wwPDB EM Validation Summary Report (i)

Sep 28, 2024 – 07:47 pm BST

PDB ID	:	6RFL
EMDB ID	:	EMD-4868
Title	:	Structure of the complete Vaccinia DNA-dependent RNA polymerase complex
Authors	:	Grimm, C.; Hillen, S.H.; Bedenk, K.; Bartuli, J.; Neyer, S.; Zhang, Q.; Huettenhofer, A.; Erlacher, M.; Dienemann, C.; Schlosser, A.; Urlaub, H.; Boettcher, B.; Szalay, A.A.; Cramer, P.; Fischer, U.
Deposited on	:	2019-04-15
Resolution	:	2.76 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:

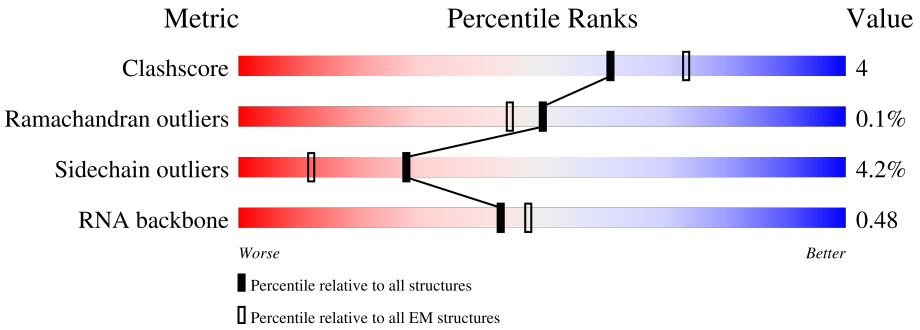
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.76 Å.

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



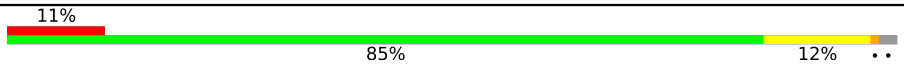
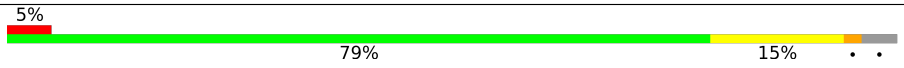
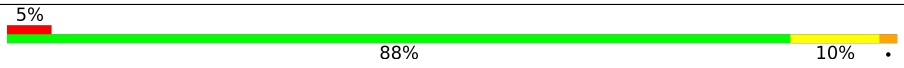
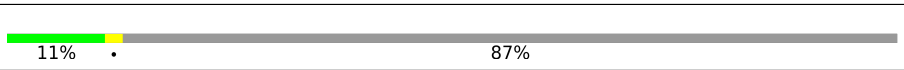
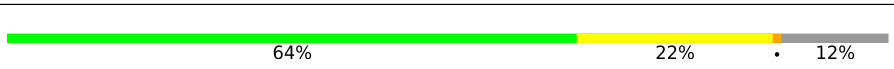
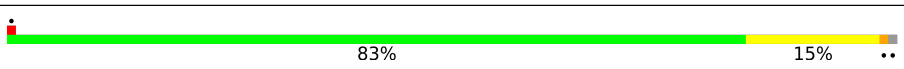
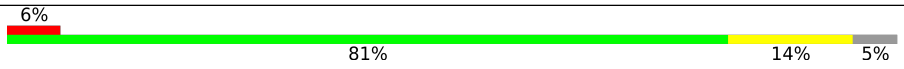
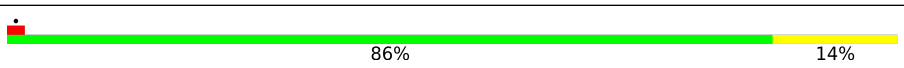
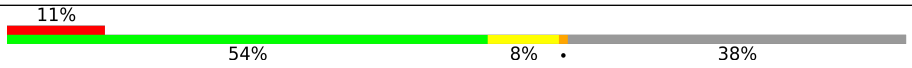
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	B	1164	82% 14%
2	E	185	83% 15%
3	F	164	57% 6% 37%
4	G	161	83% 12% 5%
5	I	795	5% 85% 11%
6	J	63	75% 22%
7	L	287	33% 80% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	O	844	
9	Q	129	
9	R	129	
10	K	710	
11	U	72	
12	A	1286	
13	Y	631	
14	C	305	
15	S	259	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 51788 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 DNA-dependent RNA polymerase subunit rpo132.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1129	9091	5794	1554	1695	48	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	184	1495	966	248	276	5	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	103	849	545	148	153	3	0	0

- Molecule 4 is a protein called DNA-dependent RNA polymerase subunit rpo18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	153	1192	753	198	235	6	0	0

- Molecule 5 is a protein called Putative H4L RNA polymerase-associated transcription factor RAP94.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	773	6446	4210	1025	1190	21	0	0

- Molecule 6 is a protein called DNA-dependent RNA polymerase subunit rpo7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	61	490	310	88	88	4	0	0

- Molecule 7 is a protein called Small subunit of mRNA capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	284	Total	C	N	O	S	0	0
			2320	1492	385	430	13		

- Molecule 8 is a protein called Large subunit of mRNA capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	826	Total	C	N	O	S	0	0
			6693	4317	1099	1259	18		

- Molecule 9 is a protein called Virion core protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	129	Total	C	N	O	S	1	0
			1056	689	165	197	5		
9	Q	124	Total	C	N	O	S	0	0
			1013	660	158	190	5		

- Molecule 10 is a protein called Transcription factor VETF 82kDa large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	91	Total	C	N	O	S	0	0
			749	476	131	133	9		

- Molecule 11 is a RNA chain called chr17.trna16-GlnTTG.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	63	Total	C	N	O	P	6	0
			1465	654	251	491	69		

- Molecule 12 is a protein called DNA-dependent RNA polymerase subunit rpo147.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	1272	Total	C	N	O	S	0	0
			10223	6578	1683	1917	45		

- Molecule 13 is a protein called Nucleoside triphosphate phosphohydrolase-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	600	Total	C	N	O	S	0	0
			4845	3105	826	889	25		

- Molecule 14 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	304	Total 2484	C 1608	N 399	O 464	S 13	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	S	161	Total 1311	C 820	N 211	O 273	P 3	S 4	0	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	B	1	Total 1	Zn 1	0
16	I	1	Total 1	Zn 1	0
16	A	2	Total 2	Zn 2	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total 1	Mg 1	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	B	28	Total 28	O 28	0
18	E	2	Total 2	O 2	0
18	F	1	Total 1	O 1	0
18	G	2	Total 2	O 2	0
18	I	3	Total 3	O 3	0
18	J	3	Total 3	O 3	0

Continued on next page...

Continued from previous page...

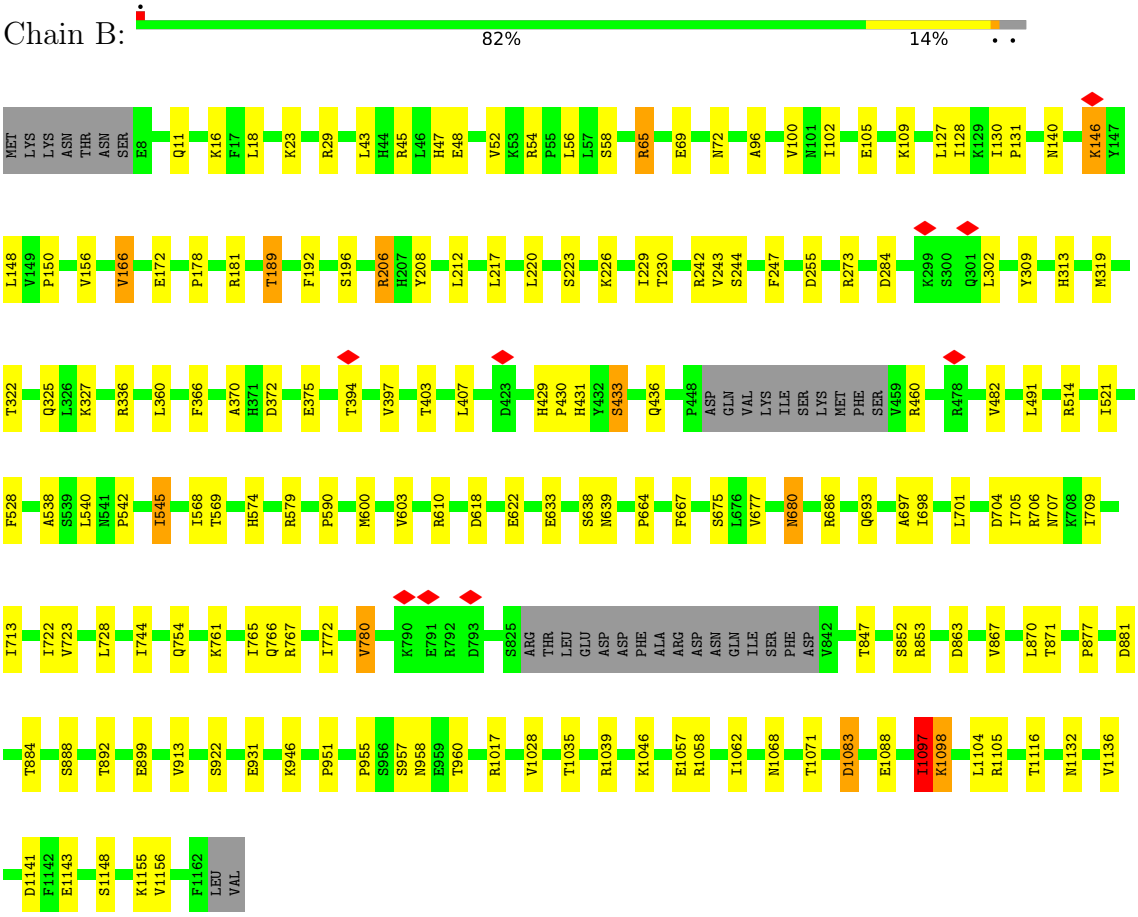
Mol	Chain	Residues	Atoms	AltConf
18	K	1	Total O 1 1	0
18	A	16	Total O 16 16	0
18	Y	2	Total O 2 2	0
18	C	3	Total O 3 3	0

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.

