Full wwPDB EM Validation Report ⓘ

Mar 11, 2024 – 12:04 AM EDT

PDB ID	:	6OMC
EMDB ID	:	EMD-20125
Title	:	capsid of T5 virion
Authors	:	Huet, A.; Duda, R.L.; Boulanger, P.; Conway, J.F.
Deposited on	:	2019-04-18
Resolution	:	3.80 Å(reported)
Based on initial model	:	2FT1

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

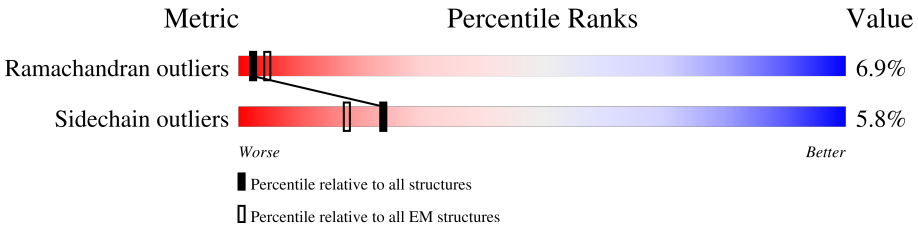
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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	A	299	30% 84% 13% ·
1	B	299	30% 87% 11% ·
1	C	299	29% 84% 13% ·
1	D	299	28% 87% 11% ·
1	E	299	31% 85% 13% ·
1	F	299	28% 84% 12% ·
1	G	299	31% 87% 11% ·
1	H	299	31% 86% 12% ·
1	I	299	29% 84% 14% ·

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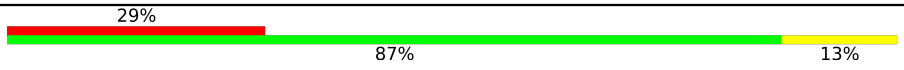
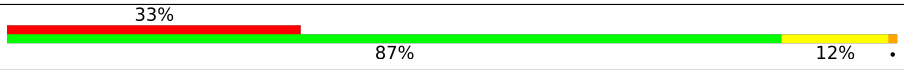
Mol	Chain	Length	Quality of chain
1	J	299	
1	K	299	
1	L	299	
1	M	299	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 60547 atoms, of which 30455 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 Major capsid protein.

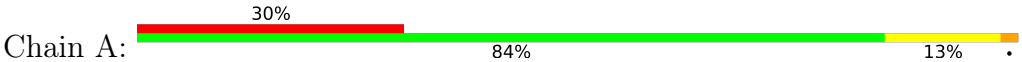
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	B	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	C	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	D	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	E	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	F	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	G	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	H	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	I	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	J	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	K	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	L	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	M	295	Total	C	H	N	O	S	0	0
			4603	1449	2315	385	449	5		

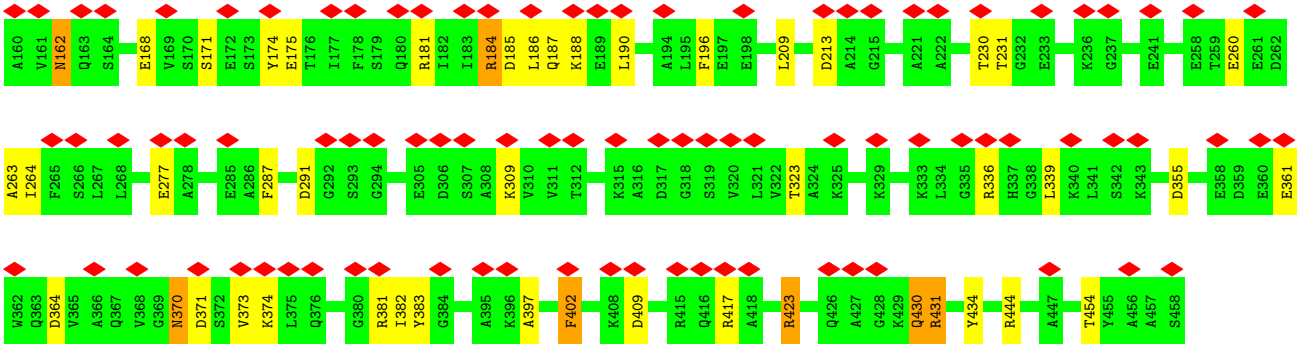
3 Residue-property plots (i)

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: Major capsid protein

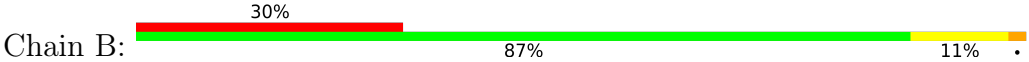
Chain A:

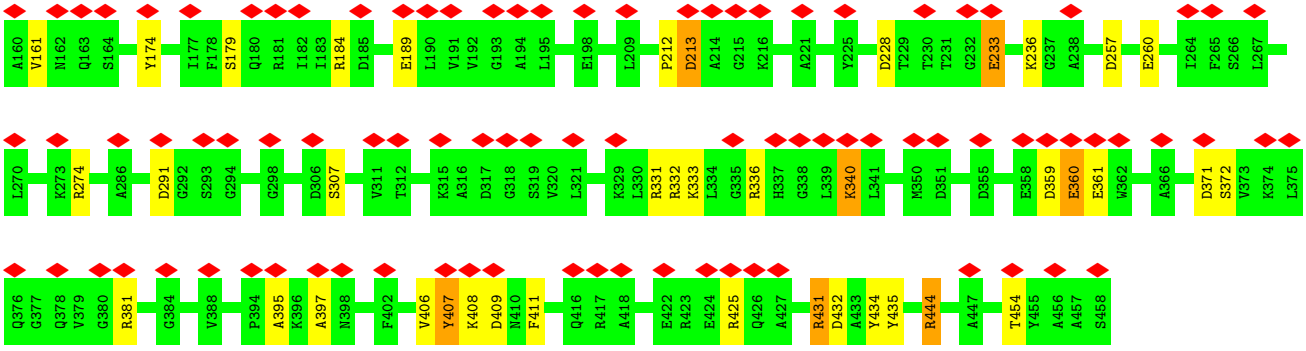




• Molecule 1: Major capsid protein

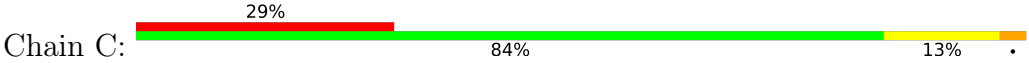
Chain B:

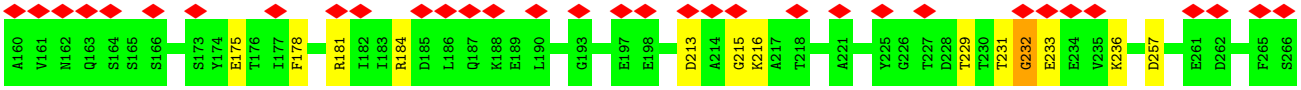


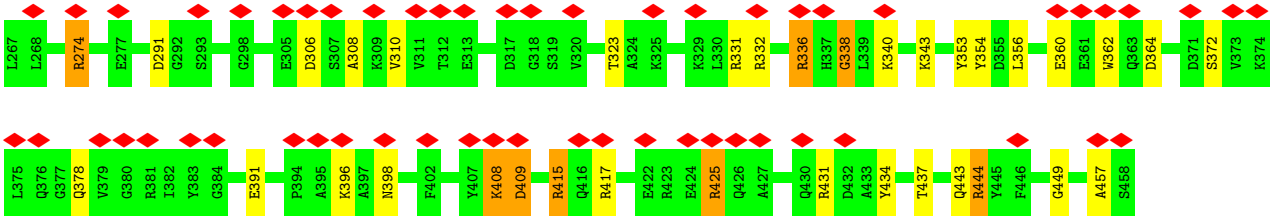


• Molecule 1: Major capsid protein

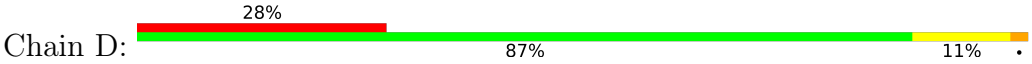
Chain C:

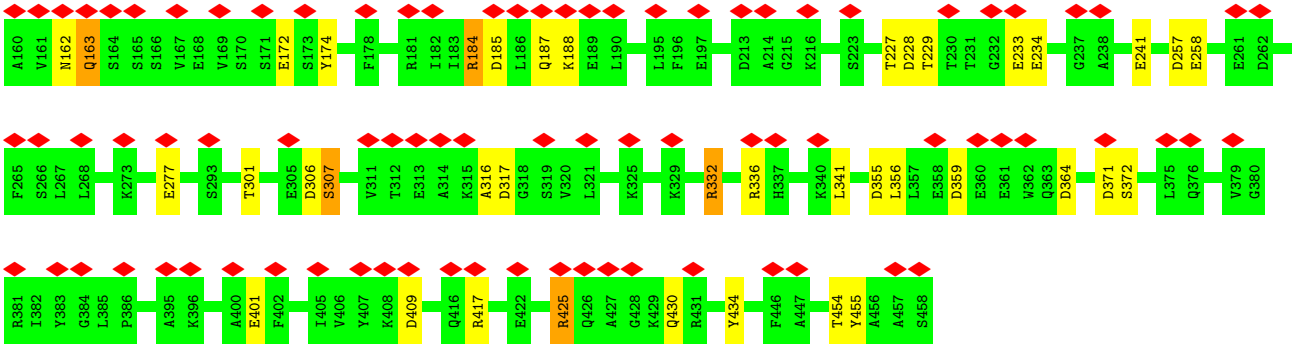




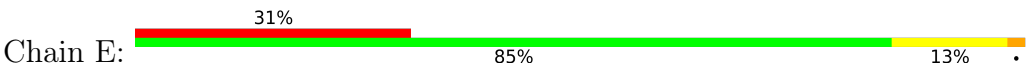


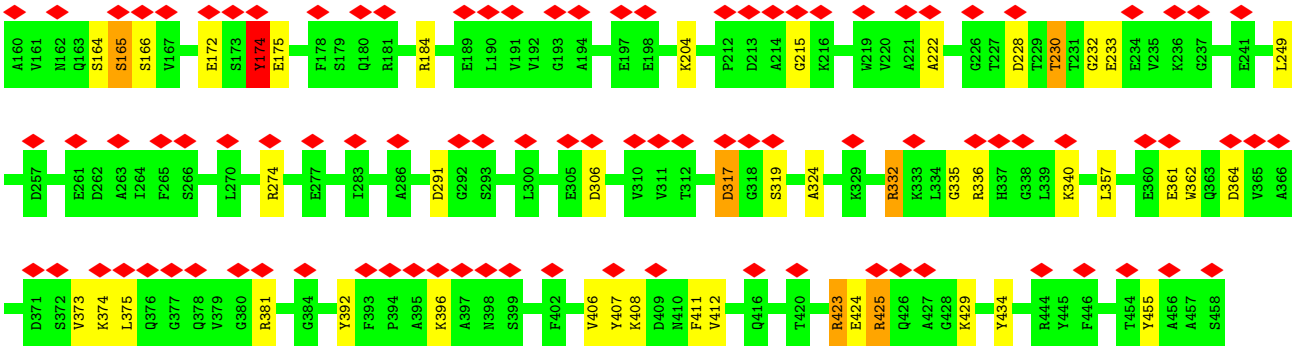
• Molecule 1: Major capsid protein



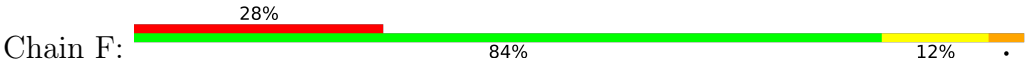


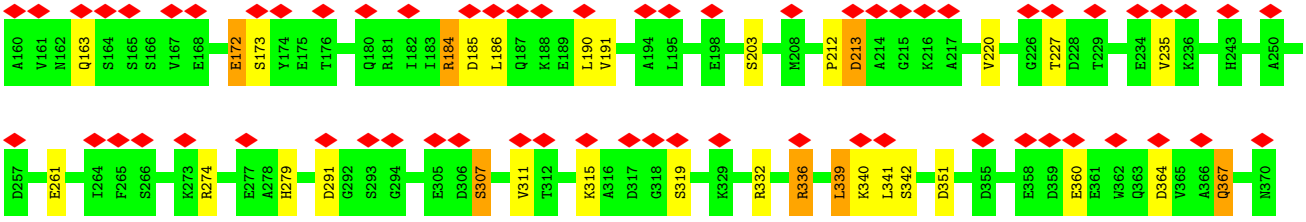
• Molecule 1: Major capsid protein

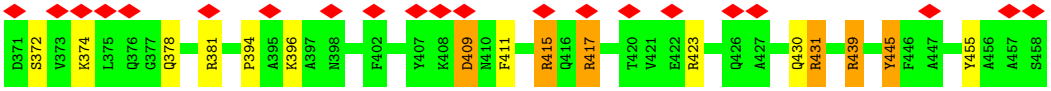




• Molecule 1: Major capsid protein

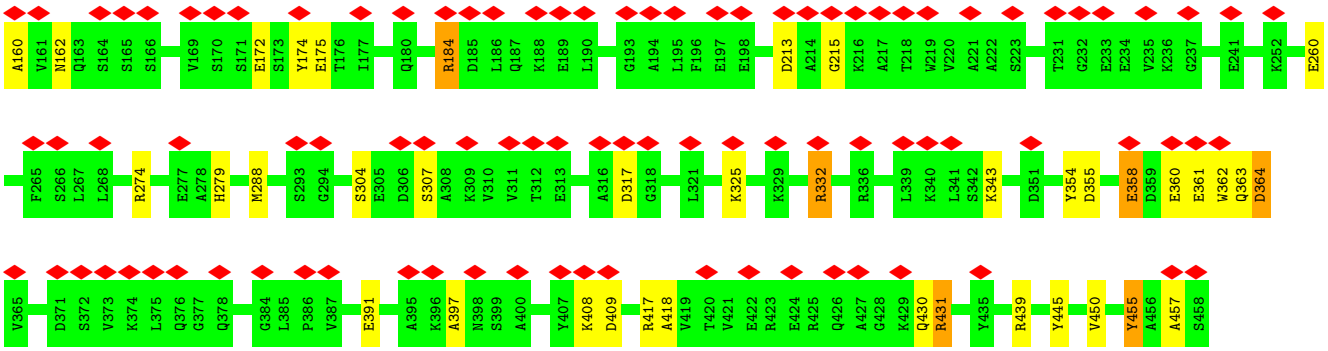






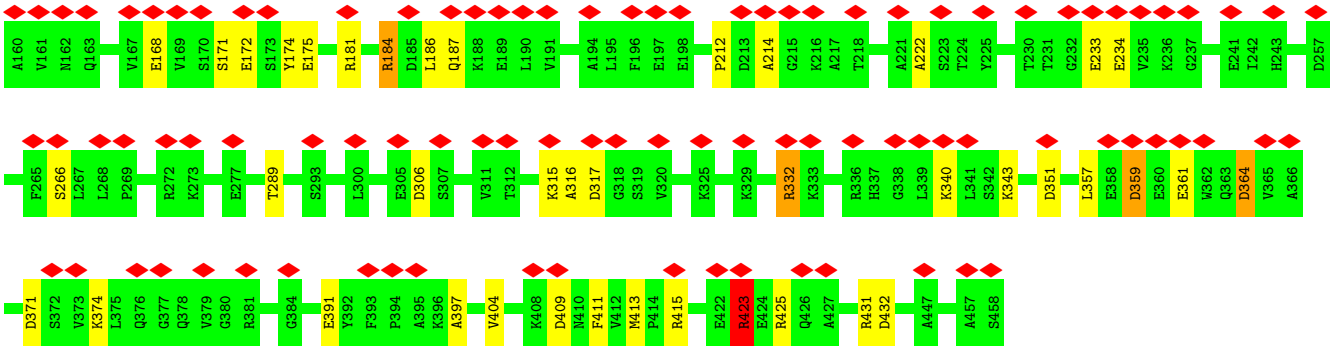
• Molecule 1: Major capsid protein

Chain G:



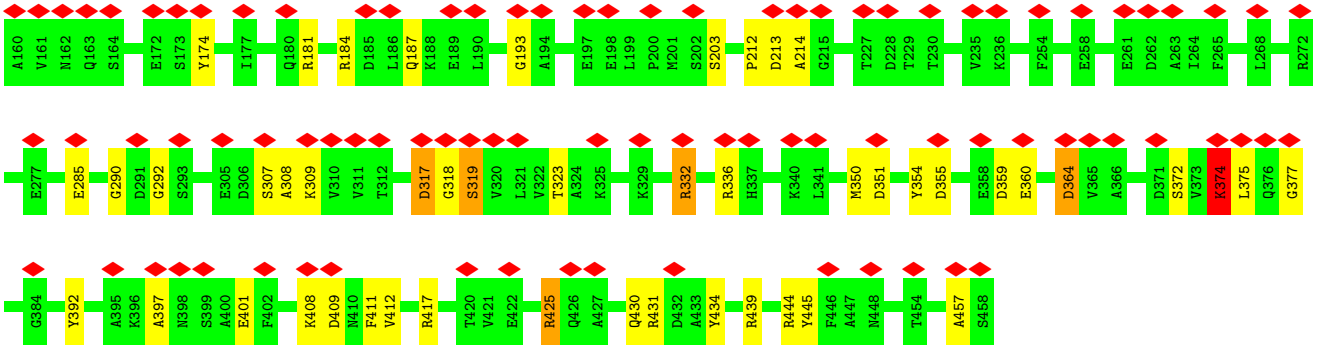
• Molecule 1: Major capsid protein

Chain H:



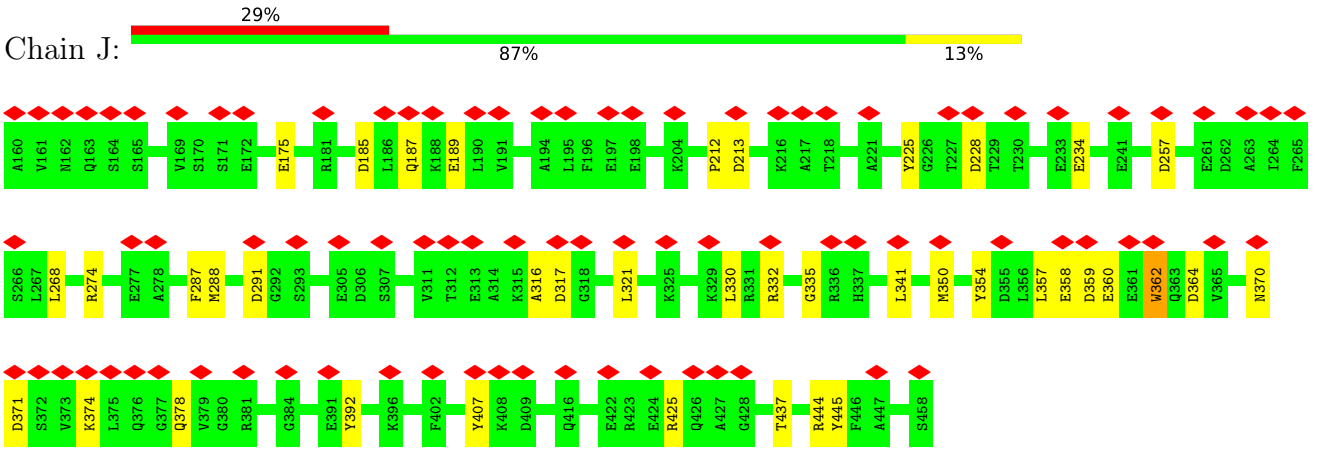
• Molecule 1: Major capsid protein

Chain I:



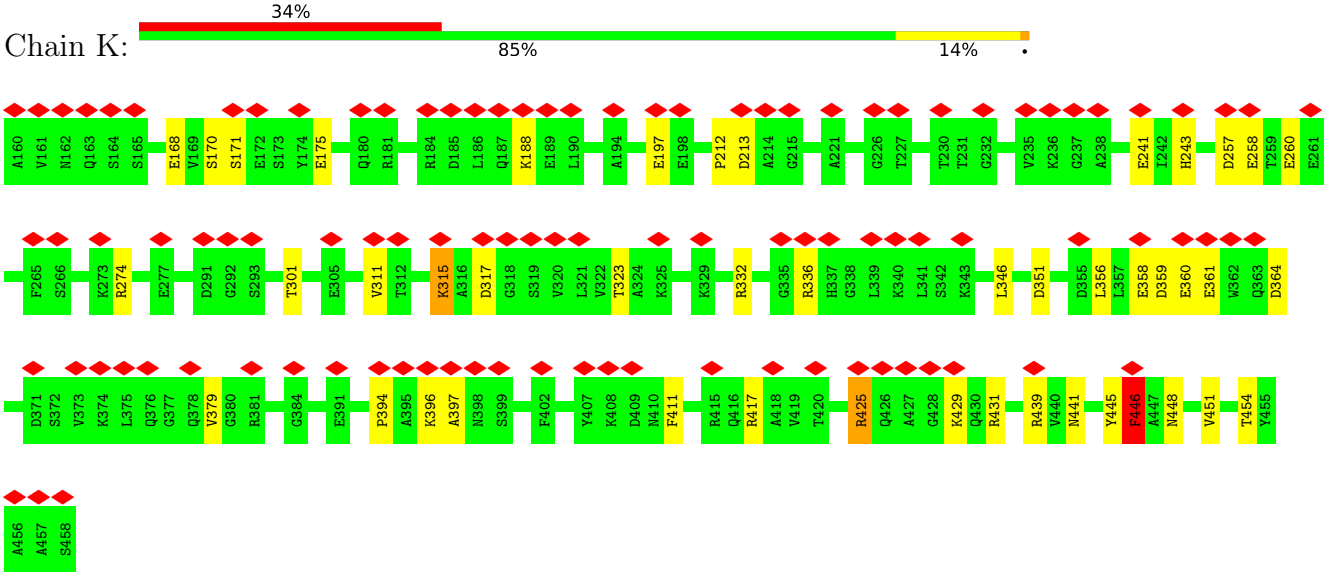
• Molecule 1: Major capsid protein

Chain J:



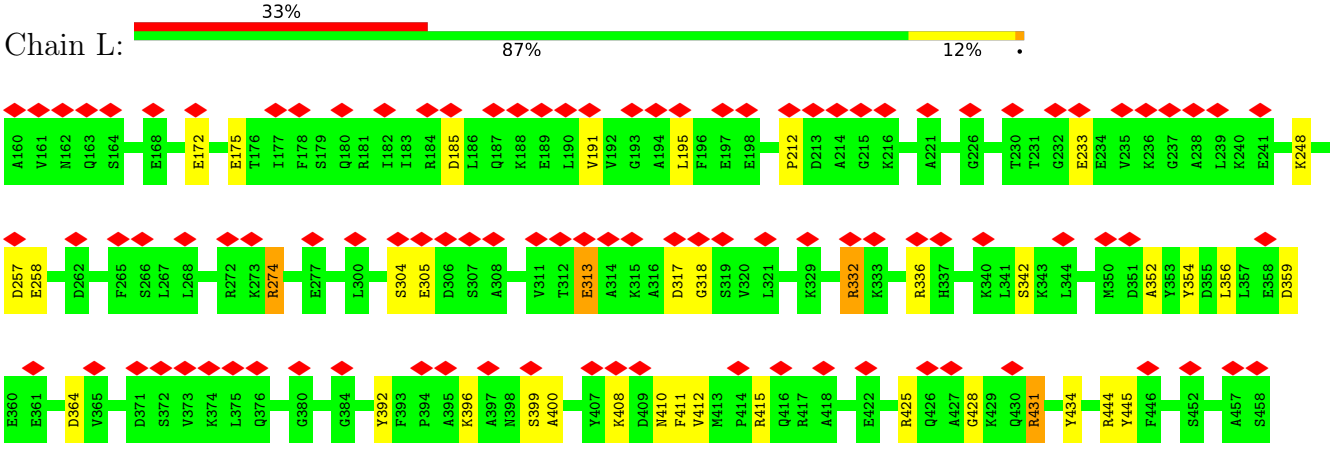
• Molecule 1: Major capsid protein

Chain K:



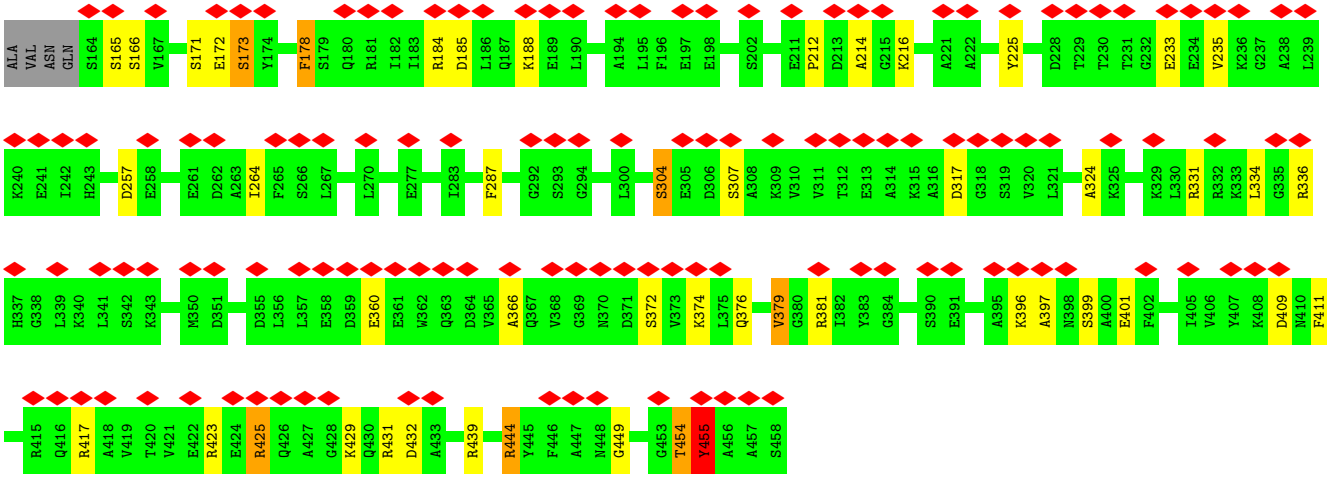
• Molecule 1: Major capsid protein

Chain L:



• Molecule 1: Major capsid protein

Chain M:


ALA VAL ASN GLN S164 S165 S166 V167 S171 E172 S173 Y174 F178 S179 Q180 R181 I182 I183 R184 D185 L186 Q187 K188 E189 L190 A194 L195 F196 E197 E198 S202 E211 P212 D213 A214 G215 K216 A221 A222 Y225 D228 T229 T230 T231 G232 E233 E234 V235 K236 G237 A238 L239
K240 E241 I242 H243 D257 E258 E261 D262 A263 I264 F265 S266 L267 L270 E277 I283 F287 G292 S293 G294 L300 S304 E305 D306 S307 A308 K309 V310 V311 T312 E313 A314 K315 A316 D317 G318 S319 V320 L321 A324 K325 K329 L330 R331 R332 K333 L334 G335 R336
H337 G338 L339 K340 L341 S342 K343 M350 D351 D355 L356 L357 E358 D359 E360 E361 W362 Q363 D364 V365 A366 Q367 V368 G369 N370 D371 S372 V373 K374 L375 Q376 V379 G380 R381 I382 Y383 G384 S390 E391 A395 K396 A397 N398 S399 A400 E401 F402 I405 V406 Y407 K408 D409 N410 F411
R415 Q416 R417 A418 V419 T420 V421 E422 R423 E424 R425 Q426 A427 G428 K429 Q430 R431 D432 A433 R439 R444 Y445 F446 A447 N448 G449 G453 T454 Y455 A456 A457 S458

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18901	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	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	32.443	Depositor
Minimum map value	-17.799	Depositor
Average map value	0.415	Depositor
Map value standard deviation	2.516	Depositor
Recommended contour level	8.5	Depositor
Map size (Å)	1013.85004, 1013.85004, 1013.85004	wwPDB
Map dimensions	751, 751, 751	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.77	0/2352	1.21	11/3178 (0.3%)
1	B	0.76	0/2352	1.22	10/3178 (0.3%)
1	C	0.79	1/2352 (0.0%)	1.25	13/3178 (0.4%)
1	D	0.77	0/2352	1.18	3/3178 (0.1%)
1	E	0.78	0/2352	1.24	13/3178 (0.4%)
1	F	0.77	0/2352	1.28	16/3178 (0.5%)
1	G	0.77	0/2352	1.24	10/3178 (0.3%)
1	H	0.76	0/2352	1.25	10/3178 (0.3%)
1	I	0.77	0/2352	1.25	14/3178 (0.4%)
1	J	0.77	0/2352	1.22	10/3178 (0.3%)
1	K	0.78	0/2352	1.25	8/3178 (0.3%)
1	L	0.77	0/2352	1.26	10/3178 (0.3%)
1	M	0.80	0/2323	1.26	16/3138 (0.5%)
All	All	0.77	1/30547 (0.0%)	1.24	144/41274 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	6
1	C	0	12
1	D	0	6
1	E	0	9
1	F	0	9
1	G	0	6
1	H	0	5
1	I	0	9
1	J	0	5
1	K	0	5
1	L	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	5
All	All	0	93

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	362	TRP	CD2-CE2	-6.33	1.33	1.41

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	415	ARG	NE-CZ-NH1	-12.74	113.93	120.30
1	H	423	ARG	NE-CZ-NH2	10.10	125.35	120.30
1	I	354	TYR	CB-CG-CD2	-9.45	115.33	121.00
1	L	431	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	G	332	ARG	NE-CZ-NH1	-9.20	115.70	120.30
1	F	431	ARG	NE-CZ-NH2	9.02	124.81	120.30
1	L	332	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	H	174	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	H	184	ARG	NE-CZ-NH2	8.61	124.60	120.30
1	I	445	TYR	CB-CG-CD2	-8.52	115.89	121.00
1	A	184	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	L	274	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	I	354	TYR	CB-CG-CD1	8.15	125.89	121.00
1	C	431	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	F	439	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	L	445	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	G	332	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	I	445	TYR	CB-CG-CD1	7.81	125.69	121.00
1	H	332	ARG	NE-CZ-NH1	-7.77	116.41	120.30
1	H	184	ARG	NE-CZ-NH1	-7.77	116.42	120.30
1	F	381	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	M	444	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	I	332	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	F	336	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	F	439	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	G	445	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	M	184	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	F	184	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	H	174	TYR	CB-CG-CD1	7.08	125.25	121.00
1	I	431	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	B	359	ASP	C-N-CA	7.07	139.36	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	445	TYR	CB-CG-CD1	7.04	125.22	121.00
1	L	445	TYR	CB-CG-CD1	7.04	125.22	121.00
1	G	274	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	I	336	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	C	444	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	A	336	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	K	274	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	F	445	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	I	444	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	E	423	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	G	439	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	E	332	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	L	444	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	E	336	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	K	425	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	C	274	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	B	360	GLU	N-CA-CB	6.50	122.30	110.60
1	E	332	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	D	184	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	J	287	PHE	CB-CG-CD1	6.42	125.29	120.80
1	E	174	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	K	446	PHE	CB-CG-CD2	-6.40	116.32	120.80
1	E	174	TYR	CB-CG-CD1	6.37	124.82	121.00
1	K	446	PHE	CB-CG-CD1	6.32	125.22	120.80
1	A	444	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	I	317	ASP	CB-CG-OD1	6.30	123.97	118.30
1	E	274	ARG	NE-CZ-NH2	6.25	123.43	120.30
1	L	257	ASP	CB-CG-OD1	6.25	123.93	118.30
1	C	415	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	E	317	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	332	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	M	425	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	K	439	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	M	178	PHE	CB-CG-CD1	6.18	125.13	120.80
1	M	381	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	J	287	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	C	336	ARG	N-CA-CB	6.09	121.57	110.60
1	L	415	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	C	354	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	I	439	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	M	184	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	F	332	ARG	NE-CZ-NH2	6.01	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	423	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	F	184	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	E	381	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	M	372	SER	N-CA-CB	5.92	119.38	110.50
1	C	362	TRP	CG-CD2-CE3	-5.88	128.60	133.90
1	J	225	TYR	CB-CG-CD1	5.88	124.53	121.00
1	E	230	THR	N-CA-CB	5.87	121.44	110.30
1	C	362	TRP	CD1-NE1-CE2	-5.85	103.74	109.00
1	J	225	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	A	402	PHE	CB-CG-CD1	5.81	124.87	120.80
1	B	444	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	J	392	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	M	307	SER	N-CA-CB	5.76	119.14	110.50
1	M	178	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	B	431	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	M	425	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	C	354	TYR	CB-CG-CD1	5.74	124.44	121.00
1	M	454	THR	C-N-CA	5.73	136.02	121.70
1	L	332	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	J	288	MET	CG-SD-CE	-5.71	91.06	100.20
1	F	374	LYS	O-C-N	-5.68	113.61	122.70
1	C	181	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	J	359	ASP	O-C-N	-5.64	113.68	122.70
1	D	307	SER	N-CA-CB	5.63	118.95	110.50
1	E	374	LYS	C-N-CA	5.63	135.78	121.70
1	B	359	ASP	O-C-N	-5.62	113.70	122.70
1	H	413	MET	CG-SD-CE	-5.60	91.24	100.20
1	F	417	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	C	184	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	M	287	PHE	CB-CG-CD1	5.59	124.71	120.80
1	I	425	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	J	359	ASP	C-N-CA	5.49	135.43	121.70
1	M	336	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	287	PHE	CB-CG-CD1	5.48	124.63	120.80
1	A	196	PHE	CB-CG-CD1	5.46	124.62	120.80
1	B	212	PRO	C-N-CA	5.45	135.32	121.70
1	A	402	PHE	CB-CG-CD2	-5.43	117.00	120.80
1	J	350	MET	CG-SD-CE	-5.43	91.51	100.20
1	I	351	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	431	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	163	GLN	N-CA-CB	5.41	120.33	110.60
1	H	359	ASP	O-C-N	-5.39	114.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	178	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	G	431	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	M	287	PHE	CB-CG-CD2	-5.35	117.06	120.80
1	M	455	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	274	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	B	435	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	F	445	TYR	CB-CG-CD1	5.28	124.17	121.00
1	C	431	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	F	336	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	331	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	J	392	TYR	CB-CG-CD1	5.22	124.13	121.00
1	L	425	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	G	417	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	I	425	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	K	425	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	E	374	LYS	O-C-N	-5.17	114.42	122.70
1	H	374	LYS	C-N-CA	5.17	134.63	121.70
1	K	336	ARG	O-C-N	-5.17	114.43	122.70
1	F	307	SER	N-CA-CB	5.16	118.24	110.50
1	F	374	LYS	C-N-CA	5.16	134.59	121.70
1	G	288	MET	CG-SD-CE	-5.15	91.96	100.20
1	G	354	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	K	171	SER	N-CA-CB	5.12	118.18	110.50
1	A	196	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	I	374	LYS	O-C-N	-5.08	114.58	122.70
1	H	214	ALA	O-C-N	-5.07	114.57	123.20
1	A	336	ARG	O-C-N	-5.05	114.62	122.70
1	E	381	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	A	287	PHE	CB-CG-CD2	-5.02	117.28	120.80

