Full wwPDB EM Validation Report (i)

Jun 20, 2024 – 02:41 AM JST

PDB ID	:	7WTS
EMDB ID	:	EMD-32799
Title	:	Cryo-EM structure of a human pre-40S ribosomal subunit - State UTP14
Authors	:	Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on	:	2022-02-05
Resolution	:	3.20 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

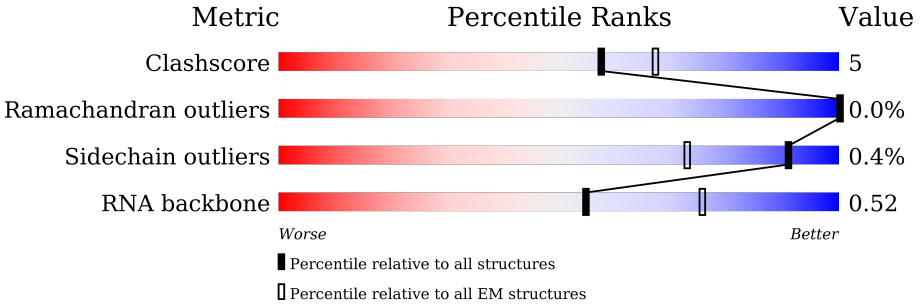
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	2	1873	48% 25% 6% 21%
2	b	84	98%
3	B	264	69% 12% 19%
4	E	263	86% 14%
5	e	59	34% 66%
6	H	194	81% 14%
7	G	249	82% 10% 8%

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Mol	Chain	Length	Quality of chain
8	Y	133	82% 11% 7%
9	x	252	69% 31%
10	X	143	83% 15%
11	W	130	90% 9%
12	u	804	78% 22%
13	O	151	83% 6% 11%
14	N	151	92% 7%
15	L	158	80% 16%
16	J	194	80% 12% 7%
17	I	208	84% 14%
18	r	125	26% 94% 6%
19	q	281	80% 20%
20	K	1297	96%
21	z	230	13% 87%
22	5	771	7% 92%
23	3	313	75% 13% 12%

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 61945 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1481	31620	14112	5672	10355	1481	0	0

- Molecule 2 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	82	640	402	118	113	7	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

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

- Molecule 4 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	262	2076	1324	386	358	8	0	0

- Molecule 5 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	20	179	110	43	25	1	0	0

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	186	1501	957	276	267	1	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	230	1862	1164	371	320	7	0	0

- Molecule 8 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Y	124	1014	641	198	170	5	0	0

- Molecule 9 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	x	175	1372	881	249	238	4	0	0

- Molecule 10 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	141	1098	693	219	183	3	0	0

- Molecule 11 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	W	129	1033	659	193	175	6	0	0

- Molecule 12 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	u	628	5060	3245	911	880	24	0	0

- Molecule 13 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	135	1009	618	198	187	6	0	0

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	149	1202	770	228	203	1	0	0

- Molecule 15 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	L	151	1229	782	230	211	6	0	0

- Molecule 16 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	J	180	1499	955	300	242	2	0	0

- Molecule 17 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	205	1682	1056	331	290	5	0	0

- Molecule 18 is a protein called Multifunctional methyltransferase subunit TRM112-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	r	118	940	601	166	166	7	0	0

- Molecule 19 is a protein called Probable 18S rRNA (guanine-N(7))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	q	226	1799	1140	316	332	11	0	0

- Molecule 20 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	K	58	468	296	86	86	0	0

- Molecule 21 is a protein called Ribosome biogenesis protein SLX9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	z	30	263	169	52	41	1	0	0

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 14 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	5	58	470	301	96	72	1	0	0

- Molecule 23 is a protein called Probable dimethyladenosine transferase.

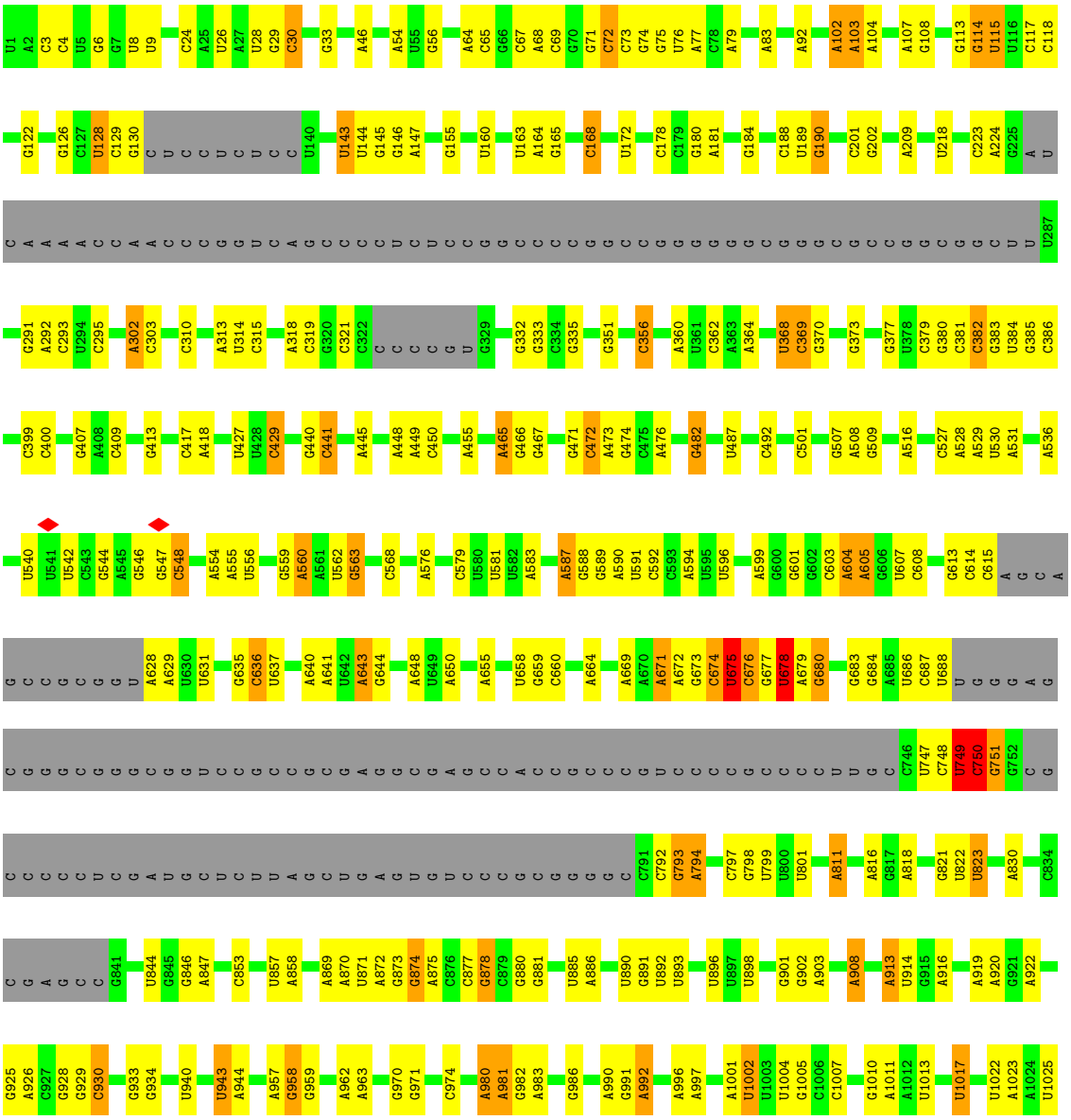
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	3	277	2200	1420	389	382	9	0	0

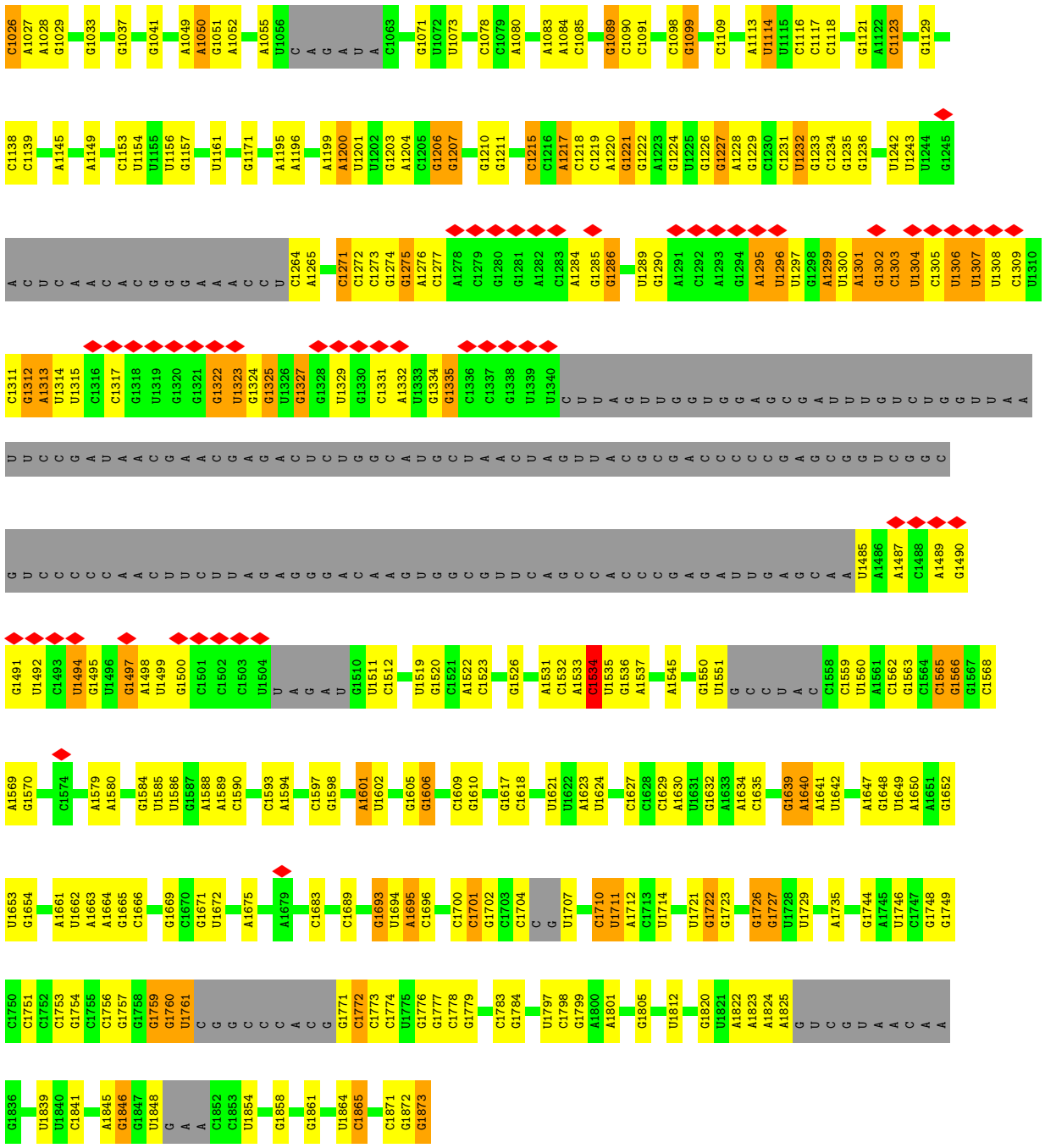
3 Residue-property plots (i)

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: 18S rRNA

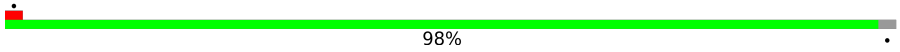
Chain 2:

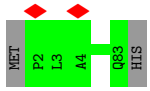




• Molecule 2: 40S ribosomal protein S27

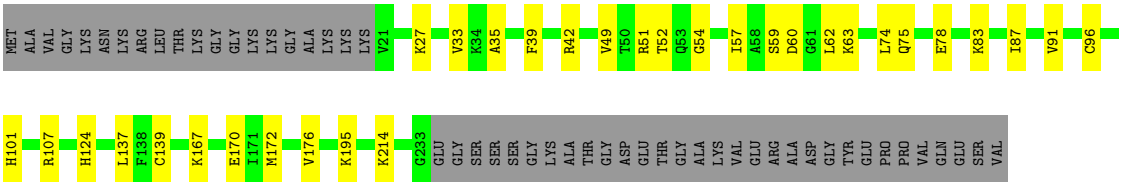
Chain b:





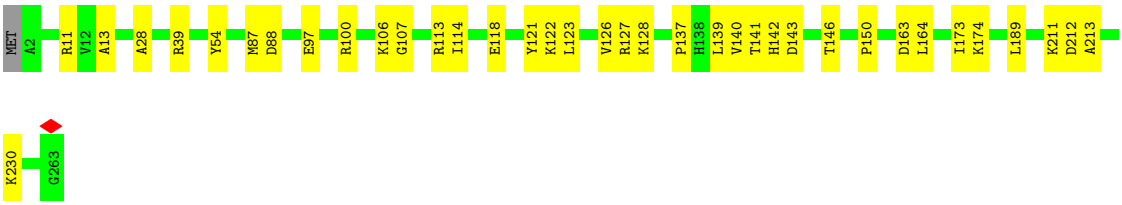
• Molecule 3: 40S ribosomal protein S3a

Chain B:



- Molecule 4: 40S ribosomal protein S4, X isoform

Chain E:

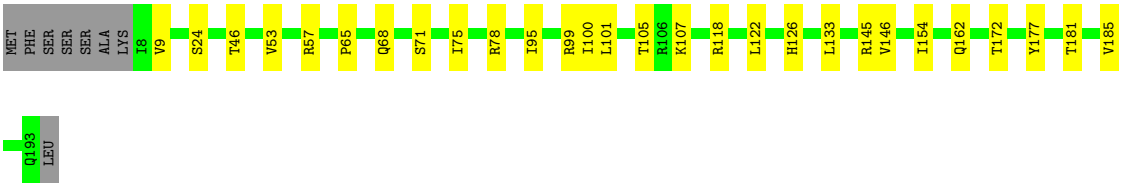


- Molecule 5: 40S ribosomal protein S30

Chain e:

- Molecule 6: 40S ribosomal protein S7

Chain H:



- Molecule 7: 40S ribosomal protein S6

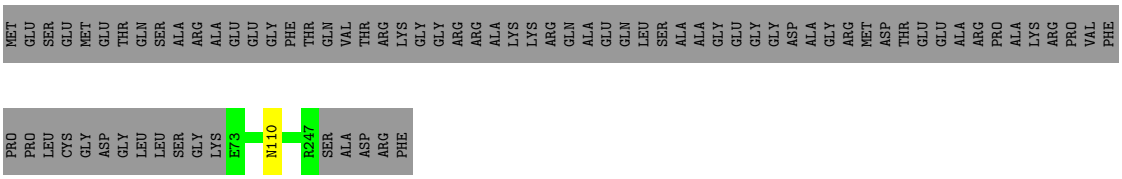
Chain G:

- Molecule 8: 40S ribosomal protein S24

Chain Y:

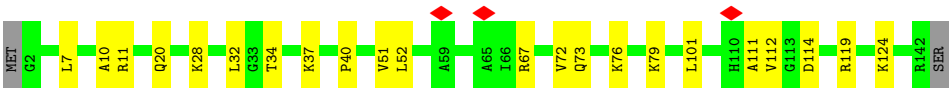
- Molecule 9: RNA-binding protein PNO1

Chain x:



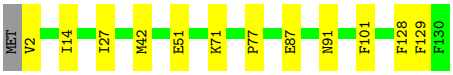
- Molecule 10: 40S ribosomal protein S23

Chain X:



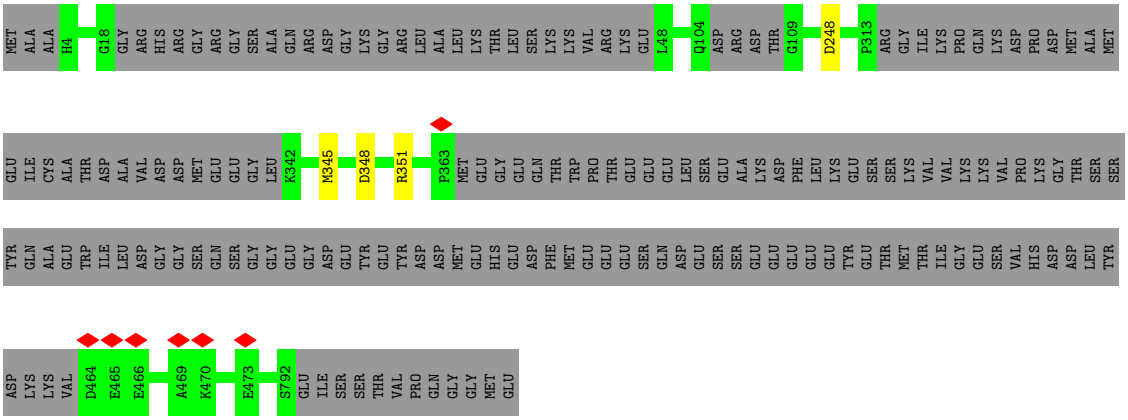
- Molecule 11: 40S ribosomal protein S15a

Chain W:



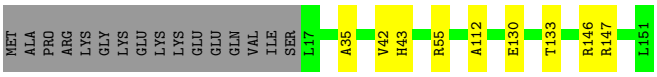
- Molecule 12: Pre-rRNA-processing protein TSR1 homolog

Chain u:



- Molecule 13: 40S ribosomal protein S14

Chain O:



- Molecule 14: 40S ribosomal protein S13

Chain N: 92% 7%

MET G2 R3 M4 H5 G10 R64 E86 H90 R104 R121 R124 R133 V150 ALA

• Molecule 15: 40S ribosomal protein S11

Chain L: 80% 16%

MET A2 K21 R22 V23 G26 K30 K38 N39 I40 G41 L42 N65 V66 S67 I68 R69 I72 G75 T85 I88 D91 R101 K104 V111 V126 R132 K136 F140 L143 K144 V145 K152 LYS GLN PHE GLN LYS PHE

• Molecule 16: 40S ribosomal protein S9

Chain J: 80% 12% 7%

MET P2 R10 E28 N39 V43 I53 R80 L81 D88 K91 E103 E107 Q113 R131 H134 I135 R136 V142 N143 I144 D158 F159 S160 L161 P164 Y165 K174 G181 GLN GLY GLY GLY ALA GLY ALA GLY ASP ASP GLU GLU GLU ASP

• Molecule 17: 40S ribosomal protein S8

Chain I: 84% 14%

MET G2 R5 R11 L29 A33 A57 V62 R74 K75 T76 Y83 N87 L90 N99 C100 I101 V102 L103 I104 D105 S106 E135 K139 K140 R141 Q146 R152 K157 L162 K170 L171 G183 R184 L190 E191 K206 GLY LYS

• Molecule 18: Multifunctional methyltransferase subunit TRM112-like protein

Chain r: 26% 94% 6%

M1 N7 R24 L25 Q26 A27 T28 E29 V30 R31 I32 C33 P34 D59 N60 L61 R62 L63 I64 Q65 K68 E79 I94 E95 G96 T97 L98 Q99 C100 P101 E102 S103 G104 R105 M106 F107 P108 I109 S110 R111 L118 SER GLU GLU GLU THR GLU SER

• Molecule 19: Probable 18S rRNA (guanine-N(7))-methyltransferase

Chain q: 80% 20%

MET ALA SER ARG GLY ARG ARG PRO GLU HIS GLY GLY PRO PRO E15 L16 V27 S30 M39 Y48 L49 P50 A139 R155 L171 G207 PRO SER THR PHE ILE PRO GLU GLY LEU SER GLU ASN GLN ASP GLU VAL GLU PRO ARG GLU SER VAL PHE THR ASN GLU

ARG PHE PRO LEU ARG MET SER ARG ARG GLY MET VAL ARG LYS SER R249 F281

• Molecule 20: RRP12-like protein

Chain K: 96%

MET GLY ARG SER GLY LYS LEU PRO SER GLY VAL SER ALA LYS LEU LYS ARG TRP LYS LYS GLY HIS SER SER ASP SER ASN PRO ALA ILE CYS ARG HIS ARG GLN ALA ALA ARG SER ARG PHE PHE SER ARG PRO SER GLY ARG SER ASP LEU THR VAL ASP ALA VAL LYS LEU HIS ASN

R1188
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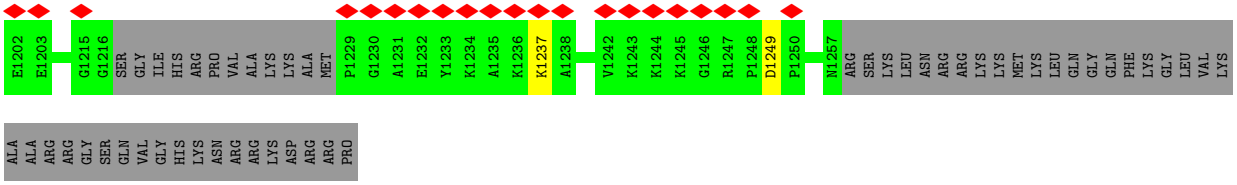
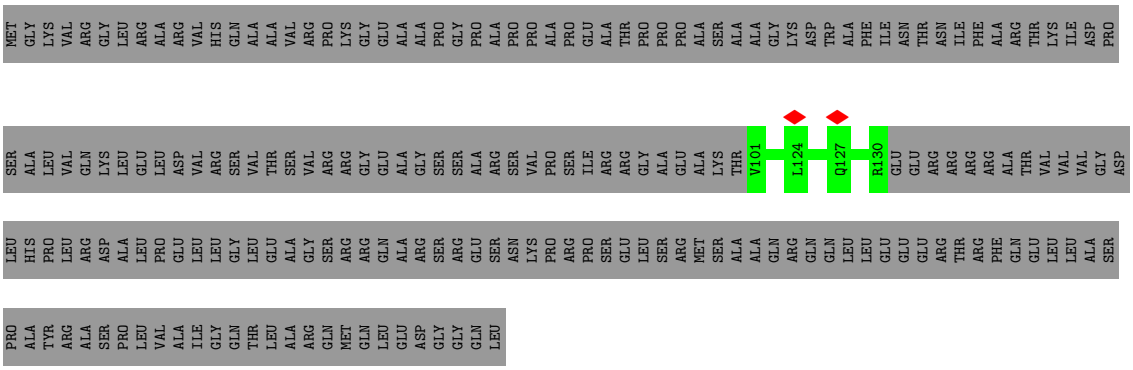
K1199
E1200
A1201



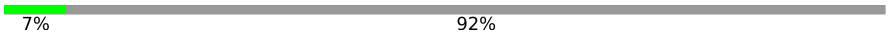
- Molecule 21: Ribosome biogenesis protein SLX9 homolog

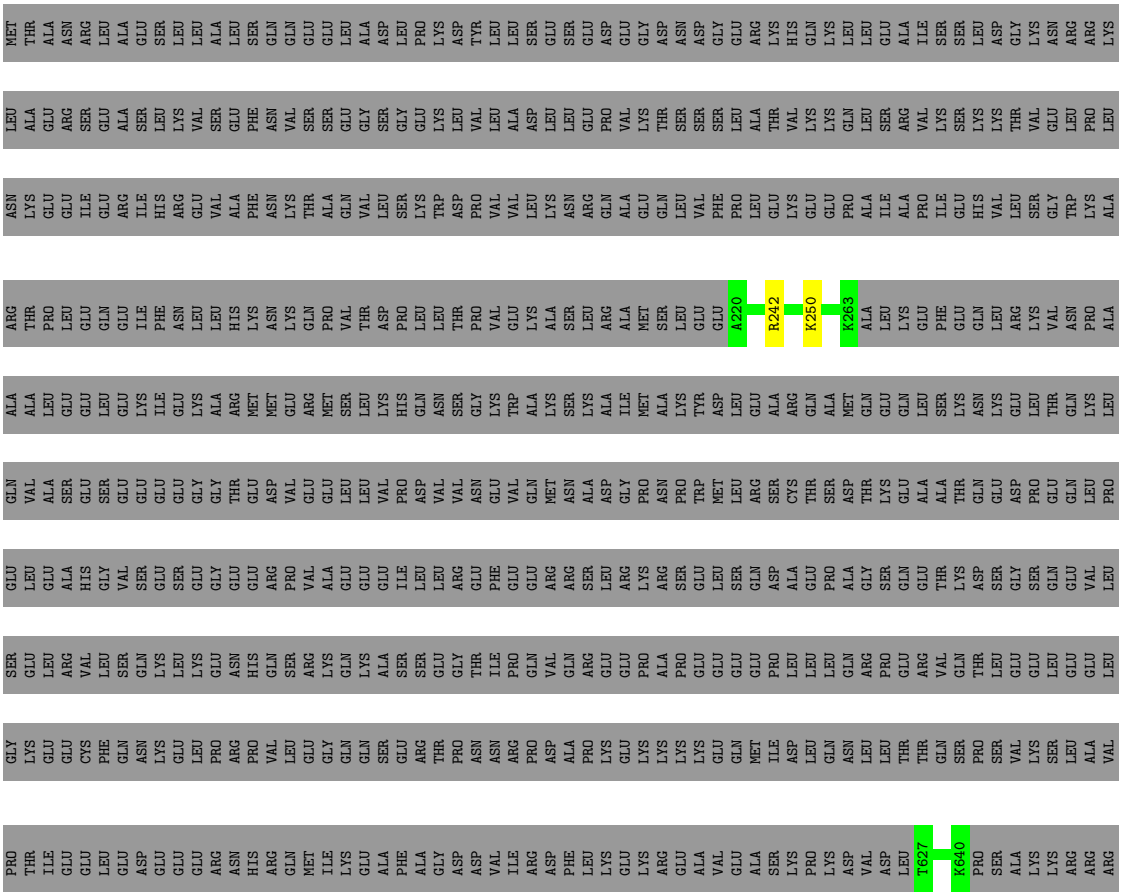
Chain z:

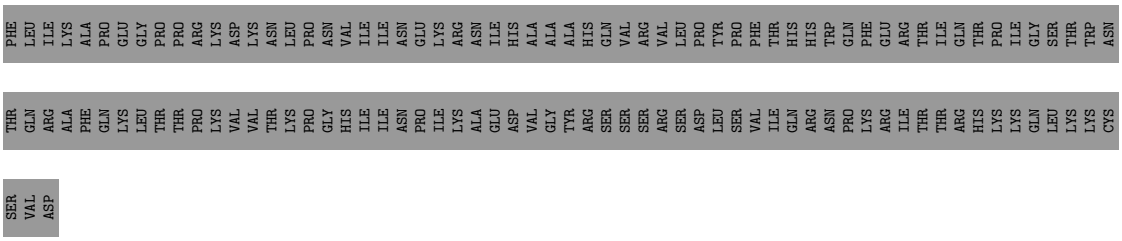


- Molecule 22: U3 small nucleolar RNA-associated protein 14 homolog A

Chain 5:

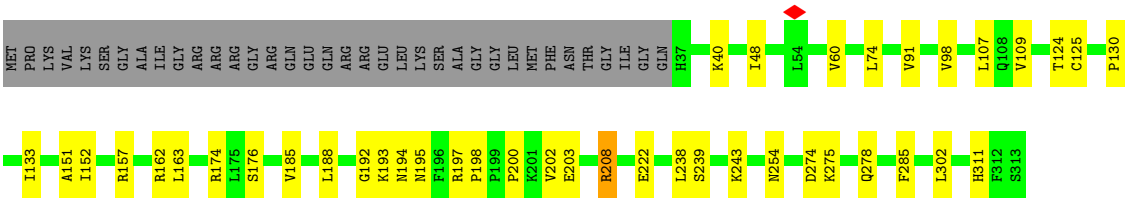






• Molecule 23: Probable dimethyladenosine transferase

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8843	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.599	Depositor
Minimum map value	-0.263	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	2	0.55	3/35348 (0.0%)	1.04	150/55069 (0.3%)
2	b	0.29	0/653	0.59	0/876
3	B	0.32	0/1756	0.62	0/2350
4	E	0.37	0/2118	0.62	1/2849 (0.0%)
5	e	0.29	0/180	0.59	0/232
6	H	0.30	0/1524	0.61	0/2042
7	G	0.32	0/1885	0.62	1/2510 (0.0%)
8	Y	0.35	0/1031	0.58	0/1370
9	x	0.31	0/1394	0.60	0/1880
10	X	0.35	0/1116	0.63	0/1490
11	W	0.36	0/1050	0.63	0/1406
12	u	0.30	0/5185	0.59	1/7003 (0.0%)
13	O	0.31	0/1022	0.69	0/1372
14	N	0.32	0/1226	0.59	0/1649
15	L	0.39	0/1250	0.62	0/1673
16	J	0.37	0/1524	0.66	0/2035
17	I	0.35	0/1711	0.62	1/2282 (0.0%)
18	r	0.27	0/961	0.62	0/1301
19	q	0.27	0/1836	0.61	1/2471 (0.0%)
20	K	0.27	0/478	0.53	0/635
21	z	0.26	0/266	0.58	0/350
22	5	0.30	0/477	0.58	0/626
23	3	0.28	0/2248	0.55	1/3045 (0.0%)
All	All	0.46	3/66239 (0.0%)	0.88	156/96516 (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
12	u	0	2
17	I	0	1