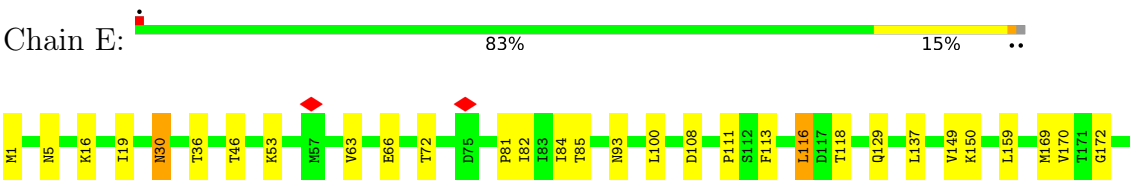
• Molecule 1: DNA-dependent RNA polymerase subunit rpo132

Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit

Chain E:

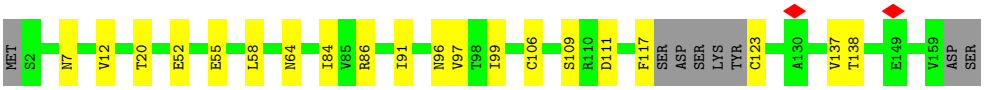


• Molecule 3: DNA-directed RNA polymerase 19 kDa subunit

Chain F:

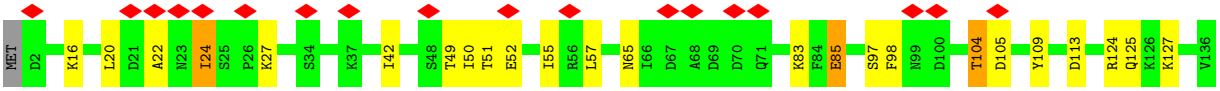
• Molecule 4: DNA-dependent RNA polymerase subunit rpo18

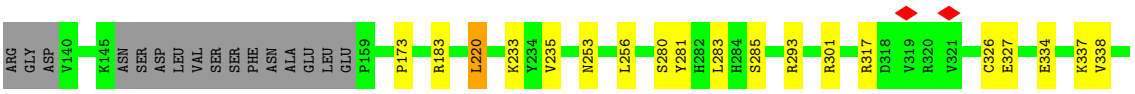
Chain G:

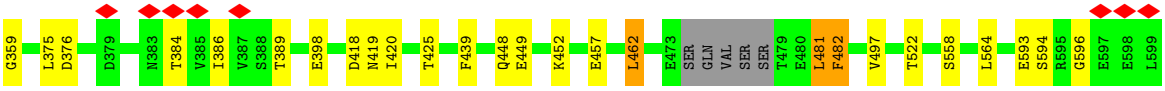


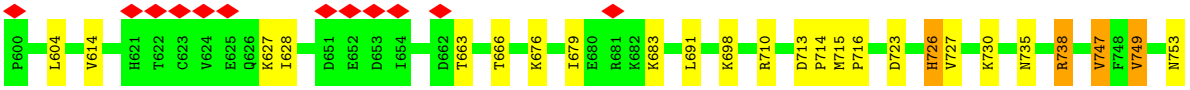
• Molecule 5: Putative H4L RNA polymerase-associated transcription factor RAP94

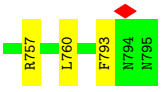
Chain I:





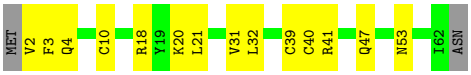






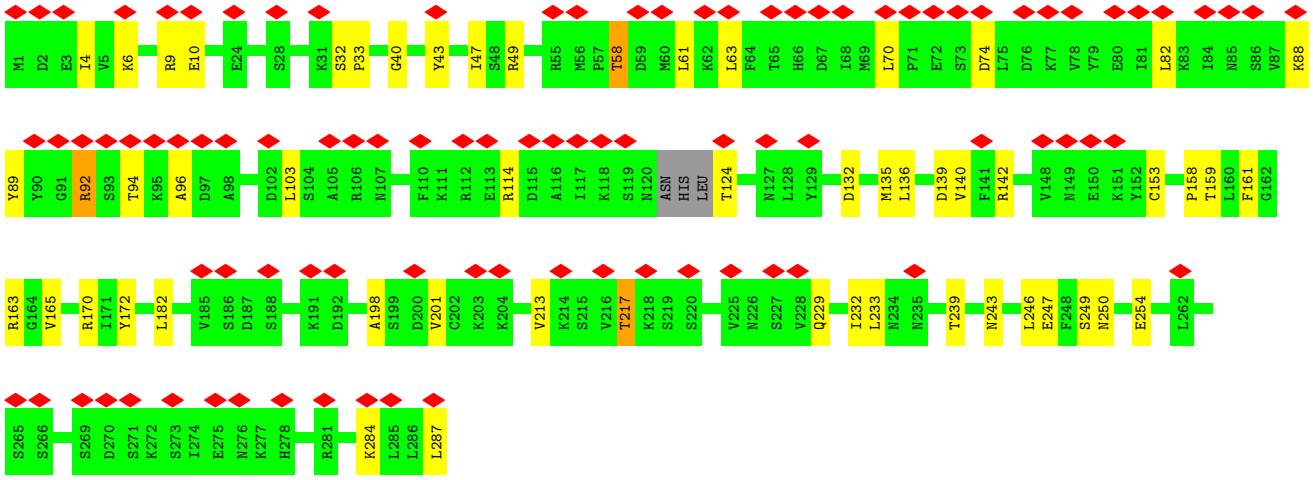
• Molecule 6: DNA-dependent RNA polymerase subunit rpo7

Chain J:



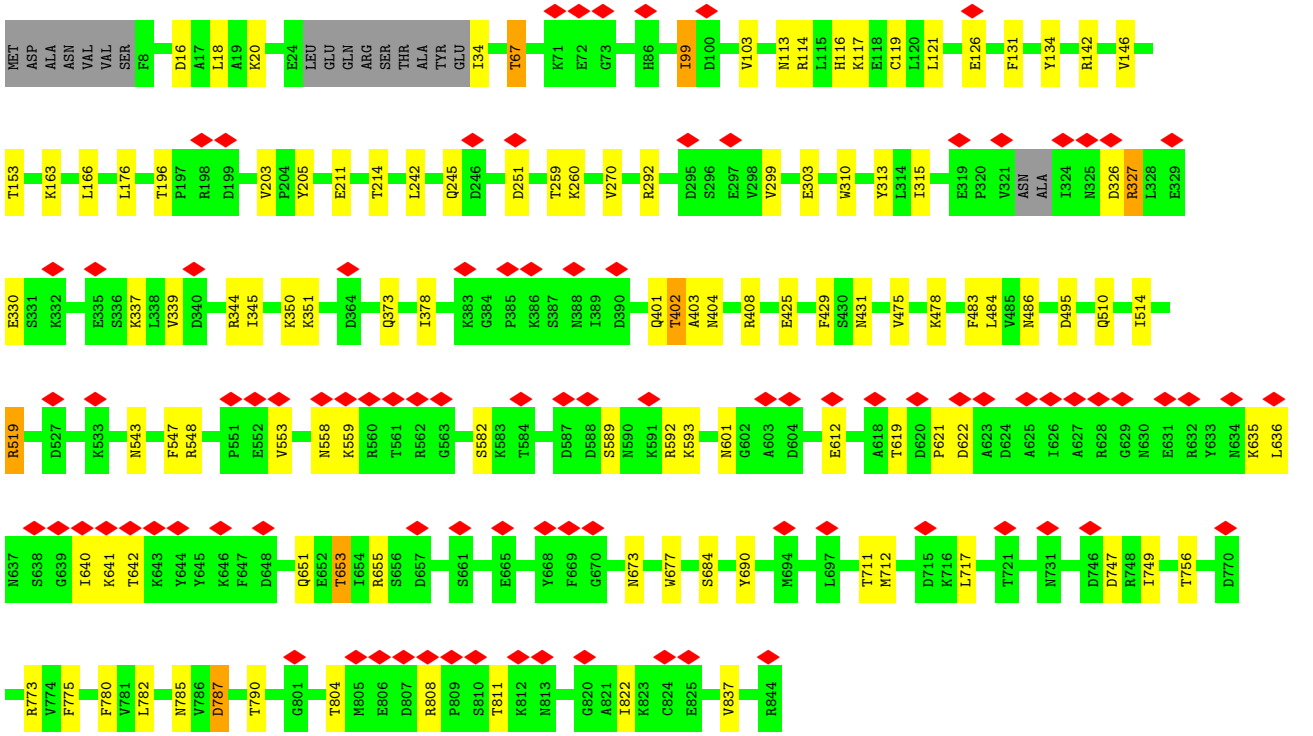
• Molecule 7: Small subunit of mRNA capping enzyme

