



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 09:06 PM EST

PDB ID : 7JQC  
EMDB ID : EMD-22433  
Title : SARS-CoV-2 Nsp1, CrPV IRES and rabbit 40S ribosome complex  
Authors : Yuan, S.; Xiong, Y.  
Deposited on : 2020-08-10  
Resolution : 3.30 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:

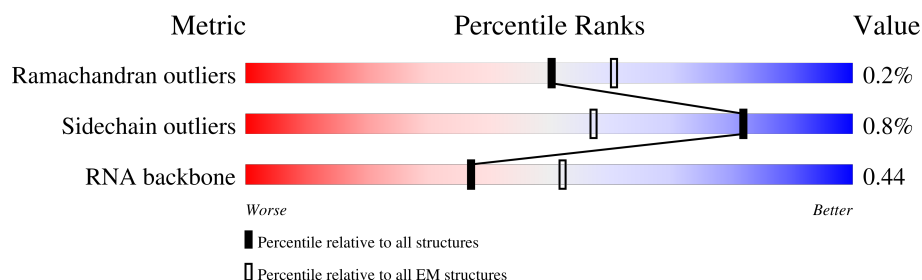
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1869	
2	a	125	
3	B	295	
4	b	115	
5	C	264	
6	D	293	
7	d	69	
8	E	243	

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Mol	Chain	Length	Quality of chain
9	f	133	
10	G	204	
11	g	156	
12	H	249	
13	h	317	
14	I	194	
15	J	208	
16	K	194	
17	L	165	
18	N	132	
19	Q	145	
20	R	146	
21	S	135	
22	T	152	
23	U	145	
24	V	119	
25	W	83	
26	Z	130	
27	F	36	
28	i	192	
29	M	263	
30	O	158	
31	P	151	
32	X	168	
33	Y	130	

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Mol	Chain	Length	Quality of chain
34	c	143	<div><div></div><div>97%</div><div></div></div>
35	e	84	<div><div>15%</div><div>95%</div><div>5%</div></div>

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 77823 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 RNA chain called rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 2 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 3 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 4 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8
b	56	ALA	VAL	conflict	UNP G1TFE8
b	109	ARG	PRO	conflict	UNP G1TFE8

- Molecule 5 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 6 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 7 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 8 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 9 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	f	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 10 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	185	Total	C	N	O	S	0	0
			1461	917	277	260	7		

- Molecule 11 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 12 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 13 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	h	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 14 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 15 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 16 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 17 is a protein called S10\_pectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 18 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 19 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	107	Total	C	N	O	S	0	0
			889	563	167	152	7		

- Molecule 20 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 21 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 22 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 23 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 24 is a protein called uS10.



Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called Host translation inhibitor nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	36	Total	C	N	O	S	0	0
			280	171	50	58	1		

- Molecule 28 is a RNA chain called Cricket paralysis virus IRES RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	143	Total	C	N	O	P	0	0
			3026	1356	518	1009	143		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	6176	C	U	conflict	GB 8895506

- Molecule 29 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	M	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 30 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	O	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 31 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 32 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 33 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

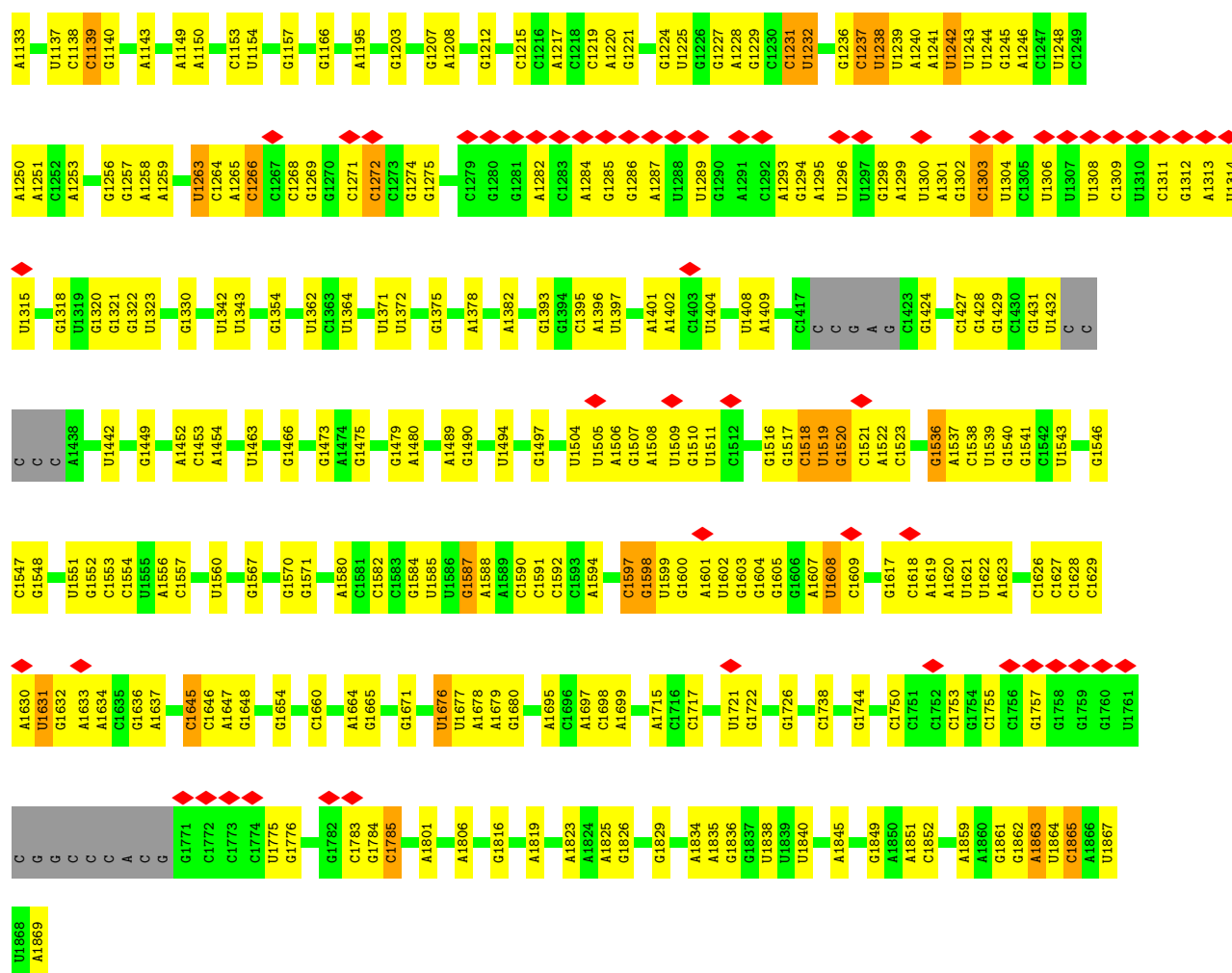
- Molecule 34 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	142	Total	C	N	O	S	0	0
			1106	698	220	184	4		

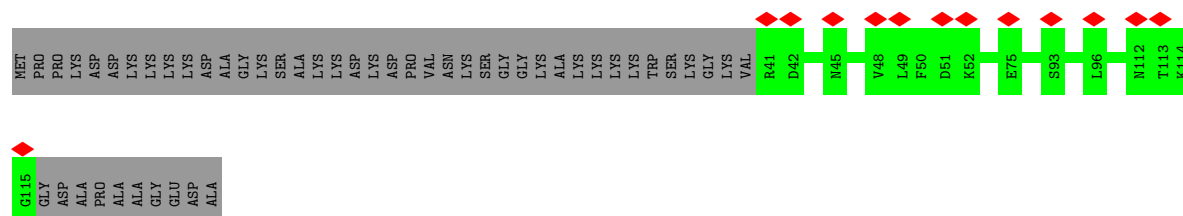
- Molecule 35 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

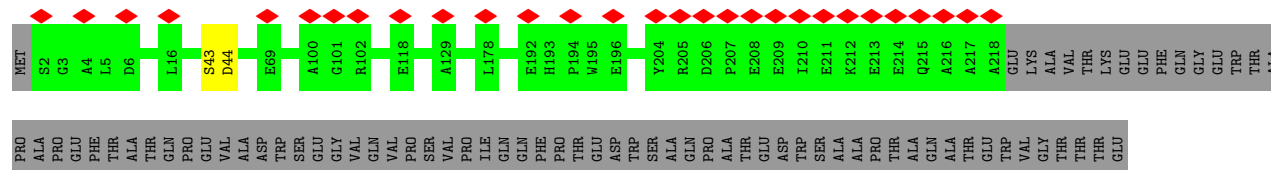
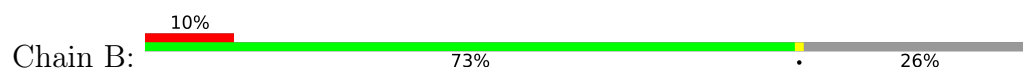




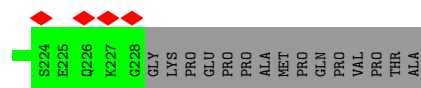
- Molecule 2: eS25



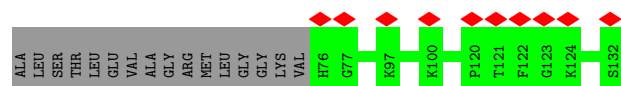
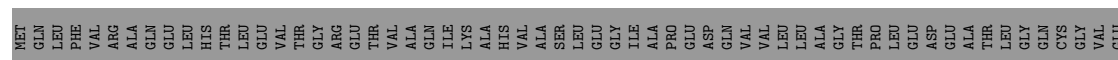
- Molecule 3: 40S ribosomal protein SA



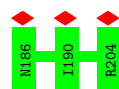
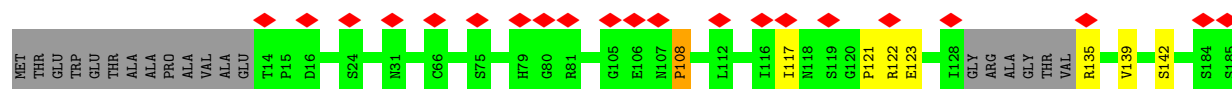
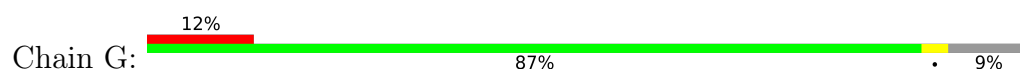




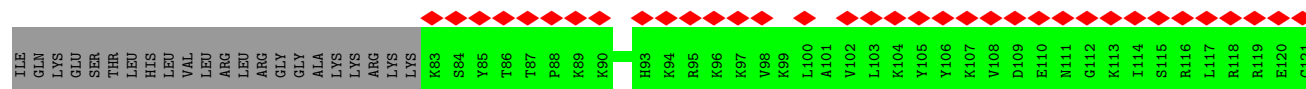
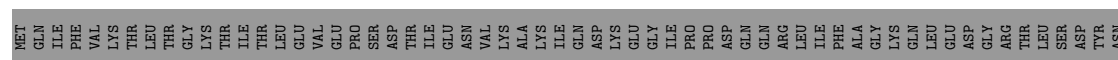
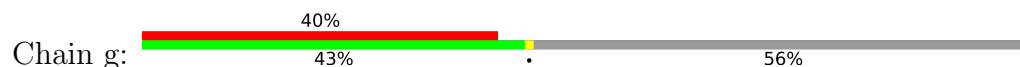
• Molecule 9: eS30