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Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	G	C1'-N9	7.43	1.59	1.48
1	2	676	C	C5-C6	-5.78	1.29	1.34
1	2	676	C	N1-C6	-5.38	1.33	1.37

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1323	U	N3-C2-O2	-14.53	112.03	122.20
1	2	501	C	N1-C2-O2	13.03	126.72	118.90
1	2	501	C	C2-N1-C1'	12.73	132.80	118.80
1	2	1773	C	N3-C2-O2	-11.98	113.52	121.90
1	2	676	C	C4-C5-C6	11.78	123.29	117.40
1	2	293	C	N1-C2-O2	11.76	125.96	118.90
1	2	501	C	N3-C2-O2	-10.58	114.49	121.90
1	2	678	U	N3-C4-O4	-10.52	112.03	119.40
1	2	1774	C	N3-C2-O2	-10.30	114.69	121.90
1	2	293	C	C2-N1-C1'	10.07	129.88	118.80
1	2	356	C	N1-C2-O2	9.84	124.81	118.90
1	2	1323	U	N1-C2-O2	9.79	129.66	122.80
1	2	676	C	N3-C4-N4	9.77	124.84	118.00
1	2	1773	C	N1-C2-O2	9.23	124.44	118.90
1	2	1865	C	N1-C2-O2	9.17	124.40	118.90
1	2	356	C	C2-N1-C1'	9.12	128.83	118.80
1	2	501	C	C6-N1-C1'	-9.01	109.99	120.80
1	2	1701	C	N3-C2-O2	-8.62	115.87	121.90
1	2	678	U	C5-C4-O4	8.40	130.94	125.90
1	2	293	C	N3-C2-O2	-8.29	116.09	121.90
1	2	1139	C	N1-C2-O2	8.28	123.87	118.90
1	2	853	C	C2-N1-C1'	8.27	127.89	118.80
1	2	356	C	N3-C2-O2	-8.15	116.20	121.90
1	2	1139	C	N3-C2-O2	-8.09	116.23	121.90
1	2	676	C	C6-N1-C1'	-7.86	111.37	120.80
1	2	1022	U	C2-N1-C1'	7.86	127.13	117.70
1	2	1641	A	N7-C8-N9	7.81	117.70	113.80
1	2	676	C	N1-C2-O2	7.80	123.58	118.90
1	2	501	C	C6-N1-C2	-7.75	117.20	120.30
1	2	1276	A	N1-C6-N6	-7.72	113.97	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1865	C	N3-C2-O2	-7.70	116.51	121.90
1	2	1590	C	N1-C2-O2	7.68	123.51	118.90
1	2	853	C	N3-C2-O2	-7.57	116.60	121.90
1	2	676	C	C5-C4-N4	-7.55	114.91	120.20
1	2	1865	C	C2-N1-C1'	7.40	126.94	118.80
1	2	1774	C	N1-C2-O2	7.34	123.31	118.90
1	2	293	C	C6-N1-C1'	-7.31	112.03	120.80
1	2	1624	U	C2-N1-C1'	7.18	126.31	117.70
1	2	676	C	C2-N1-C1'	7.13	126.65	118.80
1	2	676	C	C5-C6-N1	-7.11	117.44	121.00
1	2	4	C	C2-N1-C1'	7.10	126.61	118.80
1	2	1520	G	C4-N9-C1'	7.04	135.65	126.50
1	2	1701	C	C6-N1-C2	-7.04	117.48	120.30
1	2	1139	C	C2-N1-C1'	6.95	126.44	118.80
1	2	749	U	C2-N1-C1'	6.93	126.02	117.70
1	2	853	C	N1-C2-O2	6.90	123.04	118.90
1	2	1711	U	C5-C6-N1	6.81	126.10	122.70
1	2	427	U	C2-N1-C1'	6.80	125.86	117.70
1	2	853	C	C6-N1-C2	-6.72	117.61	120.30
1	2	407	G	C4-N9-C1'	6.67	135.18	126.50
1	2	1759	G	N1-C2-N2	-6.67	110.20	116.20
1	2	1641	A	C6-C5-N7	-6.64	127.65	132.30
1	2	1109	C	N1-C2-O2	6.63	122.88	118.90
1	2	1026	C	C2-N1-C1'	-6.58	111.56	118.80
1	2	1494	U	P-O3'-C3'	6.55	127.56	119.70
1	2	1689	C	N1-C2-O2	6.54	122.82	118.90
1	2	4	C	N1-C2-O2	6.53	122.82	118.90
1	2	1520	G	N3-C4-N9	6.53	129.91	126.00
1	2	1772	C	N1-C2-O2	6.50	122.80	118.90
1	2	1139	C	C6-N1-C2	-6.48	117.71	120.30
1	2	1520	G	N3-C4-C5	-6.47	125.36	128.60
1	2	1641	A	C8-N9-C4	-6.46	103.22	105.80
1	2	1759	G	N1-C6-O6	-6.42	116.05	119.90
1	2	427	U	N3-C2-O2	-6.33	117.77	122.20
1	2	1760	G	N1-C2-N2	-6.27	110.56	116.20
1	2	1865	C	C6-N1-C2	-6.25	117.80	120.30
1	2	356	C	C6-N1-C1'	-6.24	113.32	120.80
1	2	1532	C	N3-C2-O2	-6.22	117.54	121.90
1	2	356	C	C6-N1-C2	-6.22	117.81	120.30
1	2	1590	C	N3-C2-O2	-6.19	117.57	121.90
1	2	407	G	N3-C4-N9	6.16	129.69	126.00
1	2	1700	C	C2-N1-C1'	6.12	125.53	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	3	274	ASP	CB-CG-OD1	6.10	123.79	118.30
1	2	114	G	P-O3'-C3'	6.07	126.98	119.70
1	2	293	C	C5-C6-N1	6.00	124.00	121.00
1	2	1696	C	N3-C2-O2	-5.95	117.74	121.90
1	2	1520	G	C8-N9-C1'	-5.93	119.28	127.00
1	2	1760	G	N3-C2-N2	5.91	124.04	119.90
1	2	1759	G	N3-C2-N2	5.91	124.04	119.90
1	2	407	G	C8-N9-C1'	-5.90	119.33	127.00
1	2	1751	C	N1-C2-O2	5.89	122.43	118.90
1	2	1641	A	N3-C4-N9	5.87	132.09	127.40
1	2	1306	U	C2-N1-C1'	5.86	124.73	117.70
1	2	1624	U	N1-C2-O2	5.84	126.89	122.80
1	2	1751	C	N3-C2-O2	-5.84	117.81	121.90
1	2	178	C	N1-C2-O2	5.78	122.37	118.90
1	2	1641	A	C4-C5-C6	5.78	119.89	117.00
7	G	197	GLN	CA-CB-CG	5.78	126.11	113.40
4	E	163	ASP	CB-CG-OD1	5.75	123.47	118.30
1	2	1590	C	C2-N1-C1'	5.67	125.04	118.80
12	u	248	ASP	CB-CG-OD1	5.66	123.39	118.30
1	2	675	U	C6-N1-C2	-5.65	117.61	121.00
1	2	1689	C	N3-C2-O2	-5.62	117.97	121.90
1	2	1485	U	N1-C2-O2	5.61	126.73	122.80
1	2	472	C	C6-N1-C2	-5.61	118.06	120.30
1	2	1323	U	N1-C2-N3	5.60	118.26	114.90
1	2	675	U	C5-C6-N1	5.59	125.50	122.70
1	2	823	U	C2-N1-C1'	5.56	124.37	117.70
1	2	102	A	P-O3'-C3'	5.55	126.36	119.70
1	2	1774	C	C6-N1-C2	-5.54	118.08	120.30
1	2	293	C	C6-N1-C2	-5.53	118.09	120.30
1	2	1123	C	N1-C2-O2	5.52	122.21	118.90
1	2	441	C	C2-N1-C1'	5.51	124.86	118.80
1	2	659	G	C4-N9-C1'	5.50	133.66	126.50
1	2	321	C	C2-N1-C1'	5.49	124.84	118.80
1	2	1276	A	C5-C6-N6	5.49	128.09	123.70
1	2	1696	C	N1-C2-O2	5.46	122.18	118.90
1	2	1109	C	C2-N1-C1'	5.46	124.80	118.80
1	2	465	A	P-O3'-C3'	5.45	126.24	119.70
1	2	1689	C	C2-N1-C1'	5.40	124.74	118.80
1	2	407	G	N3-C4-C5	-5.40	125.90	128.60
1	2	143	U	P-O3'-C3'	5.39	126.16	119.70
1	2	1590	C	C6-N1-C2	-5.37	118.15	120.30
1	2	1304	U	P-O3'-C3'	5.34	126.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	877	C	C2-N1-C1'	5.34	124.67	118.80
1	2	1022	U	N3-C2-O2	-5.33	118.47	122.20
1	2	1624	U	N3-C2-O2	-5.32	118.48	122.20
1	2	30	C	C6-N1-C2	-5.30	118.18	120.30
1	2	501	C	C5-C6-N1	5.29	123.65	121.00
1	2	1534	C	P-O3'-C3'	5.29	126.05	119.70
1	2	1219	C	N1-C2-O2	5.28	122.07	118.90
1	2	1700	C	N1-C2-O2	5.28	122.07	118.90
1	2	1532	C	N1-C2-O2	5.27	122.06	118.90
1	2	1693	G	P-O3'-C3'	5.26	126.01	119.70
1	2	853	C	C6-N1-C1'	-5.26	114.49	120.80
1	2	1022	U	C6-N1-C1'	-5.25	113.85	121.20
1	2	636	C	P-O3'-C3'	5.25	126.00	119.70
1	2	1022	U	N1-C2-O2	5.24	126.47	122.80
1	2	676	C	N3-C2-O2	-5.24	118.23	121.90
1	2	579	C	N1-C2-O2	5.23	122.04	118.90
1	2	1759	G	C5-C6-O6	5.23	131.74	128.60
1	2	1311	C	N1-C2-O2	5.19	122.02	118.90
1	2	793	G	N1-C6-O6	-5.19	116.78	119.90
1	2	1485	U	N3-C2-O2	-5.19	118.57	122.20
1	2	188	C	C2-N1-C1'	5.18	124.50	118.80
17	I	29	LEU	CA-CB-CG	5.18	127.22	115.30
1	2	178	C	C2-N1-C1'	5.18	124.50	118.80
1	2	168	C	N1-C2-O2	5.17	122.00	118.90
1	2	750	C	C5-C6-N1	5.17	123.59	121.00
1	2	943	U	C5-C4-O4	-5.17	122.80	125.90
1	2	750	C	P-O3'-C3'	5.16	125.89	119.70
1	2	4	C	C6-N1-C2	-5.13	118.25	120.30
1	2	1601	A	P-O3'-C3'	5.11	125.84	119.70
1	2	1109	C	N3-C2-O2	-5.10	118.33	121.90
1	2	823	U	N3-C2-O2	-5.09	118.63	122.20
1	2	930	C	N1-C2-O2	5.09	121.95	118.90
1	2	1314	U	C2-N1-C1'	5.09	123.81	117.70
1	2	1641	A	N3-C4-C5	-5.07	123.25	126.80
1	2	114	G	OP1-P-O3'	5.05	116.31	105.20
1	2	1311	C	C2-N1-C1'	5.03	124.33	118.80
1	2	1161	U	N3-C2-O2	-5.03	118.68	122.20
1	2	1711	U	C5-C4-O4	-5.02	122.89	125.90
1	2	427	U	N1-C2-O2	5.02	126.31	122.80
1	2	1123	C	C2-N1-C1'	5.02	124.32	118.80
1	2	117	C	C6-N1-C2	-5.02	118.29	120.30
19	q	39	MET	CA-CB-CG	5.00	121.81	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	I	140	LYS	Peptide
12	u	345	MET	Peptide
12	u	348	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	31620	0	15971	244	0
2	b	640	0	665	0	0
3	B	1729	0	1803	19	0
4	E	2076	0	2177	24	0
5	e	179	0	200	0	0
6	H	1501	0	1593	18	0
7	G	1862	0	2018	15	0
8	Y	1014	0	1082	12	0
9	x	1372	0	1453	0	0
10	X	1098	0	1167	15	0
11	W	1033	0	1080	9	0
12	u	5060	0	5131	0	0
13	O	1009	0	1034	8	0
14	N	1202	0	1289	8	0
15	L	1229	0	1302	15	0
16	J	1499	0	1618	18	0
17	I	1682	0	1769	20	0
18	r	940	0	958	0	0
19	q	1799	0	1788	0	0
20	K	468	0	476	1	0
21	z	263	0	295	0	0
22	5	470	0	516	3	0
23	3	2200	0	2293	22	0
All	All	61945	0	47678	396	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 5.

