Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:02 am GMT

PDB ID	:	6GC4
EMDB ID	:	EMD-4380
Title	:	50S ribosomal subunit assembly intermediate state 3
Authors	:	Nikolay, R.; Hilal, T.; Qin, B.; Loerke, J.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on	:	2018-04-17
Resolution	:	4.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

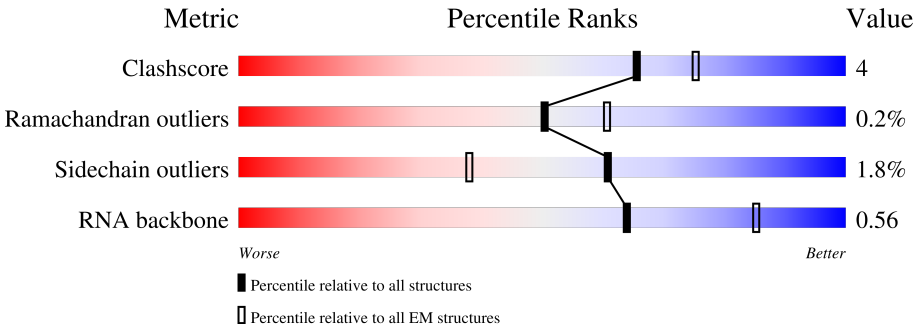
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.30 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)
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	V	94	95% 86% 13%
2	A	2904	12% 57% 28% 11%
3	C	271	26% 86% 14%
4	D	209	22% 85% 14%
5	E	201	20% 89% 11%
6	G	176	97% 85% 14%
7	J	142	9% 93% 7%

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Mol	Chain	Length	Quality of chain
8	K	122	22% 89% 11%
9	L	143	38% 83% 16%
10	N	120	7% 84% 15%
11	P	114	15% 88% 11%
12	Q	117	10% 90% 9%
13	R	103	12% 88% 12%
14	S	110	9% 85% 15%
15	T	93	11% 74% 23%
16	U	102	23% 81% 18%
17	X	77	29% 90% 10%
18	Y	63	63% 83% 16%
19	0	56	12% 91% 9%
20	2	46	15% 93%
21	O	116	19% 90% 10%
22	F	177	60% 81% 18%
23	B	119	6% 66% 30%
24	Z	58	26% 84% 16%
25	H	50	90% 86% 8% 6%
26	W	76	26% 84% 16%

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 80165 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2586	Total	C	N	O	P	0	0
			55544	24777	10247	17934	2586		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 11 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 12 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 13 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 14 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 15 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 16 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	U	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 17 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 19 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 20 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 21 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 22 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 23 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 25 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 26 is a protein called 50S ribosomal protein L27.

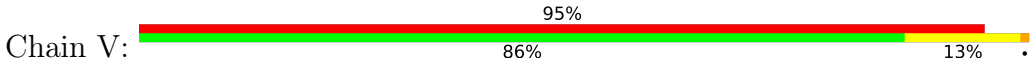
Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

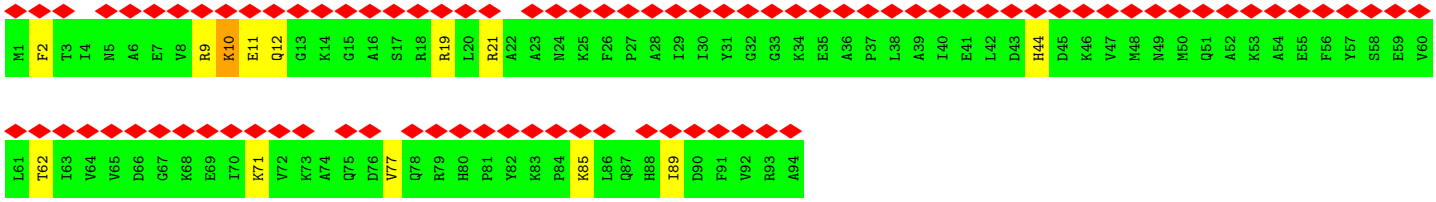
3 Residue-property plots (i)

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: 50S ribosomal protein L25

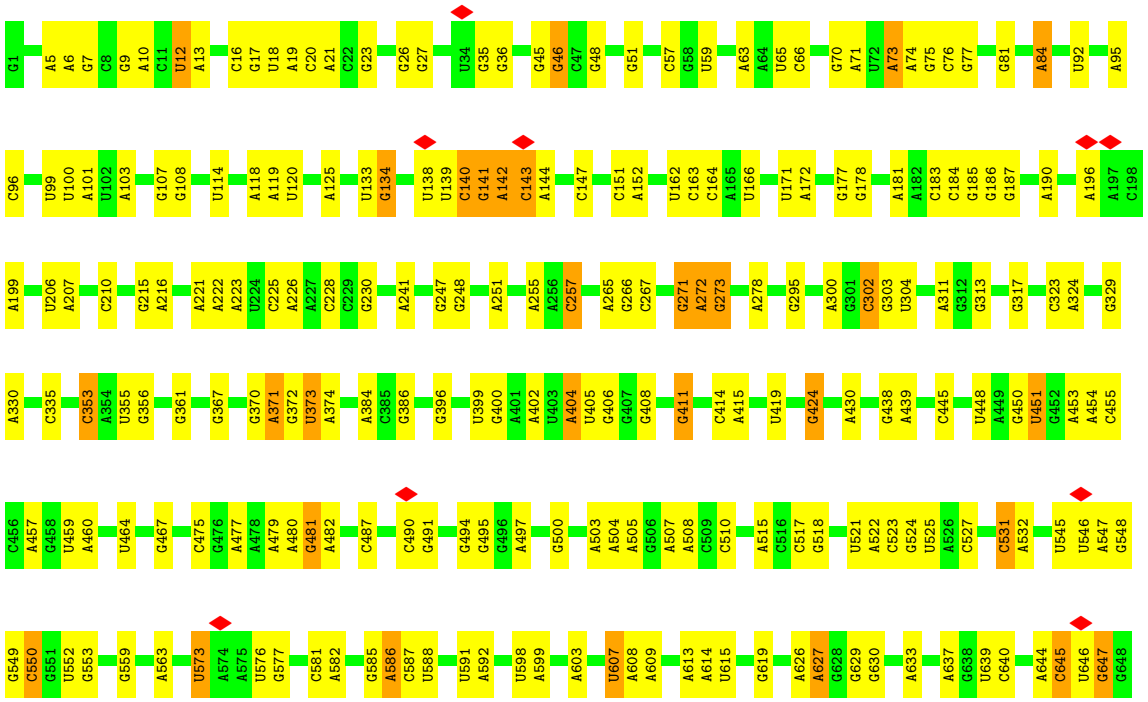
Chain V:

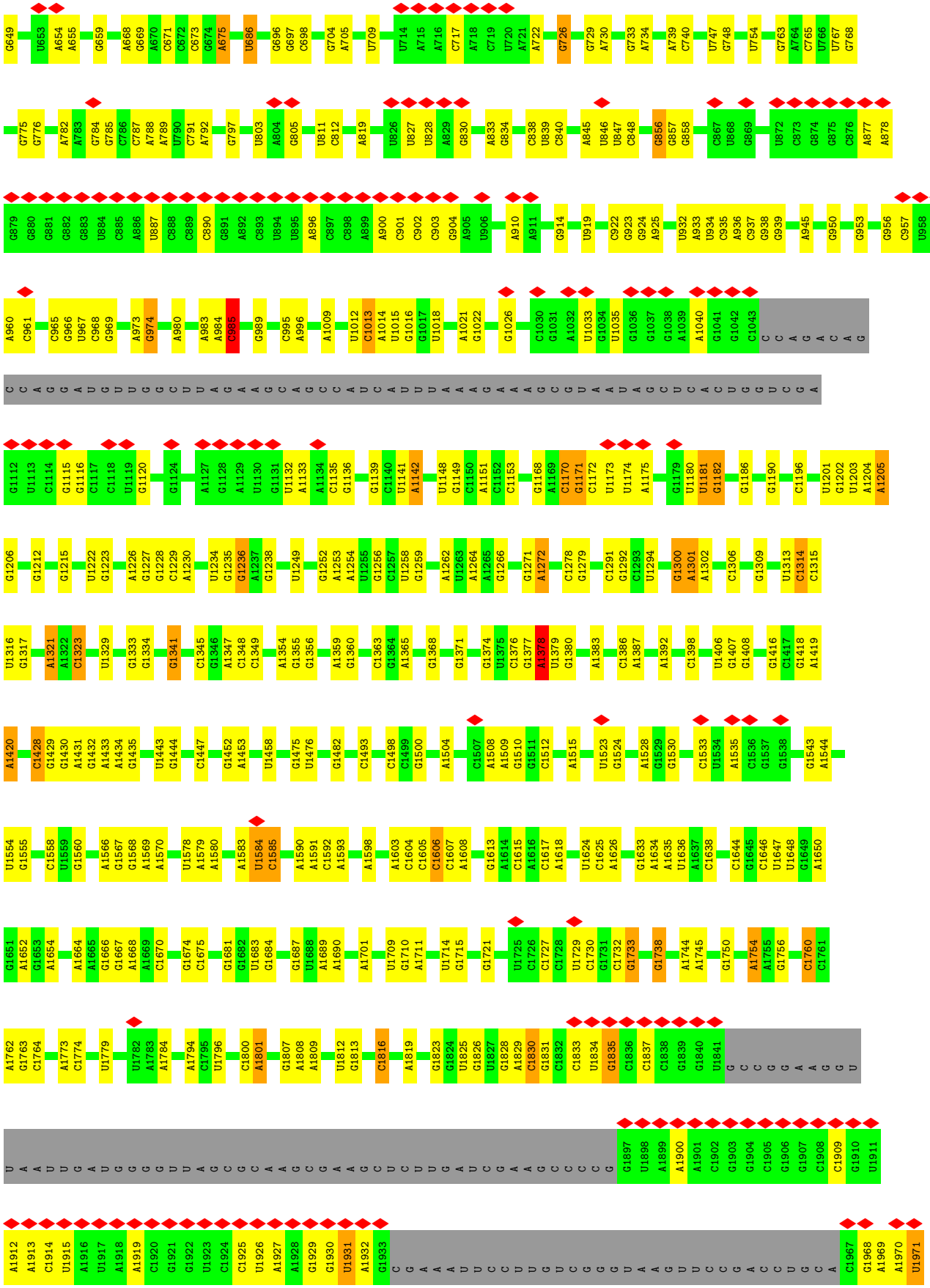


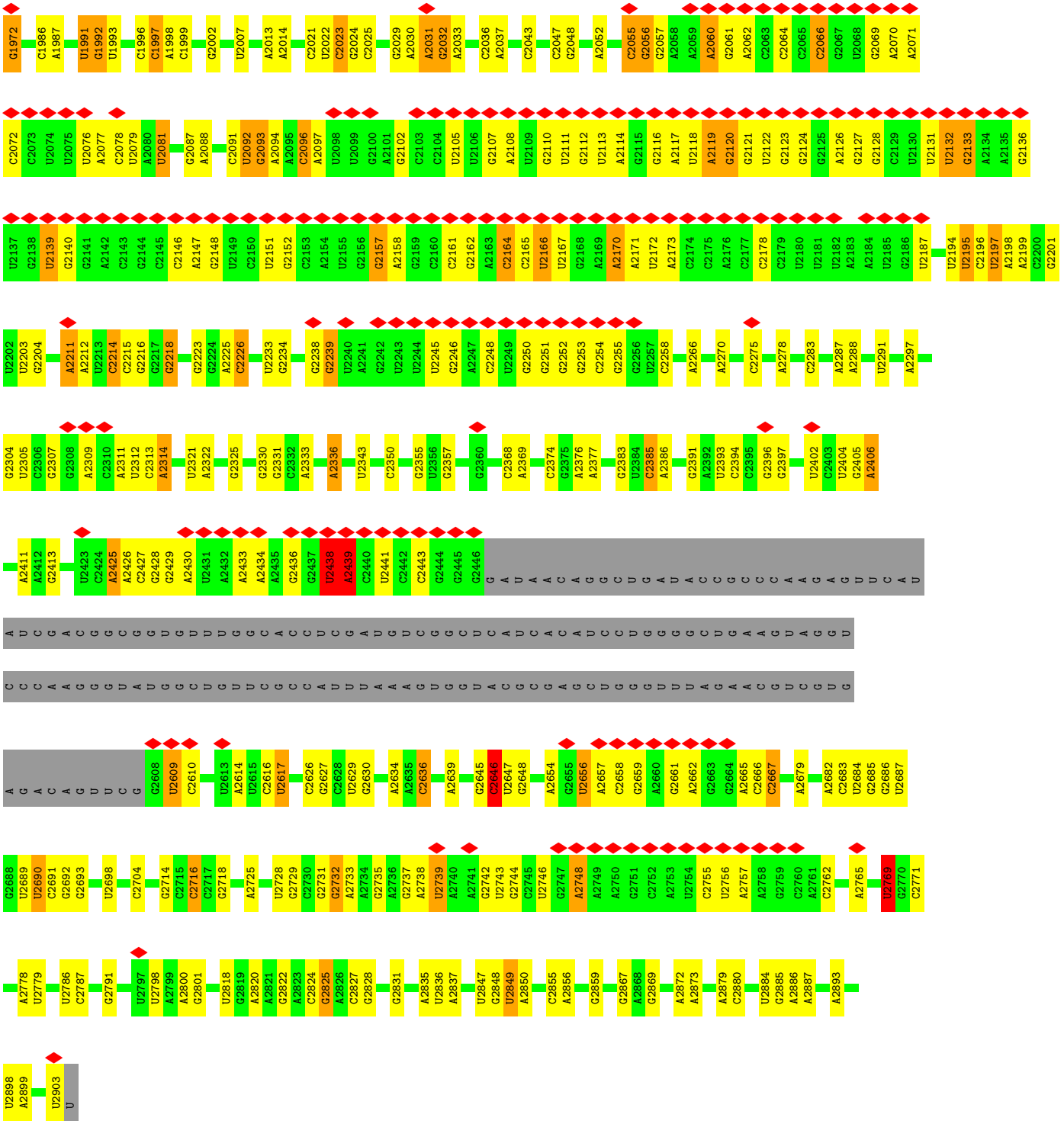


• Molecule 2: 23S ribosomal RNA

Chain A:

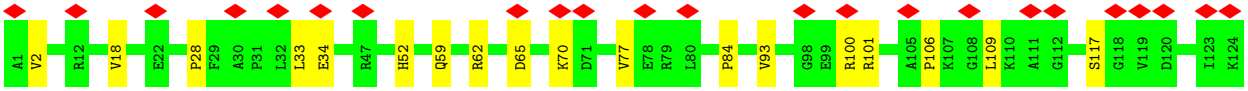


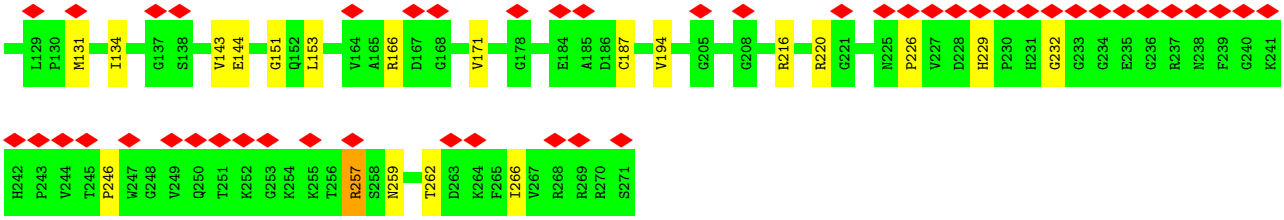




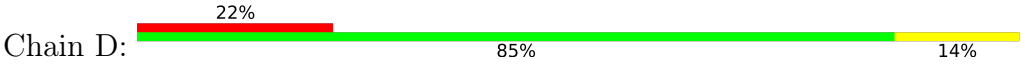
• Molecule 3: 50S ribosomal protein L2

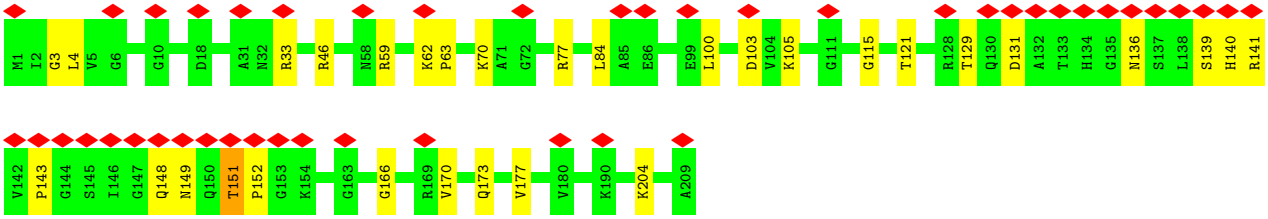
Chain C:



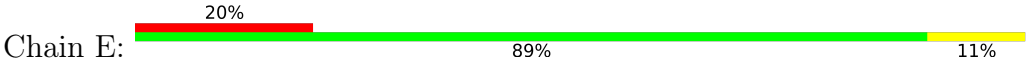


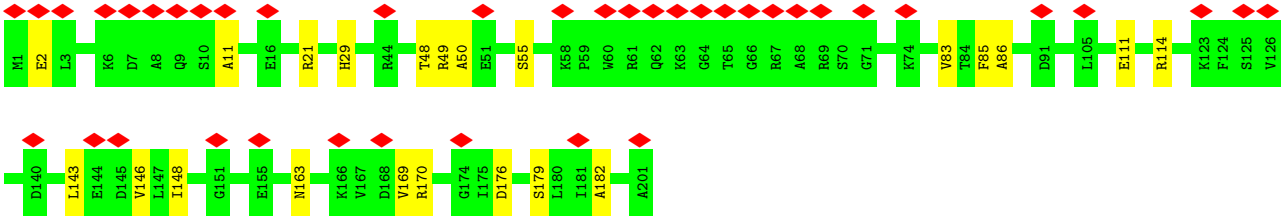
• Molecule 4: 50S ribosomal protein L3



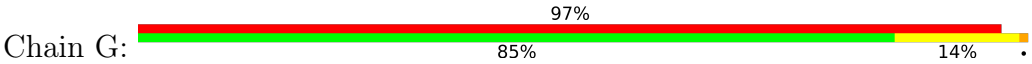


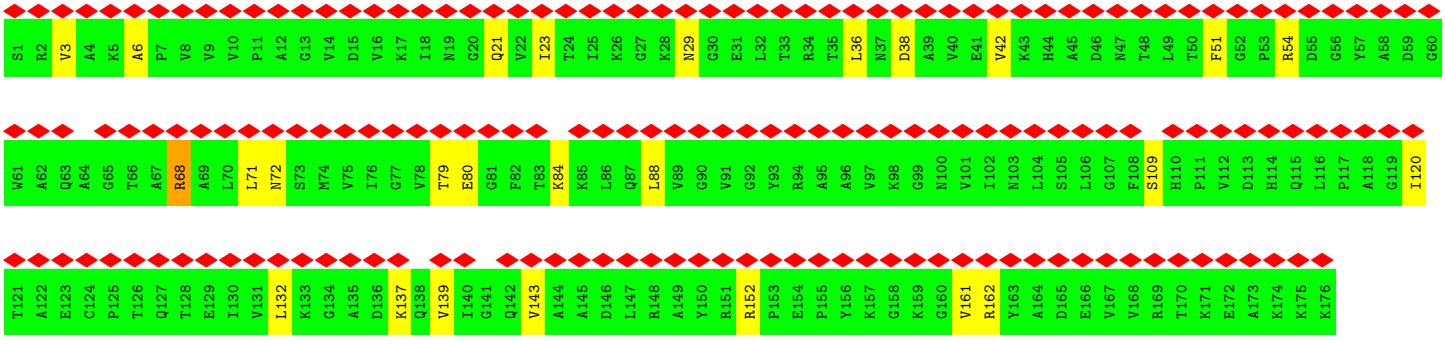
• Molecule 5: 50S ribosomal protein L4



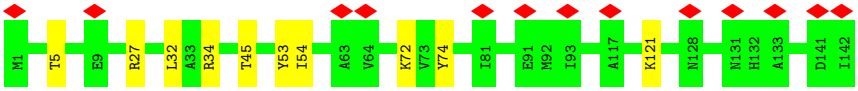


• Molecule 6: 50S ribosomal protein L6



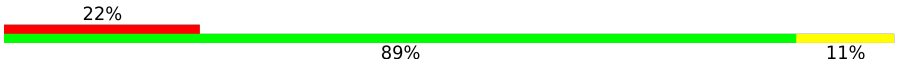


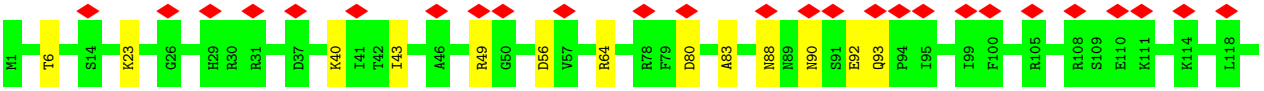
• Molecule 7: 50S ribosomal protein L13



• Molecule 8: 50S ribosomal protein L14

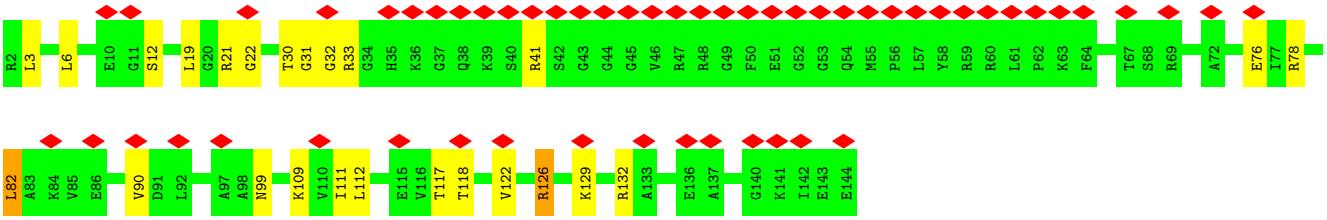
Chain K:





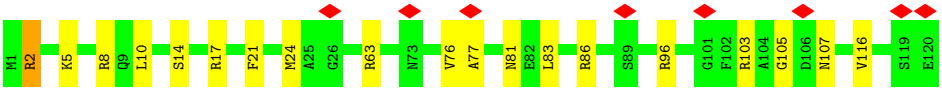
• Molecule 9: 50S ribosomal protein L15

Chain L:



• Molecule 10: 50S ribosomal protein L17

Chain N:

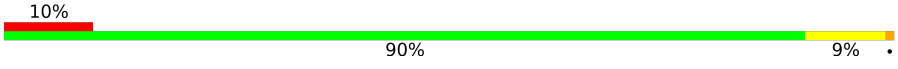


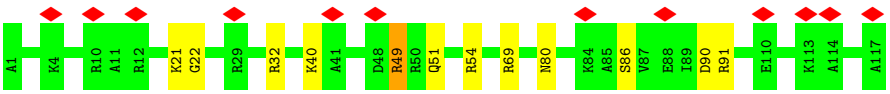
• Molecule 11: 50S ribosomal protein L19

Chain P:

• Molecule 12: 50S ribosomal protein L20

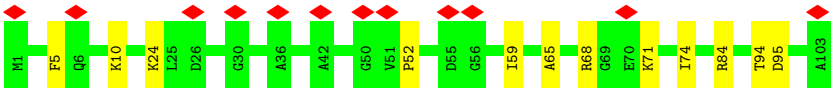
Chain Q:





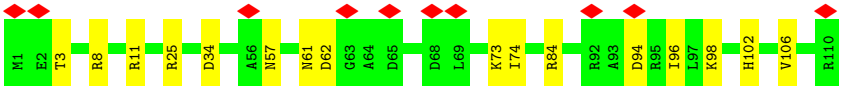
• Molecule 13: 50S ribosomal protein L21

Chain R:



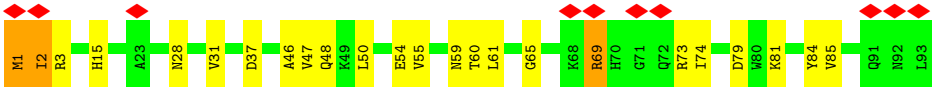
• Molecule 14: 50S ribosomal protein L22

Chain S:



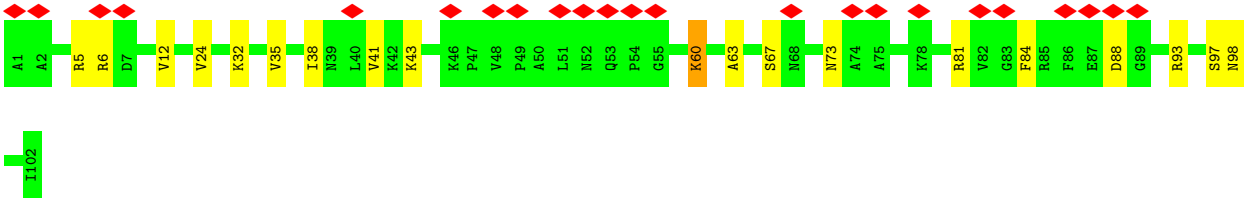
• Molecule 15: 50S ribosomal protein L23

Chain T:



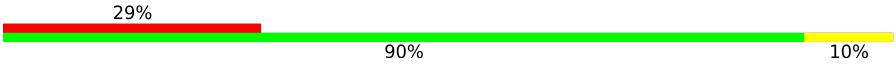
• Molecule 16: 50S ribosomal protein L24

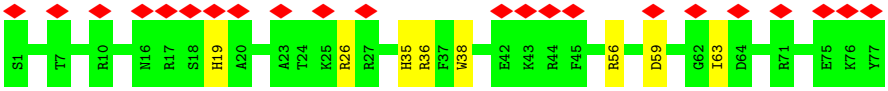
Chain U:



• Molecule 17: 50S ribosomal protein L28

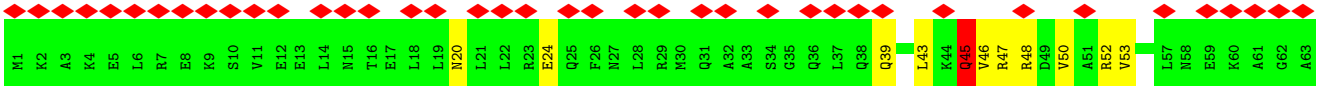
Chain X:





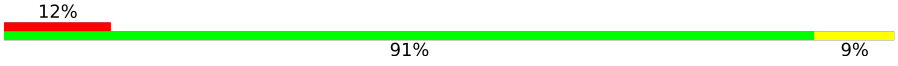
• Molecule 18: 50S ribosomal protein L29

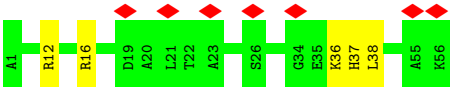
Chain Y:



• Molecule 19: 50S ribosomal protein L32

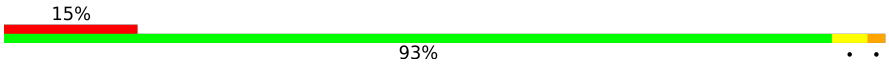
Chain 0:

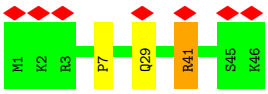




• Molecule 20: 50S ribosomal protein L34

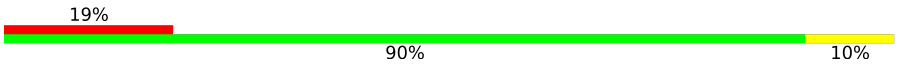
Chain 2:

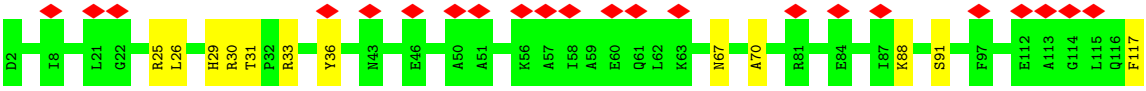




• Molecule 21: 50S ribosomal protein L18

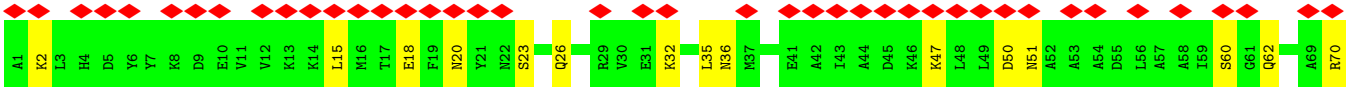
Chain O:

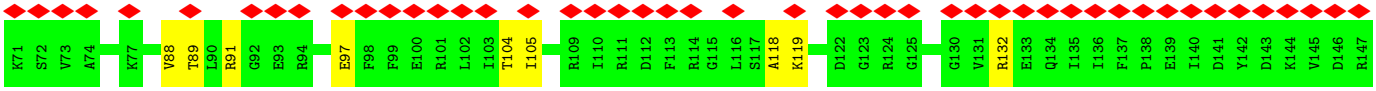


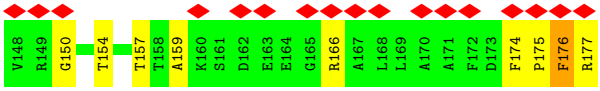


• Molecule 22: 50S ribosomal protein L5

Chain F:

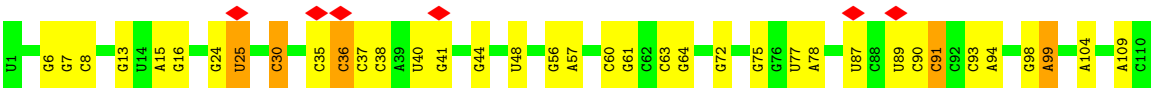


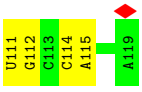




• Molecule 23: 5S ribosomal RNA

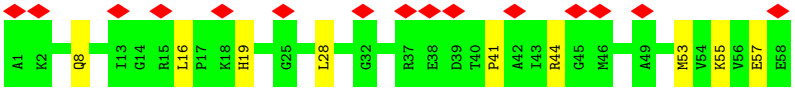
Chain B:





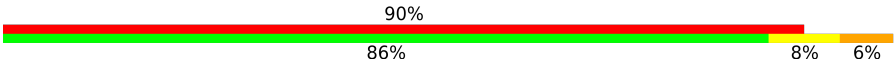
• Molecule 24: 50S ribosomal protein L30

Chain Z:



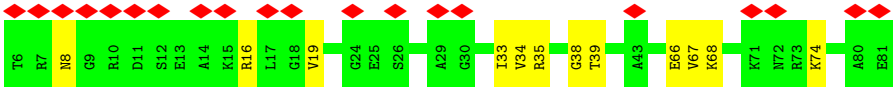
• Molecule 25: 50S ribosomal protein L9

Chain H:



• Molecule 26: 50S ribosomal protein L27

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	80645	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.942	Depositor
Minimum map value	-13.798	Depositor
Average map value	0.164	Depositor
Map value standard deviation	1.303	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	334.8, 334.8, 334.8	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

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	V	0.26	0/766	0.46	0/1025
2	A	0.27	0/62212	0.96	142/97047 (0.1%)
3	C	0.25	0/2122	0.51	0/2852
4	D	0.27	0/1586	0.54	0/2134
5	E	0.26	0/1571	0.51	0/2113
6	G	0.26	0/1343	0.49	0/1816
7	J	0.25	0/1152	0.49	0/1551
8	K	0.27	0/948	0.55	0/1268
9	L	0.28	0/1054	0.64	2/1403 (0.1%)
10	N	0.28	0/974	0.59	0/1301
11	P	0.27	0/929	0.50	0/1242
12	Q	0.30	0/960	0.48	0/1278
13	R	0.28	0/829	0.55	0/1107
14	S	0.24	0/864	0.47	0/1156
15	T	0.26	0/745	0.57	1/994 (0.1%)
16	U	0.30	0/788	0.60	1/1051 (0.1%)
17	X	0.26	0/635	0.50	0/848
18	Y	0.29	0/510	0.63	0/677
19	0	0.25	0/450	0.55	0/599
20	2	0.25	0/380	0.53	0/498
21	O	0.27	0/902	0.53	0/1209
22	F	0.31	0/1435	0.55	0/1926
23	B	0.27	0/2850	0.97	5/4444 (0.1%)
24	Z	0.25	0/453	0.50	0/605
25	H	0.31	0/389	0.74	1/523 (0.2%)
26	W	0.26	0/582	0.47	0/769
All	All	0.27	0/87429	0.88	152/131436 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
8	K	0	2
9	L	0	1
10	N	0	1
16	U	0	2
18	Y	0	1
22	F	0	2
25	H	0	1
All	All	0	11

There are no bond length outliers.