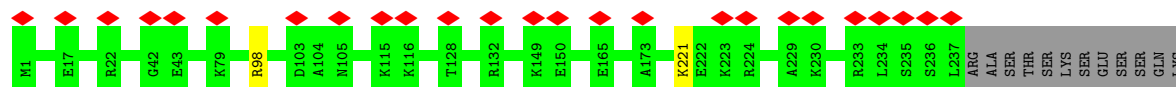
• Molecule 10: uS7



• Molecule 11: eS31

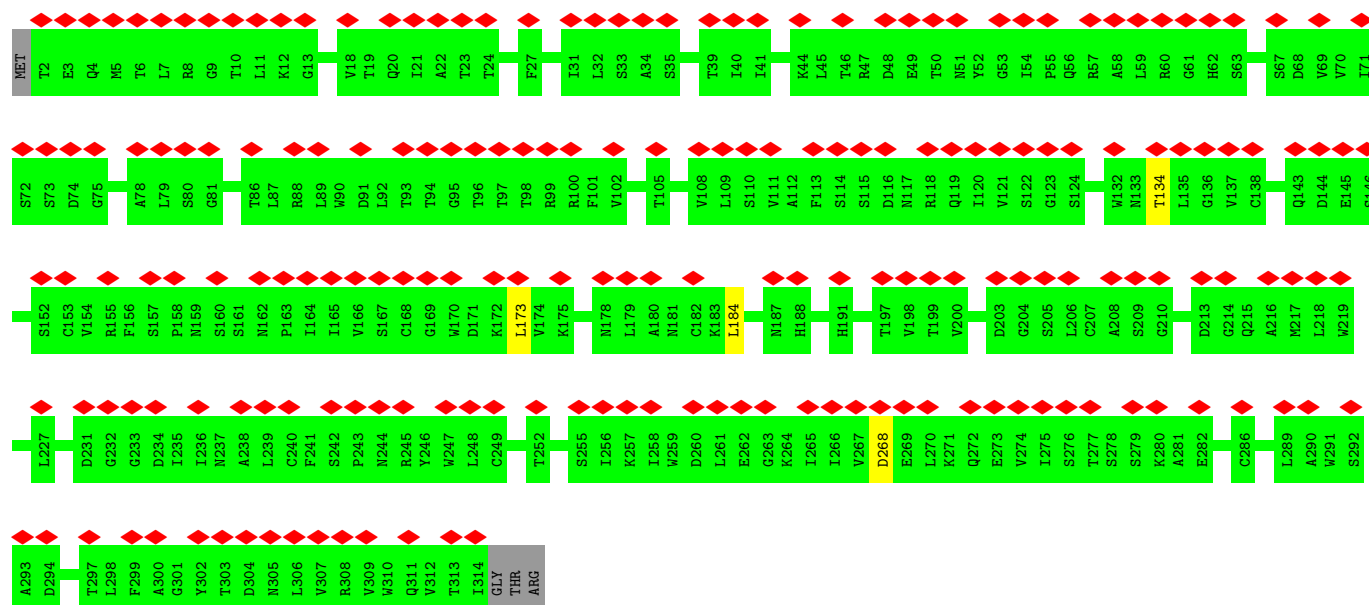


• Molecule 12: eS6



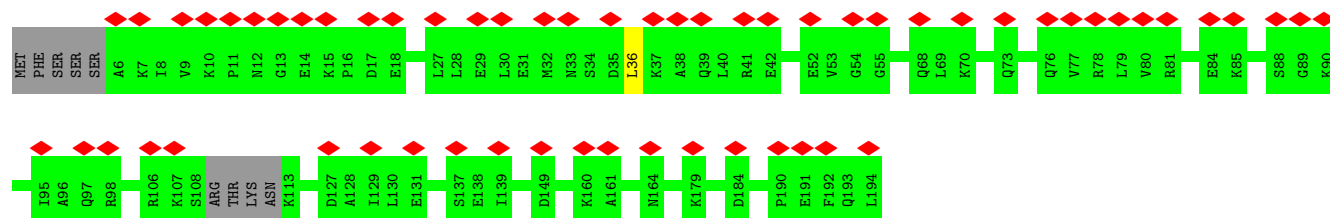
• Molecule 13: RACK1





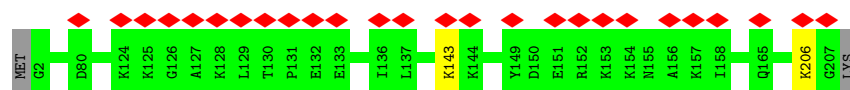
- Molecule 14: eS7

Chain I: 30% 95% 5%



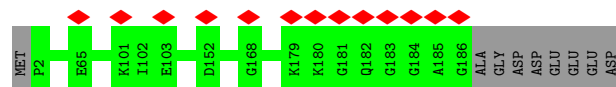
- Molecule 15: eS8

Chain J: 12% 98% 5%



- Molecule 16: uS4

Chain K: 7% 95% 5%

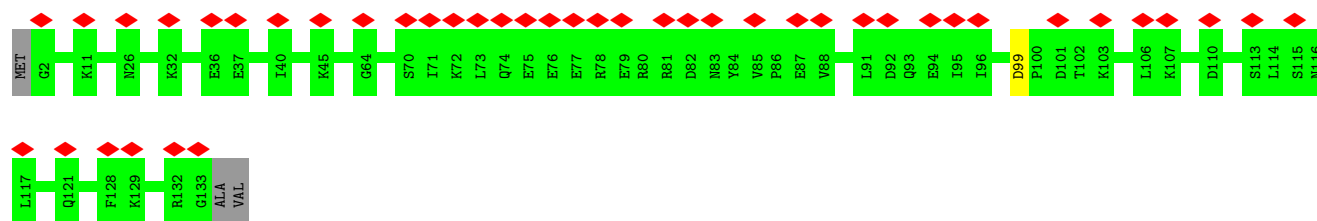


- Molecule 17: S10\_pectin domain-containing protein

Chain L: 29% 58% 42%

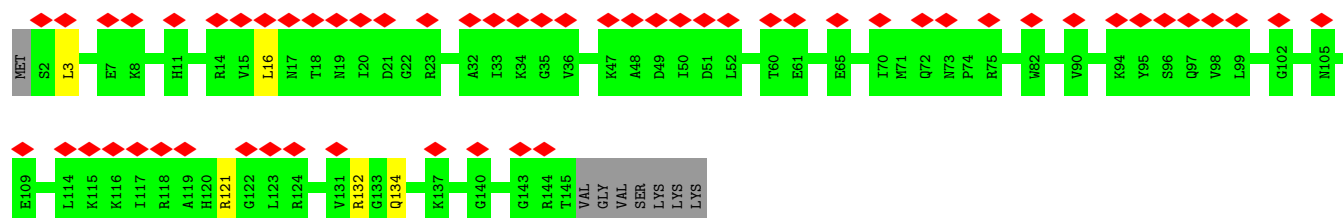






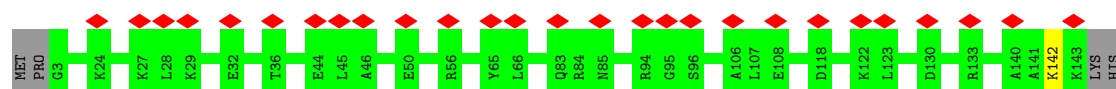
• Molecule 22: uS13

Chain T: 38% 91% 5%



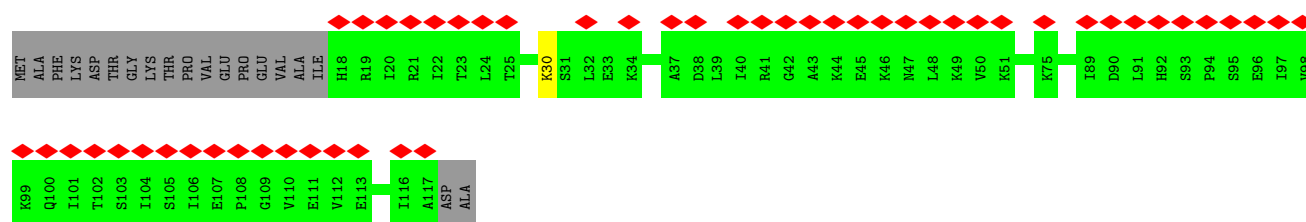
• Molecule 23: Uncharacterized protein

Chain U: 19% 97% 2%



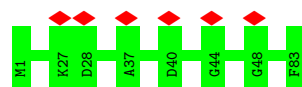
• Molecule 24: uS10

Chain V: 44% 83% 16%



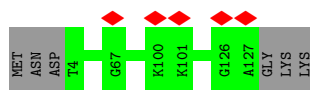
• Molecule 25: 40S ribosomal protein S21

Chain W: 7% 100% 0%

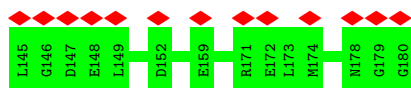


• Molecule 26: 40S ribosomal protein S24

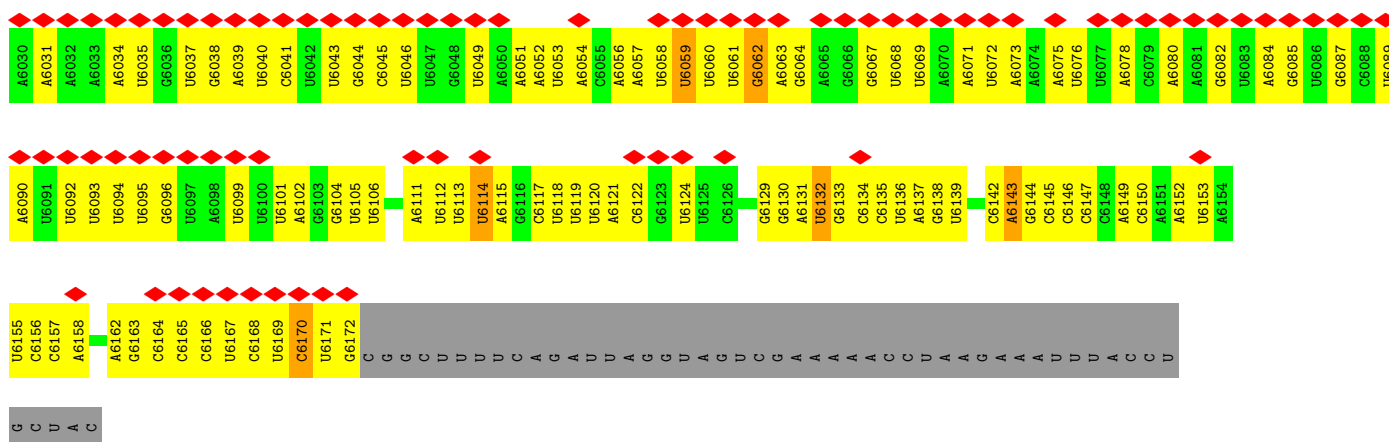
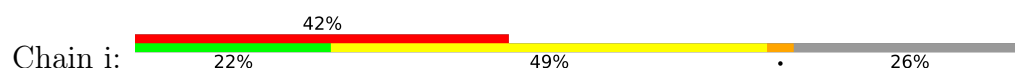
Chain Z: 95% 5% 0%



- Molecule 27: Host translation inhibitor nsp1



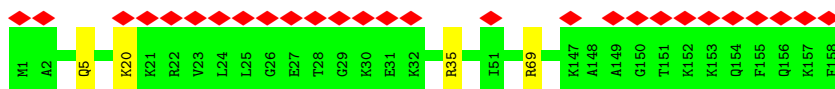
- Molecule 28: Cricket paralysis virus IRES RNA