All (396) 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)
11:W:101:PHE:O	11:W:128:PHE:HA	1.35	1.20
13:O:42:VAL:O	13:O:55:ARG:HA	1.43	1.16
1:2:748:C:H42	1:2:794:A:N6	1.45	1.14
1:2:536:A:H61	1:2:548:C:N4	1.47	1.13
1:2:536:A:N6	1:2:548:C:H42	1.47	1.13
1:2:748:C:N4	1:2:794:A:H61	1.45	1.12
1:2:1609:C:H42	1:2:1630:A:N6	1.50	1.09
1:2:24:C:H42	1:2:650:A:N6	1.52	1.08
1:2:1609:C:N4	1:2:1630:A:H61	1.50	1.08
1:2:24:C:N4	1:2:650:A:H61	1.53	1.05
1:2:1710:C:N4	1:2:1823:A:C6	2.31	0.98
1:2:678:U:H3	1:2:1027:A:H62	1.07	0.92
1:2:615:C:H42	1:2:628:A:N6	1.68	0.89
1:2:1710:C:N4	1:2:1823:A:N6	2.24	0.86
1:2:614:C:H42	1:2:629:A:N6	1.74	0.85
1:2:1652:G:H1	1:2:1672:U:H3	1.24	0.84
1:2:1215:C:H42	1:2:1220:A:H61	1.27	0.83
1:2:878:G:H1	1:2:908:A:H61	1.28	0.82
1:2:615:C:N4	1:2:628:A:H61	1.78	0.81
1:2:678:U:O4	1:2:1027:A:N7	2.13	0.81
1:2:1033:G:H1	1:2:1080:A:HO2'	1.28	0.81
1:2:1534:C:C2	1:2:1598:G:N2	2.49	0.81
1:2:614:C:N4	1:2:629:A:N6	2.31	0.79
1:2:615:C:H42	1:2:628:A:H61	1.34	0.75
6:H:177:TYR:O	6:H:181:THR:HB	1.87	0.75
1:2:748:C:H42	1:2:794:A:H61	0.77	0.75
1:2:925:G:H1	1:2:1017:U:H3	1.34	0.75
1:2:678:U:H3	1:2:1027:A:N6	1.82	0.74
1:2:1609:C:N3	1:2:1630:A:N1	2.36	0.73
1:2:1335:G:H1	1:2:1492:U:H3	1.37	0.73
1:2:749:U:O4	1:2:793:G:O6	2.08	0.72
10:X:112:VAL:HG12	10:X:114:ASP:H	1.53	0.72
1:2:103:A:OP2	1:2:356:C:N4	2.24	0.71
1:2:957:A:H3'	1:2:958:G:H21	1.55	0.70
1:2:536:A:N1	1:2:548:C:N3	2.40	0.70
16:J:159:PHE:HE2	16:J:165:TYR:HB2	1.57	0.70
1:2:1215:C:H42	1:2:1220:A:N6	1.89	0.69
1:2:1296:U:H3	1:2:1301:A:H62	1.39	0.68
1:2:1215:C:N4	1:2:1220:A:H61	1.90	0.68
1:2:919:A:OP2	14:N:64:ARG:NH2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:614:C:N4	1:2:629:A:H61	1.90	0.67
17:I:57:ALA:HB2	17:I:183:GLY:HA2	1.76	0.67
1:2:1091:C:HO2'	11:W:2:VAL:N	1.90	0.67
3:B:124:HIS:HA	3:B:137:LEU:O	1.95	0.67
1:2:536:A:H61	1:2:548:C:H42	0.74	0.66
1:2:677:G:OP1	14:N:124:ARG:NH1	2.29	0.65
1:2:1757:G:C6	1:2:1776:G:C2	2.85	0.65
1:2:1275:G:O6	1:2:1324:G:C2	2.49	0.65
1:2:1629:C:H2'	1:2:1630:A:H8	1.62	0.65
10:X:10:ALA:HB2	15:L:101:ARG:HB2	1.79	0.65
1:2:748:C:N4	1:2:794:A:N6	2.19	0.64
1:2:643:A:OP1	16:J:39:ASN:ND2	2.30	0.64
1:2:671:A:O2'	1:2:1089:G:OP2	2.14	0.64
1:2:64:A:H2	1:2:83:A:H62	1.44	0.64
1:2:1236:G:H21	1:2:1522:A:H62	1.44	0.64
1:2:507:G:OP1	8:Y:108:LYS:NZ	2.32	0.63
1:2:77:A:N7	7:G:154:ARG:NH1	2.46	0.62
10:X:11:ARG:NH2	15:L:104:LYS:O	2.32	0.62
4:E:127:ARG:HD2	4:E:142:HIS:HA	1.82	0.62
1:2:878:G:H1	1:2:908:A:N6	1.95	0.62
10:X:28:LYS:O	10:X:32:LEU:HB2	2.00	0.62
1:2:1156:U:OP1	11:W:71:LYS:NZ	2.32	0.62
1:2:1332:A:C6	1:2:1497:G:N1	2.68	0.61
1:2:943:U:H2'	1:2:944:A:H8	1.65	0.61
1:2:1534:C:C2	1:2:1598:G:C2	2.88	0.61
4:E:13:ALA:O	4:E:39:ARG:NH2	2.33	0.61
1:2:615:C:N3	1:2:628:A:N1	2.49	0.61
6:H:53:VAL:O	6:H:57:ARG:HB2	2.00	0.61
1:2:913:A:H2	6:H:99:ARG:H	1.48	0.61
3:B:33:VAL:HA	3:B:96:CYS:HB2	1.82	0.60
3:B:59:SER:HB3	3:B:63:LYS:HE2	1.82	0.60
6:H:105:THR:HG23	6:H:107:LYS:H	1.65	0.60
1:2:1606:G:H22	1:2:1632:G:H1'	1.66	0.60
3:B:49:VAL:HG21	3:B:62:LEU:HD12	1.84	0.60
6:H:154:ILE:HB	6:H:185:VAL:HG22	1.81	0.60
15:L:21:LYS:NZ	17:I:157:LYS:O	2.35	0.60
1:2:429:C:O2'	1:2:811:A:N1	2.34	0.59
1:2:1232:U:H2'	1:2:1233:G:H8	1.66	0.59
3:B:27:LYS:O	3:B:51:ARG:NE	2.36	0.59
15:L:38:LYS:NZ	15:L:66:VAL:O	2.33	0.59
7:G:56:ASN:ND2	7:G:60:GLY:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:373:G:H4'	15:L:85:THR:HG21	1.85	0.59
1:2:1761:U:O2	1:2:1771:G:N2	2.35	0.58
10:X:101:LEU:HB3	10:X:124:LYS:HB2	1.85	0.58
1:2:885:U:O2	1:2:901:G:O6	2.20	0.58
1:2:674:C:H2'	1:2:675:U:C6	2.38	0.58
1:2:1761:U:H3	1:2:1771:G:H1	1.50	0.58
1:2:560:A:H5'	16:J:174:LYS:HE3	1.86	0.58
4:E:97:GLU:OE2	4:E:113:ARG:NH1	2.37	0.58
1:2:615:C:N4	1:2:628:A:N6	2.38	0.57
1:2:507:G:OP2	8:Y:104:ARG:NH2	2.35	0.57
1:2:1226:G:H22	1:2:1640:A:H2	1.53	0.57
10:X:51:VAL:HA	10:X:72:VAL:HG12	1.85	0.57
10:X:111:ALA:HB2	10:X:119:ARG:HE	1.70	0.57
15:L:42:LEU:HD13	15:L:72:ILE:HD11	1.86	0.57
3:B:52:THR:HG22	3:B:54:GLY:H	1.69	0.57
23:3:275:LYS:HD2	23:3:278:GLN:HE21	1.69	0.57
1:2:943:U:H2'	1:2:944:A:C8	2.40	0.56
23:3:193:LYS:HB2	23:3:200:PRO:HD2	1.87	0.56
1:2:1033:G:N1	1:2:1080:A:O2'	2.32	0.56
1:2:846:G:OP1	4:E:106:LYS:NZ	2.38	0.56
1:2:928:G:H1	1:2:1013:U:H3	1.52	0.56
7:G:85:ARG:O	7:G:87:ARG:NH1	2.39	0.56
1:2:1084:A:OP1	1:2:1858:G:O2'	2.22	0.56
1:2:8:U:H3	1:2:1196:A:H62	1.54	0.56
4:E:100:ARG:NH2	4:E:121:TYR:O	2.39	0.56
1:2:749:U:C4	1:2:750:C:N4	2.74	0.56
1:2:1302:G:C6	1:2:1306:U:O4	2.59	0.56
11:W:87:GLU:O	11:W:91:ASN:ND2	2.39	0.56
1:2:1277:C:O2	1:2:1322:G:N2	2.39	0.56
1:2:1722:G:O6	1:2:1812:U:O2	2.24	0.56
16:J:107:GLU:O	16:J:113:GLN:NE2	2.35	0.56
16:J:159:PHE:CE2	16:J:165:TYR:HB2	2.39	0.55
1:2:677:G:O2'	1:2:1029:G:N2	2.40	0.55
4:E:122:LYS:HD2	4:E:164:LEU:HD21	1.88	0.55
1:2:1858:G:OP2	13:O:146:ARG:NH2	2.39	0.55
1:2:24:C:H42	1:2:650:A:H61	0.71	0.55
1:2:587:A:H5'	1:2:592:C:H41	1.72	0.55
1:2:1302:G:O6	1:2:1307:U:O4	2.25	0.55
1:2:1562:C:H2'	1:2:1563:G:H8	1.72	0.55
15:L:65:ASN:O	15:L:132:ARG:NH1	2.40	0.55
17:I:162:LEU:HD11	17:I:191:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:24:C:N3	1:2:650:A:N1	2.55	0.54
1:2:594:A:H61	1:2:643:A:H5"	1.72	0.54
4:E:88:ASP:OD1	4:E:122:LYS:NZ	2.39	0.54
4:E:173:ILE:HG23	4:E:230:LYS:HD3	1.90	0.54
1:2:218:U:O2	17:I:184:ARG:NH2	2.40	0.54
1:2:1707:U:O2'	23:3:195:ASN:OD1	2.25	0.54
7:G:21:GLU:OE1	7:G:22:ARG:NH2	2.38	0.54
1:2:818:A:OP1	16:J:80:ARG:NH2	2.39	0.54
4:E:107:GLY:HA2	4:E:189:LEU:HG	1.89	0.54
1:2:925:G:OP1	14:N:121:ARG:NH1	2.34	0.54
8:Y:5:VAL:HA	8:Y:28:LEU:O	2.08	0.54
1:2:1277:C:C2	1:2:1322:G:N2	2.76	0.54
1:2:190:G:O2'	1:2:209:A:N6	2.42	0.53
1:2:1332:A:N6	1:2:1497:G:C6	2.76	0.53
15:L:91:ASP:HB3	15:L:104:LYS:HE2	1.90	0.53
1:2:928:G:H2'	1:2:929:G:C8	2.43	0.53
1:2:368:U:OP1	1:2:369:C:O2'	2.25	0.53
1:2:992:A:OP1	22:5:242:ARG:NH1	2.41	0.53
16:J:131:ARG:NH1	16:J:143:ASN:O	2.42	0.53
3:B:137:LEU:HD11	3:B:176:VAL:HG21	1.90	0.53
1:2:303:C:O2	17:I:184:ARG:NH1	2.42	0.53
1:2:614:C:N3	1:2:629:A:N1	2.57	0.53
1:2:885:U:O2	1:2:902:G:C6	2.62	0.53
1:2:943:U:OP1	3:B:214:LYS:NZ	2.37	0.53
1:2:677:G:H1'	1:2:1029:G:H22	1.74	0.53
1:2:1701:C:H2'	1:2:1702:G:H8	1.73	0.53
1:2:318:A:H61	7:G:186:GLN:HE22	1.57	0.52
3:B:83:LYS:NZ	13:O:130:GLU:OE2	2.40	0.52
1:2:1286:G:N2	1:2:1312:G:O2'	2.43	0.52
1:2:1610:G:O6	1:2:1630:A:N6	2.42	0.52
14:N:3:ARG:HH12	14:N:10:GLY:H	1.56	0.52
16:J:134:HIS:HE1	16:J:164:PRO:HD2	1.73	0.52
1:2:1568:C:O2	1:2:1627:C:O2'	2.28	0.52
6:H:146:VAL:HG12	11:W:42:MET:HE1	1.91	0.52
4:E:212:ASP:OD1	4:E:213:ALA:N	2.40	0.52
8:Y:37:LYS:HD2	8:Y:57:VAL:HG23	1.91	0.52
3:B:62:LEU:HD22	3:B:91:VAL:HB	1.91	0.52
3:B:75:GLN:HB3	3:B:78:GLU:HB2	1.91	0.52
13:O:35:ALA:HB2	13:O:112:ALA:HB2	1.92	0.52
15:L:136:LYS:NZ	17:I:11:ARG:O	2.34	0.52
17:I:62:VAL:HG11	17:I:75:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:139:LEU:O	4:E:146:THR:HA	2.09	0.51
15:L:75:GLY:HA3	15:L:88:ILE:HD12	1.92	0.51
1:2:1331:C:N4	1:2:1499:U:H3	2.08	0.51
1:2:30:C:O2'	1:2:596:U:OP1	2.27	0.51
1:2:122:G:H21	4:E:146:THR:HG21	1.75	0.51
6:H:9:VAL:HG23	6:H:24:SER:HB3	1.92	0.51
23:3:188:LEU:HD11	23:3:208:ARG:HB2	1.92	0.51
1:2:1007:C:O2'	14:N:104:ARG:NH2	2.44	0.51
10:X:28:LYS:HG2	10:X:32:LEU:HD22	1.93	0.51
1:2:528:A:H2'	1:2:529:A:H8	1.76	0.51
1:2:913:A:OP2	6:H:99:ARG:NH2	2.41	0.51
1:2:1199:A:H5"	22:5:250:LYS:HE3	1.93	0.51
1:2:1550:G:H3'	1:2:1579:A:H61	1.76	0.51
1:2:164:A:H3'	1:2:165:G:H21	1.75	0.51
7:G:59:GLN:OE1	7:G:72:ARG:NH2	2.44	0.51
23:3:162:ARG:O	23:3:176:SER:OG	2.22	0.51
23:3:48:ILE:HG23	23:3:152:ILE:HG21	1.92	0.51
1:2:675:U:C2	1:2:676:C:H5	2.29	0.50
4:E:100:ARG:NH1	4:E:118:GLU:OE2	2.44	0.50
1:2:1649:U:H2'	1:2:1650:A:H8	1.77	0.50
1:2:640:A:H2'	1:2:641:A:C8	2.46	0.50
1:2:1227:G:N2	1:2:1635:C:O2'	2.44	0.50
10:X:7:LEU:HG	11:W:77:PRO:HB2	1.93	0.50
1:2:980:A:H2'	1:2:981:A:C8	2.46	0.50
1:2:1329:U:O2	1:2:1500:G:O6	2.30	0.50
1:2:1605:G:H21	1:2:1634:A:H62	1.60	0.49
1:2:981:A:H2'	1:2:982:G:C8	2.47	0.49
17:I:106:SER:HB3	17:I:171:LEU:HG	1.94	0.49
1:2:1296:U:O4	1:2:1301:A:N7	2.46	0.49
1:2:1050:A:OP1	1:2:1846:G:N2	2.40	0.49
6:H:46:THR:HG23	6:H:65:PRO:HD3	1.95	0.49
7:G:162:LEU:HB2	7:G:170:ARG:O	2.13	0.49
23:3:60:VAL:HA	23:3:124:THR:O	2.12	0.49
23:3:238:LEU:HD12	23:3:285:PHE:HB3	1.93	0.49
1:2:530:U:H2'	1:2:531:A:H8	1.77	0.49
1:2:1589:A:N3	1:2:1653:U:O2'	2.40	0.49
17:I:103:LEU:HD22	17:I:170:LYS:HB3	1.94	0.49
1:2:189:U:OP1	17:I:152:ARG:NH2	2.45	0.48
1:2:201:C:H3'	1:2:202:G:H8	1.78	0.48
1:2:1232:U:H3	1:2:1526:G:H1	1.59	0.48
4:E:54:TYR:O	8:Y:15:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:28:U:H2'	1:2:29:G:H8	1.78	0.48
6:H:68:GLN:O	6:H:71:SER:OG	2.23	0.48
4:E:128:LYS:HG2	4:E:140:VAL:HB	1.96	0.48
16:J:88:ASP:HB3	16:J:91:LYS:HG2	1.96	0.48
1:2:983:A:OP1	1:2:1073:U:O2'	2.25	0.48
4:E:174:LYS:HE3	4:E:174:LYS:HB3	1.69	0.48
1:2:115:U:OP1	1:2:382:C:O2'	2.28	0.47
1:2:528:A:H2'	1:2:529:A:C8	2.49	0.47
1:2:1275:G:O6	1:2:1324:G:N3	2.47	0.47
1:2:1332:A:C6	1:2:1497:G:C6	3.02	0.47
16:J:103:GLU:O	16:J:107:GLU:HG2	2.14	0.47
1:2:1013:U:OP1	1:2:1129:G:O2'	2.28	0.47
1:2:874:G:H2'	1:2:875:A:H8	1.79	0.47
1:2:974:C:O2	13:O:55:ARG:NH1	2.48	0.47
1:2:1331:C:H2'	1:2:1332:A:C8	2.49	0.47
1:2:1776:G:H2'	1:2:1777:G:C8	2.49	0.47
1:2:1286:G:H21	1:2:1313:A:H62	1.60	0.47
3:B:35:ALA:HB3	3:B:42:ARG:HA	1.96	0.47
14:N:133:ARG:HA	14:N:133:ARG:HD3	1.80	0.47
15:L:23:VAL:HG23	15:L:26:GLY:H	1.77	0.47
1:2:1726:G:H2'	1:2:1727:G:H8	1.79	0.47
1:2:1228:A:H2'	1:2:1229:G:C8	2.49	0.47
1:2:1701:C:H2'	1:2:1702:G:C8	2.50	0.47
3:B:57:ILE:HG13	3:B:60:ASP:H	1.80	0.47
14:N:86:GLU:O	14:N:90:HIS:ND1	2.47	0.47
1:2:379:C:H5'	17:I:33:ALA:HA	1.97	0.47
1:2:1776:G:H2'	1:2:1777:G:H8	1.80	0.47
1:2:1778:C:H2'	1:2:1779:G:C8	2.50	0.47
17:I:101:ILE:HD12	17:I:190:LEU:HD11	1.97	0.47
1:2:107:A:H2'	1:2:108:G:C8	2.50	0.47
1:2:380:G:N1	1:2:383:G:OP2	2.37	0.47
1:2:686:U:O2	6:H:118:ARG:NH2	2.36	0.47
1:2:857:U:H2'	1:2:858:A:C8	2.50	0.47
3:B:39:PHE:CE2	3:B:74:LEU:HD13	2.50	0.47
1:2:118:C:H1'	1:2:445:A:C5	2.50	0.46
1:2:1236:G:N2	1:2:1522:A:H62	2.09	0.46
8:Y:114:MET:O	8:Y:122:LYS:NZ	2.42	0.46
1:2:1534:C:N3	1:2:1598:G:C2	2.83	0.46
1:2:1759:G:H2'	1:2:1760:G:C8	2.50	0.46
1:2:482:G:H5'	10:X:76:LYS:HB3	1.98	0.46
1:2:1536:G:H2'	1:2:1537:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1010:G:H2'	1:2:1011:A:C8	2.50	0.46
1:2:1746:U:OP1	7:G:31:ARG:NH2	2.44	0.46
1:2:1778:C:H2'	1:2:1779:G:H8	1.81	0.46
10:X:52:LEU:HD11	10:X:73:GLN:HB2	1.98	0.46
1:2:1295:A:H2'	1:2:1296:U:H6	1.81	0.46
1:2:145:G:H2'	1:2:146:G:C8	2.51	0.46
1:2:1271:C:O2'	1:2:1303:C:O2	2.32	0.46
1:2:1297:U:N3	1:2:1300:U:OP2	2.49	0.46
7:G:52:ILE:HA	7:G:111:LEU:HD23	1.98	0.46
1:2:658:U:N3	10:X:20:GLN:O	2.41	0.45
4:E:100:ARG:HB2	4:E:114:ILE:HD13	1.96	0.45
1:2:1854:U:OP1	13:O:147:ARG:NH1	2.49	0.45
3:B:167:LYS:HA	3:B:170:GLU:HG2	1.97	0.45
1:2:562:U:H2'	1:2:563:G:C8	2.51	0.45
20:K:1249:ASP:OD1	20:K:1249:ASP:N	2.49	0.45
1:2:1025:U:OP1	1:2:1090:C:O2'	2.27	0.45
1:2:1871:C:OP1	1:2:1873:G:N1	2.49	0.45
1:2:1145:A:N3	22:5:250:LYS:NZ	2.65	0.45
1:2:1199:A:H2'	1:2:1200:A:C8	2.51	0.45
17:I:83:TYR:HB3	17:I:101:ILE:HB	1.99	0.45
1:2:1332:A:N6	1:2:1497:G:O6	2.50	0.45
23:3:192:GLY:O	23:3:195:ASN:ND2	2.45	0.45
1:2:823:U:H5	16:J:143:ASN:HB2	1.82	0.45
1:2:1228:A:H2'	1:2:1229:G:H8	1.81	0.45
1:2:223:C:H2'	1:2:224:A:C8	2.51	0.44
7:G:211:LYS:HB3	7:G:211:LYS:HE2	1.83	0.44
1:2:384:U:O4	17:I:5:ARG:NH2	2.47	0.44
1:2:527:C:H2'	1:2:528:A:H8	1.82	0.44
1:2:986:G:OP1	1:2:1001:A:O2'	2.34	0.44
7:G:38:ALA:HB1	7:G:41:LEU:HD23	1.98	0.44
7:G:57:ASP:HA	7:G:106:LEU:HA	1.99	0.44
4:E:211:LYS:HE3	4:E:211:LYS:HB3	1.83	0.44
15:L:40:ILE:HD11	15:L:143:LEU:HD22	1.98	0.44
1:2:507:G:P	8:Y:104:ARG:HH22	2.40	0.44
1:2:940:U:H3	1:2:1002:U:H3	1.66	0.44
1:2:1207:G:C2	1:2:1695:A:N6	2.86	0.44
1:2:1331:C:H42	1:2:1499:U:H3	1.64	0.44
1:2:1714:U:C2	1:2:1820:G:C2	3.04	0.44
1:2:54:A:OP1	8:Y:111:LYS:NZ	2.36	0.44
1:2:581:U:H4'	8:Y:66:GLY:HA2	1.99	0.44
1:2:1753:C:H2'	1:2:1754:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:126:HIS:CE1	6:H:181:THR:HG23	2.53	0.44
23:3:98:VAL:HG11	23:3:107:LEU:HD22	1.99	0.44
1:2:1113:A:H5"	1:2:1114:U:H4'	1.99	0.44
23:3:197:ARG:HA	23:3:198:PRO:HA	1.81	0.44
1:2:1605:G:N2	1:2:1634:A:H62	2.15	0.44
8:Y:86:GLU:OE1	8:Y:90:ARG:HD2	2.18	0.44
10:X:34:THR:HA	10:X:37:LYS:HB2	2.00	0.44
1:2:560:A:H5'	16:J:174:LYS:HB2	1.99	0.43
1:2:1098:C:H2'	1:2:1099:G:C8	2.53	0.43
1:2:1228:A:O2'	1:2:1634:A:N3	2.40	0.43
1:2:1597:C:N4	1:2:1598:G:O6	2.51	0.43
3:B:195:LYS:HB3	3:B:195:LYS:HE3	1.77	0.43
6:H:53:VAL:HG21	6:H:172:THR:HA	1.99	0.43
23:3:125:CYS:O	23:3:151:ALA:HA	2.18	0.43
3:B:139:CYS:HB3	3:B:172:MET:HE1	2.01	0.43
6:H:100:ILE:HD12	6:H:122:LEU:HD12	1.99	0.43
10:X:40:PRO:HA	10:X:79:LYS:HD2	2.01	0.43
1:2:1275:G:O6	1:2:1324:G:N2	2.51	0.43
16:J:136:ARG:HE	16:J:158:ASP:HB3	1.82	0.43
1:2:1707:U:H5'	23:3:194:ASN:HD22	1.83	0.43
4:E:126:VAL:HA	4:E:141:THR:HA	2.00	0.43
6:H:95:ILE:HD11	6:H:133:LEU:HD13	2.00	0.43
1:2:1289:U:H2'	1:2:1290:G:C8	2.54	0.43
3:B:107:ARG:NH1	13:O:133:THR:O	2.52	0.43
8:Y:99:LYS:HE3	8:Y:99:LYS:HB2	1.85	0.43
1:2:1217:A:H2'	1:2:1218:C:H6	1.84	0.43
1:2:1726:G:H2'	1:2:1727:G:C8	2.53	0.43
15:L:126:VAL:HG12	15:L:145:VAL:HG22	2.00	0.43
23:3:222:GLU:HG3	23:3:302:LEU:HD11	2.00	0.43
4:E:87:MET:HG2	4:E:123:LEU:O	2.19	0.43
23:3:239:SER:O	23:3:243:LYS:HG2	2.19	0.43
1:2:104:A:H62	1:2:356:C:H5	1.66	0.42
1:2:1037:G:H4'	1:2:1845:A:H4'	2.01	0.42
1:2:1748:G:H2'	1:2:1749:G:H8	1.83	0.42
15:L:40:ILE:HD11	15:L:68:ILE:HG13	2.00	0.42
1:2:65:C:H4'	7:G:172:LYS:HD3	2.02	0.42
1:2:1545:A:N3	1:2:1671:G:O2'	2.41	0.42
8:Y:37:LYS:HA	8:Y:40:ILE:HD12	2.02	0.42
13:O:43:HIS:HA	13:O:55:ARG:HB3	2.02	0.42
1:2:1822:A:H2'	1:2:1823:A:C8	2.54	0.42
23:3:157:ARG:HG3	23:3:203:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:115:U:O2'	1:2:381:C:O2	2.31	0.42
1:2:747:U:H2'	1:2:748:C:C6	2.55	0.42
1:2:1297:U:H3	1:2:1299:A:H3'	1.84	0.42
23:3:163:LEU:HG	23:3:185:VAL:HG21	2.02	0.42
16:J:53:ILE:HD13	16:J:81:LEU:HD21	2.01	0.42
1:2:1710:C:H41	1:2:1823:A:N6	2.14	0.42
1:2:455:A:O2'	1:2:1735:A:N3	2.42	0.42
1:2:1051:G:H2'	1:2:1052:A:C8	2.55	0.41
4:E:137:PRO:HB2	4:E:150:PRO:HD2	2.01	0.41
4:E:143:ASP:OD1	4:E:143:ASP:N	2.53	0.41
4:E:164:LEU:HD23	4:E:164:LEU:HA	1.89	0.41
17:I:76:THR:HG21	17:I:104:ILE:HD12	2.02	0.41
1:2:1272:C:OP1	1:2:1303:C:O2'	2.38	0.41
1:2:1848:U:O4	23:3:174:ARG:NE	2.53	0.41
17:I:135:GLU:O	17:I:139:LYS:HB3	2.20	0.41
1:2:1593:C:H2'	1:2:1594:A:H8	1.84	0.41
6:H:101:LEU:HD23	6:H:101:LEU:HA	1.93	0.41
1:2:71:G:H2'	1:2:72:C:O4'	2.21	0.41
1:2:399:C:H5	1:2:680:G:H5'	1.85	0.41
1:2:540:U:H2'	1:2:542:U:H5	1.86	0.41
1:2:1536:G:H2'	1:2:1537:A:H8	1.86	0.41
17:I:87:ASN:HB3	17:I:90:LEU:HG	2.02	0.41
17:I:157:LYS:HD2	17:I:157:LYS:HA	1.80	0.41
23:3:254:ASN:ND2	23:3:311:HIS:O	2.42	0.41
1:2:816:A:OP2	16:J:10:ARG:NH2	2.45	0.41
1:2:1206:G:C6	1:2:1207:G:H1'	2.56	0.41
1:2:1562:C:H2'	1:2:1563:G:C8	2.54	0.41
1:2:1797:U:H2'	1:2:1798:C:C6	2.56	0.41
4:E:11:ARG:HA	4:E:28:ALA:HB2	2.01	0.41
6:H:145:ARG:HD2	11:W:51:GLU:HB2	2.01	0.41
1:2:368:U:H3'	1:2:369:C:H2'	2.02	0.41
1:2:28:U:H2'	1:2:29:G:C8	2.56	0.41
1:2:302:A:O5'	17:I:74:ARG:NH2	2.53	0.41
1:2:1325:G:O2'	1:2:1327:G:OP2	2.29	0.41
1:2:1712:A:N1	1:2:1822:A:N6	2.69	0.41
14:N:5:HIS:NE2	14:N:121:ARG:HG3	2.36	0.41
16:J:28:GLU:HG2	16:J:43:VAL:HG11	2.02	0.41
1:2:1565:C:H2'	1:2:1566:G:C8	2.55	0.41
1:2:1710:C:H2'	1:2:1711:U:C6	2.56	0.41
1:2:1798:C:H2'	1:2:1799:G:O4'	2.21	0.41
7:G:14:LYS:HE2	7:G:124:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:134:HIS:CE1	16:J:164:PRO:HD2	2.53	0.41
1:2:128:U:H5'	1:2:129:C:H5	1.86	0.41
1:2:1606:G:H1	1:2:1632:G:H1'	1.86	0.41
7:G:44:GLU:HG2	7:G:45:TRP:CD1	2.56	0.41
11:W:71:LYS:O	11:W:129:PHE:HA	2.21	0.41
23:3:130:PRO:HD2	23:3:133:ILE:HD11	2.02	0.41
1:2:750:C:H2'	1:2:751:G:C8	2.56	0.40
1:2:885:U:O2	1:2:901:G:C6	2.75	0.40
1:2:962:A:N1	1:2:1055:A:O2'	2.54	0.40
1:2:1221:G:H2'	1:2:1222:G:H8	1.86	0.40
1:2:1334:G:H2'	1:2:1335:G:H8	1.86	0.40
16:J:142:VAL:HG12	16:J:144:ILE:H	1.86	0.40
1:2:1004:U:H2'	1:2:1005:G:C8	2.56	0.40
1:2:1051:G:H2'	1:2:1052:A:H8	1.86	0.40
1:2:1207:G:N2	1:2:1695:A:N6	2.69	0.40
3:B:87:ILE:HG22	3:B:101:HIS:HB2	2.03	0.40
6:H:75:ILE:HA	6:H:78:ARG:HH21	1.86	0.40
1:2:382:C:H2'	1:2:383:G:H8	1.87	0.40
1:2:508:A:H3'	1:2:509:G:H8	1.87	0.40
1:2:604:A:H2'	1:2:605:A:C8	2.57	0.40
1:2:675:U:C2	1:2:676:C:C5	3.09	0.40
15:L:111:VAL:HG12	15:L:140:PHE:HB2	2.03	0.40
23:3:91:VAL:HG13	23:3:109:VAL:HG11	2.03	0.40
1:2:996:A:H2'	1:2:997:A:C8	2.55	0.40
23:3:60:VAL:HG11	23:3:74:LEU:HD22	2.02	0.40
10:X:67:ARG:HA	10:X:67:ARG:HD2	1.83	0.40
11:W:14:ILE:HG13	11:W:27:ILE:HD11	2.03	0.40
17:I:141:ARG:HD2	17:I:146:GLN:CD	2.41	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	
2	b	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
3	B	211/264 (80%)	202 (96%)	9 (4%)	0	100	100
4	E	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
5	e	18/59 (30%)	18 (100%)	0	0	100	100
6	H	184/194 (95%)	176 (96%)	8 (4%)	0	100	100
7	G	228/249 (92%)	224 (98%)	4 (2%)	0	100	100
8	Y	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
9	x	173/252 (69%)	166 (96%)	7 (4%)	0	100	100
10	X	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
11	W	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
12	u	618/804 (77%)	593 (96%)	25 (4%)	0	100	100
13	O	133/151 (88%)	121 (91%)	12 (9%)	0	100	100
14	N	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
15	L	149/158 (94%)	139 (93%)	10 (7%)	0	100	100
16	J	178/194 (92%)	173 (97%)	4 (2%)	1 (1%)	25	64
17	I	203/208 (98%)	200 (98%)	3 (2%)	0	100	100
18	r	116/125 (93%)	107 (92%)	9 (8%)	0	100	100
19	q	222/281 (79%)	216 (97%)	6 (3%)	0	100	100
20	K	54/1297 (4%)	52 (96%)	2 (4%)	0	100	100
21	z	28/230 (12%)	28 (100%)	0	0	100	100
22	5	54/771 (7%)	51 (94%)	3 (6%)	0	100	100
23	3	275/313 (88%)	267 (97%)	8 (3%)	0	100	100
All	All	3719/6454 (58%)	3578 (96%)	140 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	J	161	LEU

