



## Full wwPDB EM Validation Report ⓘ

Jun 9, 2024 – 08:48 am BST

PDB ID : 8QBM  
EMDB ID : EMD-18315  
Title : Retron-Eco1 filament with ADP-ribosylated Effector (full map with 2 segments)  
Authors : Carabias del Rey, A.; Montoya, G.  
Deposited on : 2023-08-24  
Resolution : 3.09 Å(reported)  
Based on initial model : .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

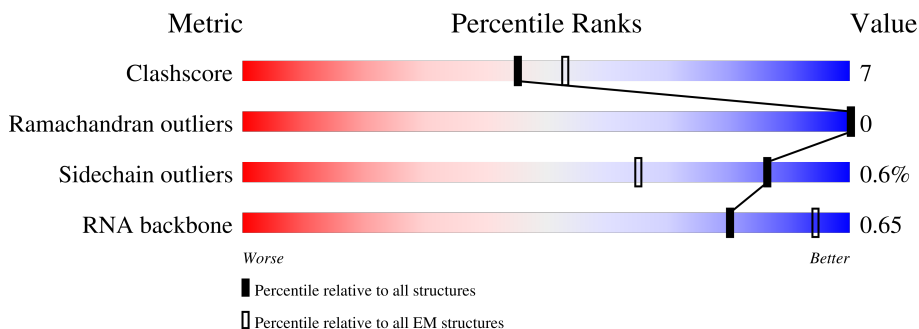
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 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 3.09 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	349	
1	I	349	
1	K	349	
1	P	349	
1	U	349	
1	Z	349	
2	C	82	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	82	
2	O	82	
2	R	82	
2	W	82	
2	b	82	
3	D	14	
3	N	14	
3	S	14	
3	X	14	
3	Y	14	
3	c	14	
4	E	307	
4	F	307	
4	G	307	
4	H	307	
4	T	307	
5	B	85	
5	J	85	
5	L	85	
5	Q	85	
5	V	85	
5	a	85	

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 39564 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 Retron Ec86 reverse transcriptase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	309	2337	1495	420	415	7	1	0
1	I	309	1531	911	310	310		1	0
1	K	309	2301	1472	411	410	8	1	0
1	P	309	1881	1179	348	351	3	1	0
1	U	309	2267	1455	406	400	6	1	0
1	Z	309	1534	912	310	312		1	0

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	321	GLY	-	expression tag	UNP P23070
A	322	SER	-	expression tag	UNP P23070
A	323	GLU	-	expression tag	UNP P23070
A	324	PHE	-	expression tag	UNP P23070
A	325	GLU	-	expression tag	UNP P23070
A	326	LEU	-	expression tag	UNP P23070
A	327	GLU	-	expression tag	UNP P23070
A	328	ASN	-	expression tag	UNP P23070
A	329	LEU	-	expression tag	UNP P23070
A	330	TYR	-	expression tag	UNP P23070
A	331	PHE	-	expression tag	UNP P23070
A	332	GLN	-	expression tag	UNP P23070
A	333	GLY	-	expression tag	UNP P23070
A	334	GLU	-	expression tag	UNP P23070
A	335	LEU	-	expression tag	UNP P23070
A	336	ARG	-	expression tag	UNP P23070
A	337	ARG	-	expression tag	UNP P23070
A	338	GLN	-	expression tag	UNP P23070

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ALA	-	expression tag	UNP P23070
A	340	SER	-	expression tag	UNP P23070
A	341	ALA	-	expression tag	UNP P23070
A	342	LEU	-	expression tag	UNP P23070
A	343	GLU	-	expression tag	UNP P23070
A	344	HIS	-	expression tag	UNP P23070
A	345	HIS	-	expression tag	UNP P23070
A	346	HIS	-	expression tag	UNP P23070
A	347	HIS	-	expression tag	UNP P23070
A	348	HIS	-	expression tag	UNP P23070
A	349	HIS	-	expression tag	UNP P23070
I	321	GLY	-	expression tag	UNP P23070
I	322	SER	-	expression tag	UNP P23070
I	323	GLU	-	expression tag	UNP P23070
I	324	PHE	-	expression tag	UNP P23070
I	325	GLU	-	expression tag	UNP P23070
I	326	LEU	-	expression tag	UNP P23070
I	327	GLU	-	expression tag	UNP P23070
I	328	ASN	-	expression tag	UNP P23070
I	329	LEU	-	expression tag	UNP P23070
I	330	TYR	-	expression tag	UNP P23070
I	331	PHE	-	expression tag	UNP P23070
I	332	GLN	-	expression tag	UNP P23070
I	333	GLY	-	expression tag	UNP P23070
I	334	GLU	-	expression tag	UNP P23070
I	335	LEU	-	expression tag	UNP P23070
I	336	ARG	-	expression tag	UNP P23070
I	337	ARG	-	expression tag	UNP P23070
I	338	GLN	-	expression tag	UNP P23070
I	339	ALA	-	expression tag	UNP P23070
I	340	SER	-	expression tag	UNP P23070
I	341	ALA	-	expression tag	UNP P23070
I	342	LEU	-	expression tag	UNP P23070
I	343	GLU	-	expression tag	UNP P23070
I	344	HIS	-	expression tag	UNP P23070
I	345	HIS	-	expression tag	UNP P23070
I	346	HIS	-	expression tag	UNP P23070
I	347	HIS	-	expression tag	UNP P23070
I	348	HIS	-	expression tag	UNP P23070
I	349	HIS	-	expression tag	UNP P23070
K	321	GLY	-	expression tag	UNP P23070
K	322	SER	-	expression tag	UNP P23070

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
K	323	GLU	-	expression tag	UNP P23070
K	324	PHE	-	expression tag	UNP P23070
K	325	GLU	-	expression tag	UNP P23070
K	326	LEU	-	expression tag	UNP P23070
K	327	GLU	-	expression tag	UNP P23070
K	328	ASN	-	expression tag	UNP P23070
K	329	LEU	-	expression tag	UNP P23070
K	330	TYR	-	expression tag	UNP P23070
K	331	PHE	-	expression tag	UNP P23070
K	332	GLN	-	expression tag	UNP P23070
K	333	GLY	-	expression tag	UNP P23070
K	334	GLU	-	expression tag	UNP P23070
K	335	LEU	-	expression tag	UNP P23070
K	336	ARG	-	expression tag	UNP P23070
K	337	ARG	-	expression tag	UNP P23070
K	338	GLN	-	expression tag	UNP P23070
K	339	ALA	-	expression tag	UNP P23070
K	340	SER	-	expression tag	UNP P23070
K	341	ALA	-	expression tag	UNP P23070
K	342	LEU	-	expression tag	UNP P23070
K	343	GLU	-	expression tag	UNP P23070
K	344	HIS	-	expression tag	UNP P23070
K	345	HIS	-	expression tag	UNP P23070
K	346	HIS	-	expression tag	UNP P23070
K	347	HIS	-	expression tag	UNP P23070
K	348	HIS	-	expression tag	UNP P23070
K	349	HIS	-	expression tag	UNP P23070
P	321	GLY	-	expression tag	UNP P23070
P	322	SER	-	expression tag	UNP P23070
P	323	GLU	-	expression tag	UNP P23070
P	324	PHE	-	expression tag	UNP P23070
P	325	GLU	-	expression tag	UNP P23070
P	326	LEU	-	expression tag	UNP P23070
P	327	GLU	-	expression tag	UNP P23070
P	328	ASN	-	expression tag	UNP P23070
P	329	LEU	-	expression tag	UNP P23070
P	330	TYR	-	expression tag	UNP P23070
P	331	PHE	-	expression tag	UNP P23070
P	332	GLN	-	expression tag	UNP P23070
P	333	GLY	-	expression tag	UNP P23070
P	334	GLU	-	expression tag	UNP P23070
P	335	LEU	-	expression tag	UNP P23070

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
P	336	ARG	-	expression tag	UNP P23070
P	337	ARG	-	expression tag	UNP P23070
P	338	GLN	-	expression tag	UNP P23070
P	339	ALA	-	expression tag	UNP P23070
P	340	SER	-	expression tag	UNP P23070
P	341	ALA	-	expression tag	UNP P23070
P	342	LEU	-	expression tag	UNP P23070
P	343	GLU	-	expression tag	UNP P23070
P	344	HIS	-	expression tag	UNP P23070
P	345	HIS	-	expression tag	UNP P23070
P	346	HIS	-	expression tag	UNP P23070
P	347	HIS	-	expression tag	UNP P23070
P	348	HIS	-	expression tag	UNP P23070
P	349	HIS	-	expression tag	UNP P23070
U	321	GLY	-	expression tag	UNP P23070
U	322	SER	-	expression tag	UNP P23070
U	323	GLU	-	expression tag	UNP P23070
U	324	PHE	-	expression tag	UNP P23070
U	325	GLU	-	expression tag	UNP P23070
U	326	LEU	-	expression tag	UNP P23070
U	327	GLU	-	expression tag	UNP P23070
U	328	ASN	-	expression tag	UNP P23070
U	329	LEU	-	expression tag	UNP P23070
U	330	TYR	-	expression tag	UNP P23070
U	331	PHE	-	expression tag	UNP P23070
U	332	GLN	-	expression tag	UNP P23070
U	333	GLY	-	expression tag	UNP P23070
U	334	GLU	-	expression tag	UNP P23070
U	335	LEU	-	expression tag	UNP P23070
U	336	ARG	-	expression tag	UNP P23070
U	337	ARG	-	expression tag	UNP P23070
U	338	GLN	-	expression tag	UNP P23070
U	339	ALA	-	expression tag	UNP P23070
U	340	SER	-	expression tag	UNP P23070
U	341	ALA	-	expression tag	UNP P23070
U	342	LEU	-	expression tag	UNP P23070
U	343	GLU	-	expression tag	UNP P23070
U	344	HIS	-	expression tag	UNP P23070
U	345	HIS	-	expression tag	UNP P23070
U	346	HIS	-	expression tag	UNP P23070
U	347	HIS	-	expression tag	UNP P23070
U	348	HIS	-	expression tag	UNP P23070

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
U	349	HIS	-	expression tag	UNP P23070
Z	321	GLY	-	expression tag	UNP P23070
Z	322	SER	-	expression tag	UNP P23070
Z	323	GLU	-	expression tag	UNP P23070
Z	324	PHE	-	expression tag	UNP P23070
Z	325	GLU	-	expression tag	UNP P23070
Z	326	LEU	-	expression tag	UNP P23070
Z	327	GLU	-	expression tag	UNP P23070
Z	328	ASN	-	expression tag	UNP P23070
Z	329	LEU	-	expression tag	UNP P23070
Z	330	TYR	-	expression tag	UNP P23070
Z	331	PHE	-	expression tag	UNP P23070
Z	332	GLN	-	expression tag	UNP P23070
Z	333	GLY	-	expression tag	UNP P23070
Z	334	GLU	-	expression tag	UNP P23070
Z	335	LEU	-	expression tag	UNP P23070
Z	336	ARG	-	expression tag	UNP P23070
Z	337	ARG	-	expression tag	UNP P23070
Z	338	GLN	-	expression tag	UNP P23070
Z	339	ALA	-	expression tag	UNP P23070
Z	340	SER	-	expression tag	UNP P23070
Z	341	ALA	-	expression tag	UNP P23070
Z	342	LEU	-	expression tag	UNP P23070
Z	343	GLU	-	expression tag	UNP P23070
Z	344	HIS	-	expression tag	UNP P23070
Z	345	HIS	-	expression tag	UNP P23070
Z	346	HIS	-	expression tag	UNP P23070
Z	347	HIS	-	expression tag	UNP P23070
Z	348	HIS	-	expression tag	UNP P23070
Z	349	HIS	-	expression tag	UNP P23070

- Molecule 2 is a RNA chain called Retron-Eco1-msr.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	61	Total	C	N	O	P	0	0
			1293	577	222	433	61		
2	M	61	Total	C	N	O	P	0	0
			1293	577	222	433	61		
2	O	61	Total	C	N	O	P	0	0
			1293	577	222	433	61		
2	R	61	Total	C	N	O	P	0	0
			1293	577	222	433	61		

*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	61	Total	C	N	O	P	0	0
			1293	577	222	433	61		
2	b	61	Total	C	N	O	P	0	0
			1293	577	222	433	61		

- Molecule 3 is a RNA chain called Retron-Eco1-A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	14	Total	C	N	O	P	0	0
			304	135	58	97	14		
3	N	14	Total	C	N	O	P	0	0
			304	135	58	97	14		
3	S	14	Total	C	N	O	P	0	0
			304	135	58	97	14		
3	X	14	Total	C	N	O	P	0	0
			304	135	58	97	14		
3	Y	14	Total	C	N	O	P	0	0
			304	135	58	97	14		
3	c	14	Total	C	N	O	P	0	0
			304	135	58	97	14		

- Molecule 4 is a protein called Retron Ec86 putative ribosyltransferase/DNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	302	Total	C	N	O	S	0	0
			2227	1437	392	391	7		
4	F	302	Total	C	N	O	S	0	0
			2109	1363	368	373	5		
4	G	124	Total	C	N	O	S	0	0
			695	424	133	137	1		
4	H	302	Total	C	N	O	S	0	0
			2038	1330	354	349	5		
4	T	302	Total	C	N	O	S	0	0
			2213	1428	389	390	6		

- Molecule 5 is a DNA chain called Retron-Eco1 msDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	85	Total	C	N	O	P	0	0
			1752	830	337	500	85		
5	J	85	Total	C	N	O	P	0	0
			1752	830	337	500	85		

Continued on next page...

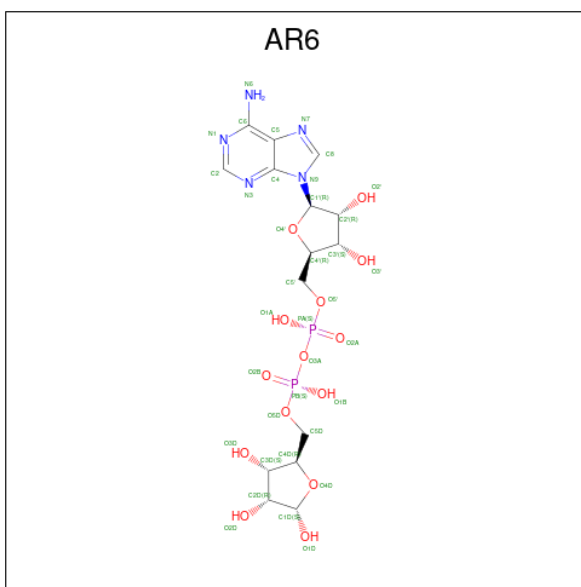
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L	43	Total	C	N	O	P	0	0
			890	422	178	247	43		
5	Q	85	Total	C	N	O	P	0	0
			1752	830	337	500	85		
5	V	85	Total	C	N	O	P	0	0
			1752	830	337	500	85		
5	a	39	Total	C	N	O	P	0	0
			808	383	163	223	39		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	Total	Mg	0
			1	1	
6	K	1	Total	Mg	0
			1	1	
6	U	1	Total	Mg	0
			1	1	

- Molecule 7 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[[[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	E	1	Total	C	N	O	P	0
			35	15	5	13	2	

Continued on next page...

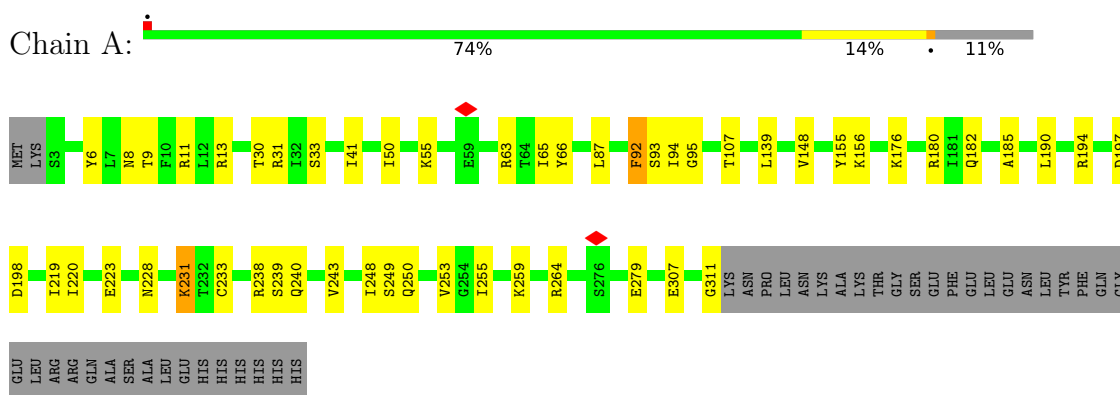
*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	F	1	Total 35	15	5	13	2	0
7	H	1	Total 35	15	5	13	2	0
7	T	1	Total 35	15	5	13	2	0

