



wwPDB EM Validation Summary Report ⓘ

Jun 4, 2025 – 04:39 PM JST

PDB ID : 8XCH / pdb_00008xch
EMDB ID : EMD-38243
Title : SARS-CoV-2 Replication-Transcription Complex has a dimer-of-dimeric architecture (ddRTC) in pre-capping initiation.
Authors : Yan, L.; Lou, Z.
Deposited on : 2023-12-09
Resolution : 3.40 Å(reported)

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

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

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
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) : 2.43.1

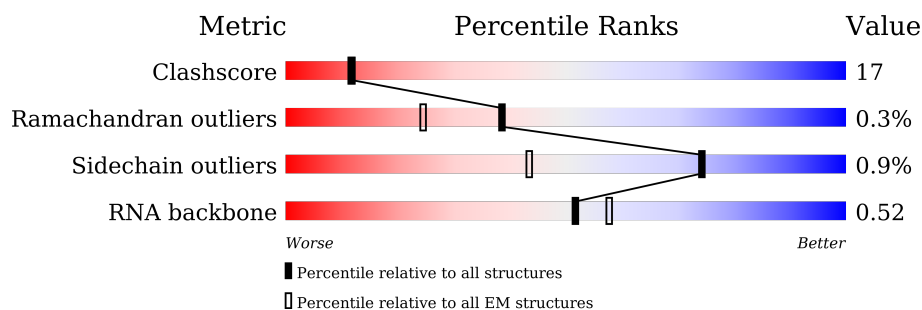
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	942	77% 21% .
1	I	942	77% 21% .
1	Q	942	74% 24% .
1	Y	942	74% 24% .
2	B	198	73% 21% . 6%
2	D	198	61% 33% 6%
2	J	198	69% 25% 6%

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Mol	Chain	Length	Quality of chain
2	L	198	
2	R	198	
2	T	198	
2	Z	198	
2	b	198	
3	C	83	
3	K	83	
3	S	83	
3	a	83	
4	E	601	
4	F	601	
4	M	601	
4	N	601	
4	U	601	
4	V	601	
4	c	601	
4	d	601	
5	G	39	
5	O	39	
5	W	39	
5	e	39	
6	H	39	
6	P	39	
6	X	39	
6	f	39	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 86774 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 Replicase polyprotein 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	926	Total	C	N	O	S	0	0
			7458	4763	1251	1390	54		
1	I	926	Total	C	N	O	S	0	0
			7458	4763	1251	1390	54		
1	Q	926	Total	C	N	O	S	0	0
			7458	4763	1251	1390	54		
1	Y	926	Total	C	N	O	S	0	0
			7458	4763	1251	1390	54		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	933	HIS	-	expression tag	UNP P0DTD1
A	934	HIS	-	expression tag	UNP P0DTD1
A	935	HIS	-	expression tag	UNP P0DTD1
A	936	HIS	-	expression tag	UNP P0DTD1
A	937	HIS	-	expression tag	UNP P0DTD1
A	938	HIS	-	expression tag	UNP P0DTD1
A	939	HIS	-	expression tag	UNP P0DTD1
A	940	HIS	-	expression tag	UNP P0DTD1
A	941	HIS	-	expression tag	UNP P0DTD1
A	942	HIS	-	expression tag	UNP P0DTD1
I	933	HIS	-	expression tag	UNP P0DTD1
I	934	HIS	-	expression tag	UNP P0DTD1
I	935	HIS	-	expression tag	UNP P0DTD1
I	936	HIS	-	expression tag	UNP P0DTD1
I	937	HIS	-	expression tag	UNP P0DTD1
I	938	HIS	-	expression tag	UNP P0DTD1
I	939	HIS	-	expression tag	UNP P0DTD1
I	940	HIS	-	expression tag	UNP P0DTD1
I	941	HIS	-	expression tag	UNP P0DTD1
I	942	HIS	-	expression tag	UNP P0DTD1
Q	933	HIS	-	expression tag	UNP P0DTD1
Q	934	HIS	-	expression tag	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	935	HIS	-	expression tag	UNP P0DTD1
Q	936	HIS	-	expression tag	UNP P0DTD1
Q	937	HIS	-	expression tag	UNP P0DTD1
Q	938	HIS	-	expression tag	UNP P0DTD1
Q	939	HIS	-	expression tag	UNP P0DTD1
Q	940	HIS	-	expression tag	UNP P0DTD1
Q	941	HIS	-	expression tag	UNP P0DTD1
Q	942	HIS	-	expression tag	UNP P0DTD1
Y	933	HIS	-	expression tag	UNP P0DTD1
Y	934	HIS	-	expression tag	UNP P0DTD1
Y	935	HIS	-	expression tag	UNP P0DTD1
Y	936	HIS	-	expression tag	UNP P0DTD1
Y	937	HIS	-	expression tag	UNP P0DTD1
Y	938	HIS	-	expression tag	UNP P0DTD1
Y	939	HIS	-	expression tag	UNP P0DTD1
Y	940	HIS	-	expression tag	UNP P0DTD1
Y	941	HIS	-	expression tag	UNP P0DTD1
Y	942	HIS	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1400	873	241	275	11		
2	D	186	Total	C	N	O	S	0	0
			1418	892	243	272	11		
2	J	187	Total	C	N	O	S	0	0
			1400	873	241	275	11		
2	L	186	Total	C	N	O	S	0	0
			1418	892	243	272	11		
2	R	187	Total	C	N	O	S	0	0
			1400	873	241	275	11		
2	T	186	Total	C	N	O	S	0	0
			1418	892	243	272	11		
2	Z	187	Total	C	N	O	S	0	0
			1400	873	241	275	11		
2	b	186	Total	C	N	O	S	0	0
			1418	892	243	272	11		

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	72	Total	C	N	O	S	0	0
			553	349	91	107	6		
3	K	72	Total	C	N	O	S	0	0
			553	349	91	107	6		
3	S	72	Total	C	N	O	S	0	0
			553	349	91	107	6		
3	a	72	Total	C	N	O	S	0	0
			553	349	91	107	6		

- Molecule 4 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	590	Total	C	N	O	S	0	0
			4602	2926	781	861	34		
4	F	596	Total	C	N	O	S	0	0
			4618	2935	781	869	33		
4	M	587	Total	C	N	O	S	1	0
			4558	2903	766	854	35		
4	N	596	Total	C	N	O	S	0	0
			4624	2938	784	869	33		
4	U	590	Total	C	N	O	S	0	0
			4602	2926	781	861	34		
4	V	596	Total	C	N	O	S	0	0
			4618	2935	781	869	33		
4	c	587	Total	C	N	O	S	1	0
			4558	2903	766	854	35		
4	d	596	Total	C	N	O	S	0	0
			4634	2944	788	869	33		

- Molecule 5 is a RNA chain called RNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	39	Total	C	N	O	P	0	0
			844	376	160	269	39		
5	O	37	Total	C	N	O	P	0	0
			802	357	152	256	37		
5	W	39	Total	C	N	O	P	0	0
			844	376	160	269	39		
5	e	38	Total	C	N	O	P	0	0
			824	367	157	262	38		

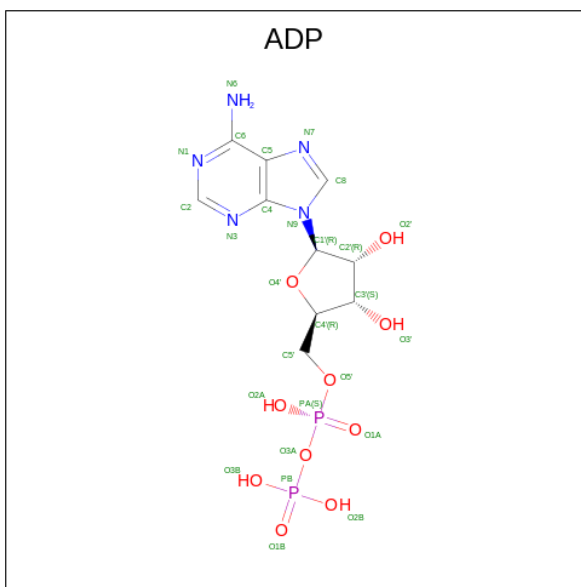
- Molecule 6 is a RNA chain called RNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	39	Total	C	N	O	P	0	0
			815	365	134	277	39		
6	P	39	Total	C	N	O	P	0	0
			815	365	134	277	39		
6	X	39	Total	C	N	O	P	0	0
			815	365	134	277	39		
6	f	38	Total	C	N	O	P	0	0
			792	355	129	270	38		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Zn	0
			2	2	
7	E	3	Total	Zn	0
			3	3	
7	F	3	Total	Zn	0
			3	3	
7	I	2	Total	Zn	0
			2	2	
7	M	3	Total	Zn	0
			3	3	
7	N	3	Total	Zn	0
			3	3	
7	Q	2	Total	Zn	0
			2	2	
7	U	3	Total	Zn	0
			3	3	
7	V	3	Total	Zn	0
			3	3	
7	Y	2	Total	Zn	0
			2	2	
7	c	3	Total	Zn	0
			3	3	
7	d	3	Total	Zn	0
			3	3	

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

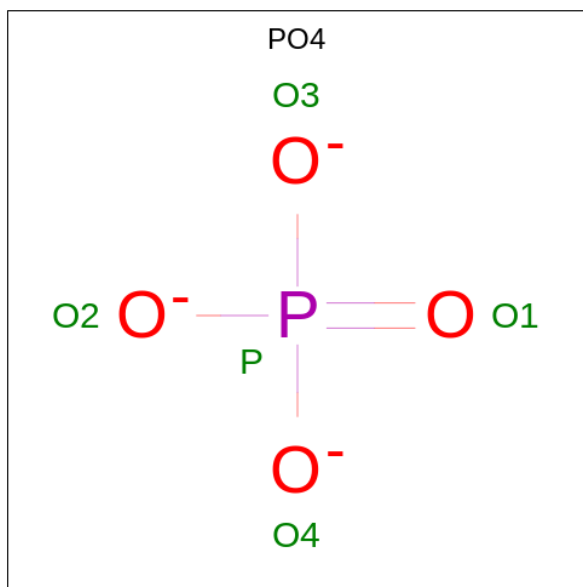


Mol	Chain	Residues	Atoms				AltConf	
8	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	d	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	I	1	Total	Mg	0
			1	1	
9	Y	1	Total	Mg	0
			1	1	

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).

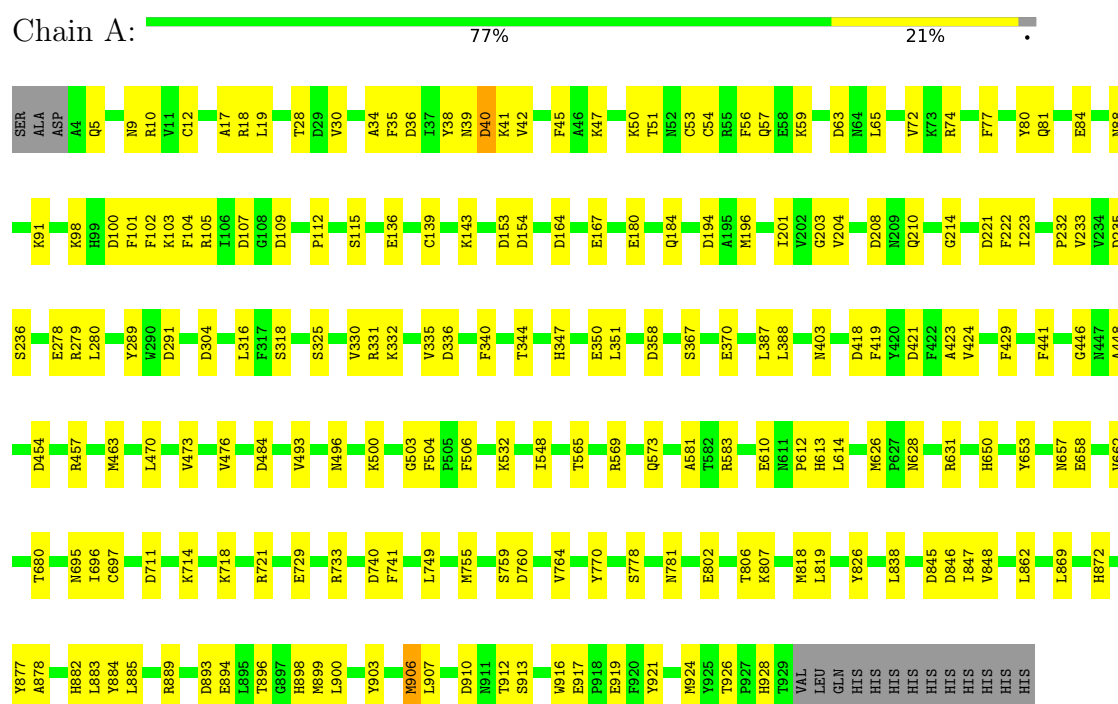


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
10	d	1	5	4	1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

