



## Full wwPDB EM Validation Report ⓘ

Dec 9, 2024 – 12:26 PM JST

PDB ID : 9JM0  
EMDB ID : EMD-61595  
Title : retron Ec86-effector fiber  
Authors : Wang, Y.J.; Guan, Z.Y.; Wang, C.; Zou, T.T.  
Deposited on : 2024-09-20  
Resolution : 2.70 Å (reported)

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>.

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

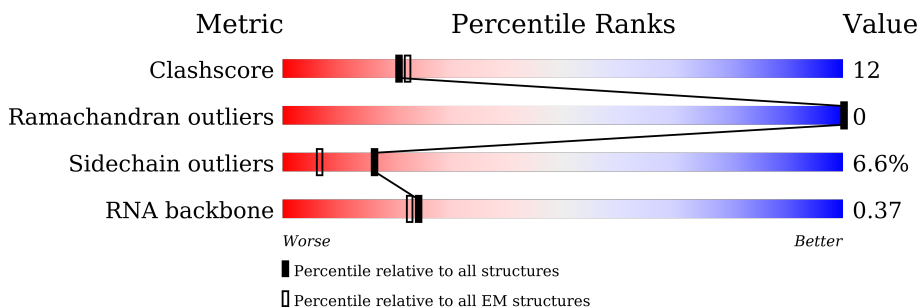
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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.






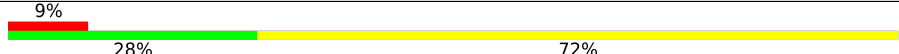
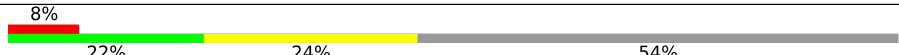
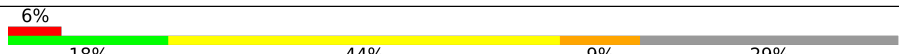
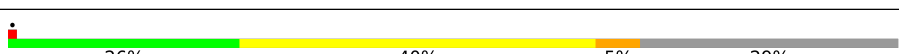
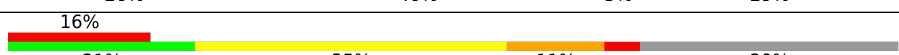
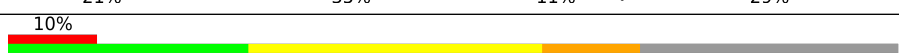
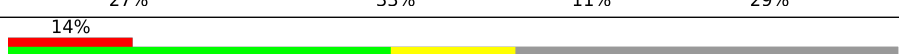
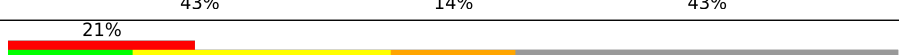
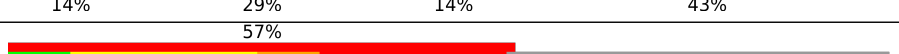

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	330	
1	B	330	
1	K	330	
1	P	330	
2	C	307	
2	J	307	
2	L	307	

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Mol	Chain	Length	Quality of chain
2	T	307	
3	D	85	
3	G	85	
3	M	85	
3	Q	85	
4	E	82	
4	H	82	
4	N	82	
4	R	82	
5	F	14	
5	I	14	
5	O	14	
5	S	14	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28012 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	314	2518	1613	450	446	9	0	0
1	B	314	2518	1613	450	446	9	0	0
1	K	314	2518	1613	450	446	9	0	0
1	P	314	2518	1613	450	446	9	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	321	LEU	-	expression tag	UNP P23070
A	322	GLU	-	expression tag	UNP P23070
A	323	HIS	-	expression tag	UNP P23070
A	324	HIS	-	expression tag	UNP P23070
A	325	HIS	-	expression tag	UNP P23070
A	326	HIS	-	expression tag	UNP P23070
A	327	HIS	-	expression tag	UNP P23070
A	328	HIS	-	expression tag	UNP P23070
A	329	HIS	-	expression tag	UNP P23070
A	330	HIS	-	expression tag	UNP P23070
B	321	LEU	-	expression tag	UNP P23070
B	322	GLU	-	expression tag	UNP P23070
B	323	HIS	-	expression tag	UNP P23070
B	324	HIS	-	expression tag	UNP P23070
B	325	HIS	-	expression tag	UNP P23070
B	326	HIS	-	expression tag	UNP P23070
B	327	HIS	-	expression tag	UNP P23070
B	328	HIS	-	expression tag	UNP P23070
B	329	HIS	-	expression tag	UNP P23070
B	330	HIS	-	expression tag	UNP P23070
K	321	LEU	-	expression tag	UNP P23070
K	322	GLU	-	expression tag	UNP P23070

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Chain	Residue	Modelled	Actual	Comment	Reference
K	323	HIS	-	expression tag	UNP P23070
K	324	HIS	-	expression tag	UNP P23070
K	325	HIS	-	expression tag	UNP P23070
K	326	HIS	-	expression tag	UNP P23070
K	327	HIS	-	expression tag	UNP P23070
K	328	HIS	-	expression tag	UNP P23070
K	329	HIS	-	expression tag	UNP P23070
K	330	HIS	-	expression tag	UNP P23070
P	321	LEU	-	expression tag	UNP P23070
P	322	GLU	-	expression tag	UNP P23070
P	323	HIS	-	expression tag	UNP P23070
P	324	HIS	-	expression tag	UNP P23070
P	325	HIS	-	expression tag	UNP P23070
P	326	HIS	-	expression tag	UNP P23070
P	327	HIS	-	expression tag	UNP P23070
P	328	HIS	-	expression tag	UNP P23070
P	329	HIS	-	expression tag	UNP P23070
P	330	HIS	-	expression tag	UNP P23070

- Molecule 2 is a protein called Retron Ec86 putative ribosyltransferase/DNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	132	1096	704	195	192	5	0	0
2	J	306	2490	1589	441	449	11	0	0
2	L	132	1096	704	195	192	5	0	0
2	T	306	2490	1589	441	449	11	0	0

- Molecule 3 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	D	85	1752	830	337	500	85	0	0
3	G	39	808	383	163	223	39	0	0
3	M	85	1752	830	337	500	85	0	0
3	Q	39	808	383	163	223	39	0	0

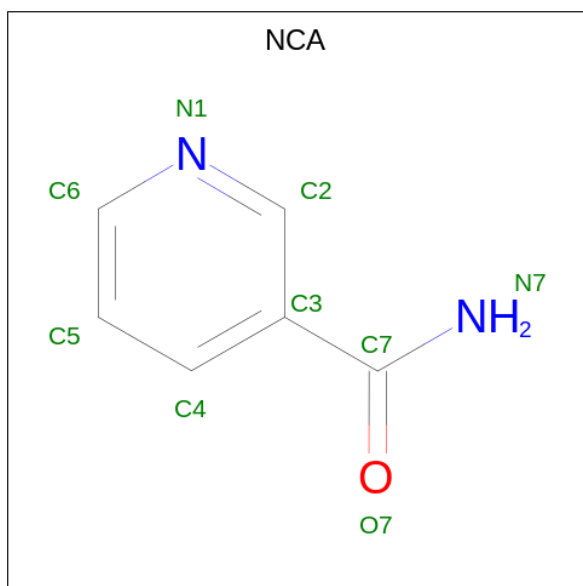
- Molecule 4 is a RNA chain called RNA (82-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	E	58	Total	C	N	O	P	0	0
			1225	547	205	415	58		
4	H	58	Total	C	N	O	P	0	0
			1225	547	205	415	58		
4	N	58	Total	C	N	O	P	0	0
			1225	547	205	415	58		
4	R	58	Total	C	N	O	P	0	0
			1225	547	205	415	58		

- Molecule 5 is a RNA chain called RNA (5'-R(P\*CP\*GP\*UP\*AP\*AP\*GP\*GP\*GP\*UP\*GP\*CP\*GP\*CP\*A)-3').

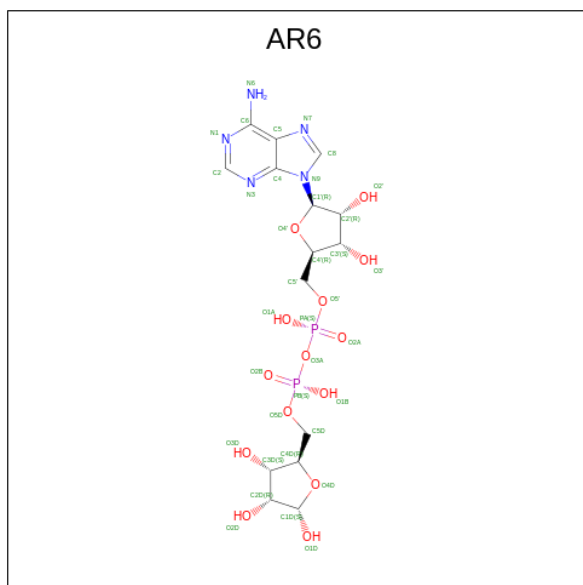
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	F	8	Total	C	N	O	P	0	0
			176	78	35	55	8		
5	I	8	Total	C	N	O	P	0	0
			176	78	35	55	8		
5	O	8	Total	C	N	O	P	0	0
			176	78	35	55	8		
5	S	8	Total	C	N	O	P	0	0
			176	78	35	55	8		

- Molecule 6 is NICOTINAMIDE (three-letter code: NCA) (formula: C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	J	1	9	6	2	1	0

- 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).

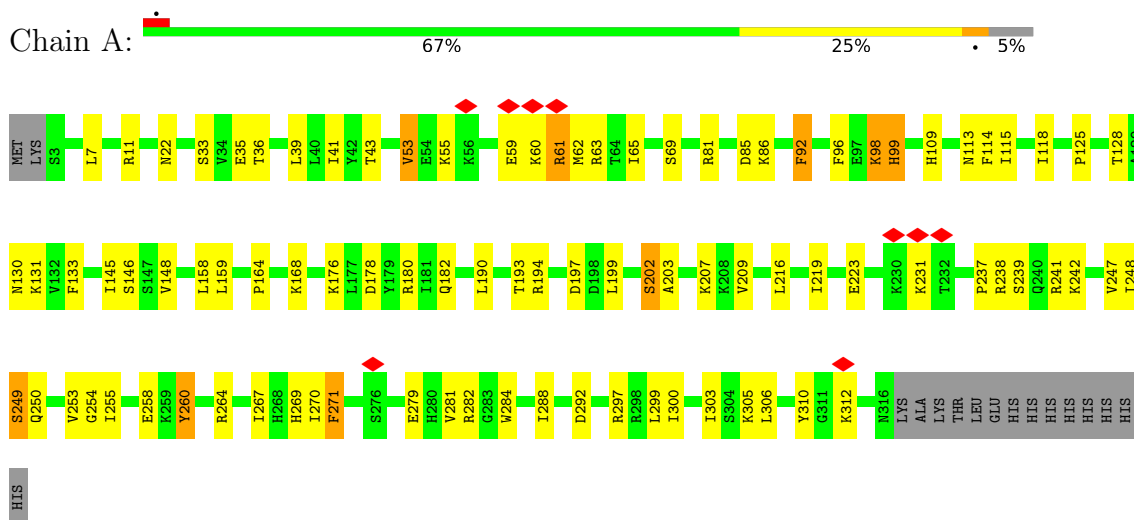


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	J	1	35	15	5	13	2	0

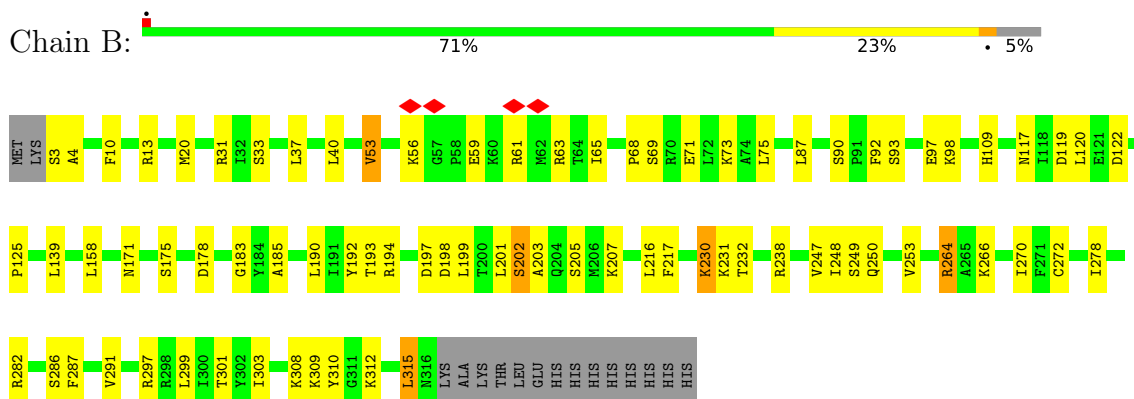
### 3 Residue-property plots i

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

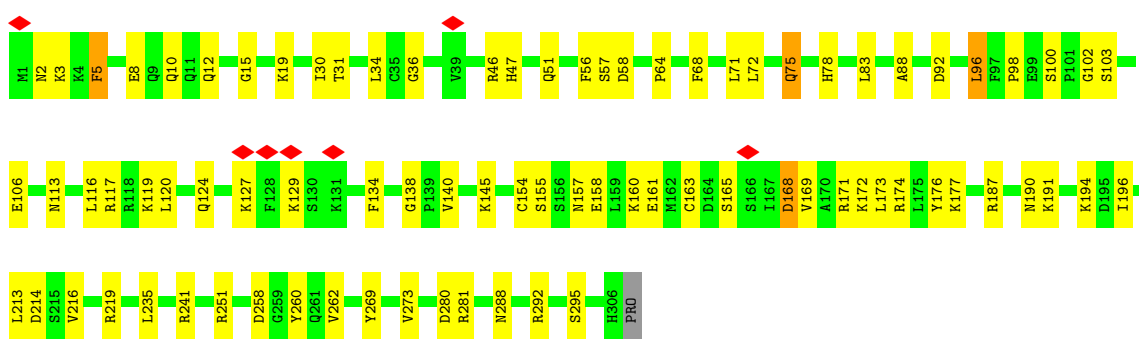


- Molecule 1: Retron Ec86 reverse transcriptase

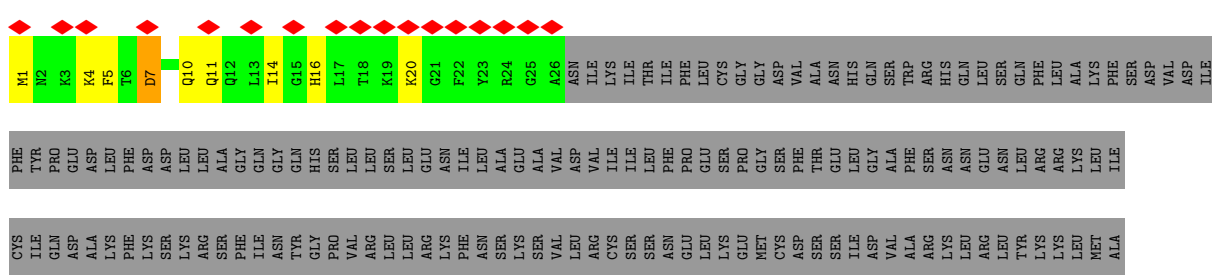
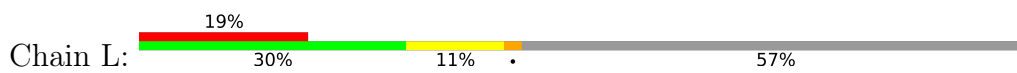




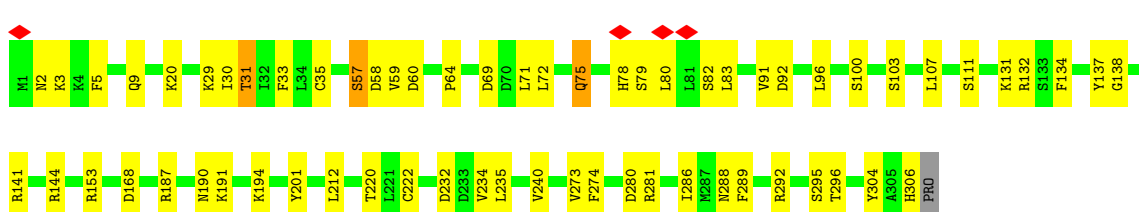
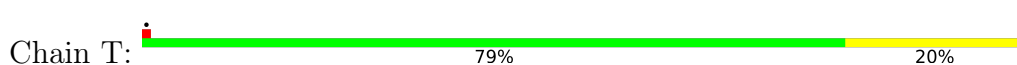