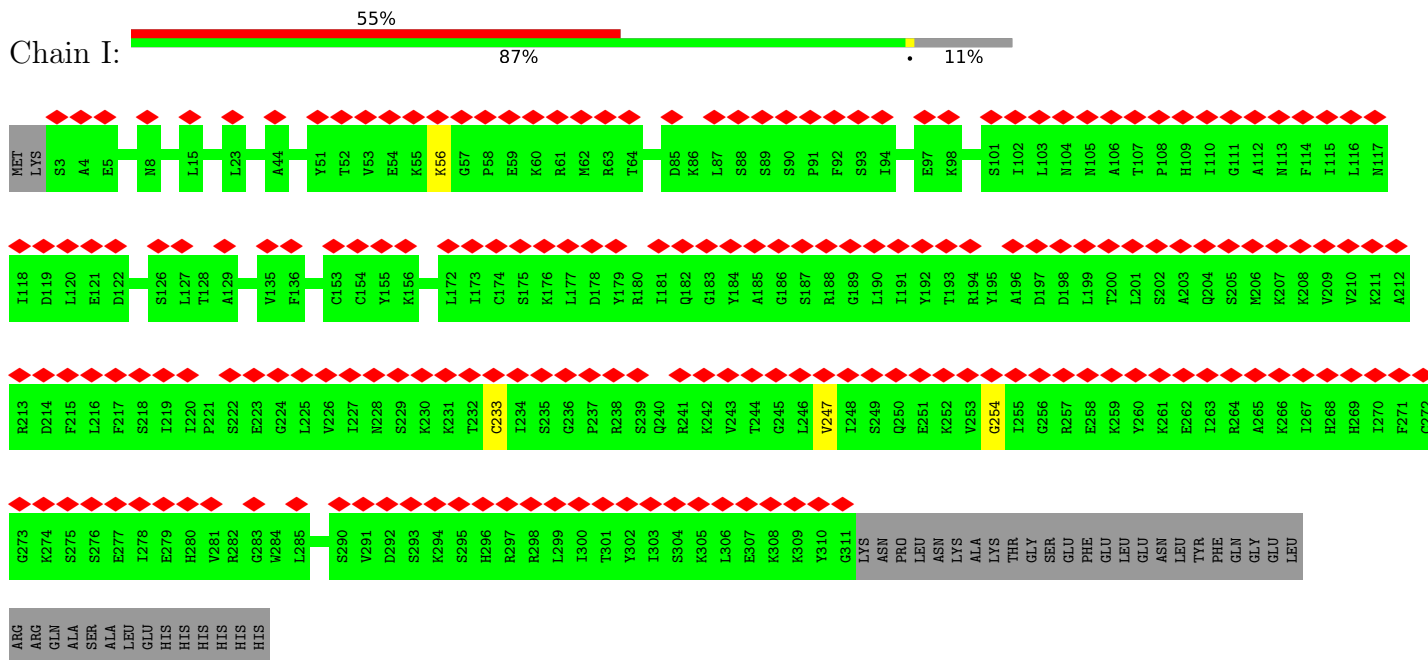
### 3 Residue-property plots [i](#)

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

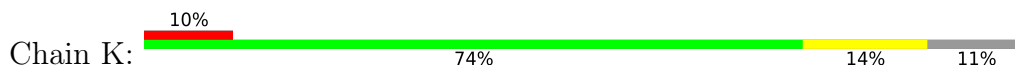
- Molecule 1: Retron Ec86 reverse transcriptase

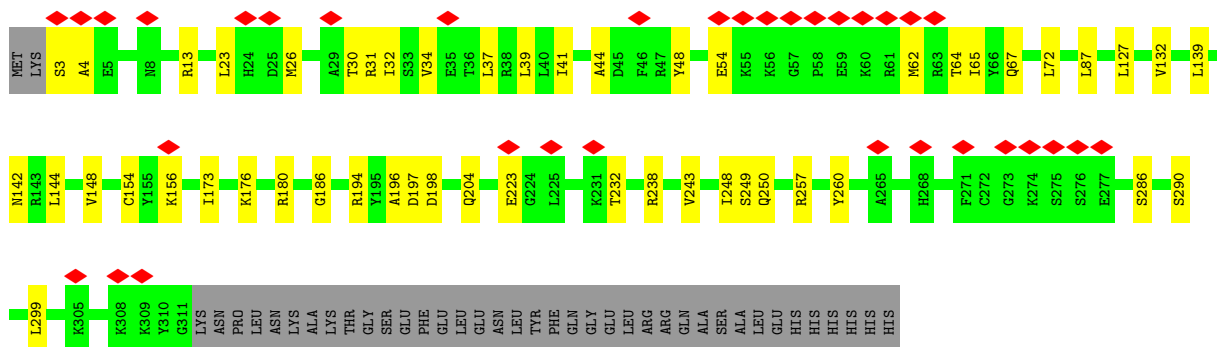


- Molecule 1: Retron Ec86 reverse transcriptase

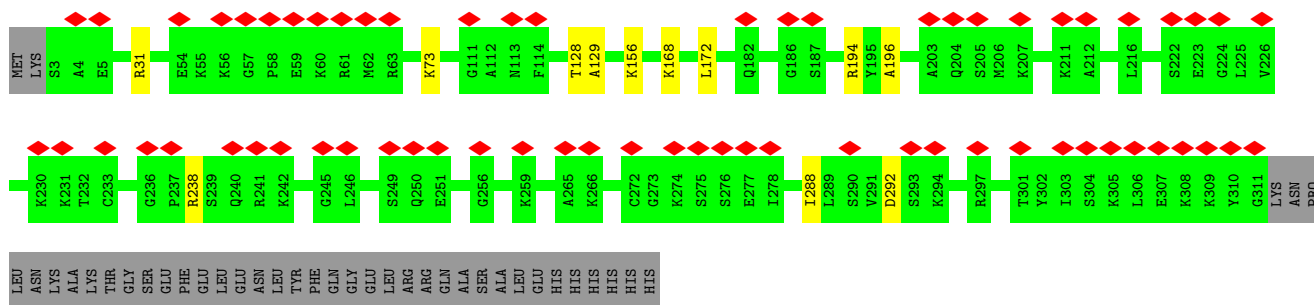
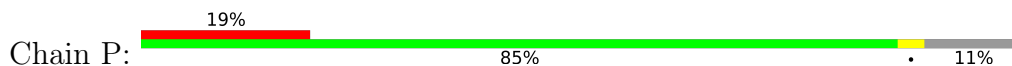


- Molecule 1: Retron Ec86 reverse transcriptase

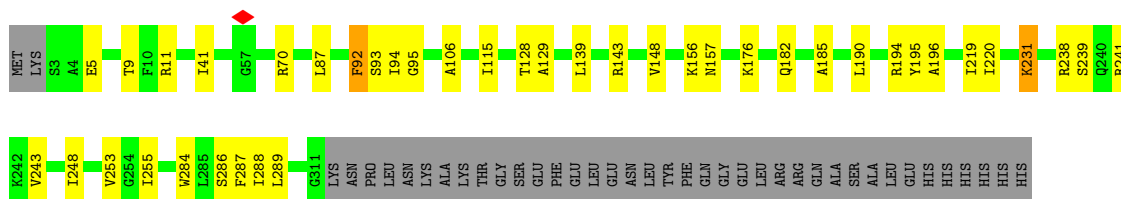
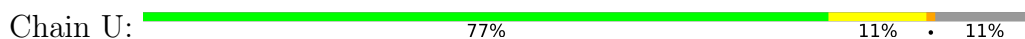




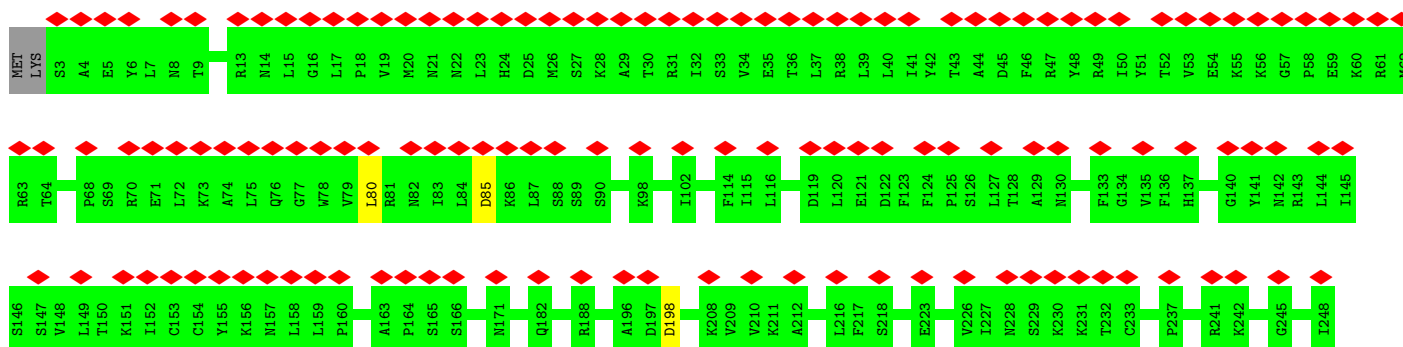
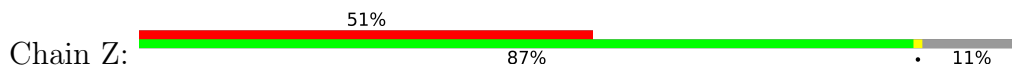
• Molecule 1: Retron Ec86 reverse transcriptase

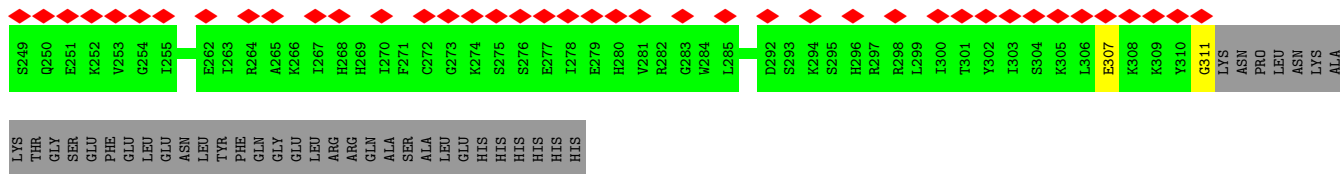


• Molecule 1: Retron Ec86 reverse transcriptase



• Molecule 1: Retron Ec86 reverse transcriptase

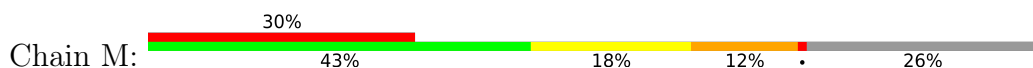




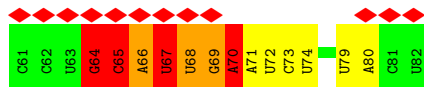
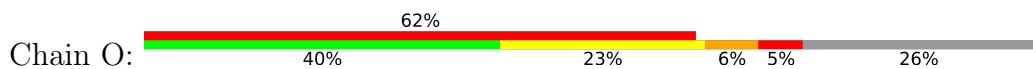
● Molecule 2: Retron-Eco1-msr



● Molecule 2: Retron-Eco1-msr



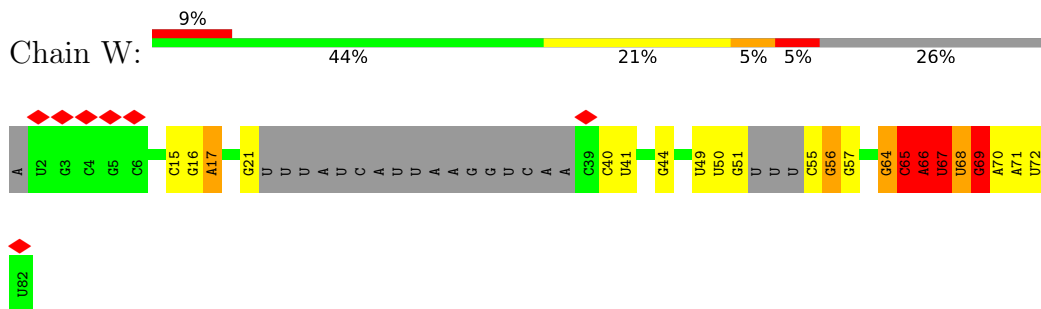
● Molecule 2: Retron-Eco1-msr



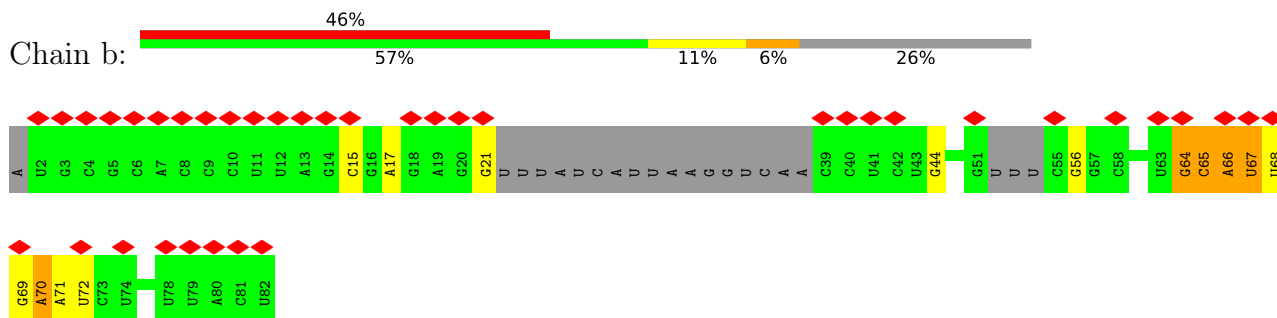
● Molecule 2: Retron-Eco1-msr



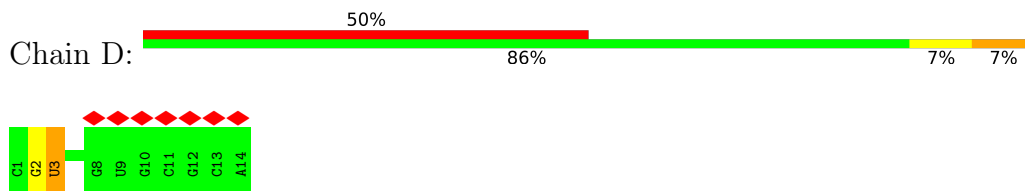
• Molecule 2: Retron-Eco1-msr



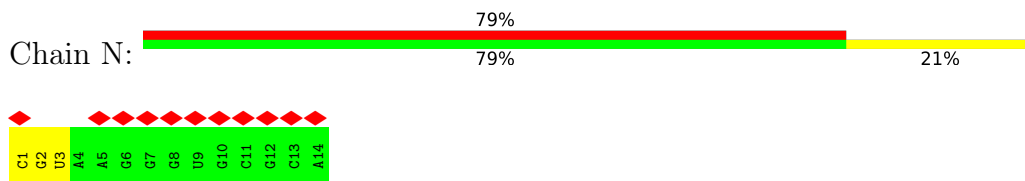
• Molecule 2: Retron-Eco1-msr



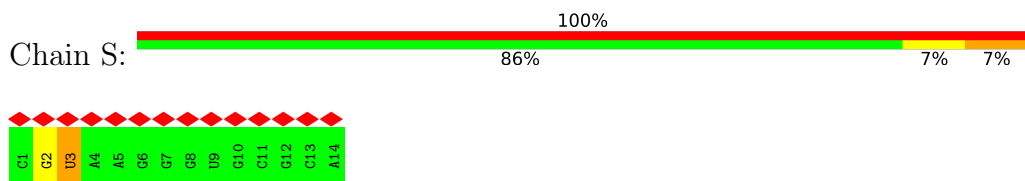
• Molecule 3: Retron-Eco1-A2



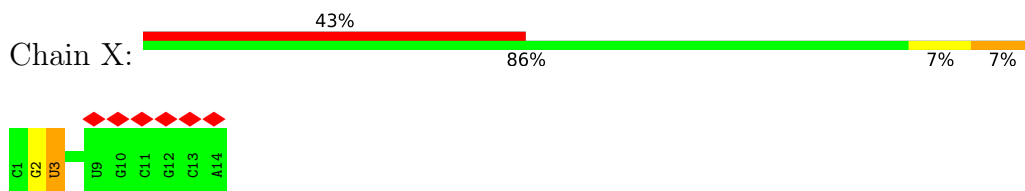
• Molecule 3: Retron-Eco1-A2



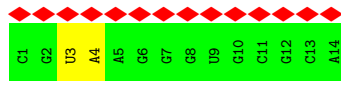
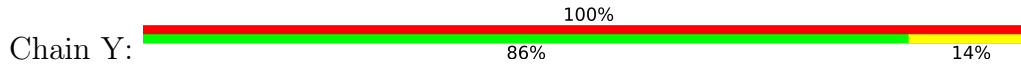
• Molecule 3: Retron-Eco1-A2



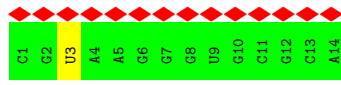
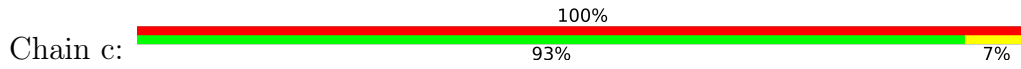
• Molecule 3: Retron-Eco1-A2



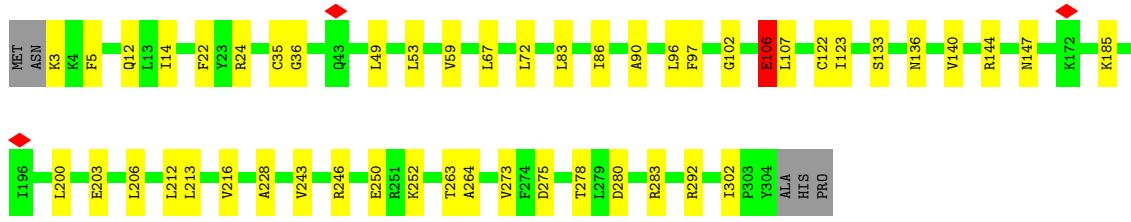
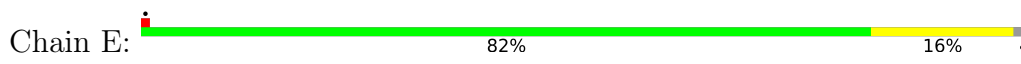
• Molecule 3: Retron-Eco1-A2



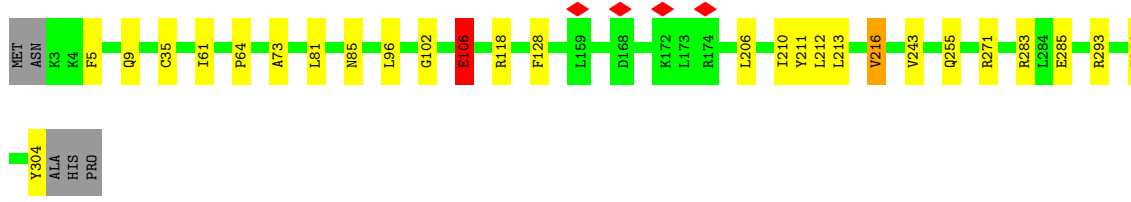
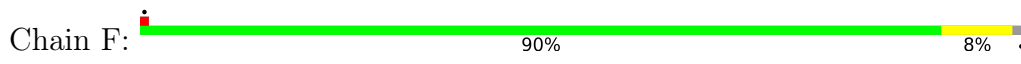
• Molecule 3: Retron-Eco1-A2