- Molecule 29: 40S ribosomal protein S4



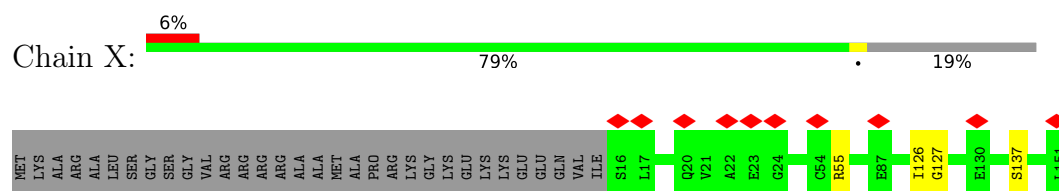
- Molecule 30: uS17



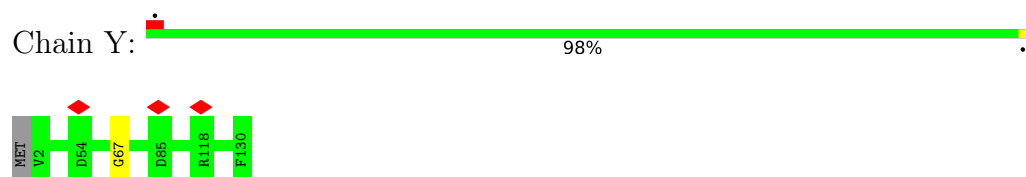
- Molecule 31: uS15



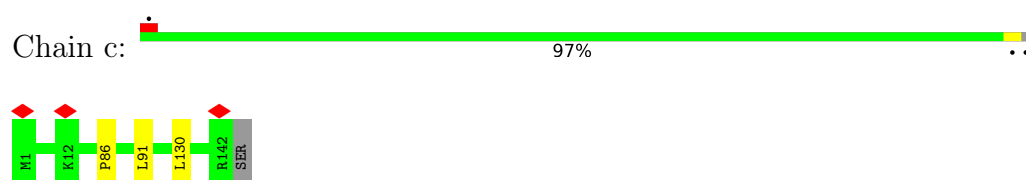
- Molecule 32: Uncharacterized protein



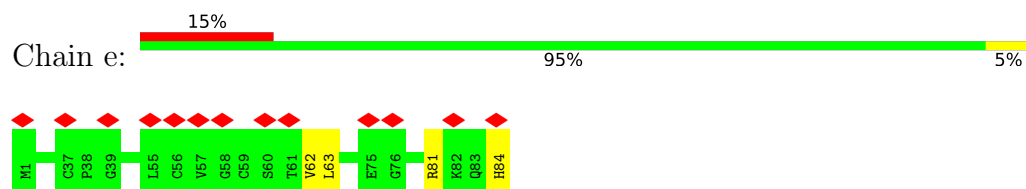
- Molecule 33: uS8



- Molecule 34: Uncharacterized protein



- Molecule 35: eS27



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48689	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.462	Depositor
Minimum map value	-0.196	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	341.75998, 341.75998, 341.75998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.068, 1.068, 1.068	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.63	0/40509	1.06	181/63128 (0.3%)
2	a	0.30	0/604	0.54	0/810
3	B	0.34	0/1747	0.53	1/2374 (0.0%)
4	b	0.38	0/828	0.49	0/1109
5	C	0.35	0/1756	0.54	0/2350
6	D	0.39	0/1753	0.51	0/2369
7	d	0.35	0/490	0.63	0/656
8	E	0.33	0/1796	0.56	1/2417 (0.0%)
9	f	0.33	0/462	0.54	0/607
10	G	0.32	0/1482	0.62	0/1992
11	g	0.32	0/567	0.55	0/753
12	H	0.30	0/1946	0.51	0/2590
13	h	0.30	0/2493	0.63	2/3394 (0.1%)
14	I	0.32	0/1510	0.58	1/2022 (0.0%)
15	J	0.36	0/1715	0.55	0/2287
16	K	0.35	0/1550	0.50	0/2069
17	L	0.30	0/834	0.50	0/1125
18	N	0.30	0/918	0.69	1/1233 (0.1%)
19	Q	0.30	0/904	0.64	0/1205
20	R	0.33	0/1146	0.62	0/1534
21	S	0.32	0/1082	0.52	0/1452
22	T	0.30	0/1208	0.65	1/1618 (0.1%)
23	U	0.32	0/1115	0.54	0/1493
24	V	0.29	0/805	0.55	0/1081
25	W	0.34	0/643	0.50	0/860
26	Z	0.34	0/1028	0.50	0/1366
27	F	0.29	0/285	0.49	0/384
28	i	0.41	0/3380	1.11	19/5259 (0.4%)
29	M	0.39	0/2125	0.61	0/2856
30	O	0.42	0/1319	0.65	0/1761
31	P	0.35	0/1232	0.56	1/1656 (0.1%)
32	X	0.36	0/1029	0.64	0/1380
33	Y	0.43	0/1051	0.58	0/1406
34	c	0.39	0/1124	0.62	1/1500 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	e	0.35	0/673	0.62	1/902 (0.1%)
All	All	0.50	0/83109	0.88	210/120998 (0.2%)

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
3	B	0	1
10	G	0	5
18	N	0	1
19	Q	0	1
20	R	0	2
22	T	0	1
31	P	0	1
32	X	0	4
34	c	0	1
35	e	0	1
All	All	0	18

There are no bond length outliers.