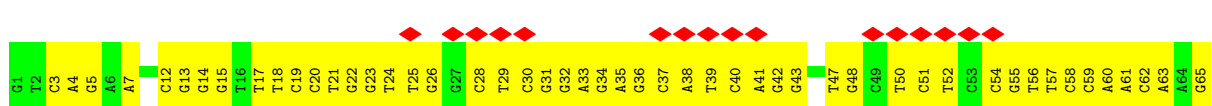
Molecule 2: Retron Ec86 putative ribosyltransferase/DNA-binding protein



Molecule 2: Retron Ec86 putative ribosyltransferase/DNA-binding protein



Molecule 3: DNA (85-MER)

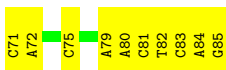




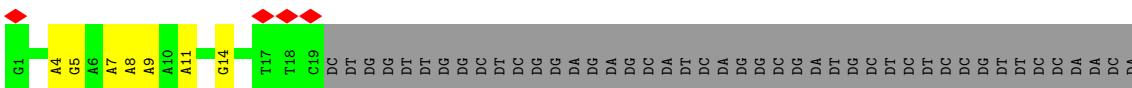
- Molecule 3: DNA (85-MER)



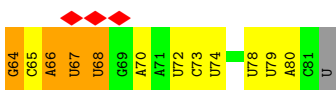
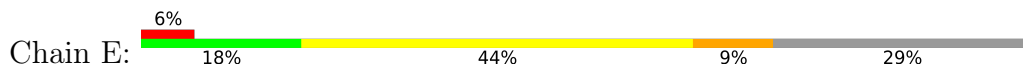
- Molecule 3: DNA (85-MER)



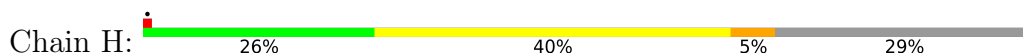
- Molecule 3: DNA (85-MER)

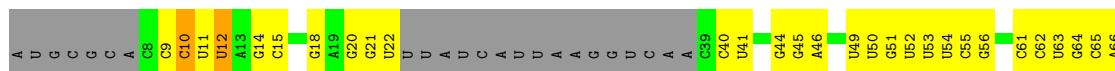


- Molecule 4: RNA (82-MER)

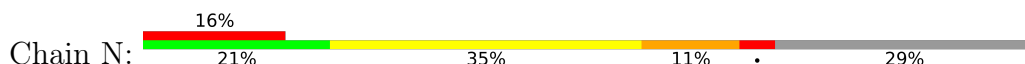


- Molecule 4: RNA (82-MER)

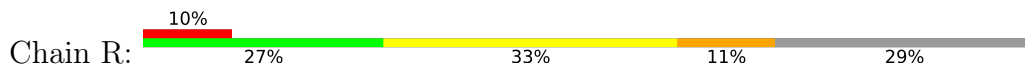




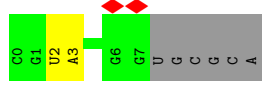
• Molecule 4: RNA (82-MER)



• Molecule 4: RNA (82-MER)



• Molecule 5: RNA (5'-R(P\*CP\*GP\*UP\*AP\*AP\*GP\*GP\*GP\*UP\*GP\*CP\*GP\*CP\*A)-3')



• Molecule 5: RNA (5'-R(P\*CP\*GP\*UP\*AP\*AP\*GP\*GP\*GP\*UP\*GP\*CP\*GP\*CP\*A)-3')

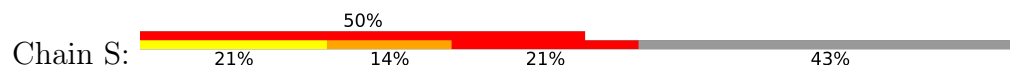


• Molecule 5: RNA (5'-R(P\*CP\*GP\*UP\*AP\*AP\*GP\*GP\*GP\*UP\*GP\*CP\*GP\*CP\*A)-3')





- Molecule 5: RNA (5'-R(P\*CP\*GP\*UP\*AP\*AP\*GP\*GP\*GP\*UP\*GP\*CP\*GP\*CP\*A)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	270375	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.187	Depositor
Minimum map value	-2.191	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.4	Depositor
Map size ( $\text{\AA}$ )	299.6, 299.6, 299.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.07, 1.07, 1.07	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: AR6, NCA

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	0.28	0/2568	0.49	0/3456
1	B	0.29	0/2568	0.49	0/3456
1	K	0.26	0/2568	0.50	0/3456
1	P	0.26	0/2568	0.48	0/3456
2	C	0.26	0/1112	0.50	0/1489
2	J	0.28	0/2531	0.49	0/3396
2	L	0.29	0/1112	0.55	0/1489
2	T	0.28	0/2531	0.49	0/3396
3	D	0.56	0/1970	0.90	0/3039
3	G	0.55	0/910	0.86	0/1400
3	M	0.52	0/1970	0.91	0/3039
3	Q	0.63	0/910	0.89	0/1400
4	E	0.25	0/1364	0.90	3/2119 (0.1%)
4	H	0.30	0/1364	0.87	3/2119 (0.1%)
4	N	0.45	2/1364 (0.1%)	1.32	23/2119 (1.1%)
4	R	0.27	0/1364	0.92	3/2119 (0.1%)
5	F	0.20	0/197	0.70	0/306
5	I	0.26	0/197	0.83	0/306
5	O	1.00	0/197	2.16	15/306 (4.9%)
5	S	0.79	0/197	1.76	4/306 (1.3%)
All	All	0.37	2/29562 (0.0%)	0.76	51/42172 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	13	A	N9-C4	8.54	1.43	1.37
4	N	13	A	C2-N3	5.23	1.38	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	13	A	C6-N1-C2	-14.94	109.64	118.60
4	N	13	A	C5-C6-N6	-14.90	111.78	123.70
4	N	13	A	C5-C6-N1	14.29	124.85	117.70
5	O	2	U	C2-N3-C4	-13.98	118.61	127.00
4	N	13	A	N3-C4-N9	13.35	138.08	127.40
5	O	2	U	C5-C4-O4	-13.29	117.93	125.90
4	N	10	C	C2-N1-C1'	-10.70	107.04	118.80
4	N	13	A	N3-C4-C5	-10.56	119.41	126.80
4	N	10	C	C6-N1-C1'	10.46	133.35	120.80
4	N	13	A	C6-C5-N7	-9.60	125.58	132.30
5	O	2	U	N3-C4-C5	9.22	120.13	114.60
4	N	13	A	C4-N9-C1'	9.02	142.54	126.30
4	N	13	A	C2-N3-C4	8.58	114.89	110.60
4	N	13	A	C8-N9-C1'	-8.52	112.37	127.70
4	N	13	A	N9-C4-C5	-8.23	102.51	105.80
5	O	6	G	C4-C5-N7	-8.23	107.51	110.80
4	N	13	A	N1-C6-N6	7.95	123.37	118.60
5	O	7	G	N9-C4-C5	7.55	108.42	105.40
5	O	6	G	C5-C6-O6	7.48	133.09	128.60
4	N	10	C	C5-C4-N4	7.42	125.39	120.20
4	N	10	C	O4'-C1'-N1	7.42	114.13	108.20
5	S	2	U	C2-N3-C4	7.17	131.30	127.00
4	N	13	A	C4-C5-N7	6.96	114.18	110.70
5	O	7	G	N1-C6-O6	-6.81	115.82	119.90
4	N	10	C	N3-C4-N4	-6.79	113.25	118.00
5	O	6	G	N3-C4-C5	-6.60	125.30	128.60
4	E	68	U	C2-N1-C1'	6.57	125.58	117.70
5	O	7	G	C5-C6-O6	6.54	132.52	128.60
4	N	13	A	C4-C5-C6	6.47	120.24	117.00
4	N	8	C	C6-N1-C2	-6.27	117.79	120.30
5	O	6	G	N1-C6-O6	-5.99	116.31	119.90
4	N	10	C	N1-C2-N3	5.94	123.36	119.20
4	R	62	C	N3-C2-O2	-5.92	117.75	121.90
5	O	7	G	C4-C5-N7	-5.82	108.47	110.80
4	E	68	U	N1-C2-O2	5.79	126.85	122.80
5	O	6	G	C5-N7-C8	5.63	107.12	104.30
4	H	10	C	N1-C2-O2	5.43	122.16	118.90
4	R	10	C	O4'-C1'-N1	5.42	112.53	108.20
4	H	65	C	C2-N1-C1'	5.36	124.70	118.80
5	O	7	G	C6-C5-N7	5.36	133.61	130.40
4	E	68	U	N3-C2-O2	-5.31	118.48	122.20
4	H	10	C	N3-C2-O2	-5.26	118.22	121.90
5	S	2	U	N3-C4-C5	-5.25	111.45	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	7	G	N3-C4-N9	-5.25	122.85	126.00
4	N	65	C	C2-N1-C1'	5.24	124.57	118.80
4	R	65	C	C2-N1-C1'	5.22	124.54	118.80
5	O	2	U	C2-N1-C1'	5.15	123.88	117.70
5	S	6	G	N3-C2-N2	5.14	123.50	119.90
4	N	8	C	C5-C4-N4	5.13	123.79	120.20
4	N	8	C	N3-C2-O2	-5.12	118.31	121.90
5	S	5	G	C8-N9-C4	-5.03	104.39	106.40

There are no chirality outliers.

There are no planarity outliers.

## 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	2518	0	2621	63	0
1	B	2518	0	2621	54	0
1	K	2518	0	2621	97	0
1	P	2518	0	2621	59	0
2	C	1096	0	1139	24	0
2	J	2490	0	2567	50	0
2	L	1096	0	1139	19	0
2	T	2490	0	2567	43	0
3	D	1752	0	952	62	0
3	G	808	0	437	22	0
3	M	1752	0	952	49	0
3	Q	808	0	437	19	0
4	E	1225	0	621	34	0
4	H	1225	0	621	19	0
4	N	1225	0	621	30	0
4	R	1225	0	621	17	0
5	F	176	0	88	2	0
5	I	176	0	88	2	0
5	O	176	0	88	14	0
5	S	176	0	88	9	0
6	J	9	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	35	0	18	4	0
All	All	28012	0	23534	599	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 12.