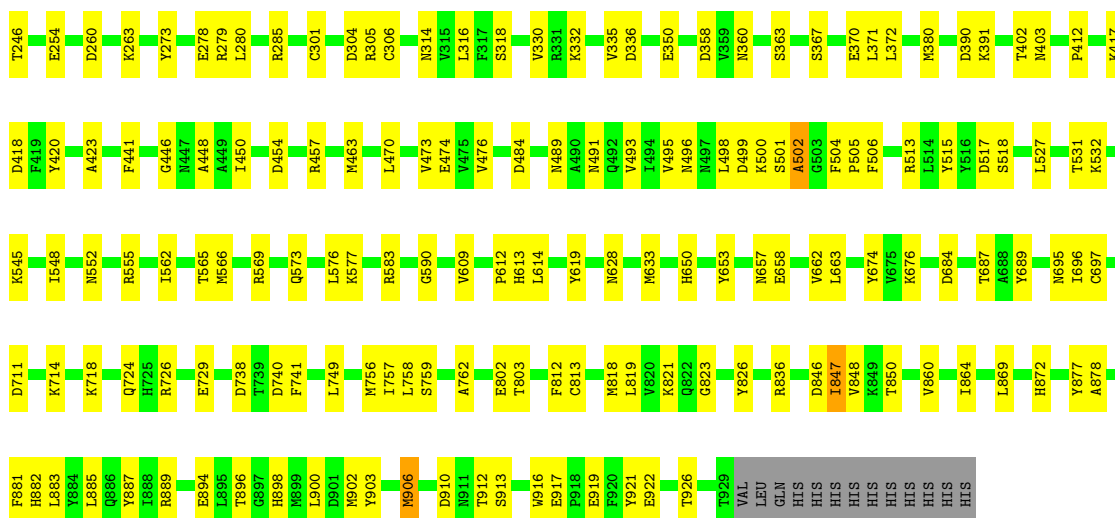
• Molecule 1: Replicase polypeptide 1ab



• Molecule 1: Replicase polypeptide 1ab

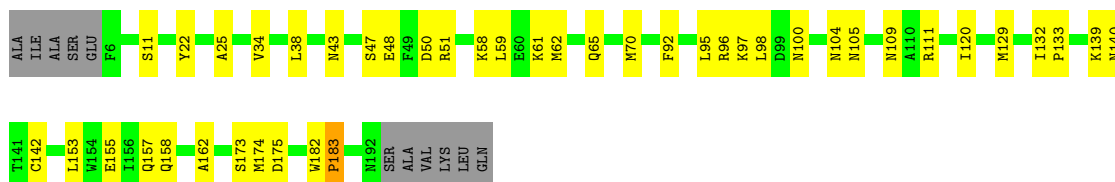






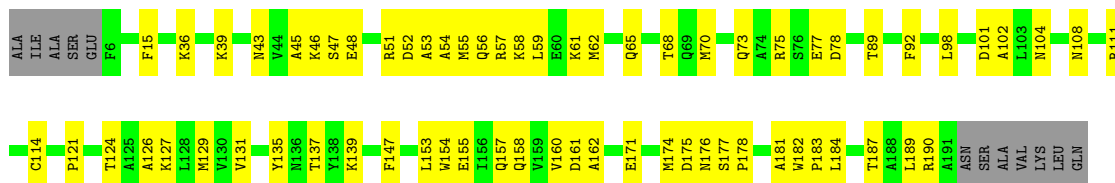
• Molecule 2: Non-structural protein 8

Chain B: 73% 21% 6%



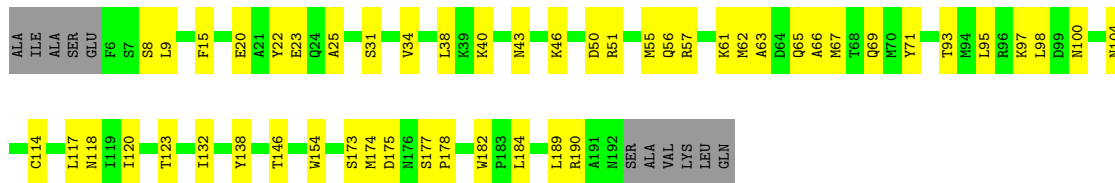
• Molecule 2: Non-structural protein 8

Chain D: 61% 33% 6%



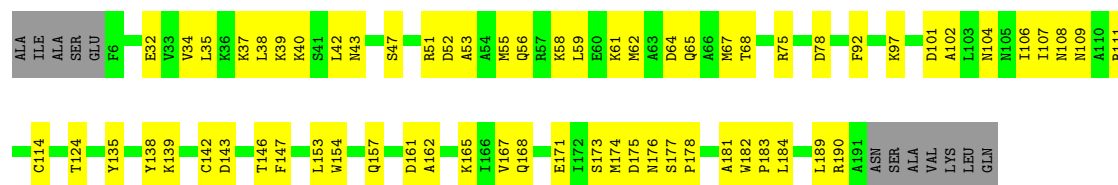
• Molecule 2: Non-structural protein 8

Chain J: 69% 25% 6%



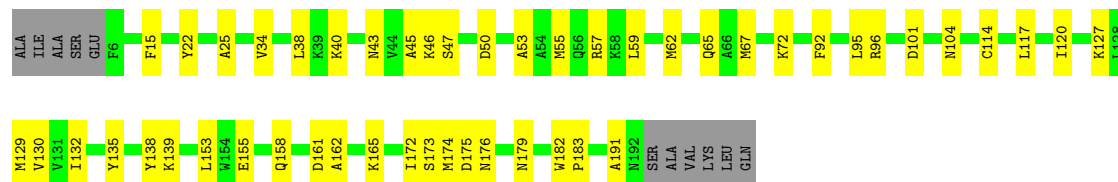
• Molecule 2: Non-structural protein 8

Chain L: 61% 33% 6%



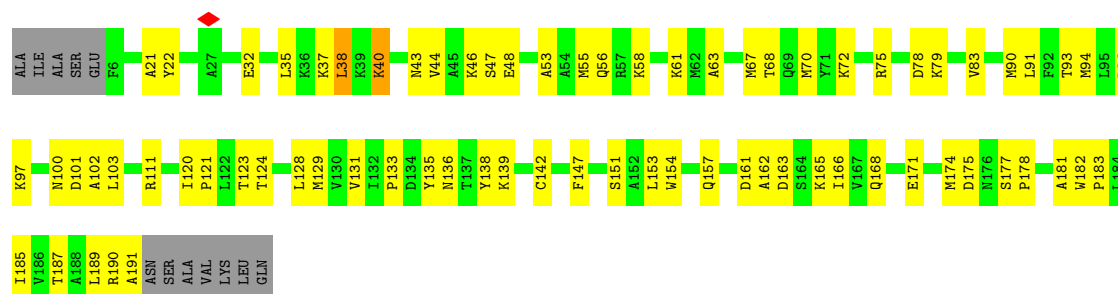
• Molecule 2: Non-structural protein 8

Chain R: 70% 25% 6%



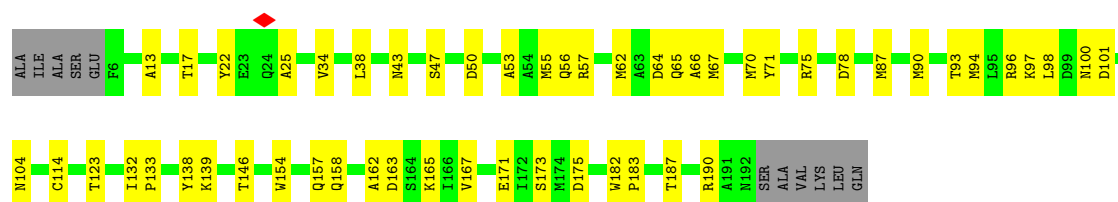
• Molecule 2: Non-structural protein 8

Chain T: 57% 36% 6%



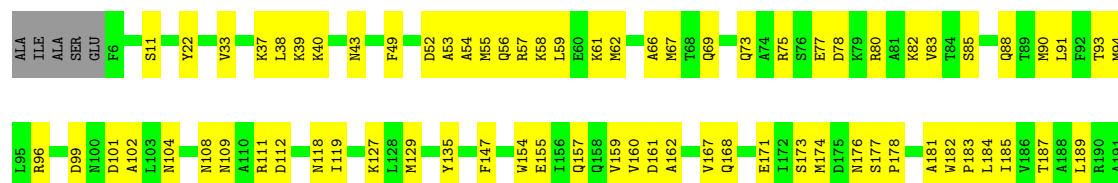
• Molecule 2: Non-structural protein 8

Chain Z: 68% 27% 6%



• Molecule 2: Non-structural protein 8

Chain b: 58% 36% 6%



ASN
SER
ALA
VAL
LYS
LEU
GLN

• Molecule 3: Non-structural protein 7

Chain C: 64% 23% 13%

SER K2 M3 S4 D5 V6 K7 L14 L15 V16 Q19 H36 A42 K43 T46 E47 A48 F49 E50 K51 M52 V53 I68 N69 K70 E73 GLU MET LEU MET LEU ASP ASN ARG ALA THR LEU GLN

• Molecule 3: Non-structural protein 7

Chain K: 65% 22% 13%

SER K2 M3 S4 D5 V6 K7 L14 L15 V16 Q19 H36 A42 K43 T46 E47 A48 F49 E50 K51 M52 V53 I68 N69 K70 E73 GLU MET LEU MET LEU ASP ASN ARG ALA THR LEU GLN

• Molecule 3: Non-structural protein 7

Chain S: 64% 23% 13%

SER K2 M3 S4 D5 V6 K7 L14 L15 V16 Q19 H36 A42 K43 T46 E47 A48 F49 E50 K51 M52 V53 I68 N69 K70 E73 GLU MET LEU MET LEU ASP ASN ARG ALA THR LEU GLN

• Molecule 3: Non-structural protein 7

Chain a: 69% 18% 13%

SER K2 M3 S4 D5 V6 K7 L14 L15 V16 Q19 H36 A42 K43 T46 E47 A48 F49 E50 K51 M52 V53 I68 N69 K70 E73 GLU MET LEU MET LEU ASP ASN ARG ALA THR LEU GLN

• Molecule 4: Helicase

Chain E: 55% 42% ..

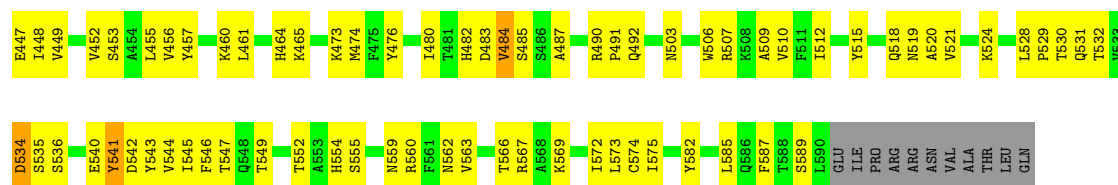
A1 V2 C5 V6 L7 C8 H9 S10 S13 T127 A18 R21 R22 C26 V34 I35 H39 K40 L43 Y48 N51 V57 Q62 L63 Y64 L65 G66 G67 M68 S69 Y70 Y71 C72 K73 S74 H75 K76 P77 P78 I79 S80 P82 L83 L92 Y93 V98

G99 S100 N101 N102 V103 T104 D105 Y120 C126 T127 E128 R129 L130 K131 L132 E136 E142 K146 L147 Y149 G150 I151 A152 T153 V154 R155 E156 V157 Q62 L63 Y64 L65 G66 G67 M68 S69 Y70 Y71 C72 K73 S74 H75 K76 P77 P78 I79 S80 P82 L83 L92 Y93 V98

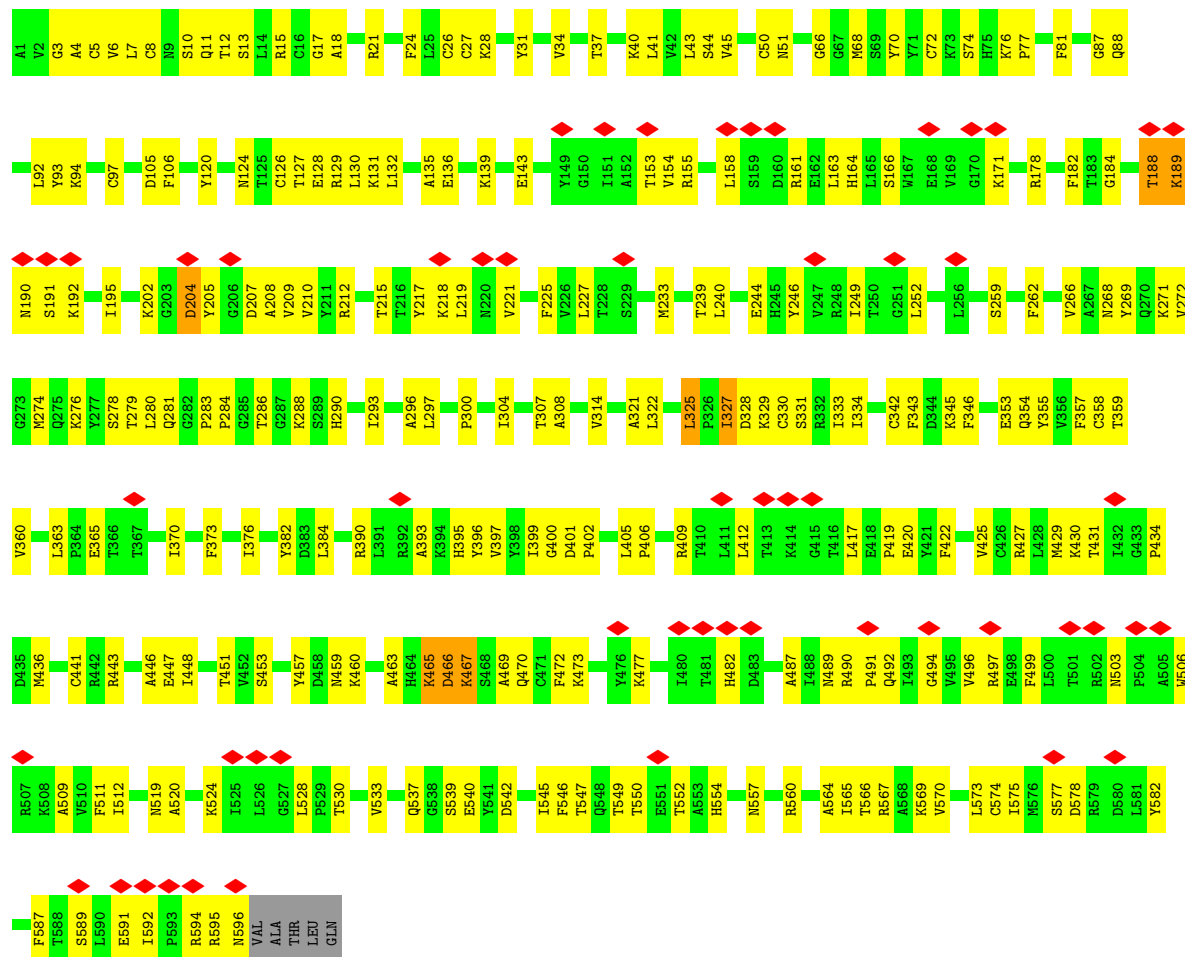
K192 I195 G196 E197 Y198 T199 F200 E201 D204 Y205 G206 D207 K208 L209 V210 Y211 R212 G213 T214 T215 K218 L219 N220 V221 G222 D223 Y224 F225 V226 L227 M233 P234 L235 E236 A237 V241 P242 Q243 E244 T249 T250 G251 P254 N257 D260 N268 Y269 V272 G273