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ARG	Sidechain
1	A	184	ARG	Sidechain
1	A	187	GLN	Peptide
1	A	370	ASN	Peptide
1	A	374	LYS	Peptide
1	A	381	ARG	Sidechain
1	A	409	ASP	Peptide
1	A	417	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	423	ARG	Sidechain
1	A	434	TYR	Sidechain
1	B	184	ARG	Sidechain
1	B	336	ARG	Sidechain
1	B	381	ARG	Sidechain
1	B	407	TYR	Sidechain
1	B	434	TYR	Sidechain
1	B	444	ARG	Sidechain
1	C	229	THR	Peptide
1	C	232	GLY	Peptide
1	C	274	ARG	Sidechain
1	C	331	ARG	Sidechain
1	C	332	ARG	Sidechain
1	C	338	GLY	Peptide
1	C	353	TYR	Sidechain
1	C	415	ARG	Sidechain
1	C	417	ARG	Sidechain
1	C	425	ARG	Sidechain
1	C	434	TYR	Sidechain
1	C	444	ARG	Sidechain
1	D	184	ARG	Sidechain
1	D	227	THR	Peptide
1	D	332	ARG	Sidechain
1	D	417	ARG	Sidechain
1	D	434	TYR	Sidechain
1	D	455	TYR	Sidechain
1	E	165	SER	Peptide
1	E	184	ARG	Sidechain
1	E	332	ARG	Sidechain
1	E	392	TYR	Sidechain
1	E	407	TYR	Sidechain
1	E	423	ARG	Sidechain
1	E	425	ARG	Sidechain
1	E	434	TYR	Sidechain
1	E	455	TYR	Sidechain
1	F	172	GLU	Peptide
1	F	184	ARG	Sidechain
1	F	212	PRO	Peptide
1	F	274	ARG	Sidechain
1	F	415	ARG	Sidechain
1	F	417	ARG	Sidechain
1	F	423	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	431	ARG	Sidechain
1	F	439	ARG	Sidechain
1	G	160	ALA	Peptide
1	G	184	ARG	Sidechain
1	G	332	ARG	Sidechain
1	G	358	GLU	Peptide
1	G	431	ARG	Peptide
1	G	455	TYR	Sidechain
1	H	181	ARG	Sidechain
1	H	332	ARG	Sidechain
1	H	423	ARG	Sidechain
1	H	425	ARG	Sidechain
1	H	431	ARG	Sidechain
1	I	181	ARG	Sidechain
1	I	184	ARG	Sidechain
1	I	290	GLY	Peptide
1	I	332	ARG	Sidechain
1	I	374	LYS	Peptide
1	I	392	TYR	Sidechain
1	I	409	ASP	Peptide
1	I	417	ARG	Sidechain
1	I	434	TYR	Sidechain
1	J	274	ARG	Sidechain
1	J	332	ARG	Sidechain
1	J	354	TYR	Sidechain
1	J	407	TYR	Sidechain
1	J	444	ARG	Sidechain
1	K	213	ASP	Peptide
1	K	358	GLU	Peptide
1	K	417	ARG	Sidechain
1	K	431	ARG	Peptide
1	K	445	TYR	Sidechain
1	L	274	ARG	Sidechain
1	L	332	ARG	Sidechain
1	L	354	TYR	Sidechain
1	L	392	TYR	Sidechain
1	L	431	ARG	Sidechain
1	L	434	TYR	Sidechain
1	M	331	ARG	Sidechain
1	M	417	ARG	Sidechain
1	M	425	ARG	Sidechain
1	M	439	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	M	444	ARG	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	A	2317	2345	2342	0	0
1	B	2317	2345	2342	0	0
1	C	2317	2345	2342	0	0
1	D	2317	2345	2342	0	0
1	E	2317	2345	2342	0	0
1	F	2317	2345	2342	0	0
1	G	2317	2345	2342	0	0
1	H	2317	2345	2342	0	0
1	I	2317	2345	2342	0	0
1	J	2317	2345	2342	0	0
1	K	2317	2345	2342	0	0
1	L	2317	2345	2342	0	0
1	M	2288	2315	2314	0	0
All	All	30092	30455	30418	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/299 (99%)	233 (78%)	42 (14%)	22 (7%)	1	16
1	B	297/299 (99%)	233 (78%)	47 (16%)	17 (6%)	1	21
1	C	297/299 (99%)	231 (78%)	45 (15%)	21 (7%)	1	17
1	D	297/299 (99%)	232 (78%)	46 (16%)	19 (6%)	1	20
1	E	297/299 (99%)	221 (74%)	54 (18%)	22 (7%)	1	16
1	F	297/299 (99%)	227 (76%)	43 (14%)	27 (9%)	1	12
1	G	297/299 (99%)	237 (80%)	43 (14%)	17 (6%)	1	21
1	H	297/299 (99%)	226 (76%)	54 (18%)	17 (6%)	1	21
1	I	297/299 (99%)	226 (76%)	48 (16%)	23 (8%)	1	15
1	J	297/299 (99%)	234 (79%)	48 (16%)	15 (5%)	2	23
1	K	297/299 (99%)	229 (77%)	47 (16%)	21 (7%)	1	17
1	L	297/299 (99%)	235 (79%)	46 (16%)	16 (5%)	2	22
1	M	293/299 (98%)	222 (76%)	42 (14%)	29 (10%)	0	10
All	All	3857/3887 (99%)	2986 (77%)	605 (16%)	266 (7%)	2	18

All (266) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	A	174	TYR
1	A	230	THR
1	A	309	LYS
1	A	364	ASP
1	A	431	ARG
1	B	213	ASP
1	B	233	GLU
1	B	236	LYS
1	B	333	LYS
1	B	340	LYS
1	C	216	LYS
1	C	336	ARG
1	C	372	SER
1	C	409	ASP
1	D	172	GLU
1	D	228	ASP
1	D	307	SER
1	D	372	SER
1	E	408	LYS

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Mol	Chain	Res	Type
1	E	429	LYS
1	F	213	ASP
1	F	235	VAL
1	F	307	SER
1	F	311	VAL
1	F	315	LYS
1	G	162	ASN
1	G	174	TYR
1	G	307	SER
1	G	361	GLU
1	G	362	TRP
1	G	364	ASP
1	H	266	SER
1	H	397	ALA
1	I	319	SER
1	I	372	SER
1	I	375	LEU
1	J	268	LEU
1	J	364	ASP
1	K	317	ASP
1	K	323	THR
1	K	361	GLU
1	L	364	ASP
1	L	408	LYS
1	M	171	SER
1	M	366	ALA
1	M	396	LYS
1	M	397	ALA
1	M	431	ARG
1	A	175	GLU
1	A	231	THR
1	A	264	ILE
1	A	323	THR
1	A	361	GLU
1	B	260	GLU
1	B	360	GLU
1	B	372	SER
1	B	397	ALA
1	B	406	VAL
1	B	411	PHE
1	C	231	THR
1	C	233	GLU

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Mol	Chain	Res	Type
1	C	236	LYS
1	C	308	ALA
1	C	343	LYS
1	C	356	LEU
1	C	364	ASP
1	C	378	GLN
1	D	174	TYR
1	D	185	ASP
1	D	188	LYS
1	D	364	ASP
1	D	425	ARG
1	E	164	SER
1	E	230	THR
1	E	335	GLY
1	E	362	TRP
1	E	364	ASP
1	E	396	LYS
1	E	412	VAL
1	E	425	ARG
1	F	186	LEU
1	F	190	LEU
1	F	203	SER
1	F	220	VAL
1	F	340	LYS
1	F	367	GLN
1	F	378	GLN
1	F	394	PRO
1	F	409	ASP
1	G	213	ASP
1	G	304	SER
1	G	317	ASP
1	G	450	VAL
1	G	455	TYR
1	H	361	GLU
1	H	364	ASP
1	I	307	SER
1	I	308	ALA
1	I	364	ASP
1	I	412	VAL
1	I	425	ARG
1	I	457	ALA
1	J	213	ASP