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	i	6118	U	C2-N1-C1'	11.36	131.33	117.70
1	A	1453	C	N1-C2-O2	11.07	125.54	118.90
1	A	356	C	N1-C2-O2	11.04	125.52	118.90
1	A	1453	C	C2-N1-C1'	10.74	130.62	118.80
1	A	1518	C	N1-C2-O2	10.57	125.25	118.90
28	i	6118	U	N1-C2-O2	10.20	129.94	122.80
1	A	1518	C	C6-N1-C2	-10.15	116.24	120.30
1	A	1518	C	N3-C2-O2	-9.96	114.93	121.90
1	A	356	C	C2-N1-C1'	9.72	129.49	118.80
1	A	1518	C	C2-N1-C1'	9.39	129.12	118.80
1	A	356	C	N3-C2-O2	-9.31	115.38	121.90
1	A	293	C	N1-C2-O2	9.30	124.48	118.90
1	A	1520	G	C4-N9-C1'	9.25	138.53	126.50
1	A	853	C	N1-C2-O2	9.05	124.33	118.90
1	A	853	C	C2-N1-C1'	9.04	128.74	118.80
28	i	6118	U	N3-C2-O2	-8.67	116.13	122.20
1	A	660	C	N1-C2-O2	8.53	124.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1453	C	N3-C2-O2	-8.39	116.03	121.90
1	A	853	C	N3-C2-O2	-8.29	116.09	121.90
1	A	1227	G	C4-N9-C1'	8.27	137.25	126.50
28	i	6118	U	C6-N1-C1'	-8.26	109.63	121.20
1	A	427	U	C2-N1-C1'	7.93	127.22	117.70
1	A	1453	C	C6-N1-C1'	-7.93	111.29	120.80
28	i	6062	G	C4-N9-C1'	7.88	136.75	126.50
1	A	1238	U	C6-N1-C2	-7.82	116.31	121.00
1	A	1520	G	C8-N9-C1'	-7.68	117.01	127.00
28	i	6143	A	P-O3'-C3'	7.60	128.82	119.70
1	A	1551	U	C2-N1-C1'	7.44	126.63	117.70
1	A	1608	U	C5-C6-N1	7.43	126.42	122.70
1	A	1636	G	C4-N9-C1'	7.42	136.14	126.50
1	A	293	C	N3-C2-O2	-7.38	116.73	121.90
1	A	293	C	C2-N1-C1'	7.33	126.87	118.80
28	i	6062	G	N3-C4-C5	-7.33	124.94	128.60
1	A	1636	G	N3-C4-C5	-7.29	124.95	128.60
1	A	630	U	C2-N1-C1'	7.21	126.35	117.70
1	A	1636	G	N3-C4-N9	7.20	130.32	126.00
28	i	6062	G	N3-C4-N9	7.10	130.26	126.00
1	A	752	G	P-O3'-C3'	7.09	128.20	119.70
1	A	627	U	P-O3'-C3'	7.05	128.16	119.70
1	A	1609	C	C5-C6-N1	7.04	124.52	121.00
1	A	1519	U	O4'-C1'-N1	7.03	113.82	108.20
1	A	1587	G	N3-C4-N9	6.96	130.18	126.00
1	A	1551	U	N3-C2-O2	-6.96	117.33	122.20
1	A	1139	C	C2-N1-C1'	6.87	126.36	118.80
1	A	1227	G	N3-C4-C5	-6.83	125.19	128.60
1	A	1227	G	C8-N9-C1'	-6.81	118.15	127.00
1	A	1629	C	N1-C2-O2	6.79	122.97	118.90
1	A	356	C	C6-N1-C1'	-6.78	112.67	120.80
8	E	176	LEU	CA-CB-CG	6.76	130.86	115.30
1	A	630	U	N1-C2-O2	6.74	127.52	122.80
1	A	1587	G	C4-N9-C1'	6.72	135.24	126.50
1	A	553	U	P-O3'-C3'	6.72	127.76	119.70
1	A	1227	G	N3-C4-N9	6.71	130.03	126.00
1	A	427	U	N1-C2-O2	6.70	127.49	122.80
1	A	1303	C	C2-N1-C1'	6.70	126.16	118.80
1	A	1518	C	C5-C6-N1	6.69	124.35	121.00
1	A	427	U	N3-C2-O2	-6.67	117.53	122.20
1	A	1551	U	N1-C2-O2	6.62	127.44	122.80
1	A	183	G	C4-N9-C1'	6.62	135.10	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1597	C	C6-N1-C2	-6.55	117.68	120.30
1	A	407	G	N3-C4-N9	6.52	129.91	126.00
1	A	1057	C	C2-N1-C1'	6.52	125.97	118.80
28	i	6062	G	C8-N9-C1'	-6.50	118.55	127.00
1	A	1242	U	N3-C2-O2	-6.46	117.68	122.20
1	A	407	G	C4-N9-C1'	6.44	134.88	126.50
1	A	1660	C	C2-N1-C1'	6.44	125.89	118.80
1	A	1863	A	O4'-C1'-N9	6.43	113.34	108.20
28	i	6134	C	C5-C6-N1	6.42	124.21	121.00
1	A	1364	U	N3-C2-O2	-6.40	117.72	122.20
3	B	44	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	1660	C	N1-C2-O2	6.34	122.71	118.90
1	A	606	G	C4-N9-C1'	6.34	134.74	126.50
1	A	1660	C	N3-C2-O2	-6.33	117.47	121.90
1	A	659	G	C4-N9-C1'	6.32	134.72	126.50
31	P	11	LEU	CA-CB-CG	6.32	129.83	115.30
1	A	1598	G	N3-C4-C5	-6.29	125.45	128.60
1	A	1272	C	C6-N1-C2	-6.29	117.78	120.30
1	A	1364	U	N1-C2-O2	6.25	127.17	122.80
1	A	183	G	N3-C4-C5	-6.24	125.48	128.60
1	A	630	U	N3-C2-O2	-6.23	117.84	122.20
1	A	356	C	C6-N1-C2	-6.23	117.81	120.30
1	A	1645	C	P-O3'-C3'	6.23	127.17	119.70
1	A	1303	C	N1-C2-O2	6.22	122.64	118.90
1	A	803	C	N1-C2-O2	6.22	122.63	118.90
1	A	823	U	C2-N1-C1'	6.21	125.15	117.70
1	A	853	C	C6-N1-C2	-6.19	117.82	120.30
1	A	606	G	N3-C4-N9	6.19	129.72	126.00
1	A	183	G	N3-C4-N9	6.18	129.71	126.00
1	A	1139	C	N1-C2-O2	6.17	122.60	118.90
1	A	853	C	C6-N1-C1'	-6.16	113.40	120.80
1	A	1364	U	C2-N1-C1'	6.15	125.08	117.70
1	A	1232	U	C5-C6-N1	6.12	125.76	122.70
1	A	73	C	N1-C2-O2	6.10	122.56	118.90
1	A	1362	U	N3-C2-O2	-6.08	117.94	122.20
1	A	1587	G	C8-N9-C1'	-6.08	119.09	127.00
1	A	1636	G	C8-N9-C1'	-6.07	119.11	127.00
1	A	1118	C	C2-N1-C1'	6.06	125.47	118.80
22	T	3	LEU	CA-CB-CG	6.05	129.21	115.30
1	A	1631	U	C6-N1-C2	-6.03	117.38	121.00
28	i	6134	C	C6-N1-C2	-6.03	117.89	120.30
1	A	606	G	N3-C4-C5	-5.99	125.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	h	173	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	1078	C	N3-C2-O2	-5.96	117.73	121.90
1	A	1520	G	N3-C4-C5	-5.96	125.62	128.60
1	A	407	G	N3-C4-C5	-5.93	125.63	128.60
1	A	1608	U	C6-N1-C2	-5.93	117.44	121.00
1	A	1536	G	N3-C4-N9	5.89	129.53	126.00
1	A	1157	G	N3-C4-C5	-5.88	125.66	128.60
1	A	1587	G	N3-C4-C5	-5.86	125.67	128.60
1	A	1598	G	C4-N9-C1'	5.86	134.12	126.50
1	A	1272	C	O4'-C1'-N1	5.86	112.88	108.20
1	A	803	C	N3-C2-O2	-5.83	117.82	121.90
1	A	1078	C	N1-C2-O2	5.83	122.40	118.90
1	A	501	C	N1-C2-O2	5.83	122.40	118.90
1	A	368	U	P-O3'-C3'	5.83	126.69	119.70
1	A	1231	C	P-O3'-C3'	5.82	126.68	119.70
1	A	1238	U	C5-C6-N1	5.81	125.61	122.70
1	A	1609	C	C6-N1-C2	-5.79	117.98	120.30
1	A	1475	G	N3-C2-N2	-5.79	115.85	119.90
1	A	627	U	OP2-P-O3'	5.78	117.91	105.20
1	A	1676	U	C5-C6-N1	5.76	125.58	122.70
1	A	823	U	N3-C2-O2	-5.75	118.17	122.20
28	i	6134	C	N1-C2-O2	5.74	122.34	118.90
1	A	915	G	O4'-C1'-N9	5.73	112.79	108.20
1	A	1636	G	C2-N3-C4	5.72	114.76	111.90
1	A	660	C	N3-C2-O2	-5.71	117.90	121.90
1	A	1139	C	N3-C2-O2	-5.71	117.90	121.90
1	A	501	C	C5-C6-N1	5.71	123.85	121.00
1	A	1629	C	C6-N1-C2	-5.69	118.02	120.30
1	A	49	C	N1-C2-O2	5.69	122.31	118.90
1	A	1509	U	C2-N1-C1'	5.67	124.50	117.70
1	A	548	C	C6-N1-C2	-5.65	118.04	120.30
1	A	1609	C	N1-C2-O2	5.64	122.28	118.90
1	A	494	C	N1-C2-O2	5.63	122.28	118.90
1	A	1157	G	N3-C4-N9	5.63	129.38	126.00
1	A	874	G	P-O3'-C3'	5.60	126.42	119.70
1	A	659	G	C8-N9-C1'	-5.60	119.72	127.00
1	A	870	A	P-O3'-C3'	5.59	126.41	119.70
1	A	494	C	C6-N1-C2	-5.58	118.07	120.30
28	i	6132	U	C2-N1-C1'	5.57	124.38	117.70
1	A	1536	G	N3-C4-C5	-5.56	125.82	128.60
1	A	687	C	N1-C2-O2	5.56	122.23	118.90
1	A	1057	C	N1-C2-O2	5.55	122.23	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	i	6062	G	C2-N3-C4	5.55	114.67	111.90
1	A	183	G	C8-N9-C1'	-5.54	119.80	127.00
1	A	532	C	P-O3'-C3'	5.54	126.34	119.70
1	A	35	C	C6-N1-C2	-5.53	118.09	120.30
1	A	1453	C	C6-N1-C2	-5.53	118.09	120.30
1	A	1268	C	N1-C2-O2	5.51	122.20	118.90
1	A	1362	U	N1-C2-O2	5.51	126.66	122.80
1	A	1266	C	N1-C2-O2	5.49	122.19	118.90
1	A	407	G	C8-N9-C1'	-5.49	119.87	127.00
1	A	1784	G	O5'-P-OP1	-5.49	100.76	105.70
1	A	1865	C	N3-C2-O2	-5.47	118.07	121.90
1	A	427	U	C6-N1-C1'	-5.44	113.58	121.20
28	i	6114	U	C5-C6-N1	5.43	125.42	122.70
1	A	1268	C	N3-C2-O2	-5.41	118.11	121.90
1	A	465	A	P-O3'-C3'	5.41	126.19	119.70
14	I	36	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	110	U	P-O3'-C3'	5.38	126.15	119.70
1	A	1242	U	N1-C2-O2	5.38	126.56	122.80
1	A	402	C	C6-N1-C2	-5.36	118.16	120.30
1	A	539	C	N1-C2-O2	5.34	122.11	118.90
35	e	63	LEU	CA-CB-CG	5.34	127.59	115.30
28	i	6118	U	C5-C6-N1	5.34	125.37	122.70
1	A	293	C	C6-N1-C1'	-5.33	114.41	120.80
1	A	823	U	N1-C2-O2	5.31	126.52	122.80
1	A	1509	U	N1-C2-O2	5.29	126.50	122.80
1	A	1865	C	N1-C2-O2	5.29	122.07	118.90
1	A	1240	A	C4-N9-C1'	5.29	135.82	126.30
13	h	184	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	1057	C	N3-C2-O2	-5.28	118.21	121.90
1	A	1509	U	N3-C2-O2	-5.28	118.51	122.20
1	A	1631	U	C5-C6-N1	5.27	125.34	122.70
1	A	37	C	N1-C2-O2	5.27	122.06	118.90
1	A	402	C	C5-C6-N1	5.25	123.62	121.00
1	A	606	G	C8-N9-C1'	-5.24	120.18	127.00
1	A	427	U	O4'-C1'-N1	5.24	112.39	108.20
18	N	85	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	1139	C	C6-N1-C1'	-5.23	114.52	120.80
1	A	1755	C	C6-N1-C2	-5.23	118.21	120.30
1	A	659	G	N3-C4-N9	5.23	129.14	126.00
1	A	1520	G	N3-C4-N9	5.23	129.14	126.00
1	A	1865	C	C2-N1-C1'	5.21	124.53	118.80
1	A	142	C	N1-C2-O2	5.20	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	C	N3-C2-O2	-5.20	118.26	121.90
1	A	1520	G	N7-C8-N9	5.19	115.70	113.10
1	A	37	C	N3-C2-O2	-5.17	118.28	121.90
28	i	6059	U	C5-C6-N1	5.16	125.28	122.70
1	A	1629	C	N3-C2-O2	-5.16	118.29	121.90
1	A	188	C	N1-C2-O2	5.16	122.00	118.90
1	A	178	C	N1-C2-O2	5.15	121.99	118.90
1	A	1518	C	C6-N1-C1'	-5.14	114.63	120.80
28	i	6044	G	C4-N9-C1'	5.13	133.18	126.50
1	A	579	C	N1-C2-O2	5.13	121.98	118.90
34	c	91	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	1785	C	N1-C2-O2	5.12	121.97	118.90
1	A	879	C	C6-N1-C2	-5.12	118.25	120.30
1	A	1453	C	C5-C6-N1	5.11	123.55	121.00
1	A	1834	A	N7-C8-N9	5.11	116.35	113.80
1	A	494	C	C2-N1-C1'	5.08	124.39	118.80
1	A	1263	U	O4'-C1'-N1	5.07	112.25	108.20
1	A	1865	C	C6-N1-C2	-5.06	118.28	120.30
1	A	73	C	N3-C2-O2	-5.06	118.36	121.90
1	A	1738	C	C6-N1-C2	-5.04	118.28	120.30
28	i	6170	C	C6-N1-C2	-5.04	118.28	120.30
1	A	1520	G	C8-N9-C4	-5.04	104.39	106.40
1	A	368	U	OP2-P-O3'	5.03	116.27	105.20
1	A	30	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1237	C	N1-C2-O2	5.01	121.91	118.90

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	43	SER	Peptide
10	G	108	PRO	Peptide
10	G	117	ILE	Peptide
10	G	121	PRO	Peptide
10	G	135	ARG	Peptide
10	G	142	SER	Peptide
18	N	76	LEU	Peptide
31	P	22	VAL	Peptide
19	Q	85	ILE	Peptide
20	R	101	ASP	Peptide
20	R	99	TYR	Peptide
22	T	134	GLN	Peptide