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	
2	b	74/76 (97%)	74 (100%)	0	100	100
3	B	194/231 (84%)	194 (100%)	0	100	100
4	E	224/225 (100%)	224 (100%)	0	100	100
5	e	18/48 (38%)	18 (100%)	0	100	100
6	H	167/174 (96%)	166 (99%)	1 (1%)	86	94
7	G	200/218 (92%)	200 (100%)	0	100	100
8	Y	108/115 (94%)	108 (100%)	0	100	100
9	x	148/208 (71%)	147 (99%)	1 (1%)	84	94
10	X	113/115 (98%)	113 (100%)	0	100	100
11	W	112/113 (99%)	112 (100%)	0	100	100
12	u	550/705 (78%)	549 (100%)	1 (0%)	93	98
13	O	105/119 (88%)	105 (100%)	0	100	100
14	N	130/131 (99%)	130 (100%)	0	100	100
15	L	135/142 (95%)	133 (98%)	2 (2%)	65	85
16	J	160/168 (95%)	160 (100%)	0	100	100
17	I	178/180 (99%)	176 (99%)	2 (1%)	73	88
18	r	105/112 (94%)	104 (99%)	1 (1%)	76	90
19	q	191/240 (80%)	191 (100%)	0	100	100
20	K	47/1094 (4%)	46 (98%)	1 (2%)	53	79
21	z	28/185 (15%)	28 (100%)	0	100	100
22	5	44/686 (6%)	44 (100%)	0	100	100
23	3	248/276 (90%)	245 (99%)	3 (1%)	71	88
All	All	3279/5561 (59%)	3267 (100%)	12 (0%)	91	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	H	162	GLN
9	x	110	ASN
12	u	351	ARG
15	L	30	LYS
15	L	69	ARG
17	I	99	ASN