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2439	A	O5'-P-OP1	-27.08	78.20	110.70
2	A	2439	A	OP1-P-OP2	-26.99	79.12	119.60
2	A	2439	A	O5'-P-OP2	16.50	130.50	110.70
2	A	2438	U	OP2-P-O3'	-15.37	71.38	105.20
2	A	2438	U	OP1-P-O3'	13.94	135.86	105.20
2	A	1313	U	C2-N1-C1'	9.05	128.56	117.70
2	A	1348	C	N1-C2-O2	8.83	124.20	118.90
2	A	2072	C	C2-N1-C1'	8.78	128.46	118.80
2	A	1313	U	N1-C2-O2	8.66	128.86	122.80
2	A	1313	U	N3-C2-O2	-8.48	116.27	122.20
2	A	12	U	N3-C2-O2	-7.71	116.80	122.20
2	A	12	U	N1-C2-O2	7.69	128.19	122.80
2	A	183	C	N1-C2-O2	7.69	123.52	118.90
2	A	2196	C	N1-C2-O2	7.43	123.36	118.90
2	A	2226	C	N1-C2-O2	7.39	123.34	118.90
2	A	12	U	C2-N1-C1'	7.26	126.41	117.70
2	A	1348	C	N3-C2-O2	-7.25	116.82	121.90
2	A	2072	C	N1-C2-O2	7.17	123.20	118.90
2	A	1774	C	N3-C2-O2	-7.08	116.94	121.90
25	H	27	ARG	C-N-CA	7.06	139.35	121.70
2	A	2096	C	C2-N1-C1'	7.04	126.54	118.80
2	A	2214	C	N1-C2-O2	6.98	123.09	118.90
2	A	550	C	C2-N1-C1'	6.93	126.42	118.80
2	A	2196	C	C2-N1-C1'	6.86	126.35	118.80
2	A	2092	U	P-O3'-C3'	6.75	127.80	119.70
2	A	985	C	N1-C2-O2	6.73	122.94	118.90
2	A	225	C	N1-C2-O2	6.65	122.89	118.90
2	A	1378	A	P-O3'-C3'	6.65	127.68	119.70
2	A	2704	C	N1-C2-O2	6.64	122.88	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2066	C	N1-C2-O2	6.59	122.86	118.90
2	A	1774	C	N1-C2-O2	6.58	122.85	118.90
2	A	2066	C	C5-C6-N1	6.57	124.28	121.00
2	A	271	G	P-O3'-C3'	6.48	127.48	119.70
2	A	1348	C	C6-N1-C2	-6.46	117.72	120.30
2	A	114	U	C2-N1-C1'	6.40	125.39	117.70
2	A	2072	C	C6-N1-C2	-6.40	117.74	120.30
2	A	919	U	N1-C2-O2	6.38	127.27	122.80
2	A	2096	C	N1-C2-O2	6.38	122.73	118.90
2	A	1348	C	C2-N1-C1'	6.26	125.68	118.80
23	B	25	U	N1-C2-O2	6.22	127.16	122.80
2	A	2769	U	N1-C2-O2	6.20	127.14	122.80
2	A	2166	U	N1-C2-O2	6.20	127.14	122.80
2	A	2066	C	C2-N3-C4	6.19	123.00	119.90
2	A	1584	U	C2-N1-C1'	6.18	125.12	117.70
2	A	2072	C	C5-C6-N1	6.17	124.09	121.00
16	U	97	SER	C-N-CA	6.15	137.07	121.70
2	A	2196	C	C6-N1-C2	-6.13	117.85	120.30
2	A	985	C	C2-N1-C1'	6.13	125.54	118.80
2	A	550	C	N1-C2-O2	6.09	122.56	118.90
2	A	183	C	N3-C2-O2	-6.08	117.64	121.90
2	A	919	U	N3-C2-O2	-6.07	117.95	122.20
2	A	2666	C	N1-C2-O2	6.05	122.53	118.90
2	A	1644	C	N1-C2-O2	6.04	122.53	118.90
2	A	445	C	N1-C2-O2	6.01	122.51	118.90
2	A	2769	U	N3-C2-O2	-5.97	118.02	122.20
2	A	2072	C	C6-N1-C1'	-5.97	113.64	120.80
2	A	1378	A	OP1-P-O3'	5.95	118.29	105.20
2	A	2196	C	N3-C2-O2	-5.91	117.76	121.90
2	A	2425	A	P-O3'-C3'	5.90	126.78	119.70
2	A	838	C	N1-C2-O2	5.88	122.43	118.90
2	A	1606	C	P-O3'-C3'	5.88	126.76	119.70
2	A	2226	C	N3-C2-O2	-5.83	117.82	121.90
9	L	82	LEU	CA-CB-CG	5.82	128.70	115.30
23	B	25	U	N3-C2-O2	-5.81	118.13	122.20
2	A	901	C	N1-C2-O2	5.80	122.38	118.90
2	A	404	A	P-O3'-C3'	5.80	126.66	119.70
2	A	1313	U	C6-N1-C1'	-5.77	113.12	121.20
2	A	323	C	C2-N1-C1'	5.75	125.12	118.80
2	A	225	C	N3-C2-O2	-5.73	117.89	121.90
2	A	1349	C	C2-N1-C1'	5.72	125.09	118.80
2	A	848	C	N1-C2-O2	5.71	122.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2214	C	N3-C2-O2	-5.68	117.92	121.90
2	A	1915	U	N1-C2-O2	5.68	126.78	122.80
2	A	1675	C	N1-C2-O2	5.66	122.30	118.90
2	A	183	C	C2-N1-C1'	5.65	125.02	118.80
2	A	1604	C	N3-C2-O2	-5.65	117.94	121.90
2	A	2617	U	N1-C2-O2	5.64	126.75	122.80
2	A	2066	C	C2-N1-C1'	5.63	124.99	118.80
2	A	2164	C	N1-C2-O2	5.62	122.27	118.90
2	A	487	C	N1-C2-O2	5.62	122.27	118.90
2	A	1170	C	N1-C2-O2	5.61	122.27	118.90
2	A	902	C	N1-C2-O2	5.60	122.26	118.90
2	A	2394	C	N1-C2-O2	5.59	122.25	118.90
2	A	1624	U	N3-C2-O2	-5.59	118.29	122.20
2	A	183	C	C6-N1-C2	-5.58	118.07	120.30
2	A	1604	C	N1-C2-O2	5.58	122.25	118.90
2	A	2636	C	C2-N1-C1'	5.57	124.93	118.80
