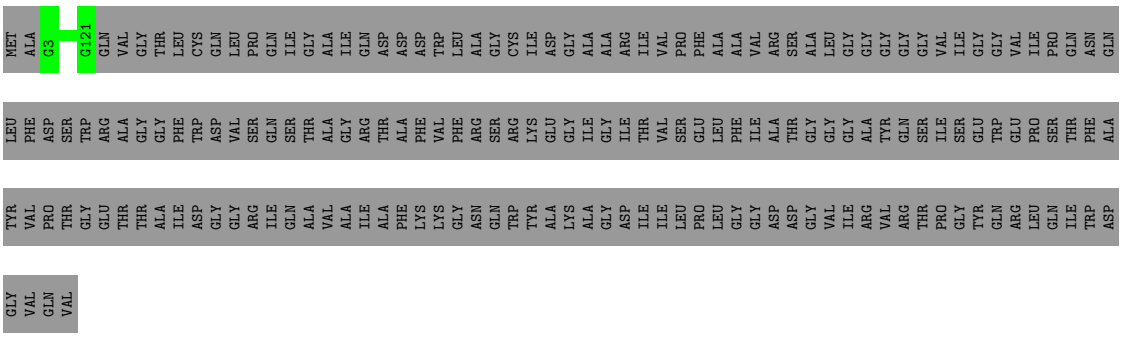
• Molecule 8: Short Tail Fibers, gp31

Chain v1:



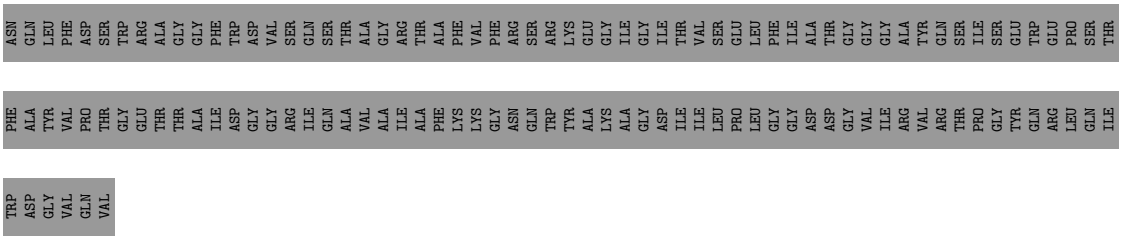
• Molecule 8: Short Tail Fibers, gp31

Chain w1:



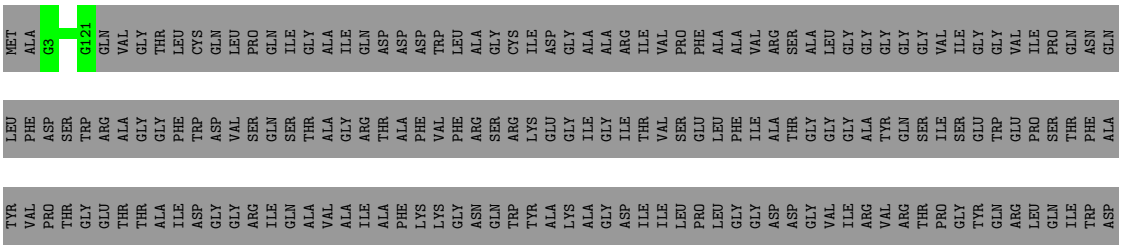
• Molecule 8: Short Tail Fibers, gp31

Chain x1:



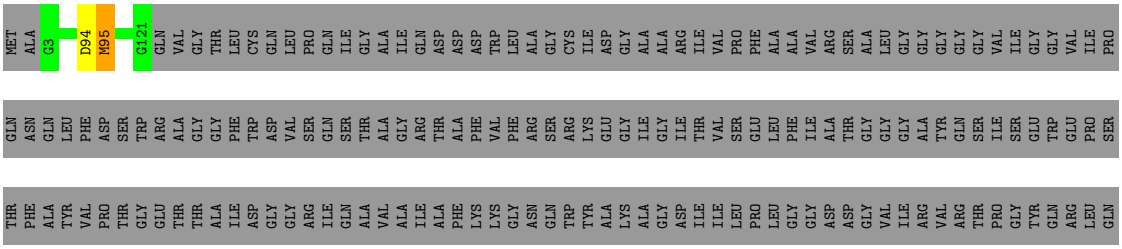
• Molecule 8: Short Tail Fibers, gp31

Chain y1:



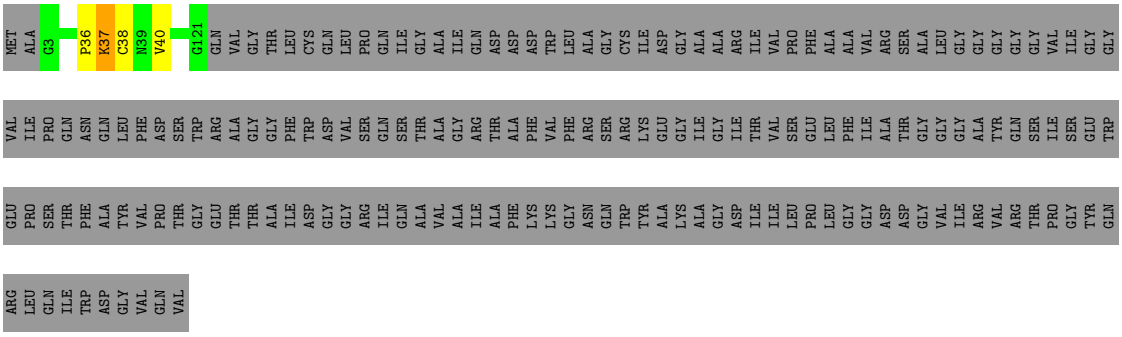
• Molecule 8: Short Tail Fibers, gp31

Chain u1:



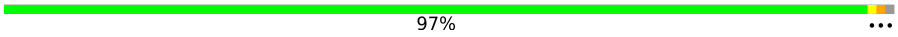
• Molecule 8: Short Tail Fibers, gp31

Chain z1:



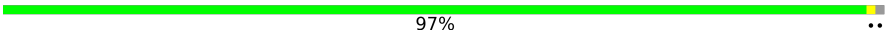
• Molecule 9: Baseplate Centerpiece, gp25

Chain U1:



• Molecule 9: Baseplate Centerpiece, gp25

Chain e1:



• Molecule 10: Baseplate Central Spike, gp27

Chain A:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14856	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.478	Depositor
Minimum map value	-0.780	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	624.24005, 624.24005, 624.24005	wwPDB
Map dimensions	578, 578, 578	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	C1	0.38	0/2598	0.57	0/3525
2	E1	0.46	0/1011	0.52	0/1382
2	a1	0.40	0/1011	0.52	0/1382
2	f1	0.38	0/1011	0.51	0/1382
2	g1	0.41	0/1011	0.52	0/1382
3	F1	0.42	0/3085	0.49	0/4207
3	G1	0.47	0/3085	0.55	0/4207
3	h1	0.42	0/3085	0.48	0/4207
3	i1	0.46	0/3085	0.54	0/4207
4	H1	0.37	0/1353	0.51	0/1831
4	j1	0.37	0/1353	0.51	0/1831
5	I1	0.41	0/3815	0.53	0/5211
5	K1	0.38	0/3781	0.51	0/5165
5	k1	0.42	0/3815	0.52	0/5211
5	m1	0.37	0/3781	0.50	0/5165
6	J1	0.44	0/2237	0.53	0/3063
6	l1	0.41	0/2237	0.50	0/3063
7	P1	0.33	0/1269	0.45	0/1755
7	Q1	0.35	0/1352	0.50	0/1868
7	R1	0.30	0/1352	0.47	0/1868
7	r1	0.33	0/1269	0.45	0/1755
7	s1	0.36	0/1352	0.46	0/1868
7	t1	0.32	0/1352	0.47	0/1868
8	S1	0.29	0/892	0.46	0/1217
8	T1	0.28	0/892	0.46	0/1217
8	V1	0.28	0/892	0.49	0/1217
8	W1	0.32	0/892	0.44	0/1217
8	X1	0.30	0/892	0.46	0/1217
8	Y1	0.29	0/892	0.45	0/1217
8	u1	0.31	0/892	0.48	0/1217
8	v1	0.30	0/892	0.47	0/1217
8	w1	0.28	0/892	0.45	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
8	x1	0.28	0/892	0.49	0/1217
8	y1	0.31	0/892	0.45	0/1217
8	z1	0.31	0/892	0.44	0/1217
9	U1	0.44	0/3093	0.49	0/4214
9	e1	0.44	0/3093	0.50	1/4214 (0.0%)
10	A	0.62	0/1320	0.91	3/1791 (0.2%)
All	All	0.40	0/67510	0.51	4/92226 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	e1	138	LEU	CA-CB-CG	5.73	128.49	115.30
10	A	116	ILE	N-CA-C	-5.73	95.53	111.00
10	A	181	ASP	CB-CG-OD2	5.18	122.96	118.30
10	A	72	GLY	N-CA-C	-5.14	100.25	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	C1	320/457 (70%)	247 (77%)	65 (20%)	8 (2%)	5 32
2	E1	129/136 (95%)	117 (91%)	12 (9%)	0	100 100
2	a1	129/136 (95%)	117 (91%)	12 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	f1	129/136 (95%)	118 (92%)	11 (8%)	0	100	100
2	g1	129/136 (95%)	118 (92%)	10 (8%)	1 (1%)	19	58
3	F1	391/396 (99%)	371 (95%)	19 (5%)	1 (0%)	41	74
3	G1	391/396 (99%)	366 (94%)	21 (5%)	4 (1%)	15	54
3	h1	391/396 (99%)	378 (97%)	10 (3%)	3 (1%)	19	58
3	i1	391/396 (99%)	363 (93%)	26 (7%)	2 (0%)	29	67
4	H1	174/178 (98%)	149 (86%)	24 (14%)	1 (1%)	25	64
4	j1	174/178 (98%)	145 (83%)	27 (16%)	2 (1%)	14	51
5	I1	496/503 (99%)	439 (88%)	56 (11%)	1 (0%)	47	79
5	K1	492/503 (98%)	421 (86%)	64 (13%)	7 (1%)	11	46
5	k1	496/503 (99%)	441 (89%)	53 (11%)	2 (0%)	34	69
5	m1	492/503 (98%)	404 (82%)	80 (16%)	8 (2%)	9	43
6	J1	283/286 (99%)	258 (91%)	20 (7%)	5 (2%)	8	41
6	l1	283/286 (99%)	253 (89%)	27 (10%)	3 (1%)	14	51
7	P1	160/587 (27%)	146 (91%)	13 (8%)	1 (1%)	25	64
7	Q1	171/587 (29%)	155 (91%)	12 (7%)	4 (2%)	6	34
7	R1	171/587 (29%)	158 (92%)	12 (7%)	1 (1%)	25	64
7	r1	160/587 (27%)	147 (92%)	12 (8%)	1 (1%)	25	64
7	s1	171/587 (29%)	158 (92%)	10 (6%)	3 (2%)	8	41
7	t1	171/587 (29%)	156 (91%)	15 (9%)	0	100	100
8	S1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	T1	117/300 (39%)	112 (96%)	4 (3%)	1 (1%)	17	56
8	V1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	W1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	X1	117/300 (39%)	107 (92%)	10 (8%)	0	100	100
8	Y1	117/300 (39%)	111 (95%)	6 (5%)	0	100	100
8	u1	117/300 (39%)	110 (94%)	6 (5%)	1 (1%)	17	56
8	v1	117/300 (39%)	107 (92%)	10 (8%)	0	100	100
8	w1	117/300 (39%)	114 (97%)	3 (3%)	0	100	100
8	x1	117/300 (39%)	105 (90%)	12 (10%)	0	100	100
8	y1	117/300 (39%)	110 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	z1	117/300 (39%)	108 (92%)	7 (6%)	2 (2%)	9 42
9	U1	392/398 (98%)	368 (94%)	21 (5%)	3 (1%)	19 58
9	e1	392/398 (98%)	361 (92%)	30 (8%)	1 (0%)	41 74
10	A	166/188 (88%)	142 (86%)	13 (8%)	11 (7%)	1 9
All	All	8648/13631 (63%)	7807 (90%)	764 (9%)	77 (1%)	21 56

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F1	375	ASP
6	J1	2	ASN
5	K1	378	PRO
7	Q1	117	ILE
7	Q1	119	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C1	281/383 (73%)	271 (96%)	10 (4%)	35 69
2	E1	115/116 (99%)	115 (100%)	0	100 100
2	a1	115/116 (99%)	115 (100%)	0	100 100
2	f1	115/116 (99%)	115 (100%)	0	100 100
2	g1	115/116 (99%)	115 (100%)	0	100 100
3	F1	330/333 (99%)	324 (98%)	6 (2%)	59 82
3	G1	330/333 (99%)	317 (96%)	13 (4%)	32 67
3	h1	330/333 (99%)	324 (98%)	6 (2%)	59 82
3	i1	330/333 (99%)	321 (97%)	9 (3%)	44 75
4	H1	145/147 (99%)	145 (100%)	0	100 100
4	j1	145/147 (99%)	145 (100%)	0	100 100
5	I1	404/408 (99%)	399 (99%)	5 (1%)	71 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	K1	400/408 (98%)	392 (98%)	8 (2%)	55 80
5	k1	404/408 (99%)	393 (97%)	11 (3%)	44 75
5	m1	400/408 (98%)	394 (98%)	6 (2%)	65 85
6	J1	245/247 (99%)	231 (94%)	14 (6%)	20 56
6	l1	245/247 (99%)	239 (98%)	6 (2%)	49 77
7	P1	129/473 (27%)	129 (100%)	0	100 100
7	Q1	138/473 (29%)	135 (98%)	3 (2%)	52 79
7	R1	138/473 (29%)	135 (98%)	3 (2%)	52 79
7	r1	129/473 (27%)	127 (98%)	2 (2%)	62 84
7	s1	138/473 (29%)	135 (98%)	3 (2%)	52 79
7	t1	138/473 (29%)	137 (99%)	1 (1%)	84 94
8	S1	97/229 (42%)	96 (99%)	1 (1%)	76 90
8	T1	97/229 (42%)	97 (100%)	0	100 100
8	V1	97/229 (42%)	95 (98%)	2 (2%)	53 79
8	W1	97/229 (42%)	97 (100%)	0	100 100
8	X1	97/229 (42%)	97 (100%)	0	100 100
8	Y1	97/229 (42%)	97 (100%)	0	100 100
8	u1	97/229 (42%)	95 (98%)	2 (2%)	53 79
8	v1	97/229 (42%)	95 (98%)	2 (2%)	53 79
8	w1	97/229 (42%)	97 (100%)	0	100 100
8	x1	97/229 (42%)	96 (99%)	1 (1%)	76 90
8	y1	97/229 (42%)	97 (100%)	0	100 100
8	z1	97/229 (42%)	94 (97%)	3 (3%)	40 72
9	U1	314/316 (99%)	308 (98%)	6 (2%)	57 81
9	e1	314/316 (99%)	309 (98%)	5 (2%)	62 84
10	A	143/162 (88%)	134 (94%)	9 (6%)	18 52
All	All	7194/10979 (66%)	7057 (98%)	137 (2%)	59 81