M274 Q275 Y277 Q281 G282 P283 P284 G285 T286 G287 K288 S289 H290 F291 V291 A292 L295 Y299 R303 V304 V305 Y306 T307 A308 V314 E319 L322 P408 R409 S430 R332 L333 L334 R339 V340 F343 F346 K347 V348 R349 L352 E353 Q354 C441 Y355 V356 F357 C358 T359 A446

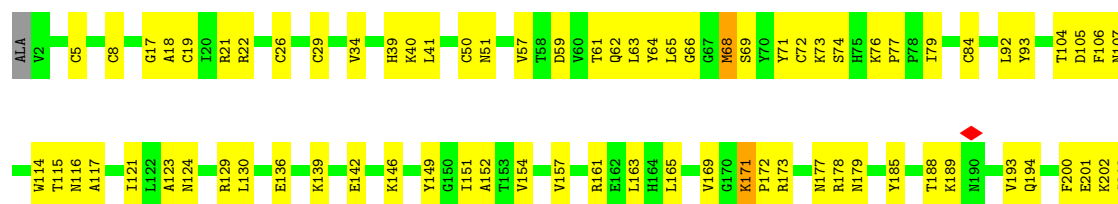
L363 T367 A368 D369 L370 V371 V372 L376 D383 L382 S385 V386 V387 N388 A389 R390 L391 R392 A393 K394 H395 V396 V397 G400 D401 Q404 L405 P406 A407 P408 R409 S430 R332 L333 L334 R339 V340 F343 F346 K347 V348 R349 L352 E353 Q354 C441 Y355 V356 F357 C358 T359 A446

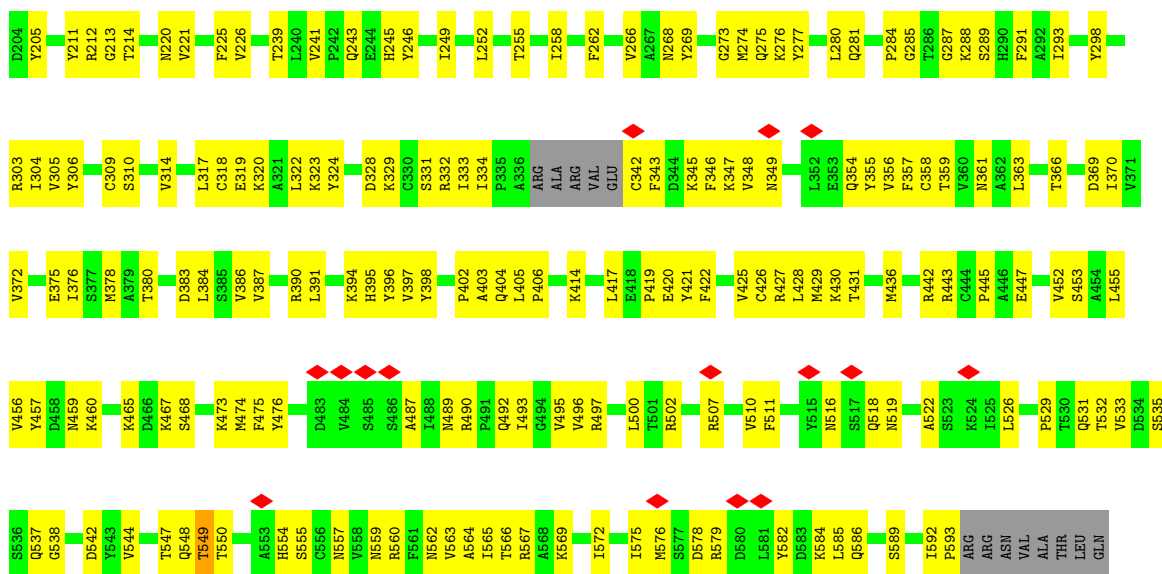


• Molecule 4: Helicase



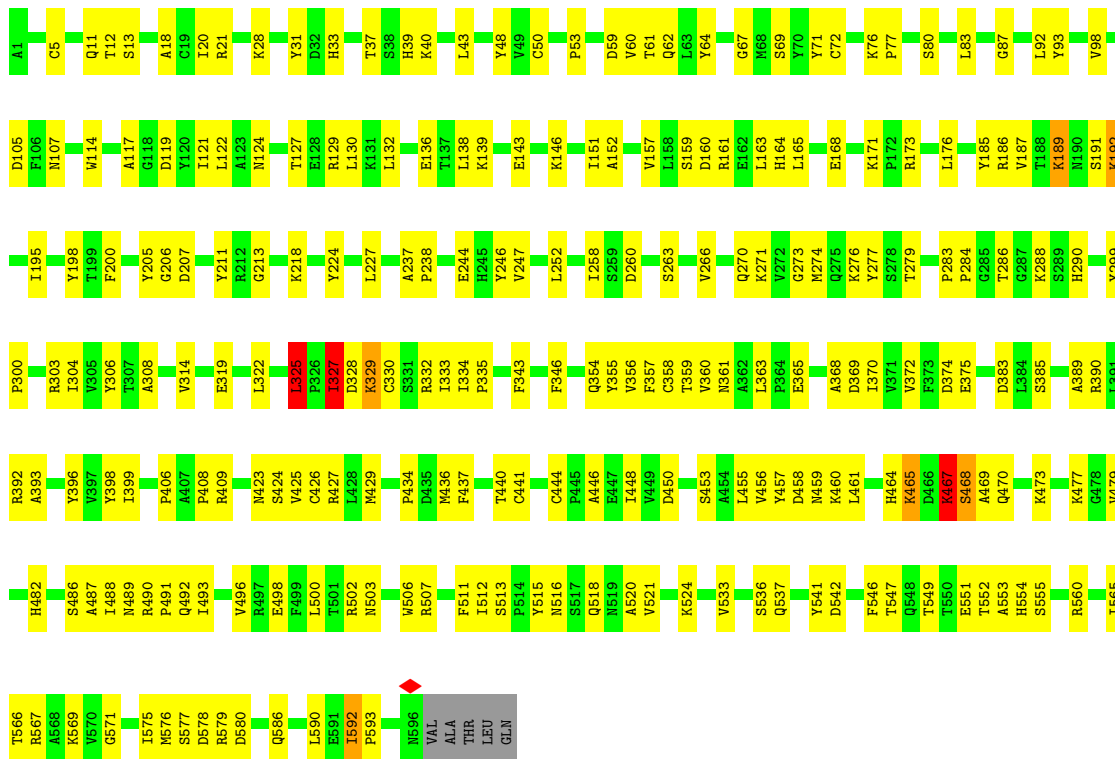
• Molecule 4: Helicase





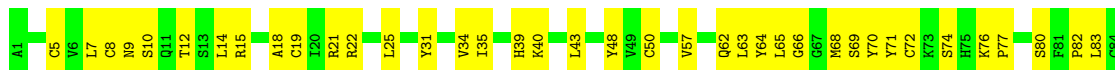
• Molecule 4: Helicase

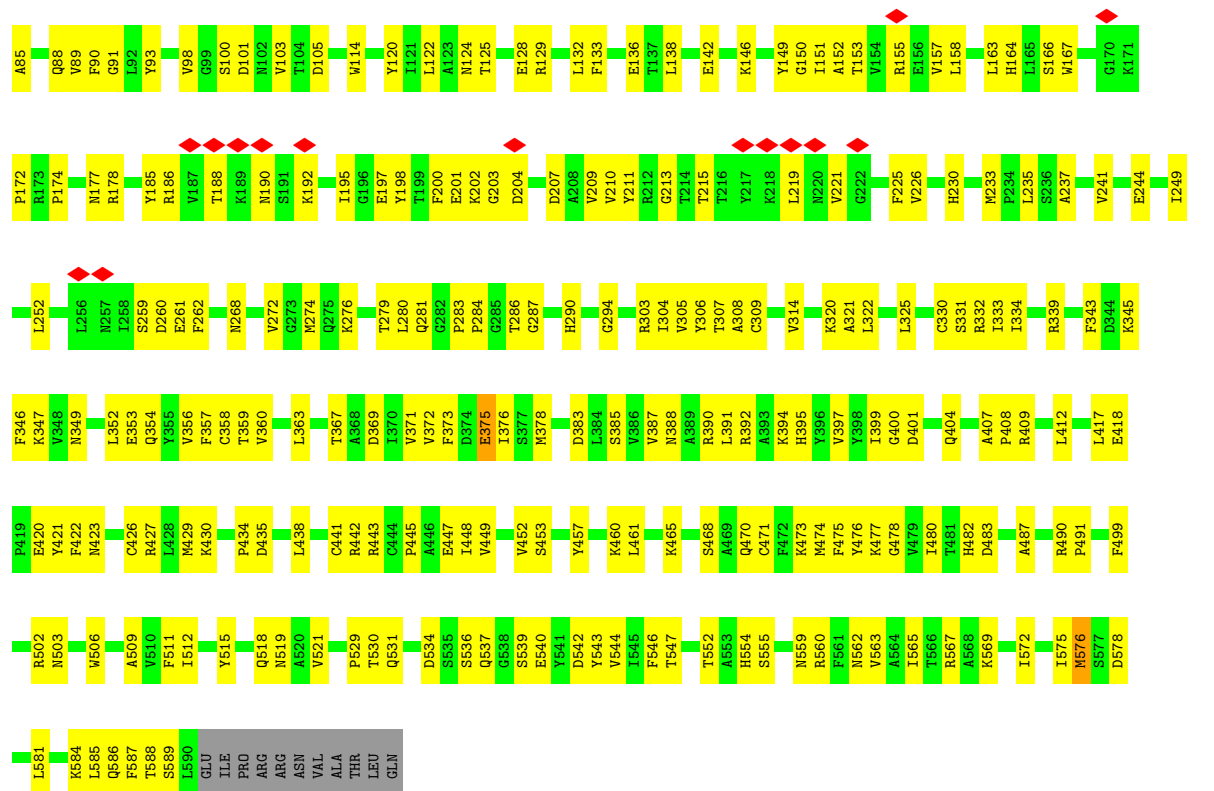
Chain N: 60% 38% ..



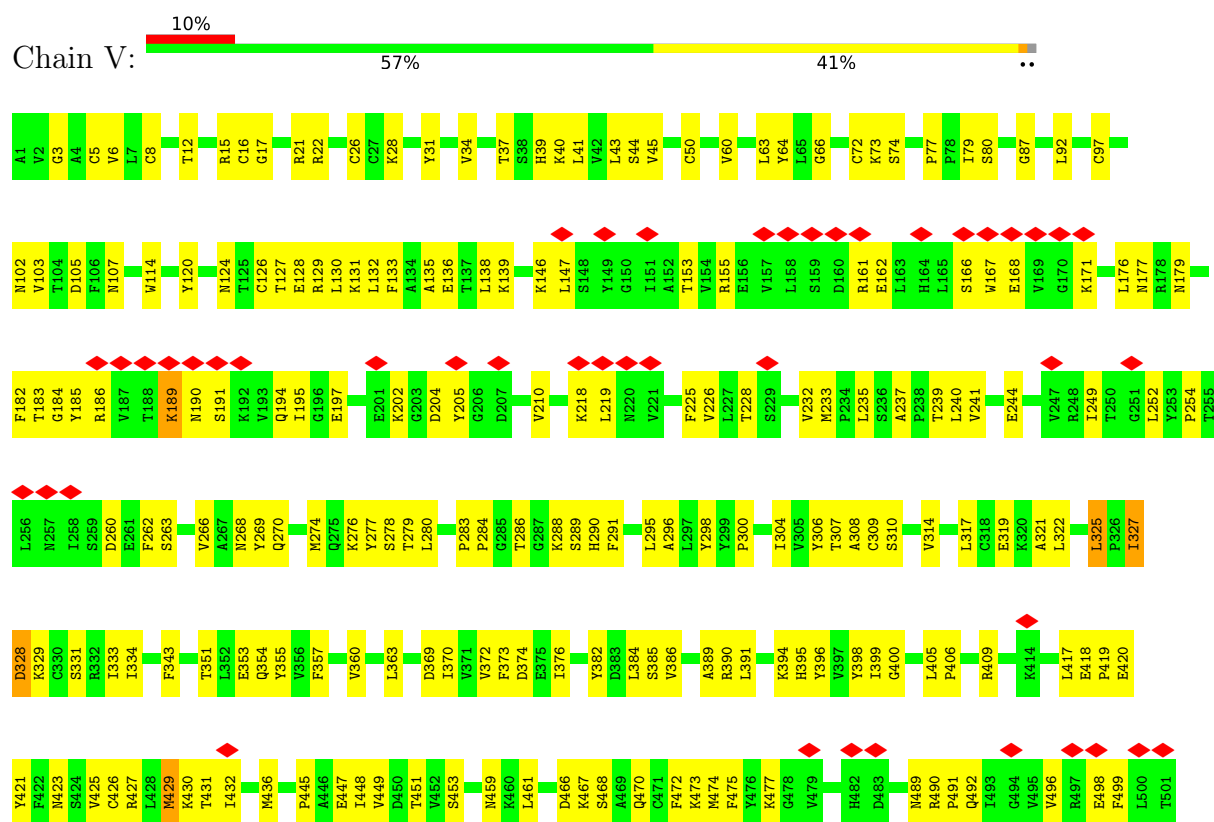
• Molecule 4: Helicase

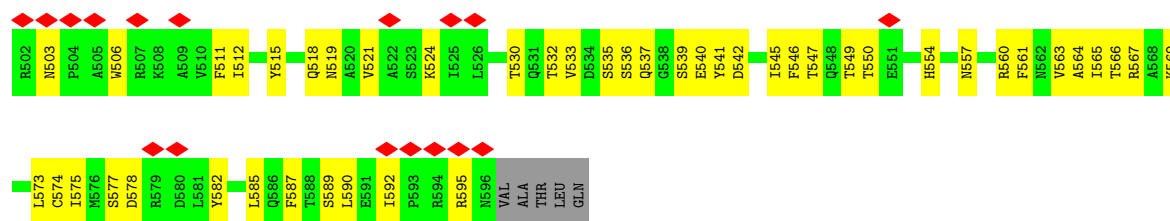
Chain U: 53% 45% .