2	A	545	U	C2-N1-C1'	5.55	124.36	117.70
2	A	166	U	N1-C2-O2	5.54	126.67	122.80
2	A	1294	U	N3-C2-O2	-5.51	118.34	122.20
2	A	1314	C	C2-N1-C1'	5.50	124.85	118.80
2	A	985	C	C6-N1-C2	-5.48	118.11	120.30
2	A	1170	C	C6-N1-C2	-5.47	118.11	120.30
2	A	2636	C	N1-C2-O2	5.43	122.16	118.90
2	A	1323	C	N1-C2-O2	5.43	122.16	118.90
2	A	1624	U	N1-C2-O2	5.42	126.60	122.80
2	A	1625	C	N1-C2-O2	5.40	122.14	118.90
2	A	2166	U	N3-C2-O2	-5.39	118.43	122.20
2	A	445	C	N3-C2-O2	-5.39	118.13	121.90
2	A	2438	U	C5-C4-O4	-5.36	122.69	125.90
2	A	2704	C	N3-C2-O2	-5.35	118.15	121.90
2	A	353	C	N1-C2-O2	5.34	122.11	118.90
2	A	2214	C	C2-N1-C1'	5.34	124.67	118.80
2	A	2646	C	N1-C2-O2	5.33	122.10	118.90
2	A	1605	C	N1-C2-O2	5.33	122.10	118.90
2	A	140	C	N1-C2-O2	5.32	122.09	118.90
2	A	2092	U	OP2-P-O3'	5.32	116.90	105.20
2	A	2617	U	N3-C2-O2	-5.30	118.49	122.20
2	A	717	C	N1-C2-O2	5.28	122.07	118.90
2	A	2226	C	C2-N1-C1'	5.27	124.60	118.80
2	A	2197	U	OP1-P-O3'	5.27	116.80	105.20
2	A	1585	C	N1-C2-O2	5.27	122.06	118.90
2	A	1915	U	N3-C2-O2	-5.26	118.52	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	640	C	C5-C6-N1	5.25	123.62	121.00
2	A	1196	C	N1-C2-O2	5.24	122.05	118.90
2	A	1349	C	C6-N1-C2	-5.24	118.20	120.30
2	A	1774	C	C6-N1-C2	-5.24	118.20	120.30
2	A	2343	U	N1-C2-O2	5.24	126.47	122.80
9	L	112	LEU	CA-CB-CG	5.22	127.30	115.30
2	A	1348	C	C5-C6-N1	5.21	123.60	121.00
2	A	1915	U	C2-N1-C1'	5.19	123.93	117.70
2	A	919	U	C2-N1-C1'	5.18	123.92	117.70
2	A	1760	C	N1-C2-O2	5.17	122.00	118.90
2	A	1830	C	N1-C2-O2	5.17	122.00	118.90
2	A	1398	C	N1-C2-O2	5.17	122.00	118.90
2	A	2066	C	C6-N1-C2	-5.17	118.23	120.30
2	A	257	C	N1-C2-O2	5.15	121.99	118.90
2	A	840	C	N1-C2-O2	5.15	121.99	118.90
2	A	1376	C	C2-N1-C1'	5.15	124.46	118.80
2	A	166	U	N3-C2-O2	-5.13	118.61	122.20
2	A	974	G	C4-N9-C1'	5.13	133.17	126.50
2	A	2226	C	C6-N1-C2	-5.13	118.25	120.30
23	B	91	C	C2-N1-C1'	5.11	124.42	118.80
2	A	1498	C	C2-N1-C1'	5.11	124.42	118.80
2	A	1644	C	N3-C2-O2	-5.11	118.33	121.90
2	A	2769	U	C2-N1-C1'	5.10	123.82	117.70
2	A	985	C	N3-C2-O2	-5.10	118.33	121.90
2	A	1830	C	C2-N1-C1'	5.09	124.40	118.80
2	A	2762	C	C2-N1-C1'	5.09	124.39	118.80
23	B	30	C	N3-C2-O2	-5.08	118.34	121.90
2	A	1512	C	N1-C2-O2	5.08	121.95	118.90
2	A	1584	U	N1-C2-O2	5.07	126.35	122.80
2	A	92	U	N1-C2-O2	5.07	126.35	122.80
2	A	2739	U	N3-C2-O2	-5.06	118.66	122.20
2	A	1625	C	N3-C2-O2	-5.06	118.36	121.90
2	A	2667	C	N1-C2-O2	5.06	121.93	118.90
23	B	25	U	C2-N1-C1'	5.05	123.76	117.70
2	A	2195	U	N3-C2-O2	-5.05	118.67	122.20
2	A	1830	C	C6-N1-C2	-5.04	118.28	120.30
2	A	2214	C	C6-N1-C2	-5.03	118.29	120.30
15	T	2	ILE	C-N-CA	5.01	134.22	121.70
2	A	2393	U	N1-C2-O2	5.01	126.31	122.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	151	THR	Peptide
22	F	174	PHE	Peptide
22	F	175	PRO	Peptide
25	H	31	VAL	Peptide
8	K	92	GLU	Peptide
8	K	93	GLN	Peptide
9	L	30	THR	Peptide
10	N	10	LEU	Peptide
16	U	6	ARG	Peptide
16	U	88	ASP	Peptide
18	Y	45	GLN	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	V	753	0	780	9	0
2	A	55544	0	27936	340	0
3	C	2083	0	2157	25	0
4	D	1565	0	1616	20	0
5	E	1552	0	1619	13	0
6	G	1323	0	1374	14	0
7	J	1129	0	1162	6	0
8	K	939	0	1012	5	0
9	L	1045	0	1117	16	0
10	N	961	0	1000	10	0
11	P	917	0	965	9	0
12	Q	947	0	1022	10	0
13	R	816	0	839	7	0
14	S	857	0	922	11	0
15	T	739	0	807	17	0
16	U	780	0	834	9	0
17	X	625	0	655	7	0
18	Y	509	0	543	6	0
19	0	444	0	461	5	0
20	2	377	0	418	3	0
21	O	892	0	923	7	0
22	F	1411	0	1447	16	0
23	B	2549	0	1291	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Z	449	0	491	4	0
25	H	384	0	405	9	0
26	W	575	0	589	10	0
All	All	80165	0	52385	512	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 4.