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	r1	175	ASP
7	t1	175	ASP

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Mol	Chain	Res	Type
10	A	38	LYS
5	K1	12	ARG
6	J1	277	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
2	a1	84	GLN
10	A	28	HIS
3	i1	355	ASN
8	z1	117	ASN
8	x1	17	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

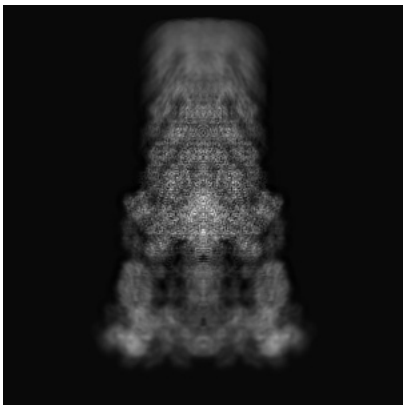
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29383. These allow visual inspection of the internal detail of the map and identification of artifacts.

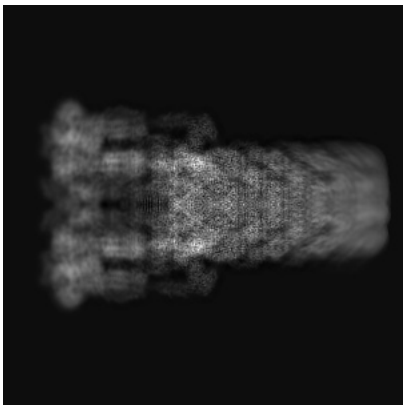
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

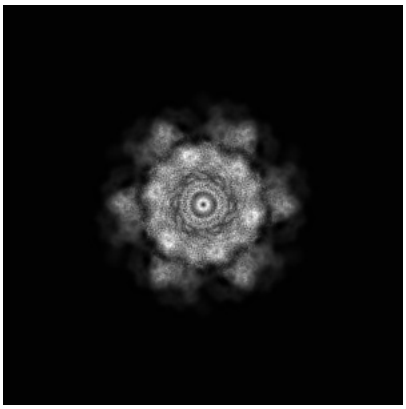
6.1.1 Primary map



X

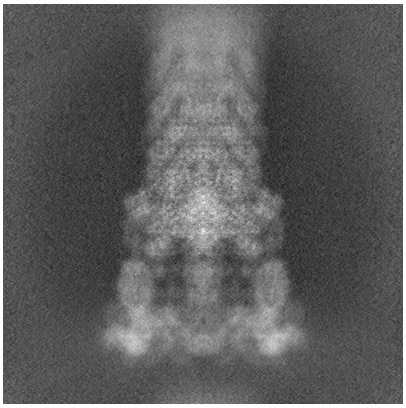


Y

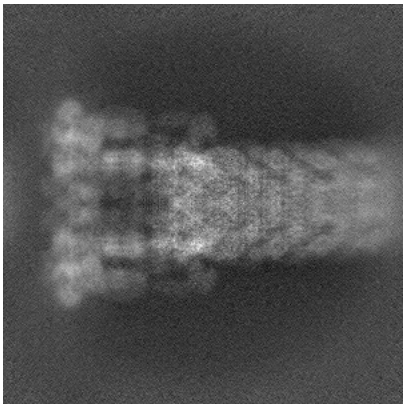


Z

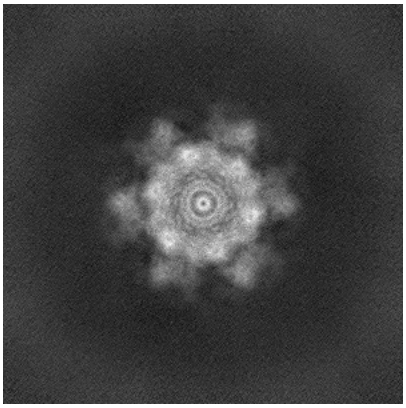
6.1.2 Raw map



X



Y

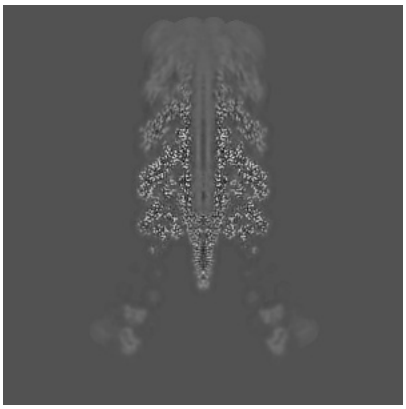


Z

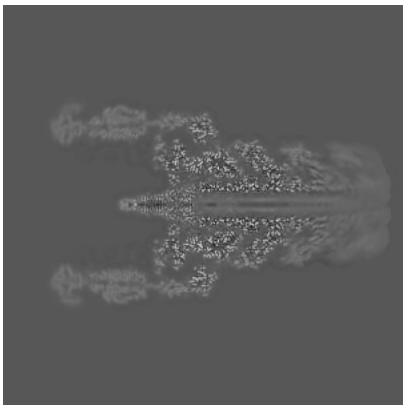
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