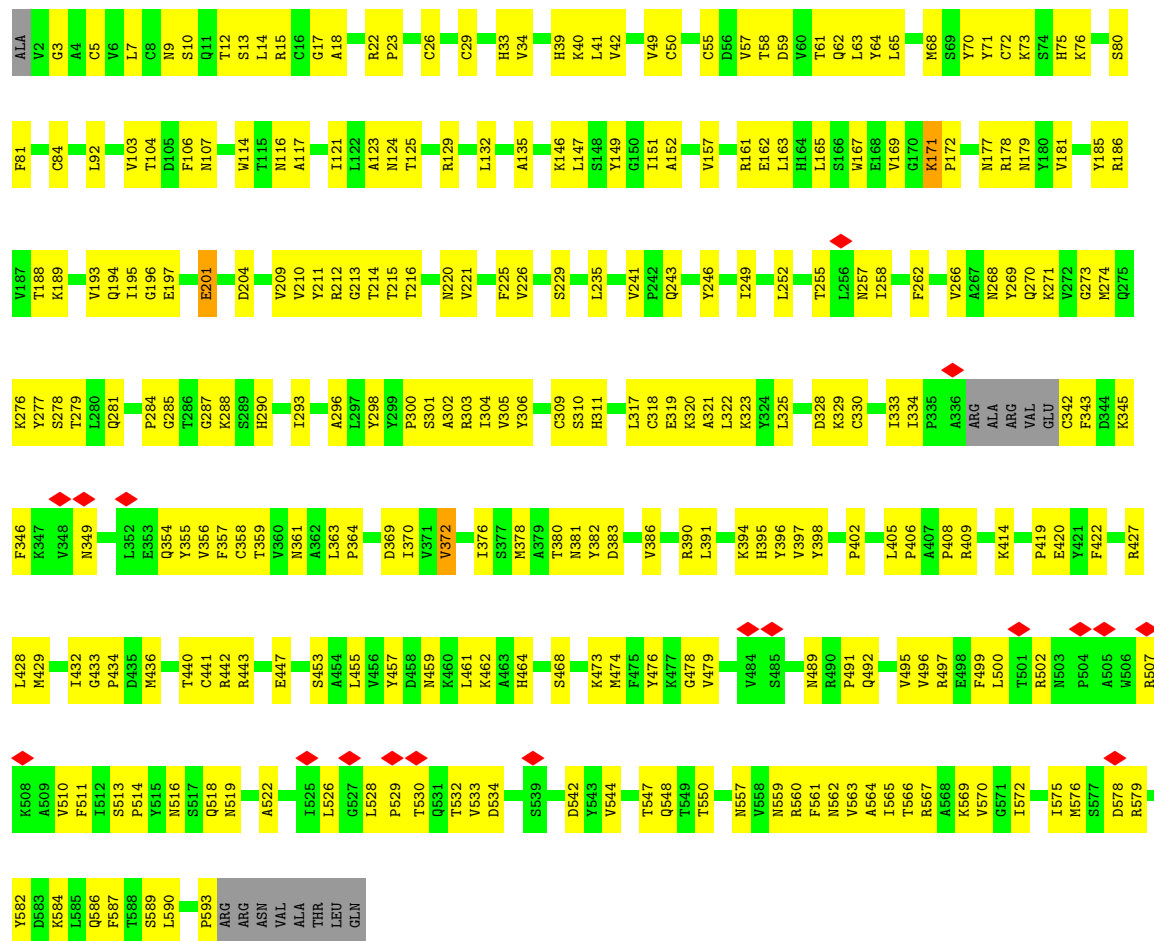
• Molecule 4: Helicase





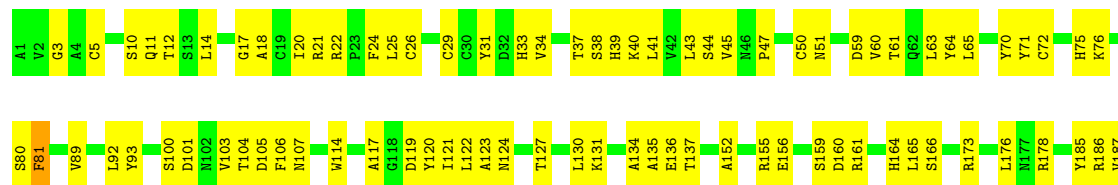
• Molecule 4: Helicase

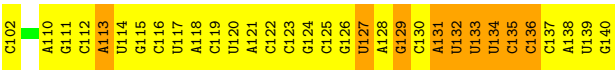
Chain c: 53% 45%



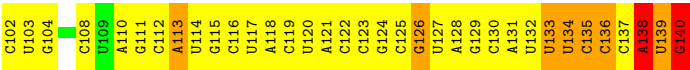
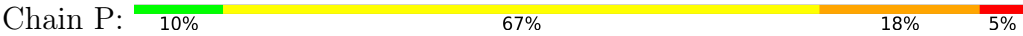
• Molecule 4: Helicase

Chain d: 53% 42%

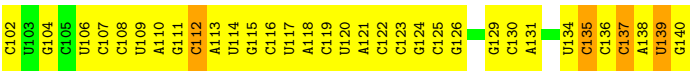




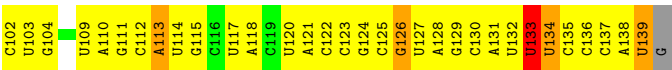
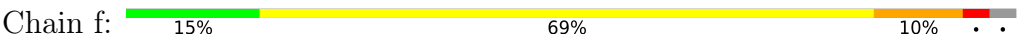
• Molecule 6: RNA (39-MER)



• Molecule 6: RNA (39-MER)



• Molecule 6: RNA (39-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213540	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.377	Depositor
Minimum map value	-1.773	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	488.32, 488.32, 488.32	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, PO4, 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	A	0.36	1/7647 (0.0%)	0.63	4/10379 (0.0%)
1	I	0.39	1/7647 (0.0%)	0.54	9/10379 (0.1%)
1	Q	0.26	0/7647	0.58	7/10379 (0.1%)
1	Y	0.26	0/7647	0.48	6/10379 (0.1%)
2	B	0.31	0/1418	0.51	0/1927
2	D	0.19	0/1437	0.47	0/1948
2	J	0.30	0/1418	0.51	0/1927
2	L	0.18	0/1437	0.41	0/1948
2	R	0.29	0/1418	0.49	0/1927
2	T	0.18	0/1437	0.48	1/1948 (0.1%)
2	Z	0.22	0/1418	0.50	0/1927
2	b	0.18	0/1437	0.44	1/1948 (0.1%)
3	C	0.25	0/556	0.45	0/749
3	K	0.25	0/556	0.43	0/749
3	S	0.18	0/556	0.47	0/749
3	a	0.15	0/556	0.34	0/749
4	E	0.27	1/4706 (0.0%)	0.53	5/6402 (0.1%)
4	F	0.23	1/4722 (0.0%)	0.52	8/6430 (0.1%)
4	M	0.16	0/4662	0.41	1/6348 (0.0%)
4	N	0.23	0/4728	0.51	6/6437 (0.1%)
4	U	0.15	0/4706	0.41	0/6402
4	V	0.16	0/4722	0.46	2/6430 (0.0%)
4	c	0.15	0/4662	0.39	0/6348
4	d	0.48	2/4738 (0.0%)	0.73	24/6448 (0.4%)
5	G	0.52	5/946 (0.5%)	0.34	0/1475
5	O	0.39	2/899 (0.2%)	0.31	0/1402
5	W	0.51	6/946 (0.6%)	0.31	0/1475
5	e	0.34	2/924 (0.2%)	0.30	0/1441
6	H	0.19	0/906	0.28	0/1406
6	P	0.44	4/906 (0.4%)	0.30	0/1406
6	X	0.38	1/906 (0.1%)	0.45	2/1406 (0.1%)
6	f	0.33	2/880 (0.2%)	0.32	0/1365

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.29	28/89191 (0.0%)	0.51	76/122633 (0.1%)

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	1
1	I	0	1
1	Q	0	2
2	B	0	1
2	J	0	1
2	R	0	1
2	Z	0	1
4	F	0	1
4	N	0	3
4	V	0	1
4	d	0	2
All	All	0	15

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	507	ASN	CA-C	-7.48	1.42	1.52
4	d	290	HIS	CA-C	-7.42	1.42	1.52
6	X	129	G	C1'-N9	-6.90	1.37	1.48
6	P	140	G	C1'-N9	-6.52	1.37	1.47
4	F	188	THR	CA-C	-6.36	1.49	1.52

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	PHE	CA-C-N	-28.86	83.77	119.84
1	A	504	PHE	C-N-CA	-28.86	83.77	119.84
1	Q	504	PHE	CA-C-N	-25.56	93.83	119.64
1	Q	504	PHE	C-N-CA	-25.56	93.83	119.64
4	d	291	PHE	N-CA-C	-15.34	94.34	113.97

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	906	MET	Peptide
2	B	182	TRP	Peptide
4	F	327	ILE	Peptide
1	I	502	ALA	Mainchain
2	J	182	TRP	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	A	7458	0	7191	133	0
1	I	7458	0	7191	148	0
1	Q	7458	0	7191	167	0
1	Y	7458	0	7191	161	0
2	B	1400	0	1372	31	0
2	D	1418	0	1427	53	0
2	J	1400	0	1372	41	0
2	L	1418	0	1427	51	0
2	R	1400	0	1372	42	0
2	T	1418	0	1427	55	0
2	Z	1400	0	1372	42	0
2	b	1418	0	1427	51	0
3	C	553	0	585	17	0
3	K	553	0	585	13	0
3	S	553	0	585	13	0
3	a	553	0	585	12	0
4	E	4602	0	4577	203	0
4	F	4618	0	4564	181	0
4	M	4558	0	4500	210	0
4	N	4624	0	4575	169	0
4	U	4602	0	4577	221	0
4	V	4618	0	4564	184	0
4	c	4558	0	4500	210	0
4	d	4634	0	4597	185	0
5	G	844	0	422	77	0
5	O	802	0	401	85	0
5	W	844	0	422	69	0
5	e	824	0	412	50	0
6	H	815	0	419	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	815	0	419	72	0
6	X	815	0	418	55	0
6	f	792	0	408	54	0
7	A	2	0	0	0	0
7	E	3	0	0	0	0
7	F	3	0	0	0	0
7	I	2	0	0	0	0
7	M	3	0	0	0	0
7	N	3	0	0	0	0
7	Q	2	0	0	0	0
7	U	3	0	0	0	0
7	V	3	0	0	0	0
7	Y	2	0	0	0	0
7	c	3	0	0	0	0
7	d	3	0	0	0	0
8	E	27	0	12	0	0
8	d	27	0	12	0	0
9	I	1	0	0	0	0
9	Y	1	0	0	0	0
10	d	5	0	0	1	0
All	All	86774	0	82099	2894	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 17.