All (599) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:402:AR6:O4'	7:J:402:AR6:C1'	1.64	1.15
1:B:109:HIS:HE2	1:B:193:THR:HG1	1.16	0.91
5:O:2:U:N3	5:O:6:G:N7	2.28	0.80
5:S:0:C:HO2'	5:S:2:U:H3	0.82	0.80
4:N:13:A:N6	5:O:6:G:C4	2.51	0.77
1:K:11:ARG:HH21	1:P:11:ARG:HG2	1.49	0.76
2:L:276:ARG:NH2	1:P:35:GLU:OE1	2.16	0.76
1:K:299:LEU:O	1:K:303:ILE:HD12	1.86	0.75
4:N:13:A:N6	5:O:6:G:C5	2.53	0.75
2:C:8:GLU:OE2	2:C:8:GLU:N	2.18	0.75
2:T:75:GLN:HE21	2:T:80:LEU:HD13	1.51	0.74
2:T:75:GLN:HE22	2:T:78:HIS:H	1.35	0.73
5:S:0:C:O2'	5:S:2:U:N3	1.99	0.73
3:D:66:DG:H2'	3:D:67:DA:C8	2.22	0.73
3:D:37:DC:H42	3:D:48:DG:H1	1.37	0.73
1:P:228:ASN:HD22	1:P:231:LYS:HB2	1.53	0.73
2:J:2:ASN:ND2	2:J:295:SER:O	2.22	0.72
1:B:40:LEU:HD21	1:B:71:GLU:HB3	1.72	0.72
1:P:257:ARG:NH1	4:R:48:G:O6	2.23	0.71
1:A:255:ILE:HD12	1:A:255:ILE:H	1.55	0.71
5:O:2:U:O4	5:O:6:G:C5	2.44	0.71
5:O:7:G:N2	5:O:7:G:OP2	2.21	0.71
2:T:2:ASN:ND2	2:T:295:SER:O	2.24	0.71
1:P:151:LYS:NZ	3:Q:9:DA:N7	2.40	0.69
3:M:67:DA:H2''	3:M:68:DA:H5''	1.72	0.69
4:E:14:G:N2	4:E:14:G:OP2	2.25	0.69
3:D:38:DA:H2''	3:D:39:DT:H5'	1.74	0.69
1:K:257:ARG:HD2	1:K:258:GLU:N	2.08	0.69
1:K:211:LYS:NZ	3:M:1:DG:OP2	2.26	0.68
3:M:65:DG:H2'	3:M:66:DG:C8	2.29	0.68
1:P:180:ARG:NH1	1:P:223:GLU:OE1	2.27	0.68
2:J:64:PRO:HG2	7:J:402:AR6:H2D	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:263:ILE:O	1:K:267:ILE:HG13	1.93	0.68
1:A:55:LYS:HD2	1:A:60:LYS:HE3	1.74	0.67
1:A:284:TRP:O	1:A:288:ILE:HG12	1.95	0.67
4:E:58:C:H2'	4:E:59:A:H8	1.59	0.67
2:L:280:ASP:OD2	1:P:33:SER:OG	2.12	0.67
2:C:288:ASN:OD1	2:C:292:ARG:NH1	2.27	0.66
4:R:43:U:HO2'	4:R:65:C:HO2'	1.41	0.66
1:P:84:LEU:HB3	1:P:168:LYS:HG2	1.77	0.66
2:J:83:LEU:HB3	6:J:401:NCA:H6	1.76	0.66
1:K:257:ARG:NH1	4:N:46:A:OP2	2.27	0.66
1:K:11:ARG:NH2	1:P:11:ARG:HG2	2.11	0.66
1:K:298:ARG:NH1	4:N:49:U:OP2	2.29	0.66
3:M:61:DA:H2''	3:M:62:DC:H5''	1.78	0.65
1:P:55:LYS:HD3	1:P:60:LYS:HG3	1.77	0.65
1:K:70:ARG:O	2:T:288:ASN:ND2	2.26	0.65
3:M:9:DA:H2''	3:M:10:DA:H5''	1.79	0.65
1:B:231:LYS:NZ	4:H:69:G:OP1	2.30	0.64
3:D:29:DT:H3	3:D:56:DT:H3	1.43	0.64
1:P:294:LYS:HD2	1:P:297:ARG:HH22	1.64	0.63
1:P:128:THR:OG1	1:P:130:ASN:OD1	2.16	0.63
3:Q:14:DG:N2	3:Q:72:DA:N1	2.46	0.63
3:D:54:DC:H1'	3:D:55:DG:C8	2.33	0.63
2:T:9:GLN:HE21	2:T:296:THR:HG23	1.63	0.63
1:A:33:SER:OG	2:J:280:ASP:OD2	2.15	0.62
1:A:194:ARG:HG3	1:A:199:LEU:HG	1.81	0.62
3:D:28:DC:H42	3:D:57:DT:H3	1.47	0.62
1:K:284:TRP:O	1:K:288:ILE:HG12	2.00	0.62
3:D:24:DT:H2''	3:D:25:DT:C5	2.34	0.62
2:J:102:GLY:O	2:J:106:GLU:HB2	2.00	0.62
2:T:31:THR:HG23	2:T:92:ASP:H	1.65	0.62
2:J:165:SER:HB3	2:J:169:VAL:HG13	1.82	0.62
2:J:30:ILE:HD11	2:J:187:ARG:HD3	1.81	0.61
1:A:118:ILE:HD12	1:A:216:LEU:HD23	1.80	0.61
1:K:257:ARG:HH21	4:N:47:U:P	2.23	0.61
3:M:83:DC:H2'	3:M:84:DA:H8	1.66	0.61
3:G:3:DC:H2'	3:G:4:DA:C8	2.36	0.61
1:K:257:ARG:HD2	1:K:258:GLU:H	1.65	0.61
1:B:286:SER:HB2	4:H:77:G:H21	1.66	0.61
1:A:180:ARG:NH1	1:A:223:GLU:OE2	2.31	0.61
2:C:292:ARG:NH2	4:H:73:C:OP1	2.29	0.61
1:K:49:ARG:HB2	3:M:75:DC:H2''	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:ASP:OD1	2:L:227:LYS:NZ	2.26	0.61
3:D:18:DT:H2'	3:D:19:DC:C6	2.36	0.61
2:T:132:ARG:NH1	2:T:137:TYR:OH	2.33	0.61
2:C:235:LEU:HD12	2:C:238:ILE:HD13	1.83	0.60
2:J:134:PHE:HB2	2:J:140:VAL:HG21	1.83	0.60
3:Q:83:DC:H2'	3:Q:84:DA:H8	1.66	0.60
1:K:111:GLY:O	1:K:204:GLN:NE2	2.27	0.60
3:M:18:DT:H2'	3:M:19:DC:C6	2.37	0.60
1:K:62:MET:SD	1:K:62:MET:N	2.67	0.60
2:J:71:LEU:HD22	2:J:235:LEU:HD22	1.83	0.60
1:K:125:PRO:HA	1:K:158:LEU:HB2	1.84	0.60
1:A:269:HIS:NE2	4:E:53:U:O2'	2.35	0.59
2:L:273:VAL:HG23	2:L:274:PHE:HD1	1.67	0.59
3:G:4:DA:H2''	3:G:5:DG:C8	2.37	0.59
3:M:60:DA:H2''	3:M:61:DA:C8	2.38	0.59
1:B:247:VAL:HG11	4:H:46:A:H5''	1.84	0.59
1:A:264:ARG:NH1	4:E:51:G:O6	2.35	0.58
1:K:33:SER:OG	2:T:280:ASP:OD2	2.14	0.58
3:D:65:DG:H2'	3:D:66:DG:C8	2.38	0.58
1:B:87:LEU:HD11	1:B:139:LEU:HD21	1.85	0.58
1:K:191:ILE:HG12	2:L:251:ARG:HE	1.68	0.58
1:A:53:VAL:HG12	1:A:63:ARG:HB3	1.86	0.58
2:T:288:ASN:OD1	2:T:292:ARG:NH1	2.35	0.58
2:C:219:ARG:O	2:C:223:GLU:HG3	2.04	0.58
3:Q:8:DA:H2''	3:Q:9:DA:C2	2.38	0.58
2:T:78:HIS:O	2:T:78:HIS:ND1	2.36	0.58
3:M:15:DG:OP1	2:T:281:ARG:NH2	2.37	0.58
3:M:62:DC:H2''	3:M:63:DA:H5'	1.86	0.58
3:Q:83:DC:H2'	3:Q:84:DA:C8	2.39	0.58
2:J:96:LEU:HD12	2:J:120:LEU:HD11	1.85	0.58
2:C:2:ASN:ND2	2:C:289:PHE:O	2.34	0.57
1:P:49:ARG:HB2	3:Q:75:DC:H2''	1.84	0.57
2:C:14:ILE:O	2:C:18:THR:OG1	2.23	0.57
1:K:251:GLU:OE2	1:K:252:LYS:HG3	2.04	0.57
1:K:185:ALA:HB1	1:K:190:LEU:HB2	1.85	0.57
5:S:3:A:O2'	5:S:5:G:O6	2.19	0.57
3:D:3:DC:H2'	3:D:4:DA:C8	2.39	0.57
3:M:4:DA:H2''	3:M:5:DG:C8	2.40	0.57
4:H:14:G:OP2	4:H:14:G:N2	2.31	0.57
2:J:288:ASN:OD1	2:J:292:ARG:NH1	2.33	0.57
3:D:17:DT:H2''	3:D:18:DT:H5''	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:38:ARG:NH2	3:Q:11:DA:OP1	2.37	0.57
1:B:194:ARG:HG3	1:B:199:LEU:HG	1.86	0.56
1:B:272:CYS:HG	1:B:310:TYR:HH	1.53	0.56
1:K:93:SER:OG	1:K:194:ARG:NH1	2.38	0.56
3:M:83:DC:H2'	3:M:84:DA:C8	2.41	0.56
5:O:6:G:N2	5:O:7:G:H5'	2.20	0.56
2:C:10:GLN:O	2:C:14:ILE:HG13	2.05	0.56
3:M:40:DC:H2''	3:M:41:DA:C8	2.40	0.56
1:B:125:PRO:HA	1:B:158:LEU:HB2	1.85	0.56
1:K:260:TYR:HE2	1:K:298:ARG:HH12	1.54	0.56
3:M:71:DC:H2''	3:M:72:DA:C8	2.40	0.56
1:B:69:SER:HB2	3:G:75:DC:H5''	1.87	0.56
1:K:309:LYS:HD3	1:K:310:TYR:HD1	1.71	0.55
1:P:247:VAL:HG11	4:R:46:A:H5''	1.87	0.55
5:S:4:A:H4'	5:S:5:G:N7	2.21	0.55
1:P:110:ILE:HG12	1:P:253:VAL:HG13	1.89	0.55
2:C:236:SER:HA	2:C:239:ILE:HD12	1.88	0.55
1:K:110:ILE:HD11	1:K:253:VAL:HG23	1.89	0.55
1:K:177:LEU:HD13	1:K:223:GLU:HG3	1.88	0.55
1:P:105:ASN:ND2	1:P:244:THR:OG1	2.39	0.55
1:A:197:ASP:OD1	1:A:197:ASP:N	2.35	0.55
1:K:231:LYS:HE2	4:N:68:U:H4'	1.89	0.55
5:S:1:G:O3'	5:S:3:A:C2	2.60	0.55
3:D:4:DA:H2''	3:D:5:DG:C8	2.41	0.54
3:Q:4:DA:H2''	3:Q:5:DG:C8	2.42	0.54
3:D:28:DC:N4	3:D:57:DT:H3	2.05	0.54
2:J:47:HIS:O	2:J:51:GLN:HG2	2.08	0.54
3:D:12:DC:H2'	3:D:13:DG:C8	2.43	0.54
3:Q:73:DG:H4'	3:Q:74:DA:OP1	2.06	0.54
3:D:38:DA:C8	3:D:39:DT:H72	2.42	0.54
3:M:17:DT:H2'	3:M:18:DT:C6	2.43	0.54
2:T:33:PHE:HB2	2:T:91:VAL:HG11	1.88	0.54
1:K:176:LYS:HZ2	1:K:180:ARG:HD2	1.72	0.54
1:B:171:ASN:OD1	1:B:194:ARG:NH2	2.41	0.54
1:K:177:LEU:HD11	1:K:220:ILE:HD13	1.88	0.54
5:O:2:U:O4	5:O:6:G:C4	2.60	0.54
2:T:232:ASP:OD1	2:T:235:LEU:HB2	2.07	0.54
1:A:270:ILE:HG12	1:A:281:VAL:HG21	1.89	0.54
1:P:194:ARG:HG3	1:P:199:LEU:HG	1.89	0.54
2:C:258:ASP:N	2:C:258:ASP:OD1	2.39	0.53
3:D:40:DC:H2''	3:D:41:DA:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:84:DA:H2'	3:M:85:DG:C8	2.43	0.53
1:P:171:ASN:HA	1:P:194:ARG:HH22	1.73	0.53
2:T:71:LEU:HD22	2:T:235:LEU:HG	1.90	0.53
1:P:178:ASP:OD2	1:P:194:ARG:NH1	2.41	0.53
1:P:237:PRO:HB2	4:R:62:C:O2'	2.08	0.53
2:J:134:PHE:HD1	2:J:140:VAL:HG11	1.73	0.53
3:M:12:DC:H2''	3:M:13:DG:C8	2.42	0.53
4:N:13:A:N1	5:O:6:G:N7	2.55	0.53
1:P:81:ARG:NH2	4:R:75:G:OP1	2.36	0.53
2:C:280:ASP:OD2	1:B:33:SER:OG	2.22	0.53
1:K:271:PHE:HZ	1:K:303:ILE:HG23	1.74	0.53
1:K:246:LEU:HB3	1:K:253:VAL:HG13	1.90	0.53
1:B:264:ARG:NH2	4:H:51:G:N7	2.52	0.52
5:O:2:U:C4	5:O:6:G:N7	2.77	0.52
4:E:58:C:H2'	4:E:59:A:C8	2.43	0.52
1:B:40:LEU:HD23	1:B:75:LEU:HD12	1.92	0.52
2:L:287:MET:HE1	1:P:32:ILE:HD11	1.91	0.52
2:L:293:ARG:NH2	4:R:76:A:OP2	2.34	0.52
2:T:191:LYS:HA	2:T:191:LYS:HE2	1.91	0.52
2:T:232:ASP:OD1	2:T:232:ASP:N	2.42	0.52
2:J:98:PRO:HA	2:J:103:SER:HB2	1.90	0.52
5:S:5:G:H2'	5:S:6:G:C2	2.45	0.52
4:N:73:C:OP1	2:T:292:ARG:NH2	2.42	0.52
2:C:199:ILE:HG23	2:C:201:TYR:H	1.75	0.52
5:F:2:U:H2'	5:F:3:A:H8	1.74	0.52
2:J:72:LEU:O	2:T:141:ARG:NH2	2.43	0.52
4:N:20:G:N2	4:N:41:U:O2	2.38	0.52
1:A:39:LEU:O	1:A:43:THR:OG1	2.25	0.52
1:K:221:PRO:HD3	1:K:227:ILE:HD11	1.92	0.52
1:B:309:LYS:HG2	1:B:310:TYR:CD1	2.44	0.52
3:M:80:DA:H2'	3:M:81:DC:C6	2.44	0.52
1:B:266:LYS:O	1:B:270:ILE:HG23	2.10	0.52
2:L:277:LYS:NZ	3:Q:14:DG:OP1	2.31	0.52
3:M:26:DG:H2''	3:M:27:DG:C8	2.44	0.52
3:Q:67:DA:H2''	3:Q:68:DA:H5'	1.92	0.52
2:T:212:LEU:HB3	2:T:286:ILE:HD12	1.92	0.52
3:D:3:DC:H2''	3:D:4:DA:O5'	2.10	0.52
1:P:92:PHE:CZ	1:P:182:GLN:HG2	2.45	0.52
1:A:41:ILE:HD13	1:A:148:VAL:HG13	1.91	0.52
1:A:238:ARG:HD2	4:E:63:U:O2'	2.10	0.52
3:D:67:DA:H2''	3:D:68:DA:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:83:DC:H2'	3:D:84:DA:H8	1.75	0.52
3:D:54:DC:H4'	3:D:55:DG:H5'	1.92	0.51
3:M:80:DA:H2'	3:M:81:DC:H6	1.73	0.51
1:A:190:LEU:HG	1:A:203:ALA:HB2	1.91	0.51
3:M:3:DC:H4'	3:M:4:DA:OP1	2.10	0.51
4:E:10:C:H2'	4:E:11:U:C6	2.46	0.51
1:B:178:ASP:OD1	1:B:192:TYR:OH	2.26	0.51
1:K:68:PRO:HG2	1:K:73:LYS:HG3	1.92	0.51
1:B:59:GLU:HB3	1:B:61:ARG:HH22	1.75	0.51
1:K:36:THR:OG1	2:T:280:ASP:OD2	2.24	0.51
3:M:19:DC:H2'	3:M:20:DC:C6	2.46	0.51
3:D:14:DG:H2''	3:D:15:DG:C8	2.46	0.51
1:A:96:PHE:HZ	3:D:85:DG:H1'	1.75	0.51
1:A:249:SER:OG	1:A:250:GLN:N	2.42	0.51
3:D:51:DC:H2'	3:D:52:DT:H72	1.91	0.51
3:D:67:DA:H2''	3:D:68:DA:H8	1.76	0.51
4:H:45:G:H2'	4:H:46:A:H8	1.74	0.51
1:K:257:ARG:NH2	4:N:47:U:OP2	2.42	0.51
3:M:81:DC:H3'	3:M:82:DT:H71	1.91	0.51
1:K:297:ARG:HG3	1:K:297:ARG:HH11	1.76	0.51
4:E:43:U:HO2'	4:E:65:C:HO2'	1.58	0.51
1:P:114:PHE:CE2	1:P:237:PRO:HD3	2.45	0.51
2:T:80:LEU:HG	2:T:83:LEU:HG	1.93	0.51
2:J:5:PHE:HB3	2:J:10:GLN:HG3	1.93	0.50
1:K:255:ILE:HD12	1:K:259:LYS:HB3	1.93	0.50
4:E:60:U:H2'	4:E:61:C:C6	2.46	0.50
4:N:66:A:H4'	4:N:67:U:O5'	2.11	0.50
1:K:297:ARG:HA	1:K:300:ILE:HG12	1.93	0.50
4:R:78:U:H2'	4:R:79:U:H6	1.77	0.50
2:T:79:SER:O	2:T:79:SER:OG	2.27	0.50
3:M:48:DG:H2''	3:M:49:DC:H5'	1.93	0.50
1:A:128:THR:OG1	1:A:130:ASN:OD1	2.16	0.50
4:E:73:C:OP1	2:J:292:ARG:NH2	2.42	0.50
3:M:3:DC:H2''	3:M:4:DA:O5'	2.12	0.50
5:S:0:C:O2'	5:S:2:U:C2	2.59	0.50
1:A:203:ALA:HB3	1:A:209:VAL:HG13	1.94	0.50
3:D:67:DA:H2''	3:D:68:DA:H5''	1.94	0.50
1:K:310:TYR:HB3	1:K:312:LYS:HZ3	1.77	0.50
3:M:79:DA:H2'	3:M:80:DA:H8	1.77	0.50
1:A:131:LYS:HG2	3:D:7:DA:C5	2.47	0.50
3:D:57:DT:H2''	3:D:58:DC:C5	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:HB2	1:B:197:ASP:HB2	1.93	0.50
1:K:264:ARG:NH2	4:N:51:G:N7	2.60	0.50
2:T:30:ILE:HG22	2:T:187:ARG:HD3	1.93	0.50
1:A:180:ARG:HH21	1:A:219:ILE:HG13	1.76	0.49
3:G:1:DG:OP1	4:H:14:G:O2'	2.24	0.49
5:F:2:U:H2'	5:F:3:A:C8	2.47	0.49
2:J:168:ASP:O	2:J:172:LYS:NZ	2.46	0.49
3:M:13:DG:H1'	3:M:14:DG:H5'	1.94	0.49
2:T:57:SER:OG	2:T:58:ASP:N	2.45	0.49
1:A:125:PRO:HA	1:A:158:LEU:HB2	1.94	0.49
4:N:60:U:H2'	4:N:61:C:C6	2.47	0.49
2:C:203:GLU:OE2	2:C:246:ARG:NH2	2.45	0.49
2:J:100:SER:H	2:J:103:SER:HG	1.60	0.49
2:L:207:LEU:HD13	2:L:269:TYR:HE1	1.77	0.49
3:M:50:DT:H2''	3:M:51:DC:C6	2.47	0.49
1:B:68:PRO:HG2	1:B:73:LYS:HG3	1.94	0.49
1:A:109:HIS:HE2	1:A:193:THR:HB	1.77	0.49
1:A:258:GLU:OE2	1:A:258:GLU:N	2.28	0.49
3:D:15:DG:OP1	2:J:281:ARG:NH2	2.43	0.49
2:J:124:GLN:HB2	2:J:134:PHE:CZ	2.46	0.49
2:T:79:SER:O	2:T:82:SER:OG	2.29	0.49
1:A:92:PHE:CZ	1:A:182:GLN:HG2	2.48	0.49
2:C:247:LEU:HB3	2:C:253:ILE:HG12	1.95	0.49
1:K:213:ARG:NH1	1:K:214:ASP:OD1	2.43	0.49
2:C:13:LEU:HG	2:C:17:LEU:HD22	1.95	0.49
2:J:57:SER:OG	2:J:58:ASP:N	2.46	0.48
1:K:55:LYS:HB3	1:K:60:LYS:HB3	1.94	0.48
3:M:51:DC:H2''	3:M:52:DT:H71	1.95	0.48
2:J:155:SER:HB2	2:J:158:GLU:HG3	1.94	0.48
2:L:223:GLU:O	2:L:227:LYS:HG3	2.14	0.48
3:Q:66:DG:H2''	3:Q:67:DA:C8	2.48	0.48
1:A:238:ARG:NE	4:E:66:A:N1	2.62	0.48
3:D:42:DG:H1'	3:D:43:DG:H5'	1.95	0.48
4:E:39:C:HO2'	4:E:40:C:H5	1.60	0.48
3:Q:70:DA:H2''	3:Q:71:DC:H5'	1.95	0.48
4:E:78:U:H2'	4:E:79:U:H6	1.78	0.48
4:H:45:G:H2'	4:H:46:A:C8	2.48	0.48
3:Q:84:DA:H2'	3:Q:85:DG:C8	2.48	0.48
3:D:37:DC:H2''	3:D:38:DA:H8	1.78	0.48
1:B:93:SER:OG	1:B:194:ARG:NH1	2.46	0.48
3:D:62:DC:H2'	3:D:63:DA:C5	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG12	1:B:63:ARG:HB3	1.95	0.48
1:K:274:LYS:HB3	1:K:274:LYS:HE3	1.53	0.48
2:T:29:LYS:HG2	2:T:58:ASP:HB2	1.94	0.48
3:G:83:DC:H2'	3:G:84:DA:C8	2.49	0.48
1:K:101:SER:OG	1:K:102:ILE:N	2.45	0.48
2:L:288:ASN:HB2	1:P:74:ALA:HB2	1.96	0.48
3:M:23:DG:C8	3:M:24:DT:H72	2.49	0.48
2:T:194:LYS:HG3	2:T:201:TYR:CE2	2.49	0.48
1:A:279:GLU:OE2	1:A:282:ARG:NH2	2.39	0.48
3:D:23:DG:H2''	3:D:24:DT:H5'	1.95	0.48
1:B:278:ILE:HG23	1:B:315:LEU:HD23	1.96	0.48
1:B:272:CYS:SG	1:B:310:TYR:OH	2.68	0.48
3:G:3:DC:H2''	3:G:4:DA:O5'	2.14	0.48
2:J:75:GLN:NE2	2:J:78:HIS:O	2.47	0.48
1:K:255:ILE:HD13	1:K:288:ILE:HD12	1.96	0.48
3:M:45:DG:H2''	3:M:46:DA:OP2	2.12	0.48
2:T:222:CYS:HA	2:T:240:VAL:HG21	1.96	0.48
1:A:98:LYS:HB3	1:A:99:HIS:ND1	2.28	0.47
1:K:288:ILE:O	1:K:292:ASP:N	2.44	0.47
3:M:18:DT:H2'	3:M:19:DC:H6	1.77	0.47
1:B:65:ILE:HD12	4:H:70:A:C2	2.49	0.47
1:B:299:LEU:O	1:B:303:ILE:HG13	2.14	0.47
1:K:267:ILE:HA	1:K:270:ILE:HG22	1.95	0.47
3:M:37:DC:H2''	3:M:38:DA:H8	1.79	0.47
3:D:37:DC:H2''	3:D:38:DA:C8	2.48	0.47
1:B:31:ARG:HG3	1:B:31:ARG:HH11	1.80	0.47
2:J:31:THR:HG23	2:J:92:ASP:H	1.80	0.47
1:K:178:ASP:OD2	1:K:194:ARG:NH1	2.47	0.47
1:A:36:THR:OG1	2:J:280:ASP:OD2	2.29	0.47
1:K:278:ILE:HD12	1:K:279:GLU:H	1.79	0.47
4:H:10:C:H2'	4:H:11:U:C6	2.49	0.47
1:K:305:LYS:NZ	4:N:51:G:OP1	2.46	0.47
5:O:2:U:N3	5:O:6:G:C8	2.82	0.47
1:A:164:PRO:HA	4:E:74:U:H5'	1.97	0.47
1:K:237:PRO:HB2	4:N:62:C:O2'	2.15	0.47
1:K:278:ILE:O	1:K:282:ARG:HD3	2.15	0.47
3:M:15:DG:H2''	3:M:16:DT:H5'	1.96	0.47
4:E:12:U:H2'	4:E:13:A:C8	2.49	0.47
4:E:48:G:O6	4:E:59:A:N6	2.48	0.47
3:G:70:DA:H1'	3:G:71:DC:H5'	1.97	0.47
1:A:59:GLU:HG3	1:A:61:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:HIS:ND1	1:A:202:SER:HB3	2.29	0.47
3:D:3:DC:H4'	3:D:4:DA:OP1	2.15	0.47
3:D:83:DC:H2'	3:D:84:DA:C8	2.50	0.47
4:E:11:U:H2'	4:E:12:U:C6	2.49	0.47
4:E:66:A:H4'	4:E:67:U:O5'	2.14	0.47
1:K:106:ALA:HB1	1:K:248:ILE:HD11	1.96	0.47
2:T:144:ARG:HE	2:T:153:ARG:HH22	1.60	0.47
3:G:14:DG:H2''	3:G:15:DG:C8	2.50	0.46
4:N:13:A:H4'	4:N:14:G:OP1	2.15	0.46
2:T:273:VAL:HG12	2:T:274:PHE:CD2	2.51	0.46
1:B:266:LYS:HG2	4:H:54:U:C4	2.50	0.46
2:J:173:LEU:O	2:J:177:LYS:HG3	2.15	0.46
1:P:273:GLY:O	1:P:274:LYS:HG2	2.15	0.46
1:A:255:ILE:HD12	1:A:255:ILE:N	2.25	0.46
3:D:59:DC:H2''	3:D:60:DA:C8	2.51	0.46
1:P:265:ALA:HB2	4:R:55:C:N4	2.31	0.46
2:C:224:LEU:HD23	2:C:224:LEU:HA	1.74	0.46
3:D:25:DT:H1'	3:D:26:DG:C8	2.50	0.46
1:B:117:ASN:ND2	1:B:198:ASP:OD1	2.43	0.46
3:G:12:DC:H2'	3:G:13:DG:C8	2.50	0.46
3:Q:73:DG:H2''	3:Q:74:DA:O5'	2.15	0.46
3:G:3:DC:H4'	3:G:4:DA:OP1	2.16	0.46
2:J:157:ASN:O	2:J:161:GLU:HG2	2.15	0.46
4:N:44:G:C4	4:N:45:G:C8	3.04	0.46
1:P:63:ARG:HG2	1:P:65:ILE:HD11	1.97	0.46
1:B:31:ARG:HG3	1:B:31:ARG:NH1	2.30	0.46
4:R:8:C:O2'	4:R:9:C:H5'	2.16	0.46
4:R:64:G:H5'	4:R:65:C:C6	2.51	0.46
1:B:171:ASN:HA	1:B:194:ARG:HH22	1.80	0.46
2:J:88:ALA:O	2:J:119:LYS:NZ	2.43	0.46
1:K:271:PHE:CZ	1:K:303:ILE:HG23	2.51	0.46
3:M:35:DA:H2''	3:M:36:DG:C8	2.51	0.46
1:P:171:ASN:OD1	1:P:194:ARG:NH2	2.48	0.46
1:A:267:ILE:HG21	1:A:303:ILE:HG22	1.97	0.45
3:D:19:DC:H2'	3:D:20:DC:C6	2.50	0.45
1:B:308:LYS:HE2	1:B:308:LYS:HB3	1.76	0.45
1:P:65:ILE:HD12	4:R:70:A:C2	2.50	0.45
1:A:297:ARG:O	1:A:300:ILE:HG13	2.15	0.45
4:H:61:C:H2'	4:H:62:C:C6	2.51	0.45
3:M:41:DA:H2''	3:M:42:DG:H8	1.81	0.45
1:P:59:GLU:OE2	1:P:60:LYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:241:ARG:NH2	2:J:260:TYR:OH	2.48	0.45
1:K:278:ILE:HD12	1:K:279:GLU:HG2	1.98	0.45
4:N:10:C:HO2'	4:N:11:U:H5	1.64	0.45
1:A:61:ARG:O	1:A:61:ARG:HG2	2.16	0.45
4:E:41:U:H2'	4:E:42:C:C6	2.52	0.45
2:J:5:PHE:CE1	2:J:213:LEU:HD21	2.52	0.45
2:J:34:LEU:HD12	2:J:46:ARG:HG3	1.97	0.45
1:K:81:ARG:NH2	4:N:75:G:OP1	2.33	0.45
3:M:25:DT:H2''	3:M:26:DG:C8	2.51	0.45
3:D:58:DC:H1'	3:D:59:DC:H5'	1.97	0.45
2:T:30:ILE:HD11	2:T:59:VAL:HG22	1.99	0.45
3:D:34:DG:H2''	3:D:35:DA:C8	2.52	0.45
2:J:113:ASN:HB3	2:J:116:LEU:HB2	1.97	0.45
1:K:11:ARG:NH1	1:K:15:LEU:HD11	2.32	0.45
1:K:171:ASN:HA	1:K:194:ARG:HH22	1.82	0.45
3:G:15:DG:H2'	3:G:16:DT:H72	1.97	0.45
1:K:278:ILE:HD12	1:K:279:GLU:N	2.32	0.45
3:M:17:DT:H3'	3:M:18:DT:H71	1.98	0.45
1:A:242:LYS:HB2	1:A:242:LYS:HE3	1.81	0.44
4:H:49:U:H2'	4:H:50:U:C6	2.53	0.44
3:M:56:DT:H2'	3:M:57:DT:H71	1.98	0.44
1:A:258:GLU:OE1	4:E:45:G:H5'	2.17	0.44
1:A:299:LEU:O	1:A:303:ILE:HG23	2.18	0.44
2:J:36:GLY:O	7:J:402:AR6:O3D	2.35	0.44
2:J:56:PHE:HZ	2:J:176:TYR:HE2	1.64	0.44
1:K:228:ASN:HD22	1:K:231:LYS:HD2	1.82	0.44
3:D:21:DT:H4'	3:D:22:DG:H5'	1.99	0.44
3:D:60:DA:H1'	3:D:61:DA:C4	2.53	0.44
4:E:16:G:N1	4:E:64:G:O4'	2.50	0.44
5:I:2:U:H2'	5:I:3:A:C8	2.52	0.44
2:J:72:LEU:HD13	2:J:83:LEU:HD12	1.99	0.44
2:J:269:TYR:O	2:J:273:VAL:HG22	2.18	0.44
1:K:213:ARG:O	1:K:217:PHE:HD1	2.00	0.44
1:P:68:PRO:HG2	1:P:73:LYS:HG3	1.98	0.44
1:P:97:GLU:OE1	1:P:168:LYS:NZ	2.51	0.44
1:A:65:ILE:HD12	4:E:70:A:C2	2.52	0.44
1:A:248:ILE:HG12	1:A:253:VAL:HG12	1.99	0.44
3:D:33:DA:H2''	3:D:34:DG:C8	2.53	0.44
1:K:38:ARG:NH2	3:M:11:DA:OP1	2.42	0.44
1:P:116:LEU:HB2	1:P:209:VAL:HG13	1.99	0.44
1:P:270:ILE:HD12	1:P:278:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:48:G:C6	4:E:59:A:N6	2.85	0.44
3:G:8:DA:H2''	3:G:9:DA:C2	2.52	0.44
3:G:73:DG:H2''	3:G:74:DA:C8	2.53	0.44
1:K:127:LEU:HD12	1:K:159:LEU:HD12	2.00	0.44
1:P:105:ASN:OD1	1:P:195:TYR:HB2	2.17	0.44
2:J:8:GLU:O	2:J:12:GLN:HG3	2.17	0.44
1:K:197:ASP:OD1	1:K:197:ASP:N	2.42	0.44
4:N:39:C:HO2'	4:N:40:C:H5	1.64	0.44
3:D:21:DT:H1'	3:D:22:DG:C8	2.53	0.44
1:B:56:LYS:HB3	4:H:69:G:C2	2.52	0.44
1:B:178:ASP:OD2	1:B:194:ARG:NH1	2.51	0.44
3:G:84:DA:H2'	3:G:85:DG:C8	2.53	0.44
1:K:255:ILE:HG13	1:K:256:GLY:N	2.33	0.44
2:L:237:LYS:HA	2:L:237:LYS:HD3	1.72	0.44
1:P:133:PHE:HZ	1:P:143:ARG:HD2	1.83	0.44
4:R:63:U:H5'	4:R:64:G:OP1	2.18	0.44
1:K:194:ARG:HG3	1:K:199:LEU:HG	2.00	0.44
1:K:240:GLN:HB2	4:N:46:A:OP1	2.18	0.44
3:M:38:DA:H1'	3:M:39:DT:H5'	2.00	0.44
2:T:2:ASN:HB3	2:T:289:PHE:CE1	2.53	0.44
2:T:30:ILE:HG23	2:T:187:ARG:HH11	1.83	0.44
2:C:253:ILE:HD12	2:C:260:TYR:HB3	2.00	0.43
3:D:35:DA:H2''	3:D:36:DG:C8	2.53	0.43
3:D:59:DC:H2''	3:D:60:DA:OP2	2.17	0.43
1:P:151:LYS:HZ2	3:Q:9:DA:H62	1.65	0.43
1:A:69:SER:HB3	3:D:75:DC:H5'	1.98	0.43
2:C:213:LEU:HB2	2:C:216:VAL:HG22	2.00	0.43
3:G:66:DG:H1'	3:G:67:DA:C5	2.52	0.43
4:N:58:C:H2'	4:N:59:A:H8	1.83	0.43
3:D:33:DA:H2''	3:D:34:DG:H8	1.83	0.43
2:T:35:CYS:HB2	2:T:96:LEU:HG	2.00	0.43
1:K:128:THR:OG1	1:K:130:ASN:OD1	2.18	0.43
1:K:260:TYR:HE2	1:K:298:ARG:NH1	2.15	0.43
4:R:48:G:C6	4:R:59:A:N6	2.85	0.43
2:T:304:TYR:CE2	2:T:306:HIS:HB3	2.53	0.43
1:A:260:TYR:O	1:A:260:TYR:HD1	2.00	0.43
2:C:250:GLU:HG2	2:C:252:LYS:HE2	2.00	0.43
5:O:2:U:C4	5:O:6:G:C8	3.07	0.43
4:R:66:A:H4'	4:R:67:U:O5'	2.18	0.43
1:A:305:LYS:NZ	4:E:51:G:OP2	2.45	0.43
1:K:211:LYS:HA	1:K:211:LYS:HD2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:286:SER:HB2	4:N:77:G:H21	1.84	0.43
2:L:252:LYS:HG2	2:L:266:GLY:HA2	2.01	0.43
1:A:178:ASP:OD2	1:A:194:ARG:NH1	2.52	0.43
1:K:244:THR:HB	3:M:84:DA:H4'	1.99	0.43
1:K:304:SER:O	1:K:307:GLU:HG3	2.19	0.43
3:D:36:DG:H2''	3:D:37:DC:C6	2.54	0.43
1:K:190:LEU:HB3	1:K:201:LEU:HD22	2.00	0.43
1:P:217:PHE:CZ	1:P:232:THR:HG21	2.54	0.43
2:T:64:PRO:O	2:T:69:ASP:HB2	2.18	0.43
3:D:23:DG:H2''	3:D:24:DT:H2'	2.01	0.43
5:S:5:G:C8	5:S:5:G:H3'	2.54	0.43
3:D:60:DA:H2''	3:D:61:DA:C8	2.53	0.43
4:E:64:G:H5'	4:E:65:C:C5	2.54	0.43
3:G:69:DA:H2''	3:G:70:DA:N7	2.33	0.43
2:J:258:ASP:N	2:J:258:ASP:OD1	2.51	0.43
1:K:164:PRO:HA	4:N:74:U:H5'	2.00	0.43
1:K:308:LYS:HB3	1:K:308:LYS:HE3	1.73	0.43
2:L:209:CYS:SG	2:L:210:ILE:N	2.92	0.43
1:P:203:ALA:HB3	1:P:209:VAL:HG23	2.01	0.43
1:A:115:ILE:HD12	1:A:241:ARG:HB3	2.00	0.42
4:E:61:C:H2'	4:E:62:C:C6	2.54	0.42
1:B:217:PHE:CZ	1:B:232:THR:HG21	2.54	0.42
5:I:5:G:H2'	5:I:6:G:C5	2.54	0.42
2:L:20:LYS:HB2	2:L:20:LYS:HE2	1.76	0.42
3:M:58:DC:H2''	3:M:59:DC:C5	2.54	0.42
5:O:7:G:H21	5:O:7:G:P	2.38	0.42
1:P:289:LEU:HB2	1:P:296:HIS:CG	2.54	0.42
2:C:269:TYR:O	2:C:273:VAL:HG22	2.19	0.42
3:D:50:DT:H2''	3:D:51:DC:C6	2.54	0.42
1:B:98:LYS:HE2	4:H:75:G:H5''	1.99	0.42
1:P:123:PHE:CG	1:P:197:ASP:HB3	2.54	0.42
1:A:113:ASN:HB2	1:A:114:PHE:CD1	2.55	0.42
1:A:176:LYS:HG3	1:B:10:PHE:HZ	1.84	0.42
1:P:263:ILE:HG13	1:P:288:ILE:HD11	2.01	0.42
1:P:286:SER:HB2	4:R:77:G:H21	1.85	0.42
1:A:306:LEU:O	1:A:310:TYR:HB2	2.19	0.42
1:B:238:ARG:HB2	4:H:63:U:O2'	2.20	0.42
3:G:16:DT:H2''	3:G:17:DT:H5''	2.02	0.42
3:G:83:DC:H2'	3:G:84:DA:H8	1.83	0.42
1:K:92:PHE:CZ	1:K:182:GLN:HG2	2.54	0.42
1:K:190:LEU:HD23	1:K:203:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:248:ILE:HD12	1:K:253:VAL:HG22	1.99	0.42
1:K:256:GLY:O	1:K:260:TYR:N	2.40	0.42
2:L:253:ILE:HD11	2:L:260:TYR:HB3	2.02	0.42
3:M:34:DG:H2''	3:M:35:DA:C8	2.53	0.42
1:A:239:SER:HA	4:E:66:A:N6	2.35	0.42
1:A:247:VAL:N	1:A:254:GLY:O	2.51	0.42
1:A:288:ILE:O	1:A:292:ASP:N	2.52	0.42
2:C:8:GLU:O	2:C:12:GLN:HG3	2.20	0.42
4:H:11:U:H2'	4:H:12:U:C6	2.55	0.42
2:L:250:GLU:O	2:L:251:ARG:HB2	2.19	0.42
3:M:42:DG:H1'	3:M:43:DG:H5'	2.00	0.42
1:P:271:PHE:CD2	1:P:306:LEU:HB3	2.54	0.42
3:D:47:DT:H1'	3:D:48:DG:H5'	2.02	0.42
4:E:64:G:H5'	4:E:65:C:C4	2.54	0.42
3:G:15:DG:H8	3:G:15:DG:H5''	1.85	0.42
2:J:30:ILE:CD1	2:J:187:ARG:HD3	2.48	0.42
1:K:264:ARG:HG3	1:K:302:TYR:CE2	2.55	0.42
1:K:302:TYR:CE1	1:K:306:LEU:HD22	2.55	0.42
3:D:84:DA:H2'	3:D:85:DG:C8	2.54	0.42
1:K:44:ALA:HB1	1:K:72:LEU:HD21	2.01	0.42
4:N:58:C:H2'	4:N:59:A:C8	2.55	0.42
4:R:78:U:H2'	4:R:79:U:C6	2.55	0.42
2:C:24:ARG:HD3	2:C:275:ASP:HB2	2.01	0.42
2:C:238:ILE:O	2:C:241:ARG:HB2	2.20	0.42
3:D:24:DT:H1'	3:D:25:DT:C2	2.55	0.42
1:P:244:THR:HG22	3:Q:84:DA:H4'	2.02	0.42
2:T:107:LEU:O	2:T:111:SER:OG	2.31	0.42
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.85	0.42
1:A:239:SER:OG	4:E:65:C:O5'	2.38	0.42
1:A:300:ILE:O	1:A:303:ILE:HG13	2.20	0.42
1:B:309:LYS:HE3	1:B:309:LYS:HB2	1.77	0.42
2:J:68:PHE:HA	2:J:71:LEU:HB2	2.01	0.42
1:P:284:TRP:CD1	3:Q:82:DT:H4'	2.55	0.42
1:B:287:PHE:O	1:B:291:VAL:HG22	2.20	0.41
2:J:129:LYS:HA	2:J:129:LYS:HD2	1.76	0.41
1:K:299:LEU:O	1:K:302:TYR:HB3	2.20	0.41
2:L:11:GLN:OE1	2:L:11:GLN:HA	2.19	0.41
3:M:84:DA:H2'	3:M:85:DG:H8	1.85	0.41
1:P:75:LEU:HD12	1:P:75:LEU:HA	1.87	0.41
1:A:130:ASN:HD22	3:D:7:DA:H2''	1.85	0.41
1:A:133:PHE:CE2	1:A:146:SER:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:GLY:HA3	3:G:4:DA:OP1	2.20	0.41
2:J:3:LYS:HE3	2:J:3:LYS:HB3	1.85	0.41
2:J:171:ARG:H	2:J:171:ARG:HD2	1.85	0.41
5:O:0:C:H3'	5:O:1:G:H8	1.84	0.41
1:P:48:TYR:OH	1:P:160:PRO:HG2	2.20	0.41
1:P:118:ILE:HD12	1:P:216:LEU:HD12	2.01	0.41
2:T:75:GLN:HB3	2:T:80:LEU:HD22	2.02	0.41
3:D:62:DC:H2'	3:D:63:DA:C4	2.56	0.41
2:J:15:GLY:O	2:J:19:LYS:HE2	2.20	0.41
1:K:280:HIS:CD2	1:K:284:TRP:HD1	2.38	0.41
1:P:178:ASP:OD1	1:P:192:TYR:OH	2.18	0.41
1:A:270:ILE:HD12	1:A:271:PHE:HD1	1.84	0.41
1:B:3:SER:OG	1:B:4:ALA:N	2.52	0.41
1:B:230:LYS:NZ	4:H:68:U:O3'	2.53	0.41
2:J:138:GLY:HA2	2:T:72:LEU:HD13	2.02	0.41
1:K:74:ALA:HB2	2:T:288:ASN:ND2	2.35	0.41
1:P:288:ILE:O	1:P:292:ASP:N	2.50	0.41
4:E:45:G:H2'	4:E:46:A:H8	1.86	0.41
1:B:217:PHE:HZ	1:B:232:THR:HG21	1.85	0.41
3:M:22:DG:H2'	3:M:23:DG:N7	2.35	0.41
1:A:237:PRO:HB2	4:E:62:C:O2'	2.20	0.41
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.91	0.41
1:B:249:SER:OG	1:B:250:GLN:N	2.53	0.41
1:K:270:ILE:HG23	1:K:271:PHE:HD1	1.85	0.41
4:N:13:A:N6	5:O:6:G:C8	2.80	0.41
1:P:37:LEU:HD23	1:P:37:LEU:HA	1.91	0.41
1:A:81:ARG:NH1	1:A:85:ASP:OD2	2.50	0.41
3:D:5:DG:OP1	1:B:13:ARG:NH2	2.39	0.41
3:D:30:DC:H2'	3:D:31:DG:OP2	2.19	0.41
4:E:59:A:H2'	4:E:60:U:C6	2.56	0.41
1:B:185:ALA:HB1	1:B:190:LEU:HB2	2.03	0.41
1:K:56:LYS:HG3	4:N:69:G:H21	1.85	0.41
4:R:41:U:H2'	4:R:42:C:C6	2.56	0.41
1:B:190:LEU:HD23	1:B:203:ALA:HB2	2.03	0.41
1:B:248:ILE:HD13	1:B:253:VAL:HG12	2.02	0.41
1:P:27:SER:HB2	1:P:32:ILE:O	2.21	0.41
1:P:28:LYS:HE3	1:P:28:LYS:HB3	1.87	0.41
1:P:134:GLY:HA3	3:Q:7:DA:H1'	2.03	0.41
1:A:145:ILE:HD13	1:A:145:ILE:HA	1.87	0.41
3:D:51:DC:H2'	3:D:52:DT:C7	2.51	0.41
1:B:202:SER:OG	2:J:251:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:O	1:B:301:THR:HG23	2.20	0.41
7:J:402:AR6:O2'	2:T:131:LYS:HD2	2.21	0.41
1:K:72:LEU:HD12	1:K:72:LEU:HA	1.88	0.41
1:K:297:ARG:O	1:K:300:ILE:HG12	2.21	0.41
2:T:100:SER:H	2:T:103:SER:HG	1.66	0.41
2:C:5:PHE:HD1	2:C:5:PHE:HA	1.65	0.41
1:K:255:ILE:HG13	1:K:256:GLY:H	1.86	0.41
1:K:259:LYS:O	1:K:263:ILE:HD12	2.21	0.41
4:N:16:G:H2'	4:N:17:A:H8	1.86	0.41
3:D:32:DG:H2''	3:D:33:DA:OP2	2.20	0.40
2:J:134:PHE:CD1	2:J:140:VAL:HG11	2.54	0.40
1:K:123:PHE:CG	1:K:197:ASP:HB3	2.56	0.40
1:K:132:VAL:HB	1:K:150:THR:HG23	2.03	0.40
3:M:60:DA:H2''	3:M:61:DA:N7	2.36	0.40
2:J:196:ILE:HD12	2:J:196:ILE:HA	1.90	0.40
1:K:30:THR:HG22	1:K:78:TRP:CE2	2.56	0.40
1:K:87:LEU:HD11	1:K:139:LEU:HD11	2.03	0.40
1:K:309:LYS:HD3	1:K:310:TYR:CD1	2.52	0.40
4:N:44:G:O2'	4:N:45:G:H8	2.04	0.40
1:P:115:ILE:HD12	1:P:241:ARG:HB3	2.04	0.40
4:E:79:U:C2	4:E:80:A:C8	3.10	0.40
2:J:31:THR:HG22	2:J:194:LYS:HE3	2.04	0.40
1:P:118:ILE:HG12	1:P:232:THR:HG23	2.03	0.40
1:A:288:ILE:HG12	1:A:288:ILE:H	1.77	0.40
3:D:60:DA:H2''	3:D:61:DA:N7	2.37	0.40
4:E:41:U:H2'	4:E:42:C:H6	1.87	0.40
1:B:201:LEU:HD13	1:B:216:LEU:HD11	2.02	0.40
1:B:207:LYS:HB3	1:B:207:LYS:HE3	1.87	0.40
3:G:66:DG:H1'	3:G:67:DA:C4	2.56	0.40
3:G:80:DA:H2''	3:G:81:DC:H6	1.86	0.40
1:K:239:SER:HB2	4:N:65:C:H5'	2.02	0.40
2:L:10:GLN:O	2:L:14:ILE:HG23	2.21	0.40
5:S:5:G:H3'	5:S:5:G:H8	1.87	0.40
2:T:134:PHE:O	2:T:138:GLY:N	2.54	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	312/330 (94%)	301 (96%)	11 (4%)	0	100	100
1	B	312/330 (94%)	302 (97%)	10 (3%)	0	100	100
1	K	312/330 (94%)	298 (96%)	14 (4%)	0	100	100
1	P	312/330 (94%)	302 (97%)	10 (3%)	0	100	100
2	C	126/307 (41%)	123 (98%)	3 (2%)	0	100	100
2	J	304/307 (99%)	285 (94%)	19 (6%)	0	100	100
2	L	126/307 (41%)	125 (99%)	1 (1%)	0	100	100
2	T	304/307 (99%)	291 (96%)	13 (4%)	0	100	100
All	All	2108/2548 (83%)	2027 (96%)	81 (4%)	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	281/296 (95%)	262 (93%)	19 (7%)	13	32
1	B	281/296 (95%)	266 (95%)	15 (5%)	19	43
1	K	281/296 (95%)	258 (92%)	23 (8%)	9	23
1	P	281/296 (95%)	267 (95%)	14 (5%)	20	46
2	C	120/278 (43%)	113 (94%)	7 (6%)	17	39
2	J	277/278 (100%)	260 (94%)	17 (6%)	15	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	120/278 (43%)	99 (82%)	21 (18%)	1	4
2	T	277/278 (100%)	266 (96%)	11 (4%)	27	55
All	All	1918/2296 (84%)	1791 (93%)	127 (7%)	16	33

