



## wwPDB EM Validation Summary Report ⓘ

Dec 9, 2025 – 12:58 am GMT

PDB ID : 9R78 / pdb\_00009r78  
EMDB ID : EMD-53736  
Title : Human Adenovirus D 10 Capsid Structure  
Authors : Waraich, K.; Mundy, R.M.; Bates, E.A.; da Fonseca, P.; Morris, E.; Rizkallah, P.J.; Baker, A.T.; Young, M.T.; Parker, A.L.; Bhella, D.  
Deposited on : 2025-05-14  
Resolution : 3.30 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](mailto: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>.

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

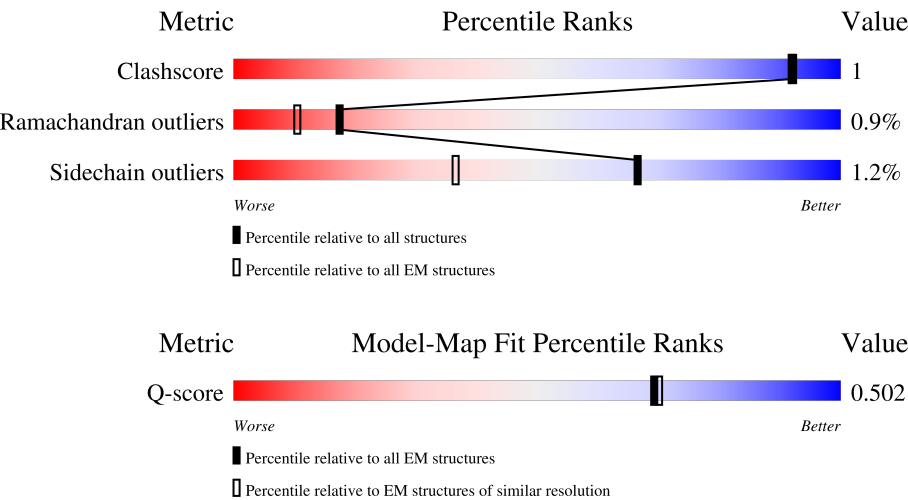
EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.47

# 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 3.30 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.



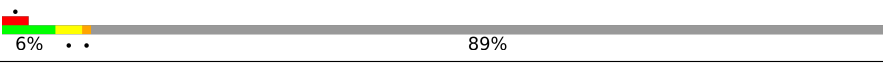
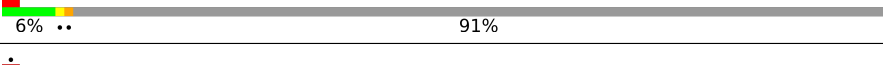

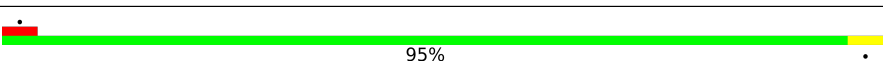
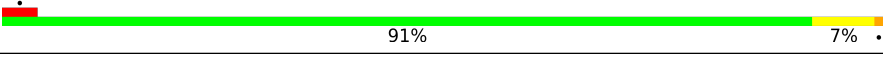
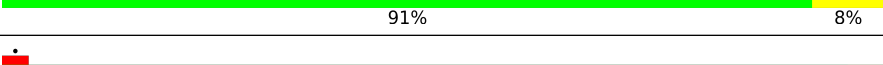
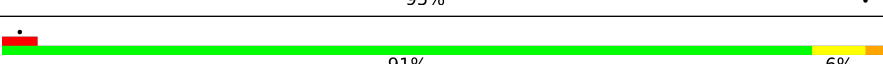
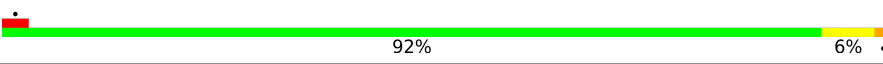
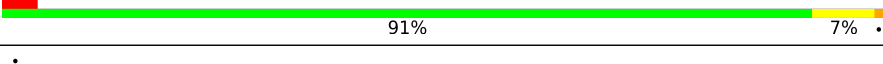
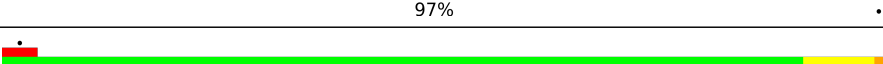
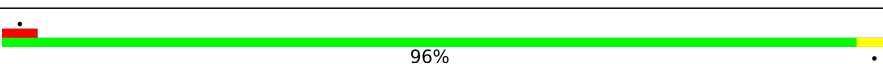
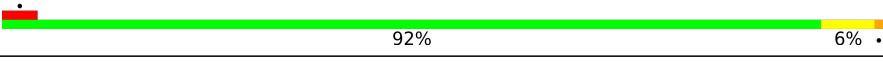
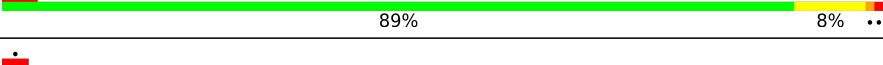


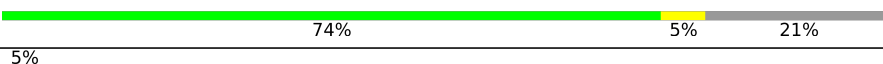

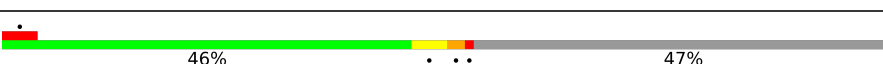





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15087 ( 2.80 - 3.80 )

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  $\geq 3$ , 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	1	234	<div><div></div><div>6% .</div><div>91%</div></div>
1	2	234	<div><div></div><div>6%</div><div>93%</div></div>
1	3	234	<div><div></div><div>. 5%</div><div>91%</div></div>
1	4	234	<div><div></div><div>. .</div><div>95%</div></div>

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Mol	Chain	Length	Quality of chain
1	5	234	
1	6	234	
1	7	234	
1	8	234	
2	A	941	
2	B	941	
2	C	941	
2	D	941	
2	E	941	
2	F	941	
2	G	941	
2	H	941	
2	I	941	
2	J	941	
2	K	941	
2	L	941	
3	M	519	
4	N	559	
5	O	227	
5	P	227	
6	Q	134	
6	R	134	
6	S	134	
6	T	134	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 198096 atoms, of which 96875 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 Pre-protein VI.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	22	Total	C	H	N	O	S	0	0
			340	112	163	33	31	1		
1	2	16	Total	C	H	N	O	S	0	0
			216	68	103	20	24	1		
1	3	21	Total	C	H	N	O	S	0	0
			325	107	157	32	28	1		
1	4	11	Total	C	H	N	O	S	0	0
			172	58	81	18	14	1		
1	5	25	Total	C	H	N	O	S	0	0
			393	128	191	36	36	2		
1	6	20	Total	C	H	N	O	S	0	0
			309	102	148	31	27	1		
1	7	27	Total	C	H	N	O	S	0	0
			415	134	204	39	37	1		
1	8	17	Total	C	H	N	O	S	0	0
			271	90	131	26	23	1		

- Molecule 2 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	B	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	C	941	Total	C	H	N	O	S	0	0
			14640	4751	7149	1264	1441	35		
2	D	941	Total	C	H	N	O	S	0	0
			14640	4751	7149	1264	1441	35		
2	E	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	F	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	G	941	Total	C	H	N	O	S	0	0
			14640	4751	7149	1264	1441	35		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	I	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	J	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	K	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	L	939	Total	C	H	N	O	S	0	0
			14604	4741	7129	1262	1439	33		

- Molecule 3 is a protein called Penton protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	472	Total	C	H	N	O	S	0	0
			7509	2410	3715	642	728	14		

- Molecule 4 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	N	281	Total	C	H	N	O	S	0	0
			4346	1354	2170	397	422	3		

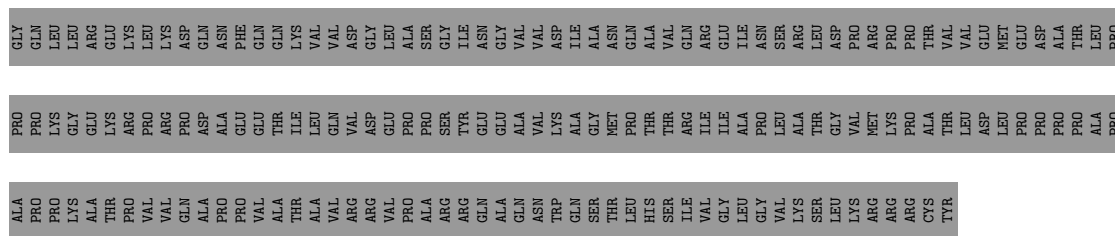
- Molecule 5 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	O	177	Total	C	H	N	O	S	0	0
			2706	868	1329	237	267	5		
5	P	180	Total	C	H	N	O	S	0	0
			2727	874	1338	240	270	5		

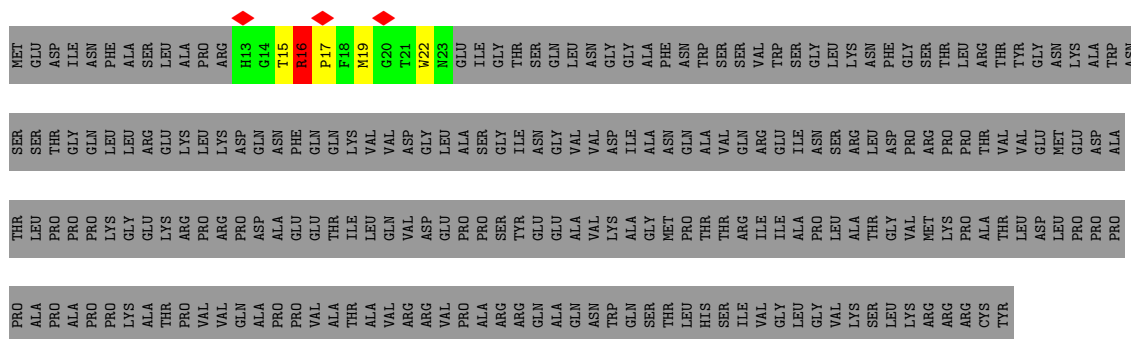
- Molecule 6 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Q	39	Total	C	H	N	O		0	0
			619	188	317	52	62			
6	R	36	Total	C	H	N	O		0	0
			579	175	294	51	59			
6	S	71	Total	C	H	N	O	S	0	0
			1017	305	513	88	109	2		
6	T	32	Total	C	H	N	O		0	0
			516	154	261	48	53			