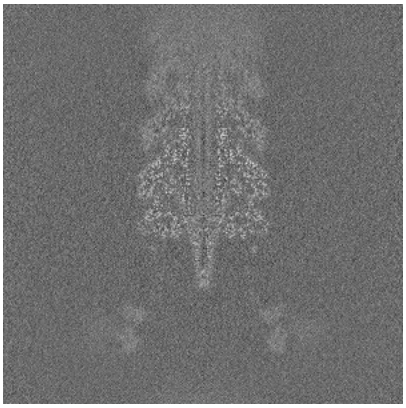
X Index: 289



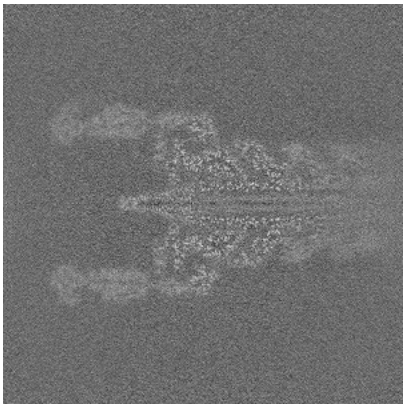
Y Index: 289

Z Index: 289

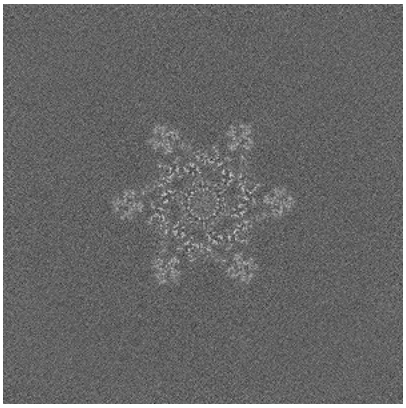
6.2.2 Raw map



X Index: 289



Y Index: 289

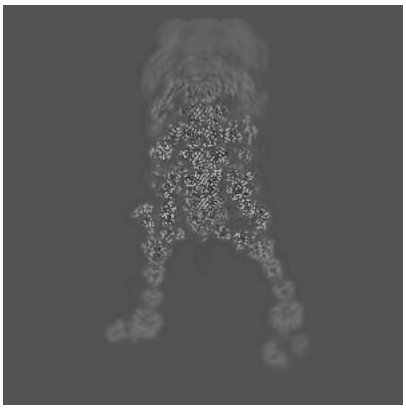


Z Index: 289

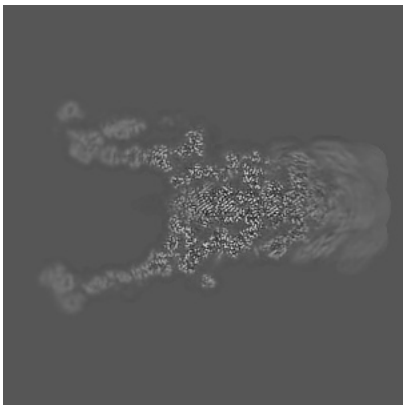
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

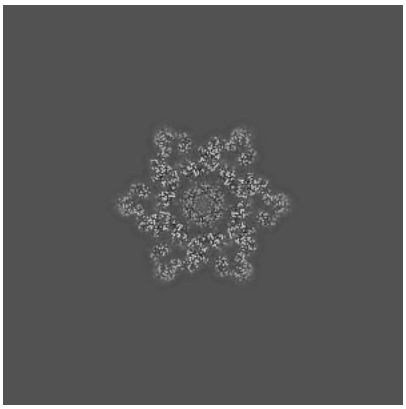
6.3.1 Primary map



X Index: 310

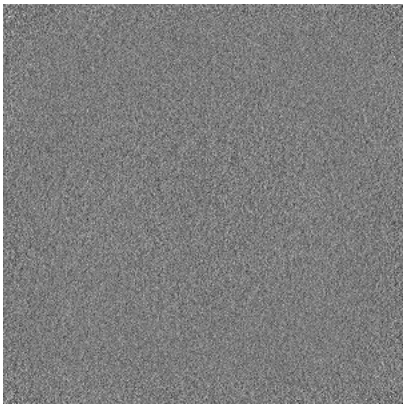


Y Index: 268

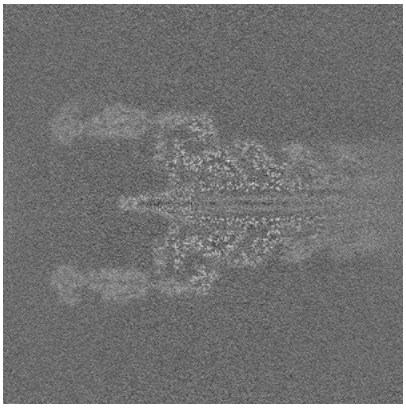


Z Index: 276

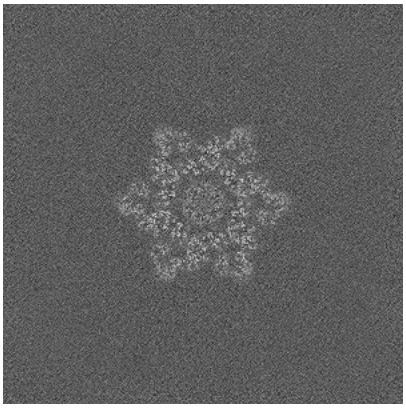
6.3.2 Raw map



X Index: 0



Y Index: 289

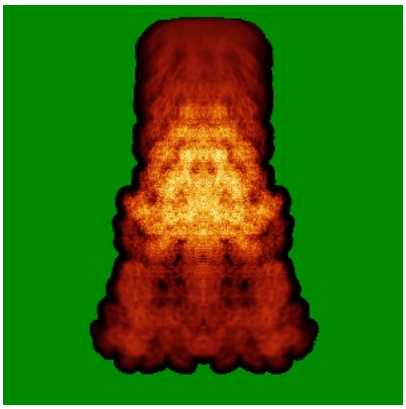


Z Index: 276

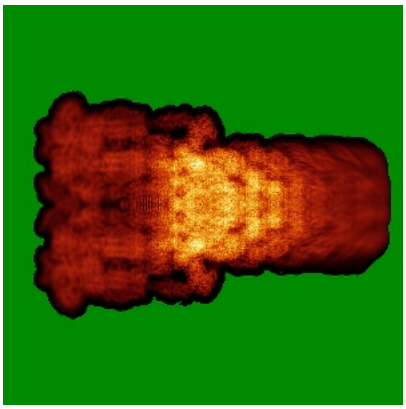
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

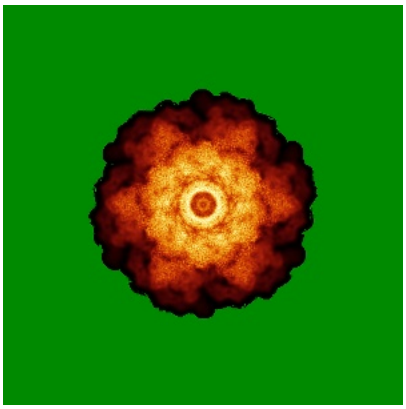
6.4.1 Primary map



X

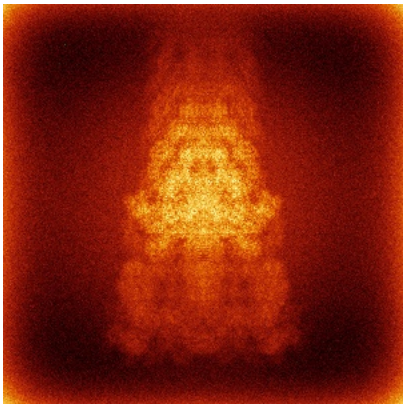


Y

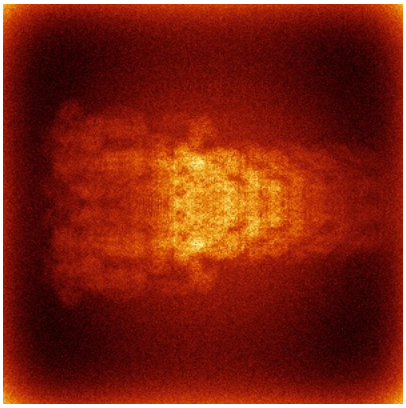


Z

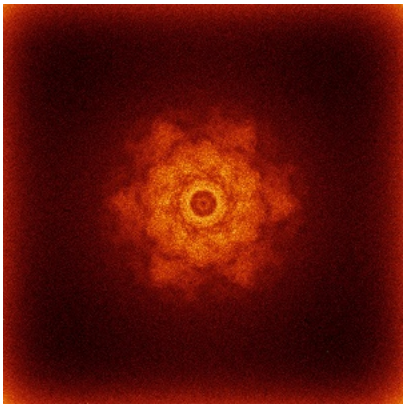
6.4.2 Raw map



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.