Chain L:



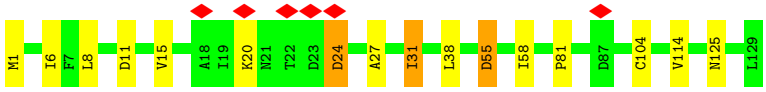
• Molecule 8: Large subunit of mRNA capping enzyme

Chain O:



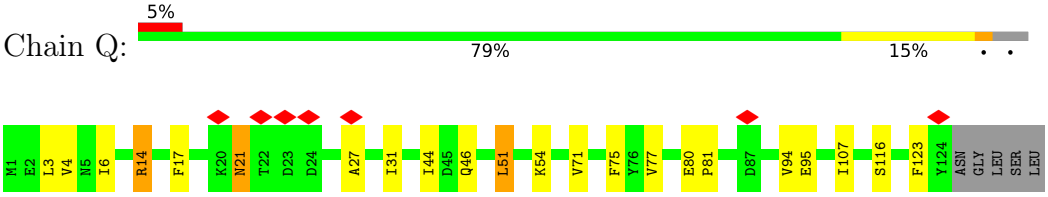
• Molecule 9: Virion core protein

Chain R:



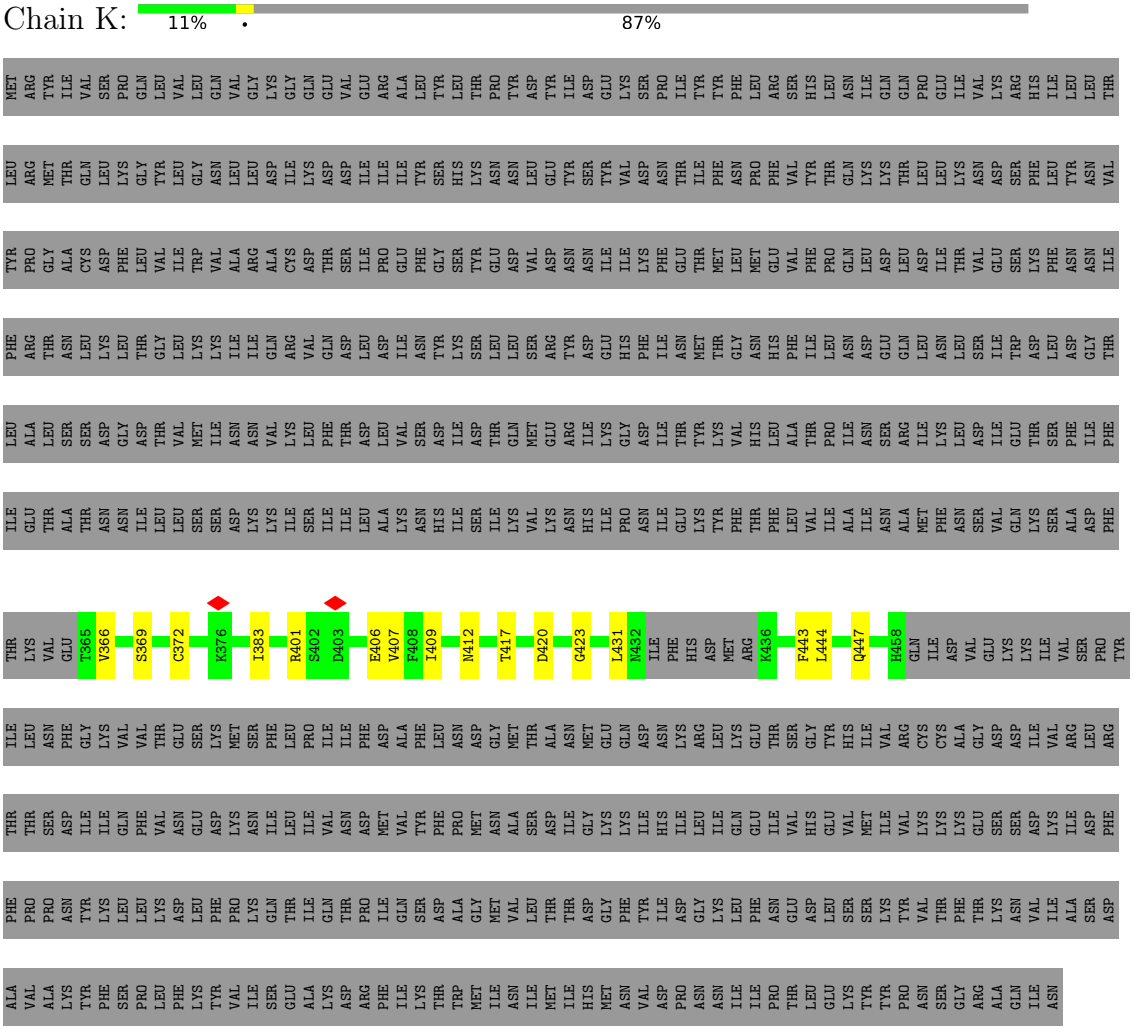
• Molecule 9: Virion core protein

Chain Q:



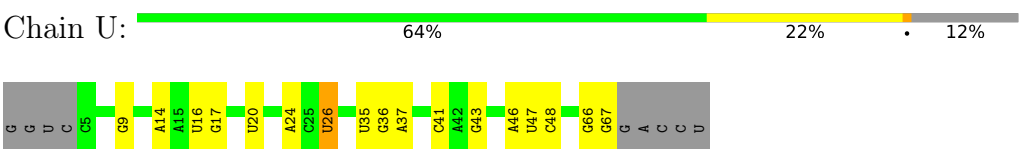
• Molecule 10: Transcription factor VETF 82kDa large subunit

Chain K:



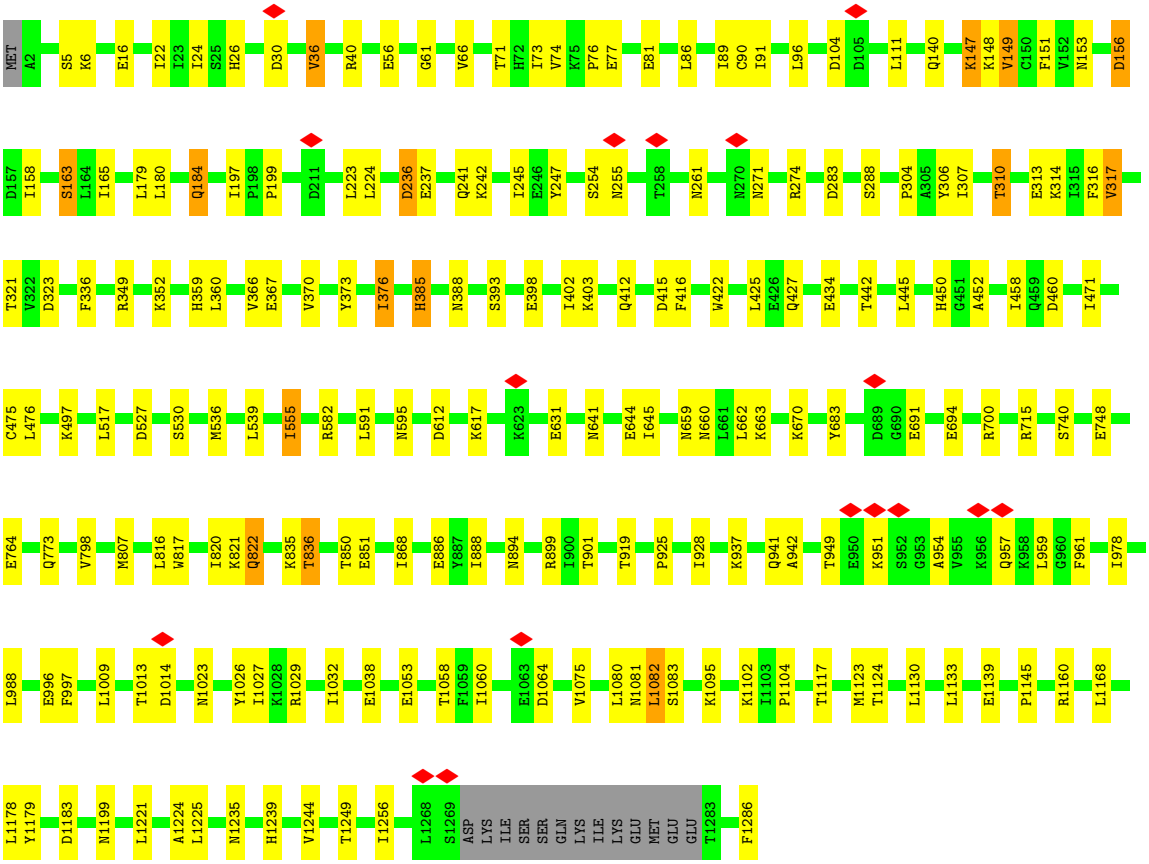
• Molecule 11: chr17.trna16-GlnTTG

Chain U:



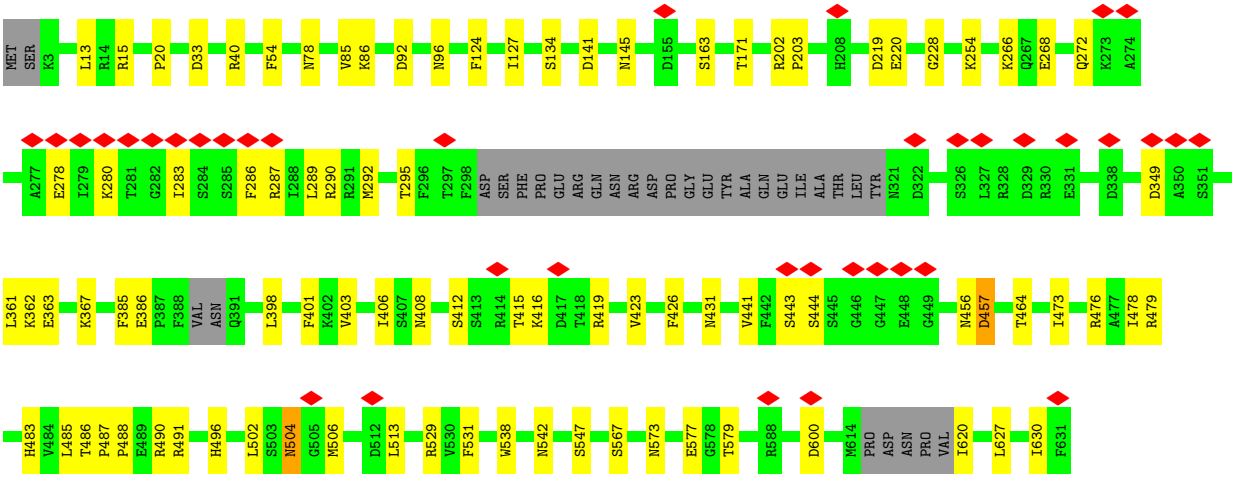
• Molecule 12: DNA-dependent RNA polymerase subunit rpo147

Chain A:



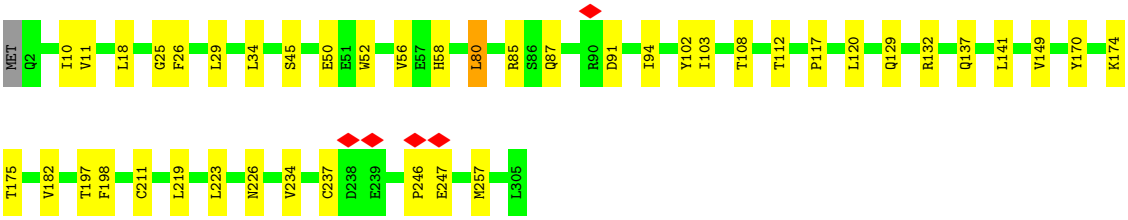
• Molecule 13: Nucleoside triphosphate phosphohydrolase-I

Chain Y:

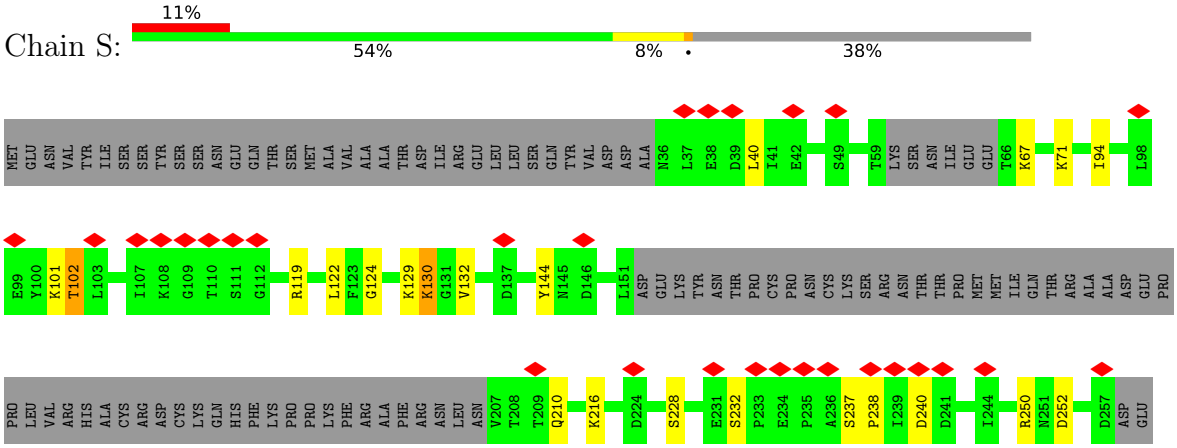


• Molecule 14: DNA-directed RNA polymerase 35 kDa subunit

Chain C:



• Molecule 15: DNA-directed RNA polymerase 30 kDa polypeptide



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	618338	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.562	Depositor
Minimum map value	-0.348	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	536.004, 536.004, 536.004	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.32	0/9281	0.52	0/12537
2	E	0.30	0/1522	0.56	0/2069
3	F	0.31	0/863	0.47	0/1158
4	G	0.32	0/1209	0.51	0/1639
5	I	0.30	0/6590	0.50	1/8918 (0.0%)
6	J	0.33	0/494	0.53	0/663
7	L	0.27	0/2365	0.47	0/3189
8	O	0.27	0/6832	0.48	0/9238
9	Q	0.29	0/1035	0.48	0/1402
9	R	0.30	0/1081	0.50	0/1463
10	K	0.28	0/767	0.49	0/1030
11	U	0.37	0/1635	1.04	10/2545 (0.4%)
12	A	0.32	0/10429	0.51	1/14098 (0.0%)
13	Y	0.28	0/4936	0.48	0/6638
14	C	0.32	0/2540	0.52	1/3440 (0.0%)
15	S	0.27	0/1302	0.51	0/1749
All	All	0.30	0/52881	0.53	13/71776 (0.0%)

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	B	0	1
2	E	0	1
5	I	0	1
7	L	1	0
12	A	0	3
All	All	1	6

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	220	LEU	CA-CB-CG	6.49	130.23	115.30
11	U	36[A]	G	C4-N9-C1'	6.34	134.74	126.50
11	U	36[B]	G	C4-N9-C1'	6.34	134.74	126.50
11	U	36[A]	G	N3-C4-C5	-5.98	125.61	128.60
11	U	36[B]	G	N3-C4-C5	-5.98	125.61	128.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	L	12	THR	CB

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	147	LYS	Peptide
12	A	458	ILE	Peptide
1	B	1097	ILE	Peptide
2	E	116	LEU	Peptide
5	I	481	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	9091	0	9146	100	0
2	E	1495	0	1548	15	0
3	F	849	0	874	8	0
4	G	1192	0	1181	9	0
5	I	6446	0	6502	53	0
6	J	490	0	530	6	0
7	L	2320	0	2363	28	0
8	O	6693	0	6766	48	0
9	Q	1013	0	998	11	0
9	R	1056	0	1056	11	0
10	K	749	0	727	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	U	1465	0	738	5	0
12	A	10223	0	10337	107	0
13	Y	4845	0	4911	50	0
14	C	2484	0	2470	24	0
15	S	1311	0	1268	15	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	1	0	0	0	0
17	A	1	0	0	0	0
18	A	16	0	0	1	0
18	B	28	0	0	0	0
18	C	3	0	0	0	0
18	E	2	0	0	0	0
18	F	1	0	0	0	0
18	G	2	0	0	0	0
18	I	3	0	0	0	0
18	J	3	0	0	0	0
18	K	1	0	0	0	0
18	Y	2	0	0	0	0
All	All	51788	0	51415	433	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 4.