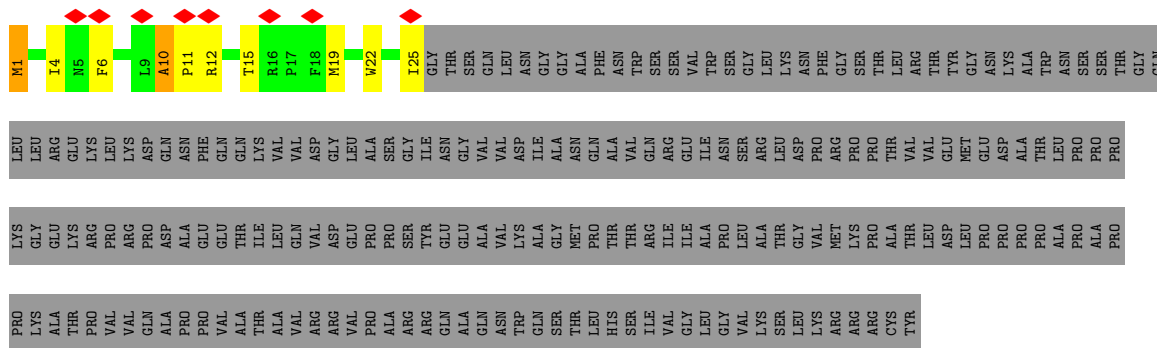




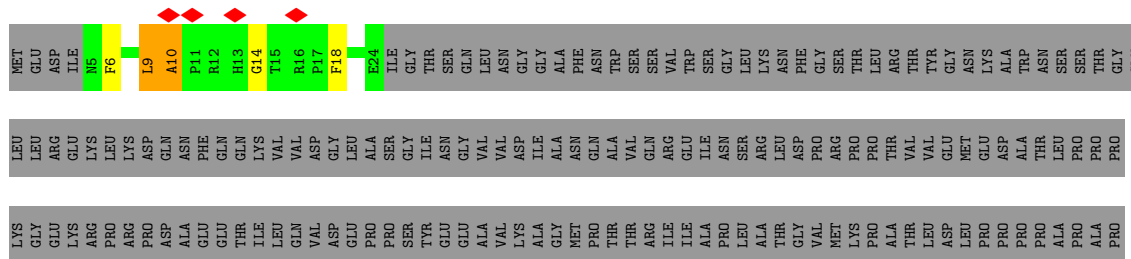
- Molecule 1: Pre-protein VI



- Molecule 1: Pre-protein VI

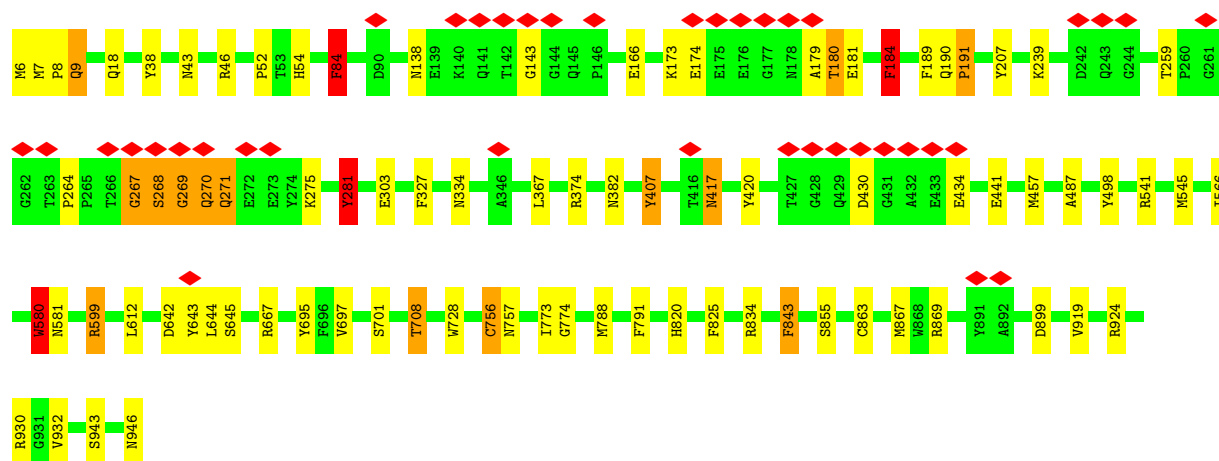


- Molecule 1: Pre-protein VI



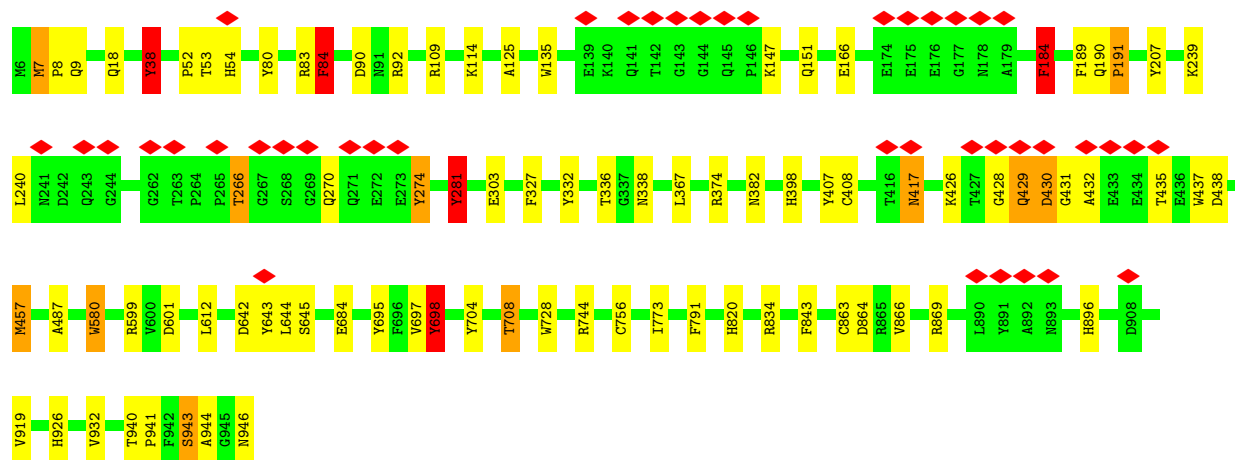






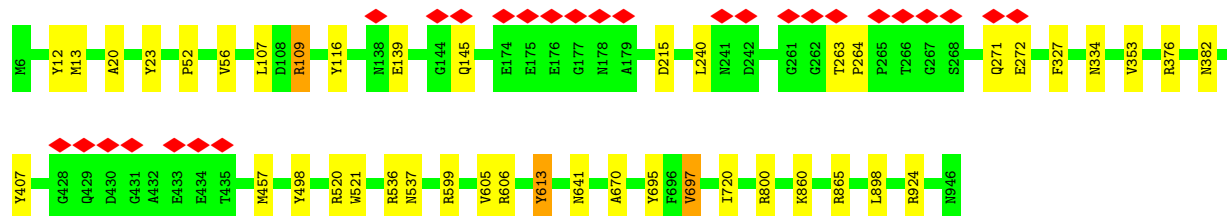
• Molecule 2: Hexon protein

Chain C: 91% 8% ..



• Molecule 2: Hexon protein

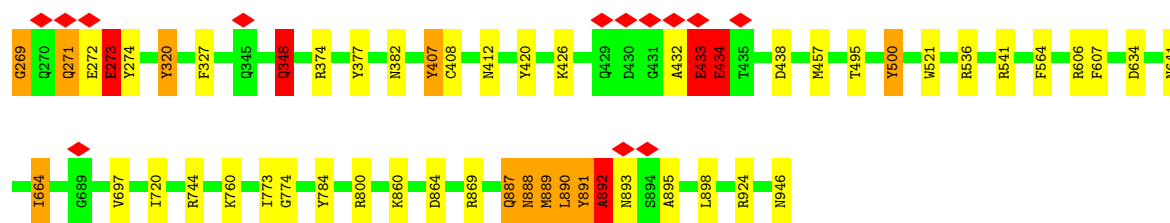
Chain D: 95% 5% .



• Molecule 2: Hexon protein

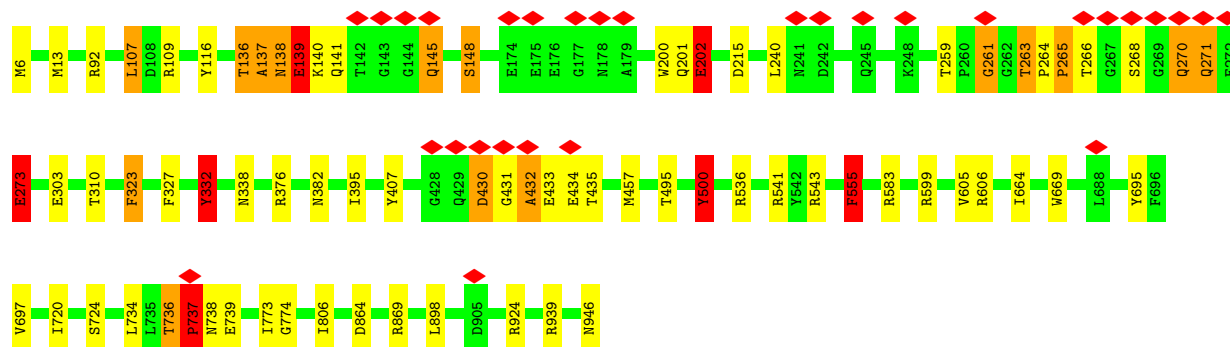
Chain E: 91% 6% ..





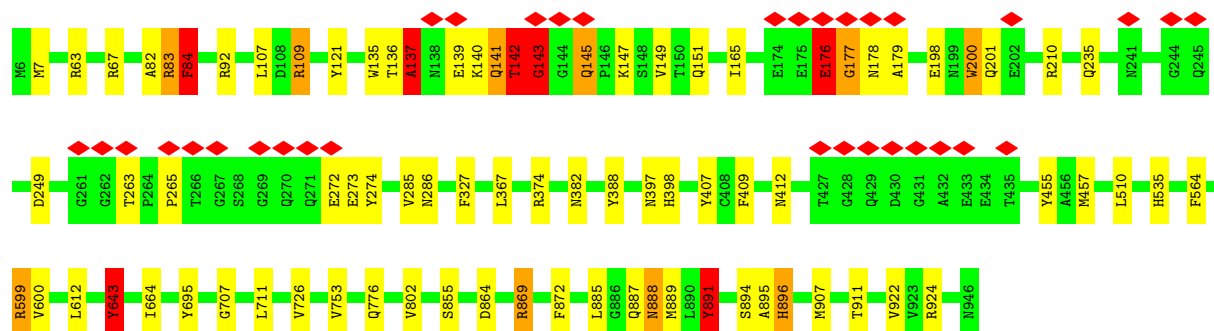
- Molecule 2: Hexon protein

Chain F: 92% 6% ..



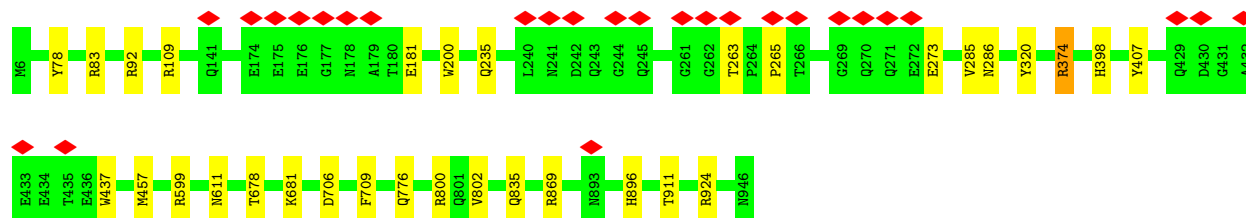
- Molecule 2: Hexon protein

Chain G: 91% 7% ..