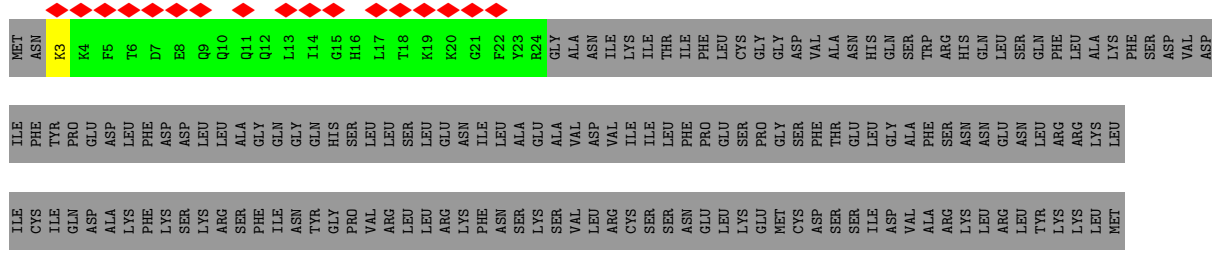
• Molecule 4: Retron Ec86 putative ribosyltransferase/DNA-binding protein



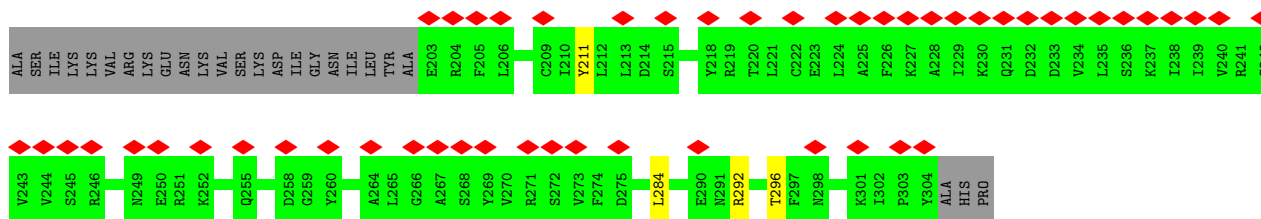
• Molecule 4: Retron Ec86 putative ribosyltransferase/DNA-binding protein



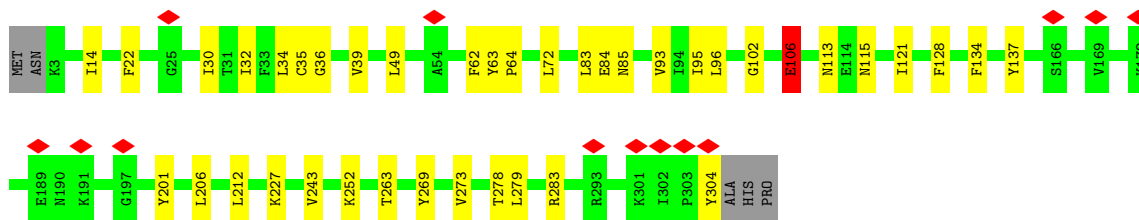
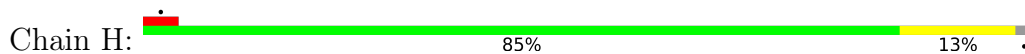
• Molecule 4: Retron Ec86 putative ribosyltransferase/DNA-binding protein



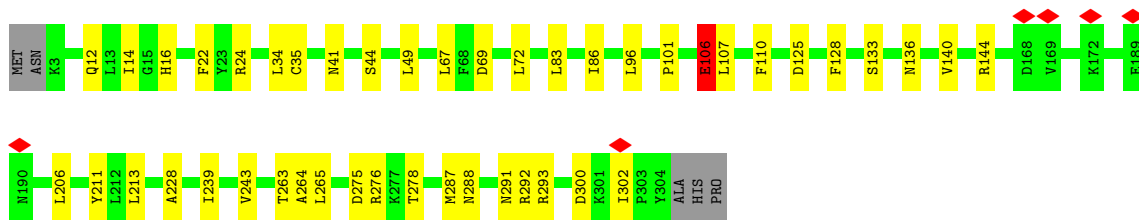
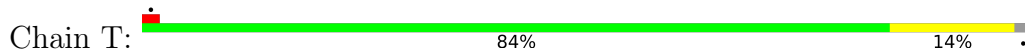




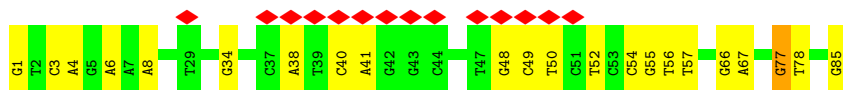
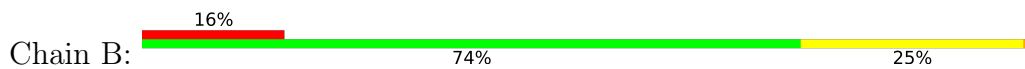
• Molecule 4: Retron Ec86 putative ribosyltransferase/DNA-binding protein



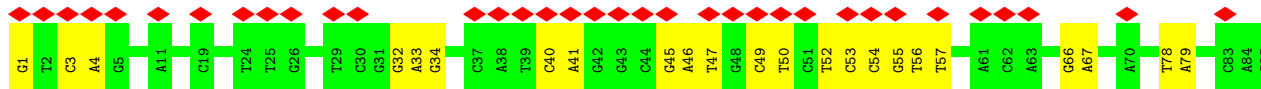
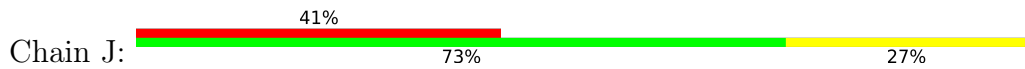
• Molecule 4: Retron Ec86 putative ribosyltransferase/DNA-binding protein



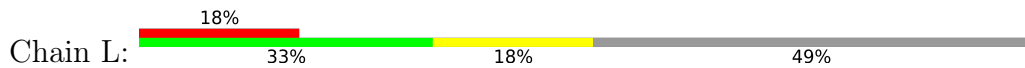
• Molecule 5: Retron-Eco1 msDNA

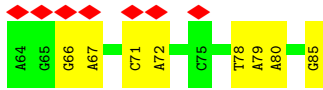
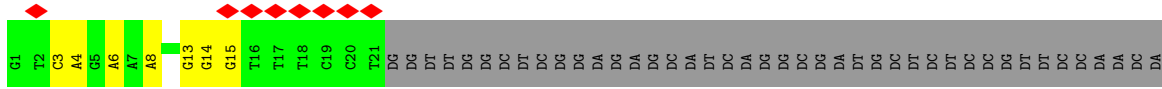


• Molecule 5: Retron-Eco1 msDNA

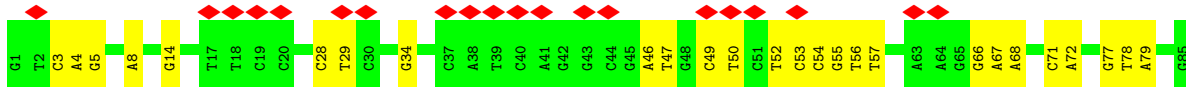


• Molecule 5: Retron-Eco1 msDNA

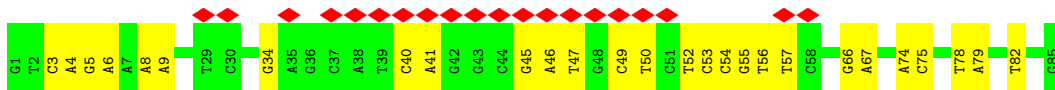




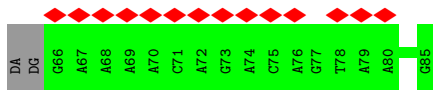
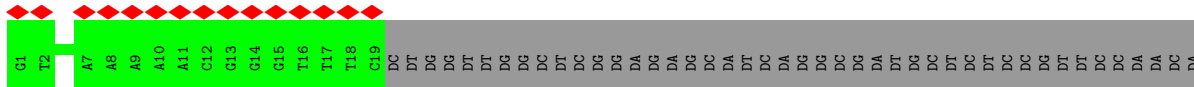
• Molecule 5: Retron-Eco1 msDNA



• Molecule 5: Retron-Eco1 msDNA



• Molecule 5: Retron-Eco1 msDNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	232272	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	39	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	80.312	Depositor
Minimum map value	-58.426	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	7.0	Depositor
Map size (Å)	499.2, 499.2, 499.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AR6

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	0.31	0/2383	0.49	0/3231
1	I	0.24	0/1530	0.41	0/2129
1	K	0.26	0/2346	0.50	0/3187
1	P	0.25	0/1914	0.43	0/2642
1	U	0.30	0/2313	0.48	0/3148
1	Z	0.24	0/1533	0.42	0/2133
2	C	0.39	0/1440	0.99	8/2236 (0.4%)
2	M	0.36	0/1440	0.93	5/2236 (0.2%)
2	O	0.34	0/1440	0.90	4/2236 (0.2%)
2	R	0.36	0/1440	0.89	5/2236 (0.2%)
2	W	0.36	0/1440	0.96	4/2236 (0.2%)
2	b	0.36	0/1440	0.91	5/2236 (0.2%)
3	D	0.19	0/340	0.71	0/529
3	N	0.16	0/340	0.70	0/529
3	S	0.16	0/340	0.71	0/529
3	X	0.21	0/340	0.73	0/529
3	Y	0.13	0/340	0.68	0/529
3	c	0.15	0/340	0.70	0/529
4	E	0.34	1/2266 (0.0%)	0.55	1/3081 (0.0%)
4	F	0.34	1/2144 (0.0%)	0.50	2/2932 (0.1%)
4	G	0.24	0/699	0.46	0/965
4	H	0.33	1/2073 (0.0%)	0.48	1/2845 (0.0%)
4	T	0.33	1/2251 (0.0%)	0.50	0/3062
5	B	0.56	0/1970	0.87	1/3039 (0.0%)
5	J	0.52	0/1970	0.85	0/3039
5	L	0.51	0/1002	0.81	0/1542
5	Q	0.52	0/1970	0.85	0/3039
5	V	0.54	0/1970	0.84	0/3039
5	a	0.50	0/910	0.81	0/1400
All	All	0.37	4/41924 (0.0%)	0.71	36/61043 (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
4	E	0	1
4	F	0	1
4	H	0	1
4	T	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	106	GLU	CD-OE2	8.19	1.34	1.25
4	T	106	GLU	CD-OE1	8.14	1.34	1.25
4	H	106	GLU	CD-OE2	8.11	1.34	1.25
4	F	106	GLU	CD-OE1	7.64	1.34	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	106	GLU	O-C-N	-13.75	100.70	122.70
2	C	65	C	P-O3'-C3'	-10.52	107.08	119.70
2	M	65	C	P-O3'-C3'	-9.91	107.81	119.70
2	C	64	G	P-O3'-C3'	-9.88	107.85	119.70
2	M	64	G	P-O3'-C3'	-9.34	108.49	119.70
2	C	67	U	P-O3'-C3'	-8.45	109.56	119.70
4	F	106	GLU	O-C-N	-8.25	109.50	122.70
2	M	70	A	P-O3'-C3'	-8.19	109.87	119.70
2	M	66	A	P-O3'-C3'	-8.16	109.91	119.70
2	b	64	G	P-O3'-C3'	-8.07	110.02	119.70
2	R	64	G	P-O3'-C3'	-8.06	110.03	119.70
4	H	106	GLU	O-C-N	-8.01	109.89	122.70
2	W	65	C	P-O3'-C3'	-7.97	110.13	119.70
2	W	67	U	P-O3'-C3'	-7.87	110.25	119.70
2	b	67	U	P-O3'-C3'	-7.77	110.37	119.70
2	W	69	G	P-O3'-C3'	-7.47	110.73	119.70
2	W	66	A	P-O3'-C3'	-7.44	110.77	119.70
2	O	67	U	P-O3'-C3'	-7.41	110.81	119.70
2	C	63	U	P-O3'-C3'	-7.33	110.91	119.70
2	C	66	A	P-O3'-C3'	-7.14	111.14	119.70
2	b	70	A	P-O3'-C3'	-7.05	111.24	119.70

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	65	C	P-O3'-C3'	-6.82	111.51	119.70
2	C	68	U	P-O3'-C3'	6.78	127.83	119.70
2	R	66	A	P-O3'-C3'	-6.75	111.60	119.70
2	R	67	U	P-O3'-C3'	-6.62	111.76	119.70
2	b	66	A	P-O3'-C3'	-6.42	112.00	119.70
2	C	62	C	P-O3'-C3'	-6.04	112.45	119.70
2	R	69	G	P-O3'-C3'	-5.94	112.57	119.70
5	B	77	DG	P-O3'-C3'	-5.92	112.60	119.70
4	F	106	GLU	CA-C-O	-5.61	108.31	120.10
2	O	64	G	P-O3'-C3'	-5.60	112.98	119.70
2	C	69	G	P-O3'-C3'	-5.47	113.13	119.70
2	R	65	C	P-O3'-C3'	-5.29	113.35	119.70
2	O	70	A	P-O3'-C3'	-5.26	113.38	119.70
2	M	4	C	P-O3'-C3'	-5.14	113.53	119.70
2	b	65	C	P-O3'-C3'	-5.06	113.62	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	106	GLU	Mainchain
4	F	106	GLU	Mainchain
4	H	106	GLU	Mainchain
4	T	106	GLU	Mainchain

## 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	2337	0	2302	44	0
1	I	1531	0	668	4	0
1	K	2301	0	2239	38	0
1	P	1881	0	1362	8	0
1	U	2267	0	2155	38	0
1	Z	1534	0	670	2	0
2	C	1293	0	657	34	0
2	M	1293	0	657	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	1293	0	657	26	0
2	R	1293	0	657	16	0
2	W	1293	0	657	25	0
2	b	1293	0	657	0	0
3	D	304	0	153	1	0
3	N	304	0	153	1	0
3	S	304	0	153	1	0
3	X	304	0	153	1	0
3	Y	304	0	153	1	0
3	c	304	0	153	0	0
4	E	2227	0	2115	40	0
4	F	2109	0	1890	22	0
4	G	695	0	399	4	0
4	H	2038	0	1771	29	0
4	T	2213	0	2090	33	0
5	B	1752	0	952	19	0
5	J	1752	0	952	17	0
5	L	890	0	482	13	0
5	Q	1752	0	952	19	0
5	V	1752	0	952	21	0
5	a	808	0	437	0	0
6	A	1	0	0	0	0
6	K	1	0	0	0	0
6	U	1	0	0	0	0
7	E	35	0	19	4	0
7	F	35	0	19	2	0
7	H	35	0	19	3	0
7	T	35	0	19	5	0
All	All	39564	0	27324	416	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 7.

All (416) 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)
4:E:133:SER:CB	7:T:401:AR6:H1'	1.94	0.97
2:O:49:U:H3	2:O:57:G:H1	1.15	0.94
2:R:49:U:H3	2:R:57:G:H1	1.13	0.90
2:R:50:U:H3	2:R:56:G:H1	1.18	0.90
2:M:49:U:H3	2:M:57:G:H1	1.16	0.89