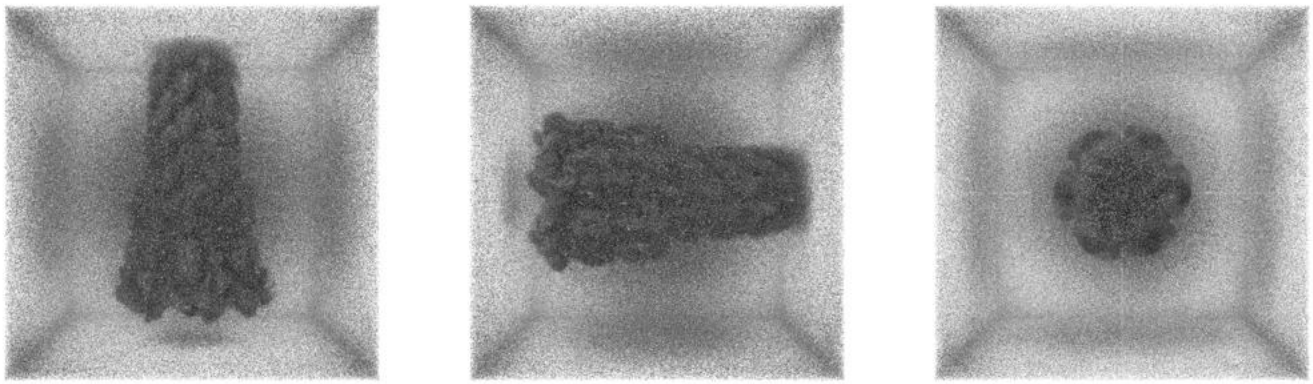
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



X Y Z

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.

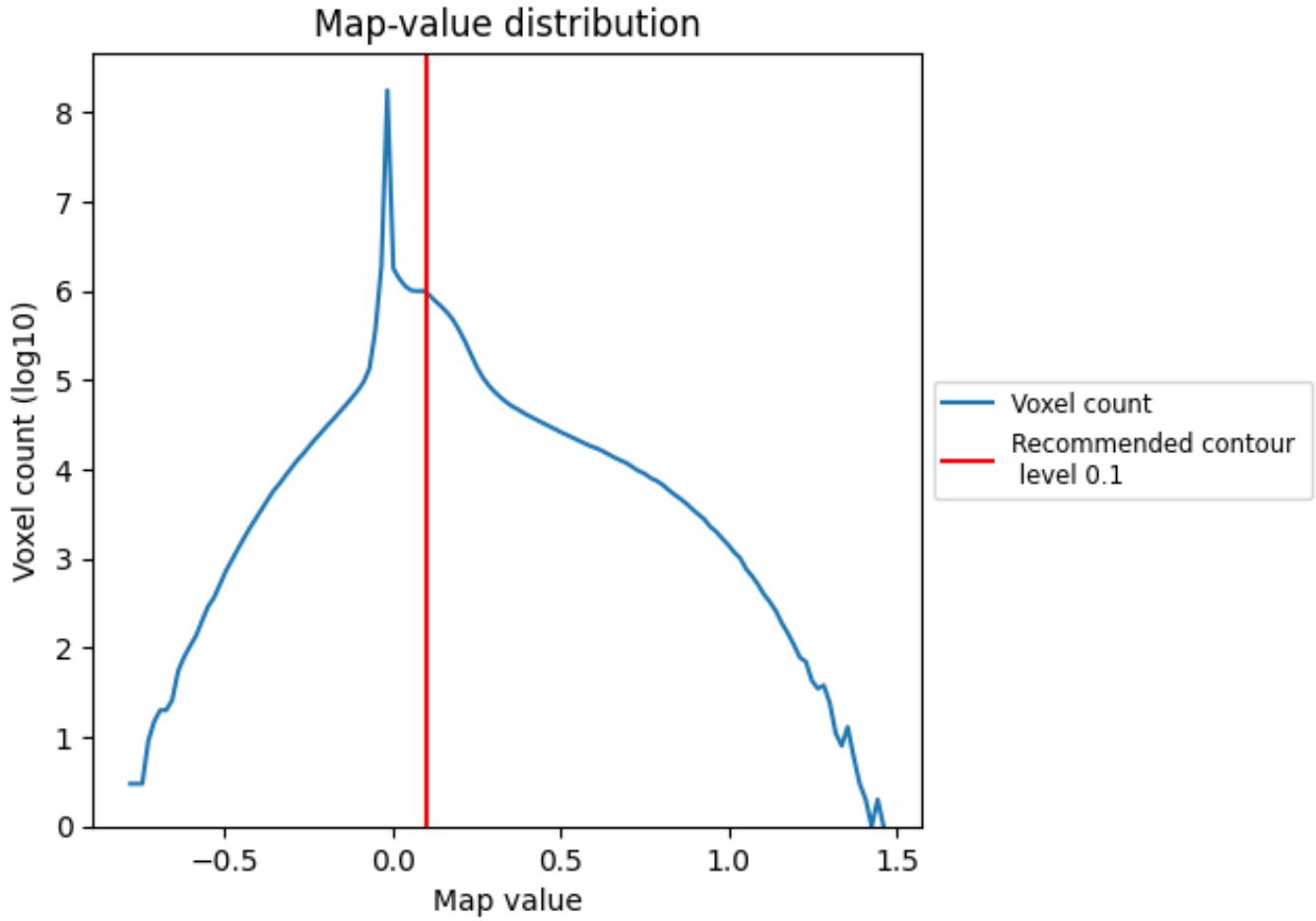
6.6 Mask visualisation (i)