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	ARG
1	A	22	ASN
1	A	35	GLU
1	A	53	VAL
1	A	61	ARG
1	A	62	MET
1	A	86	LYS
1	A	92	PHE
1	A	98	LYS
1	A	99	HIS
1	A	168	LYS
1	A	202	SER
1	A	207	LYS
1	A	231	LYS
1	A	249	SER
1	A	260	TYR
1	A	271	PHE
1	A	312	LYS
2	C	5	PHE
2	C	7	ASP
2	C	214	ASP
2	C	216	VAL
2	C	250	GLU
2	C	268	SER
2	C	293	ARG
1	B	20	MET
1	B	53	VAL
1	B	90	SER
1	B	92	PHE
1	B	97	GLU
1	B	119	ASP
1	B	122	ASP
1	B	175	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	202	SER
1	B	205	SER
1	B	230	LYS
1	B	264	ARG
1	B	282	ARG
1	B	312	LYS
1	B	315	LEU
2	J	5	PHE
2	J	75	GLN
2	J	96	LEU
2	J	117	ARG
2	J	127	LYS
2	J	145	LYS
2	J	154	CYS
2	J	160	LYS
2	J	163	CYS
2	J	168	ASP
2	J	174	ARG
2	J	190	ASN
2	J	191	LYS
2	J	214	ASP
2	J	216	VAL
2	J	219	ARG
2	J	262	VAL
1	K	11	ARG
1	K	20	MET
1	K	55	LYS
1	K	60	LYS
1	K	62	MET
1	K	113	ASN
1	K	122	ASP
1	K	143	ARG
1	K	175	SER
1	K	206	MET
1	K	207	LYS
1	K	214	ASP
1	K	231	LYS
1	K	239	SER
1	K	242	LYS
1	K	251	GLU
1	K	252	LYS
1	K	257	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	264	ARG
1	K	272	CYS
1	K	297	ARG
1	K	308	LYS
1	K	312	LYS
2	L	1	MET
2	L	4	LYS
2	L	5	PHE
2	L	7	ASP
2	L	16	HIS
2	L	200	LEU
2	L	204	ARG
2	L	209	CYS
2	L	214	ASP
2	L	215	SER
2	L	216	VAL
2	L	218	TYR
2	L	226	PHE
2	L	241	ARG
2	L	250	GLU
2	L	254	LEU
2	L	256	MET
2	L	269	TYR
2	L	276	ARG
2	L	280	ASP
2	L	306	HIS
1	P	5	GLU
1	P	24	HIS
1	P	38	ARG
1	P	48	TYR
1	P	61	ARG
1	P	85	ASP
1	P	92	PHE
1	P	101	SER
1	P	119	ASP
1	P	197	ASP
1	P	198	ASP
1	P	253	VAL
1	P	305	LYS
1	P	306	LEU
2	T	3	LYS
2	T	5	PHE