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:50:U:H3	2:W:56:G:H1	1.22	0.88
2:C:49:U:H3	2:C:57:G:H1	1.22	0.87
2:M:50:U:H3	2:M:56:G:H1	1.22	0.86
2:C:50:U:H3	2:C:56:G:H1	1.25	0.84
2:W:49:U:H3	2:W:57:G:H1	1.19	0.84
4:H:36:GLY:O	7:H:401:AR6:O3D	1.98	0.82
4:E:133:SER:HB3	7:T:401:AR6:H1'	1.61	0.80
4:F:102:GLY:O	4:F:106:GLU:HG3	1.82	0.80
1:A:233:CYS:SG	2:C:67:U:C4	2.74	0.79
4:H:102:GLY:O	4:H:106:GLU:HG3	1.86	0.75
1:K:194:ARG:NH1	1:K:196:ALA:O	2.20	0.75
2:C:55:C:O2'	2:C:56:G:OP2	2.04	0.75
1:K:144:LEU:O	1:K:148:VAL:HG23	1.87	0.74
4:E:36:GLY:O	7:E:401:AR6:O3D	2.00	0.74
4:E:102:GLY:O	4:E:106:GLU:HG3	1.87	0.74
4:G:211:TYR:O	1:K:31:ARG:NH1	2.20	0.73
2:O:50:U:H3	2:O:56:G:H1	1.37	0.72
1:U:93:SER:OG	1:U:194:ARG:NH2	2.24	0.70
1:K:257:ARG:NH2	2:M:48:G:O6	2.25	0.70
2:M:71:A:C2	2:M:73:C:C2	2.79	0.69
1:A:93:SER:OG	1:A:194:ARG:NH1	2.27	0.68
1:U:176:LYS:NZ	5:V:6:DA:OP2	2.26	0.67
4:E:133:SER:HB2	7:T:401:AR6:H1'	1.76	0.67
1:K:44:ALA:HB1	1:K:72:LEU:HD21	1.78	0.66
1:K:67:GLN:N	1:K:67:GLN:OE1	2.29	0.66
4:G:3:LYS:NZ	4:G:292:ARG:O	2.29	0.66
1:P:194:ARG:NH1	1:P:196:ALA:O	2.28	0.65
1:K:127:LEU:HD12	1:K:173:ILE:HG21	1.78	0.65
4:E:3:LYS:NZ	4:E:292:ARG:O	2.29	0.65
2:W:55:C:O2'	2:W:56:G:OP2	2.10	0.65
1:A:180:ARG:NH1	1:A:223:GLU:OE2	2.29	0.65
1:A:228:ASN:ND2	1:A:231:LYS:HG3	2.12	0.65
2:R:55:C:O2'	2:R:56:G:OP2	2.13	0.64
4:E:72:LEU:HD12	4:E:83:LEU:HD12	1.77	0.64
1:P:73:LYS:NZ	5:Q:77:DG:OP1	2.30	0.64
1:A:176:LYS:NZ	5:B:6:DA:OP2	2.31	0.64
2:O:43:U:C5	2:O:65:C:C6	2.87	0.63
1:A:231:LYS:NZ	1:A:231:LYS:HB3	2.13	0.63
4:H:39:VAL:HG21	4:H:63:TYR:CE1	2.34	0.63
2:R:75:G:N7	4:T:293:ARG:NH2	2.47	0.63
4:F:293:ARG:NE	2:W:75:G:OP2	2.32	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:LYS:O	5:L:8:DA:N6	2.31	0.62
4:H:72:LEU:HD23	4:H:83:LEU:HD12	1.82	0.62
2:R:70:A:C6	2:R:71:A:C6	2.86	0.62
4:H:84:GLU:OE1	4:H:113:ASN:ND2	2.31	0.62
1:A:233:CYS:SG	2:C:67:U:N3	2.73	0.62
1:P:156:LYS:O	5:Q:8:DA:N6	2.33	0.62
2:C:43:U:C5	2:C:65:C:C6	2.88	0.62
4:T:72:LEU:HD23	4:T:83:LEU:HD12	1.82	0.62
4:H:85:ASN:OD1	4:H:115:ASN:ND2	2.33	0.61
1:A:8:ASN:OD1	1:A:11:ARG:NH2	2.32	0.61
4:H:49:LEU:O	4:H:49:LEU:HD13	2.01	0.61
2:C:66:A:C2	2:C:67:U:C2	2.89	0.60
4:F:64:PRO:HG2	7:F:401:AR6:H2D	1.82	0.60
4:E:67:LEU:HD13	4:E:67:LEU:O	2.02	0.60
4:E:203:GLU:OE1	4:E:246:ARG:NH1	2.35	0.60
5:J:34:DG:N2	5:J:52:DT:O2	2.35	0.60
2:R:43:U:C5	2:R:65:C:C5	2.89	0.59
4:E:147:ASN:OD1	4:E:185:LYS:HD3	2.02	0.59
1:K:238:ARG:O	2:M:44:G:N2	2.31	0.59
4:T:67:LEU:HD13	4:T:67:LEU:O	2.01	0.59
4:F:206:LEU:HD12	4:F:243:VAL:HG11	1.85	0.59
4:F:213:LEU:HD12	4:F:216:VAL:HG22	1.83	0.59
4:E:72:LEU:HD12	4:E:83:LEU:CD1	2.33	0.59
1:A:13:ARG:NH2	5:V:5:DG:OP1	2.35	0.59
4:E:212:LEU:O	4:E:283:ARG:NH1	2.36	0.59
2:R:16:G:C8	2:R:64:G:C6	2.91	0.58
1:K:197:ASP:OD1	1:K:198:ASP:N	2.36	0.58
2:W:16:G:C8	2:W:64:G:C6	2.91	0.58
3:X:2:G:O2'	3:X:3:U:OP2	2.19	0.58
2:R:66:A:C2	2:R:67:U:C2	2.92	0.58
5:V:34:DG:N2	5:V:52:DT:O2	2.37	0.57
5:B:34:DG:N2	5:B:52:DT:O2	2.38	0.56
1:A:248:ILE:HD13	1:A:253:VAL:HG12	1.87	0.56
2:C:73:C:OP1	4:E:292:ARG:NH2	2.38	0.56
2:O:43:U:C5	2:O:65:C:C5	2.94	0.56
2:W:16:G:O2'	2:W:17:A:O5'	2.23	0.56
2:M:16:G:O4'	2:M:64:G:N2	2.39	0.56
1:P:128:THR:OG1	1:P:129:ALA:N	2.39	0.56
1:U:243:VAL:O	1:U:243:VAL:HG23	2.06	0.56
2:O:16:G:H21	2:O:66:A:H62	1.53	0.55
1:U:156:LYS:O	5:V:8:DA:N6	2.38	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:O	5:B:8:DA:N6	2.39	0.55
5:J:78:DT:H4'	5:J:79:DA:OP1	2.07	0.55
2:R:73:C:OP1	4:T:292:ARG:NH2	2.40	0.55
1:U:128:THR:HG22	1:U:129:ALA:H	1.71	0.55
2:M:55:C:O2'	2:M:56:G:OP2	2.21	0.54
2:O:16:G:O4'	2:O:64:G:N2	2.40	0.54
4:E:263:THR:HG22	4:E:264:ALA:N	2.22	0.54
1:I:233:CYS:CB	2:O:67:U:C4	2.91	0.54
2:W:66:A:C2	2:W:67:U:C2	2.96	0.54
2:C:43:U:C5	2:C:65:C:C5	2.96	0.54
5:Q:78:DT:H4'	5:Q:79:DA:OP1	2.08	0.54
1:A:30:THR:O	1:A:31:ARG:HB2	2.08	0.54
1:K:48:TYR:HE2	1:K:72:LEU:HD23	1.73	0.54
1:I:233:CYS:CB	2:O:67:U:C5	2.92	0.53
1:A:243:VAL:HG23	1:A:243:VAL:O	2.06	0.53
4:E:24:ARG:O	4:E:24:ARG:HG2	2.08	0.53
1:K:3:SER:OG	1:K:4:ALA:N	2.42	0.53
1:U:157:ASN:OD1	1:U:157:ASN:O	2.25	0.53
5:L:78:DT:H4'	5:L:79:DA:OP1	2.08	0.53
4:E:213:LEU:HD11	4:E:216:VAL:HG23	1.91	0.53
4:H:252:LYS:O	4:H:263:THR:OG1	2.27	0.53
1:K:180:ARG:NH1	1:K:223:GLU:OE2	2.40	0.53
1:K:249:SER:OG	1:K:250:GLN:N	2.41	0.53
1:K:176:LYS:NZ	5:L:6:DA:OP2	2.42	0.53
1:A:197:ASP:OD1	5:B:85:DG:O3'	2.23	0.53
2:O:70:A:C6	2:O:71:A:C2	2.97	0.53
5:V:78:DT:H4'	5:V:79:DA:OP1	2.09	0.53
1:U:5:GLU:O	1:U:9:THR:HG23	2.09	0.52
4:T:206:LEU:HD12	4:T:243:VAL:HG11	1.90	0.52
4:H:212:LEU:HD21	4:H:279:LEU:HD23	1.92	0.52
4:H:64:PRO:HG2	7:H:401:AR6:H2D	1.92	0.52
2:R:66:A:N1	2:R:67:U:C2	2.77	0.52
1:A:107:THR:HG22	4:F:255:GLN:O	2.10	0.52
4:H:93:VAL:HG21	4:H:121:ILE:HD12	1.91	0.52
4:H:14:ILE:HD13	4:H:227:LYS:HB2	1.92	0.52
4:E:206:LEU:HD12	4:E:243:VAL:HG11	1.92	0.52
4:T:34:LEU:HD11	4:T:49:LEU:HD12	1.91	0.52
1:K:87:LEU:HD11	1:K:139:LEU:HD11	1.92	0.52
4:T:206:LEU:CD1	4:T:243:VAL:HG11	2.39	0.52
4:E:49:LEU:HD22	4:E:97:PHE:HZ	1.74	0.51
4:E:133:SER:HB3	7:T:401:AR6:C1'	2.36	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:140:VAL:O	4:T:144:ARG:HG3	2.11	0.51
1:A:11:ARG:CD	1:U:11:ARG:HH12	2.23	0.51
4:H:206:LEU:HD12	4:H:243:VAL:HG11	1.91	0.51
2:O:70:A:H2'	2:O:71:A:O4'	2.10	0.51
5:J:3:DC:H4'	5:J:4:DA:OP1	2.10	0.51
1:A:33:SER:OG	4:E:280:ASP:OD2	2.20	0.51
2:W:70:A:H2'	2:W:71:A:O4'	2.11	0.51
5:Q:3:DC:H4'	5:Q:4:DA:OP1	2.10	0.50
1:K:26:MET:O	1:K:30:THR:HG22	2.10	0.50
1:P:238:ARG:O	2:R:44:G:N2	2.42	0.50
5:L:3:DC:H4'	5:L:4:DA:OP1	2.10	0.50
1:A:249:SER:OG	1:A:250:GLN:N	2.43	0.50
4:T:41:ASN:ND2	4:T:44:SER:OG	2.44	0.50
1:U:231:LYS:HE2	2:W:69:G:OP2	2.12	0.50
7:H:401:AR6:PB	7:H:401:AR6:H4'	2.52	0.50
1:I:56:LYS:CB	2:O:69:G:O2'	2.59	0.50
1:K:286:SER:OG	2:M:78:U:O4'	2.30	0.50
1:Z:307:GLU:O	1:Z:311:GLY:N	2.45	0.50
4:T:96:LEU:HD21	4:T:107:LEU:HB2	1.94	0.50
2:W:67:U:H3'	2:W:68:U:C5'	2.42	0.50
4:H:39:VAL:HG21	4:H:63:TYR:HE1	1.76	0.49
2:M:68:U:H2'	2:M:69:G:H21	1.77	0.49
2:W:69:G:H2'	2:W:69:G:N3	2.26	0.49
5:Q:49:DC:H2'	5:Q:50:DT:H71	1.94	0.49
2:O:73:C:H2'	2:O:74:U:O2	2.12	0.49
1:A:13:ARG:NH1	5:V:5:DG:OP1	2.44	0.49
1:K:64:THR:C	1:K:65:ILE:HD13	2.32	0.49
5:Q:34:DG:N2	5:Q:52:DT:O2	2.45	0.49
4:T:239:ILE:O	4:T:243:VAL:HG12	2.12	0.49
4:F:106:GLU:HG2	4:H:134:PHE:CE2	2.48	0.49
1:K:13:ARG:NH2	5:Q:5:DG:OP1	2.40	0.49
4:E:213:LEU:HD11	4:E:216:VAL:CG2	2.43	0.48
5:B:3:DC:H4'	5:B:4:DA:OP1	2.13	0.48
1:K:243:VAL:HG23	1:K:248:ILE:HD12	1.95	0.48
1:U:248:ILE:HD13	1:U:253:VAL:HG12	1.96	0.48
5:J:49:DC:H2'	5:J:50:DT:H71	1.95	0.48
5:V:46:DA:H2'	5:V:47:DT:H71	1.94	0.48
4:E:246:ARG:HG2	4:E:246:ARG:HH11	1.79	0.48
2:O:16:G:O2'	2:O:17:A:O5'	2.28	0.48
2:C:16:G:O2'	2:C:17:A:O5'	2.27	0.48
2:O:43:U:H5	2:O:65:C:C5	2.29	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:255:ILE:HG21	1:U:288:ILE:HD13	1.96	0.48
1:A:11:ARG:HD2	1:U:11:ARG:HH12	1.79	0.48
3:D:2:G:O2'	3:D:3:U:OP2	2.23	0.48
4:E:35:CYS:HB2	4:E:96:LEU:HD13	1.95	0.48
4:F:9:GLN:NE2	4:F:296:THR:OG1	2.38	0.48
4:F:118:ARG:HG2	4:F:118:ARG:HH11	1.79	0.48
4:H:32:ILE:HG23	4:H:95:ILE:HD13	1.95	0.48
1:K:62:MET:HA	1:K:62:MET:HE3	1.95	0.48
2:M:17:A:HO2'	2:M:18:G:H8	1.60	0.48
4:E:140:VAL:O	4:E:144:ARG:HG3	2.14	0.48
1:A:198:ASP:OD1	1:A:198:ASP:O	2.32	0.47
4:F:213:LEU:CD1	4:F:216:VAL:HG22	2.44	0.47
2:R:43:U:C5	2:R:65:C:C6	3.01	0.47
1:U:248:ILE:CD1	1:U:253:VAL:HG12	2.44	0.47
5:V:3:DC:H4'	5:V:4:DA:OP1	2.14	0.47
2:M:68:U:C2'	2:M:69:G:H21	2.27	0.47
5:V:3:DC:H2''	5:V:4:DA:O5'	2.13	0.47
4:E:14:ILE:HD12	4:E:228:ALA:HB2	1.96	0.47
5:J:45:DG:H2'	5:J:46:DA:C8	2.50	0.47
4:T:276:ARG:NH2	5:Q:14:DG:OP1	2.44	0.47
2:W:16:G:HO2'	2:W:17:A:C5'	2.26	0.47
5:B:3:DC:H2''	5:B:4:DA:O5'	2.14	0.47
2:O:13:A:N1	3:Y:4:A:N6	2.63	0.47
5:V:3:DC:H2'	5:V:4:DA:C8	2.49	0.47
4:T:263:THR:HG22	4:T:264:ALA:N	2.30	0.47
1:U:143:ARG:NH2	5:V:9:DA:OP1	2.39	0.47
1:U:255:ILE:HD13	1:U:288:ILE:HD12	1.96	0.47
4:F:128:PHE:N	4:F:128:PHE:CD1	2.82	0.47
5:Q:46:DA:H2'	5:Q:47:DT:H71	1.97	0.47
4:F:285:GLU:OE2	1:U:70:ARG:NH2	2.48	0.46
1:U:231:LYS:NZ	1:U:231:LYS:HB3	2.30	0.46
5:B:77:DG:H1'	5:B:78:DT:C6	2.50	0.46
1:A:41:ILE:HD13	1:A:148:VAL:HG13	1.96	0.46
1:A:233:CYS:SG	2:C:67:U:C5	3.09	0.46
1:I:247:VAL:N	1:I:254:GLY:O	2.47	0.46
4:T:14:ILE:HD12	4:T:228:ALA:HB2	1.97	0.46
5:B:49:DC:H2'	5:B:50:DT:H71	1.97	0.46
5:L:3:DC:H2''	5:L:4:DA:O5'	2.15	0.46
2:C:16:G:C5	2:C:64:G:C4	3.02	0.46
4:F:73:ALA:HB2	4:H:137:TYR:CE1	2.50	0.46
1:U:87:LEU:HD11	1:U:139:LEU:HD11	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:3:DC:H2'	5:J:4:DA:O5'	2.16	0.46
1:A:63:ARG:HG3	1:A:65:ILE:HD11	1.98	0.46
2:C:69:G:N3	2:C:69:G:H2'	2.31	0.46
5:B:3:DC:H2'	5:B:4:DA:C8	2.49	0.46
1:A:94:ILE:HG22	1:A:95:GLY:N	2.31	0.46
4:F:212:LEU:O	4:F:283:ARG:NH1	2.49	0.46
1:A:185:ALA:HB1	1:A:190:LEU:HB2	1.98	0.46
1:A:50:ILE:HD12	1:A:66:TYR:CD2	2.51	0.46
1:A:55:LYS:HE2	1:A:63:ARG:NH2	2.31	0.46
2:C:66:A:OP2	2:C:66:A:C8	2.69	0.46
1:K:142:ASN:OD1	1:K:142:ASN:N	2.49	0.46
2:O:70:A:N1	2:O:71:A:N3	2.64	0.46
1:A:238:ARG:O	2:C:44:G:N2	2.41	0.45
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.15	0.45
2:O:43:U:C2	2:O:65:C:O2'	2.67	0.45
2:O:64:G:H3'	2:O:65:C:H5'	1.98	0.45
4:T:16:HIS:NE2	4:T:300:ASP:OD1	2.48	0.45
4:T:22:PHE:HD1	4:T:278:THR:HG21	1.82	0.45
5:V:49:DC:H2'	5:V:50:DT:H71	1.97	0.45
5:V:74:DA:H3'	5:V:75:DC:H5''	1.98	0.45
1:A:155:TYR:OH	1:A:156:LYS:NZ	2.50	0.45
1:A:264:ARG:HH12	2:C:50:U:H5	1.64	0.45
4:G:296:THR:N	5:L:78:DT:OP1	2.43	0.45
1:U:195:TYR:O	1:U:196:ALA:HB3	2.17	0.45
4:H:269:TYR:O	4:H:273:VAL:HG12	2.16	0.45
4:T:35:CYS:HB2	4:T:96:LEU:HD13	1.98	0.45
1:U:115:ILE:HD12	1:U:241:ARG:HB3	1.98	0.45
5:Q:28:DC:H2'	5:Q:29:DT:H71	1.99	0.45
5:J:56:DT:H2''	5:J:57:DT:H71	1.98	0.45
4:E:49:LEU:HD22	4:E:97:PHE:CZ	2.52	0.45
1:P:288:ILE:O	1:P:292:ASP:N	2.49	0.45
1:A:255:ILE:HG22	1:A:259:LYS:HB2	1.98	0.45
4:F:61:ILE:N	4:F:61:ILE:HD12	2.32	0.45
4:T:287:MET:O	4:T:291:ASN:HB2	2.17	0.45
4:T:288:ASN:OD1	4:T:292:ARG:NH1	2.50	0.45
2:C:17:A:C2	2:C:65:C:H2'	2.52	0.45
1:K:286:SER:HB3	2:M:77:G:H21	1.82	0.45
2:R:70:A:C2	2:R:71:A:C4	3.05	0.45
1:U:231:LYS:HB3	1:U:231:LYS:HZ2	1.81	0.45
1:U:255:ILE:HD13	1:U:288:ILE:CD1	2.47	0.45
1:K:290:SER:OG	2:M:77:G:O4'	2.35	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:A:H3'	2:C:67:U:C5'	2.48	0.44
4:H:30:ILE:CG2	4:H:32:ILE:HD11	2.47	0.44
1:A:233:CYS:SG	2:C:67:U:C2	3.10	0.44
1:K:132:VAL:HG21	1:K:154:CYS:SG	2.57	0.44
5:L:66:DG:C2	5:L:67:DA:C5	3.05	0.44
5:Q:66:DG:C2	5:Q:67:DA:C5	3.05	0.44
4:F:35:CYS:HB2	4:F:96:LEU:HD13	1.99	0.44
5:Q:56:DT:H2''	5:Q:57:DT:H72	1.98	0.44
4:F:296:THR:O	1:U:70:ARG:NH2	2.50	0.44
1:K:204:GLN:OE1	1:K:204:GLN:HA	2.17	0.44
2:M:16:G:O2'	2:M:17:A:O5'	2.31	0.44
5:Q:3:DC:H2''	5:Q:4:DA:O5'	2.17	0.44
2:O:4:C:N4	2:O:5:G:O6	2.51	0.44
5:V:40:DC:H2''	5:V:41:DA:C8	2.53	0.44
1:A:11:ARG:HD2	1:U:11:ARG:HH22	1.83	0.44
2:C:16:G:HO2'	2:C:17:A:P	2.40	0.44
4:E:206:LEU:CD1	4:E:243:VAL:HG11	2.48	0.44
2:M:50:U:C2	2:M:57:G:C2	3.06	0.44
4:T:24:ARG:O	4:T:24:ARG:HG2	2.18	0.44
4:H:212:LEU:O	4:H:283:ARG:NH1	2.50	0.44
4:T:106:GLU:O	4:T:110:PHE:CG	2.71	0.43
1:Z:80:LEU:O	1:Z:85:ASP:N	2.49	0.43
5:J:1:DG:N2	5:J:3:DC:H41	2.15	0.43
5:L:14:DG:H1'	5:L:15:DG:C8	2.52	0.43
1:K:197:ASP:OD1	5:L:85:DG:O3'	2.33	0.43
1:A:243:VAL:O	1:A:243:VAL:CG2	2.66	0.43
2:C:16:G:C8	2:C:64:G:C6	3.06	0.43
4:E:90:ALA:HB1	4:E:200:LEU:HD12	2.00	0.43
4:E:122:CYS:C	4:E:123:ILE:HD12	2.38	0.43
1:U:239:SER:HB2	2:W:65:C:OP2	2.18	0.43
5:J:54:DC:C2	5:J:55:DG:N7	2.87	0.43
2:O:79:U:N3	2:O:80:A:N7	2.66	0.43
3:S:2:G:O2'	3:S:3:U:OP2	2.26	0.43
1:U:238:ARG:CG	2:W:65:C:OP1	2.66	0.43
1:A:92:PHE:CZ	1:A:182:GLN:HG2	2.53	0.43
4:E:22:PHE:HD1	4:E:278:THR:HG21	1.83	0.43
5:L:13:DG:H2''	5:L:14:DG:C8	2.53	0.43
4:E:275:ASP:HB3	4:E:278:THR:HG22	2.00	0.43
4:E:83:LEU:O	4:E:86:ILE:HG13	2.18	0.43
4:E:96:LEU:HD21	4:E:107:LEU:HB2	2.00	0.43
1:K:37:LEU:HD22	1:K:41:ILE:HD11	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:168:LYS:O	1:P:172:LEU:HD13	2.19	0.43
1:U:92:PHE:CZ	1:U:182:GLN:HG2	2.54	0.43
2:W:65:C:H3'	2:W:66:A:N7	2.33	0.43
2:W:66:A:P	2:W:66:A:C8	3.12	0.43
5:V:55:DG:H1'	5:V:56:DT:H5'	2.01	0.43
2:C:70:A:C2	2:C:71:A:C4	3.07	0.43
1:K:37:LEU:O	1:K:41:ILE:HG13	2.18	0.43
5:J:53:DC:H2''	5:J:54:DC:C5	2.54	0.43
5:J:66:DG:C2	5:J:67:DA:C5	3.06	0.43
1:A:87:LEU:HD11	1:A:139:LEU:HD11	2.00	0.43
1:K:186:GLY:O	4:T:265:LEU:HD21	2.19	0.43
5:B:40:DC:H2''	5:B:41:DA:C8	2.54	0.43
5:V:53:DC:H2''	5:V:54:DC:C5	2.54	0.43
4:H:62:PHE:HZ	4:H:201:TYR:CE1	2.37	0.43
2:O:68:U:O2'	2:O:69:G:O5'	2.37	0.43
1:U:185:ALA:HB1	1:U:190:LEU:HB2	2.00	0.43
2:C:17:A:H4'	2:C:66:A:H61	1.83	0.42
4:E:12:GLN:NE2	4:E:302:ILE:HD12	2.34	0.42
4:E:273:VAL:O	4:E:273:VAL:HG13	2.19	0.42
5:J:32:DG:H2''	5:J:33:DA:C8	2.54	0.42
5:L:71:DC:H2''	5:L:72:DA:N7	2.34	0.42
2:C:16:G:HO2'	2:C:17:A:C5'	2.31	0.42
4:F:304:TYR:OH	5:V:79:DA:O3'	2.38	0.42
4:H:304:TYR:HB2	5:J:78:DT:H73	1.99	0.42
5:Q:55:DG:H1'	5:Q:56:DT:H5'	2.01	0.42
4:E:53:LEU:HD12	4:E:59:VAL:HG21	2.02	0.42
4:H:22:PHE:HD1	4:H:278:THR:HG21	1.83	0.42
1:K:23:LEU:HB3	1:K:34:VAL:HG23	2.01	0.42
2:O:42:C:H2'	2:O:43:U:C6	2.54	0.42
2:O:70:A:N1	2:O:71:A:C2	2.88	0.42
1:U:289:LEU:HD12	1:U:289:LEU:O	2.19	0.42
5:B:38:DA:C2	5:B:48:DG:C2	3.08	0.42
2:O:17:A:HO2'	2:O:18:G:H8	1.66	0.42
5:J:40:DC:H2''	5:J:41:DA:C8	2.54	0.42
1:A:307:GLU:O	1:A:311:GLY:N	2.51	0.42
4:F:81:LEU:O	4:F:85:ASN:ND2	2.53	0.42
5:V:66:DG:C2	5:V:67:DA:C5	3.07	0.42
2:C:12:U:O4	2:C:13:A:N6	2.53	0.42
4:F:210:ILE:HA	4:F:216:VAL:HG21	2.02	0.42
2:R:70:A:N1	2:R:71:A:C2	2.88	0.42
4:T:12:GLN:NE2	4:T:302:ILE:HD12	2.35	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:55:DG:H1'	5:J:56:DT:H5'	2.01	0.42
3:N:1:C:N4	3:N:2:G:O6	2.52	0.42
1:U:284:TRP:O	1:U:288:ILE:HG12	2.19	0.42
1:K:62:MET:HA	1:K:62:MET:CE	2.50	0.42
1:K:260:TYR:HE1	1:K:299:LEU:CD2	2.33	0.42
2:W:66:A:N3	2:W:66:A:H2'	2.34	0.42
2:W:74:U:O5'	2:W:74:U:O2	2.38	0.42
2:C:16:G:N7	2:C:64:G:C5	2.88	0.42
2:C:72:U:H1'	5:B:77:DG:H5''	2.02	0.42
4:T:275:ASP:OD1	4:T:276:ARG:N	2.53	0.42
2:W:66:A:C8	2:W:66:A:O5'	2.72	0.42
5:Q:53:DC:H2''	5:Q:54:DC:C5	2.55	0.42
1:A:239:SER:OG	1:A:240:GLN:N	2.53	0.41
2:C:65:C:H2'	2:C:65:C:O2	2.19	0.41
4:T:125:ASP:OD1	4:T:128:PHE:CD2	2.73	0.41
2:W:67:U:H3'	2:W:68:U:H5'	2.02	0.41
5:Q:14:DG:N2	5:Q:72:DA:C2	2.88	0.41
4:F:73:ALA:HB2	4:H:137:TYR:CD1	2.55	0.41
2:R:68:U:O2'	2:R:69:G:N3	2.41	0.41
4:T:101:PRO:HG2	7:T:401:AR6:H8	2.02	0.41
2:C:17:A:N6	2:C:65:C:N3	2.68	0.41
7:E:401:AR6:PB	7:E:401:AR6:H4'	2.60	0.41
4:E:67:LEU:HD13	4:E:67:LEU:C	2.41	0.41
4:H:34:LEU:HD21	4:H:49:LEU:HD12	2.02	0.41
2:O:64:G:H4'	2:O:65:C:O2	2.20	0.41
5:B:66:DG:C2	5:B:67:DA:C5	3.08	0.41
7:E:401:AR6:H2	4:T:136:ASN:OD1	2.19	0.41
1:K:232:THR:O	2:M:67:U:C5	2.73	0.41
2:C:68:U:C5	2:C:69:G:C5	3.08	0.41
4:E:250:GLU:HG3	4:E:252:LYS:HD3	2.01	0.41
1:U:94:ILE:HG22	1:U:95:GLY:N	2.35	0.41
2:W:66:A:C8	2:W:66:A:OP2	2.73	0.41
5:B:49:DC:C2'	5:B:50:DT:H71	2.51	0.41
5:B:55:DG:H1'	5:B:56:DT:H5'	2.03	0.41
5:B:77:DG:N3	5:B:78:DT:C2	2.89	0.41
2:C:74:U:O5'	2:C:74:U:O2	2.38	0.41
1:U:106:ALA:HA	1:U:243:VAL:HG21	2.02	0.41
4:H:35:CYS:HB2	4:H:96:LEU:HD13	2.03	0.41
4:T:69:ASP:OD1	4:T:69:ASP:C	2.58	0.41
5:V:56:DT:H2''	5:V:57:DT:H72	2.02	0.41
1:A:11:ARG:CD	1:U:11:ARG:HH22	2.34	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ILE:HG13	1:A:220:ILE:N	2.35	0.41
4:H:212:LEU:HD21	4:H:279:LEU:CD2	2.50	0.41
1:K:39:LEU:HB2	5:L:13:DG:H4'	2.02	0.41
2:M:71:A:C2	2:M:73:C:O2	2.73	0.41
2:M:71:A:N1	2:M:73:C:O2	2.54	0.41
2:O:66:A:C5'	2:O:67:U:OP2	2.69	0.41
1:U:219:ILE:HG13	1:U:220:ILE:N	2.34	0.41
1:U:286:SER:HB3	2:W:77:G:H21	1.86	0.41
5:B:56:DT:C2'	5:B:57:DT:H72	2.51	0.41
1:A:55:LYS:HE3	1:A:63:ARG:HB3	2.03	0.41
4:E:133:SER:OG	4:E:136:ASN:OD1	2.39	0.41
7:E:401:AR6:H4'	7:E:401:AR6:O1B	2.21	0.41
4:H:32:ILE:HD13	4:H:93:VAL:CG1	2.51	0.41
1:P:31:ARG:HD2	4:T:211:TYR:CE1	2.56	0.41
2:R:70:A:N6	2:R:71:A:N6	2.69	0.41
2:W:16:G:HO2'	2:W:17:A:P	2.41	0.41
5:L:79:DA:C4	5:L:80:DA:C8	3.09	0.41
1:K:54:GLU:HA	1:K:62:MET:HE3	2.02	0.40
4:T:69:ASP:OD1	4:T:69:ASP:O	2.39	0.40
1:U:41:ILE:HD13	1:U:148:VAL:HG13	2.03	0.40
1:U:157:ASN:O	1:U:157:ASN:CG	2.60	0.40
2:W:66:A:C3'	2:W:67:U:H4'	2.50	0.40
5:J:46:DA:H2'	5:J:47:DT:H71	2.03	0.40
2:C:14:G:O2'	5:B:1:DG:P	2.80	0.40
2:C:17:A:HO2'	2:C:18:G:H8	1.69	0.40
2:C:65:C:O2	2:C:65:C:C2'	2.66	0.40
4:E:246:ARG:NH1	4:E:246:ARG:HG2	2.36	0.40
7:F:401:AR6:C2	4:H:128:PHE:HB3	2.52	0.40
4:G:284:LEU:HD21	1:K:32:ILE:HD13	2.03	0.40
2:M:12:U:O4	2:M:13:A:N6	2.54	0.40
4:T:276:ARG:NH1	5:Q:14:DG:OP1	2.53	0.40
5:Q:71:DC:H2''	5:Q:72:DA:N7	2.36	0.40
4:F:211:TYR:OH	4:F:271:ARG:NE	2.50	0.40
2:W:40:C:H2'	2:W:41:U:C6	2.57	0.40
1:A:6:TYR:O	1:A:9:THR:HG22	2.21	0.40
5:J:3:DC:H2'	5:J:4:DA:C8	2.56	0.40
5:Q:67:DA:C2	5:Q:68:DA:C5	3.10	0.40
5:V:45:DG:H2'	5:V:46:DA:C8	2.56	0.40
4:T:83:LEU:O	4:T:86:ILE:HG13	2.21	0.40
4:T:133:SER:OG	4:T:136:ASN:OD1	2.38	0.40
1:U:287:PHE:HB2	5:V:82:DT:O2	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:54:DC:C2	5:B:55:DG:N7	2.90	0.40