The worst 5 of 2894 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)
5:G:3:A:N6	6:H:133:U:H3	0.94	1.43
5:O:3:A:N1	4:U:482:HIS:HB3	1.19	1.40
5:G:3:A:N6	6:H:133:U:N3	1.71	1.39
5:O:3:A:N1	5:O:4:A:C6	1.94	1.36
5:O:3:A:C6	5:O:4:A:N6	1.99	1.29

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	924/942 (98%)	849 (92%)	73 (8%)	2 (0%)	44	72
1	I	924/942 (98%)	846 (92%)	76 (8%)	2 (0%)	44	72
1	Q	924/942 (98%)	851 (92%)	71 (8%)	2 (0%)	44	72
1	Y	924/942 (98%)	861 (93%)	61 (7%)	2 (0%)	44	72
2	B	185/198 (93%)	170 (92%)	14 (8%)	1 (0%)	25	54
2	D	184/198 (93%)	174 (95%)	10 (5%)	0	100	100
2	J	185/198 (93%)	173 (94%)	12 (6%)	0	100	100
2	L	184/198 (93%)	175 (95%)	9 (5%)	0	100	100
2	R	185/198 (93%)	175 (95%)	9 (5%)	1 (0%)	25	54
2	T	184/198 (93%)	171 (93%)	13 (7%)	0	100	100
2	Z	185/198 (93%)	173 (94%)	11 (6%)	1 (0%)	25	54
2	b	184/198 (93%)	176 (96%)	8 (4%)	0	100	100
3	C	70/83 (84%)	68 (97%)	2 (3%)	0	100	100
3	K	70/83 (84%)	68 (97%)	2 (3%)	0	100	100
3	S	70/83 (84%)	65 (93%)	5 (7%)	0	100	100
3	a	70/83 (84%)	69 (99%)	1 (1%)	0	100	100
4	E	588/601 (98%)	517 (88%)	67 (11%)	4 (1%)	19	47
4	F	594/601 (99%)	517 (87%)	77 (13%)	0	100	100
4	M	584/601 (97%)	528 (90%)	53 (9%)	3 (0%)	25	54
4	N	594/601 (99%)	531 (89%)	60 (10%)	3 (0%)	25	54
4	U	588/601 (98%)	537 (91%)	49 (8%)	2 (0%)	37	66
4	V	594/601 (99%)	532 (90%)	61 (10%)	1 (0%)	44	72
4	c	584/601 (97%)	534 (91%)	47 (8%)	3 (0%)	25	54
4	d	594/601 (99%)	514 (86%)	72 (12%)	8 (1%)	10	33
All	All	10172/10492 (97%)	9274 (91%)	863 (8%)	35 (0%)	38	66

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	847	ILE
1	I	40	ASP
1	I	847	ILE
4	M	171	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	817/833 (98%)	817 (100%)	0	100	100
1	I	817/833 (98%)	817 (100%)	0	100	100
1	Q	817/833 (98%)	815 (100%)	2 (0%)	92	96
1	Y	817/833 (98%)	816 (100%)	1 (0%)	92	97
2	B	146/167 (87%)	144 (99%)	2 (1%)	62	77
2	D	150/167 (90%)	150 (100%)	0	100	100
2	J	146/167 (87%)	146 (100%)	0	100	100
2	L	150/167 (90%)	150 (100%)	0	100	100
2	R	146/167 (87%)	145 (99%)	1 (1%)	81	88
2	T	150/167 (90%)	148 (99%)	2 (1%)	65	78
2	Z	146/167 (87%)	145 (99%)	1 (1%)	81	88
2	b	150/167 (90%)	150 (100%)	0	100	100
3	C	67/77 (87%)	66 (98%)	1 (2%)	60	76
3	K	67/77 (87%)	67 (100%)	0	100	100
3	S	67/77 (87%)	67 (100%)	0	100	100
3	a	67/77 (87%)	67 (100%)	0	100	100
4	E	513/523 (98%)	503 (98%)	10 (2%)	52	71
4	F	512/523 (98%)	504 (98%)	8 (2%)	58	75
4	M	506/523 (97%)	503 (99%)	3 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	513/523 (98%)	503 (98%)	10 (2%)	52	71
4	U	513/523 (98%)	511 (100%)	2 (0%)	89	93
4	V	512/523 (98%)	507 (99%)	5 (1%)	73	83
4	c	506/523 (97%)	503 (99%)	3 (1%)	84	90
4	d	515/523 (98%)	488 (95%)	27 (5%)	19	45
All	All	8810/9160 (96%)	8732 (99%)	78 (1%)	74	86

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	258	ILE
4	d	536	SER
4	d	262	PHE
4	d	440	THR
4	d	560	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
4	U	51	ASN
1	Y	713	ASN
4	V	11	GLN
1	Y	158	ASN
2	Z	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	G	39/39 (100%)	7 (17%)	2 (5%)
5	O	36/39 (92%)	4 (11%)	2 (5%)
5	W	39/39 (100%)	7 (17%)	2 (5%)
5	e	37/39 (94%)	7 (18%)	0
6	H	38/39 (97%)	14 (36%)	0
6	P	38/39 (97%)	7 (18%)	1 (2%)
6	X	38/39 (97%)	7 (18%)	0
6	f	37/39 (94%)	7 (18%)	0
All	All	302/312 (96%)	60 (19%)	7 (2%)

5 of 60 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	G	-2	A
5	G	-1	U
5	G	0	G
5	G	4	A
5	G	18	G

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	O	24	U
6	P	139	U
5	W	24	U
5	W	-3	C
5	O	1	G

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](#)

Of 37 ligands modelled in this entry, 34 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
10	PO4	d	705	-	4,4,4	1.01	0	6,6,6	0.59	0
8	ADP	d	704	-	24,29,29	0.93	1 (4%)	29,45,45	1.51	4 (13%)
8	ADP	E	704	-	24,29,29	1.01	1 (4%)	29,45,45	1.72	6 (20%)

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
8	ADP	d	704	-	-	4/12/32/32	0/3/3/3
8	ADP	E	704	-	-	4/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	704	ADP	C5-C4	2.39	1.47	1.40
8	d	704	ADP	C5-C4	2.16	1.46	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	704	ADP	PA-O3A-PB	-3.95	119.28	132.83
8	d	704	ADP	PA-O3A-PB	-3.45	120.99	132.83
8	d	704	ADP	C3'-C2'-C1'	3.34	106.00	100.98
8	E	704	ADP	O2B-PB-O3A	3.28	115.65	104.64
8	E	704	ADP	C3'-C2'-C1'	3.23	105.85	100.98

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	704	ADP	C5'-O5'-PA-O3A
8	d	704	ADP	C5'-O5'-PA-O1A
8	E	704	ADP	PB-O3A-PA-O5'
8	E	704	ADP	C5'-O5'-PA-O1A
8	d	704	ADP	C5'-O5'-PA-O2A

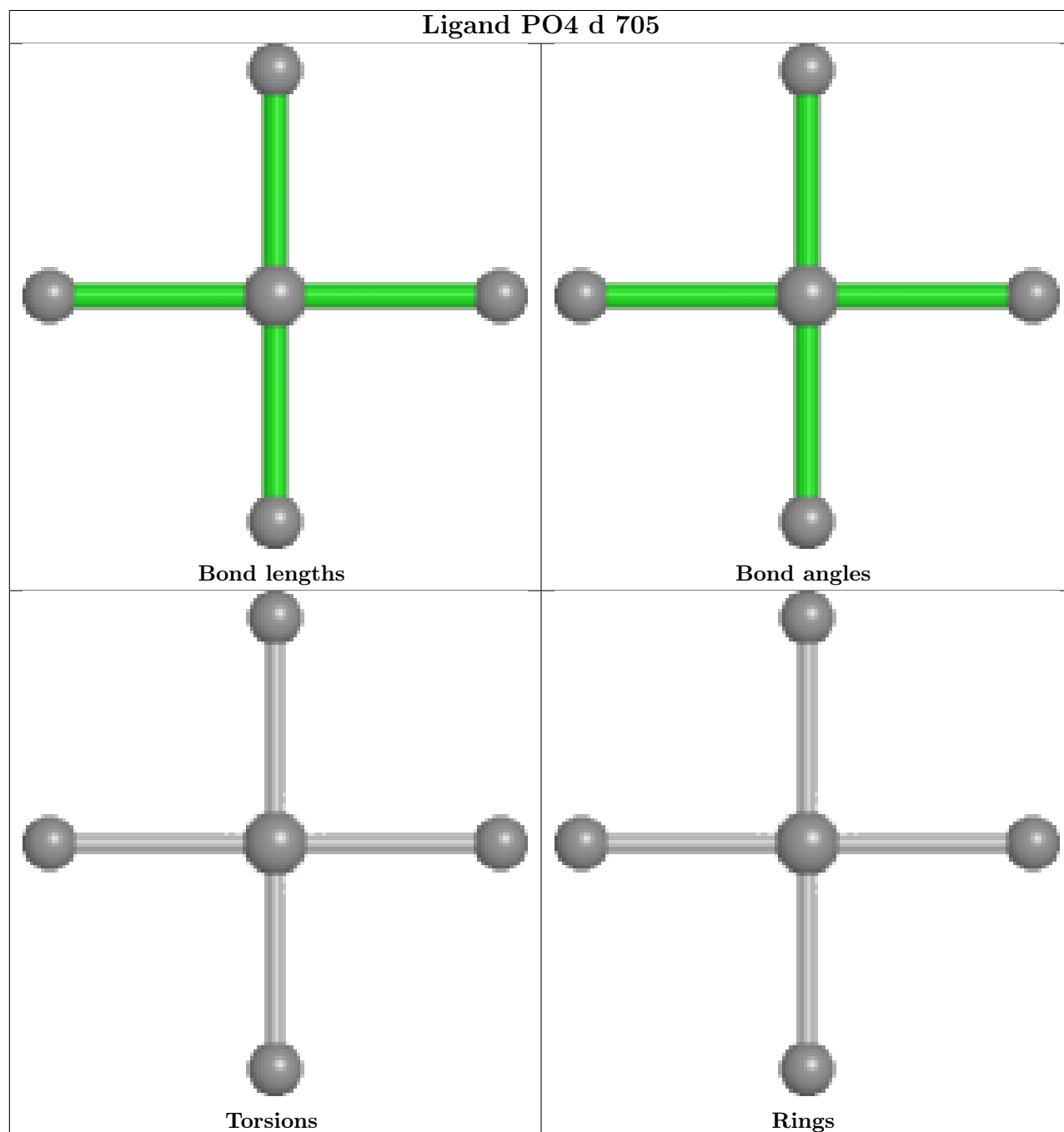
There are no ring outliers.

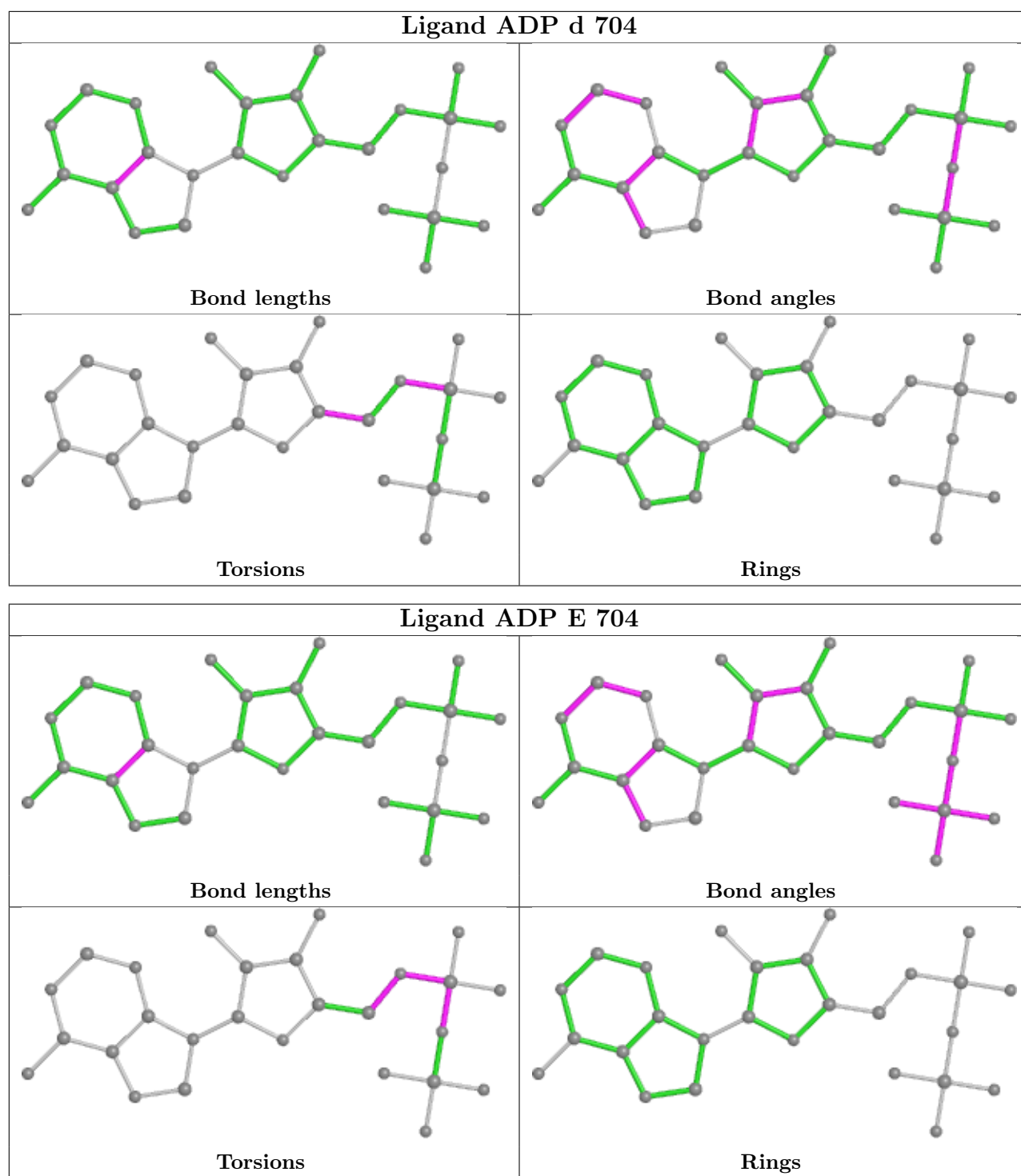
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	d	705	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

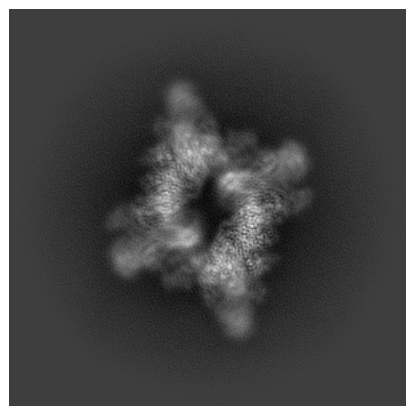
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38243. These allow visual inspection of the internal detail of the map and identification of artifacts.