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

7 Map analysis

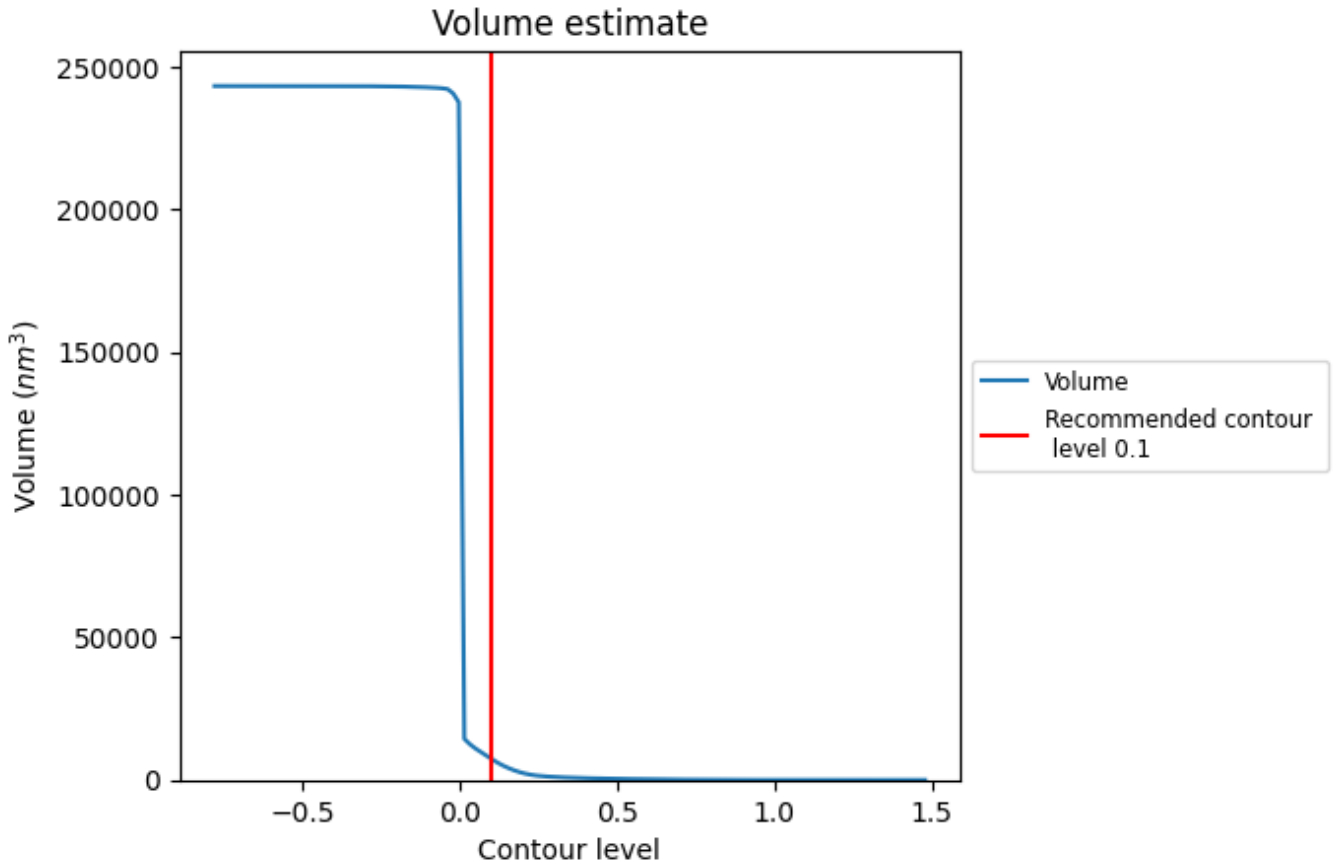
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

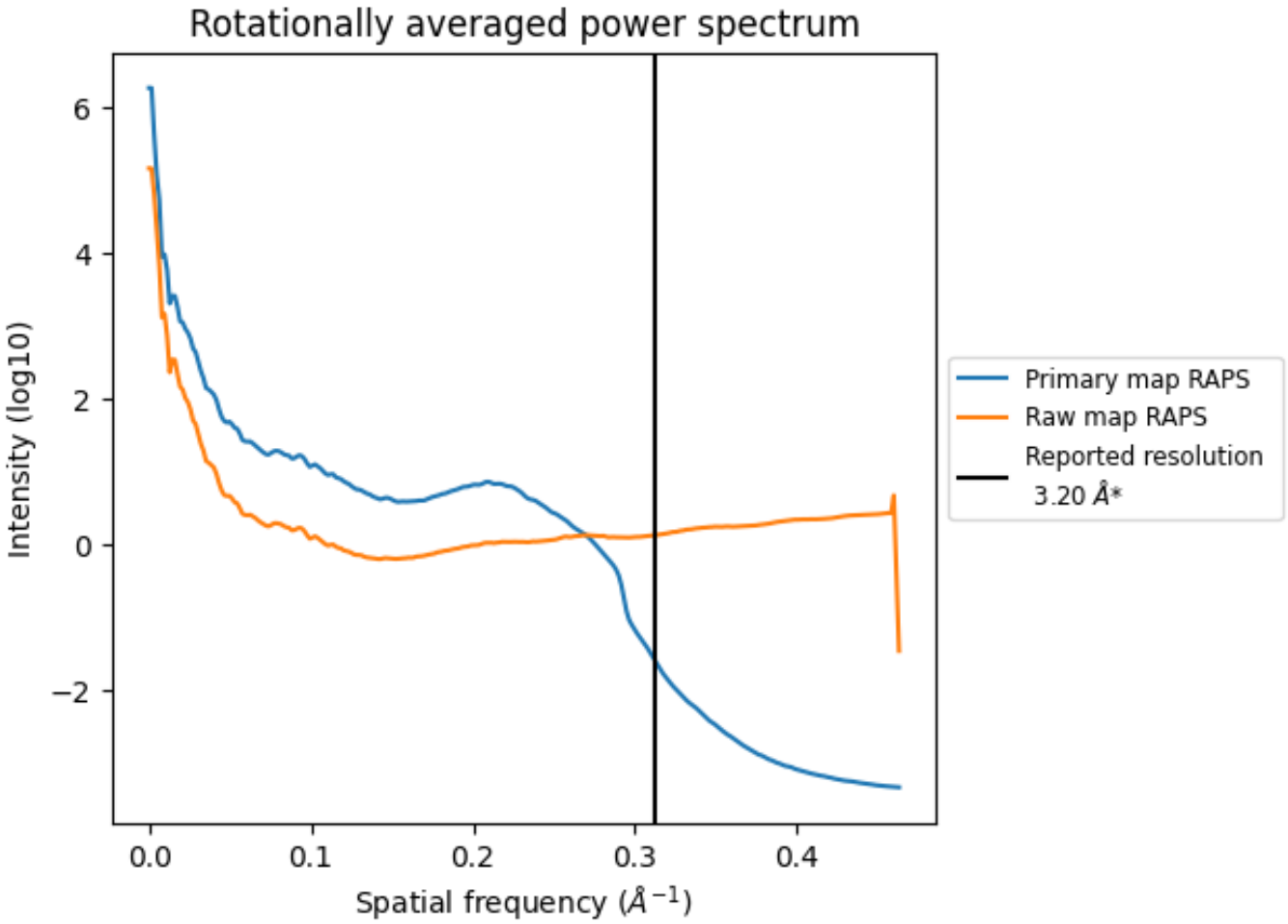
7.2 Volume estimate (i)



The volume at the recommended contour level is 7391 nm^3; this corresponds to an approximate mass of 6676 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 (i)