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	308/349 (88%)	300 (97%)	8 (3%)	0	100	100
1	I	308/349 (88%)	305 (99%)	3 (1%)	0	100	100
1	K	308/349 (88%)	300 (97%)	8 (3%)	0	100	100
1	P	308/349 (88%)	301 (98%)	7 (2%)	0	100	100
1	U	308/349 (88%)	298 (97%)	10 (3%)	0	100	100
1	Z	308/349 (88%)	306 (99%)	2 (1%)	0	100	100
4	E	300/307 (98%)	295 (98%)	5 (2%)	0	100	100
4	F	300/307 (98%)	293 (98%)	7 (2%)	0	100	100
4	G	120/307 (39%)	119 (99%)	1 (1%)	0	100	100
4	H	300/307 (98%)	296 (99%)	4 (1%)	0	100	100
4	T	300/307 (98%)	295 (98%)	5 (2%)	0	100	100
All	All	3168/3629 (87%)	3108 (98%)	60 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	239/311 (77%)	237 (99%)	2 (1%)	81	92
1	K	232/311 (75%)	232 (100%)	0	100	100
1	P	107/311 (34%)	107 (100%)	0	100	100
1	U	217/311 (70%)	215 (99%)	2 (1%)	78	91
1	Z	1/311 (0%)	0	1 (100%)	0	0
4	E	212/278 (76%)	211 (100%)	1 (0%)	88	94
4	F	178/278 (64%)	176 (99%)	2 (1%)	73	89
4	G	21/278 (8%)	21 (100%)	0	100	100
4	H	156/278 (56%)	156 (100%)	0	100	100
4	T	208/278 (75%)	207 (100%)	1 (0%)	88	94
All	All	1571/2945 (53%)	1562 (99%)	9 (1%)	86	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	PHE
1	A	231	LYS
4	E	5	PHE
4	F	5	PHE
4	F	216	VAL
4	T	213	LEU
1	U	92	PHE
1	U	231	LYS
1	Z	198	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	47	HIS
1	P	280	HIS

### 5.3.3 RNA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	58/82 (70%)	16 (27%)	5 (8%)
2	M	58/82 (70%)	13 (22%)	3 (5%)
2	O	58/82 (70%)	12 (20%)	4 (6%)
2	R	58/82 (70%)	12 (20%)	4 (6%)
2	W	58/82 (70%)	13 (22%)	4 (6%)
2	b	58/82 (70%)	14 (24%)	0
3	D	13/14 (92%)	1 (7%)	0
3	N	13/14 (92%)	1 (7%)	0
3	S	13/14 (92%)	1 (7%)	0
3	X	13/14 (92%)	1 (7%)	0
3	Y	13/14 (92%)	1 (7%)	0
3	c	13/14 (92%)	1 (7%)	0
All	All	426/576 (73%)	86 (20%)	20 (4%)

All (86) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	15	C
2	C	17	A
2	C	21	G
2	C	44	G
2	C	49	U
2	C	51	G
2	C	56	G
2	C	63	U
2	C	64	G
2	C	65	C
2	C	66	A
2	C	67	U
2	C	68	U
2	C	69	G
2	C	70	A
2	C	72	U
3	D	3	U
2	M	15	C
2	M	17	A
2	M	44	G
2	M	56	G
2	M	64	G
2	M	65	C
2	M	66	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	M	67	U
2	M	68	U
2	M	69	G
2	M	70	A
2	M	71	A
2	M	72	U
3	N	3	U
2	O	15	C
2	O	17	A
2	O	21	G
2	O	44	G
2	O	56	G
2	O	64	G
2	O	65	C
2	O	66	A
2	O	67	U
2	O	69	G
2	O	70	A
2	O	72	U
2	R	15	C
2	R	17	A
2	R	21	G
2	R	44	G
2	R	56	G
2	R	64	G
2	R	65	C
2	R	66	A
2	R	67	U
2	R	68	U
2	R	69	G
2	R	72	U
3	S	3	U
2	W	15	C
2	W	17	A
2	W	21	G
2	W	44	G
2	W	51	G
2	W	56	G
2	W	64	G
2	W	65	C
2	W	66	A
2	W	67	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	W	68	U
2	W	69	G
2	W	72	U
3	X	3	U
3	Y	3	U
2	b	15	C
2	b	17	A
2	b	21	G
2	b	44	G
2	b	56	G
2	b	64	G
2	b	65	C
2	b	66	A
2	b	67	U
2	b	68	U
2	b	69	G
2	b	70	A
2	b	71	A
2	b	72	U
3	c	3	U

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	64	G
2	C	65	C
2	C	66	A
2	C	67	U
2	C	68	U
2	M	67	U
2	M	68	U
2	M	69	G
2	O	65	C
2	O	66	A
2	O	68	U
2	O	69	G
2	R	65	C
2	R	66	A
2	R	68	U
2	R	69	G
2	W	65	C
2	W	66	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	W	67	U
2	W	68	U

## 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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
7	AR6	T	401	4	33,38,39	0.66	0	37,58,60	0.85	2 (5%)
7	AR6	H	401	4	33,38,39	0.66	0	37,58,60	0.78	2 (5%)
7	AR6	F	401	4	33,38,39	0.71	0	37,58,60	0.74	2 (5%)
7	AR6	E	401	4	33,38,39	0.67	0	37,58,60	0.73	1 (2%)

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
7	AR6	T	401	4	-	9/18/51/54	0/4/4/4
7	AR6	H	401	4	-	8/18/51/54	0/4/4/4
7	AR6	F	401	4	-	10/18/51/54	0/4/4/4

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AR6	E	401	4	-	6/18/51/54	0/4/4/4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	401	AR6	C1D-O4D-C4D	-2.64	102.00	108.16
7	T	401	AR6	C1D-O4D-C4D	-2.54	102.24	108.16
7	T	401	AR6	C5-C6-N6	2.38	123.96	120.35
7	F	401	AR6	C5-C6-N6	2.34	123.92	120.35
7	E	401	AR6	C5-C6-N6	2.31	123.86	120.35
7	H	401	AR6	C5-C6-N6	2.22	123.72	120.35
7	F	401	AR6	C1D-O4D-C4D	-2.16	103.11	108.16

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	401	AR6	C5D-O5D-PB-O1B
7	E	401	AR6	C5D-O5D-PB-O3A
7	F	401	AR6	C5'-O5'-PA-O1A
7	F	401	AR6	C3'-C4'-C5'-O5'
7	F	401	AR6	C3D-C4D-C5D-O5D
7	F	401	AR6	O4D-C4D-C5D-O5D
7	H	401	AR6	C5D-O5D-PB-O1B
7	H	401	AR6	C5D-O5D-PB-O3A
7	T	401	AR6	C5'-O5'-PA-O1A
7	T	401	AR6	C5'-O5'-PA-O2A
7	T	401	AR6	C3'-C4'-C5'-O5'
7	T	401	AR6	C3D-C4D-C5D-O5D
7	F	401	AR6	O4'-C4'-C5'-O5'
7	H	401	AR6	O4'-C4'-C5'-O5'
7	T	401	AR6	O4D-C4D-C5D-O5D
7	H	401	AR6	C3'-C4'-C5'-O5'
7	T	401	AR6	O4'-C4'-C5'-O5'
7	H	401	AR6	PA-O3A-PB-O2B
7	T	401	AR6	C4'-C5'-O5'-PA
7	E	401	AR6	C4'-C5'-O5'-PA
7	F	401	AR6	PB-O3A-PA-O5'
7	F	401	AR6	C5'-O5'-PA-O3A
7	H	401	AR6	C4'-C5'-O5'-PA

Continued on next page...