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Mol	Chain	Res	Type
17	I	139	LYS
18	r	7	ASN
20	K	1237	LYS
23	3	40	LYS
23	3	202	VAL
23	3	208	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
6	H	162	GLN
6	H	165	ASN
9	x	217	ASN
12	u	104	GLN
12	u	670	GLN
23	3	278	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1465/1873 (78%)	321 (21%)	28 (1%)

All (321) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	6	G
1	2	9	U
1	2	26	U
1	2	33	G
1	2	46	A
1	2	56	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U

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Mol	Chain	Res	Type
1	2	79	A
1	2	92	A
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	128	U
1	2	130	G
1	2	143	U
1	2	144	U
1	2	147	A
1	2	155	G
1	2	160	U
1	2	163	U
1	2	168	C
1	2	172	U
1	2	181	A
1	2	184	G
1	2	190	G
1	2	291	G
1	2	292	A
1	2	295	C
1	2	302	A
1	2	310	C
1	2	313	A
1	2	315	C
1	2	319	C
1	2	332	G
1	2	333	G
1	2	335	G
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	368	U
1	2	369	C
1	2	370	G
1	2	377	G
1	2	382	C
1	2	385	G
1	2	386	C

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Mol	Chain	Res	Type
1	2	400	C
1	2	409	C
1	2	413	G
1	2	418	A
1	2	429	C
1	2	441	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	465	A
1	2	466	G
1	2	467	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	487	U
1	2	492	C
1	2	516	A
1	2	544	G
1	2	546	G
1	2	547	G
1	2	548	C
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	563	G
1	2	568	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	599	A
1	2	601	G
1	2	603	C

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Mol	Chain	Res	Type
1	2	604	A
1	2	605	A
1	2	607	U
1	2	608	C
1	2	613	G
1	2	631	U
1	2	635	G
1	2	637	U
1	2	643	A
1	2	644	G
1	2	648	A
1	2	655	A
1	2	660	C
1	2	664	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	674	C
1	2	675	U
1	2	678	U
1	2	679	A
1	2	680	G
1	2	683	G
1	2	684	G
1	2	687	C
1	2	688	U
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	794	A
1	2	797	C
1	2	798	G
1	2	799	U
1	2	801	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	844	U
1	2	847	A

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Mol	Chain	Res	Type
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	880	G
1	2	881	G
1	2	886	A
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	896	U
1	2	898	U
1	2	903	A
1	2	908	A
1	2	913	A
1	2	914	U
1	2	916	A
1	2	920	A
1	2	922	A
1	2	926	A
1	2	930	C
1	2	933	G
1	2	934	G
1	2	959	G
1	2	963	A
1	2	970	G
1	2	971	G
1	2	981	A
1	2	990	A
1	2	991	G
1	2	992	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1026	C
1	2	1028	A
1	2	1041	G
1	2	1049	A

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Mol	Chain	Res	Type
1	2	1050	A
1	2	1071	G
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1089	G
1	2	1099	G
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1121	G
1	2	1123	C
1	2	1138	C
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1171	G
1	2	1195	A
1	2	1200	A
1	2	1201	U
1	2	1203	G
1	2	1204	A
1	2	1206	G
1	2	1207	G
1	2	1210	G
1	2	1211	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1234	C
1	2	1235	G
1	2	1242	U
1	2	1243	U
1	2	1265	A
1	2	1271	C
1	2	1273	C
1	2	1274	G

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Mol	Chain	Res	Type
1	2	1275	G
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1296	U
1	2	1299	A
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1305	C
1	2	1307	U
1	2	1308	U
1	2	1309	C
1	2	1312	G
1	2	1313	A
1	2	1315	U
1	2	1317	C
1	2	1322	G
1	2	1323	U
1	2	1325	G
1	2	1327	G
1	2	1335	G
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1491	G
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1512	C
1	2	1519	U
1	2	1523	C
1	2	1531	A
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1551	U
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1569	A
1	2	1570	G

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Mol	Chain	Res	Type
1	2	1580	A
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1588	A
1	2	1601	A
1	2	1602	U
1	2	1606	G
1	2	1617	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1639	G
1	2	1640	A
1	2	1642	U
1	2	1647	A
1	2	1648	G
1	2	1654	G
1	2	1661	A
1	2	1662	U
1	2	1663	A
1	2	1664	A
1	2	1665	G
1	2	1666	C
1	2	1669	G
1	2	1675	A
1	2	1683	C
1	2	1694	U
1	2	1695	A
1	2	1704	C
1	2	1710	C
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1727	G
1	2	1729	U
1	2	1744	G
1	2	1756	C
1	2	1761	U
1	2	1772	C
1	2	1783	C
1	2	1784	G

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Mol	Chain	Res	Type
1	2	1801	A
1	2	1805	G
1	2	1824	A
1	2	1825	A
1	2	1839	U
1	2	1841	C
1	2	1846	G
1	2	1861	G
1	2	1864	U
1	2	1865	C
1	2	1872	G
1	2	1873	G

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	417	C
1	2	440	G
1	2	465	A
1	2	604	A
1	2	636	C
1	2	750	C
1	2	870	A
1	2	958	G
1	2	980	A
1	2	1231	C
1	2	1264	C
1	2	1295	A
1	2	1304	U
1	2	1494	U
1	2	1497	G
1	2	1511	U
1	2	1534	C
1	2	1565	C
1	2	1601	A

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Mol	Chain	Res	Type
1	2	1693	G
1	2	1726	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 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.

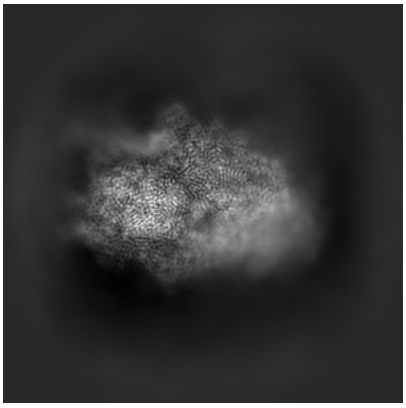
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32799. These allow visual inspection of the internal detail of the map and identification of artifacts.

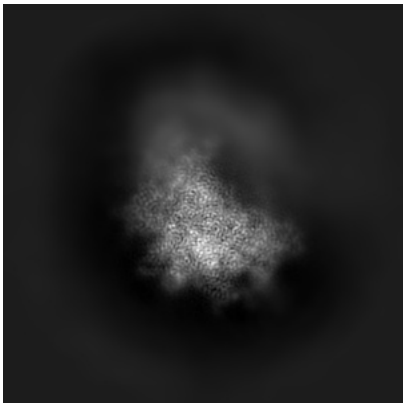
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

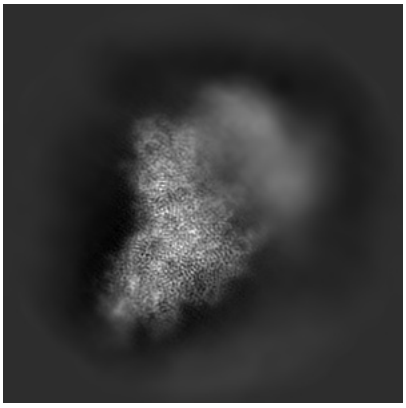
6.1.1 Primary map



X



Y

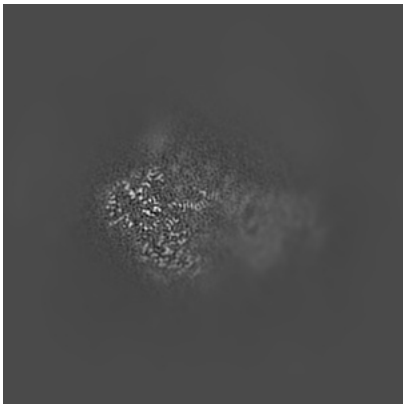


Z

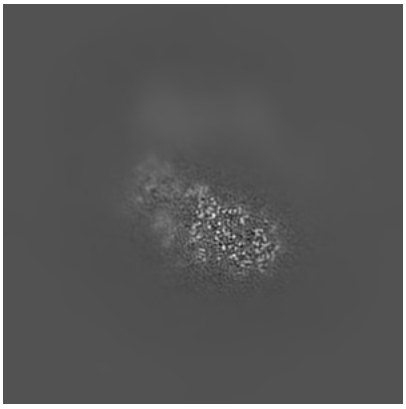
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

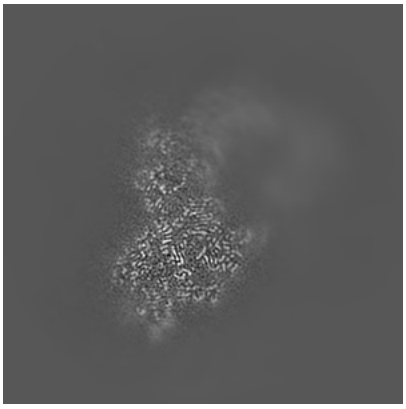
6.2.1 Primary map



X Index: 180



Y Index: 180

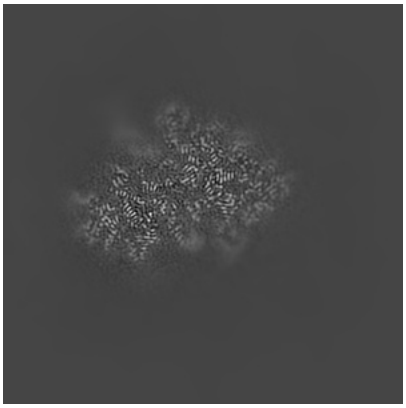


Z Index: 180

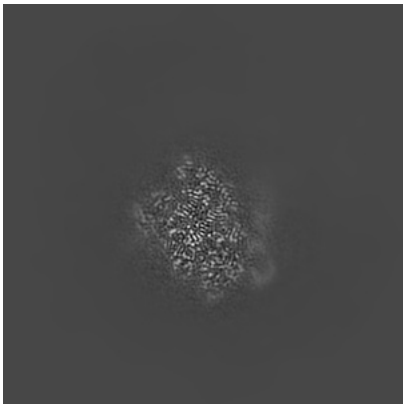
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

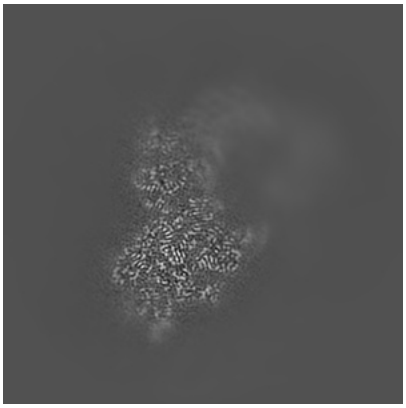
6.3.1 Primary map



X Index: 143



Y Index: 132

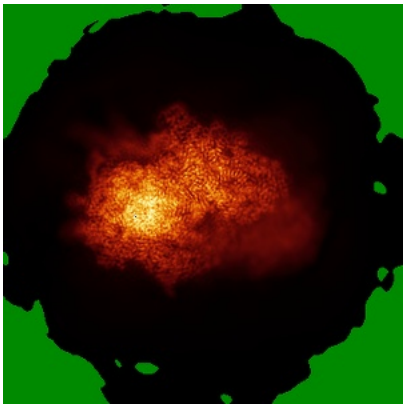


Z Index: 181

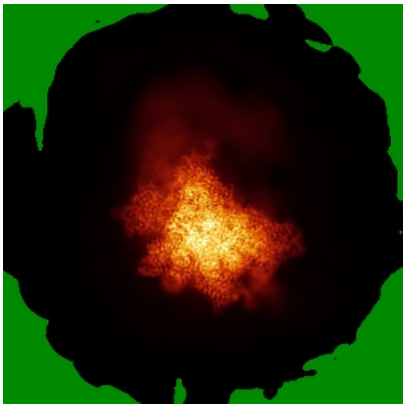
The images above show the largest variance slices of the map in three orthogonal directions.