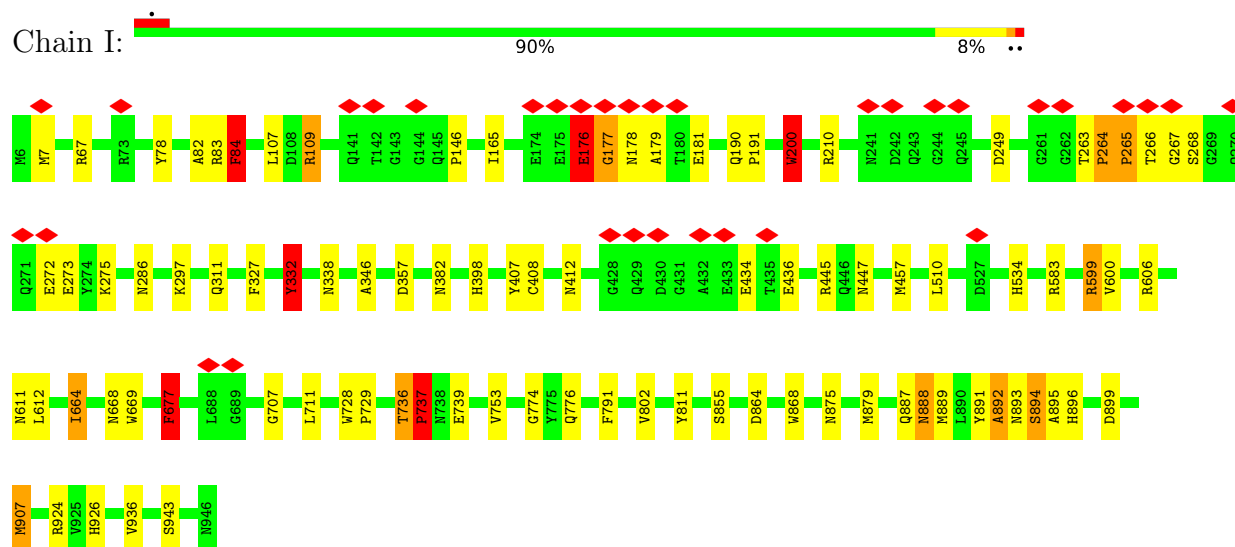


- Molecule 2: Hexon protein

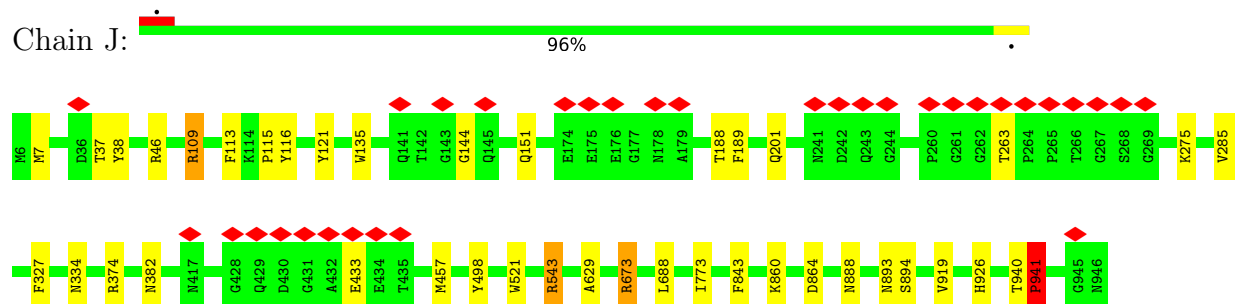
Chain H: 97%



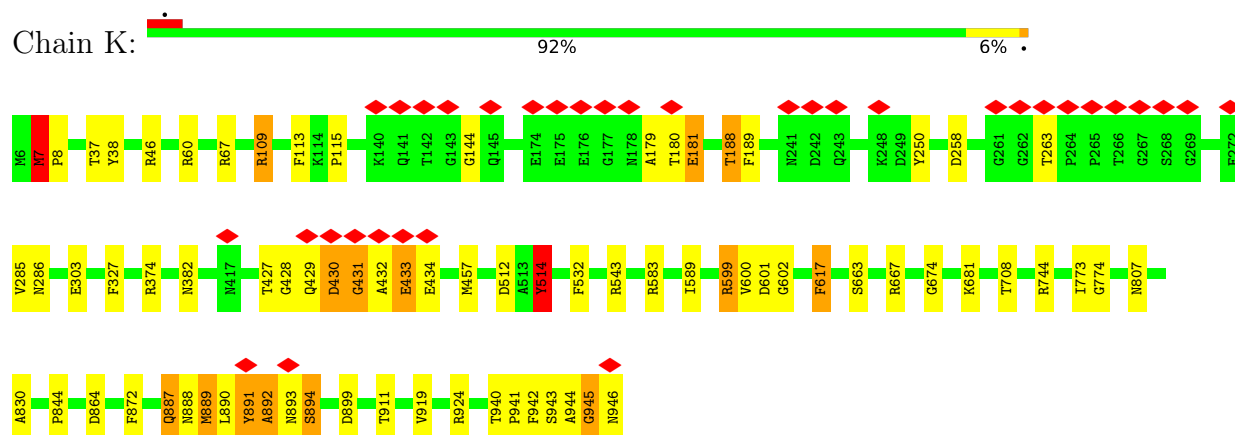
- Molecule 2: Hexon protein



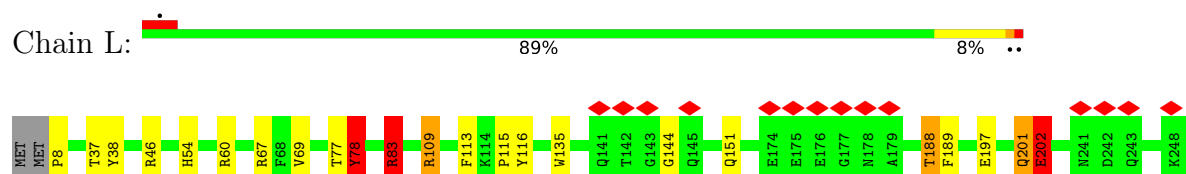
- Molecule 2: Hexon protein

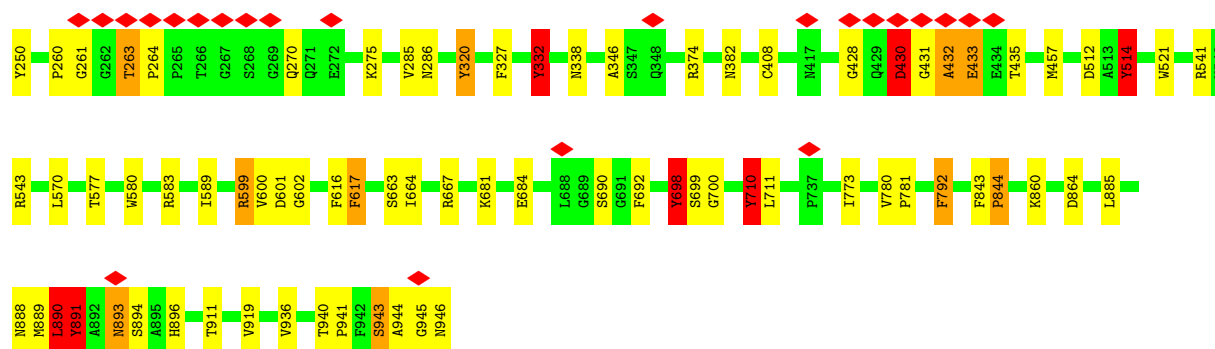


- Molecule 2: Hexon protein

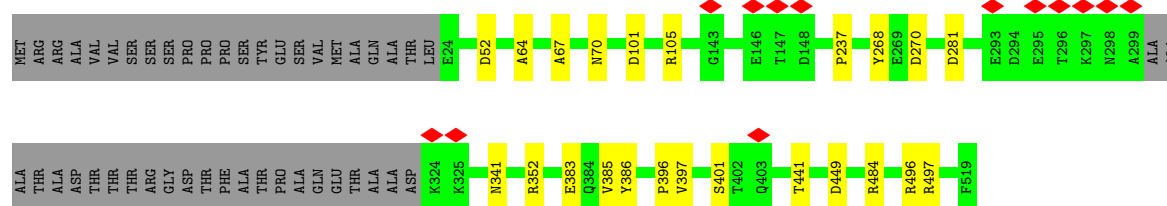


- Molecule 2: Hexon protein

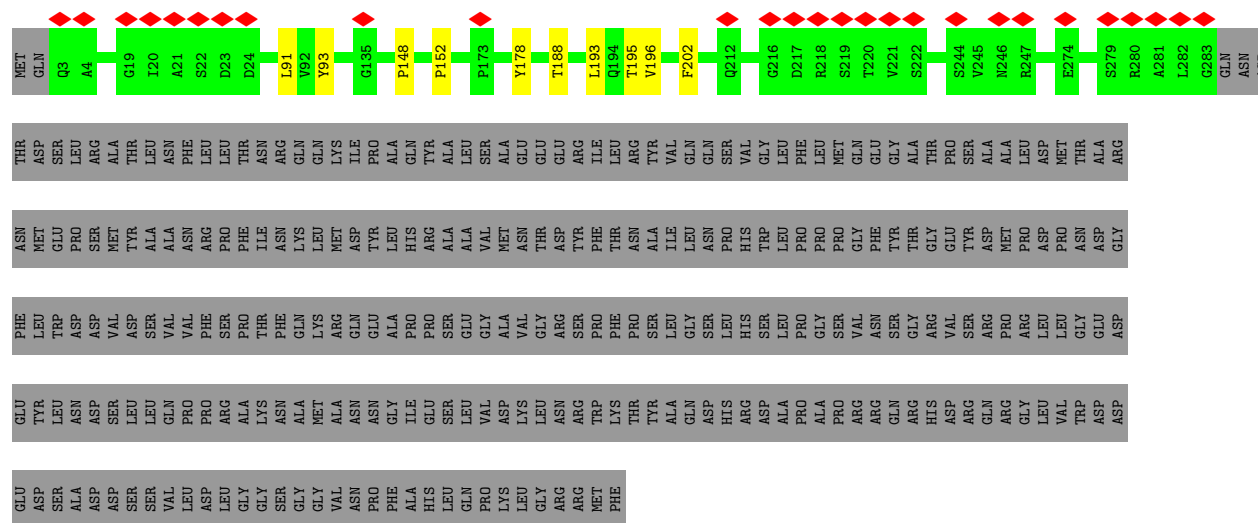




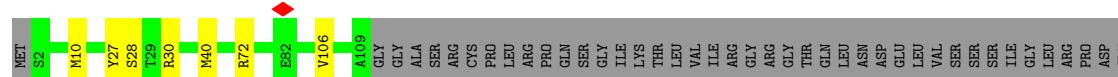
- Molecule 3: Penton protein

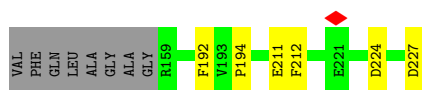


- Molecule 4: Pre-hexon-linking protein IIIa

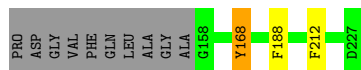
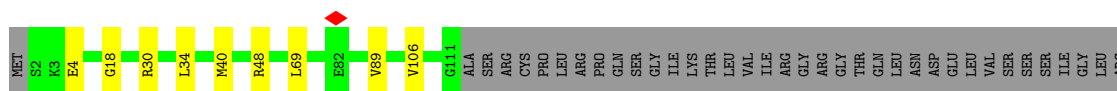