*Continued from previous page...*

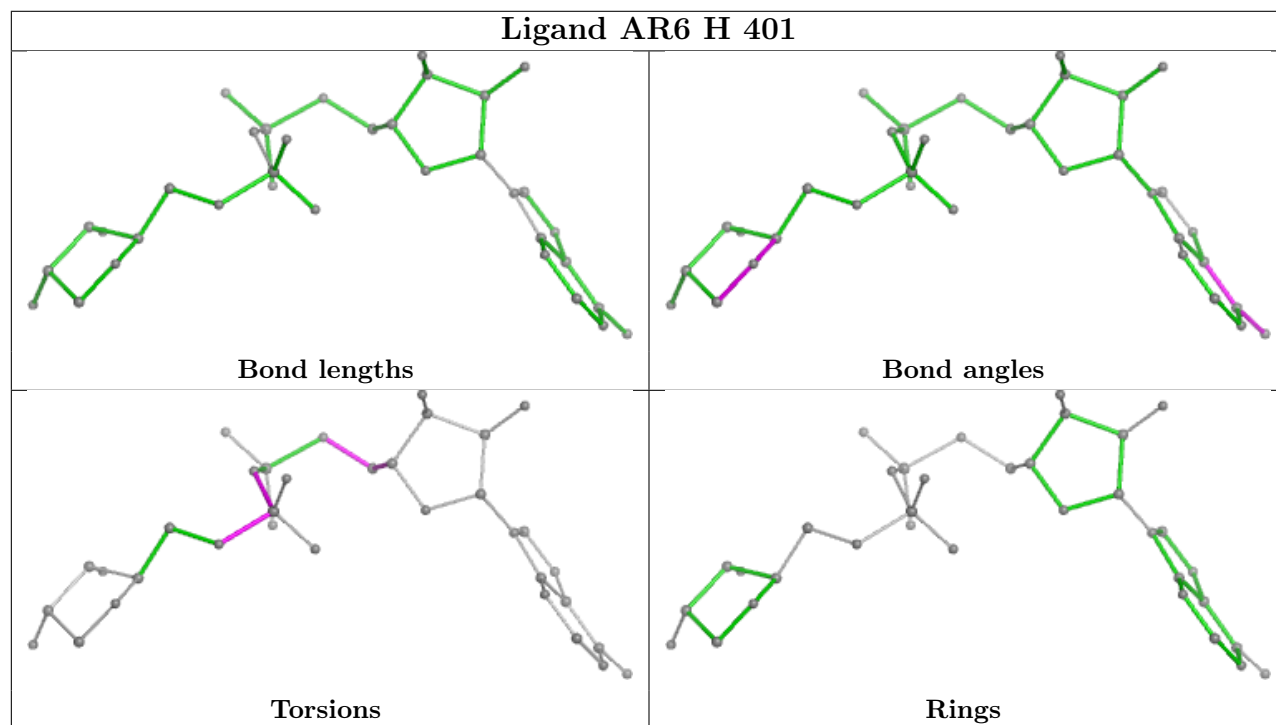
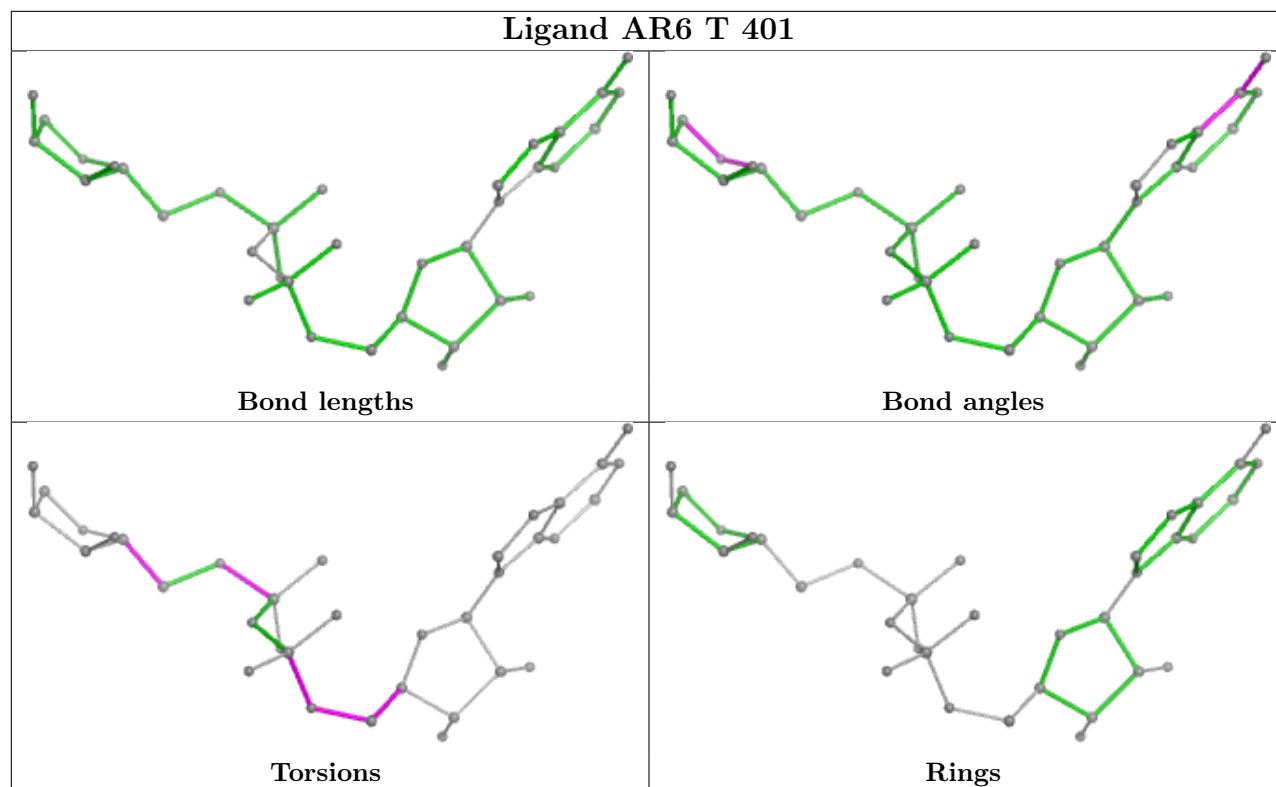
Mol	Chain	Res	Type	Atoms
7	E	401	AR6	C5D-O5D-PB-O2B
7	F	401	AR6	C5'-O5'-PA-O2A
7	H	401	AR6	C5D-O5D-PB-O2B
7	H	401	AR6	PA-O3A-PB-O1B
7	T	401	AR6	C5'-O5'-PA-O3A
7	E	401	AR6	O4'-C4'-C5'-O5'
7	E	401	AR6	PA-O3A-PB-O1B
7	F	401	AR6	PB-O3A-PA-O2A
7	F	401	AR6	C5D-O5D-PB-O2B
7	T	401	AR6	C5D-O5D-PB-O2B

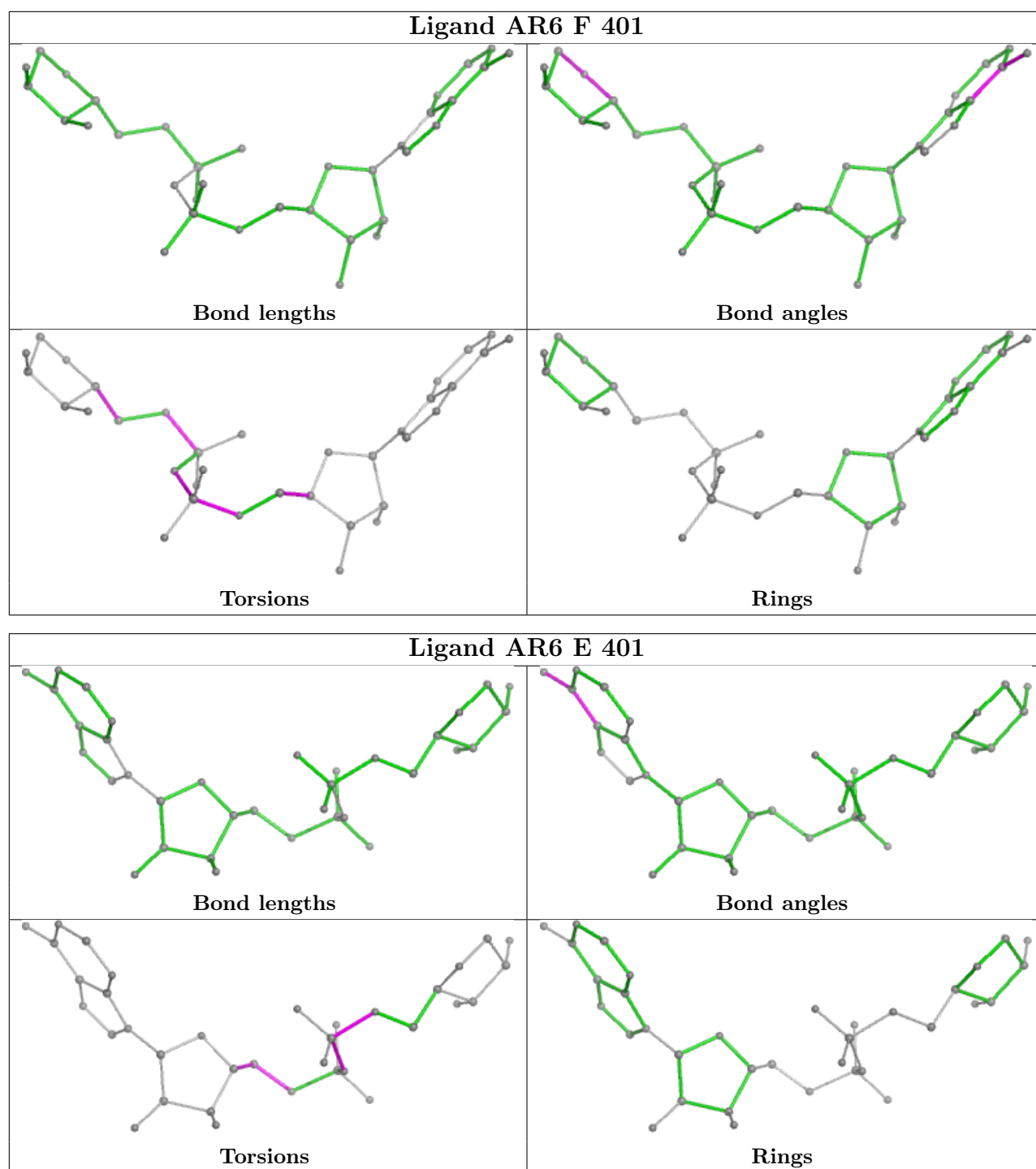
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	401	AR6	5	0
7	H	401	AR6	3	0
7	F	401	AR6	2	0
7	E	401	AR6	4	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

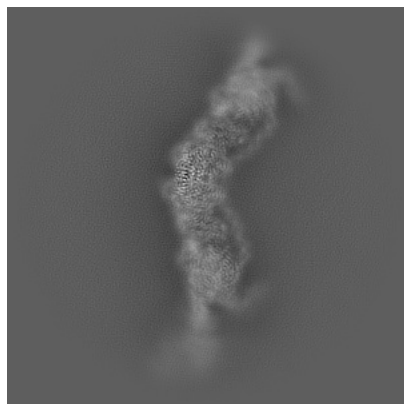
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18315. These allow visual inspection of the internal detail of the map and identification of artifacts.

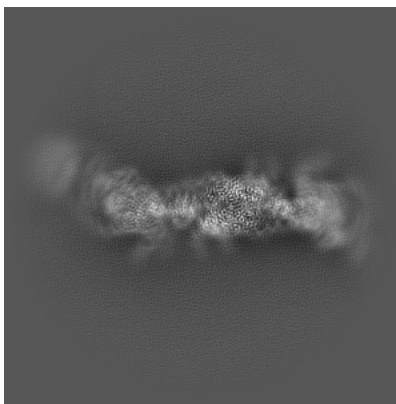
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

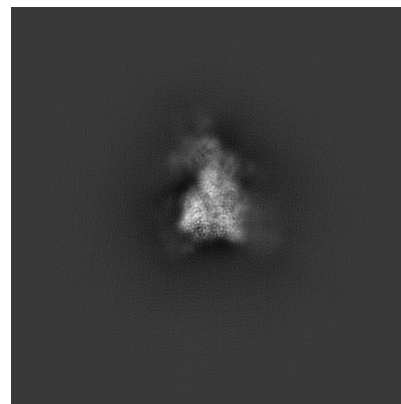
#### 6.1.1 Primary map



X

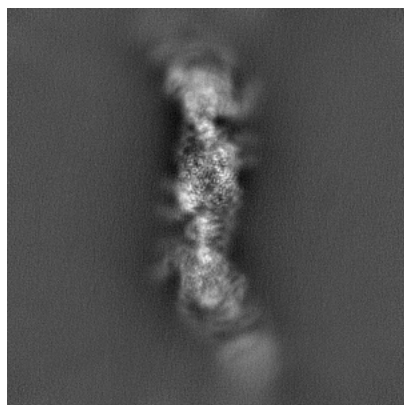


Y

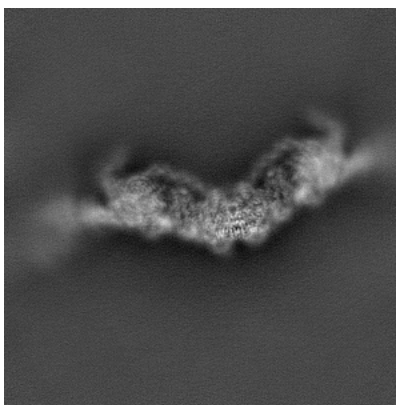


Z

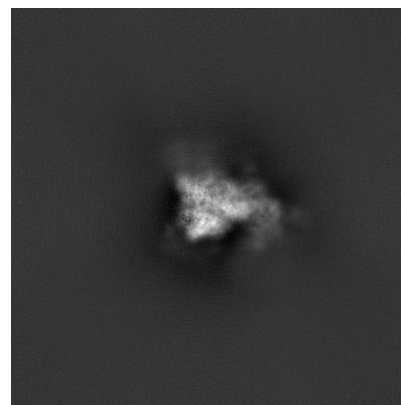
#### 6.1.2 Raw map



X



Y

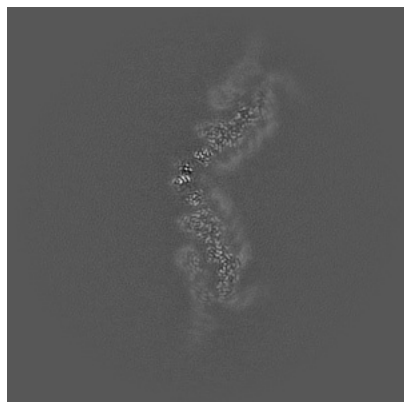


Z

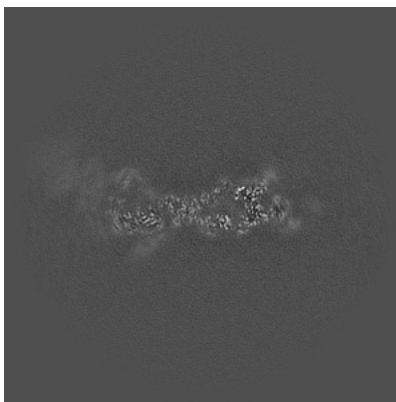
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

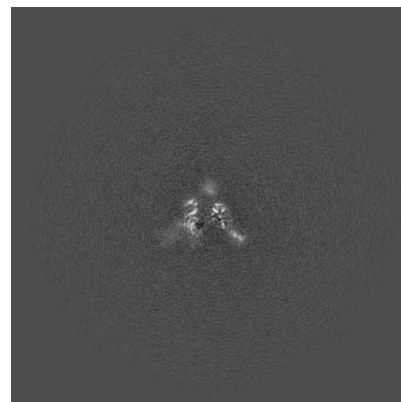
### 6.2.1 Primary map



X Index: 300

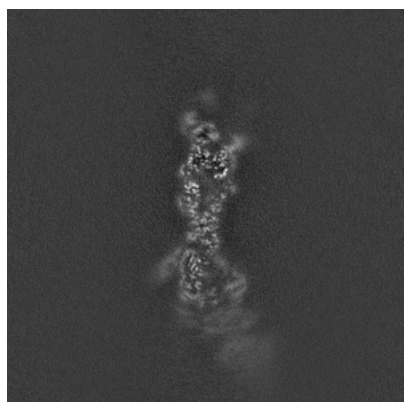


Y Index: 300

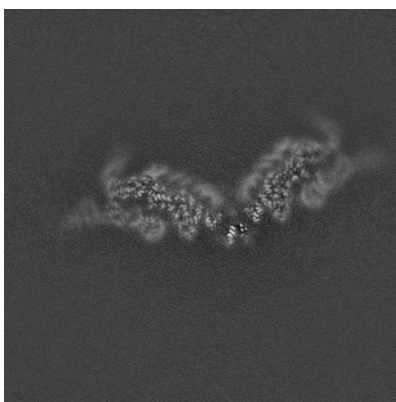


Z Index: 300

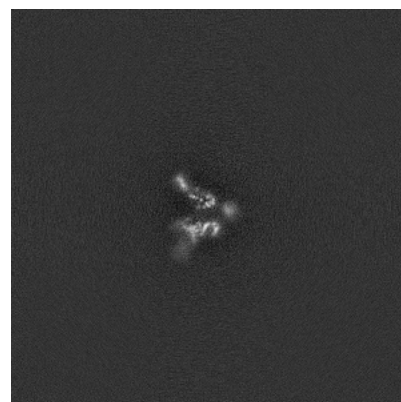
### 6.2.2 Raw map



X Index: 300



Y Index: 300

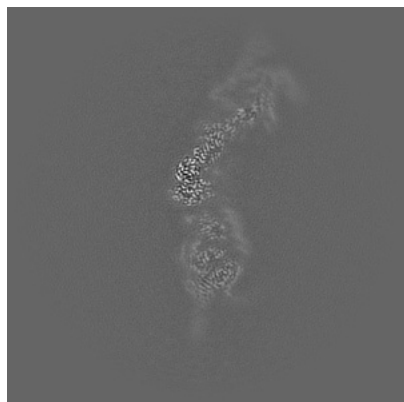


Z Index: 300

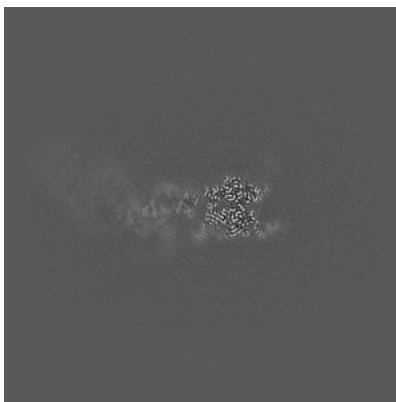
The images above show central slices of the map in three orthogonal directions.