The worst 5 of 433 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:L:43:TYR:O	7:L:47:ILE:HB	1.75	0.85
14:C:25:GLY:O	14:C:29:LEU:HB2	1.85	0.75
12:A:817:TRP:O	12:A:821:LYS:HB3	1.89	0.72
13:Y:268:GLU:HG2	13:Y:272:GLN:HE22	1.57	0.69
5:I:233:LYS:HB2	11:U:41:C:H5'	1.78	0.65

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	B	1123/1164 (96%)	1046 (93%)	76 (7%)	1 (0%)	48	70
2	E	182/185 (98%)	164 (90%)	17 (9%)	1 (0%)	25	41
3	F	101/164 (62%)	95 (94%)	6 (6%)	0	100	100
4	G	149/161 (92%)	136 (91%)	13 (9%)	0	100	100
5	I	765/795 (96%)	715 (94%)	49 (6%)	1 (0%)	48	70
6	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
7	L	280/287 (98%)	267 (95%)	13 (5%)	0	100	100
8	O	820/844 (97%)	794 (97%)	26 (3%)	0	100	100
9	Q	122/129 (95%)	118 (97%)	4 (3%)	0	100	100
9	R	128/129 (99%)	121 (94%)	7 (6%)	0	100	100
10	K	87/710 (12%)	81 (93%)	6 (7%)	0	100	100
12	A	1268/1286 (99%)	1184 (93%)	84 (7%)	0	100	100
13	Y	592/631 (94%)	556 (94%)	36 (6%)	0	100	100
14	C	302/305 (99%)	278 (92%)	24 (8%)	0	100	100
15	S	152/259 (59%)	132 (87%)	19 (12%)	1 (1%)	19	32
All	All	6130/7112 (86%)	5743 (94%)	383 (6%)	4 (0%)	50	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	118	THR
5	I	482	PHE
1	B	1098	LYS
15	S	238	PRO

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	B	1030/1064 (97%)	997 (97%)	33 (3%)	34	55
2	E	174/175 (99%)	168 (97%)	6 (3%)	32	54
3	F	94/151 (62%)	92 (98%)	2 (2%)	48	69
4	G	136/144 (94%)	130 (96%)	6 (4%)	24	43
5	I	735/755 (97%)	703 (96%)	32 (4%)	24	43
6	J	60/62 (97%)	55 (92%)	5 (8%)	9	17
7	L	269/272 (99%)	256 (95%)	13 (5%)	21	39
8	O	759/774 (98%)	720 (95%)	39 (5%)	20	36
9	Q	116/121 (96%)	108 (93%)	8 (7%)	13	23
9	R	122/121 (101%)	116 (95%)	6 (5%)	21	38
10	K	87/665 (13%)	80 (92%)	7 (8%)	10	18
12	A	1143/1157 (99%)	1089 (95%)	54 (5%)	22	40
13	Y	545/573 (95%)	529 (97%)	16 (3%)	37	59
14	C	286/287 (100%)	279 (98%)	7 (2%)	44	65
15	S	146/237 (62%)	143 (98%)	3 (2%)	48	69
All	All	5702/6558 (87%)	5465 (96%)	237 (4%)	27	44

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	O	475	VAL
13	Y	464	THR
10	K	369	SER
13	Y	441	VAL
15	S	132	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	447	GLN
12	A	940	GLN
12	A	167	GLN
12	A	611	ASN
12	A	994	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	U	56/72 (77%)	11 (19%)	0

5 of 11 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	U	9	G
11	U	14	A
11	U	16	U
11	U	17	G
11	U	24	A

There are no RNA pucker outliers to report.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
15	SEP	S	232	15	8,9,10	1.55	1 (12%)	8,12,14	1.53	2 (25%)
15	SEP	S	228	15	8,9,10	1.52	1 (12%)	8,12,14	1.56	2 (25%)
15	SEP	S	237	15	8,9,10	1.53	1 (12%)	8,12,14	1.60	2 (25%)

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
15	SEP	S	232	15	-	4/5/8/10	-
15	SEP	S	228	15	-	4/5/8/10	-
15	SEP	S	237	15	-	3/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	S	232	SEP	P-O1P	3.39	1.61	1.50
15	S	228	SEP	P-O1P	3.33	1.61	1.50
15	S	237	SEP	P-O1P	3.31	1.61	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	S	237	SEP	P-OG-CB	-3.16	109.60	118.30
15	S	228	SEP	OG-CB-CA	2.93	111.00	108.14
15	S	232	SEP	OG-CB-CA	2.82	110.89	108.14
15	S	237	SEP	OG-CB-CA	2.79	110.86	108.14
15	S	228	SEP	P-OG-CB	-2.76	110.69	118.30

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	S	228	SEP	CB-OG-P-O2P
15	S	228	SEP	CB-OG-P-O3P
15	S	232	SEP	CA-CB-OG-P
15	S	232	SEP	CB-OG-P-O2P
15	S	232	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

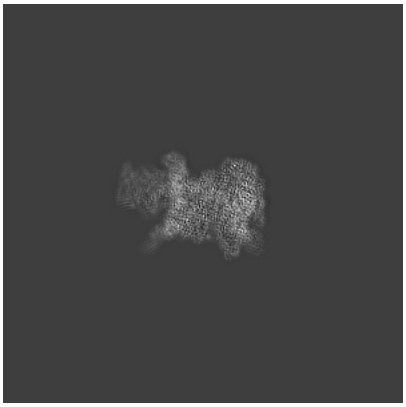
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4868. These allow visual inspection of the internal detail of the map and identification of artifacts.

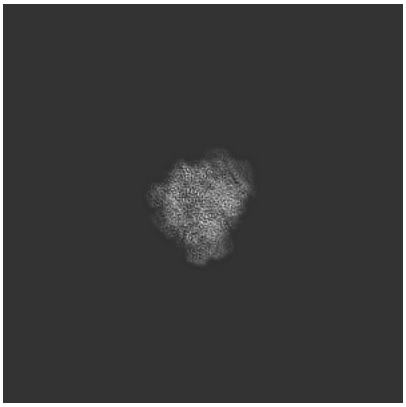
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

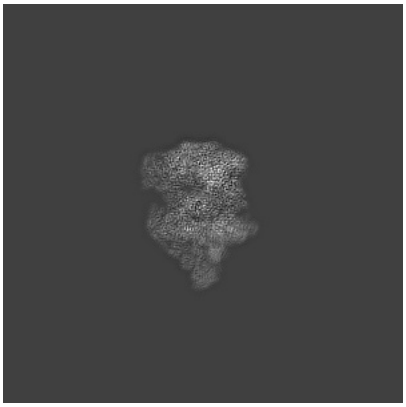
6.1.1 Primary map



X



Y

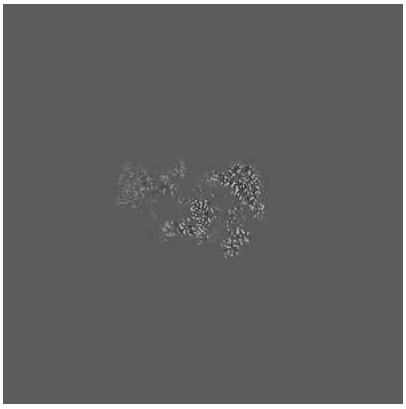


Z

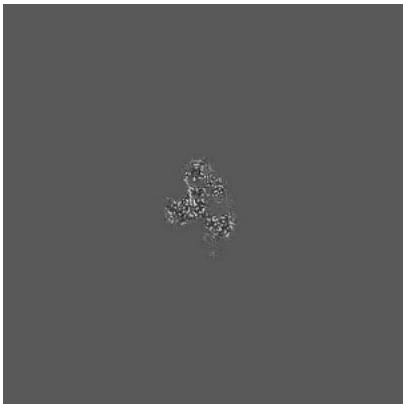
The images above show the map projected in three orthogonal directions.

6.2 Central slices

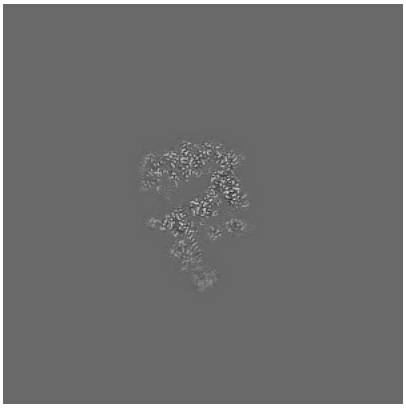
6.2.1 Primary map



X Index: 252



Y Index: 252

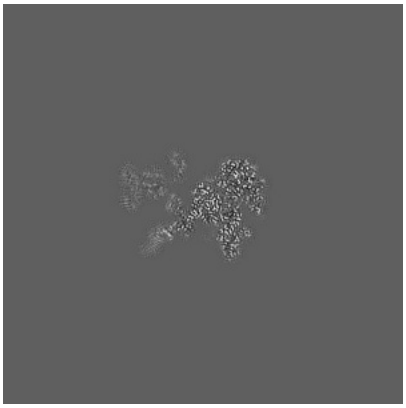


Z Index: 252

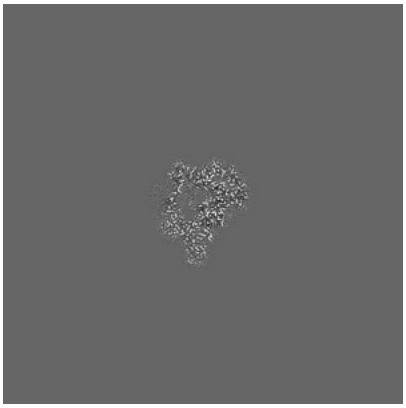
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