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Mol	Chain	Res	Type
1	J	321	LEU
1	J	371	ASP
1	K	257	ASP
1	K	315	LYS
1	K	411	PHE
1	L	313	GLU
1	L	336	ARG
1	L	356	LEU
1	L	411	PHE
1	L	412	VAL
1	M	173	SER
1	M	225	TYR
1	M	235	VAL
1	M	264	ILE
1	M	317	ASP
1	M	324	ALA
1	M	334	LEU
1	M	379	VAL
1	M	411	PHE
1	A	162	ASN
1	A	263	ALA
1	A	371	ASP
1	A	382	ILE
1	A	397	ALA
1	B	407	TYR
1	C	215	GLY
1	C	232	GLY
1	C	398	ASN
1	C	457	ALA
1	D	233	GLU
1	D	258	GLU
1	D	336	ARG
1	D	430	GLN
1	E	172	GLU
1	E	174	TYR
1	E	204	LYS
1	E	222	ALA
1	E	232	GLY
1	E	319	SER
1	E	340	LYS
1	E	361	GLU
1	E	411	PHE

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Mol	Chain	Res	Type
1	F	227	THR
1	F	319	SER
1	F	336	ARG
1	F	339	LEU
1	F	364	ASP
1	G	215	GLY
1	G	397	ALA
1	H	175	GLU
1	H	233	GLU
1	H	317	ASP
1	H	340	LYS
1	H	371	ASP
1	I	292	GLY
1	I	359	ASP
1	I	374	LYS
1	I	377	GLY
1	I	411	PHE
1	J	341	LEU
1	J	357	LEU
1	J	425	ARG
1	J	445	TYR
1	K	188	LYS
1	K	212	PRO
1	K	258	GLU
1	K	356	LEU
1	K	364	ASP
1	K	394	PRO
1	K	396	LYS
1	K	397	ALA
1	K	425	ARG
1	K	454	THR
1	L	318	GLY
1	L	352	ALA
1	L	400	ALA
1	L	428	GLY
1	M	185	ASP
1	M	360	GLU
1	M	374	LYS
1	A	168	GLU
1	A	186	LEU
1	A	430	GLN
1	B	228	ASP

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Mol	Chain	Res	Type
1	B	395	ALA
1	C	408	LYS
1	C	449	GLY
1	D	162	ASN
1	D	229	THR
1	D	371	ASP
1	E	324	ALA
1	F	341	LEU
1	F	342	SER
1	F	372	SER
1	F	411	PHE
1	F	445	TYR
1	F	455	TYR
1	G	343	LYS
1	G	418	ALA
1	H	168	GLU
1	H	222	ALA
1	H	359	ASP
1	H	411	PHE
1	I	212	PRO
1	I	318	GLY
1	I	430	GLN
1	J	316	ALA
1	K	260	GLU
1	K	446	PHE
1	L	212	PRO
1	L	317	ASP
1	L	399	SER
1	M	166	SER
1	M	216	LYS
1	M	304	SER
1	M	429	LYS
1	M	449	GLY
1	M	455	TYR
1	A	213	ASP
1	B	174	TYR
1	B	431	ARG
1	C	425	ARG
1	D	317	ASP
1	D	341	LEU
1	F	430	GLN
1	G	457	ALA

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Mol	Chain	Res	Type
1	H	316	ALA
1	H	409	ASP
1	I	174	TYR
1	I	187	GLN
1	I	203	SER
1	I	214	ALA
1	I	397	ALA
1	J	187	GLN
1	J	317	ASP
1	J	362	TRP
1	K	379	VAL
1	K	448	ASN
1	L	410	ASN
1	M	188	LYS
1	M	214	ALA
1	M	376	GLN
1	M	399	SER
1	A	185	ASP
1	B	161	VAL
1	C	213	ASP
1	D	316	ALA
1	G	430	GLN
1	H	171	SER
1	K	170	SER
1	M	165	SER
1	F	191	VAL
1	H	212	PRO
1	L	191	VAL
1	C	338	GLY
1	E	215	GLY
1	I	193	GLY
1	J	335	GLY
1	J	212	PRO
1	A	373	VAL
1	E	373	VAL
1	M	212	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	A	250/250 (100%)	235 (94%)	15 (6%)	19	50
1	B	250/250 (100%)	235 (94%)	15 (6%)	19	50
1	C	250/250 (100%)	236 (94%)	14 (6%)	21	52
1	D	250/250 (100%)	234 (94%)	16 (6%)	17	48
1	E	250/250 (100%)	236 (94%)	14 (6%)	21	52
1	F	250/250 (100%)	236 (94%)	14 (6%)	21	52
1	G	250/250 (100%)	236 (94%)	14 (6%)	21	52
1	H	250/250 (100%)	233 (93%)	17 (7%)	16	47
1	I	250/250 (100%)	238 (95%)	12 (5%)	25	56
1	J	250/250 (100%)	235 (94%)	15 (6%)	19	50
1	K	250/250 (100%)	233 (93%)	17 (7%)	16	47
1	L	250/250 (100%)	237 (95%)	13 (5%)	23	54
1	M	247/250 (99%)	235 (95%)	12 (5%)	25	55
All	All	3247/3250 (100%)	3059 (94%)	188 (6%)	24	51

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	188	LYS
1	A	190	LEU
1	A	209	LEU
1	A	260	GLU
1	A	277	GLU
1	A	291	ASP
1	A	339	LEU
1	A	355	ASP
1	A	370	ASN
1	A	383	TYR
1	A	402	PHE
1	A	423	ARG
1	A	430	GLN
1	A	454	THR
1	B	179	SER
1	B	189	GLU
1	B	213	ASP

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Mol	Chain	Res	Type
1	B	233	GLU
1	B	257	ASP
1	B	291	ASP
1	B	307	SER
1	B	340	LYS
1	B	361	GLU
1	B	371	ASP
1	B	408	LYS
1	B	409	ASP
1	B	425	ARG
1	B	432	ASP
1	B	454	THR
1	C	175	GLU
1	C	257	ASP
1	C	291	ASP
1	C	306	ASP
1	C	310	VAL
1	C	323	THR
1	C	340	LYS
1	C	360	GLU
1	C	391	GLU
1	C	396	LYS
1	C	408	LYS
1	C	409	ASP
1	C	437	THR
1	C	443	GLN
1	D	163	GLN
1	D	187	GLN
1	D	234	GLU
1	D	241	GLU
1	D	257	ASP
1	D	277	GLU
1	D	301	THR
1	D	306	ASP
1	D	332	ARG
1	D	355	ASP
1	D	356	LEU
1	D	359	ASP
1	D	401	GLU
1	D	409	ASP
1	D	425	ARG
1	D	454	THR

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Mol	Chain	Res	Type
1	E	165	SER
1	E	166	SER
1	E	174	TYR
1	E	175	GLU
1	E	228	ASP
1	E	233	GLU
1	E	249	LEU
1	E	291	ASP
1	E	306	ASP
1	E	317	ASP
1	E	357	LEU
1	E	375	LEU
1	E	406	VAL
1	E	424	GLU
1	F	163	GLN
1	F	172	GLU
1	F	173	SER
1	F	185	ASP
1	F	213	ASP
1	F	261	GLU
1	F	279	HIS
1	F	291	ASP
1	F	339	LEU
1	F	351	ASP
1	F	360	GLU
1	F	367	GLN
1	F	396	LYS
1	F	409	ASP
1	G	172	GLU
1	G	175	GLU
1	G	184	ARG
1	G	260	GLU
1	G	279	HIS
1	G	325	LYS
1	G	355	ASP
1	G	358	GLU
1	G	360	GLU
1	G	363	GLN
1	G	364	ASP
1	G	391	GLU
1	G	408	LYS
1	G	409	ASP

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Mol	Chain	Res	Type
1	H	172	GLU
1	H	184	ARG
1	H	186	LEU
1	H	187	GLN
1	H	234	GLU
1	H	289	THR
1	H	306	ASP
1	H	315	LYS
1	H	343	LYS
1	H	351	ASP
1	H	357	LEU
1	H	364	ASP
1	H	391	GLU
1	H	404	VAL
1	H	415	ARG
1	H	423	ARG
1	H	432	ASP
1	I	213	ASP
1	I	285	GLU
1	I	309	LYS
1	I	317	ASP
1	I	319	SER
1	I	323	THR
1	I	350	MET
1	I	355	ASP
1	I	360	GLU
1	I	364	ASP
1	I	401	GLU
1	I	408	LYS
1	J	175	GLU
1	J	185	ASP
1	J	189	GLU
1	J	228	ASP
1	J	234	GLU
1	J	257	ASP
1	J	291	ASP
1	J	330	LEU
1	J	358	GLU
1	J	360	GLU
1	J	362	TRP
1	J	370	ASN
1	J	374	LYS

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Mol	Chain	Res	Type
1	J	378	GLN
1	J	437	THR
1	K	168	GLU
1	K	175	GLU
1	K	197	GLU
1	K	241	GLU
1	K	243	HIS
1	K	301	THR
1	K	311	VAL
1	K	315	LYS
1	K	332	ARG
1	K	346	LEU
1	K	351	ASP
1	K	359	ASP
1	K	360	GLU
1	K	429	LYS
1	K	441	ASN
1	K	446	PHE
1	K	451	VAL
1	L	172	GLU
1	L	175	GLU
1	L	185	ASP
1	L	195	LEU
1	L	233	GLU
1	L	248	LYS
1	L	258	GLU
1	L	304	SER
1	L	305	GLU
1	L	313	GLU
1	L	342	SER
1	L	359	ASP
1	L	396	LYS
1	M	172	GLU
1	M	173	SER
1	M	178	PHE
1	M	233	GLU
1	M	257	ASP
1	M	304	SER
1	M	379	VAL
1	M	401	GLU
1	M	409	ASP
1	M	432	ASP

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Mol	Chain	Res	Type
1	M	454	THR
1	M	455	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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.

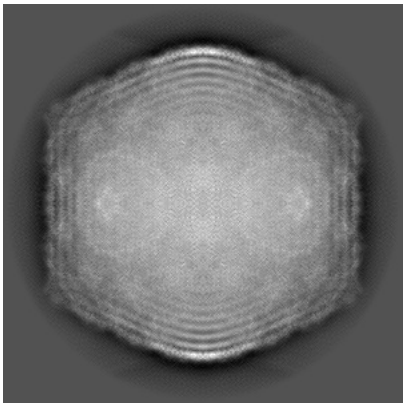
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20125. These allow visual inspection of the internal detail of the map and identification of artifacts.