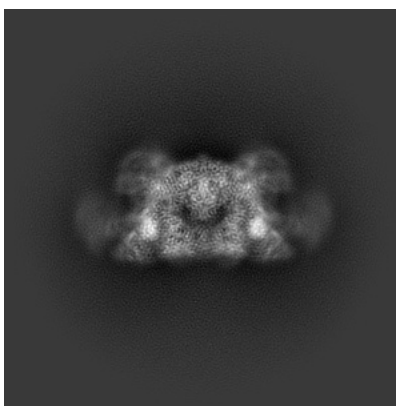
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

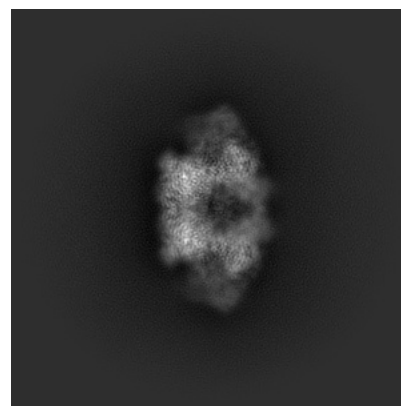
6.1.1 Primary map



X

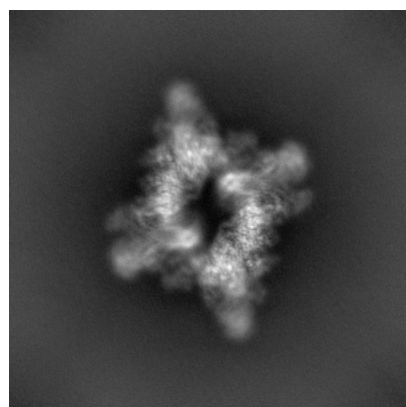


Y

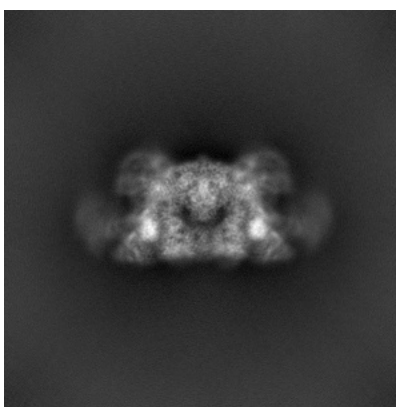


Z

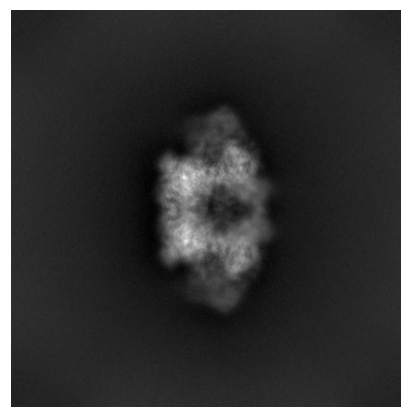
6.1.2 Raw map



X



Y

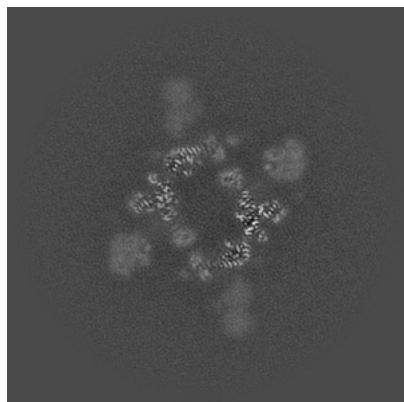


Z

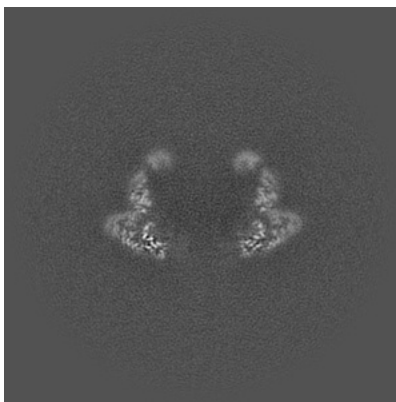
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

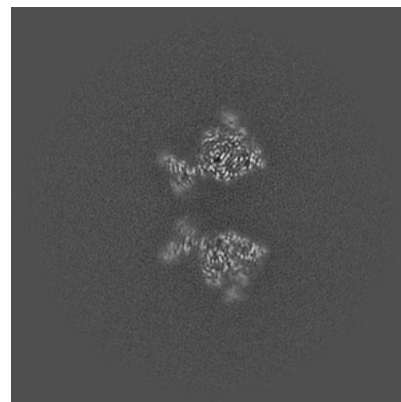
6.2.1 Primary map



X Index: 224

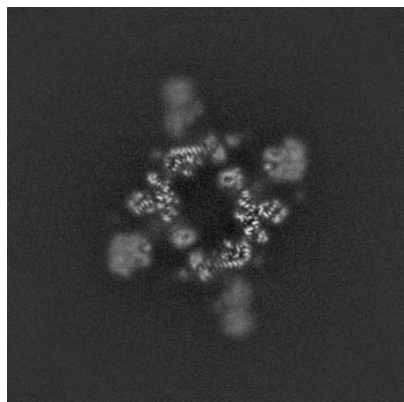


Y Index: 224

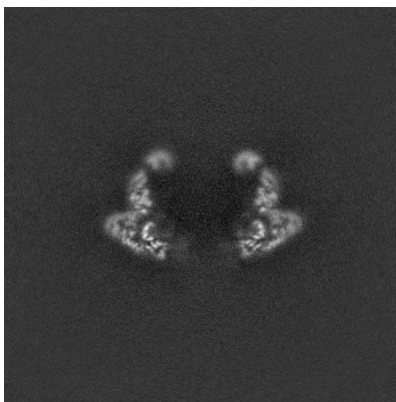


Z Index: 224

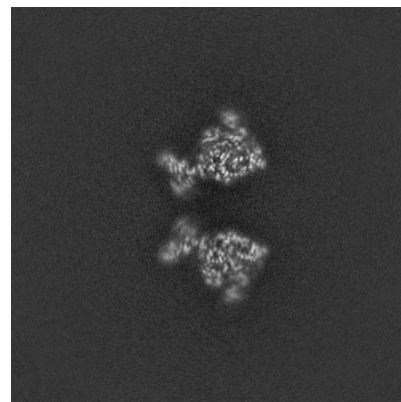
6.2.2 Raw map



X Index: 224



Y Index: 224

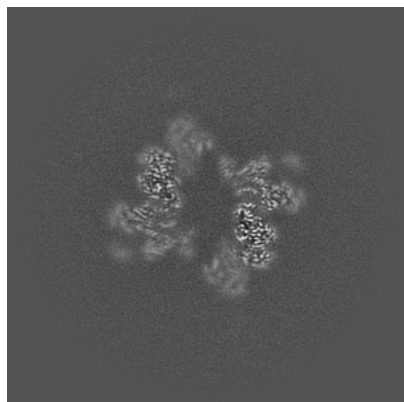


Z Index: 224

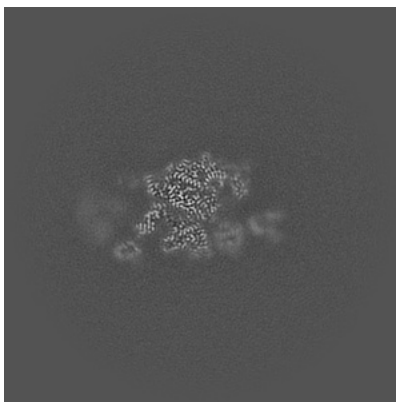
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

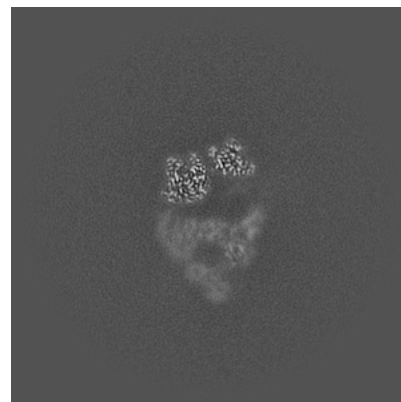
6.3.1 Primary map



X Index: 250

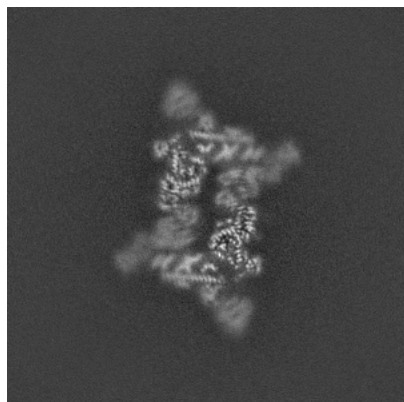


Y Index: 270

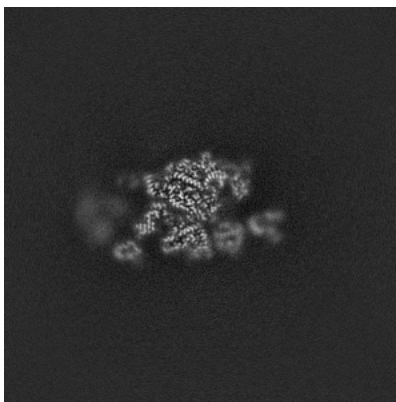


Z Index: 187

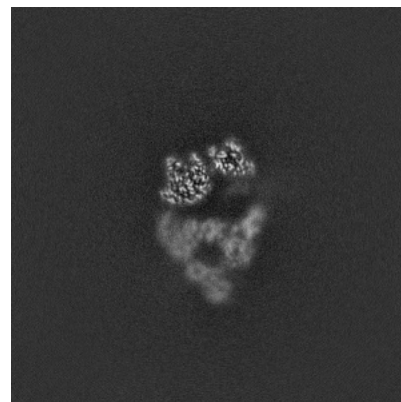
6.3.2 Raw map



X Index: 196



Y Index: 270

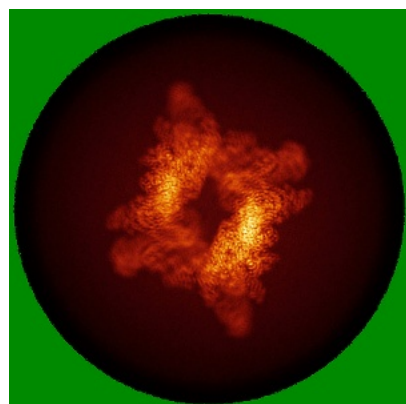


Z Index: 186

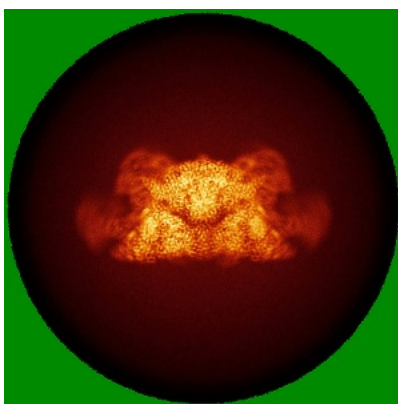
The images above show the largest variance slices of the map in three orthogonal directions.

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

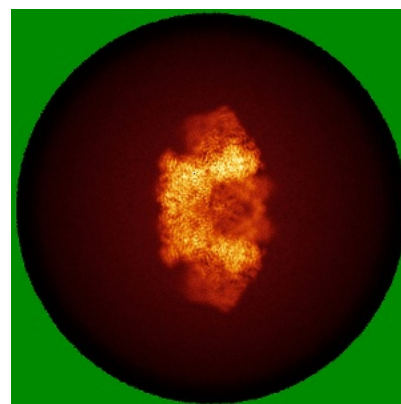
6.4.1 Primary map



X

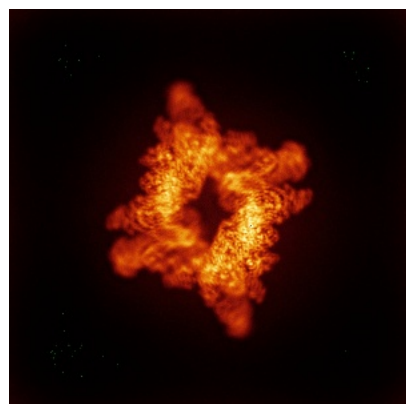


Y

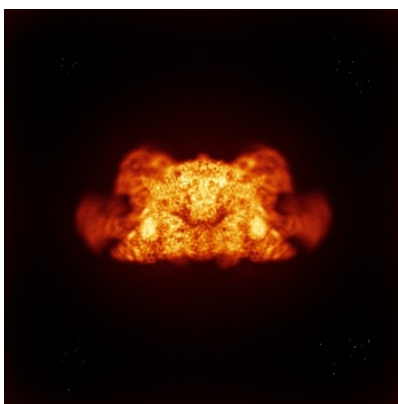


Z

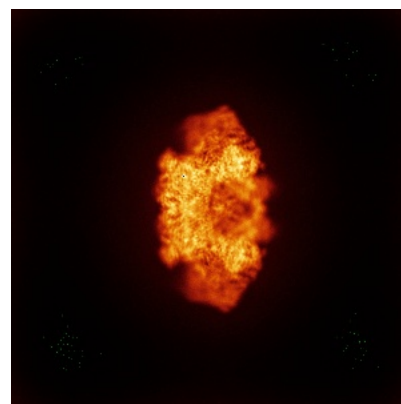
6.4.2 Raw map



X



Y

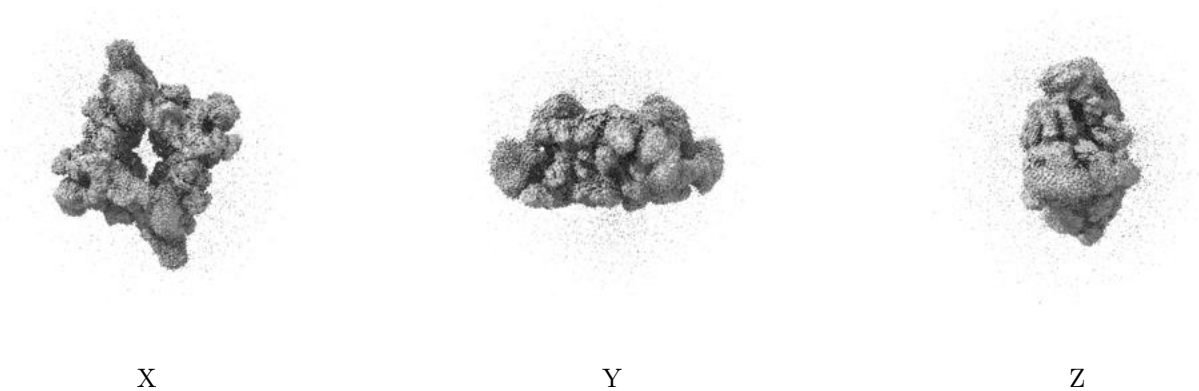


Z

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

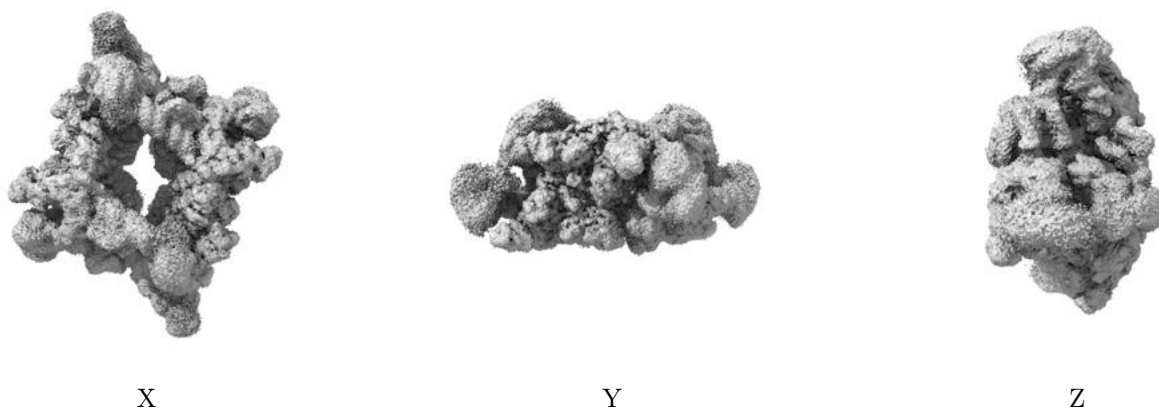
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