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

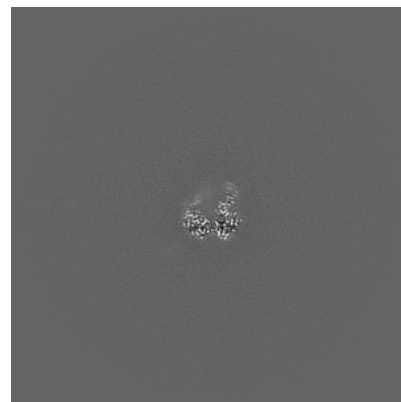
### 6.3.1 Primary map



X Index: 287



Y Index: 275

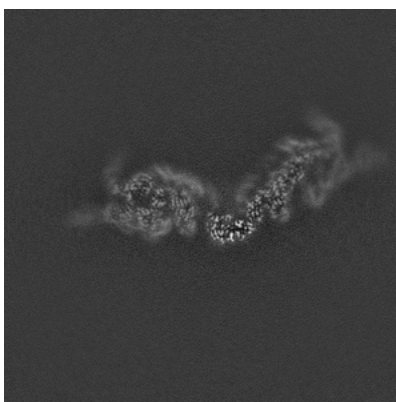


Z Index: 348

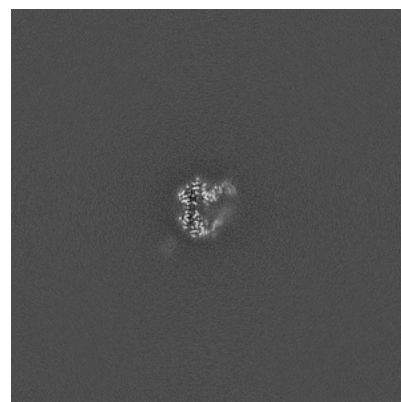
### 6.3.2 Raw map



X Index: 276



Y Index: 291

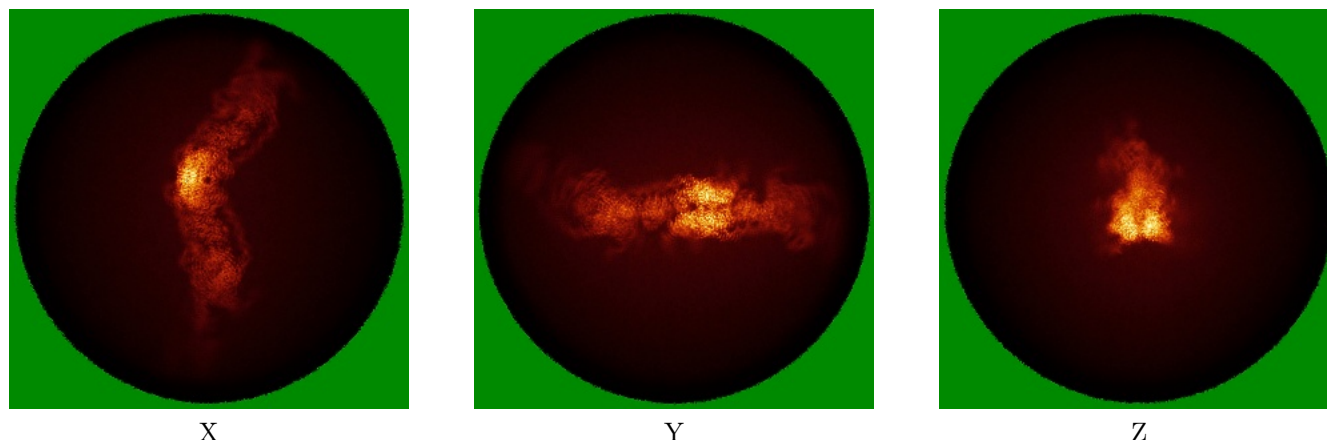


Z Index: 348

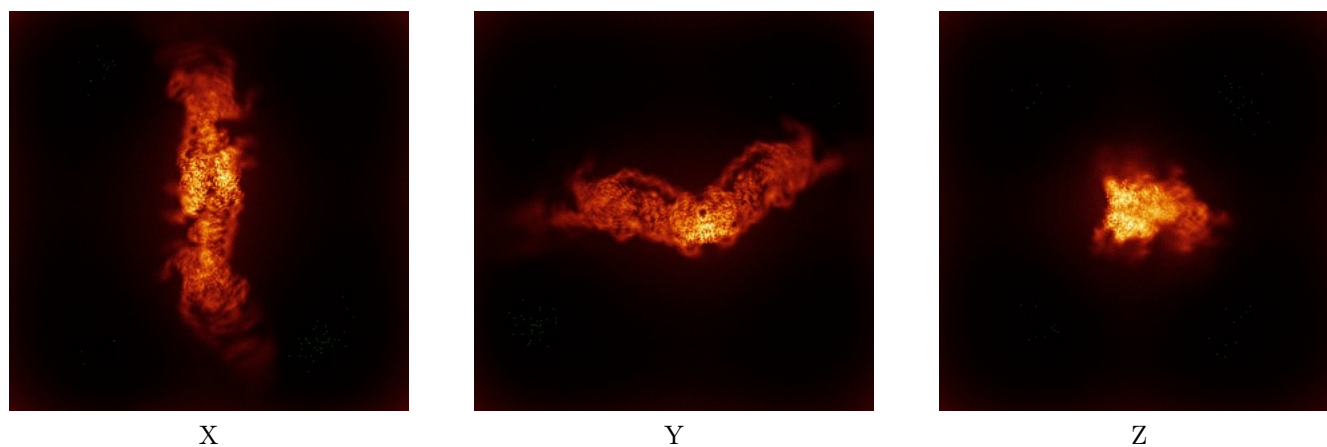
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



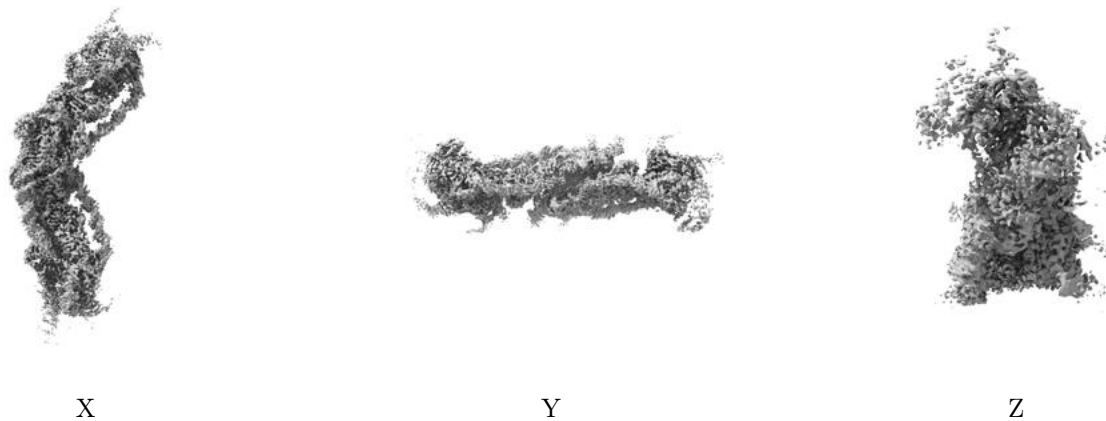
### 6.4.2 Raw map



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.

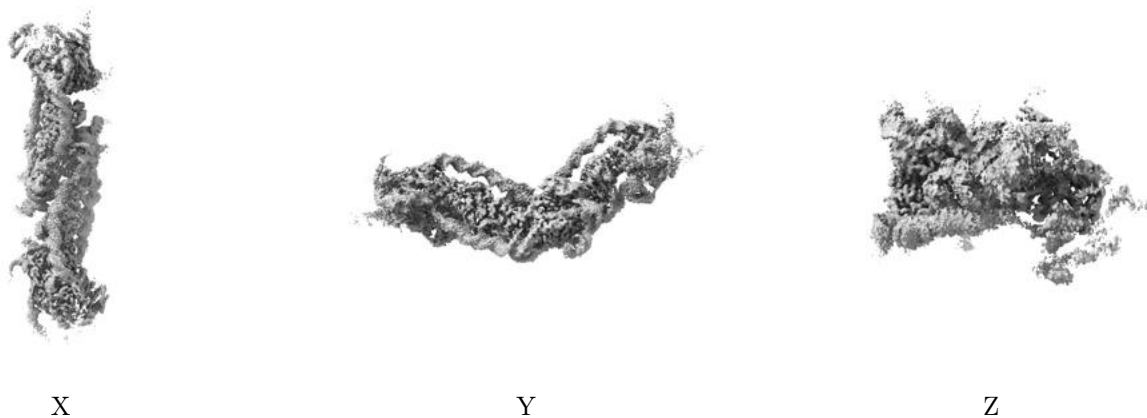
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. 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](#)

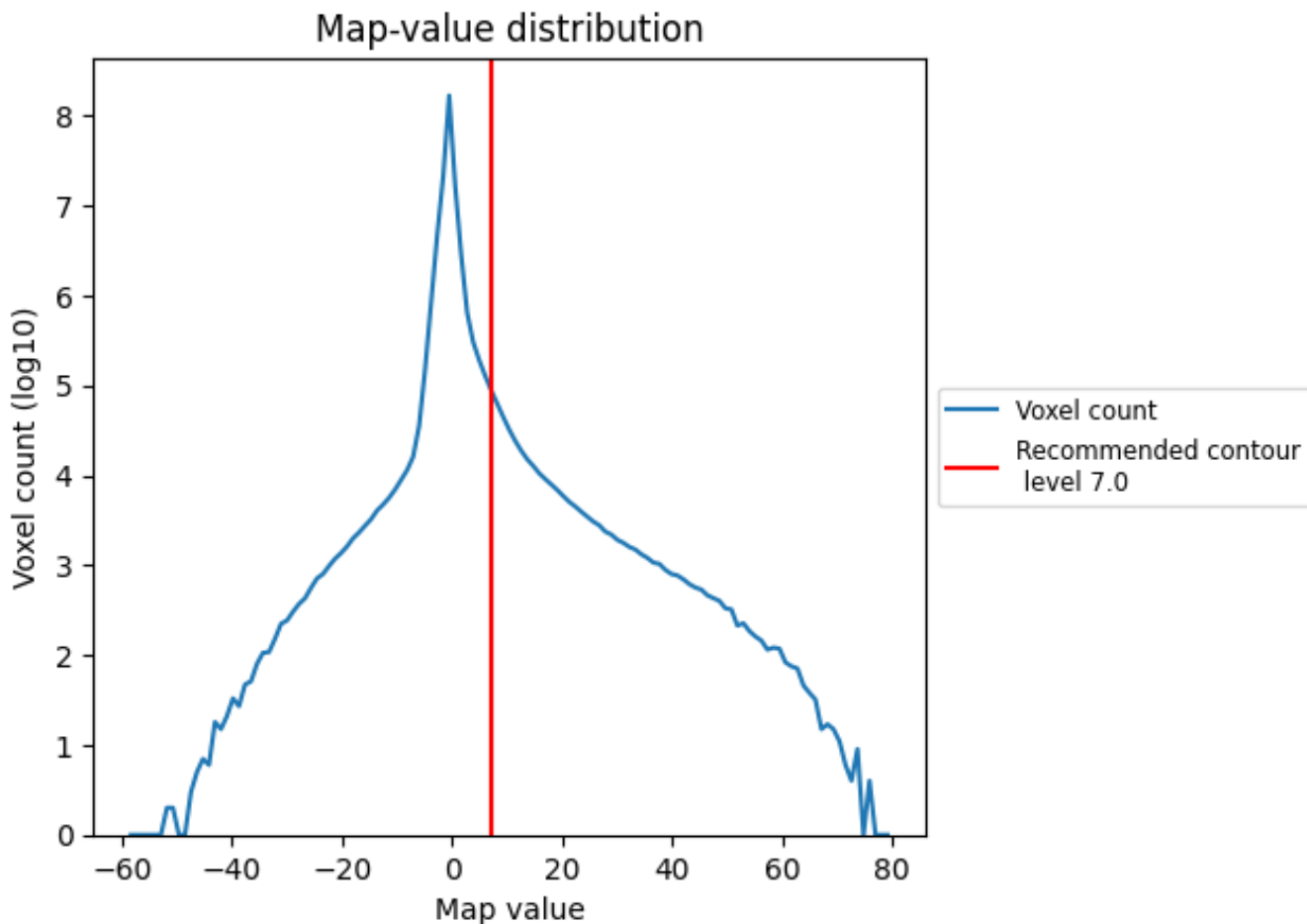
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

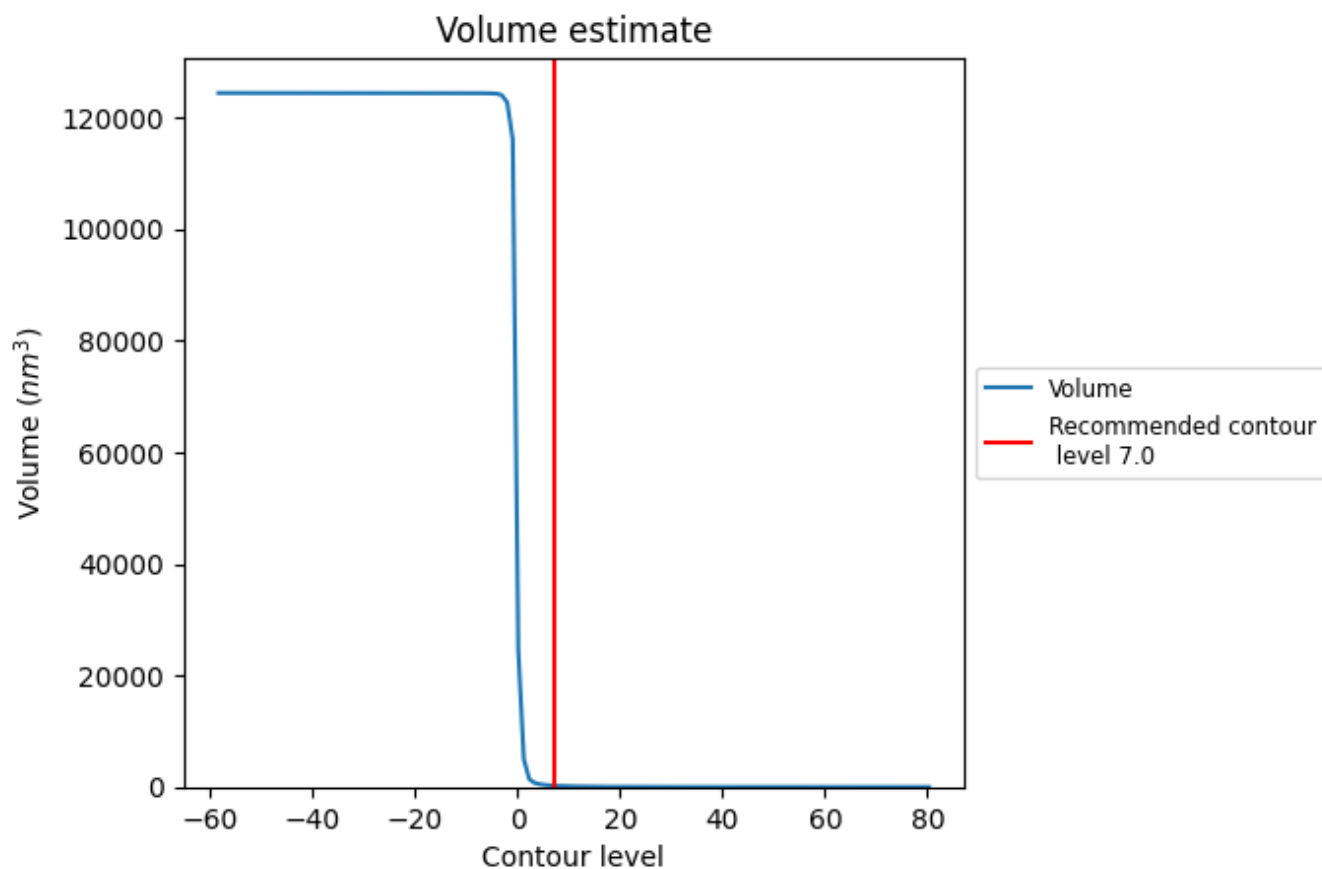
This section contains the results of statistical analysis of the map.