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Mol	Chain	Res	Type
2	T	20	LYS
2	T	31	THR
2	T	57	SER
2	T	60	ASP
2	T	75	GLN
2	T	168	ASP
2	T	190	ASN
2	T	220	THR
2	T	234	VAL

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

Mol	Chain	Res	Type
1	P	105	ASN
2	T	75	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	56/82 (68%)	17 (30%)	1 (1%)
4	H	56/82 (68%)	20 (35%)	0
4	N	56/82 (68%)	22 (39%)	1 (1%)
4	R	56/82 (68%)	21 (37%)	1 (1%)
5	F	7/14 (50%)	0	0
5	I	7/14 (50%)	4 (57%)	0
5	O	7/14 (50%)	6 (85%)	0
5	S	7/14 (50%)	6 (85%)	1 (14%)
All	All	252/384 (65%)	96 (38%)	4 (1%)

All (96) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	E	9	C
4	E	15	C
4	E	16	G
4	E	20	G
4	E	21	G
4	E	22	U
4	E	41	U
4	E	44	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	E	52	U
4	E	53	U
4	E	55	C
4	E	56	G
4	E	64	G
4	E	66	A
4	E	67	U
4	E	68	U
4	E	72	U
4	H	9	C
4	H	12	U
4	H	15	C
4	H	18	G
4	H	20	G
4	H	21	G
4	H	22	U
4	H	40	C
4	H	41	U
4	H	44	G
4	H	52	U
4	H	53	U
4	H	55	C
4	H	56	G
4	H	64	G
4	H	66	A
4	H	67	U
4	H	68	U
4	H	69	G
4	H	72	U
5	I	4	A
5	I	5	G
5	I	6	G
5	I	7	G
4	N	9	C
4	N	10	C
4	N	13	A
4	N	14	G
4	N	15	C
4	N	16	G
4	N	20	G
4	N	21	G
4	N	22	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	N	41	U
4	N	44	G
4	N	52	U
4	N	53	U
4	N	55	C
4	N	56	G
4	N	59	A
4	N	64	G
4	N	65	C
4	N	66	A
4	N	67	U
4	N	69	G
4	N	72	U
5	O	1	G
5	O	2	U
5	O	3	A
5	O	4	A
5	O	6	G
5	O	7	G
4	R	10	C
4	R	11	U
4	R	12	U
4	R	13	A
4	R	14	G
4	R	15	C
4	R	16	G
4	R	20	G
4	R	21	G
4	R	22	U
4	R	41	U
4	R	44	G
4	R	52	U
4	R	53	U
4	R	55	C
4	R	59	A
4	R	64	G
4	R	66	A
4	R	67	U
4	R	69	G
4	R	72	U
5	S	1	G
5	S	2	U