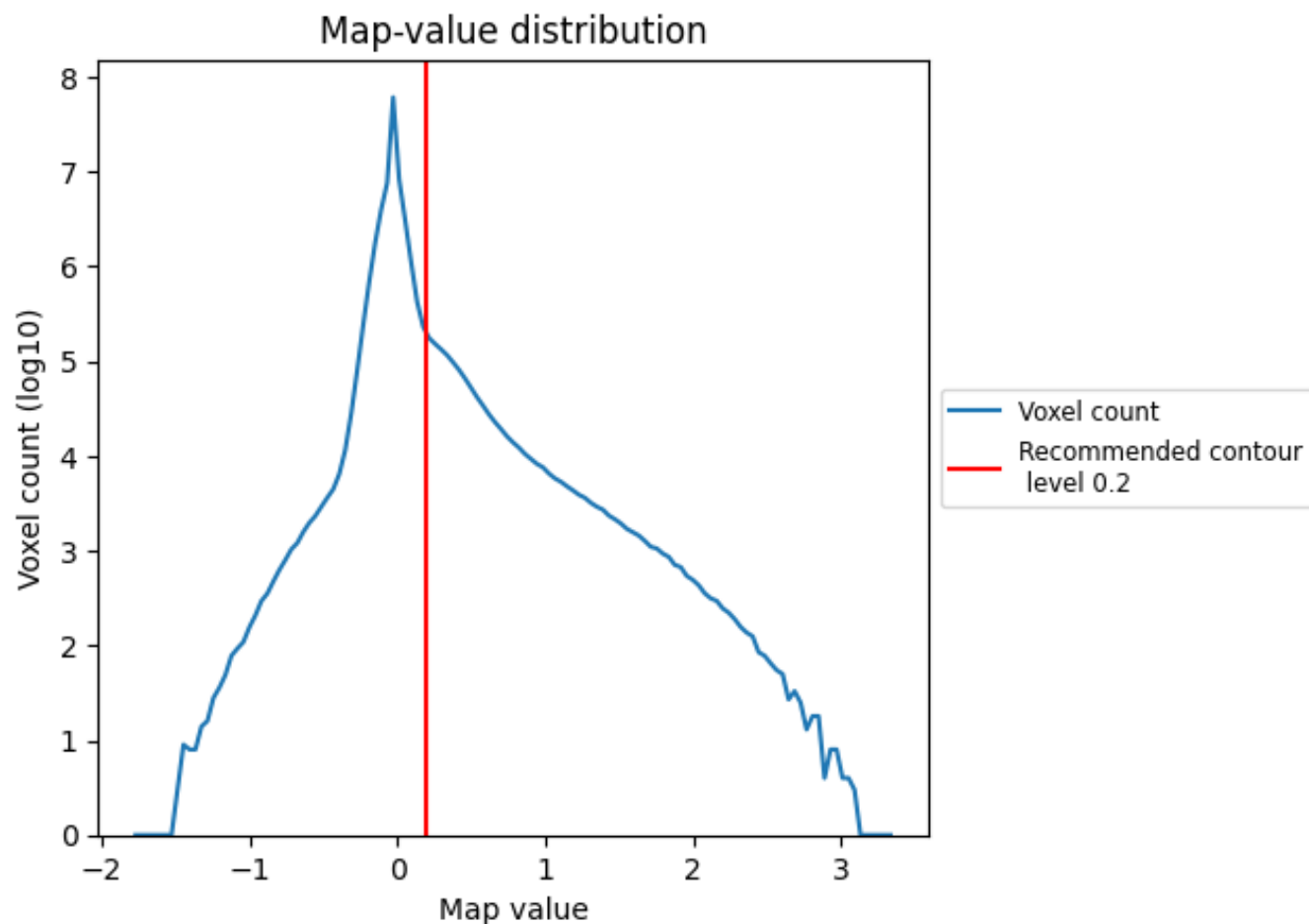
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

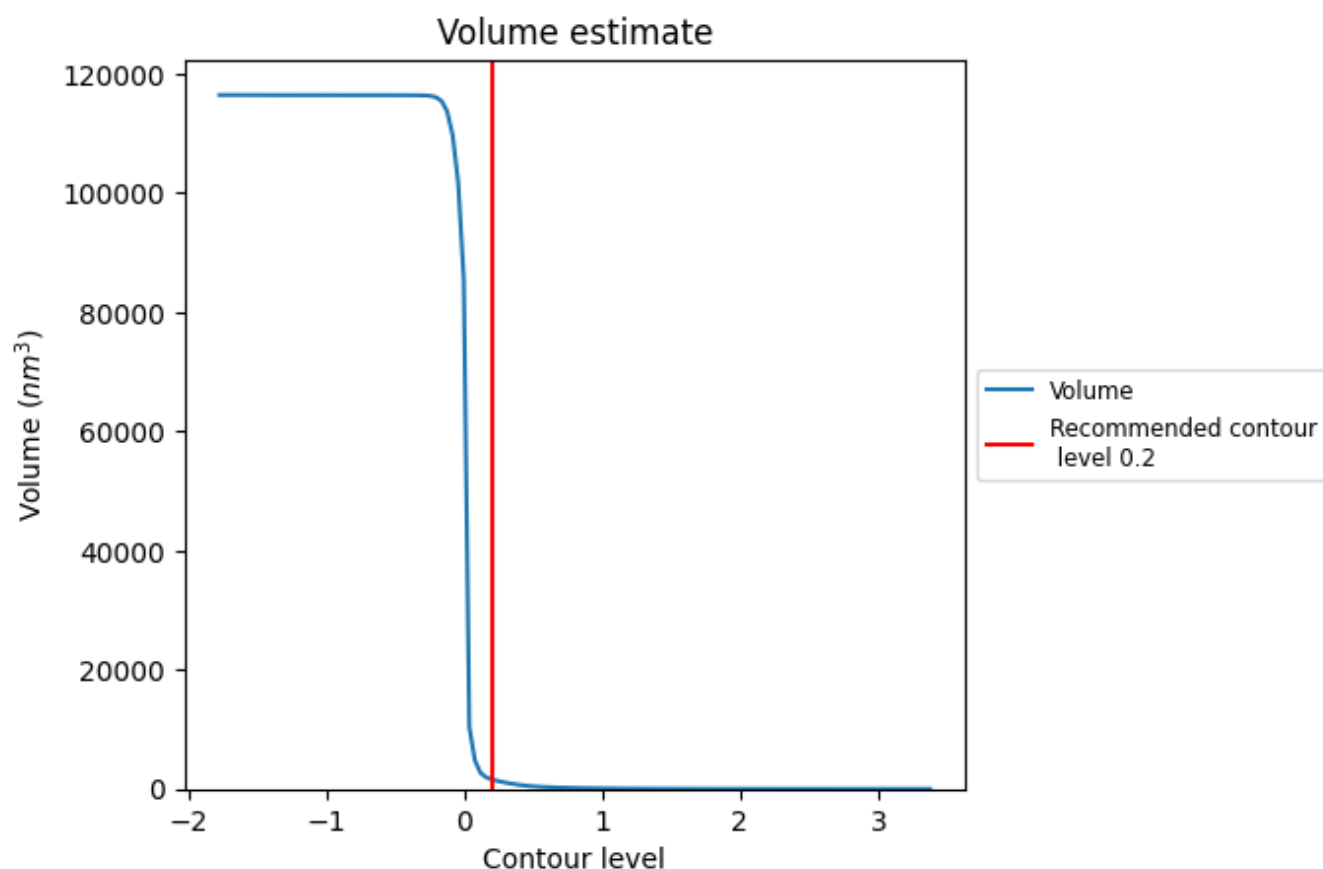
This section contains the results of statistical analysis of the map.

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.

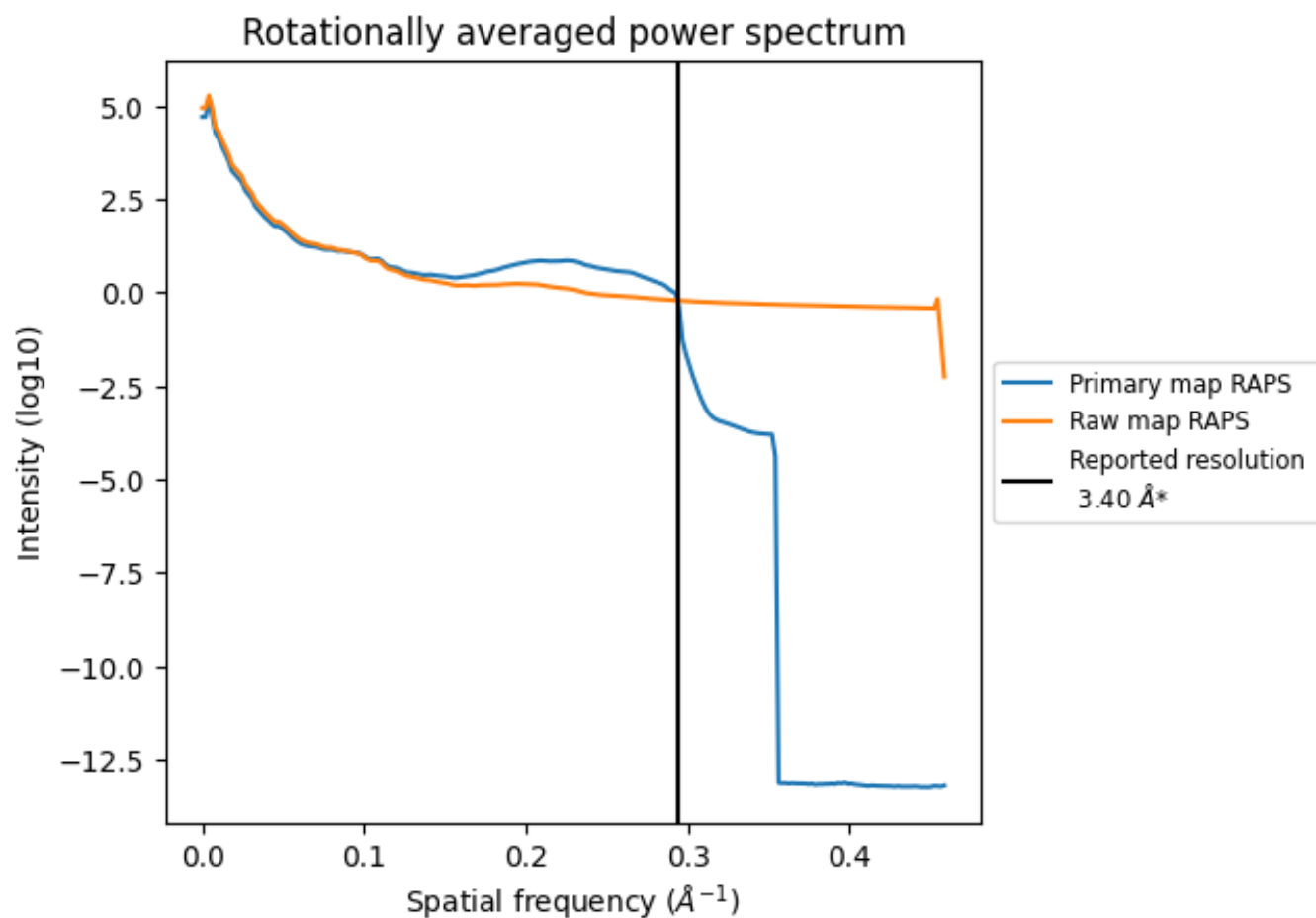
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1598 nm³; this corresponds to an approximate mass of 1443 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 ⓘ