- Molecule 5: Pre-hexon-linking protein VIII

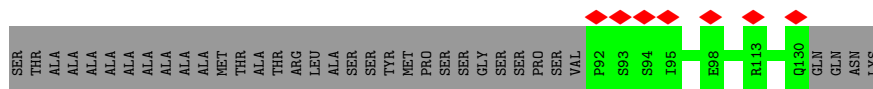
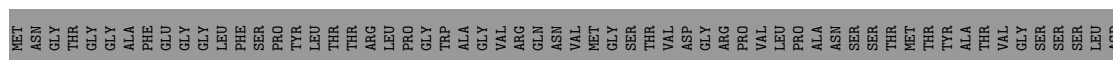




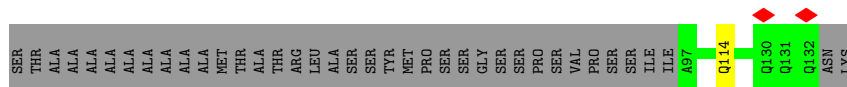
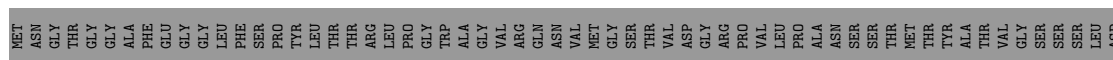
- Molecule 5: Pre-hexon-linking protein VIII



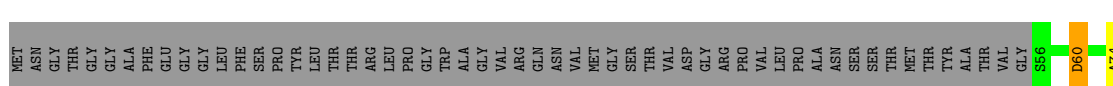
- Molecule 6: Hexon-interlacing protein



- Molecule 6: Hexon-interlacing protein



- Molecule 6: Hexon-interlacing protein



- Molecule 6: Hexon-interlacing protein



MET	ASN	GLY	THR	GLY	GLY	ALA	PHE	GLU	GLY	GLY	LEU	PHE	SER	PRO	TYR	LEU	THR	THR	ARG	LEU	PRO	GLY	TRP	ALA	GLY	VAL	ARG	GLN	ASN	VAL	MET	GLY	SER	SER	THR	THR	ASP	GLY	ARG	PRO	VAL	LEU	PRO	ALA	ASN	SER	SER	THR	MET	THR	TYR	ALA	THR	VAL	GLY	SER	SER	SER	LEU	ASP
SER	THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	MET	THR	ALA	THR	ARG	LEU	ALA	SER	SER	TYR	PRO	MET	PRO	SER	SER	GLY	SER	SER	PRO	SER	VAL	PRO	SER	SER	ILE	ILE	ALA	GLU	GLU	LYS	LEU	LEU	A103	L104	L105	A106	E107	R113	Q114	L115	Q121	L125	R126	Q132	N133	K134				

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0216	Depositor
Map size (Å)	1193.76, 1193.76, 1193.76	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.658, 1.658, 1.658	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	1	1.07	0/183	1.86	2/248 (0.8%)
1	2	1.21	0/114	1.66	0/153
1	3	1.08	0/174	2.10	6/236 (2.5%)
1	4	0.97	0/95	2.10	3/128 (2.3%)
1	5	0.90	0/208	1.64	1/281 (0.4%)
1	6	1.15	0/167	1.70	1/226 (0.4%)
1	7	1.04	0/217	1.71	3/294 (1.0%)
1	8	1.04	0/144	1.65	2/193 (1.0%)
2	A	0.73	0/7696	1.31	20/10469 (0.2%)
2	B	0.85	12/7696 (0.2%)	1.51	72/10469 (0.7%)
2	C	0.75	0/7696	1.48	76/10469 (0.7%)
2	D	0.72	0/7696	1.29	12/10469 (0.1%)
2	E	0.78	2/7696 (0.0%)	1.55	89/10469 (0.9%)
2	F	0.75	0/7696	1.46	58/10469 (0.6%)
2	G	0.74	0/7696	1.51	74/10469 (0.7%)
2	H	0.72	0/7696	1.30	15/10469 (0.1%)
2	I	0.74	0/7696	1.49	69/10469 (0.7%)
2	J	0.73	0/7696	1.32	21/10469 (0.2%)
2	K	0.75	0/7696	1.49	62/10469 (0.6%)
2	L	0.75	0/7680	1.49	72/10448 (0.7%)
3	M	0.74	0/3887	1.35	9/5290 (0.2%)
4	N	0.75	0/2212	1.38	1/3011 (0.0%)
5	O	0.77	0/1414	1.37	4/1929 (0.2%)
5	P	0.77	0/1426	1.40	4/1944 (0.2%)
6	Q	0.64	0/302	1.29	0/406
6	R	0.60	0/284	1.27	0/381
6	S	0.91	0/505	1.63	5/683 (0.7%)
6	T	0.67	0/254	1.34	0/339
All	All	0.76	14/103922 (0.0%)	1.44	681/141349 (0.5%)

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	3	0	1
2	A	0	4
2	B	0	13
2	C	0	14
2	D	0	9
2	E	0	14
2	F	0	17
2	G	0	16
2	H	0	8
2	I	0	8
2	J	0	9
2	K	0	11
2	L	0	17
3	M	0	4
4	N	0	1
5	O	0	3
All	All	0	149

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	180	THR	CA-CB	-17.48	1.23	1.53
2	B	180	THR	CB-OG1	-16.99	1.16	1.43
2	E	200	TRP	NE1-CE2	-13.87	1.22	1.37
2	B	180	THR	C-O	-11.58	1.09	1.23
2	B	181	GLU	CD-OE2	-9.87	1.06	1.25

The worst 5 of 681 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	179	ALA	N-CA-C	22.79	137.12	112.97
2	G	177	GLY	CA-C-N	12.95	139.25	122.16
2	G	177	GLY	C-N-CA	12.95	139.25	122.16
2	K	431	GLY	CA-C-N	12.90	144.53	123.37
2	K	431	GLY	C-N-CA	12.90	144.53	123.37

There are no chirality outliers.

5 of 149 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	19	MET	Peptide
2	A	140	LYS	Peptide

*Continued on next page...*

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Mol	Chain	Res	Type	Group
2	A	407	TYR	Sidechain
2	A	433	GLU	Peptide
2	A	80	TYR	Sidechain

## 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	1	177	163	162	2	0
1	2	113	103	102	0	0
1	3	168	157	156	2	0
1	4	91	81	80	2	0
1	5	202	191	191	3	0
1	6	161	148	147	1	0
1	7	211	204	203	1	0
1	8	140	131	129	1	0
2	A	7491	7148	7145	11	0
2	B	7491	7148	7145	22	0
2	C	7491	7149	7146	21	0
2	D	7491	7149	7146	12	0
2	E	7491	7148	7145	33	0
2	F	7491	7148	7145	37	0
2	G	7491	7149	7146	26	0
2	H	7491	7148	7145	4	0
2	I	7491	7148	7145	39	0
2	J	7491	7148	7145	12	0
2	K	7491	7148	7145	26	0
2	L	7475	7129	7129	50	0
3	M	3794	3715	3712	2	0
4	N	2176	2170	2169	2	0
5	O	1377	1329	1327	4	0
5	P	1389	1338	1336	4	0
6	Q	302	317	317	0	0
6	R	285	294	293	0	0
6	S	504	513	511	3	0
6	T	255	261	260	0	0
All	All	101221	96875	96822	281	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 281 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)
2:F:734:LEU:HB2	2:F:737:PRO:CG	2.12	0.79
2:F:495:THR:HA	2:F:500:TYR:CD2	2.20	0.77
2:B:191:PRO:HG3	2:B:281:TYR:CD2	2.22	0.73
2:F:495:THR:HG22	2:F:500:TYR:CE2	2.26	0.71
2:I:736:THR:H	2:I:737:PRO:CD	2.06	0.69

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	1	20/234 (8%)	16 (80%)	4 (20%)	0	100	100
1	2	14/234 (6%)	9 (64%)	4 (29%)	1 (7%)	1	7
1	3	19/234 (8%)	9 (47%)	7 (37%)	3 (16%)	0	1
1	4	9/234 (4%)	4 (44%)	4 (44%)	1 (11%)	0	2
1	5	23/234 (10%)	14 (61%)	5 (22%)	4 (17%)	0	1
1	6	18/234 (8%)	10 (56%)	5 (28%)	3 (17%)	0	1
1	7	25/234 (11%)	17 (68%)	5 (20%)	3 (12%)	0	1
1	8	13/234 (6%)	8 (62%)	5 (38%)	0	100	100
2	A	939/941 (100%)	883 (94%)	53 (6%)	3 (0%)	37	66
2	B	939/941 (100%)	881 (94%)	49 (5%)	9 (1%)	13	42
2	C	939/941 (100%)	886 (94%)	45 (5%)	8 (1%)	14	44
2	D	939/941 (100%)	877 (93%)	59 (6%)	3 (0%)	37	66

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	939/941 (100%)	866 (92%)	59 (6%)	14 (2%)	8	33
2	F	939/941 (100%)	875 (93%)	53 (6%)	11 (1%)	11	38
2	G	939/941 (100%)	881 (94%)	49 (5%)	9 (1%)	13	42
2	H	939/941 (100%)	888 (95%)	50 (5%)	1 (0%)	48	76
2	I	939/941 (100%)	879 (94%)	50 (5%)	10 (1%)	12	40
2	J	939/941 (100%)	880 (94%)	54 (6%)	5 (0%)	25	56
2	K	939/941 (100%)	879 (94%)	50 (5%)	10 (1%)	12	40
2	L	937/941 (100%)	881 (94%)	48 (5%)	8 (1%)	14	44
3	M	468/519 (90%)	438 (94%)	30 (6%)	0	100	100
4	N	279/559 (50%)	254 (91%)	23 (8%)	2 (1%)	19	50
5	O	173/227 (76%)	163 (94%)	10 (6%)	0	100	100
5	P	176/227 (78%)	162 (92%)	14 (8%)	0	100	100
6	Q	37/134 (28%)	37 (100%)	0	0	100	100
6	R	34/134 (25%)	33 (97%)	1 (3%)	0	100	100
6	S	67/134 (50%)	53 (79%)	10 (15%)	4 (6%)	1	9
6	T	30/134 (22%)	30 (100%)	0	0	100	100
All	All	12671/15232 (83%)	11813 (93%)	746 (6%)	112 (1%)	17	44

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	16	ARG
1	5	6	PHE
1	6	10	ALA
2	B	268	SER
2	B	269	GLY

### 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	1	18/195 (9%)	14 (78%)	4 (22%)	1	3
1	2	11/195 (6%)	10 (91%)	1 (9%)	7	27
1	3	17/195 (9%)	15 (88%)	2 (12%)	4	17
1	4	9/195 (5%)	7 (78%)	2 (22%)	1	3
1	5	21/195 (11%)	17 (81%)	4 (19%)	1	5
1	6	16/195 (8%)	15 (94%)	1 (6%)	15	41
1	7	22/195 (11%)	18 (82%)	4 (18%)	1	6
1	8	14/195 (7%)	14 (100%)	0	100	100
2	A	813/813 (100%)	805 (99%)	8 (1%)	73	84
2	B	813/813 (100%)	804 (99%)	9 (1%)	70	82
2	C	813/813 (100%)	801 (98%)	12 (2%)	60	77
2	D	813/813 (100%)	805 (99%)	8 (1%)	73	84
2	E	813/813 (100%)	802 (99%)	11 (1%)	62	78
2	F	813/813 (100%)	804 (99%)	9 (1%)	70	82
2	G	813/813 (100%)	807 (99%)	6 (1%)	81	88
2	H	813/813 (100%)	807 (99%)	6 (1%)	81	88
2	I	813/813 (100%)	807 (99%)	6 (1%)	81	88
2	J	813/813 (100%)	809 (100%)	4 (0%)	86	91
2	K	813/813 (100%)	809 (100%)	4 (0%)	86	91
2	L	811/813 (100%)	798 (98%)	13 (2%)	58	76
3	M	426/461 (92%)	420 (99%)	6 (1%)	62	78
4	N	236/473 (50%)	233 (99%)	3 (1%)	65	79
5	O	152/190 (80%)	150 (99%)	2 (1%)	65	79
5	P	152/190 (80%)	147 (97%)	5 (3%)	33	60
6	Q	33/102 (32%)	33 (100%)	0	100	100
6	R	30/102 (29%)	29 (97%)	1 (3%)	33	60
6	S	54/102 (53%)	51 (94%)	3 (6%)	17	45
6	T	27/102 (26%)	25 (93%)	2 (7%)	11	34
All	All	10992/13038 (84%)	10856 (99%)	136 (1%)	66	80

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	341	ASN
3	M	441	THR
6	R	114	GLN
2	D	139	GLU
2	D	13	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	464	ASN
2	L	134	GLN
2	I	893	ASN
2	J	558	GLN
2	L	365	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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.