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

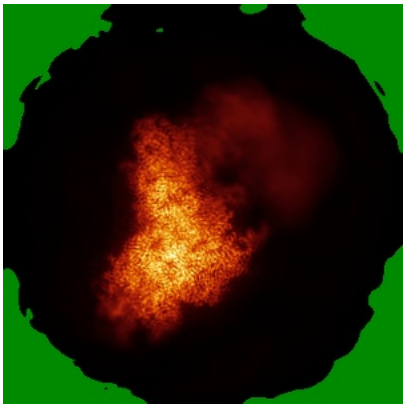
6.4.1 Primary map



X



Y

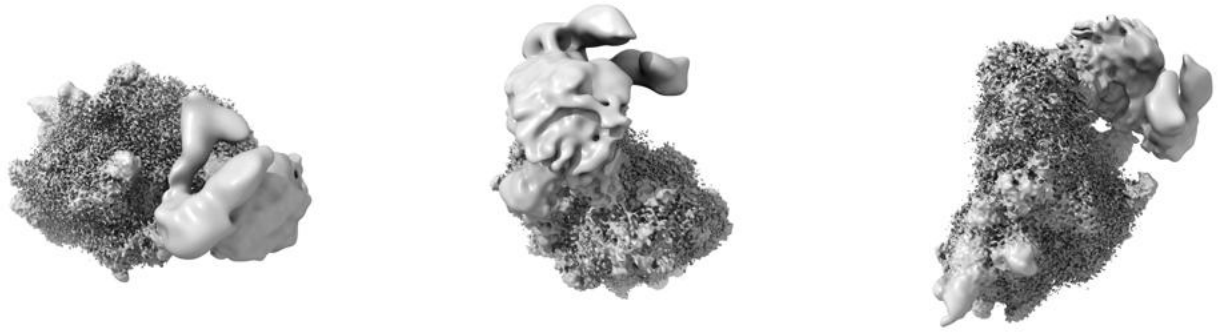


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

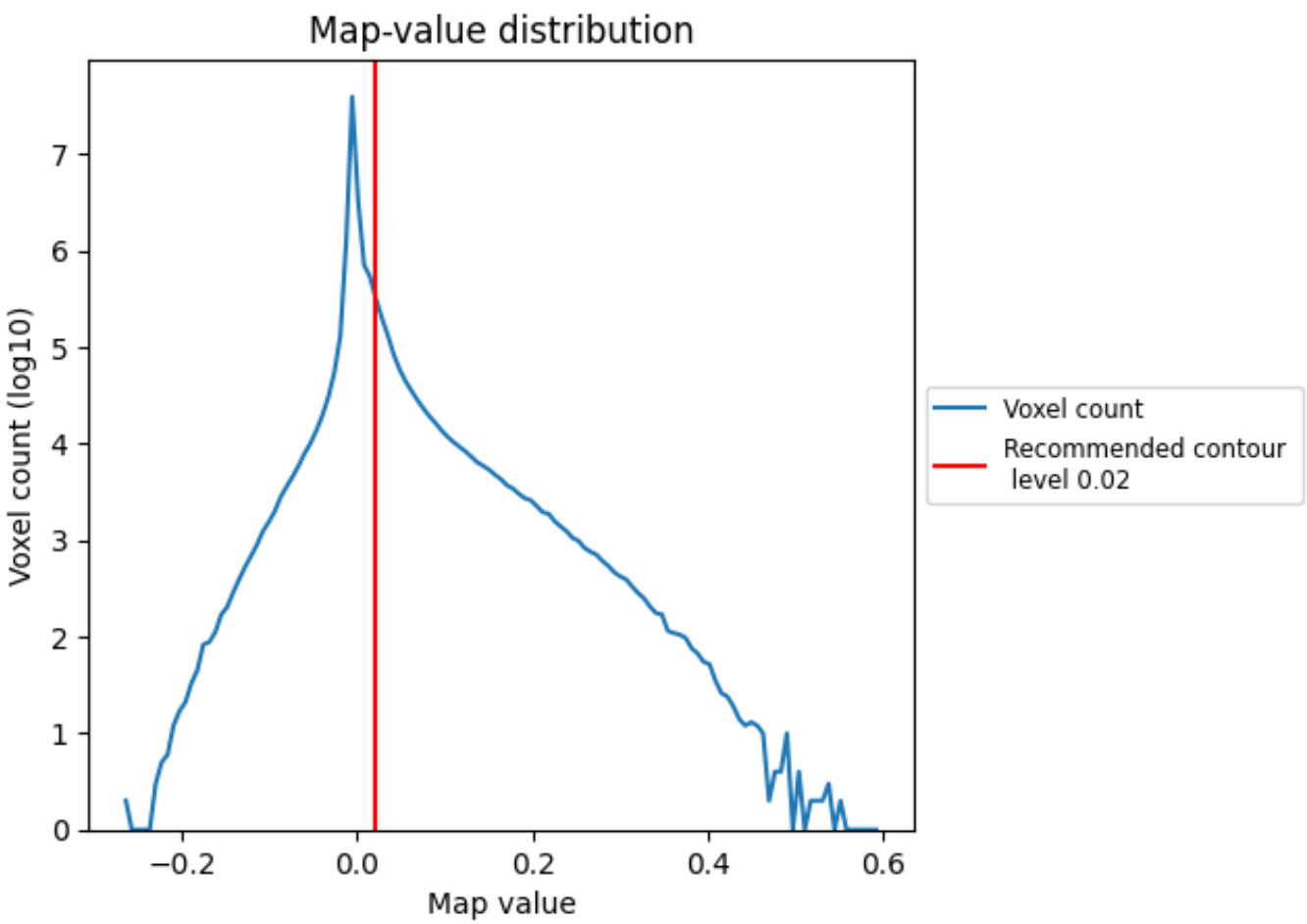
6.6 Mask visualisation (i)

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

7 Map analysis (i)

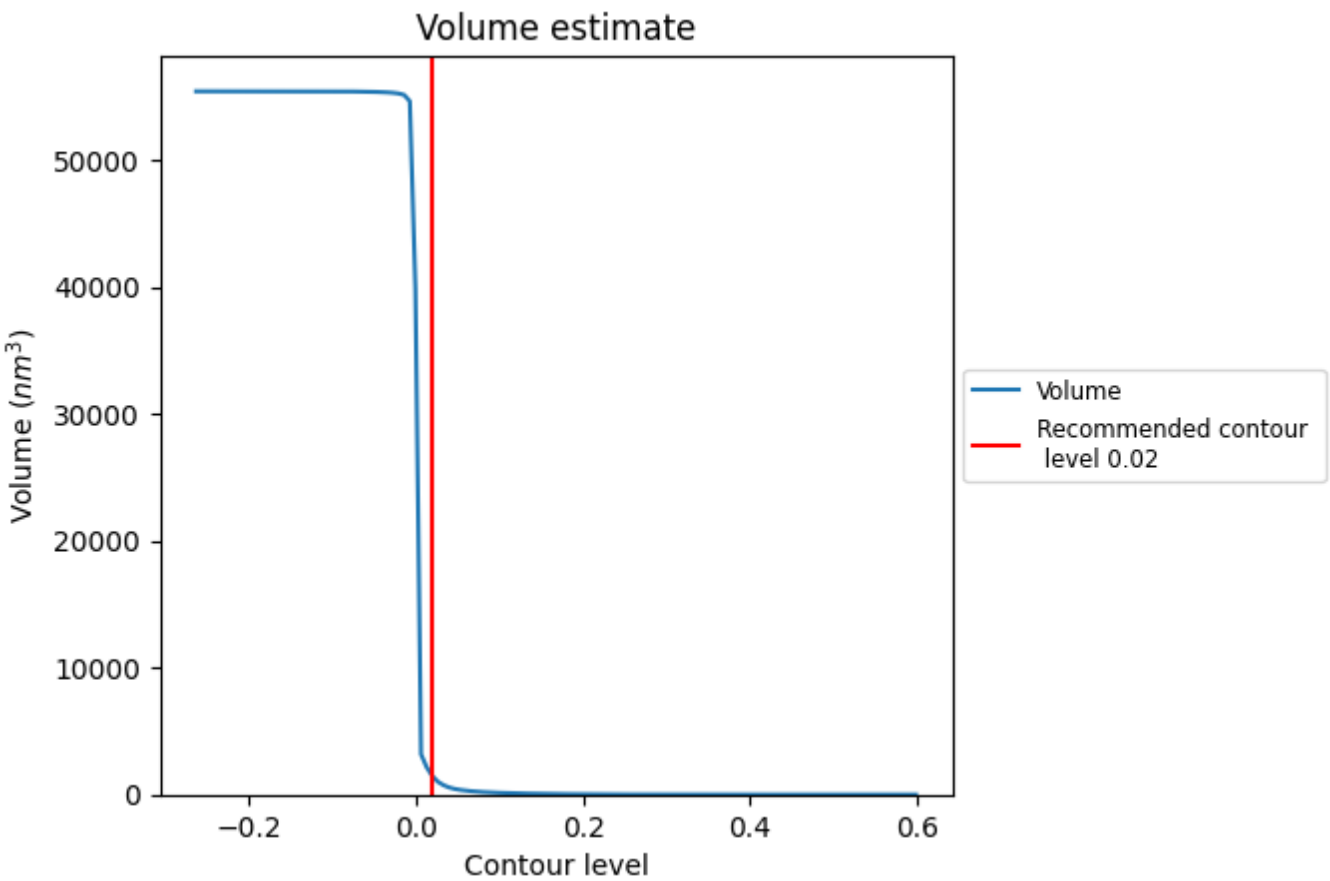
This section contains the results of statistical analysis of the map.

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.

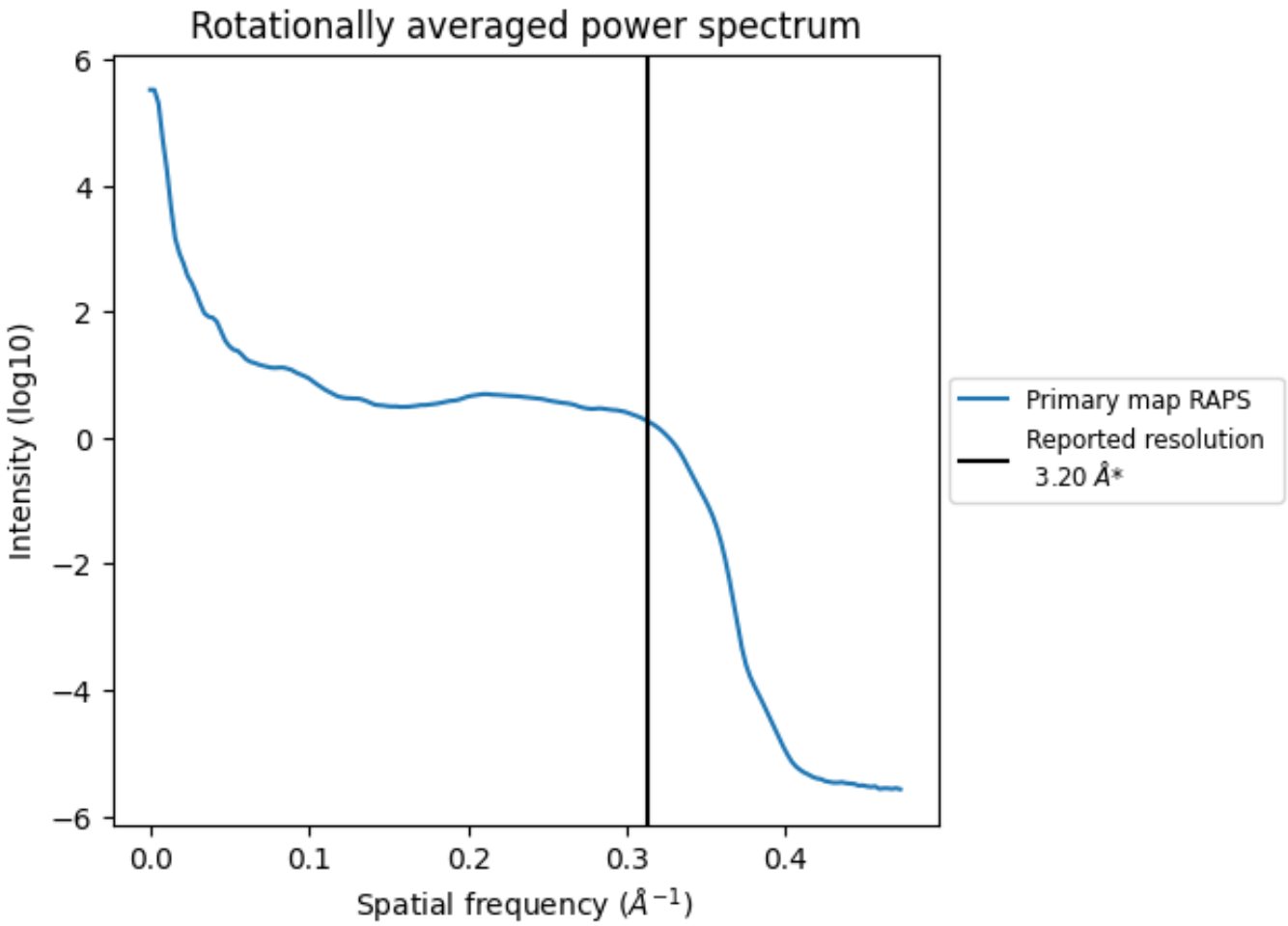
7.2 Volume estimate (i)