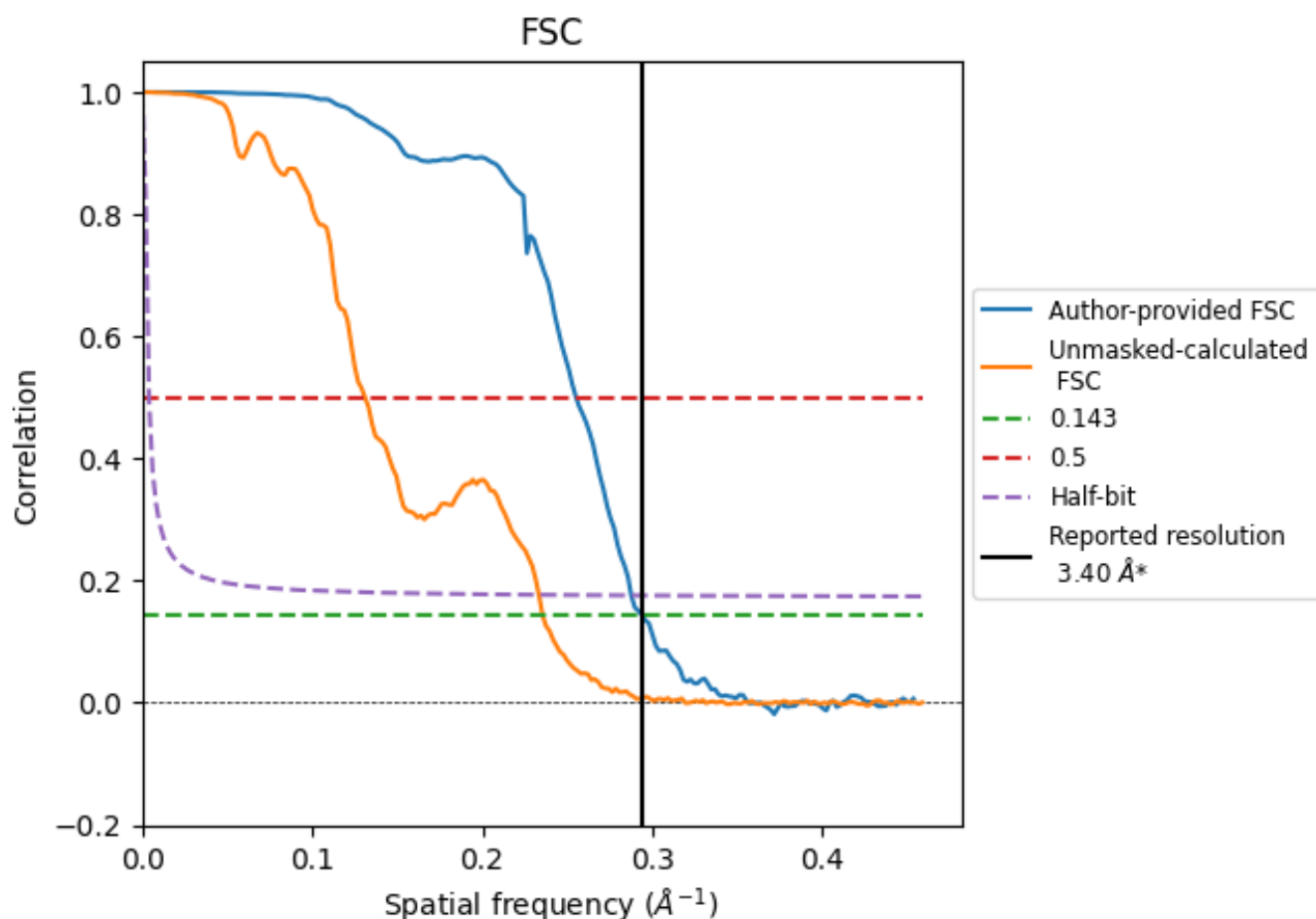


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

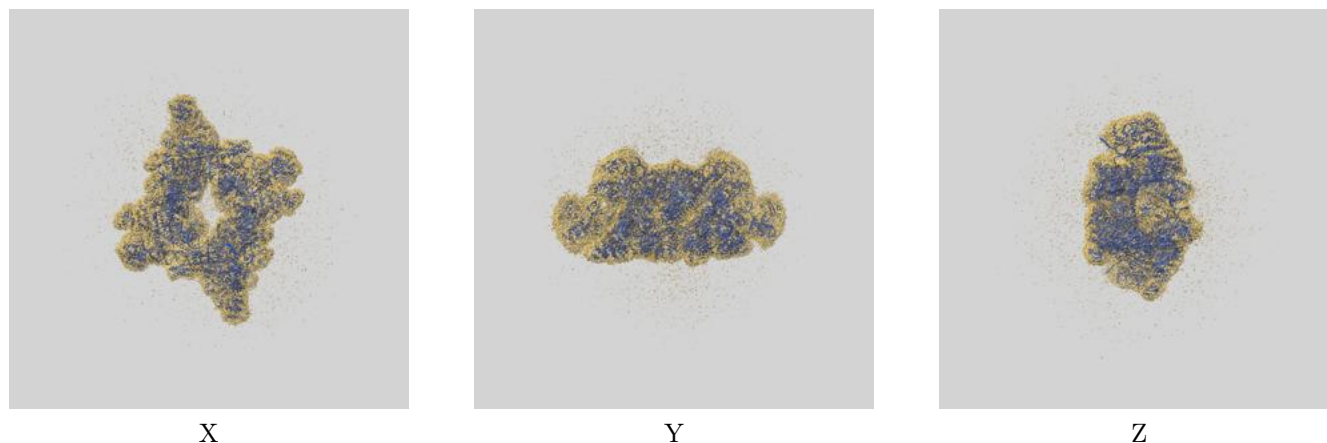
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.92	3.48
Unmasked-calculated*	4.25	7.63	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.25 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

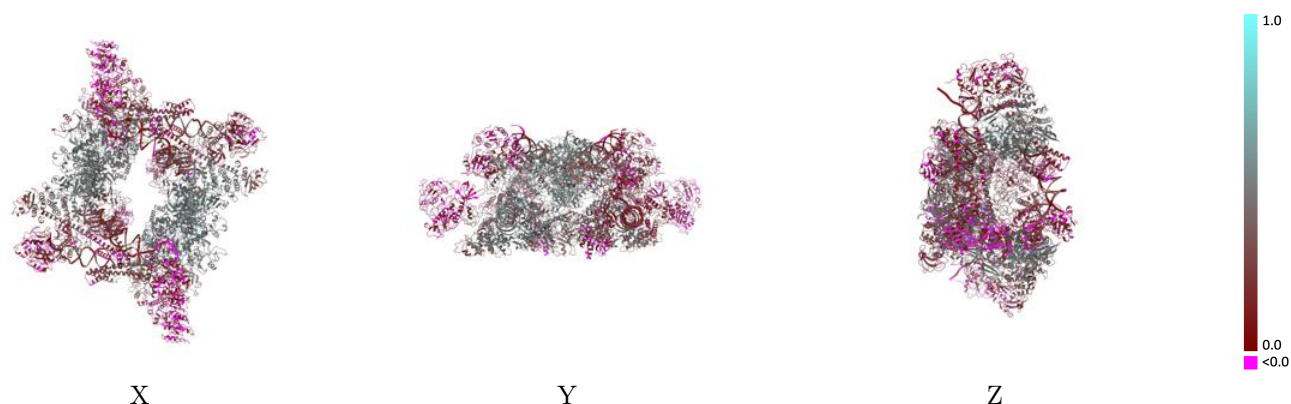
This section contains information regarding the fit between EMDB map EMD-38243 and PDB model 8XCH. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



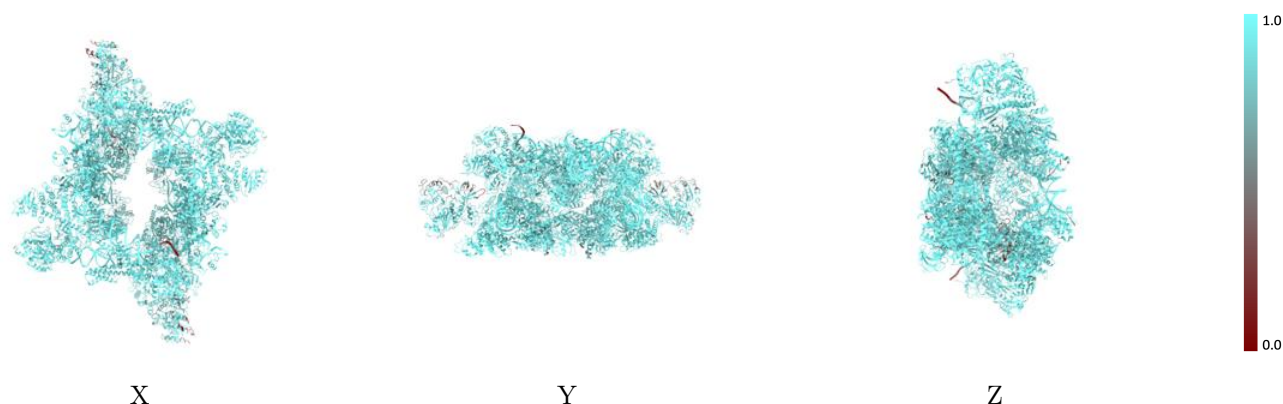
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



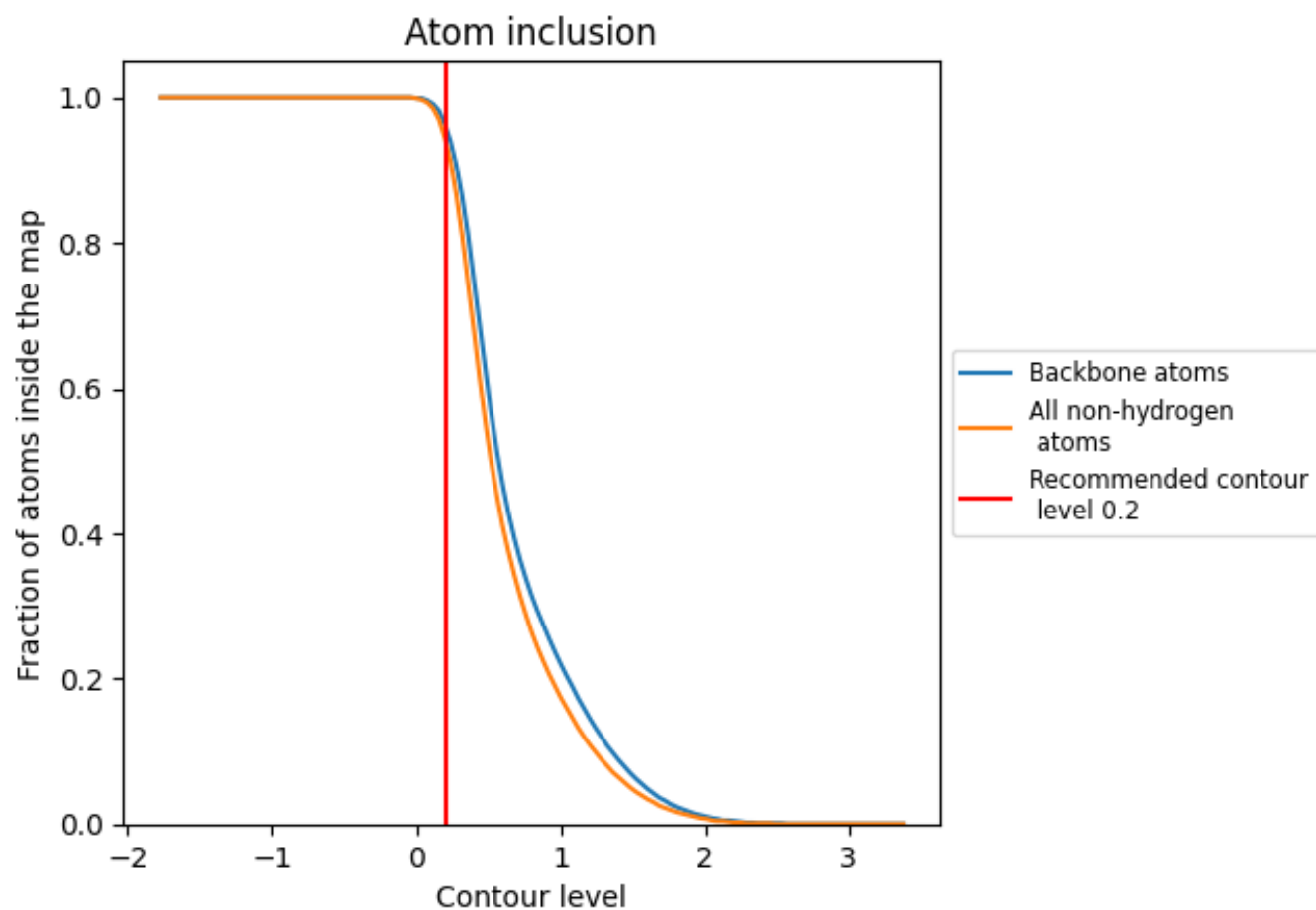
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9440	 0.3000
A	 0.9810	 0.4930
B	 0.9800	 0.4090
C	 0.9840	 0.4400
D	 0.9690	 0.2950
E	 0.9170	 0.1630
F	 0.8240	 0.0940
G	 0.9360	 0.2540
H	 0.9960	 0.2690
I	 0.9800	 0.4980
J	 0.9810	 0.4140
K	 0.9910	 0.4450
L	 0.9710	 0.3030
M	 0.9120	 0.1980
N	 0.9680	 0.2010
O	 0.9390	 0.2220
P	 0.9980	 0.2510
Q	 0.9810	 0.4580
R	 0.9680	 0.3730
S	 0.9750	 0.3770
T	 0.9650	 0.2280
U	 0.9150	 0.1610
V	 0.8220	 0.0800
W	 0.9180	 0.2190
X	 0.9990	 0.2530
Y	 0.9780	 0.4700
Z	 0.9650	 0.3440
a	 0.9780	 0.3840
b	 0.9710	 0.2330
c	 0.8980	 0.1460
d	 0.9660	 0.1590
e	 0.8900	 0.1980
f	 0.9950	 0.2490