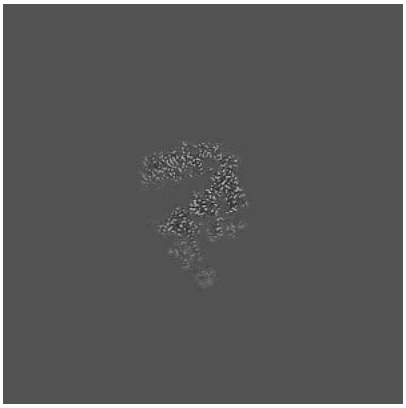
6.3.1 Primary map



X Index: 262



Y Index: 302

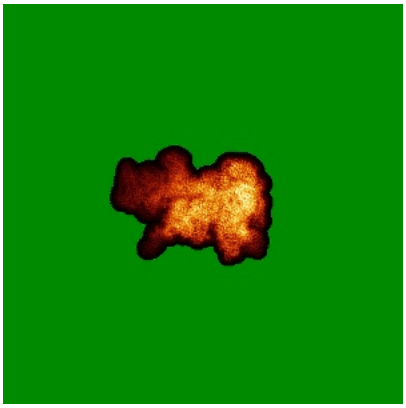


Z Index: 248

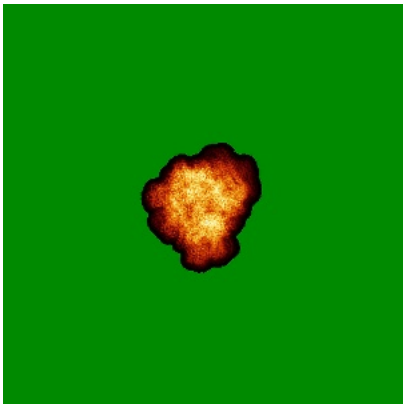
The images above show the largest variance slices of the map in three orthogonal directions.

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

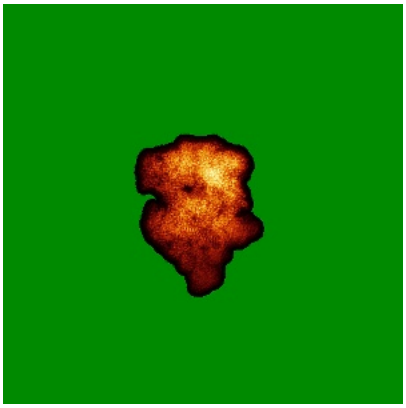
6.4.1 Primary map



X



Y



Z

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

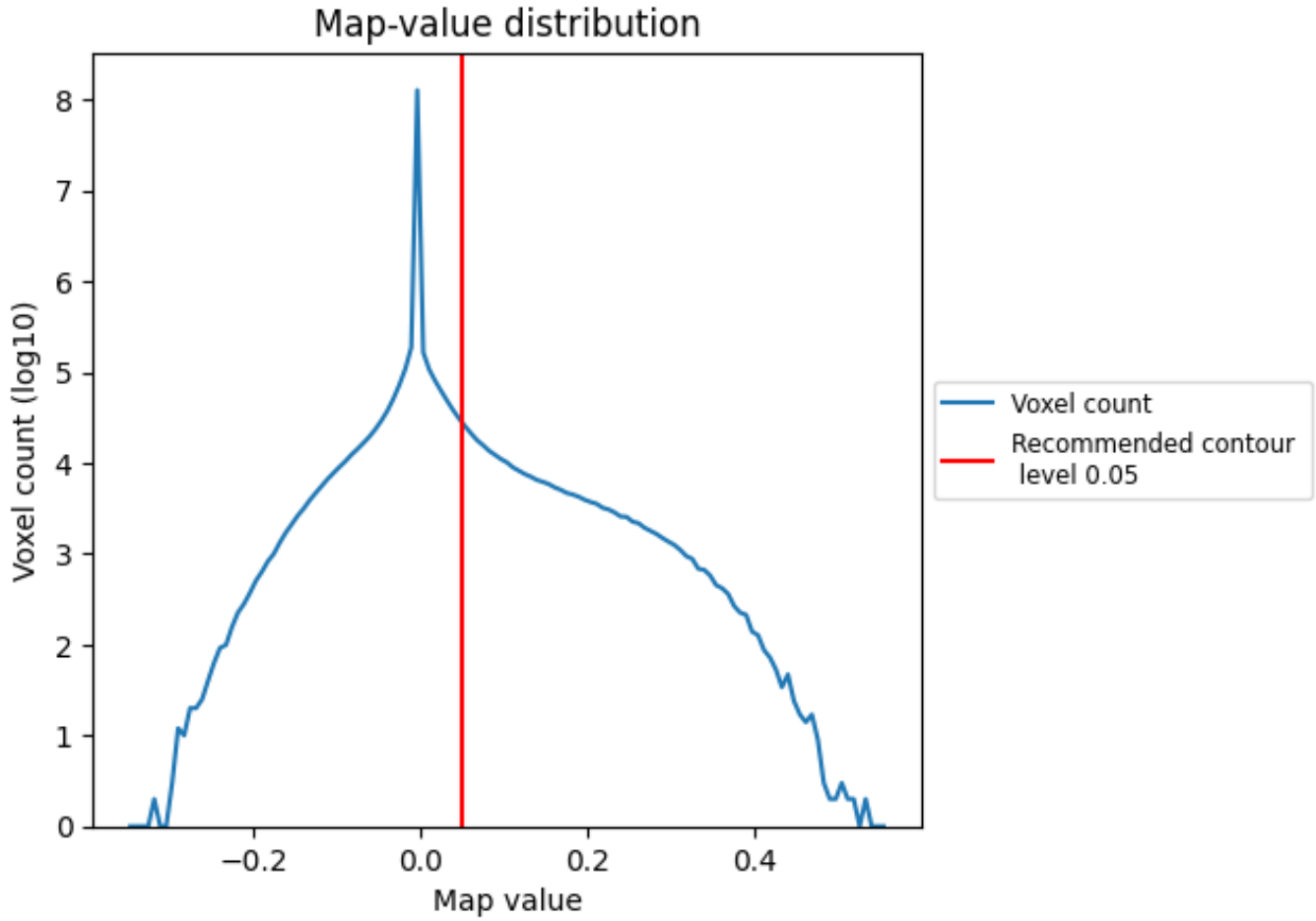
6.6 Mask visualisation (i)

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

7 Map analysis

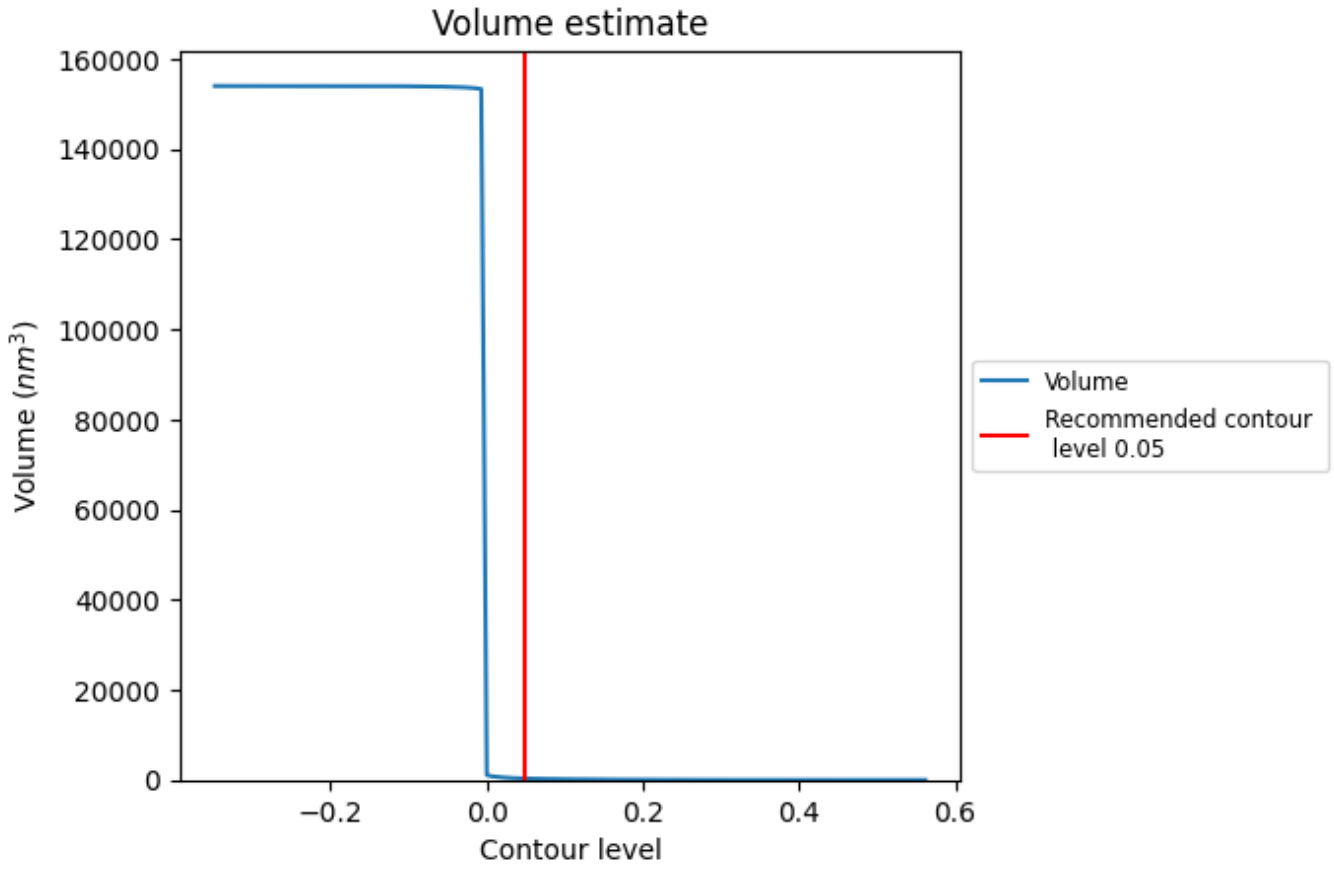
This section contains the results of statistical analysis of the map.