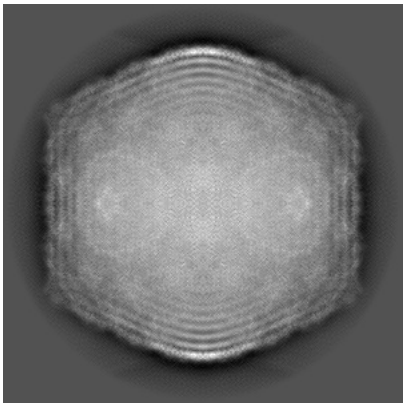
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

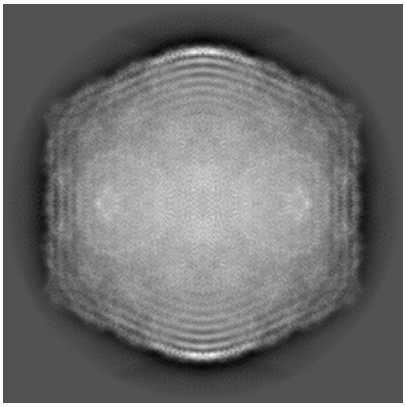
6.1.1 Primary map



X



Y

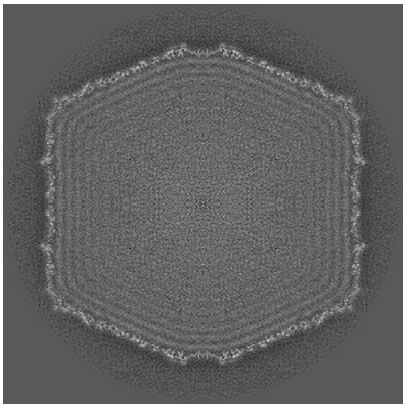


Z

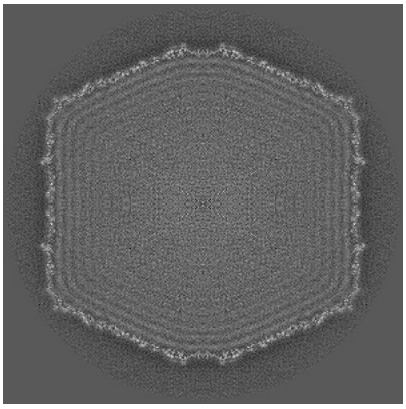
The images above show the map projected in three orthogonal directions.

6.2 Central slices

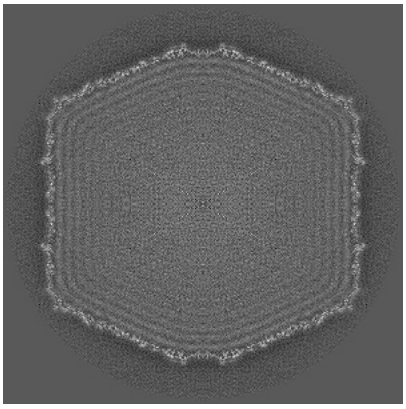
6.2.1 Primary map



X Index: 375



Y Index: 375

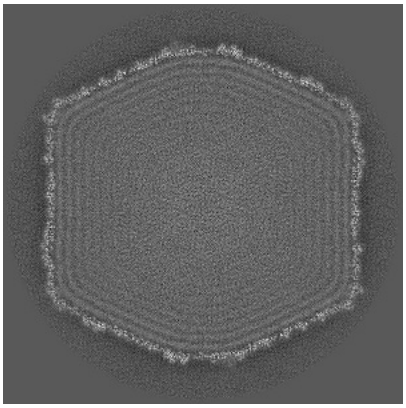


Z Index: 375

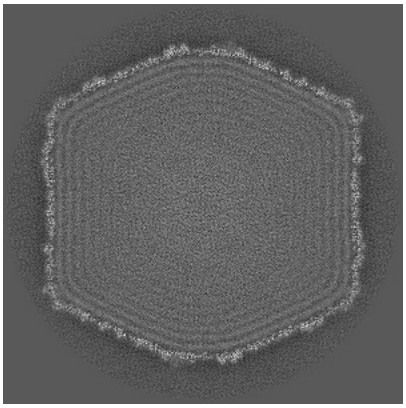
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

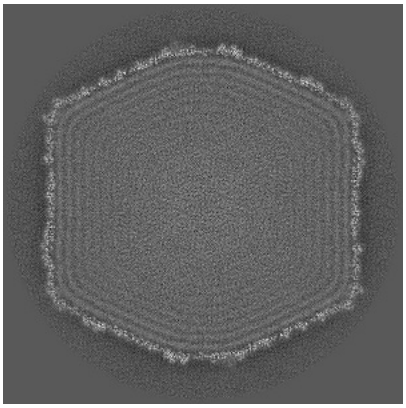
6.3.1 Primary map



X Index: 382



Y Index: 368

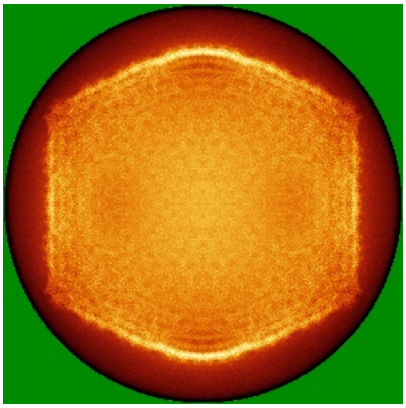


Z Index: 382

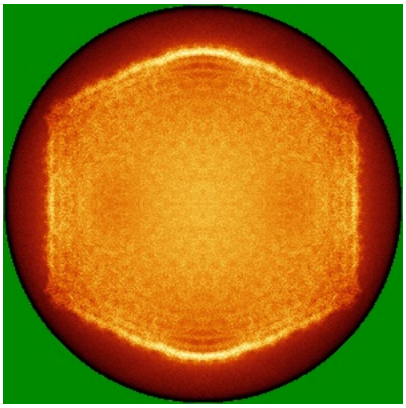
The images above show the largest variance slices of the map in three orthogonal directions.

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

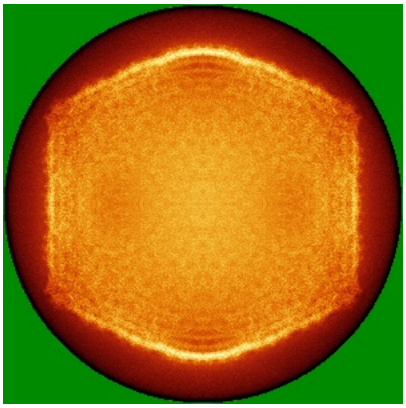
6.4.1 Primary map



X



Y

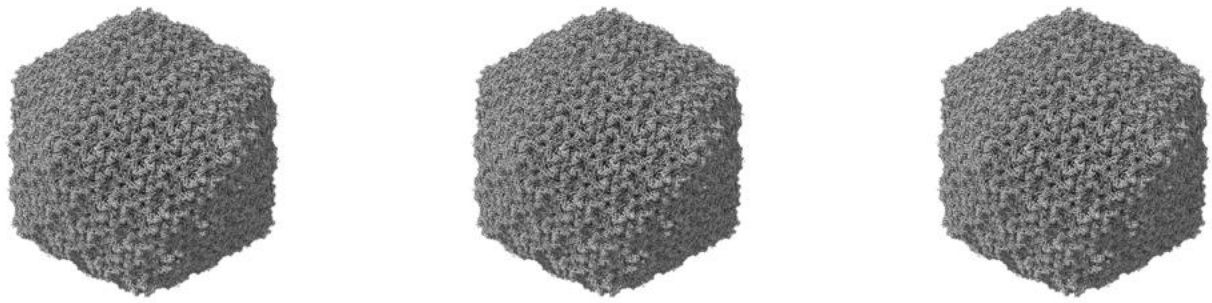


Z

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

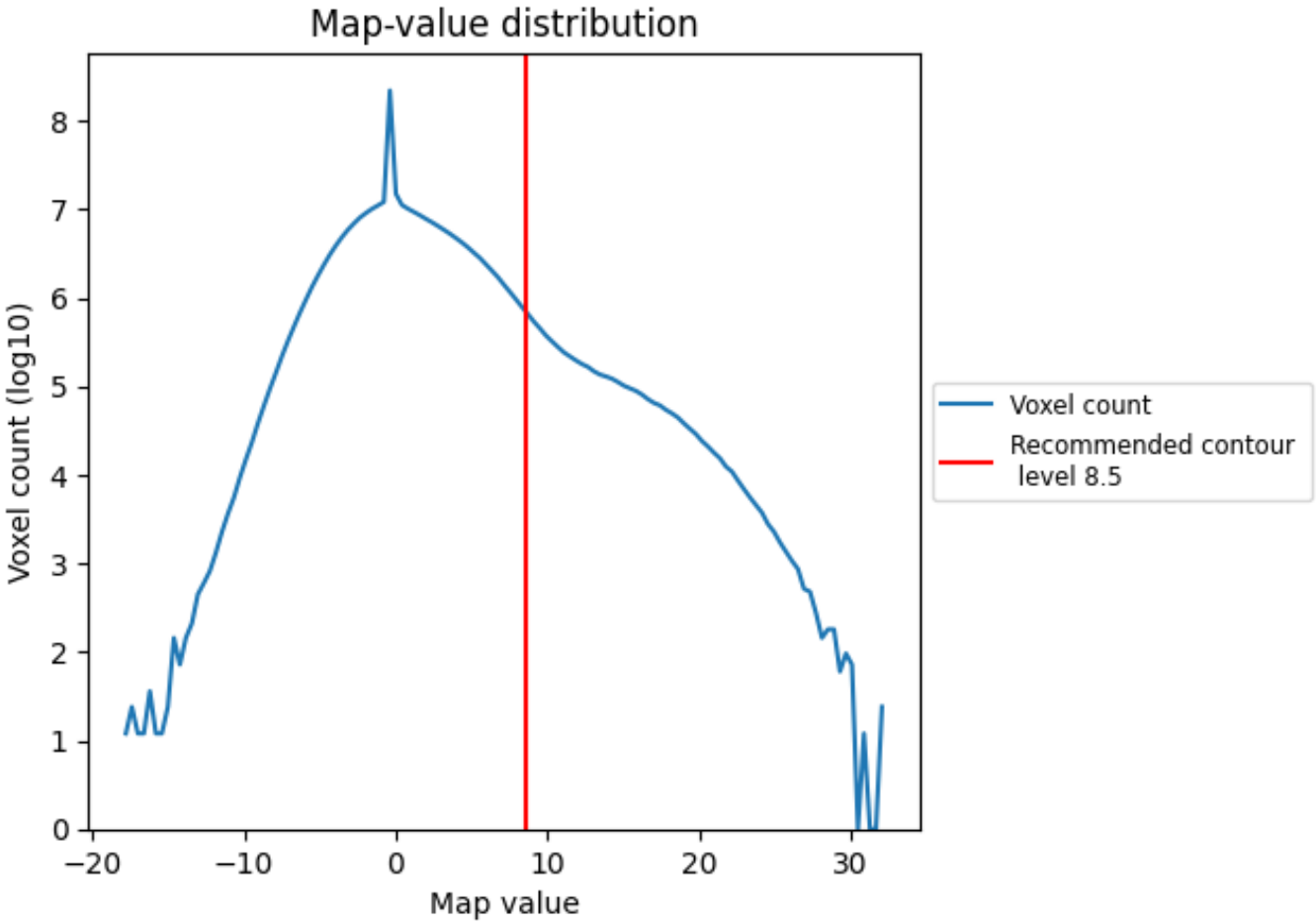
6.6 Mask visualisation (i)