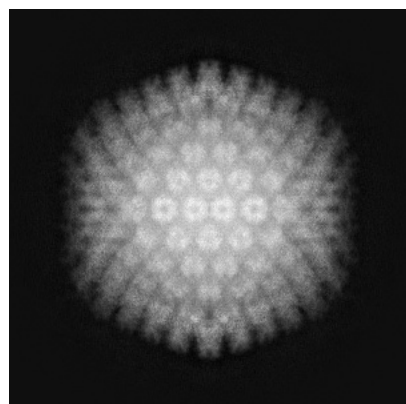
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53736. These allow visual inspection of the internal detail of the map and identification of artifacts.

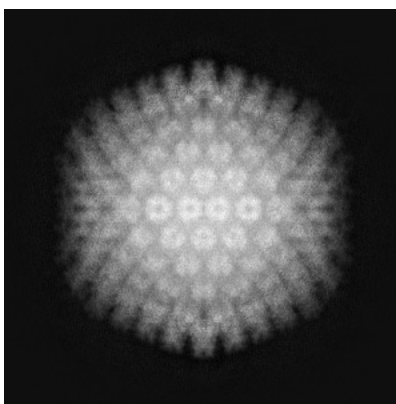
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

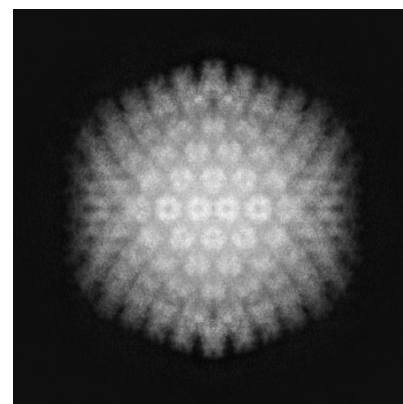
#### 6.1.1 Primary map



X

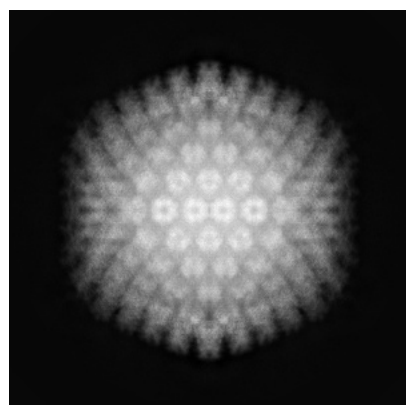


Y

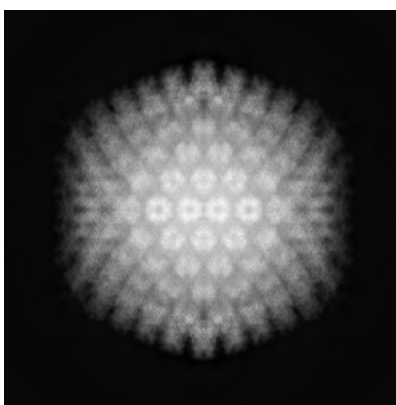


Z

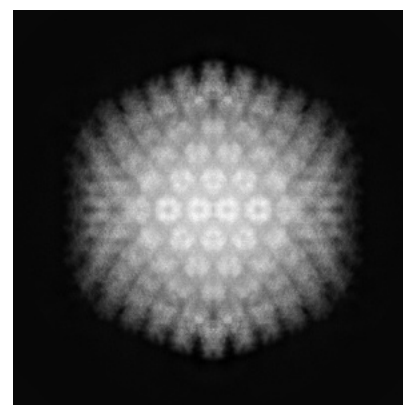
#### 6.1.2 Raw map



X



Y



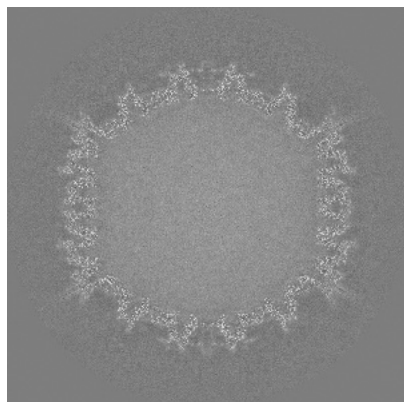
Z

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

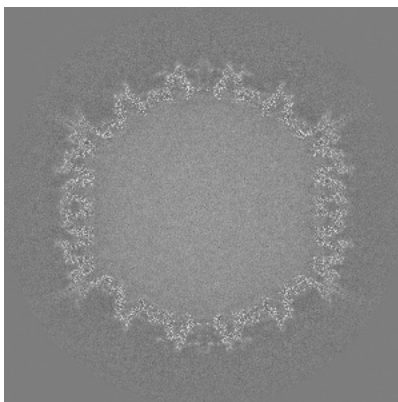


## 6.2 Central slices [i](#)

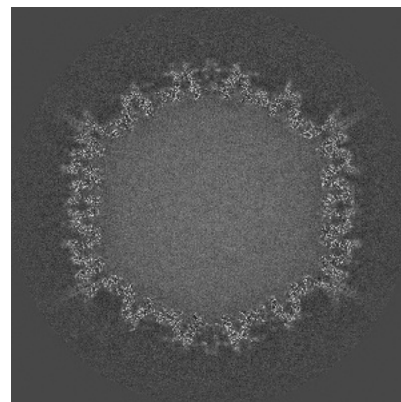
### 6.2.1 Primary map



X Index: 360

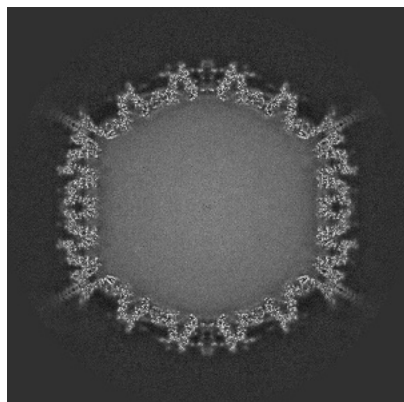


Y Index: 360

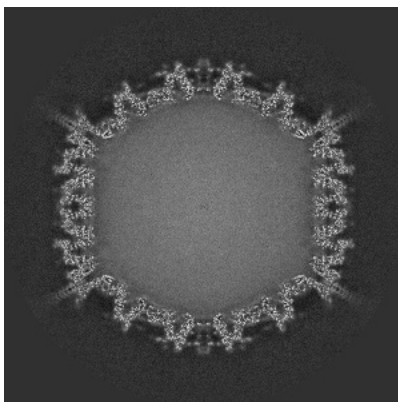


Z Index: 360

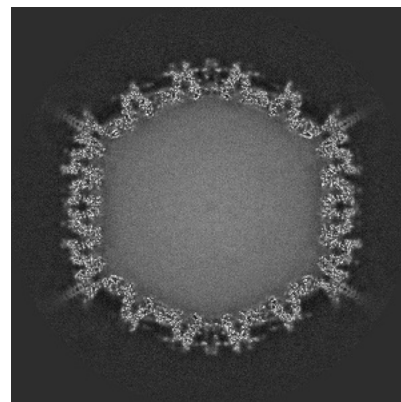
### 6.2.2 Raw map



X Index: 360



Y Index: 360



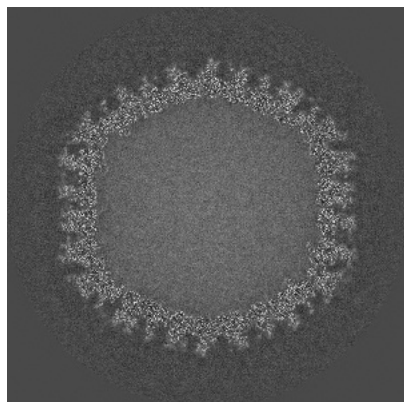
Z Index: 360

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

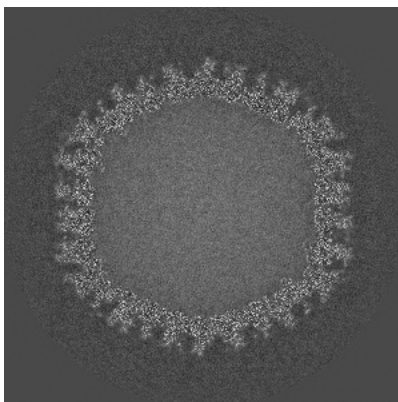


## 6.3 Largest variance slices [i](#)

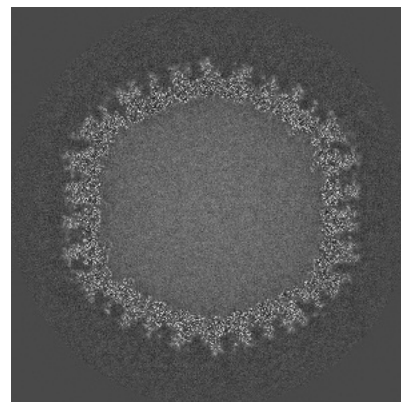
### 6.3.1 Primary map



X Index: 348