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Mol	Chain	Res	Type	Group
32	X	126	ILE	Peptide
32	X	127	GLY	Peptide
32	X	137	SER	Peptide
32	X	55	ARG	Peptide
34	c	86	PRO	Peptide
35	e	62	VAL	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	
2	a	73/125 (58%)	66 (90%)	7 (10%)	0	100	100
3	B	215/295 (73%)	207 (96%)	8 (4%)	0	100	100
4	b	99/115 (86%)	94 (95%)	5 (5%)	0	100	100
5	C	211/264 (80%)	198 (94%)	13 (6%)	0	100	100
6	D	219/293 (75%)	215 (98%)	4 (2%)	0	100	100
7	d	60/69 (87%)	56 (93%)	4 (7%)	0	100	100
8	E	226/243 (93%)	216 (96%)	10 (4%)	0	100	100
9	f	55/133 (41%)	51 (93%)	4 (7%)	0	100	100
10	G	181/204 (89%)	154 (85%)	24 (13%)	3 (2%)	9	35
11	g	66/156 (42%)	58 (88%)	8 (12%)	0	100	100
12	H	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
13	h	311/317 (98%)	275 (88%)	36 (12%)	0	100	100
14	I	181/194 (93%)	175 (97%)	6 (3%)	0	100	100
15	J	204/208 (98%)	189 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	K	183/194 (94%)	177 (97%)	6 (3%)	0	100	100
17	L	94/165 (57%)	87 (93%)	7 (7%)	0	100	100
18	N	115/132 (87%)	107 (93%)	7 (6%)	1 (1%)	17	48
19	Q	105/145 (72%)	88 (84%)	17 (16%)	0	100	100
20	R	140/146 (96%)	122 (87%)	18 (13%)	0	100	100
21	S	130/135 (96%)	120 (92%)	10 (8%)	0	100	100
22	T	142/152 (93%)	119 (84%)	23 (16%)	0	100	100
23	U	139/145 (96%)	130 (94%)	9 (6%)	0	100	100
24	V	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
25	W	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
26	Z	122/130 (94%)	119 (98%)	3 (2%)	0	100	100
27	F	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
29	M	261/263 (99%)	230 (88%)	31 (12%)	0	100	100
30	O	156/158 (99%)	136 (87%)	19 (12%)	1 (1%)	25	57
31	P	148/151 (98%)	138 (93%)	9 (6%)	1 (1%)	22	54
32	X	134/168 (80%)	112 (84%)	22 (16%)	0	100	100
33	Y	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	19	51
34	c	140/143 (98%)	130 (93%)	9 (6%)	1 (1%)	22	54
35	e	82/84 (98%)	73 (89%)	9 (11%)	0	100	100
All	All	4767/5544 (86%)	4399 (92%)	360 (8%)	8 (0%)	50	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	G	123	GLU
31	P	23	PRO
18	N	55	ASN
10	G	122	ARG
34	c	130	LEU
10	G	108	PRO
30	O	5	GLN
33	Y	67	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	a	66/103 (64%)	66 (100%)	0	100	100
3	B	180/245 (74%)	180 (100%)	0	100	100
4	b	88/98 (90%)	86 (98%)	2 (2%)	50	73
5	C	194/231 (84%)	194 (100%)	0	100	100
6	D	187/225 (83%)	185 (99%)	2 (1%)	73	85
7	d	55/62 (89%)	52 (94%)	3 (6%)	21	52
8	E	190/202 (94%)	188 (99%)	2 (1%)	73	85
9	f	47/106 (44%)	47 (100%)	0	100	100
10	G	155/170 (91%)	154 (99%)	1 (1%)	86	91
11	g	61/140 (44%)	60 (98%)	1 (2%)	62	79
12	H	207/218 (95%)	205 (99%)	2 (1%)	76	86
13	h	272/275 (99%)	270 (99%)	2 (1%)	84	90
14	I	165/174 (95%)	165 (100%)	0	100	100
15	J	178/180 (99%)	176 (99%)	2 (1%)	73	85
16	K	161/168 (96%)	161 (100%)	0	100	100
17	L	87/136 (64%)	87 (100%)	0	100	100
18	N	99/108 (92%)	96 (97%)	3 (3%)	41	68
19	Q	97/130 (75%)	97 (100%)	0	100	100
20	R	117/121 (97%)	117 (100%)	0	100	100
21	S	119/121 (98%)	118 (99%)	1 (1%)	81	89
22	T	125/132 (95%)	122 (98%)	3 (2%)	49	73
23	U	111/115 (96%)	110 (99%)	1 (1%)	78	87
24	V	92/107 (86%)	91 (99%)	1 (1%)	73	85
25	W	67/67 (100%)	67 (100%)	0	100	100
26	Z	107/112 (96%)	107 (100%)	0	100	100
27	F	29/31 (94%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	M	225/225 (100%)	223 (99%)	2 (1%)	78	87
30	O	142/142 (100%)	139 (98%)	3 (2%)	53	75
31	P	130/131 (99%)	129 (99%)	1 (1%)	81	89
32	X	106/130 (82%)	106 (100%)	0	100	100
33	Y	112/113 (99%)	112 (100%)	0	100	100
34	c	114/115 (99%)	114 (100%)	0	100	100
35	e	76/76 (100%)	74 (97%)	2 (3%)	46	71
All	All	4161/4709 (88%)	4127 (99%)	34 (1%)	82	89

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	b	15	ARG
4	b	46	GLU
6	D	167	ARG
6	D	209	VAL
7	d	13	ARG
7	d	66	ARG
7	d	67	ARG
8	E	18	LYS
8	E	76	ARG
10	G	139	VAL
11	g	138	ARG
12	H	98	ARG
12	H	221	LYS
13	h	134	THR
13	h	268	ASP
15	J	143	LYS
15	J	206	LYS
18	N	40	LYS
18	N	63	LYS
18	N	101	ARG
21	S	99	ASP
22	T	16	LEU
22	T	121	ARG
22	T	132	ARG
23	U	142	LYS
24	V	30	LYS
29	M	67	GLN
29	M	166	THR

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Mol	Chain	Res	Type
30	O	20	LYS
30	O	35	ARG
30	O	69	ARG
31	P	67	THR
35	e	81	ARG
35	e	84	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	45	ASN
2	a	106	GLN
3	B	70	ASN
3	B	215	GLN
4	b	17	HIS
5	C	101	HIS
5	C	158	HIS
6	D	113	GLN
6	D	134	ASN
7	d	29	GLN
7	d	45	ASN
9	f	110	GLN
10	G	74	ASN
10	G	137	GLN
10	G	148	ASN
12	H	146	ASN
13	h	76	GLN
13	h	104	HIS
16	K	111	GLN
19	Q	32	GLN
19	Q	54	HIS
19	Q	104	GLN
20	R	29	ASN
20	R	86	GLN
21	S	26	ASN
21	S	48	ASN
22	T	42	HIS
22	T	101	ASN
24	V	28	ASN
25	W	35	ASN
27	F	178	ASN
29	M	36	HIS

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Mol	Chain	Res	Type
29	M	50	ASN
29	M	142	HIS
30	O	5	GLN
30	O	154	GLN
31	P	5	HIS
31	P	90	HIS
31	P	123	HIS
32	X	43	HIS
34	c	61	GLN
35	e	26	GLN
35	e	51	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1685/1869 (90%)	473 (28%)	16 (0%)
28	i	142/192 (73%)	98 (69%)	0
All	All	1827/2061 (88%)	571 (31%)	16 (0%)

All (571) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	C
1	A	4	C
1	A	17	C
1	A	25	A
1	A	33	G
1	A	41	G
1	A	46	A
1	A	55	U
1	A	56	G
1	A	58	C
1	A	62	G
1	A	65	C
1	A	67	C
1	A	68	A
1	A	71	G
1	A	73	C
1	A	74	G
1	A	76	U

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Mol	Chain	Res	Type
1	A	77	A
1	A	79	A
1	A	92	A
1	A	99	A
1	A	103	A
1	A	110	U
1	A	111	A
1	A	113	G
1	A	115	U
1	A	126	G
1	A	130	G
1	A	142	C
1	A	143	U
1	A	146	G
1	A	147	A
1	A	156	G
1	A	157	U
1	A	162	C
1	A	163	U
1	A	170	A
1	A	171	A
1	A	172	U
1	A	175	A
1	A	183	G
1	A	184	G
1	A	188	C
1	A	190	G
1	A	192	C
1	A	206	G
1	A	208	G
1	A	209	A
1	A	304	C
1	A	305	U
1	A	306	C
1	A	307	G
1	A	308	G
1	A	309	G
1	A	312	G
1	A	319	C
1	A	320	G
1	A	347	G
1	A	351	G

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Mol	Chain	Res	Type
1	A	362	C
1	A	364	A
1	A	368	U
1	A	369	C
1	A	370	G
1	A	381	C
1	A	382	C
1	A	385	G
1	A	386	C
1	A	398	A
1	A	400	C
1	A	407	G
1	A	408	A
1	A	409	C
1	A	417	C
1	A	418	A
1	A	426	A
1	A	438	G
1	A	441	C
1	A	447	A
1	A	448	A
1	A	450	C
1	A	465	A
1	A	466	G
1	A	467	G
1	A	471	G
1	A	472	C
1	A	473	A
1	A	474	G
1	A	482	G
1	A	487	U
1	A	492	C
1	A	501	C
1	A	502	C
1	A	508	A
1	A	509	G
1	A	516	A
1	A	531	A
1	A	532	C
1	A	533	A
1	A	534	G
1	A	536	A

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Mol	Chain	Res	Type
1	A	537	C
1	A	538	U
1	A	541	U
1	A	542	U
1	A	544	G
1	A	547	G
1	A	548	C
1	A	549	C
1	A	551	U
1	A	554	A
1	A	556	U
1	A	559	G
1	A	560	A
1	A	561	A
1	A	562	U
1	A	568	C
1	A	576	A
1	A	583	A
1	A	585	C
1	A	587	A
1	A	588	G
1	A	589	G
1	A	590	A
1	A	591	U
1	A	592	C
1	A	593	C
1	A	603	C
1	A	604	A
1	A	605	A
1	A	606	G
1	A	607	U
1	A	614	C
1	A	615	C
1	A	617	G
1	A	626	G
1	A	627	U
1	A	628	A
1	A	631	U
1	A	634	A
1	A	635	G
1	A	643	A
1	A	644	G

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Mol	Chain	Res	Type
1	A	655	A
1	A	659	G
1	A	660	C
1	A	662	G
1	A	664	A
1	A	668	A
1	A	669	A
1	A	671	A
1	A	672	A
1	A	673	G
1	A	684	G
1	A	688	U
1	A	691	G
1	A	693	A
1	A	696	G
1	A	730	C
1	A	731	G
1	A	752	G
1	A	753	C
1	A	754	G
1	A	755	C
1	A	796	G
1	A	797	C
1	A	798	G
1	A	799	U
1	A	801	U
1	A	810	A
1	A	811	A
1	A	821	G
1	A	822	U
1	A	823	U
1	A	830	A
1	A	845	G
1	A	847	A
1	A	852	G
1	A	853	C
1	A	859	G
1	A	870	A
1	A	871	U
1	A	872	A
1	A	873	G
1	A	874	G

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Mol	Chain	Res	Type
1	A	875	A
1	A	879	C
1	A	887	U
1	A	888	U
1	A	889	U
1	A	891	G
1	A	892	U
1	A	895	G
1	A	896	U
1	A	898	U
1	A	909	G
1	A	913	A
1	A	914	U
1	A	920	A
1	A	933	G
1	A	943	U
1	A	954	U
1	A	959	G
1	A	971	G
1	A	978	G
1	A	985	G
1	A	990	A
1	A	992	A
1	A	999	G
1	A	1002	U
1	A	1008	A
1	A	1017	U
1	A	1023	A
1	A	1050	A
1	A	1055	A
1	A	1060	A
1	A	1061	U
1	A	1062	A
1	A	1080	A
1	A	1081	U
1	A	1083	A
1	A	1085	C
1	A	1115	U
1	A	1116	C
1	A	1117	C
1	A	1118	C
1	A	1121	G

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Mol	Chain	Res	Type
1	A	1123	C
1	A	1133	A
1	A	1138	C
1	A	1139	C
1	A	1140	G
1	A	1143	A
1	A	1149	A
1	A	1150	A
1	A	1153	C
1	A	1154	U
1	A	1166	G
1	A	1195	A
1	A	1203	G
1	A	1207	G
1	A	1208	A
1	A	1212	G
1	A	1215	C
1	A	1217	A
1	A	1219	C
1	A	1220	A
1	A	1221	G
1	A	1224	G
1	A	1225	U
1	A	1228	A
1	A	1229	G
1	A	1231	C
1	A	1232	U
1	A	1236	G
1	A	1237	C
1	A	1238	U
1	A	1239	U
1	A	1241	A
1	A	1242	U
1	A	1243	U
1	A	1244	U
1	A	1245	G
1	A	1246	A
1	A	1248	U
1	A	1250	A
1	A	1251	A
1	A	1253	A
1	A	1256	G

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Mol	Chain	Res	Type
1	A	1257	G
1	A	1258	A
1	A	1259	A
1	A	1263	U
1	A	1264	C
1	A	1265	A
1	A	1266	C
1	A	1269	G
1	A	1271	C
1	A	1272	C
1	A	1274	G
1	A	1275	G
1	A	1282	A
1	A	1284	A
1	A	1285	G
1	A	1286	G
1	A	1287	A
1	A	1289	U
1	A	1293	A
1	A	1294	G
1	A	1295	A
1	A	1296	U
1	A	1298	G
1	A	1299	A
1	A	1300	U
1	A	1301	A
1	A	1302	G
1	A	1303	C
1	A	1304	U
1	A	1306	U
1	A	1308	U
1	A	1309	C
1	A	1311	C
1	A	1312	G
1	A	1313	A
1	A	1314	U
1	A	1315	U
1	A	1318	G
1	A	1320	G
1	A	1321	G
1	A	1322	G
1	A	1323	U