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

7 Map analysis

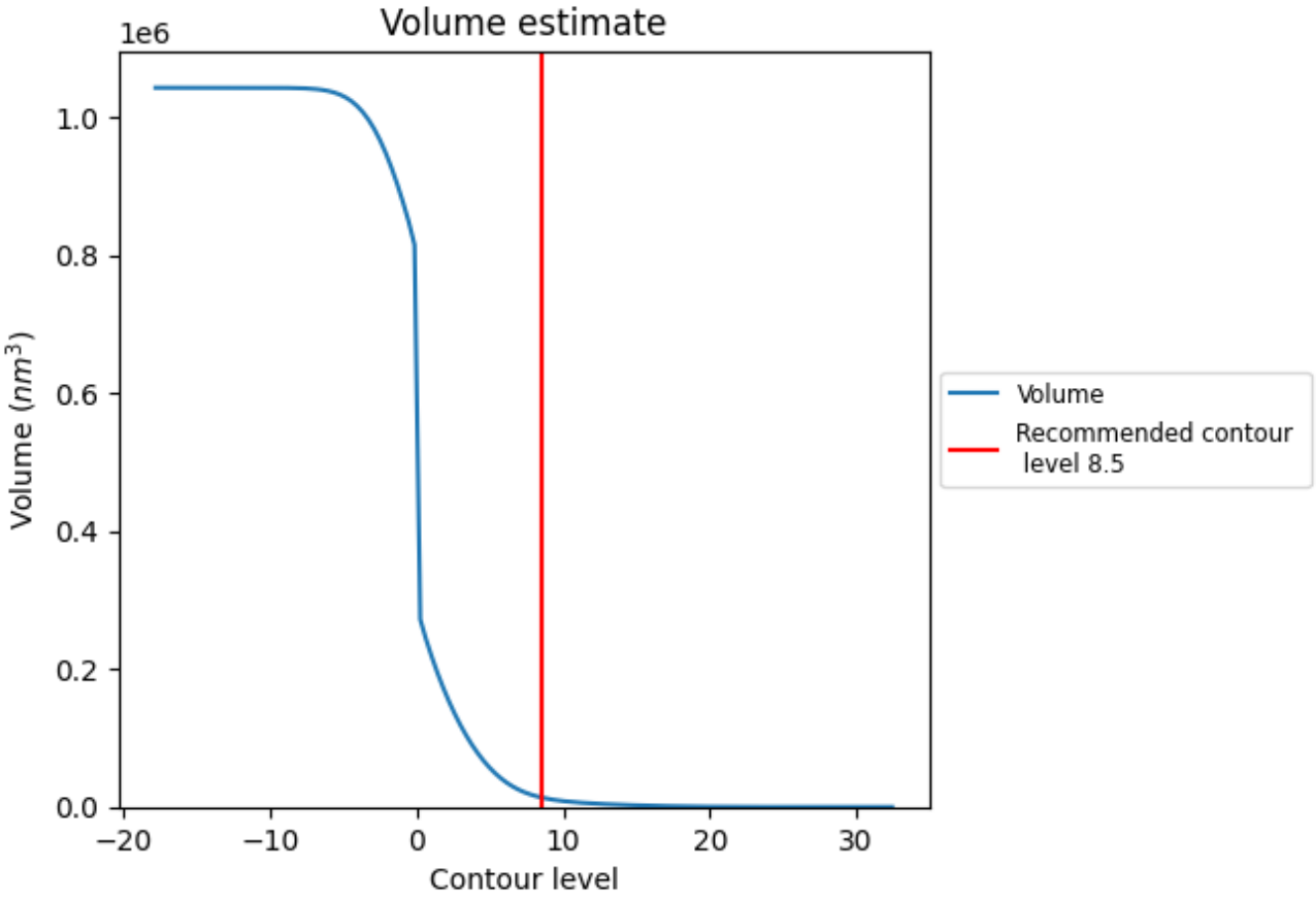
This section contains the results of statistical analysis of the map.

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.

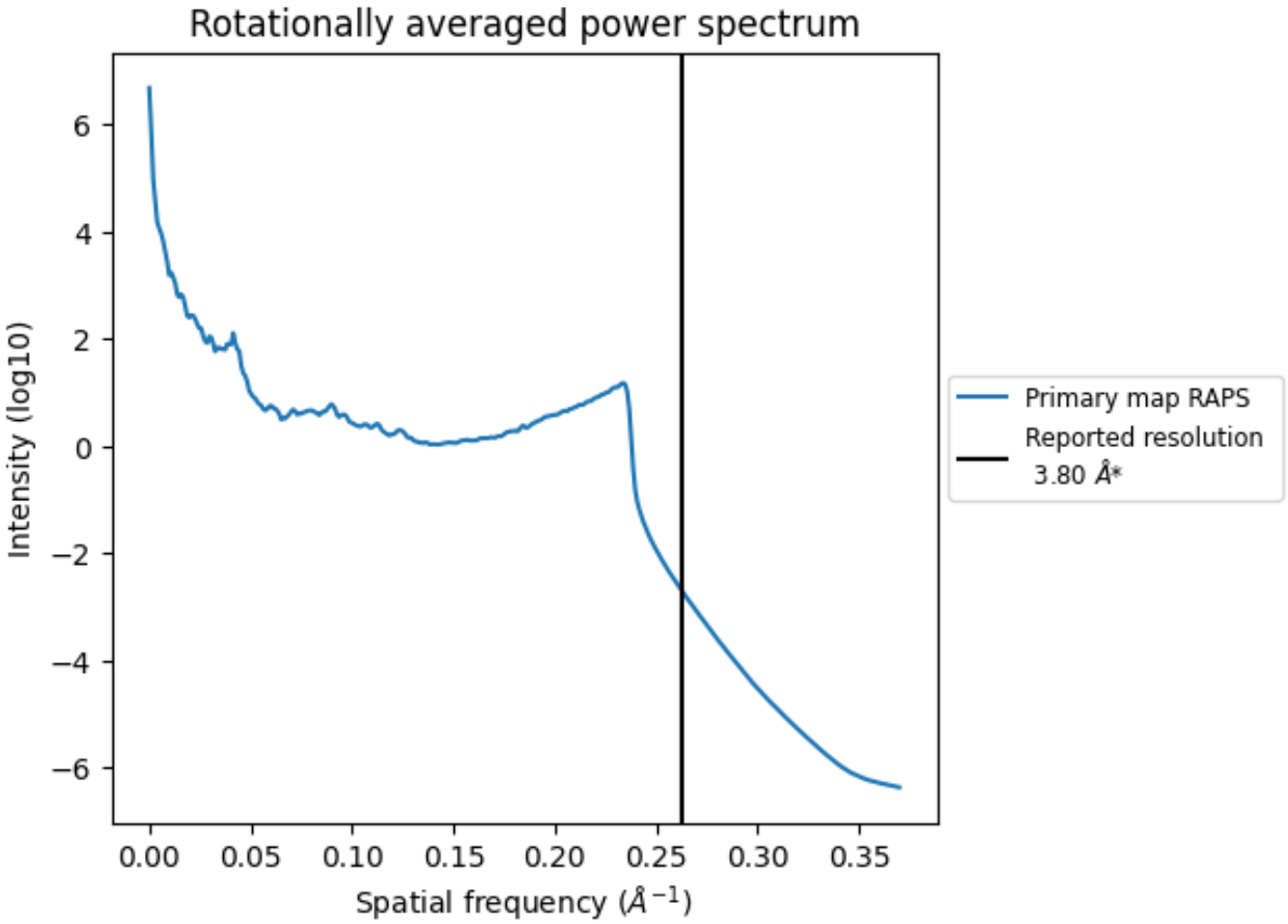
7.2 Volume estimate (i)



The volume at the recommended contour level is 13798 nm^3; this corresponds to an approximate mass of 12464 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)

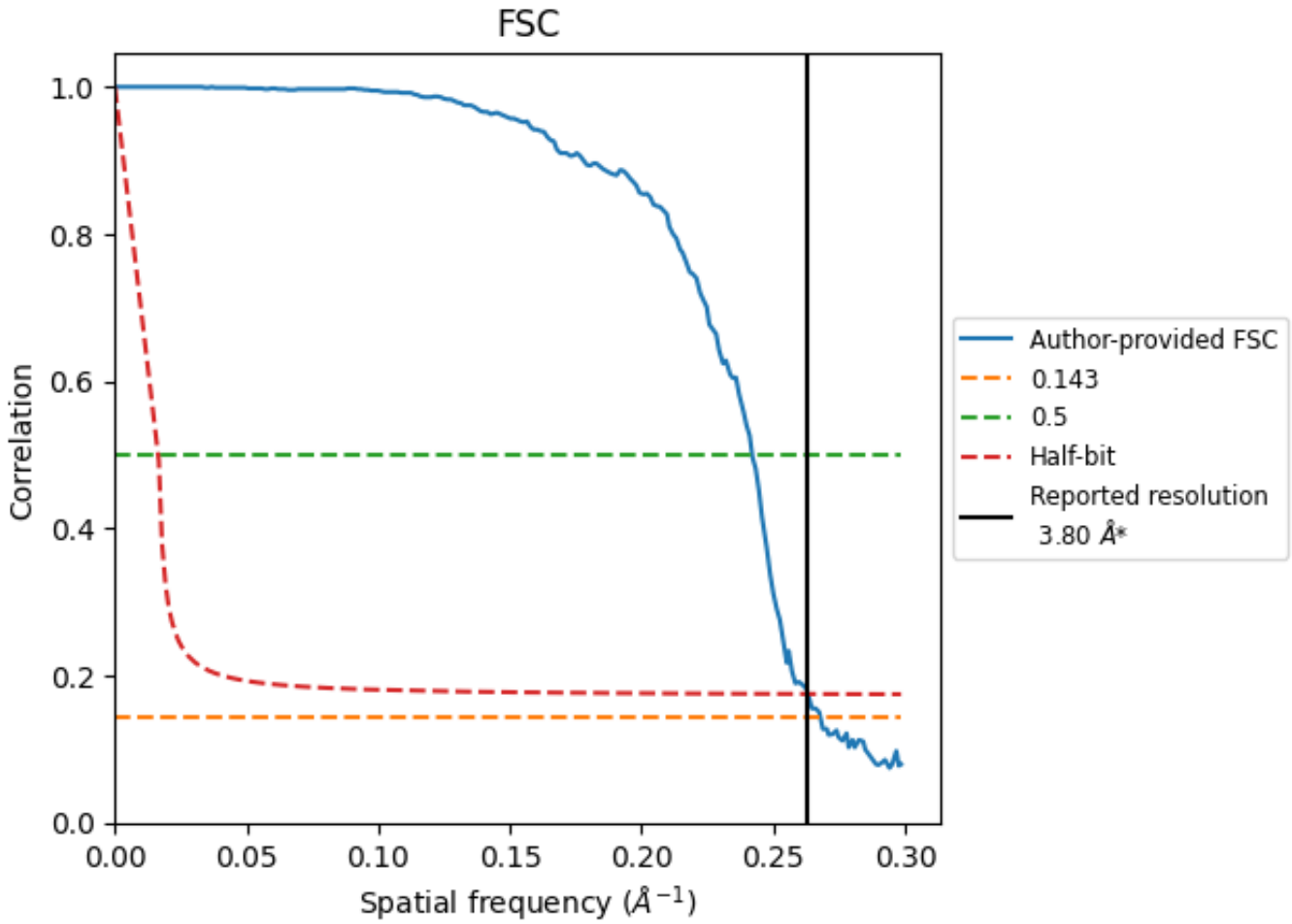


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.73	4.13	3.80
Unmasked-calculated*	-	-	-