### 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.

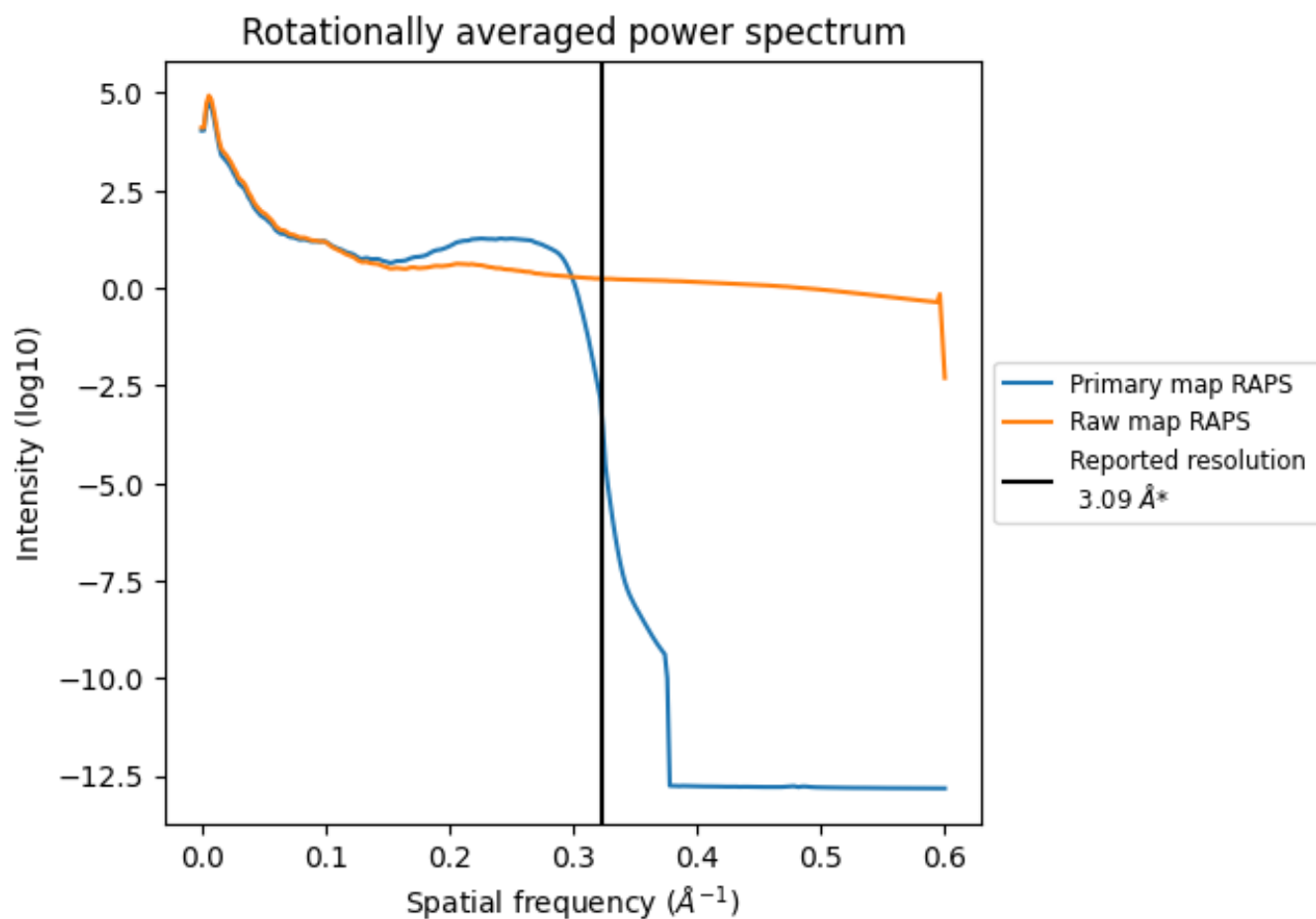
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $232 \text{ nm}^3$ ; this corresponds to an approximate mass of 209 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](#)

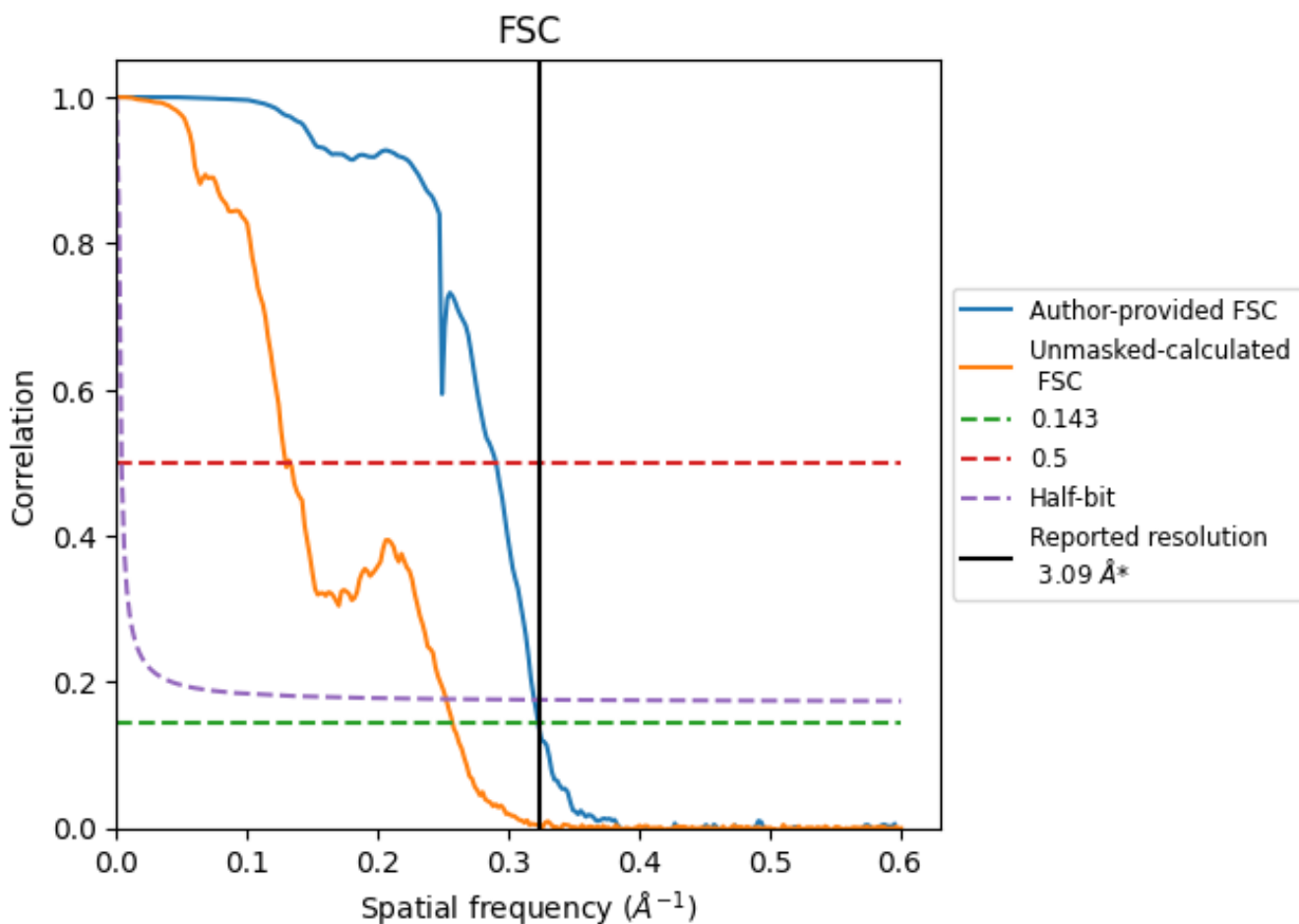


\*Reported resolution corresponds to spatial frequency of 0.324 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.324  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

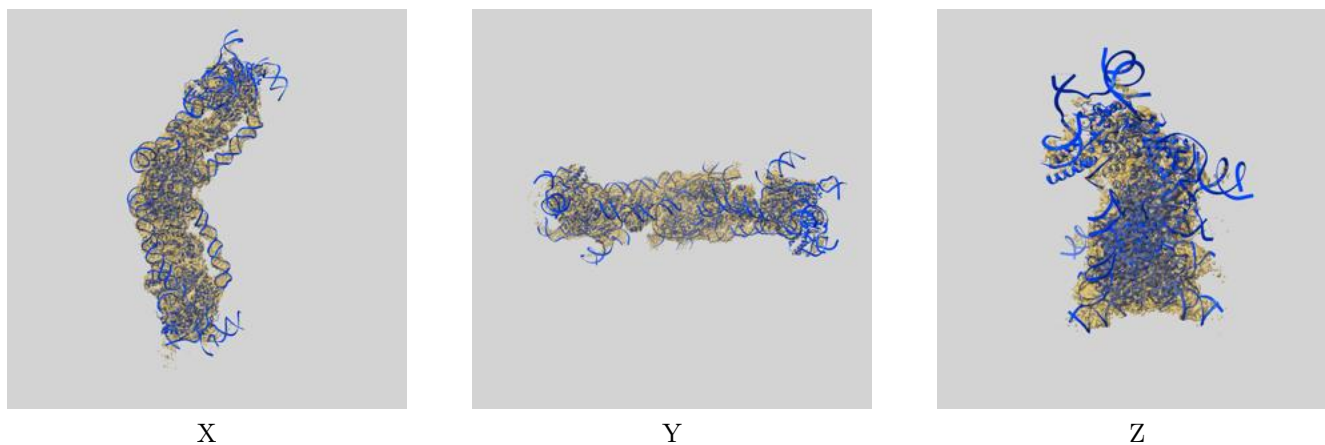
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.10	3.44	3.12
Unmasked-calculated*	3.88	7.72	3.96

\*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 3.88 differs from the reported value 3.09 by more than 10 %

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

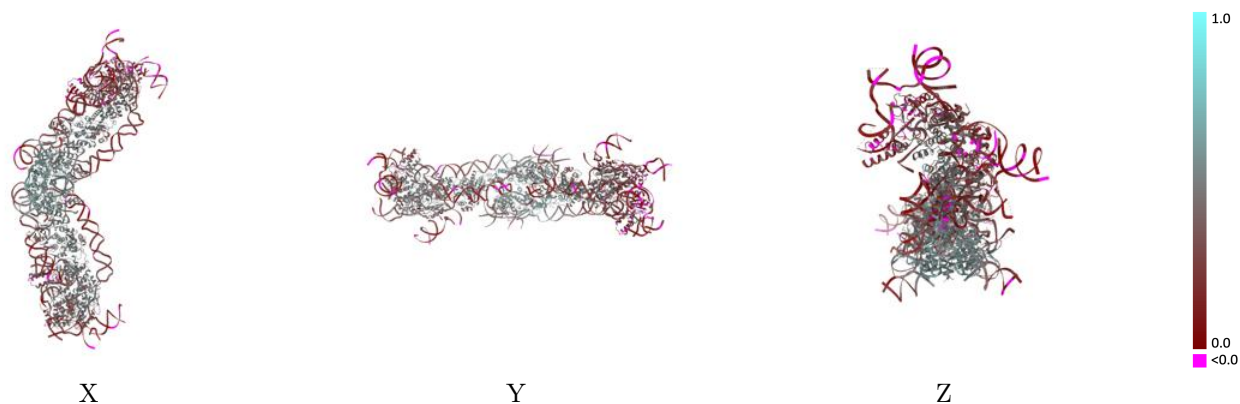
This section contains information regarding the fit between EMDB map EMD-18315 and PDB model 8QBM. Per-residue inclusion information can be found in section 3 on page 12.

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



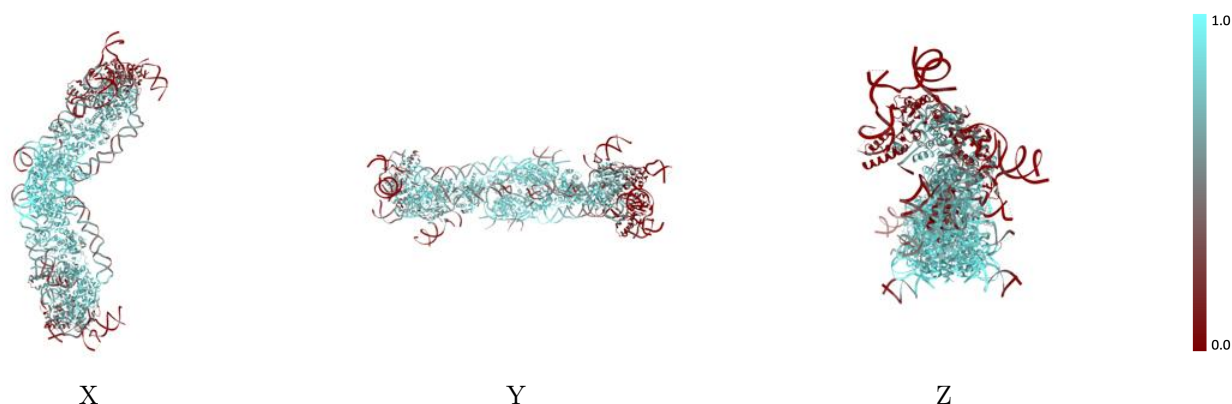
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



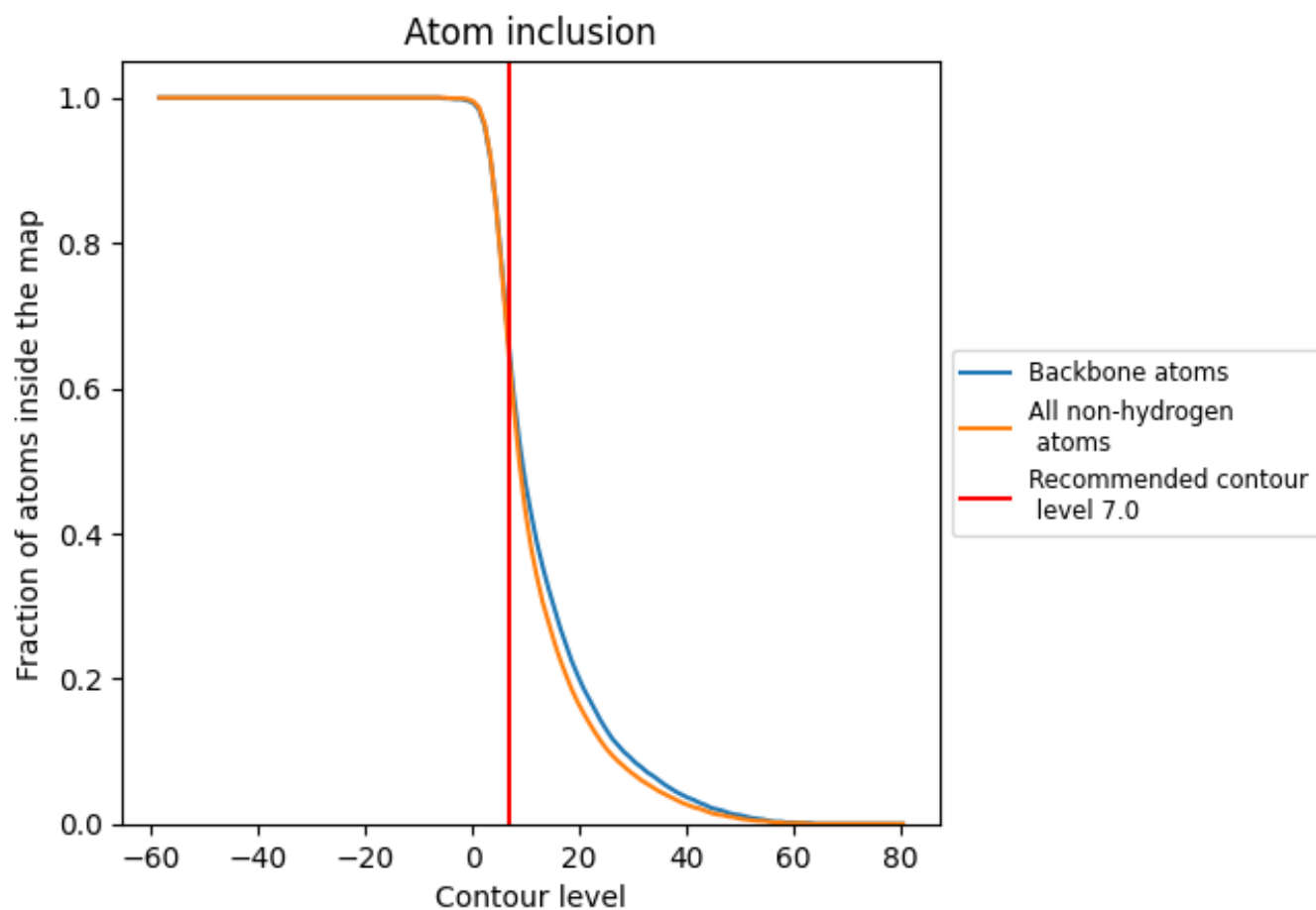
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7.0).

## 9.4 Atom inclusion [i](#)































































At the recommended contour level, 64% of all backbone atoms, 63% 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 (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6290	 0.3650
A	 0.9190	 0.5500
B	 0.7230	 0.3400
C	 0.7420	 0.3570
D	 0.4540	 0.2100
E	 0.8800	 0.5050
F	 0.8900	 0.5290
G	 0.4330	 0.3690
H	 0.8020	 0.4770
I	 0.3540	 0.2790
J	 0.4390	 0.1900
K	 0.7100	 0.4390
L	 0.5130	 0.2910
M	 0.4650	 0.2420
N	 0.1740	 0.1490
O	 0.1620	 0.1490
P	 0.7190	 0.4470
Q	 0.5850	 0.2440
R	 0.3230	 0.2290
S	 0.0620	 0.1090
T	 0.8110	 0.4860
U	 0.9250	 0.5520
V	 0.6770	 0.3560
W	 0.7640	 0.3530
X	 0.5330	 0.2890
Y	 0.0230	 0.1150
Z	 0.4200	 0.2860
a	 0.2470	 0.1740
b	 0.3020	 0.1500
c	 0.0720	 0.0910