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Mol	Chain	Res	Type
1	A	1330	G
1	A	1342	U
1	A	1343	U
1	A	1354	G
1	A	1371	U
1	A	1372	U
1	A	1375	G
1	A	1378	A
1	A	1382	A
1	A	1393	G
1	A	1396	A
1	A	1397	U
1	A	1401	A
1	A	1402	A
1	A	1404	U
1	A	1408	U
1	A	1409	A
1	A	1424	G
1	A	1427	C
1	A	1428	G
1	A	1429	G
1	A	1431	G
1	A	1432	U
1	A	1442	U
1	A	1449	G
1	A	1452	A
1	A	1454	A
1	A	1463	U
1	A	1466	G
1	A	1473	G
1	A	1479	G
1	A	1480	A
1	A	1489	A
1	A	1490	G
1	A	1494	U
1	A	1497	G
1	A	1504	U
1	A	1505	U
1	A	1506	A
1	A	1507	G
1	A	1508	A
1	A	1510	G

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Mol	Chain	Res	Type
1	A	1511	U
1	A	1516	G
1	A	1517	G
1	A	1518	C
1	A	1519	U
1	A	1520	G
1	A	1521	C
1	A	1522	A
1	A	1523	C
1	A	1536	G
1	A	1537	A
1	A	1538	C
1	A	1539	U
1	A	1540	G
1	A	1541	G
1	A	1543	U
1	A	1546	G
1	A	1547	C
1	A	1548	G
1	A	1552	G
1	A	1553	C
1	A	1554	C
1	A	1556	A
1	A	1557	C
1	A	1560	U
1	A	1567	G
1	A	1570	G
1	A	1571	G
1	A	1580	A
1	A	1582	C
1	A	1584	G
1	A	1585	U
1	A	1587	G
1	A	1588	A
1	A	1590	C
1	A	1591	C
1	A	1592	C
1	A	1594	A
1	A	1597	C
1	A	1598	G
1	A	1599	U
1	A	1600	G

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Mol	Chain	Res	Type
1	A	1601	A
1	A	1602	U
1	A	1603	G
1	A	1604	G
1	A	1605	G
1	A	1607	A
1	A	1608	U
1	A	1617	G
1	A	1618	C
1	A	1619	A
1	A	1620	A
1	A	1621	U
1	A	1622	U
1	A	1623	A
1	A	1626	C
1	A	1627	C
1	A	1628	C
1	A	1630	A
1	A	1631	U
1	A	1632	G
1	A	1633	A
1	A	1634	A
1	A	1637	A
1	A	1646	C
1	A	1647	A
1	A	1648	G
1	A	1654	G
1	A	1664	A
1	A	1665	G
1	A	1671	G
1	A	1676	U
1	A	1677	U
1	A	1678	A
1	A	1679	A
1	A	1680	G
1	A	1695	A
1	A	1697	A
1	A	1698	C
1	A	1699	A
1	A	1715	A
1	A	1717	C
1	A	1721	U

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Mol	Chain	Res	Type
1	A	1722	G
1	A	1726	G
1	A	1744	G
1	A	1750	C
1	A	1753	C
1	A	1757	G
1	A	1775	U
1	A	1776	G
1	A	1783	C
1	A	1785	C
1	A	1801	A
1	A	1806	A
1	A	1816	G
1	A	1819	A
1	A	1823	A
1	A	1825	A
1	A	1826	G
1	A	1829	G
1	A	1835	A
1	A	1836	G
1	A	1838	U
1	A	1840	U
1	A	1845	A
1	A	1849	G
1	A	1851	A
1	A	1852	C
1	A	1859	A
1	A	1861	G
1	A	1862	G
1	A	1863	A
1	A	1864	U
1	A	1865	C
1	A	1867	U
1	A	1869	A
28	i	6031	A
28	i	6034	A
28	i	6035	U
28	i	6037	U
28	i	6038	G
28	i	6039	A
28	i	6040	U
28	i	6041	C

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Mol	Chain	Res	Type
28	i	6043	U
28	i	6045	C
28	i	6046	U
28	i	6049	U
28	i	6051	A
28	i	6052	A
28	i	6053	U
28	i	6054	A
28	i	6056	A
28	i	6057	A
28	i	6058	U
28	i	6059	U
28	i	6060	U
28	i	6061	U
28	i	6062	G
28	i	6063	A
28	i	6064	G
28	i	6067	G
28	i	6068	U
28	i	6069	U
28	i	6071	A
28	i	6072	U
28	i	6073	A
28	i	6075	A
28	i	6076	U
28	i	6078	A
28	i	6080	A
28	i	6082	G
28	i	6084	A
28	i	6085	G
28	i	6087	G
28	i	6089	U
28	i	6090	A
28	i	6092	U
28	i	6093	U
28	i	6094	U
28	i	6095	U
28	i	6096	G
28	i	6099	U
28	i	6101	U
28	i	6102	A
28	i	6104	G

*Continued on next page...*

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Mol	Chain	Res	Type
28	i	6105	U
28	i	6106	U
28	i	6111	A
28	i	6112	U
28	i	6113	U
28	i	6114	U
28	i	6115	A
28	i	6117	C
28	i	6119	U
28	i	6120	U
28	i	6121	A
28	i	6122	C
28	i	6124	U
28	i	6129	G
28	i	6130	G
28	i	6131	A
28	i	6132	U
28	i	6133	G
28	i	6135	C
28	i	6136	U
28	i	6137	A
28	i	6138	G
28	i	6139	U
28	i	6142	C
28	i	6143	A
28	i	6144	G
28	i	6145	C
28	i	6146	C
28	i	6147	C
28	i	6149	A
28	i	6150	C
28	i	6152	A
28	i	6153	U
28	i	6155	U
28	i	6156	C
28	i	6157	C
28	i	6158	A
28	i	6162	A
28	i	6163	G
28	i	6164	C
28	i	6165	C
28	i	6166	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
28	i	6167	U
28	i	6168	C
28	i	6169	U
28	i	6170	C
28	i	6171	U
28	i	6172	G

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	24	C
1	A	110	U
1	A	303	C
1	A	368	U
1	A	465	A
1	A	532	C
1	A	553	U
1	A	561	A
1	A	627	U
1	A	752	G
1	A	870	A
1	A	874	G
1	A	1137	U
1	A	1395	C
1	A	1520	G
1	A	1645	C

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



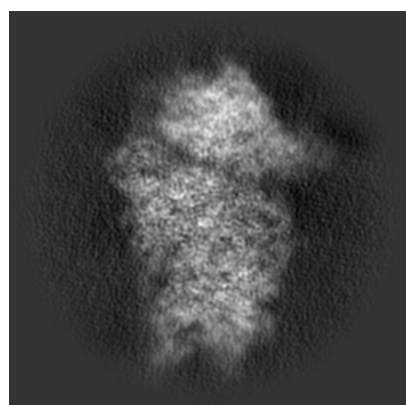
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22433. These allow visual inspection of the internal detail of the map and identification of artifacts.

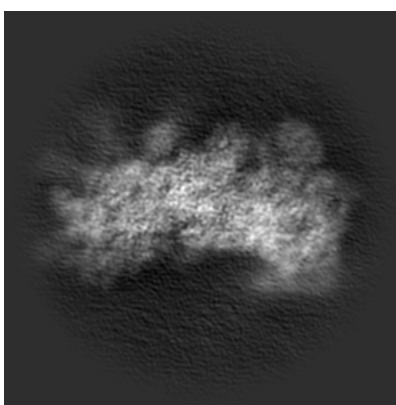
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

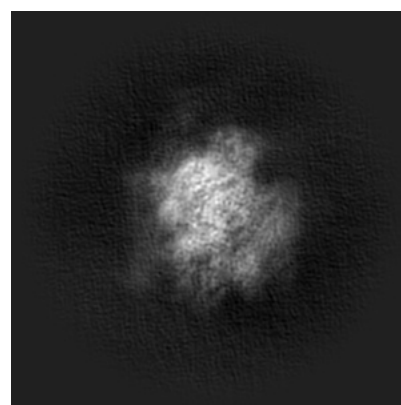
#### 6.1.1 Primary map



X



Y

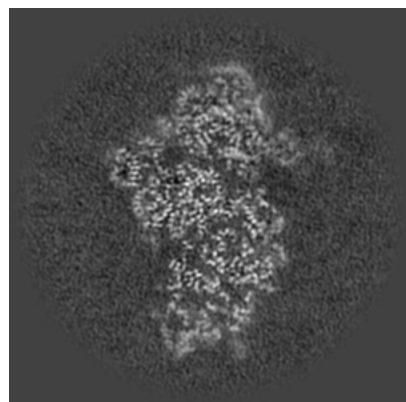


Z

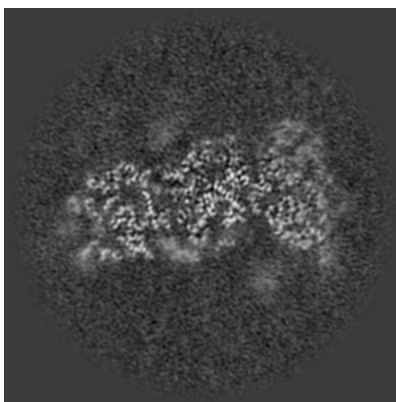
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

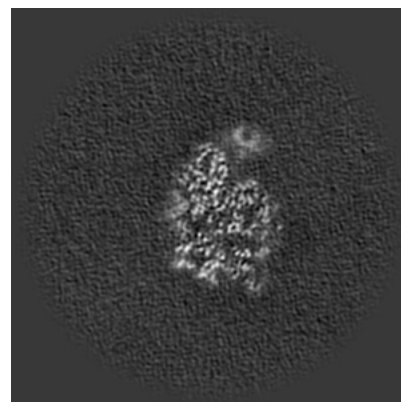
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

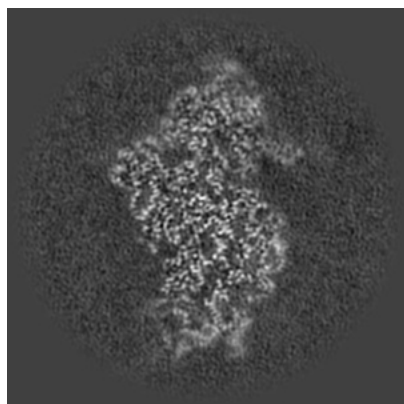


Z Index: 160

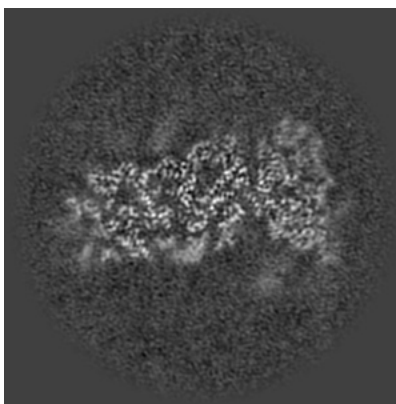
The images above show central slices of the map in three orthogonal directions.