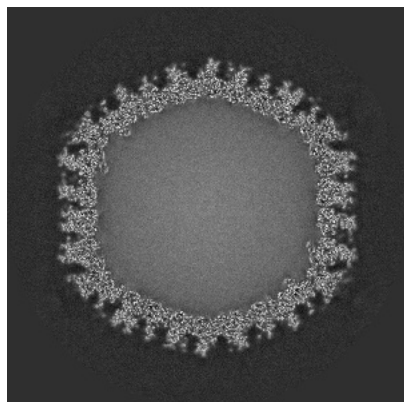


Y Index: 348

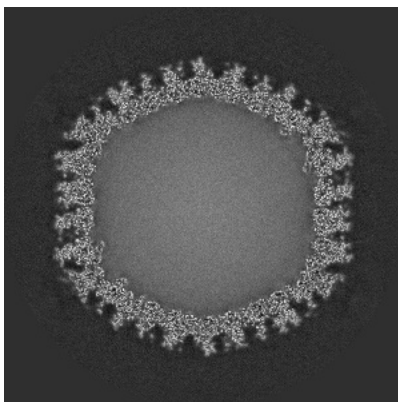


Z Index: 371

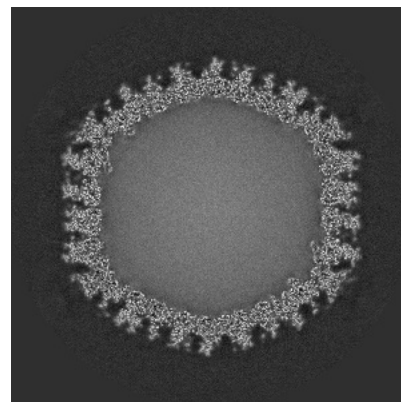
### 6.3.2 Raw map



X Index: 348



Y Index: 372

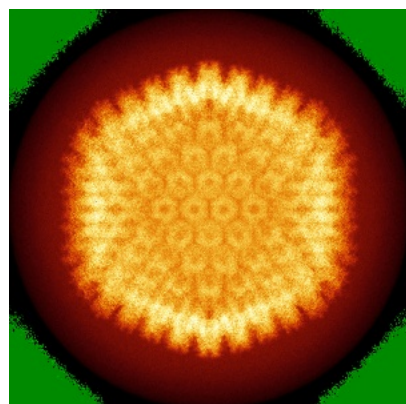


Z Index: 347

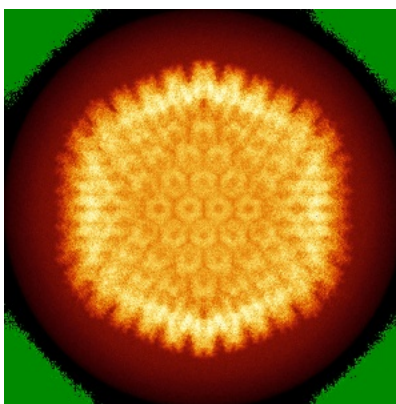
The images above show the largest variance slices of the map in three orthogonal directions.

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

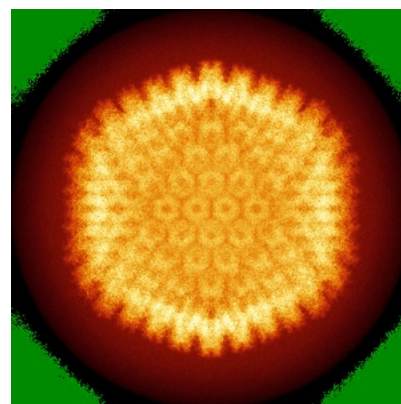
### 6.4.1 Primary map



X

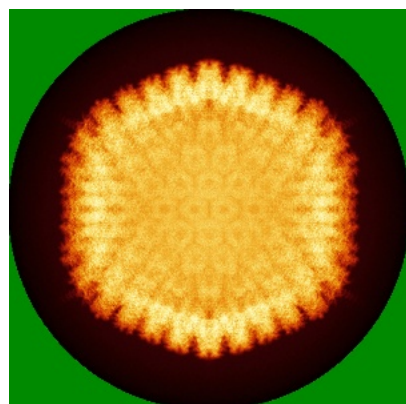


Y

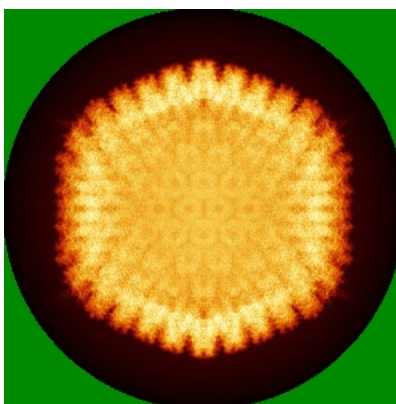


Z

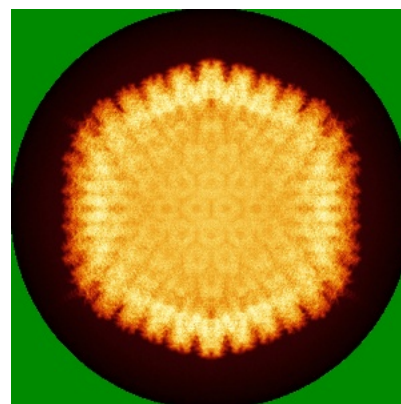
### 6.4.2 Raw map



X



Y

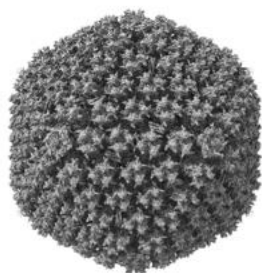


Z

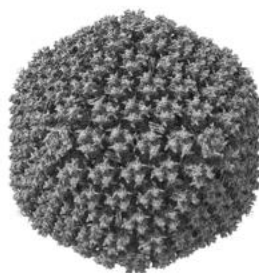
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

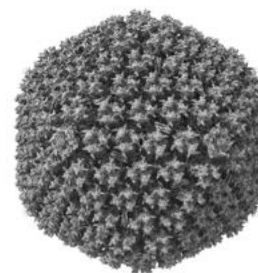
### 6.5.1 Primary map



X



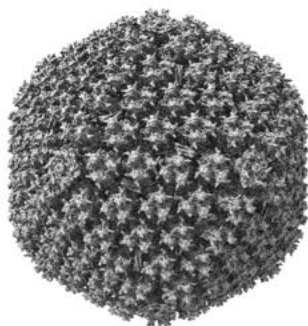
Y



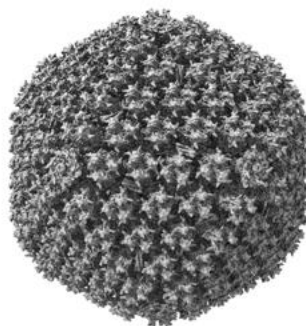
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

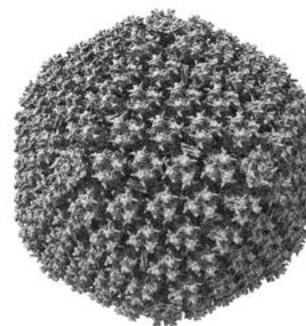
### 6.5.2 Raw map



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.

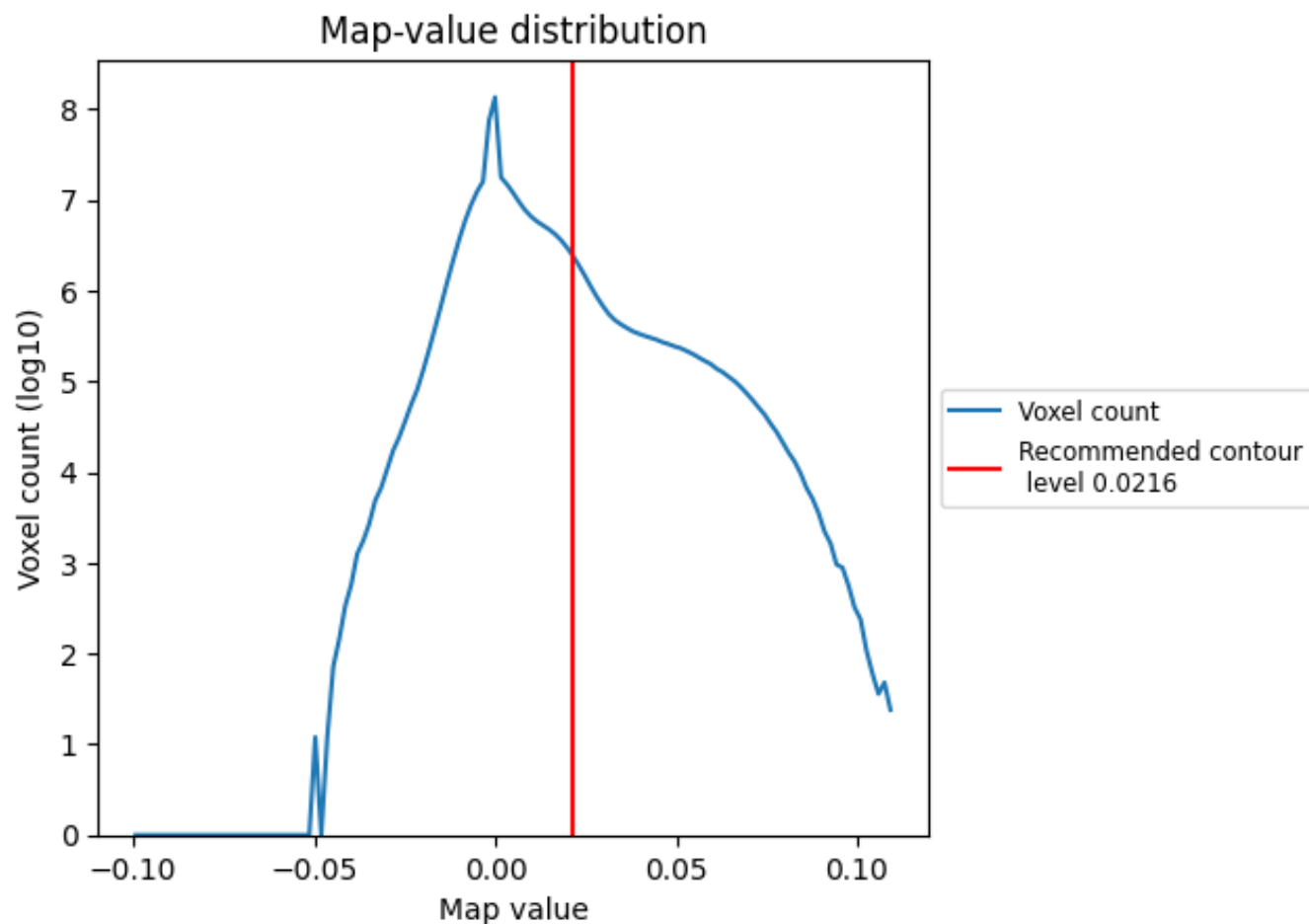
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