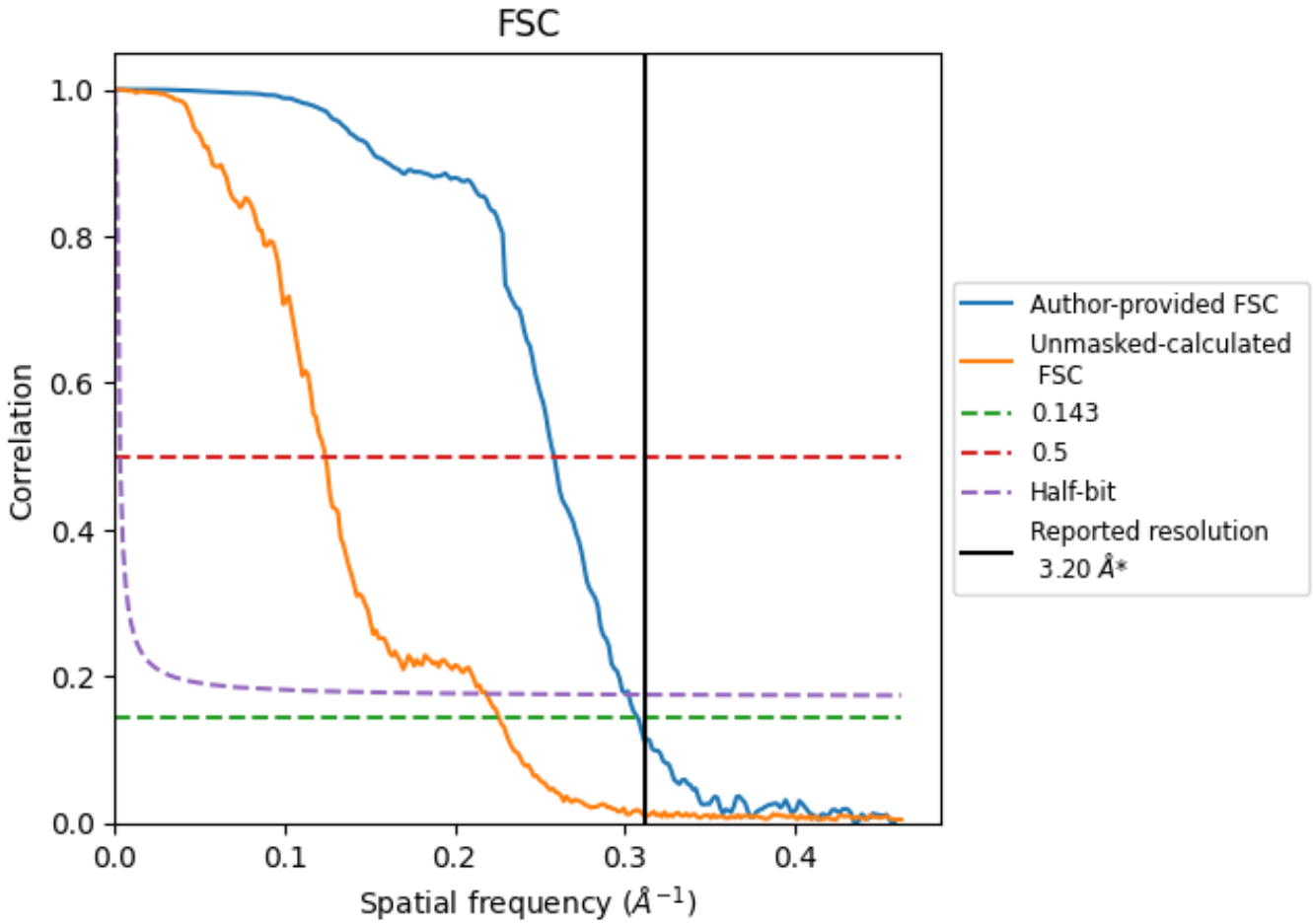


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.25	3.87	3.31
Unmasked-calculated*	4.42	8.07	4.58

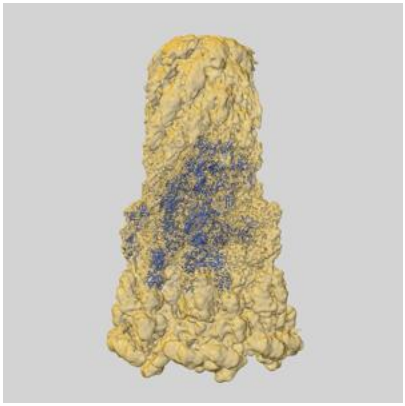
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.2 by more than 10 %

9 Map-model fit

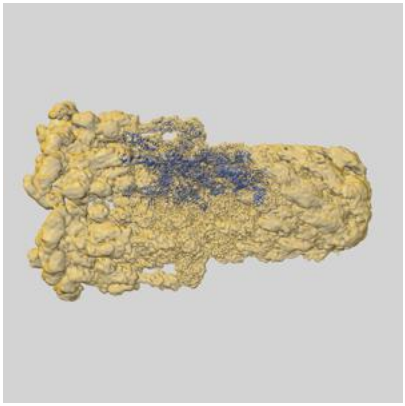
This section contains information regarding the fit between EMDB map EMD-29383 and PDB model 8FQC. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

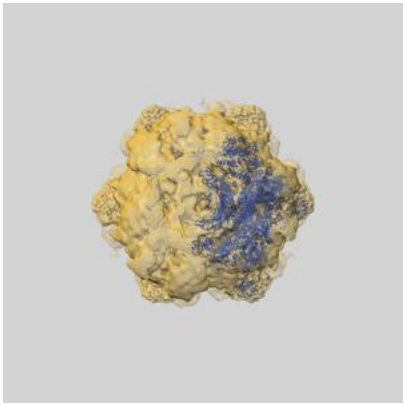
9.1.1 Map-model overlay



X

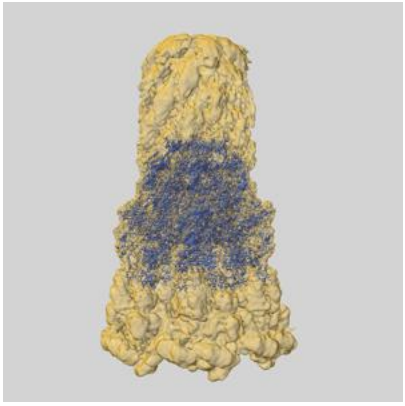


Y

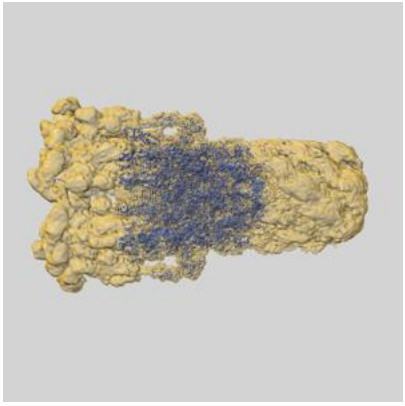


Z

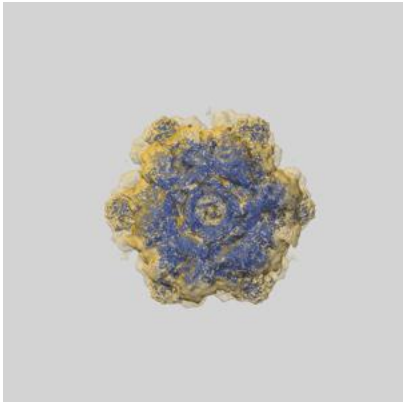
9.1.2 Map-model assembly overlay



X



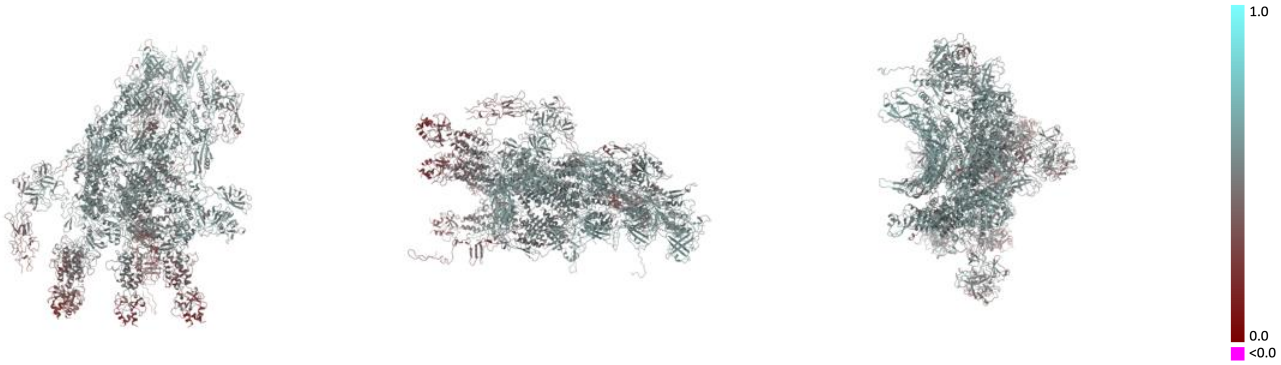
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