The volume at the recommended contour level is 1425 nm^3; this corresponds to an approximate mass of 1288 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)

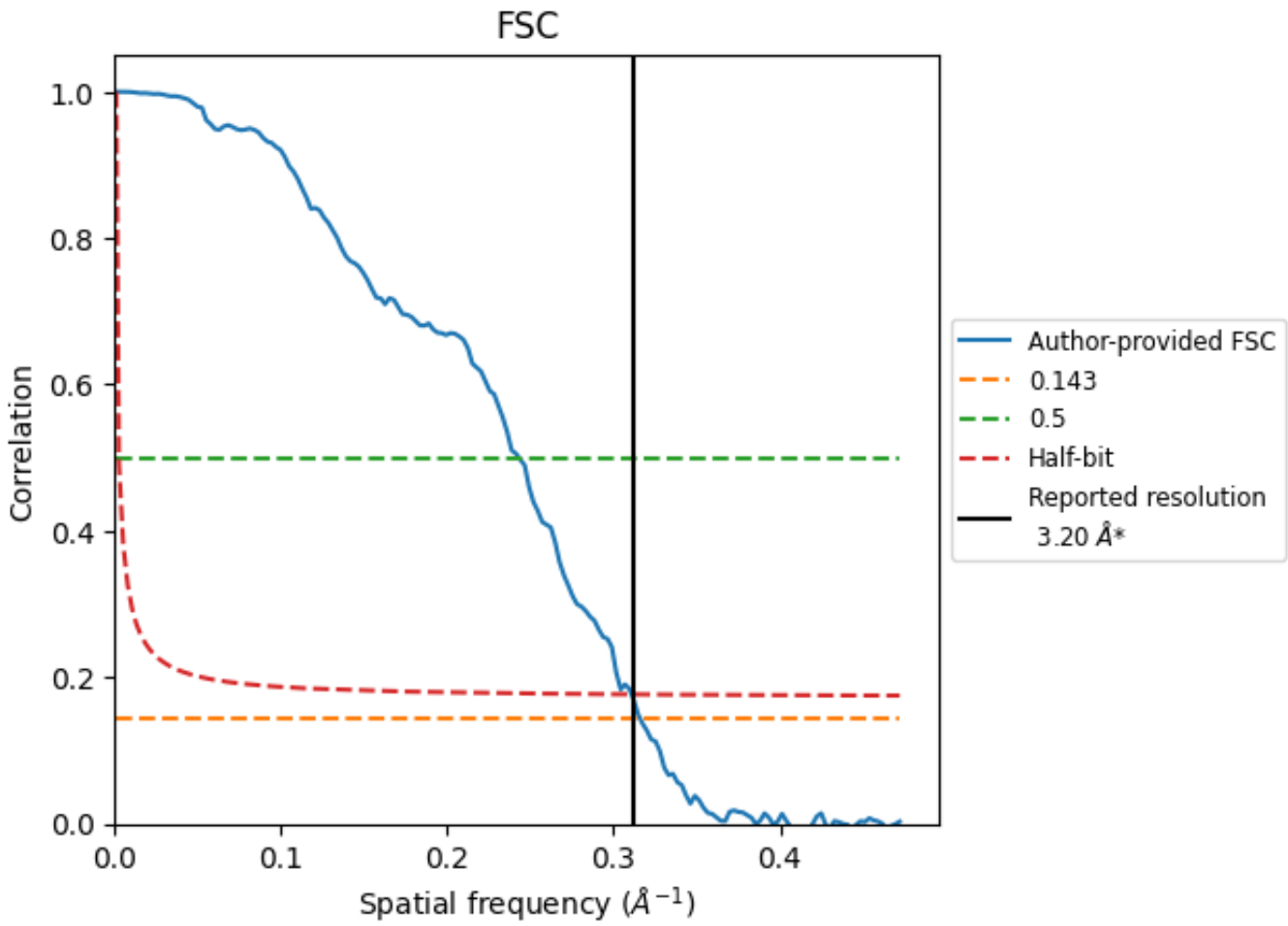


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

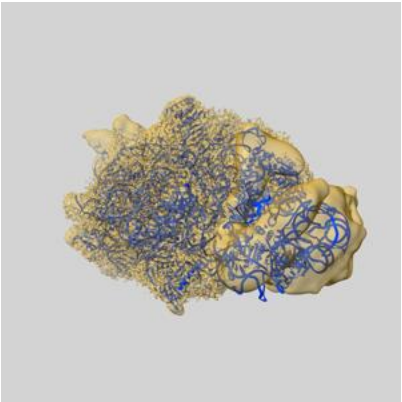
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.16	4.11	3.22
Unmasked-calculated*	-	-	-

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

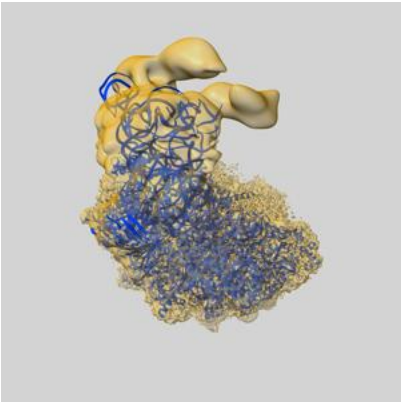
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32799 and PDB model 7WTS. Per-residue inclusion information can be found in section 3 on page 8.

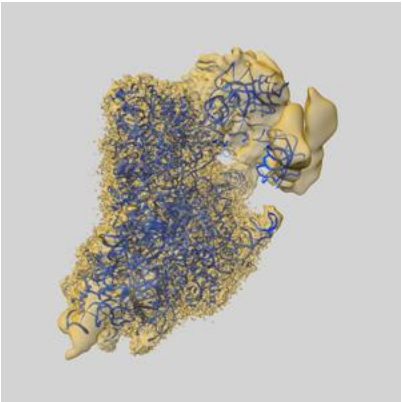
9.1 Map-model overlay (i)



X



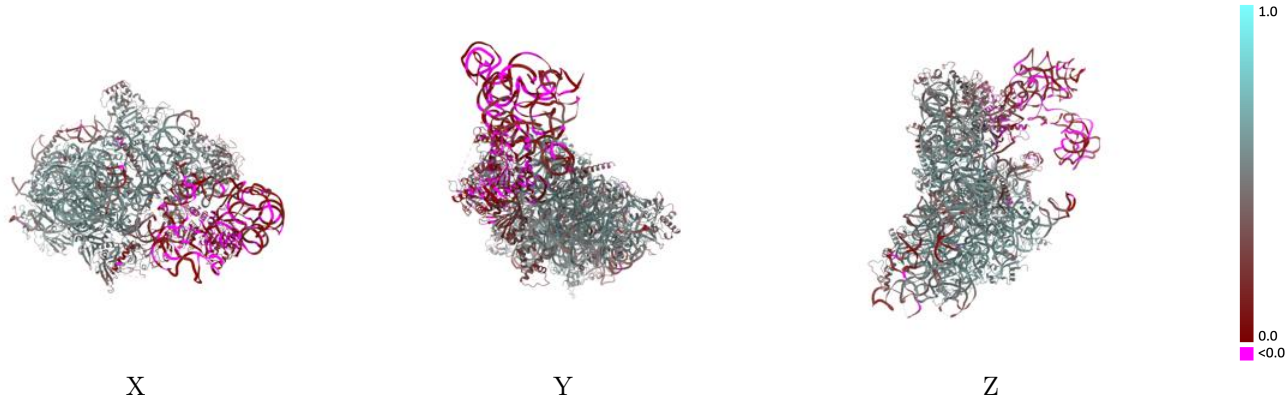
Y



Z

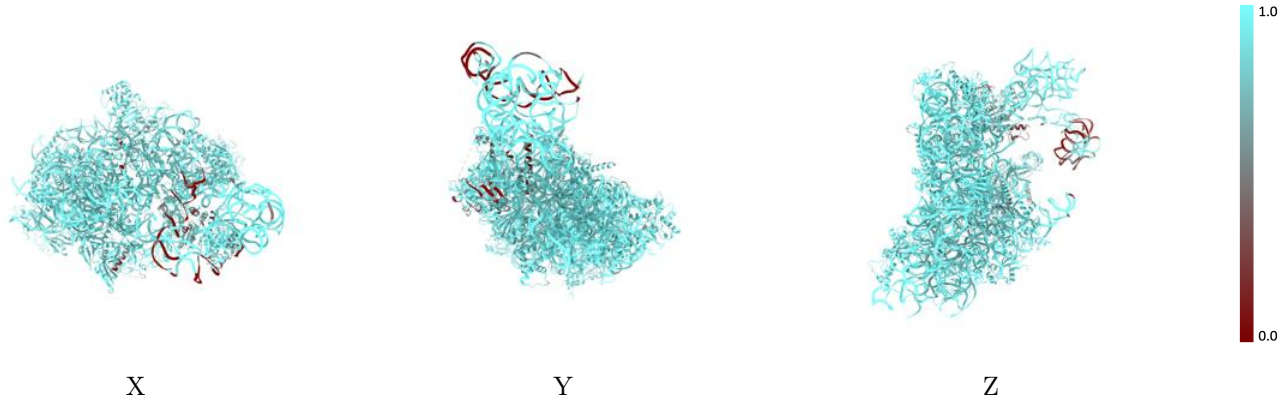
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



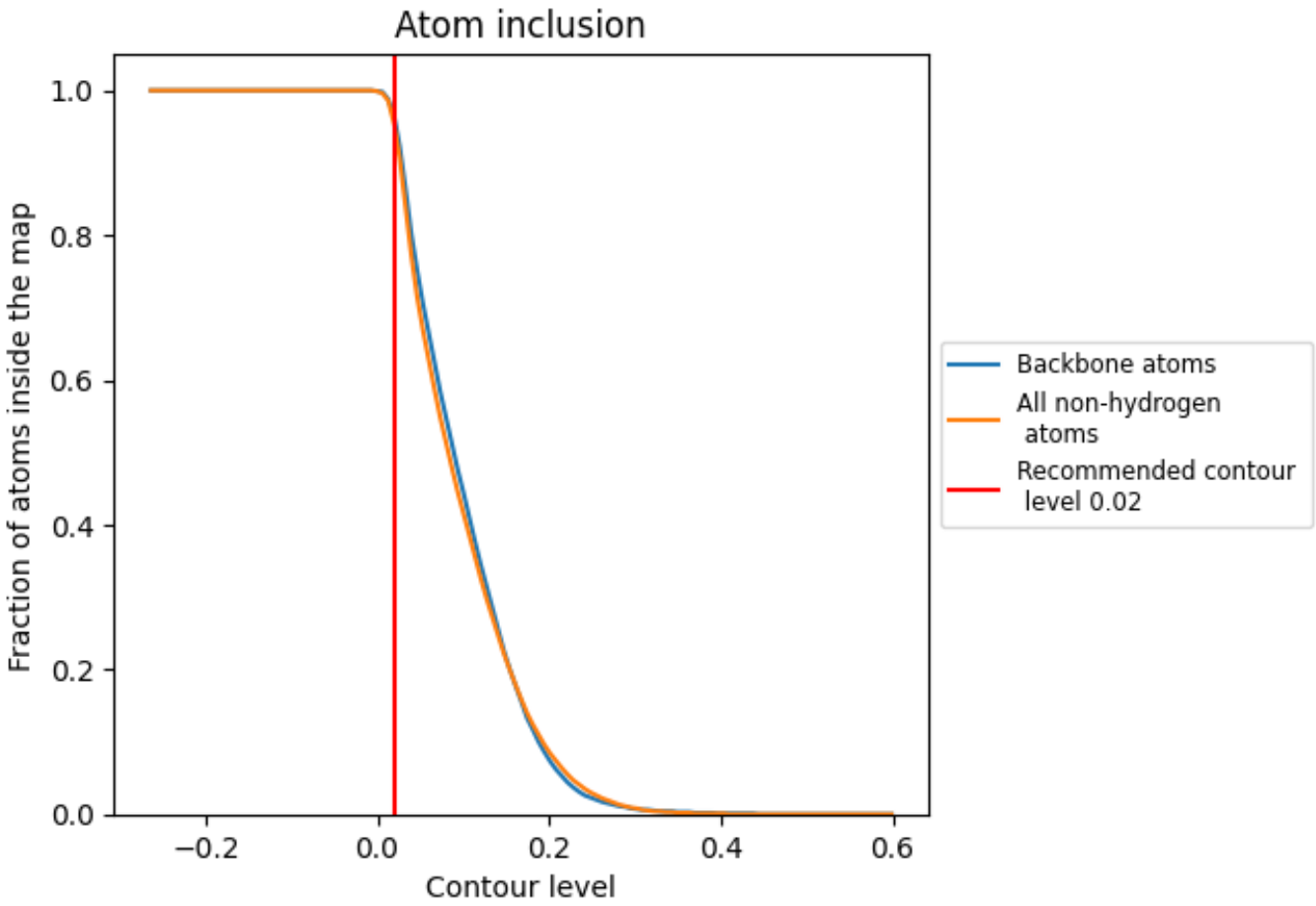
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.4290
2	0.9540	0.4190
3	0.9300	0.2860
5	0.9540	0.4520
B	0.9790	0.4840
E	0.9910	0.5850
G	0.9890	0.5070
H	0.9700	0.4340
I	0.9860	0.5400
J	0.9960	0.5710
K	0.4440	0.0430
L	0.9800	0.5660
N	0.9880	0.5430
O	0.9670	0.4500
W	0.9960	0.5720
X	0.9620	0.5150
Y	0.9920	0.5680
b	0.9630	0.5110
e	1.0000	0.5740
q	0.9140	0.1080
r	0.6490	0.0580
u	0.9570	0.4190
x	0.9810	0.4740
z	0.7850	0.3270