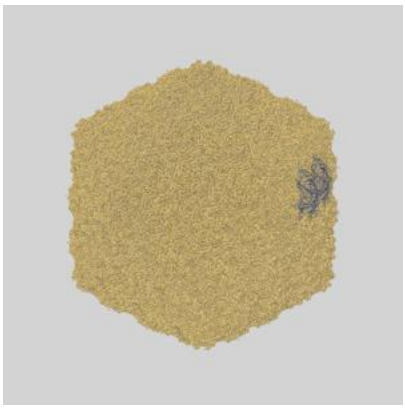
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

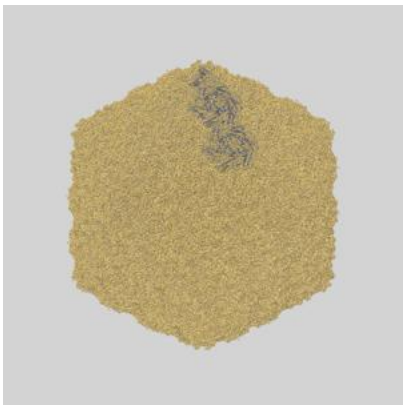
This section contains information regarding the fit between EMDB map EMD-20125 and PDB model 6OMC. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

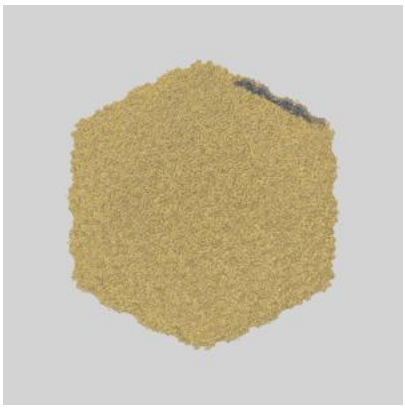
9.1.1 Map-model overlay



X

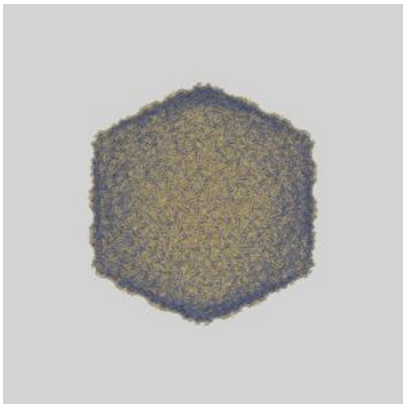


Y

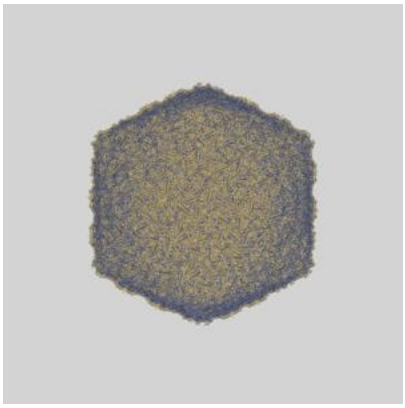


Z

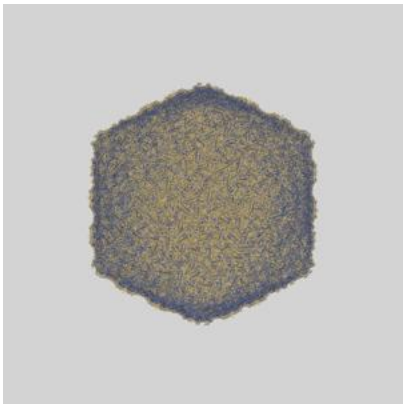
9.1.2 Map-model assembly overlay



X



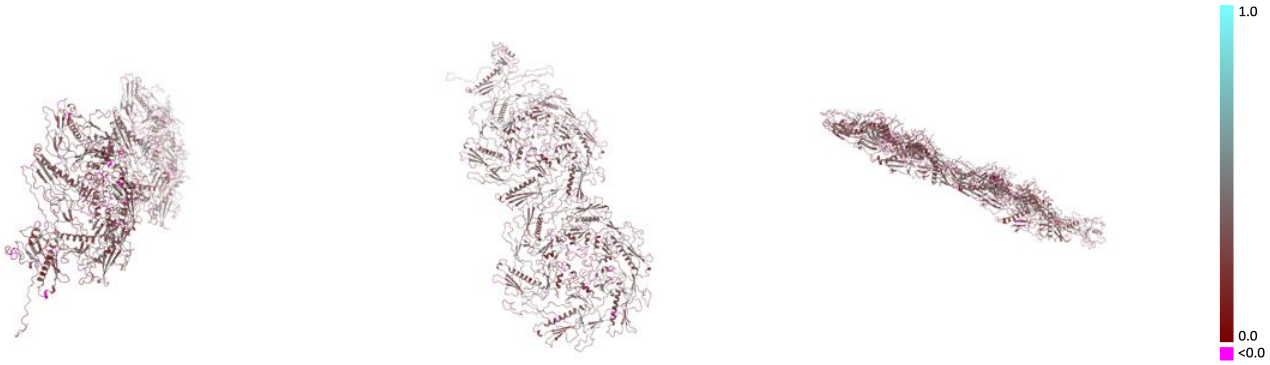
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.5 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.

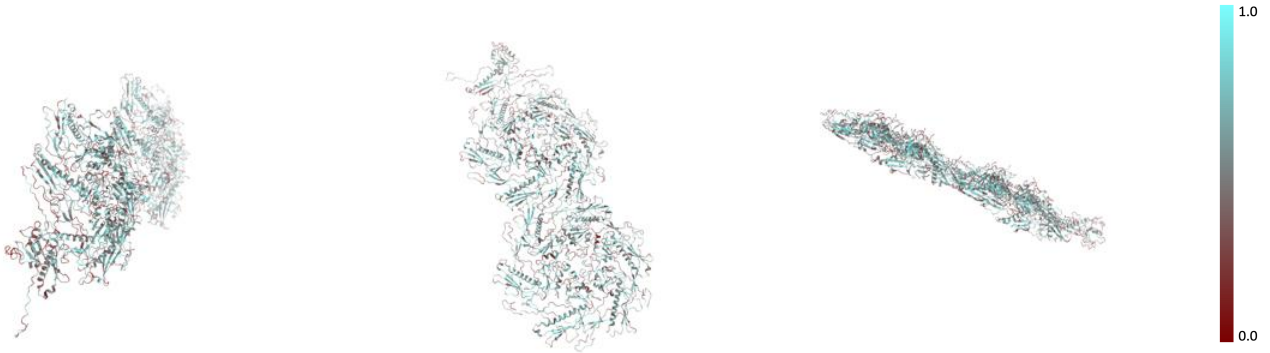
9.2 Q-score mapped to coordinate model



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.

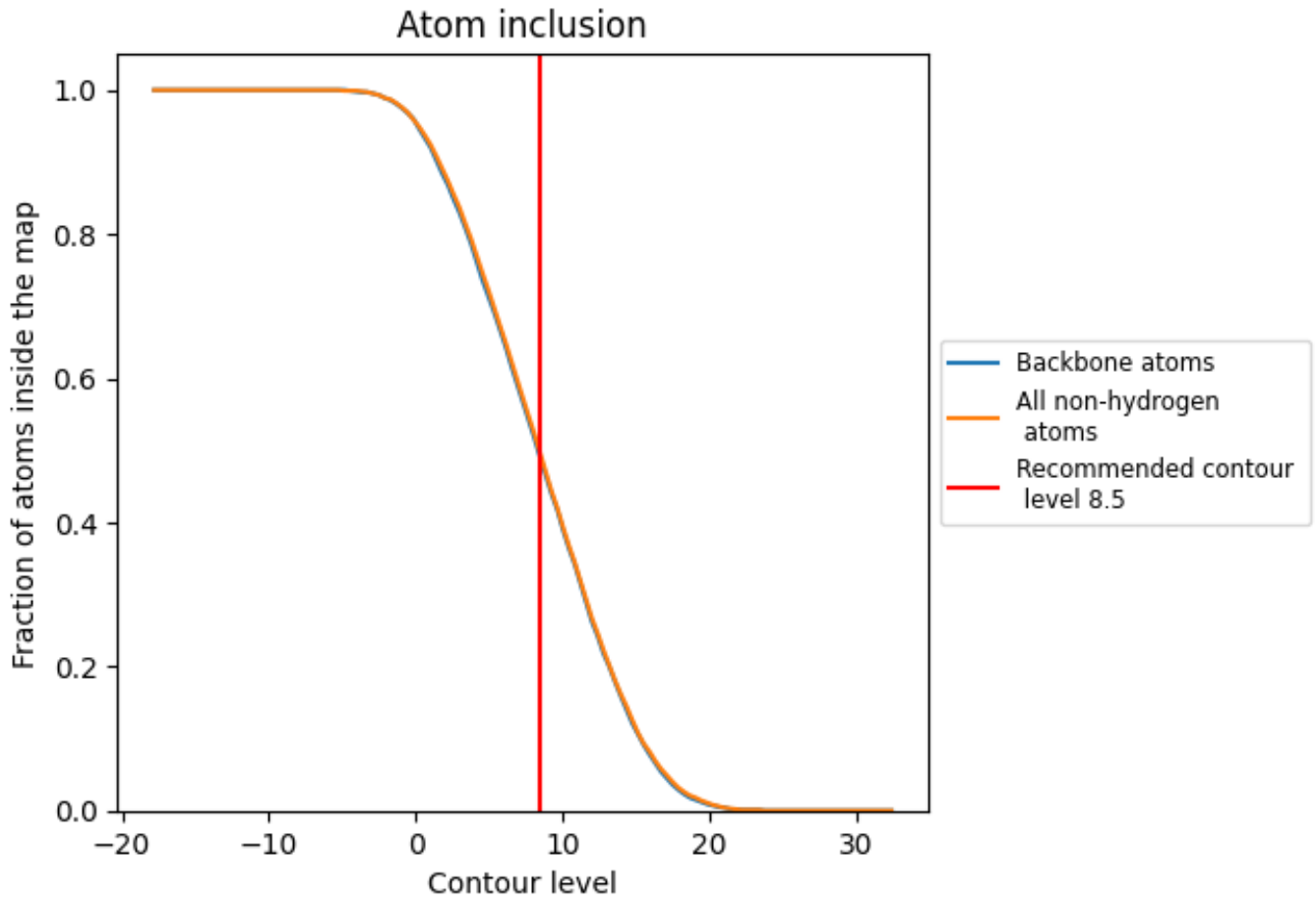
9.3 Atom inclusion mapped to coordinate model



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 (8.5).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 50% 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 (8.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4960	0.2770
A	0.5090	0.2790
B	0.5130	0.2810
C	0.5080	0.2690
D	0.5210	0.2690
E	0.5090	0.2660
F	0.5220	0.2790
G	0.4980	0.2730
H	0.5210	0.2800
I	0.5240	0.2790
J	0.5210	0.2890
K	0.4950	0.2840
L	0.4920	0.2840
M	0.4110	0.2650