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

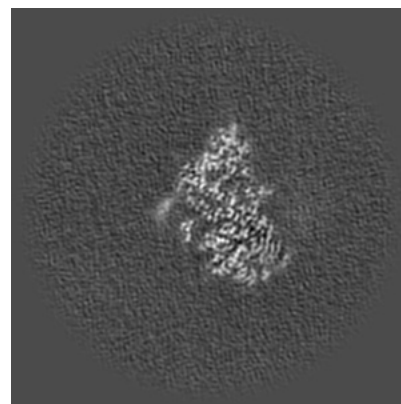
### 6.3.1 Primary map



X Index: 164



Y Index: 158



Z Index: 142

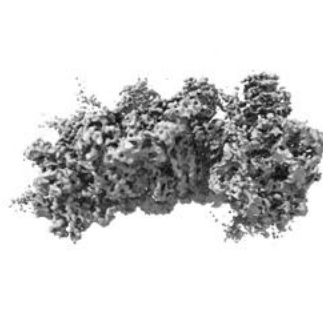
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

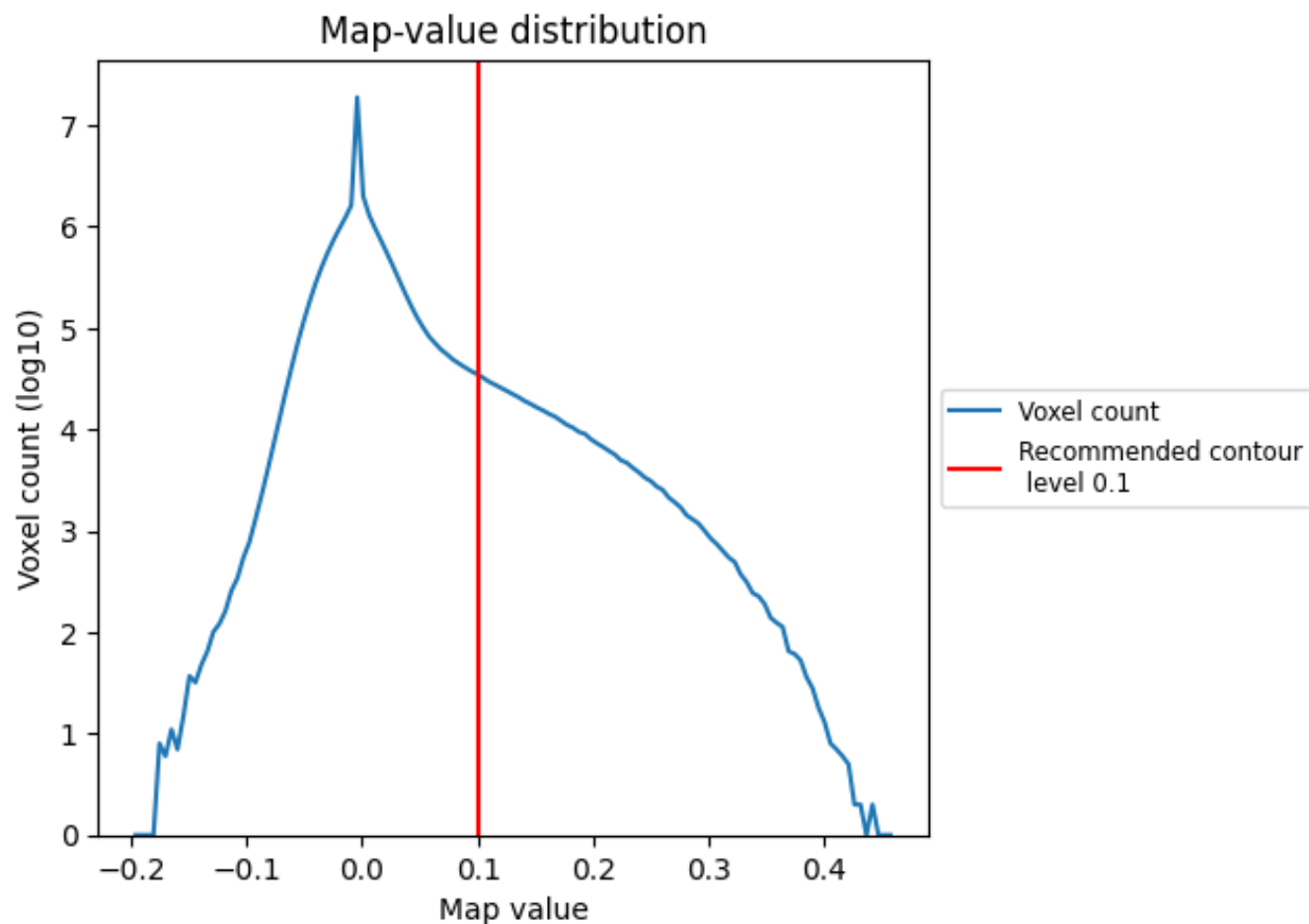
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

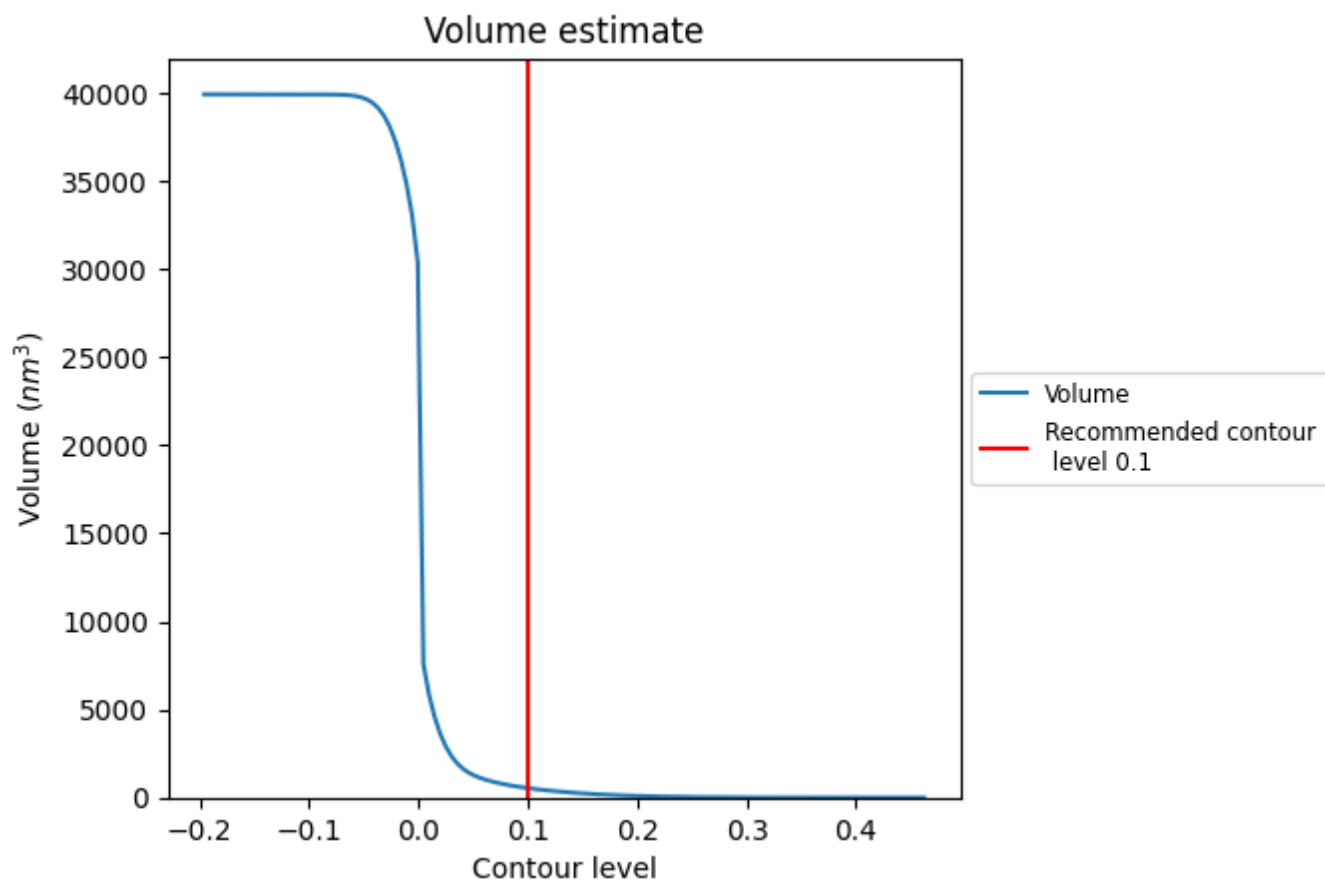
This section contains the results of statistical analysis of the map.

### 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.

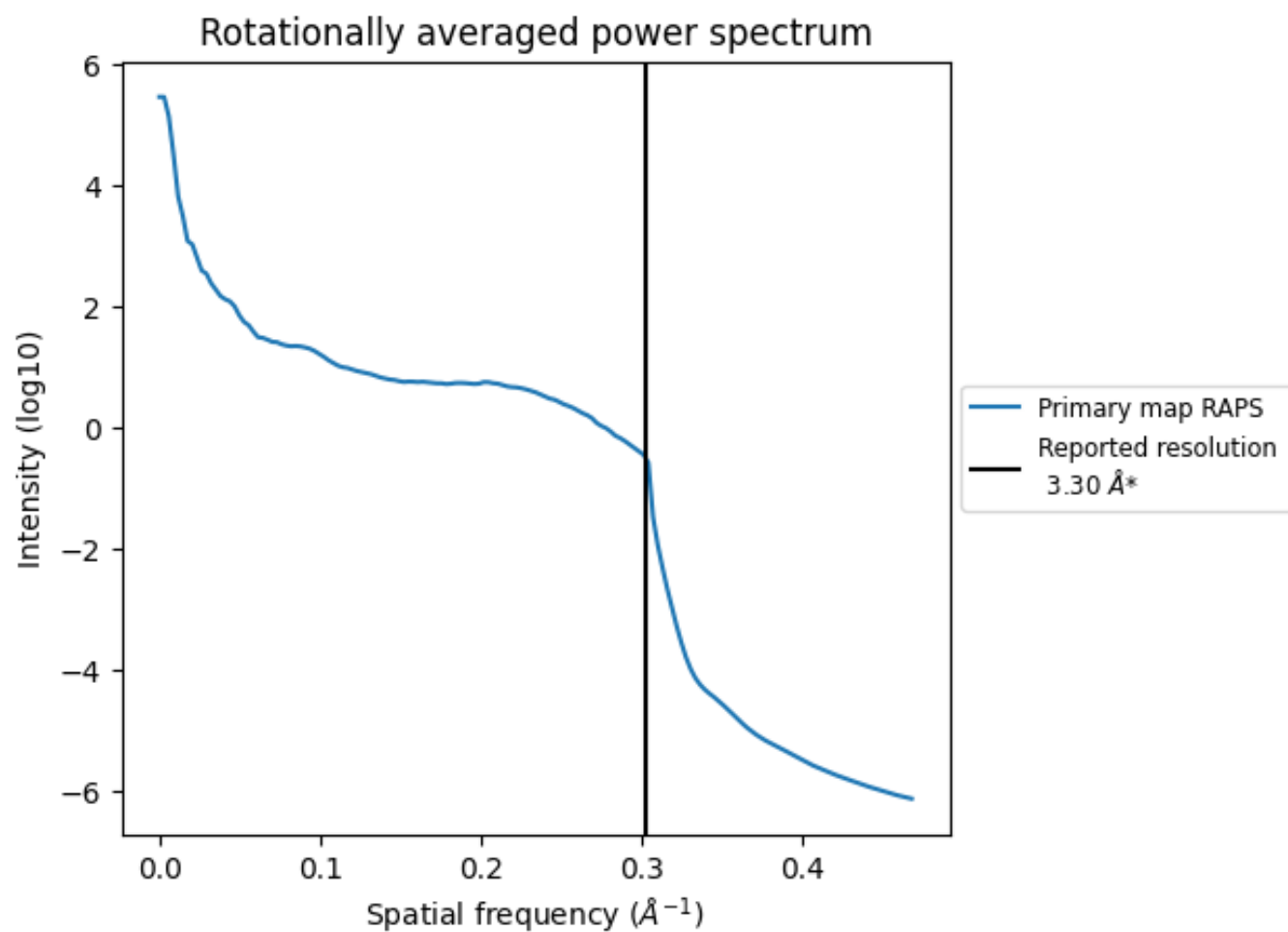
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 537 nm<sup>3</sup>; this corresponds to an approximate mass of 485 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