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.

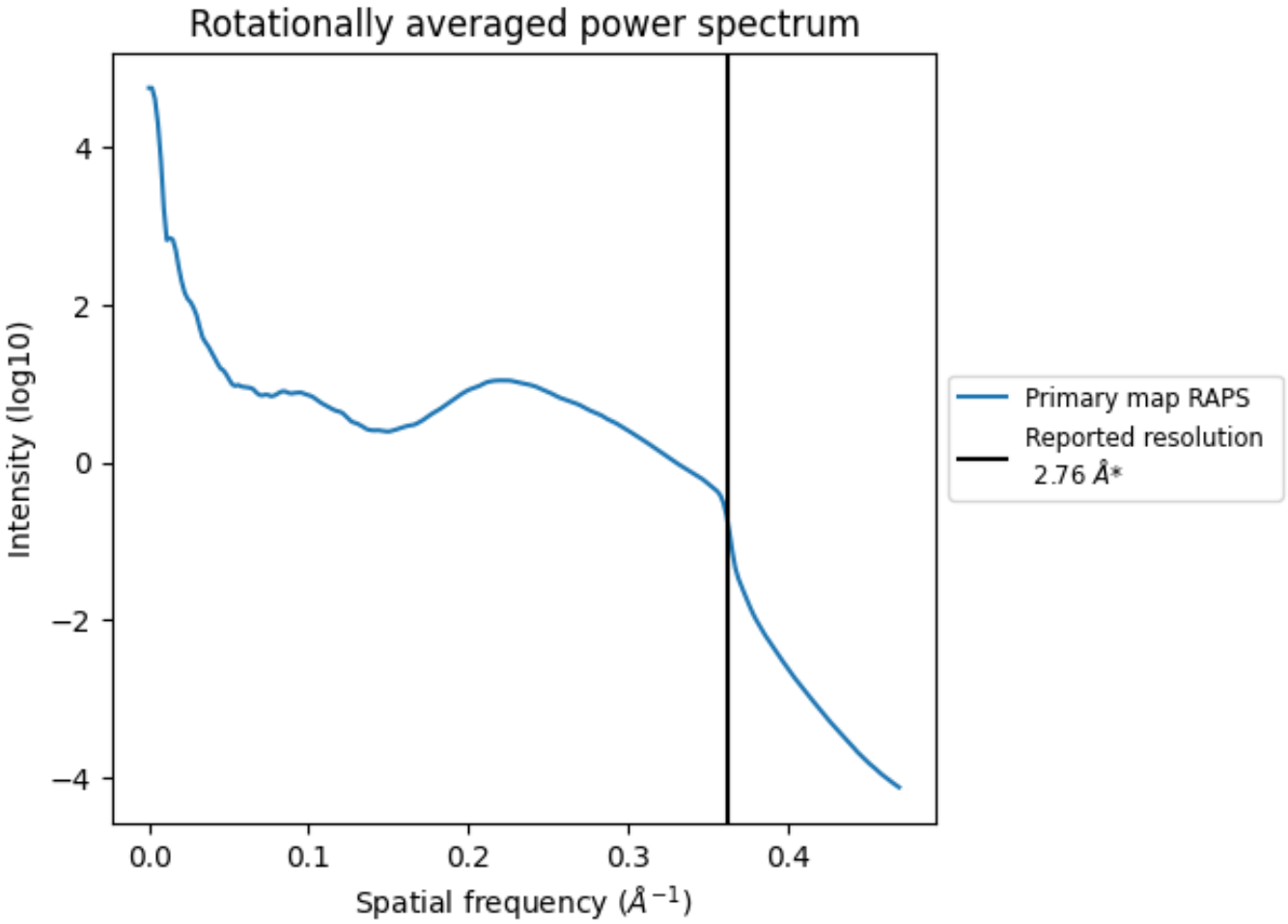
7.2 Volume estimate (i)



The volume at the recommended contour level is 314 nm^3; this corresponds to an approximate mass of 284 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)

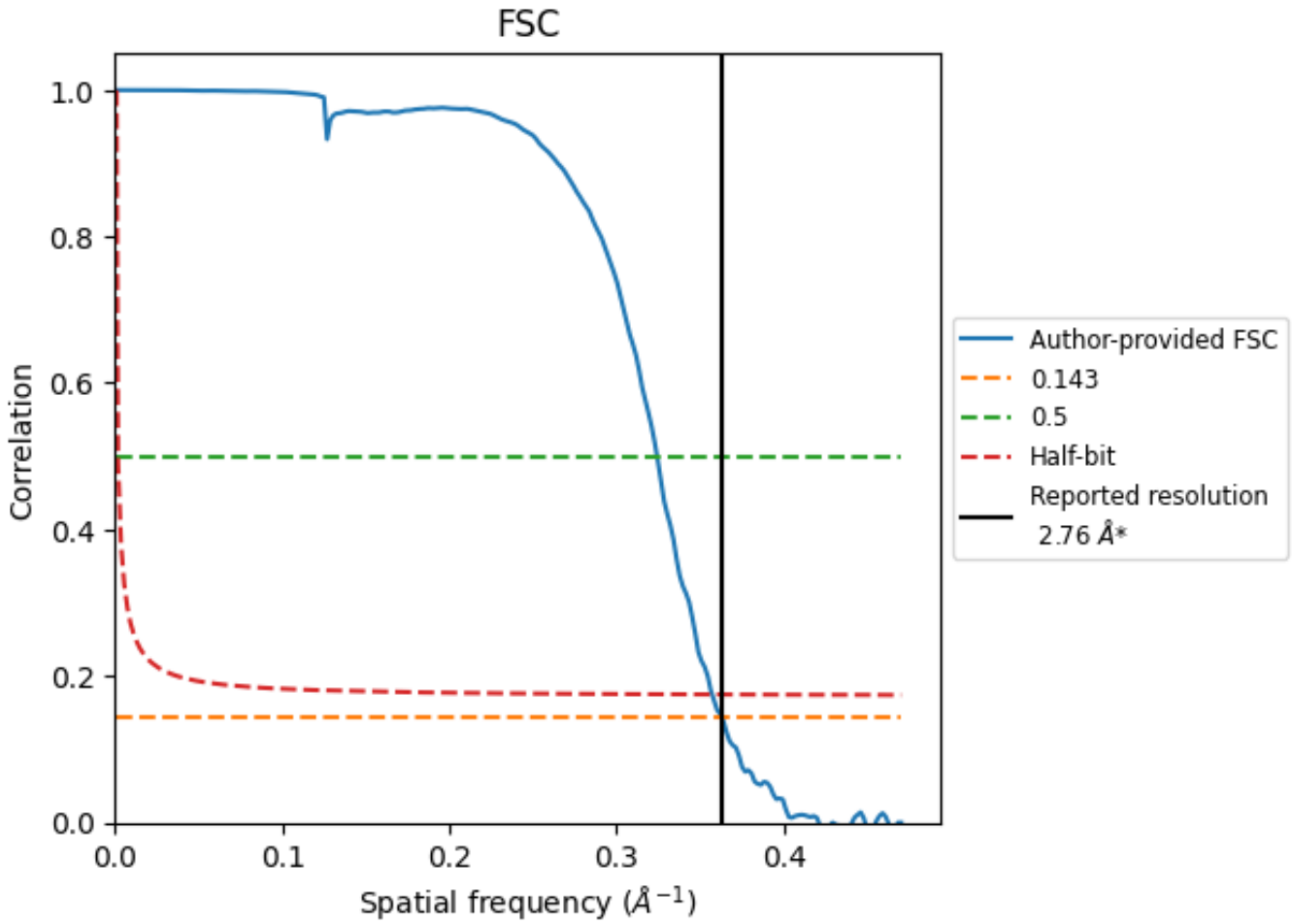


*Reported resolution corresponds to spatial frequency of 0.362 Å^{-1}

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 0.362 Å^{-1}

8.2 Resolution estimates (i)

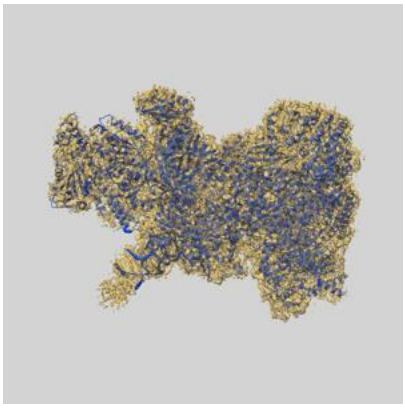
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.08	2.80
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

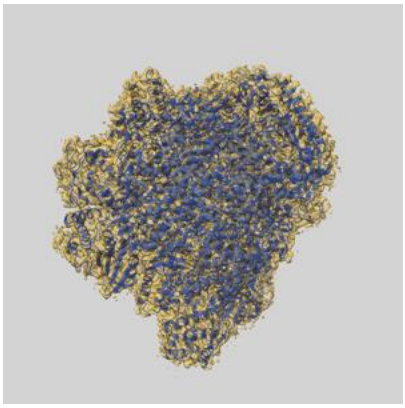
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4868 and PDB model 6RFL. Per-residue inclusion information can be found in section 3 on page 8.