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Mol	Chain	Res	Type
5	S	3	A
5	S	5	G
5	S	6	G
5	S	7	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	E	66	A
4	N	66	A
4	R	66	A
5	S	5	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NCA	J	401	-	9,9,9	0.32	0	11,11,11	0.40	0
7	AR6	J	402	2	33,38,39	5.18	15 (45%)	37,58,60	2.59	8 (21%)

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
6	NCA	J	401	-	-	0/4/4/4	0/1/1/1
7	AR6	J	402	2	-	10/18/51/54	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	402	AR6	O4'-C1'	17.09	1.64	1.41
7	J	402	AR6	C2'-C1'	-13.77	1.32	1.53
7	J	402	AR6	C2D-C3D	-10.99	1.35	1.53
7	J	402	AR6	O4D-C4D	-8.43	1.30	1.44
7	J	402	AR6	O4D-C1D	7.79	1.61	1.43
7	J	402	AR6	O4'-C4'	-6.64	1.30	1.45
7	J	402	AR6	C1D-C2D	4.17	1.58	1.51
7	J	402	AR6	O3'-C3'	-4.15	1.33	1.43
7	J	402	AR6	C3D-C4D	3.93	1.63	1.53
7	J	402	AR6	O2D-C2D	3.26	1.50	1.43
7	J	402	AR6	C6-N6	2.73	1.44	1.34
7	J	402	AR6	C5-C4	-2.33	1.34	1.40
7	J	402	AR6	C3'-C4'	2.24	1.58	1.53
7	J	402	AR6	C2-N3	2.23	1.35	1.32
7	J	402	AR6	PA-O5'	2.04	1.67	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	402	AR6	C5-C6-N6	10.05	135.62	120.35
7	J	402	AR6	N6-C6-N1	-6.87	104.32	118.57
7	J	402	AR6	N3-C2-N1	-5.66	119.83	128.68
7	J	402	AR6	C1D-C2D-C3D	4.13	107.93	101.63
7	J	402	AR6	PB-O3A-PA	-3.13	122.10	132.83
7	J	402	AR6	C3'-C2'-C1'	2.79	105.19	100.98
7	J	402	AR6	O4D-C4D-C3D	2.75	107.14	104.70
7	J	402	AR6	O2D-C2D-C3D	-2.20	107.09	111.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	402	AR6	C5'-O5'-PA-O2A
7	J	402	AR6	C5'-O5'-PA-O3A

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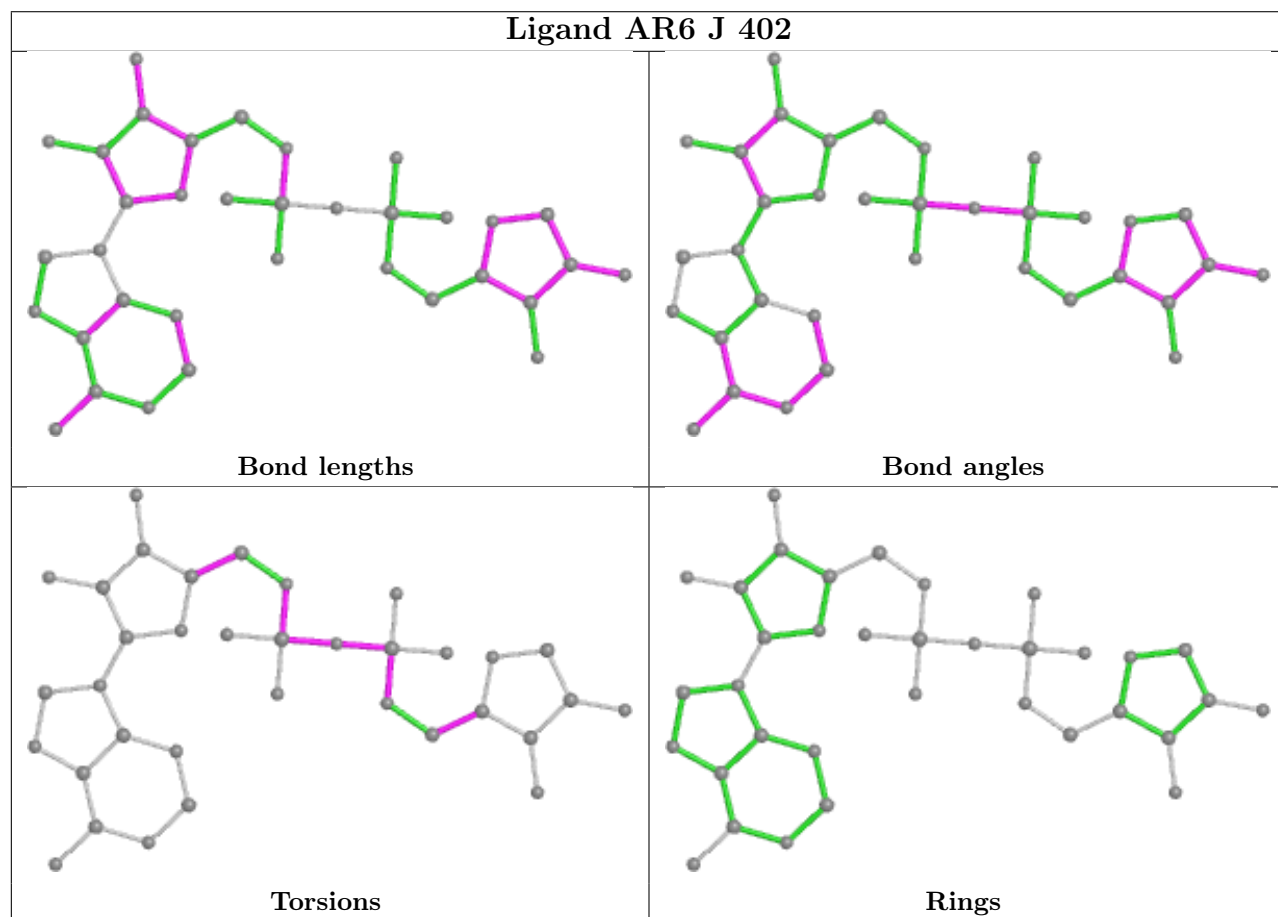
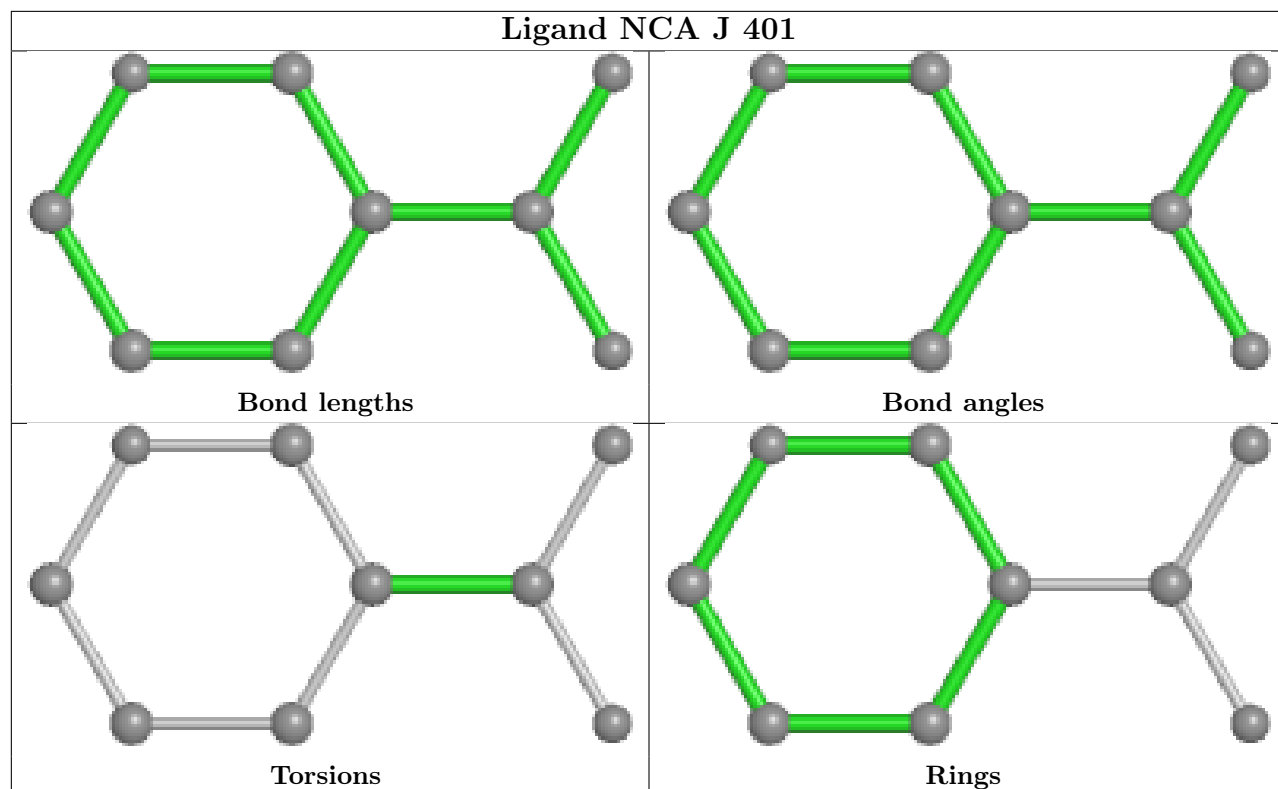
Mol	Chain	Res	Type	Atoms
7	J	402	AR6	C3'-C4'-C5'-O5'
7	J	402	AR6	C3D-C4D-C5D-O5D
7	J	402	AR6	O4D-C4D-C5D-O5D
7	J	402	AR6	O4'-C4'-C5'-O5'
7	J	402	AR6	PB-O3A-PA-O5'
7	J	402	AR6	C5D-O5D-PB-O3A
7	J	402	AR6	PA-O3A-PB-O1B
7	J	402	AR6	C5D-O5D-PB-O1B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	401	NCA	1	0
7	J	402	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.

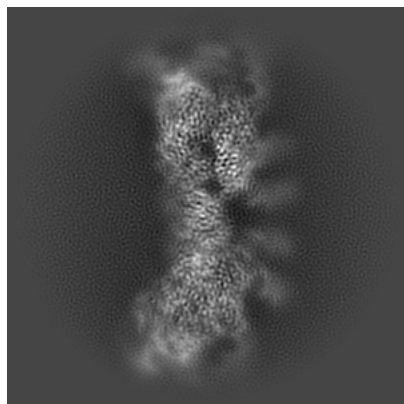
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61595. These allow visual inspection of the internal detail of the map and identification of artifacts.

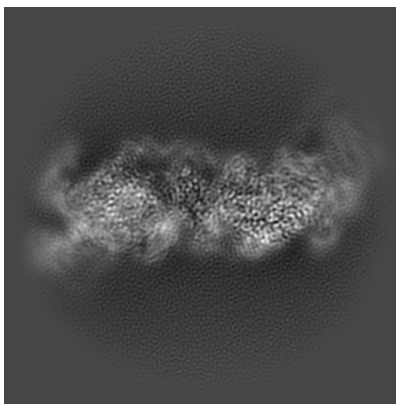
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

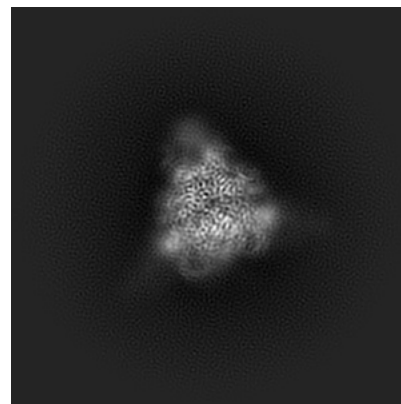
#### 6.1.1 Primary map



X

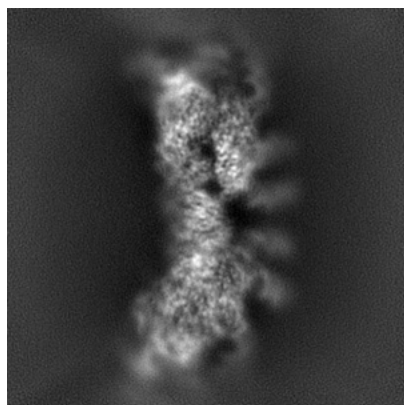


Y

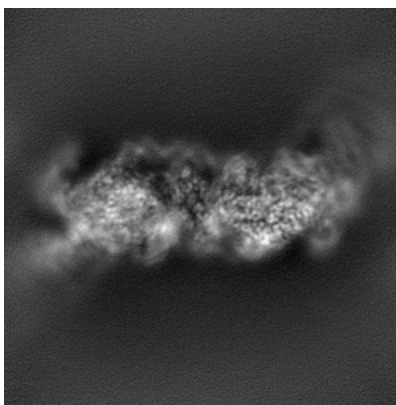


Z

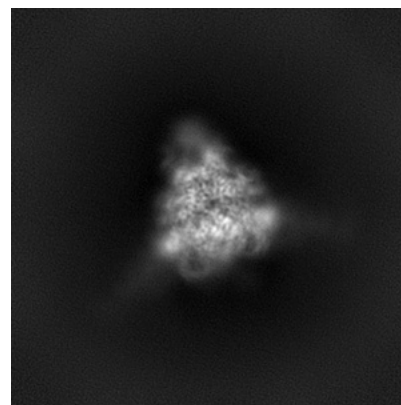
#### 6.1.2 Raw map



X



Y

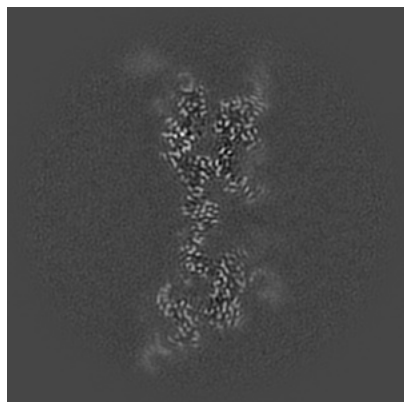


Z

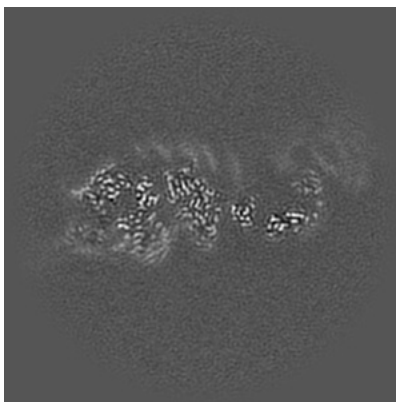
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

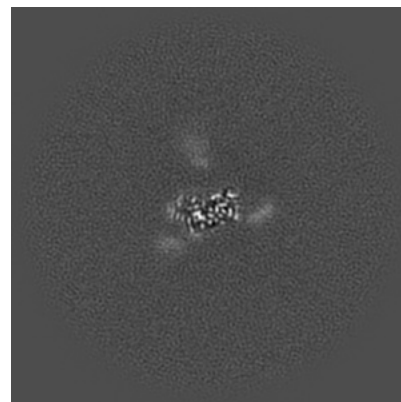
### 6.2.1 Primary map



X Index: 140

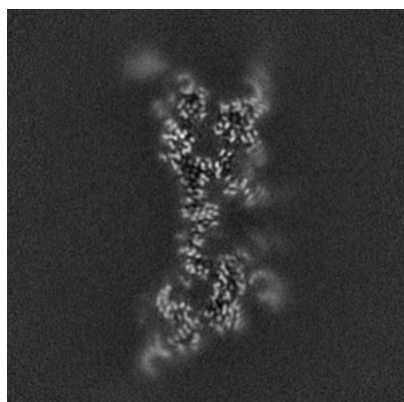


Y Index: 140

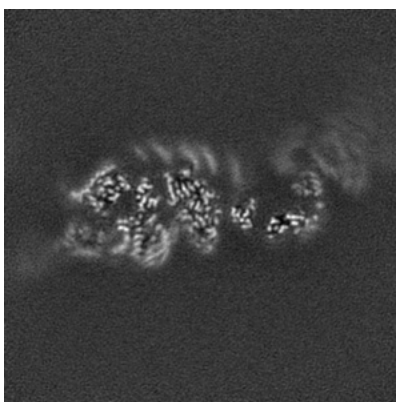


Z Index: 140

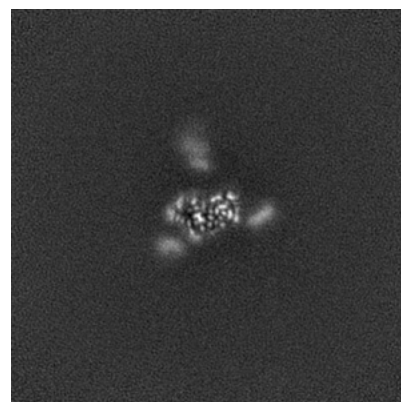
### 6.2.2 Raw map



X Index: 140



Y Index: 140

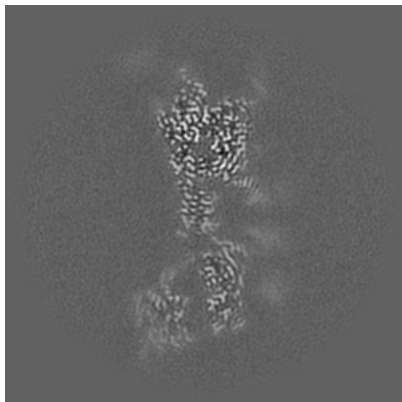


Z Index: 140

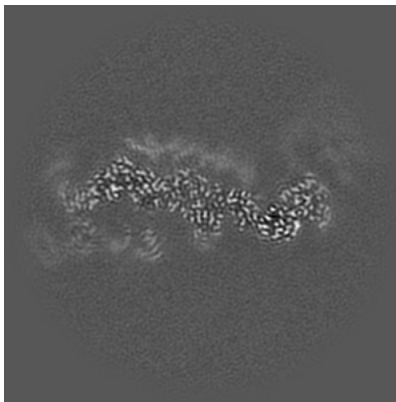
The images above show central slices of the map in three orthogonal directions.