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

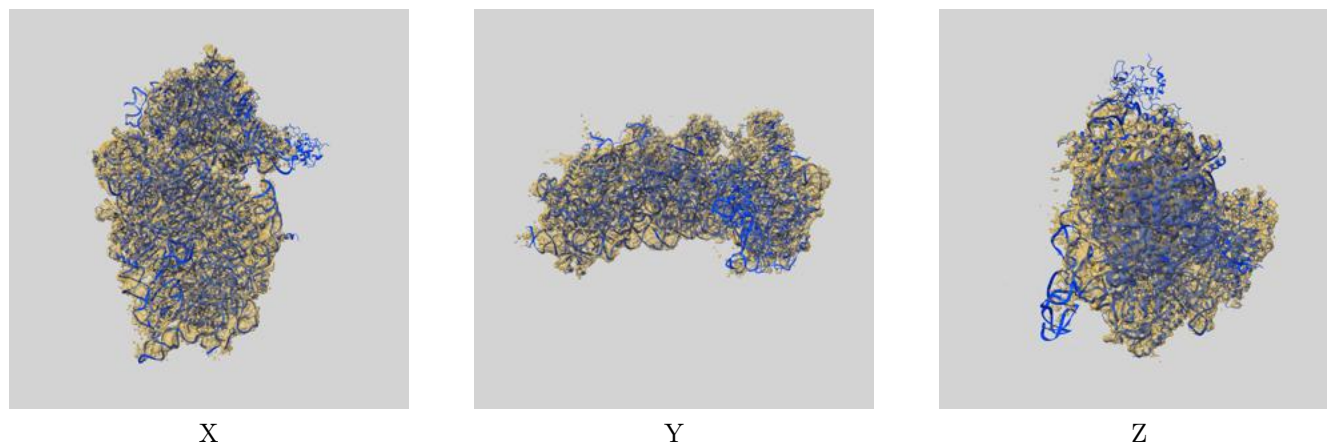
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

This section contains information regarding the fit between EMDB map EMD-22433 and PDB model 7JQC. Per-residue inclusion information can be found in section [3](#) on page [11](#).

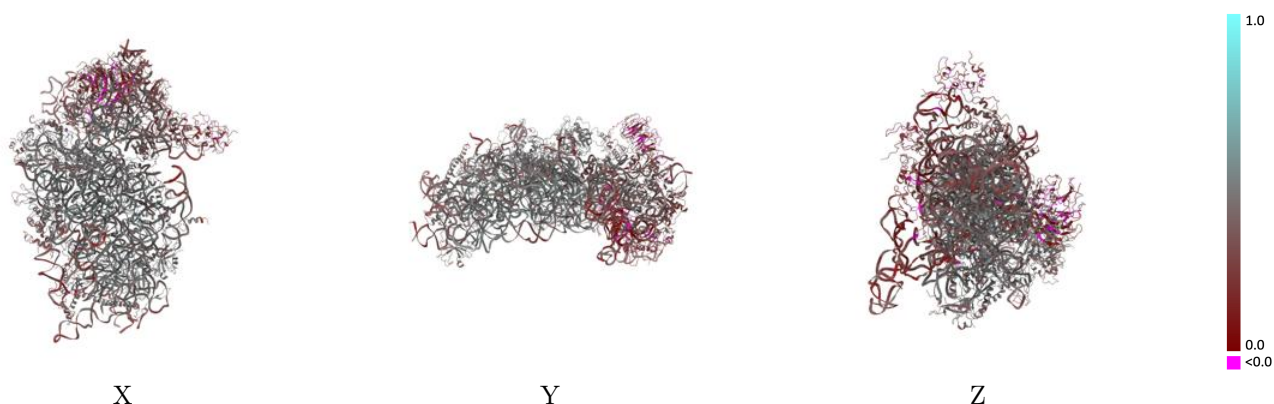
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

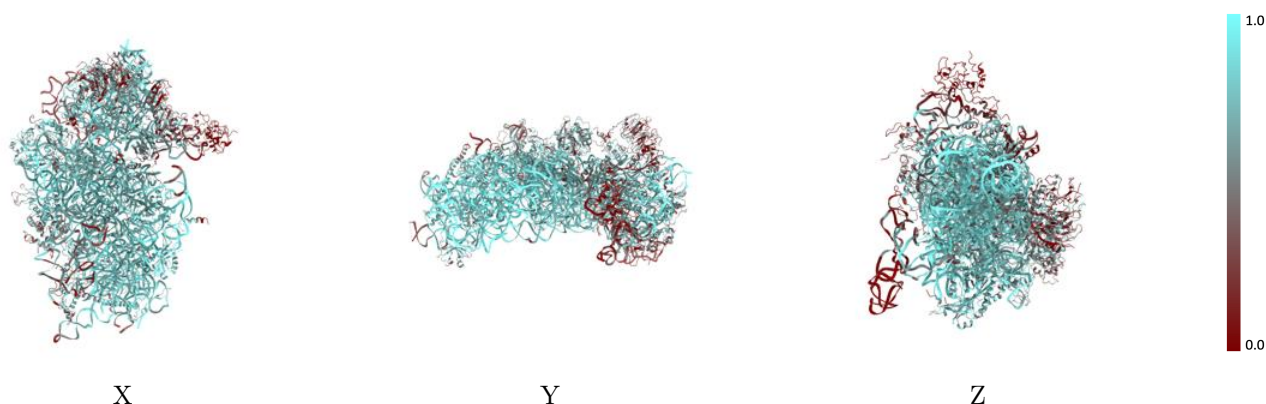


## 9.2 Q-score mapped to coordinate model [i](#)



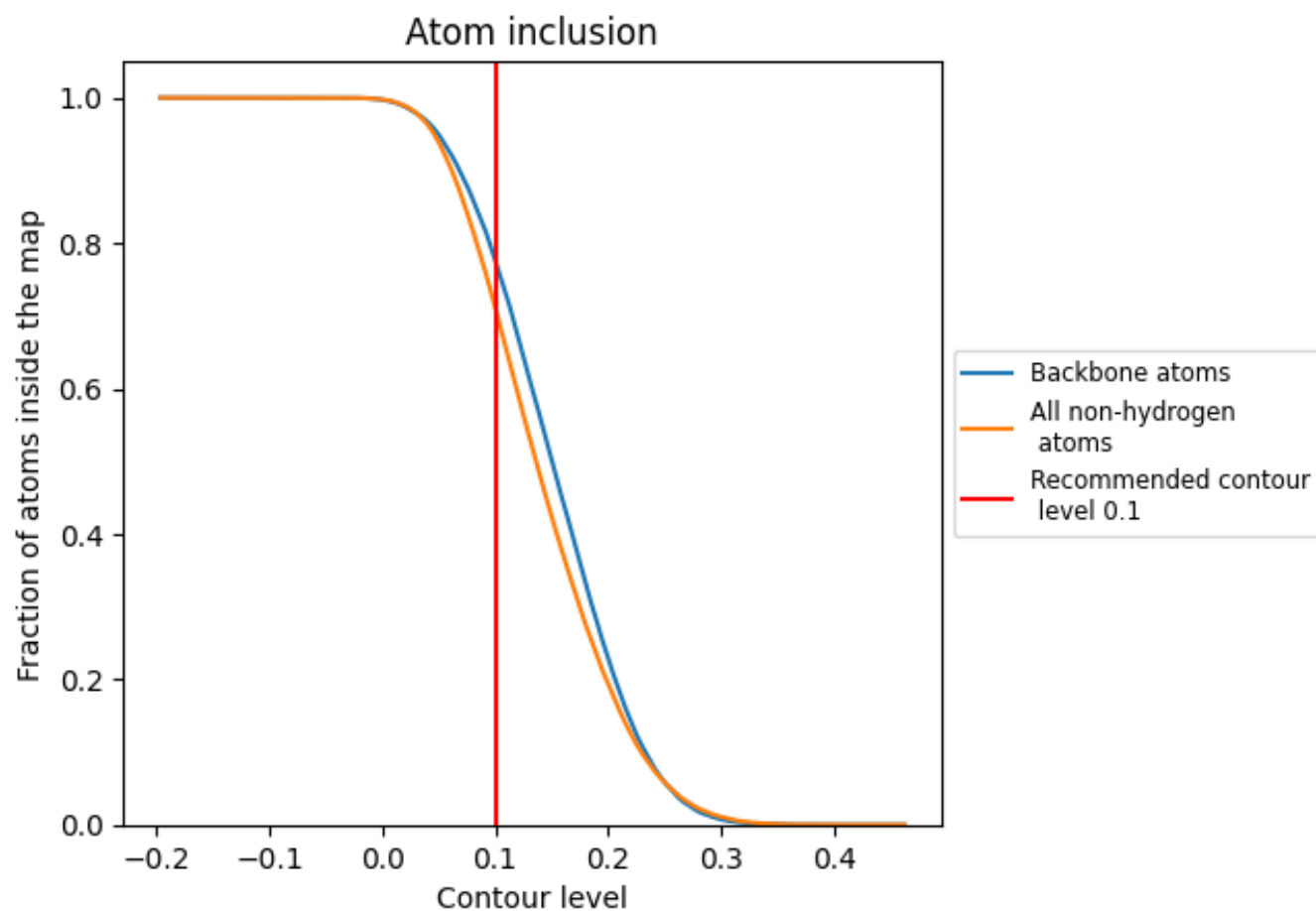
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7122	 0.3990
A	 0.8532	 0.4170
B	 0.6603	 0.4520
C	 0.7393	 0.4440
D	 0.7138	 0.4750
E	 0.4962	 0.3640
F	 0.5292	 0.4300
G	 0.6688	 0.3560
H	 0.6906	 0.4210
I	 0.4942	 0.3990
J	 0.6951	 0.4440
K	 0.7427	 0.4610
L	 0.4063	 0.3260
M	 0.7807	 0.4730
N	 0.0078	 0.2270
O	 0.6193	 0.4400
P	 0.7253	 0.4560
Q	 0.3802	 0.2580
R	 0.5668	 0.3310
S	 0.5356	 0.4120
T	 0.4812	 0.2520
U	 0.6251	 0.3080
V	 0.3773	 0.3610
W	 0.6720	 0.4610
X	 0.7538	 0.4390
Y	 0.7455	 0.4940
Z	 0.8022	 0.4510
a	 0.6552	 0.3090
b	 0.7657	 0.4830
c	 0.7646	 0.4840
d	 0.6979	 0.4230
e	 0.6337	 0.4420
f	 0.6614	 0.4430
g	 0.0963	 0.2380
h	 0.3287	 0.1990
i	 0.3695	 0.2450