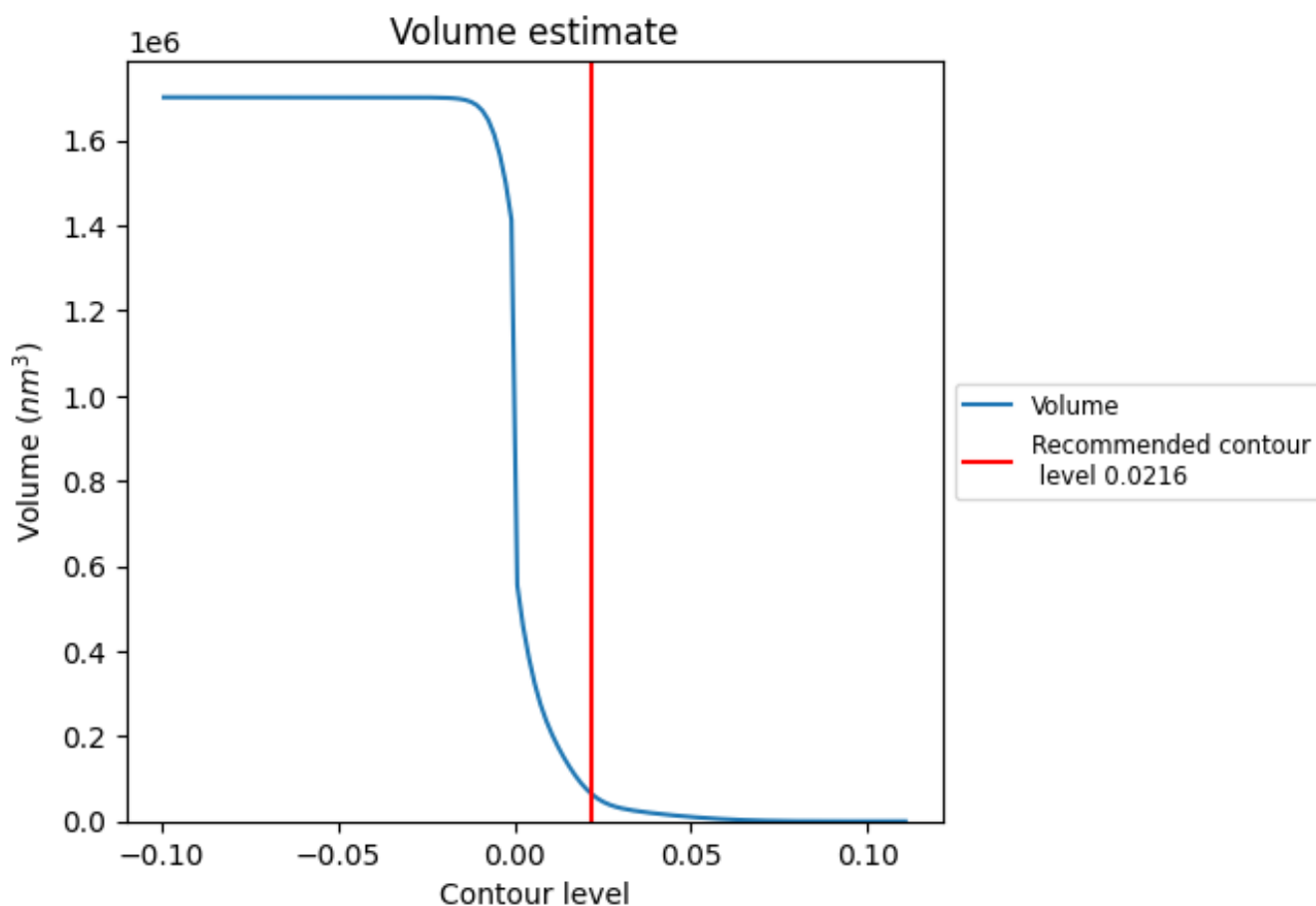
This section contains the results of statistical analysis of the map.

### 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.

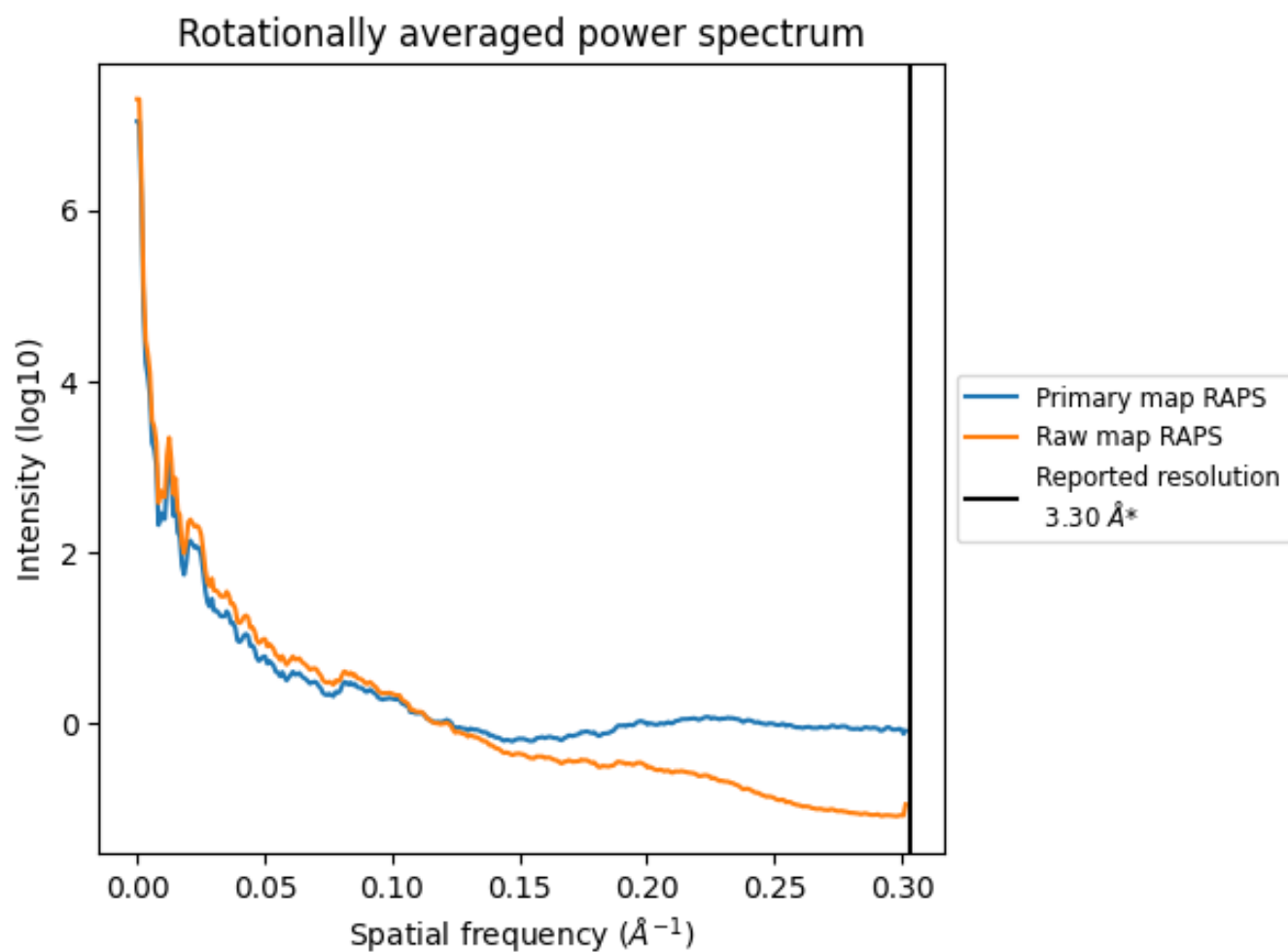
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66526 nm<sup>3</sup>; this corresponds to an approximate mass of 60095 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 ⓘ



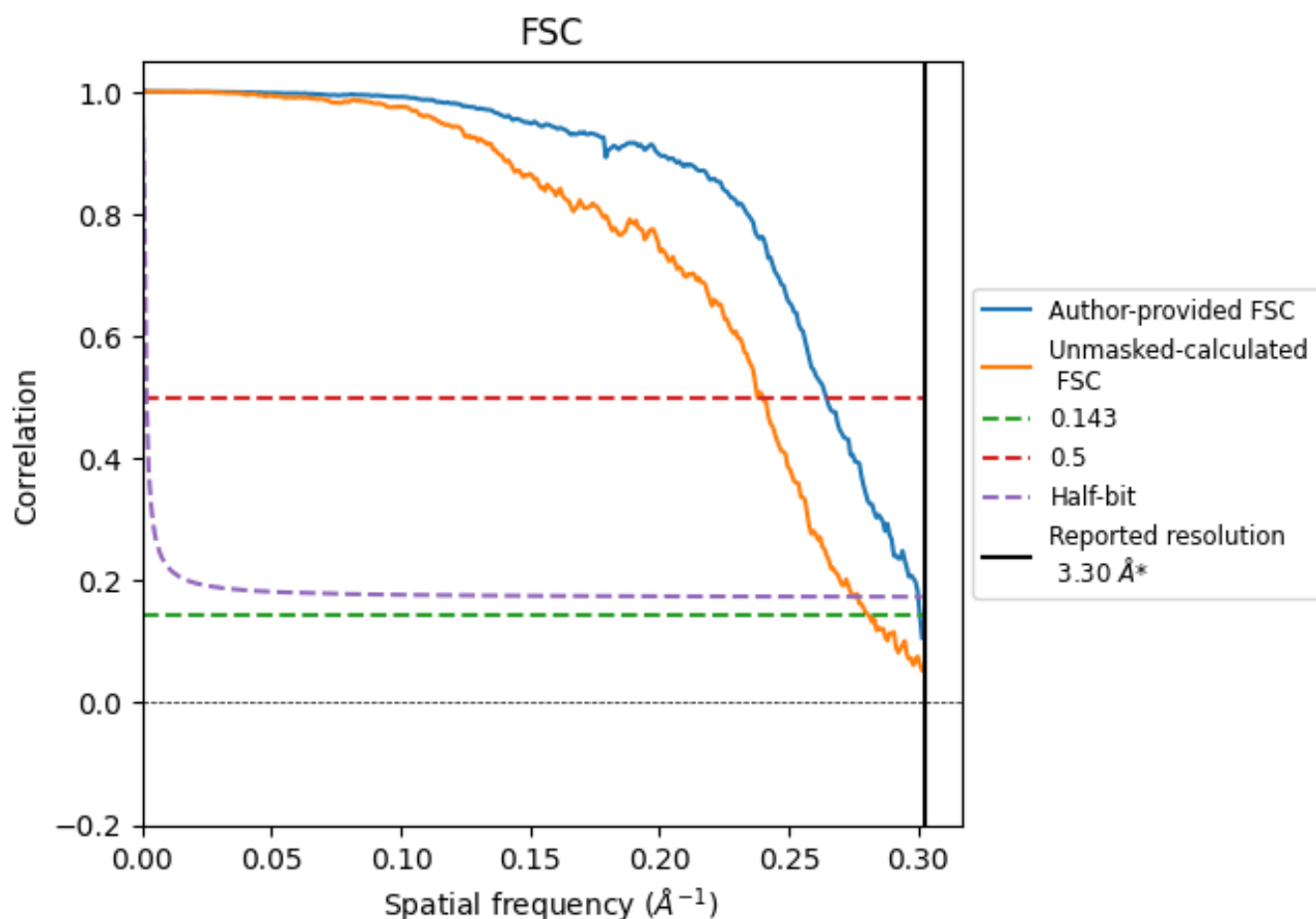
\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>



## 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 0.303  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.78	3.33
Unmasked-calculated*	3.56	4.20	3.63