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

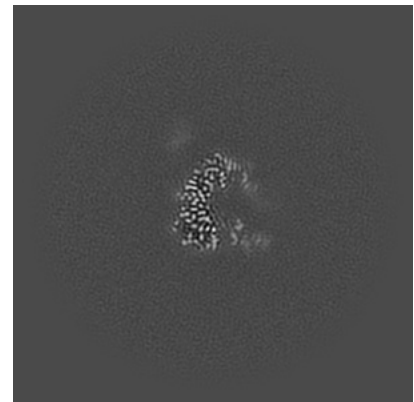
### 6.3.1 Primary map



X Index: 134

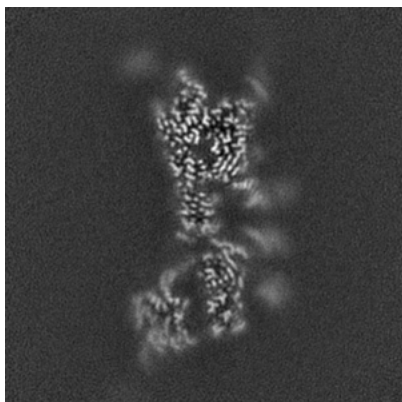


Y Index: 132

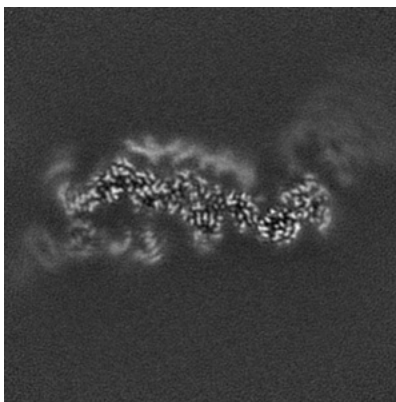


Z Index: 190

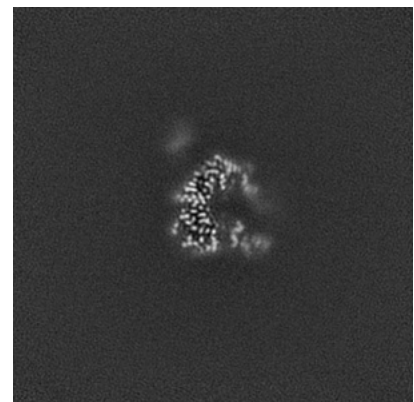
### 6.3.2 Raw map



X Index: 134



Y Index: 132

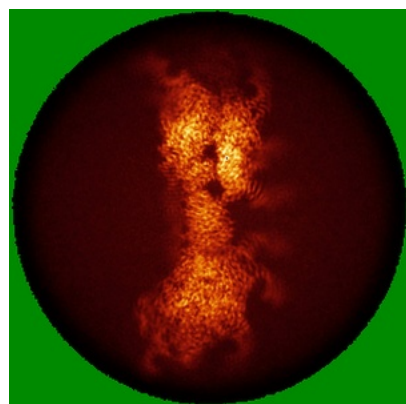


Z Index: 190

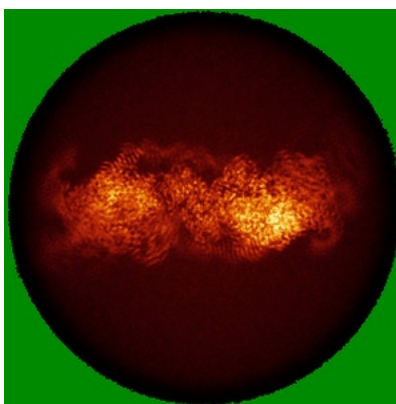
The images above show the largest variance slices of the map in three orthogonal directions.

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

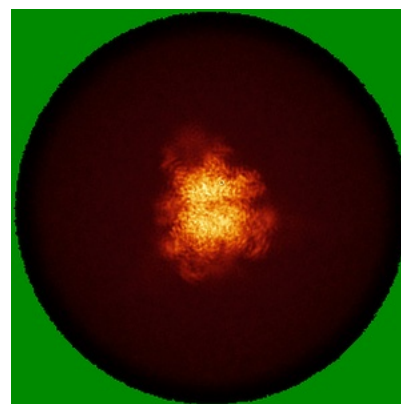
### 6.4.1 Primary map



X

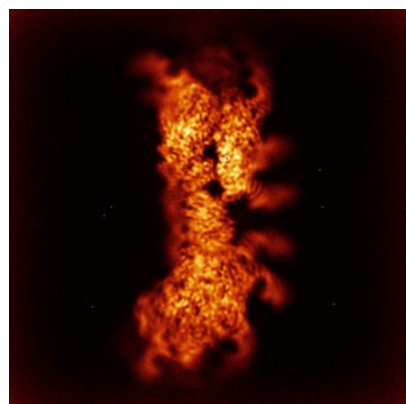


Y

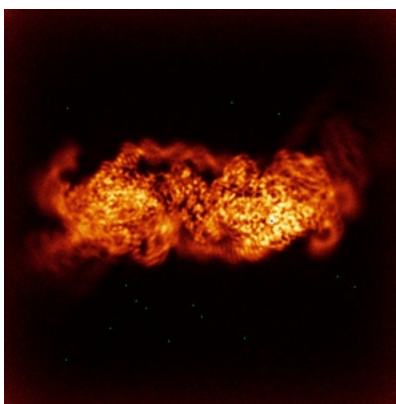


Z

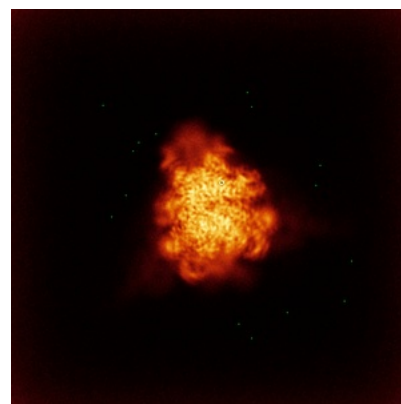
### 6.4.2 Raw map



X



Y



Z

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

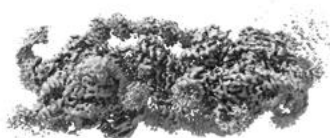


## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

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

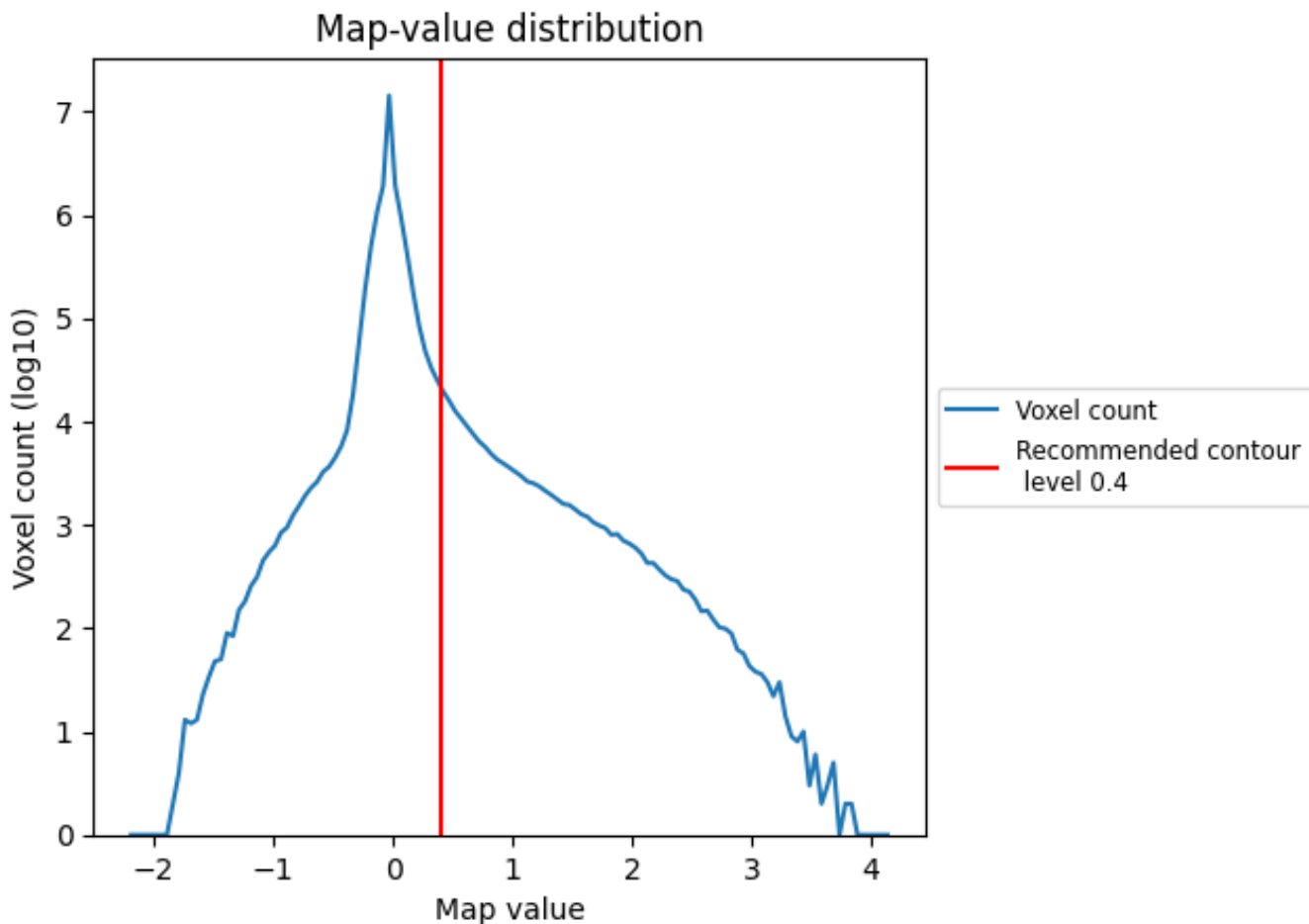
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

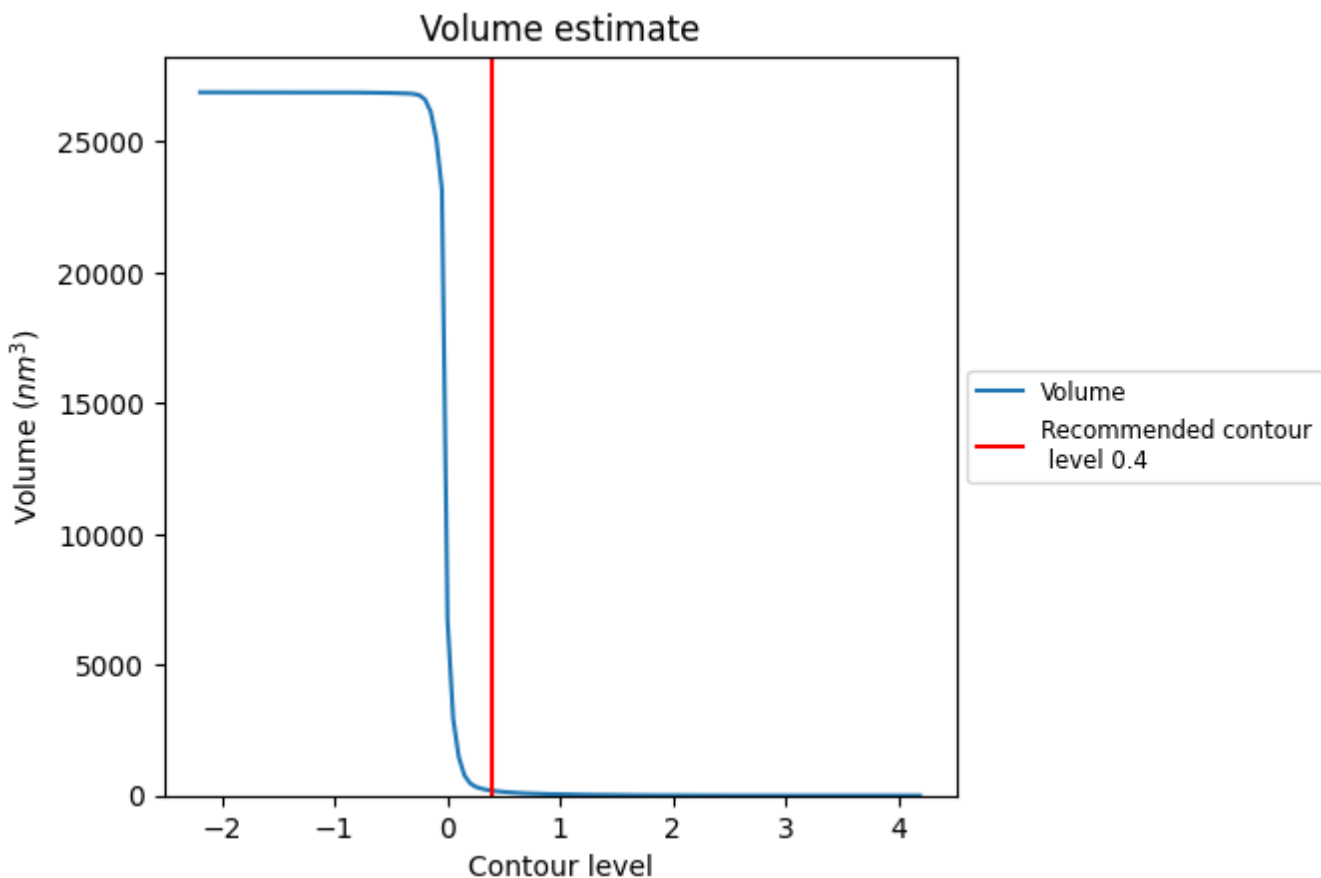
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