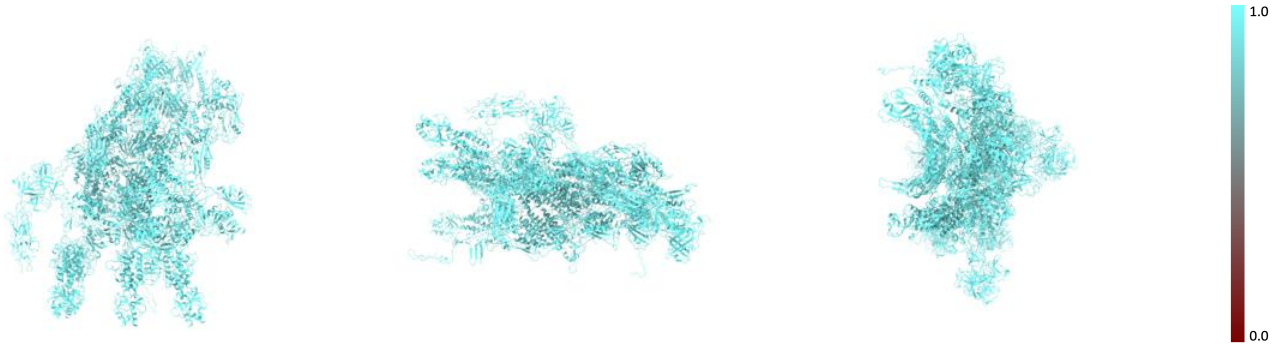
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

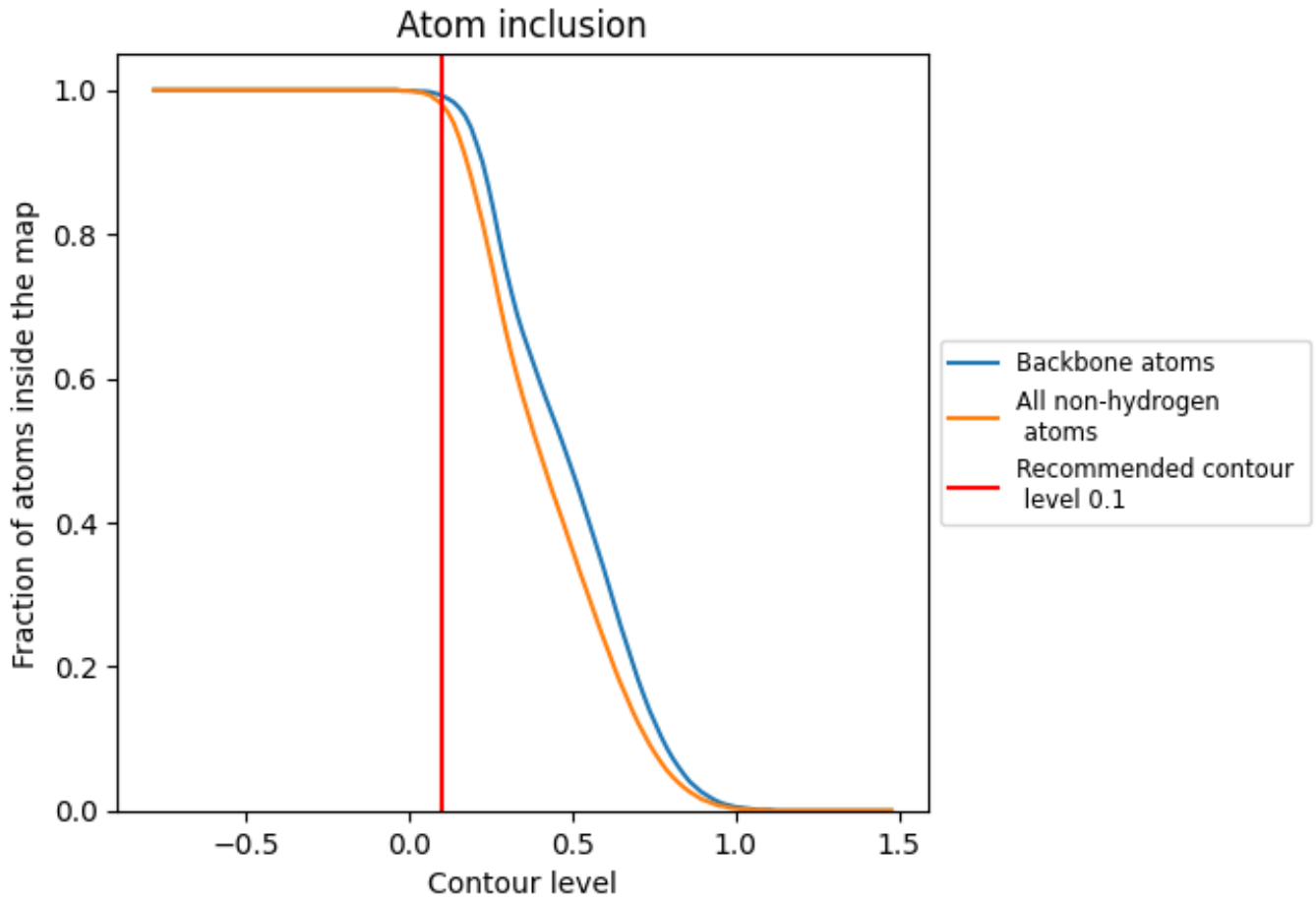
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9810	0.4980
A	0.9070	0.3820
C1	0.9400	0.4770
E1	0.9870	0.5640
F1	0.9840	0.5370
G1	0.9880	0.5390
H1	0.9770	0.5290
I1	0.9860	0.5410
J1	0.9880	0.5400
K1	0.9790	0.4980
P1	0.9880	0.4520
Q1	0.9890	0.4560
R1	0.9820	0.4260
S1	0.9780	0.3790
T1	0.9900	0.3780
U1	0.9780	0.5470
V1	0.9820	0.3670
W1	0.9910	0.4300
X1	0.9860	0.4260
Y1	0.9900	0.4110
a1	0.9840	0.5560
e1	0.9790	0.5530
f1	0.9910	0.5590
g1	0.9820	0.5630
h1	0.9840	0.5390
i1	0.9860	0.5380
j1	0.9780	0.5300
k1	0.9890	0.5440
l1	0.9840	0.5380
m1	0.9800	0.5010
r1	0.9860	0.4470
s1	0.9890	0.4560
t1	0.9870	0.4320
u1	0.9830	0.4140
v1	0.9760	0.3780

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
w1	0.9820	0.3860
x1	0.9680	0.3610
y1	0.9850	0.4160
z1	0.9780	0.4070