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

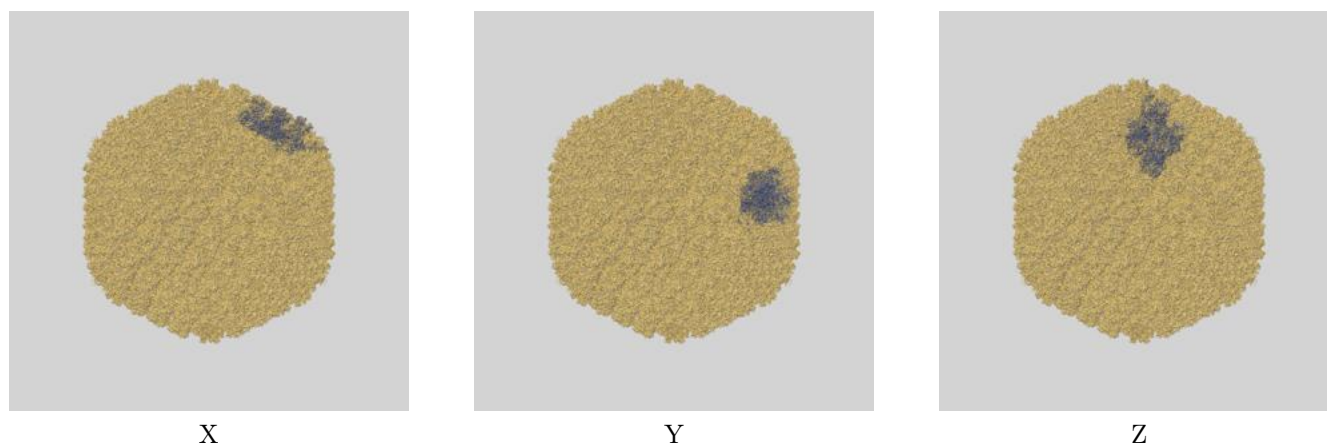


## 9 Map-model fit [i](#)

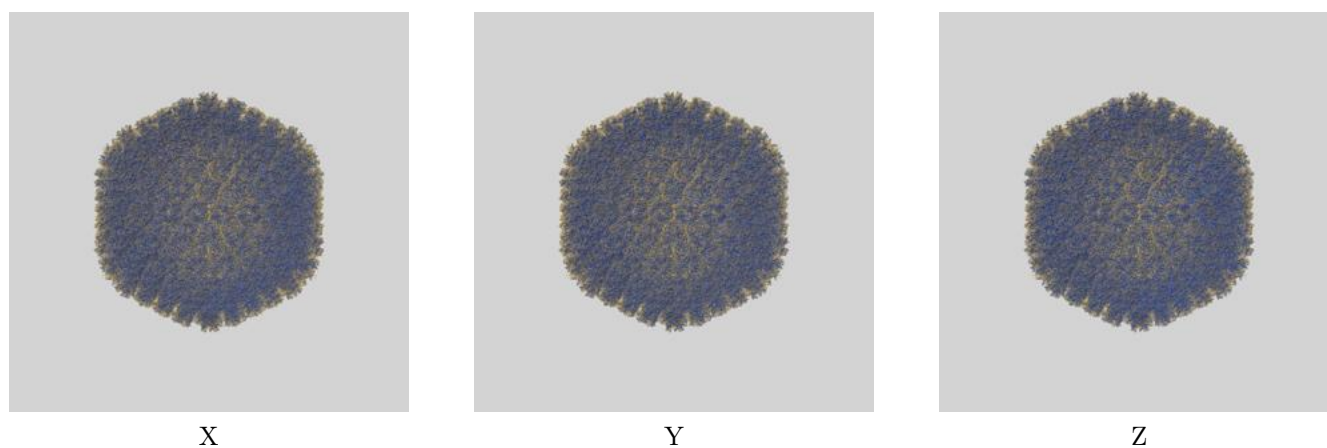
This section contains information regarding the fit between EMDB map EMD-53736 and PDB model 9R78. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

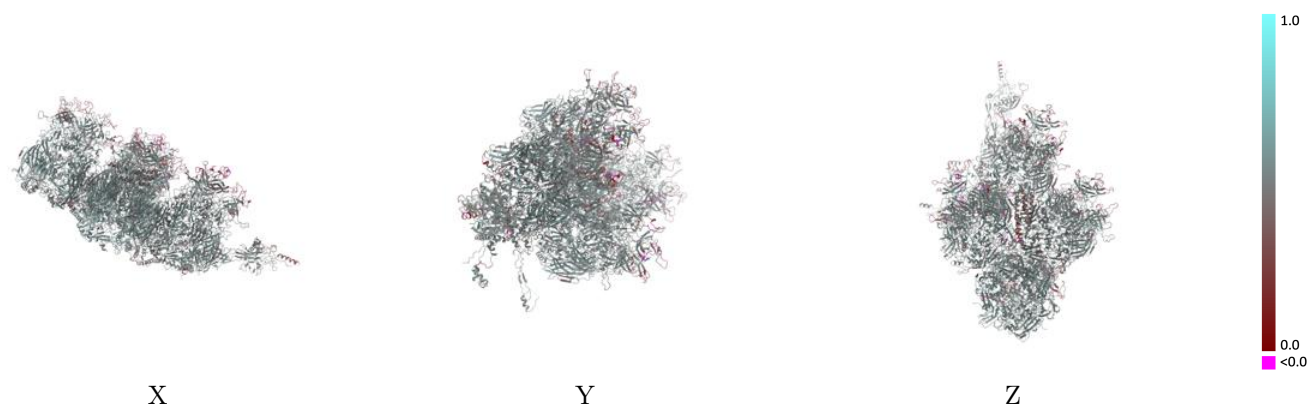


#### 9.1.2 Map-model assembly overlay [i](#)



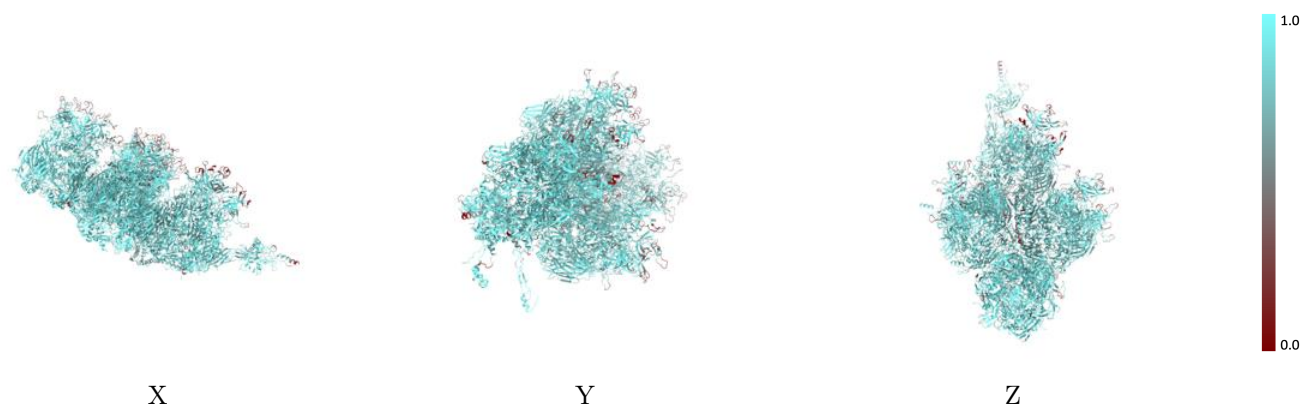
The images above show the 3D surface view of the map at the recommended contour level 0.0216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



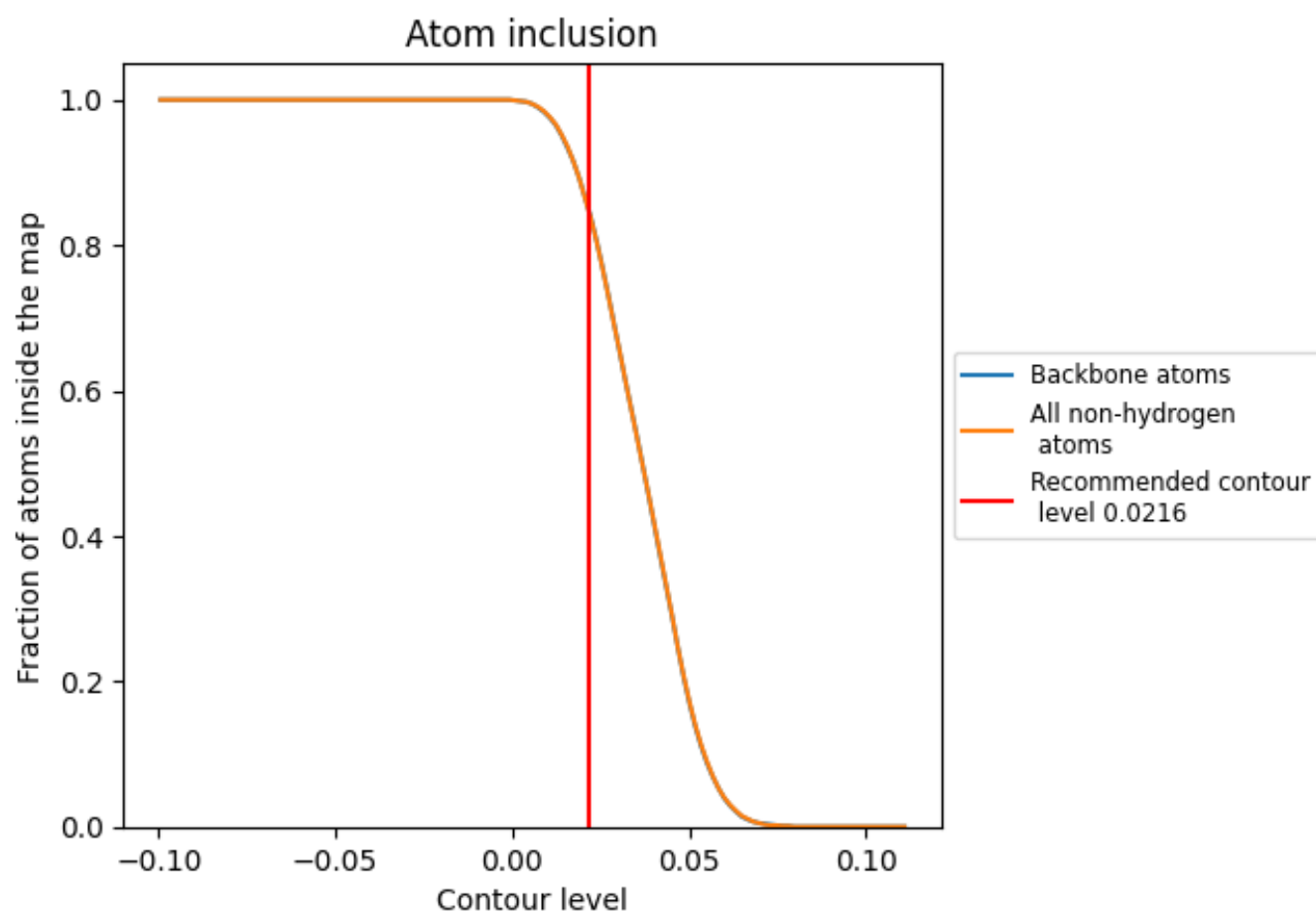
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0216).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.0216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.5020
1	 0.8200	 0.4290
2	 0.5540	 0.4150
3	 0.7120	 0.3890
4	 0.6820	 0.3790
5	 0.5890	 0.3710
6	 0.5770	 0.3260
7	 0.5970	 0.3490
8	 0.6220	 0.3830
A	 0.8600	 0.5100
B	 0.8450	 0.4910
C	 0.8450	 0.4920
D	 0.8810	 0.5240
E	 0.8630	 0.5010
F	 0.8680	 0.5070
G	 0.8690	 0.5070
H	 0.8820	 0.5290
I	 0.8610	 0.5050
J	 0.8700	 0.5180
K	 0.8610	 0.4990
L	 0.8600	 0.4990
M	 0.8080	 0.4860
N	 0.7300	 0.4460
O	 0.8910	 0.5260
P	 0.8900	 0.5220
Q	 0.5870	 0.3250
R	 0.7080	 0.4060
S	 0.7770	 0.4120
T	 0.4940	 0.2850