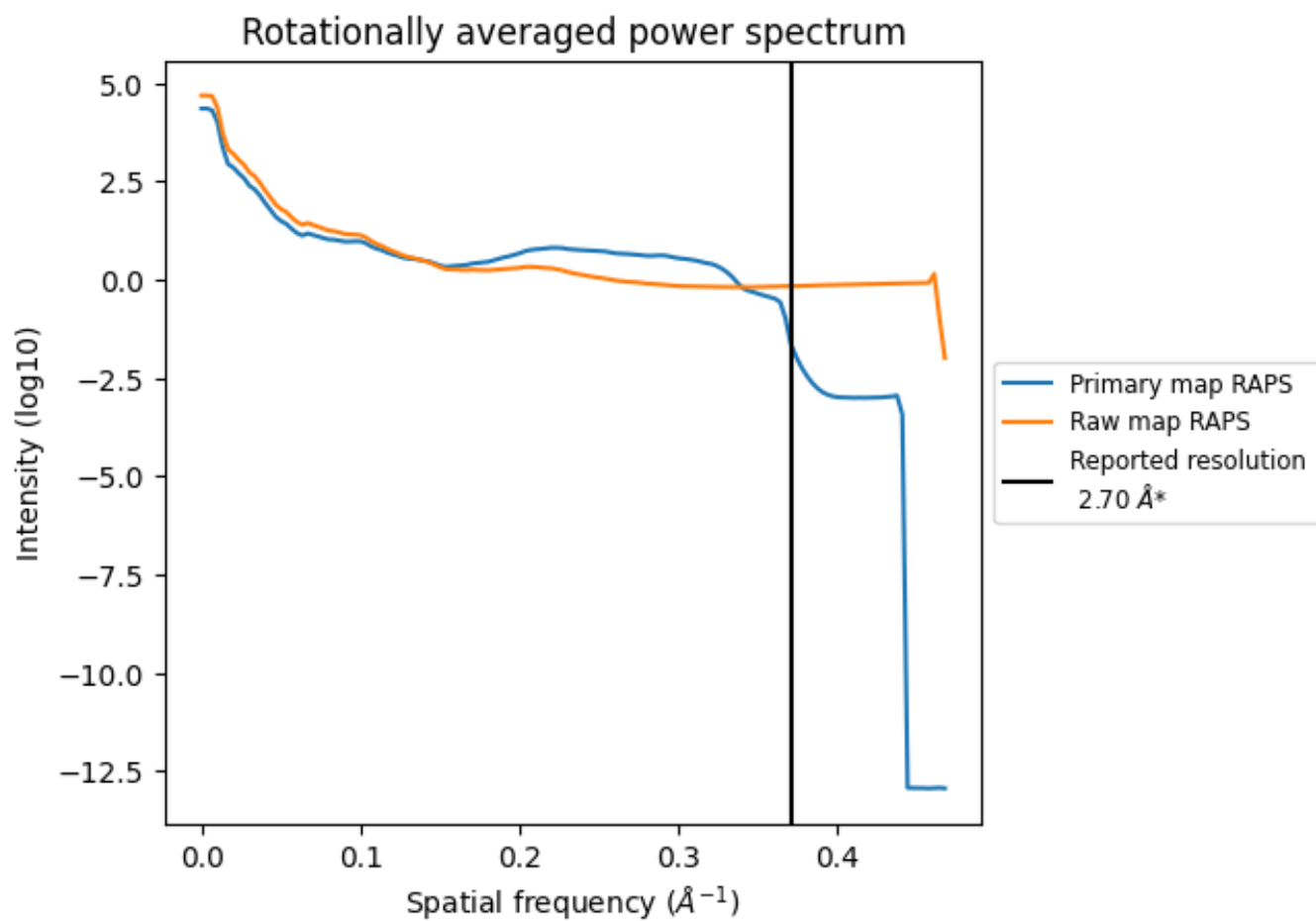
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $185 \text{ nm}^3$ ; this corresponds to an approximate mass of 168 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](#)

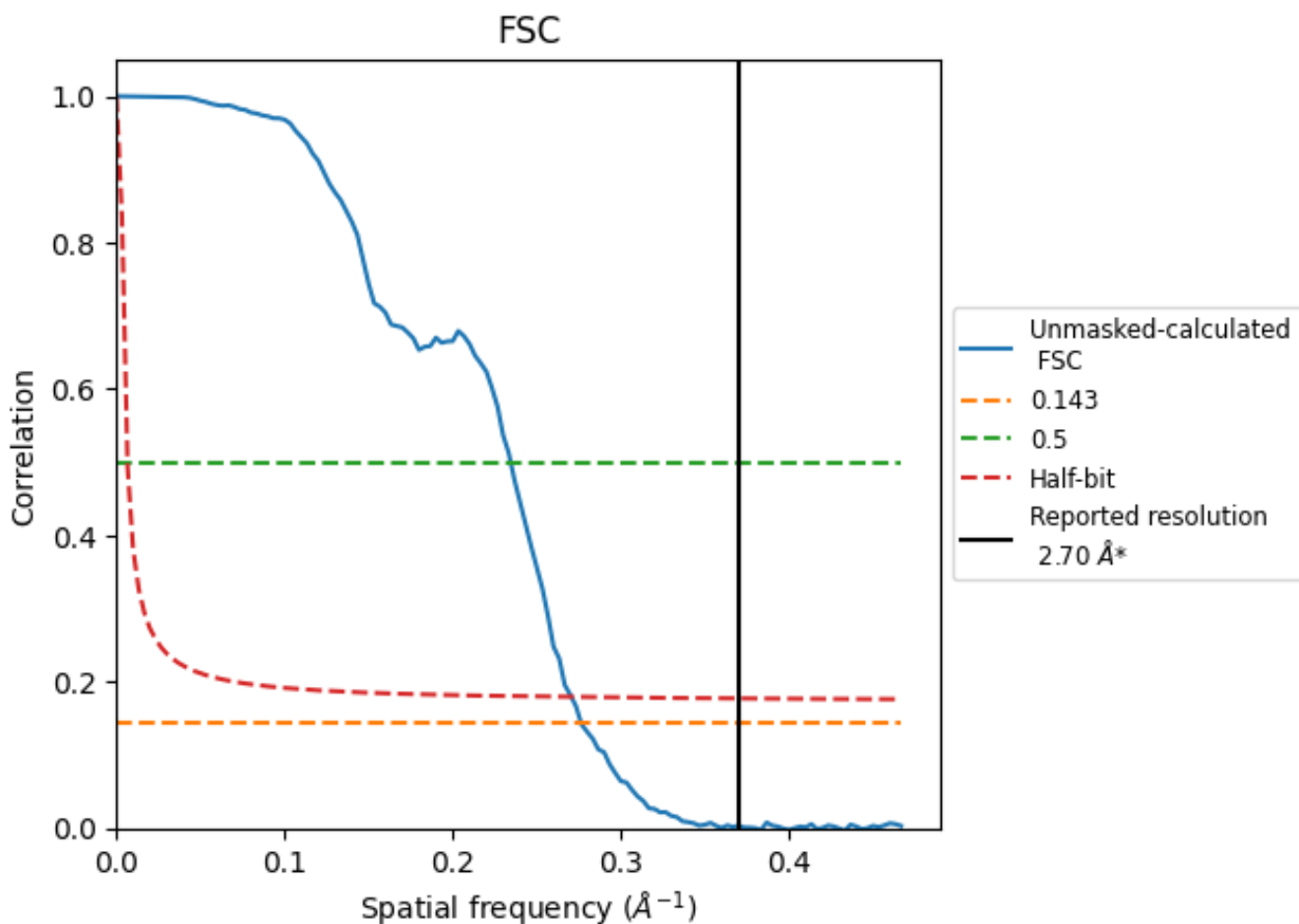


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 0.370 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

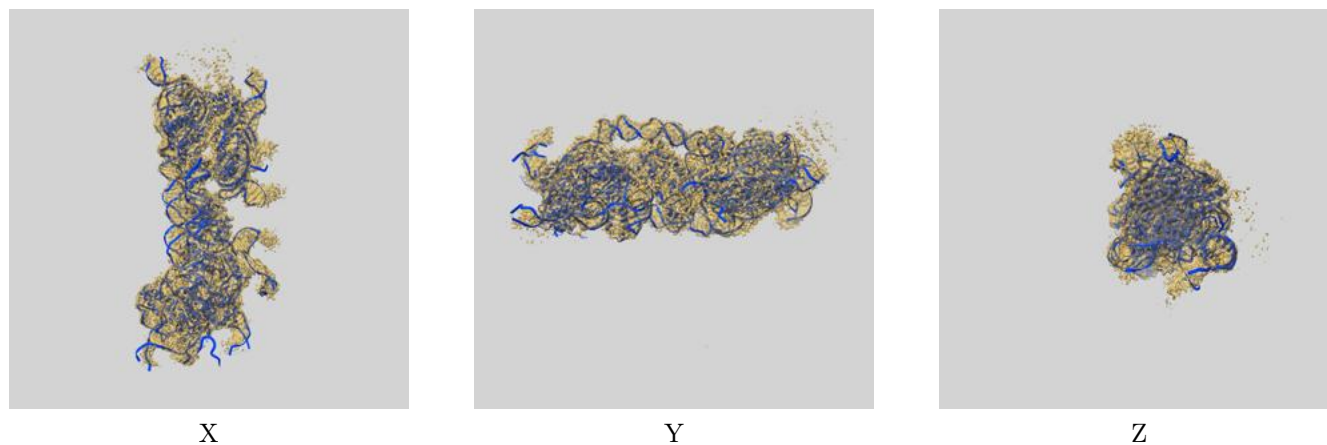
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.26	3.69

\*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 3.61 differs from the reported value 2.7 by more than 10 %

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

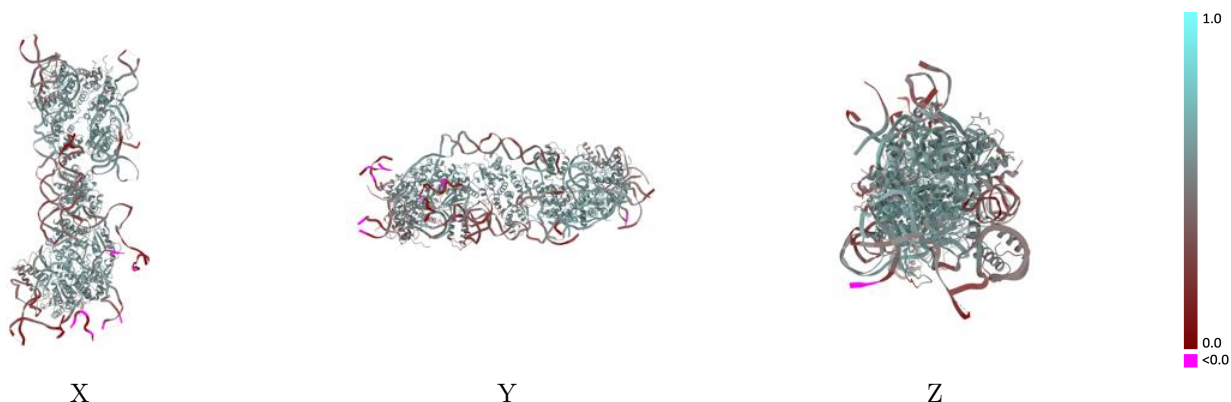
This section contains information regarding the fit between EMDB map EMD-61595 and PDB model 9JM0. Per-residue inclusion information can be found in section 3 on page 8.

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



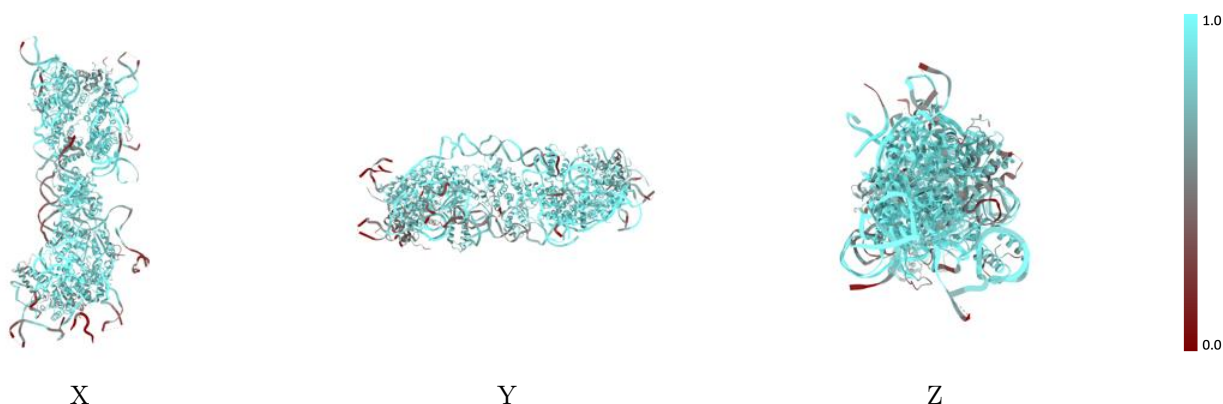
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

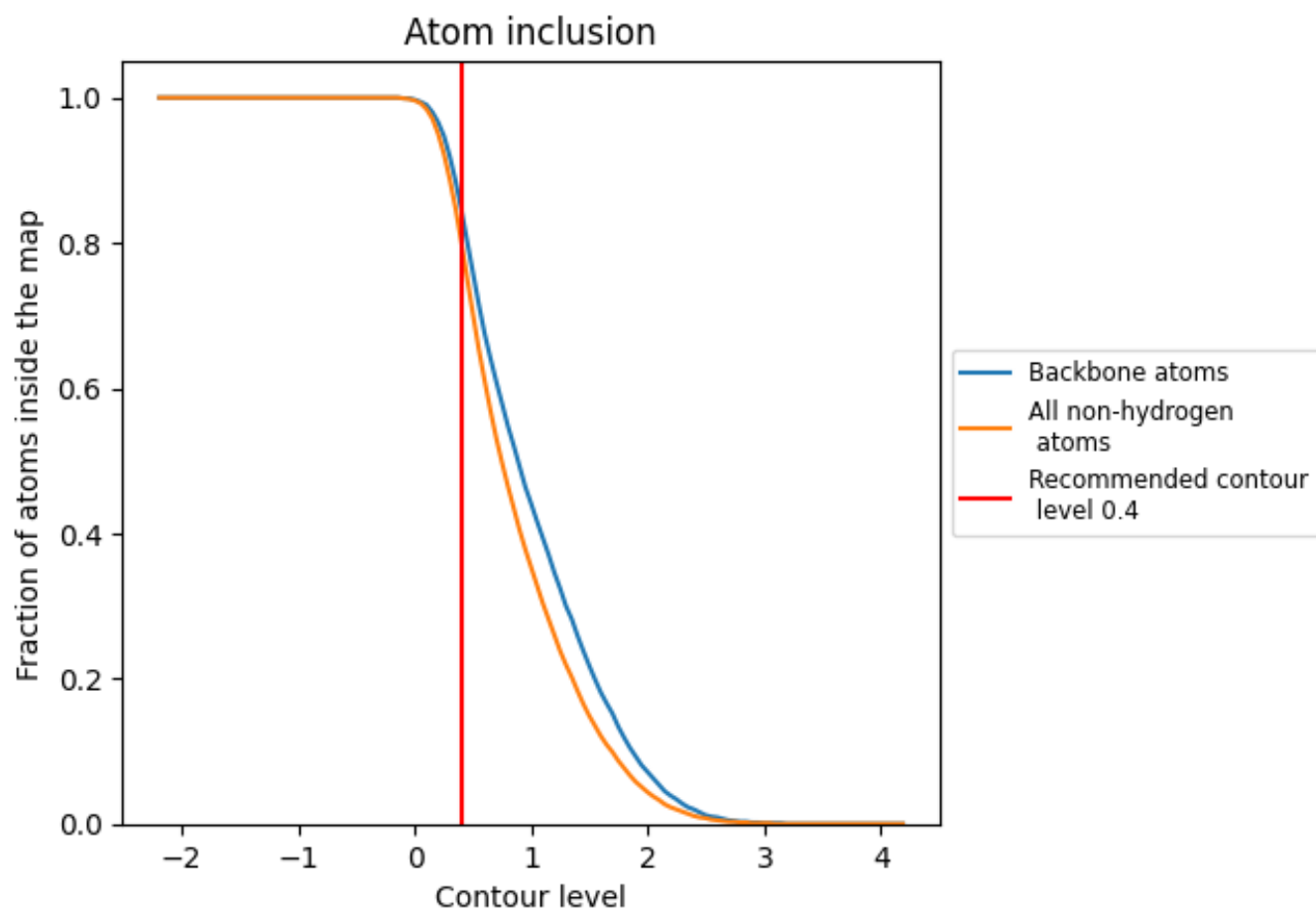
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.4).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.4920
A	 0.8930	 0.5680
B	 0.9280	 0.5970
C	 0.6790	 0.5310
D	 0.7040	 0.4110
E	 0.7940	 0.4140
F	 0.5740	 0.2870
G	 0.8800	 0.5330
H	 0.8900	 0.5060
I	 0.6310	 0.3710
J	 0.8840	 0.5750
K	 0.8320	 0.5320
L	 0.4640	 0.4360
M	 0.7820	 0.4170
N	 0.6410	 0.2900
O	 0.0510	 0.0080
P	 0.8420	 0.5250
Q	 0.7290	 0.3820
R	 0.7240	 0.3490
S	 0.2220	 0.0610
T	 0.8900	 0.5810