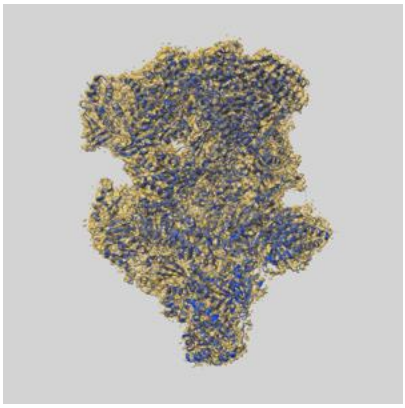
9.1 Map-model overlay



X



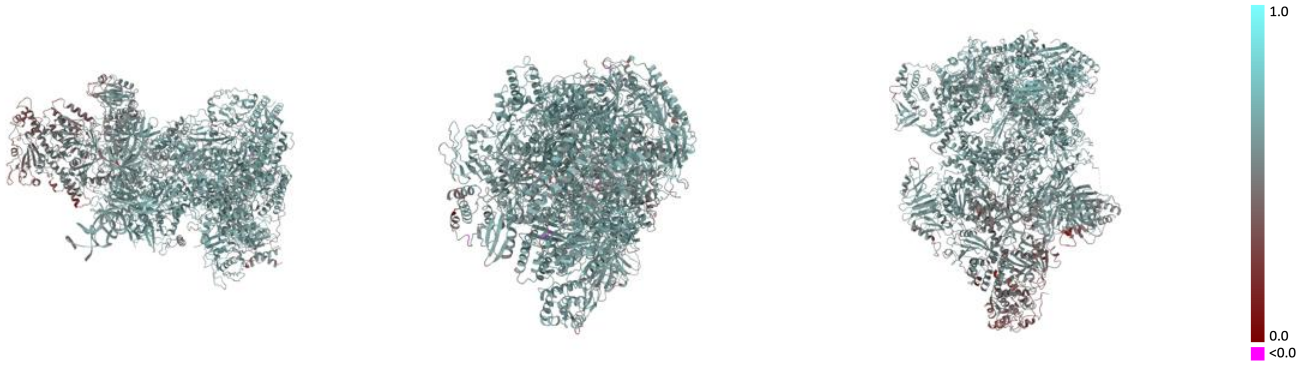
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

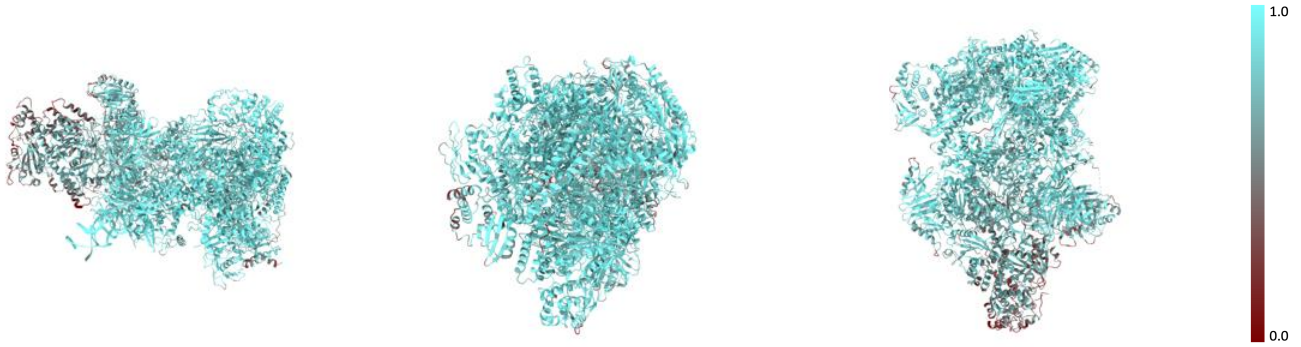
9.2 Q-score mapped to coordinate model (i)



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.

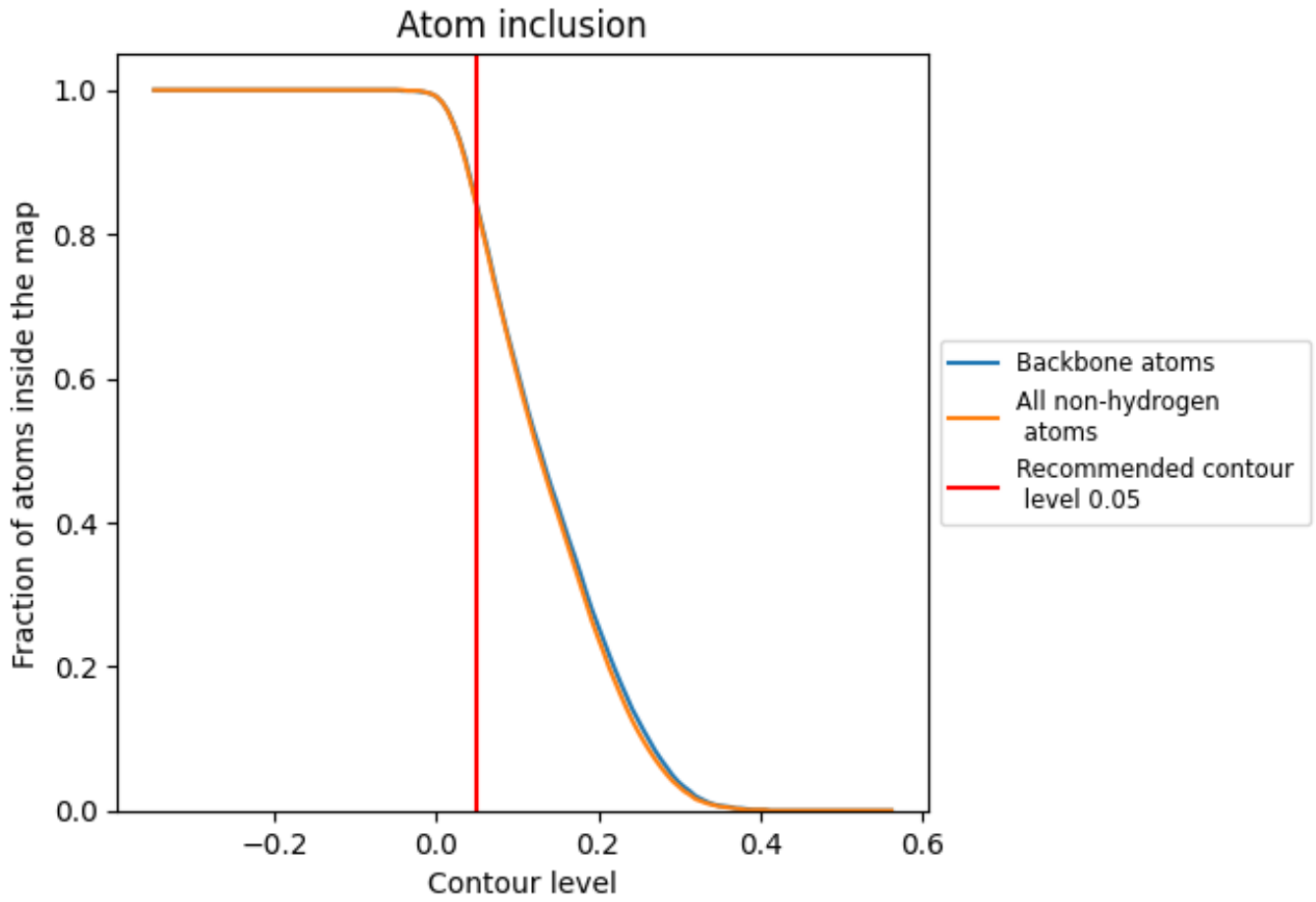
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8390	0.5720
A	0.9090	0.6090
B	0.9240	0.6120
C	0.9150	0.6000
E	0.9080	0.5940
F	0.9420	0.6250
G	0.8990	0.5960
I	0.8350	0.5680
J	0.9440	0.6110
K	0.8380	0.5710
L	0.5190	0.4060
O	0.7180	0.5210
Q	0.7870	0.5500
R	0.8380	0.5670
S	0.6680	0.5120
U	0.9300	0.5630
Y	0.8060	0.5610