All (512) 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)
2:A:2735:G:H1	2:A:2769:U:H3	1.18	0.90
2:A:950:G:H1	2:A:967:U:H3	1.18	0.87
2:A:1418:G:H21	2:A:1580:A:H62	1.39	0.69
21:O:31:THR:HG22	21:O:33:ARG:H	1.59	0.67
10:N:77:ALA:O	10:N:81:ASN:HB2	1.94	0.67
15:T:59:ASN:HB2	15:T:84:TYR:HB2	1.77	0.67
2:A:2081:U:H3	2:A:2239:G:H1	1.40	0.67
2:A:1796:U:H3	2:A:1823:G:H1	1.42	0.66
2:A:585:G:H21	2:A:1254:A:H62	1.43	0.65
23:B:30:C:H1'	23:B:57:A:H61	1.61	0.65
2:A:2093:G:H4'	25:H:24:GLY:HA3	1.80	0.64
15:T:1:MET:HG2	15:T:2:ILE:HD12	1.80	0.63
23:B:72:G:H21	23:B:104:A:H62	1.46	0.63
22:F:35:LEU:HB2	22:F:88:VAL:HB	1.81	0.61
5:E:48:THR:HG23	5:E:50:ALA:H	1.65	0.61
2:A:671:C:H41	9:L:41:ARG:HA	1.66	0.61
2:A:1434:A:H2'	2:A:1435:G:H8	1.66	0.60
2:A:1834:U:H5"	2:A:1835:G:H5'	1.84	0.60
2:A:2131:U:H5'	2:A:2132:U:H5"	1.83	0.60
2:A:2313:C:H2'	2:A:2314:A:H8	1.67	0.60
2:A:304:U:H3	2:A:313:G:H1	1.50	0.60
2:A:517:C:H5"	19:0:12:ARG:HH12	1.67	0.60
3:C:28:PRO:HG2	3:C:33:LEU:HD11	1.84	0.59
2:A:1986:C:H2'	2:A:1987:A:H8	1.67	0.59
12:Q:49:ARG:HH22	13:R:74:ILE:HG13	1.66	0.59
16:U:43:LYS:HB2	16:U:60:LYS:HZ2	1.67	0.59
2:A:19:A:H5"	12:Q:21:LYS:HE3	1.85	0.59
2:A:371:A:N6	2:A:402:A:OP2	2.35	0.59
4:D:115:GLY:HA2	4:D:166:GLY:HA3	1.85	0.59
14:S:25:ARG:NH1	14:S:74:ILE:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:21:GLN:HB3	6:G:36:LEU:HB2	1.85	0.58
2:A:2032:G:N2	4:D:151:THR:OG1	2.36	0.58
4:D:131:ASP:O	4:D:136:ASN:ND2	2.36	0.58
2:A:494:G:H21	14:S:57:ASN:HD21	1.49	0.58
2:A:2656:U:O2	2:A:2665:A:N7	2.36	0.58
2:A:1997:C:H5"	4:D:141:ARG:HH12	1.69	0.58
2:A:2355:G:N3	26:W:35:ARG:NH2	2.51	0.58
3:C:257:ARG:HH22	3:C:262:THR:HG23	1.68	0.58
9:L:76:GLU:HG3	9:L:111:ILE:HD13	1.85	0.58
15:T:60:THR:HB	15:T:81:LYS:HD2	1.86	0.57
26:W:33:ILE:HG22	26:W:34:VAL:HG23	1.86	0.57
2:A:937:C:H2'	2:A:938:G:H8	1.69	0.57
2:A:2002:G:OP1	10:N:17:ARG:NH2	2.37	0.57
2:A:2133:G:N2	2:A:2157:G:O2'	2.36	0.57
4:D:103:ASP:OD1	4:D:105:LYS:NZ	2.38	0.57
2:A:1153:C:OP1	12:Q:91:ARG:NH2	2.38	0.57
21:O:29:HIS:HB3	21:O:36:TYR:HB2	1.87	0.56
2:A:1334:G:OP1	15:T:69:ARG:NH2	2.38	0.56
2:A:609:A:H62	2:A:619:G:H21	1.54	0.56
4:D:121:THR:HG21	4:D:143:PRO:HG3	1.88	0.56
2:A:709:U:H3	2:A:722:A:H61	1.53	0.56
22:F:118:ALA:O	22:F:166:ARG:NH1	2.39	0.56
2:A:2278:A:H5"	26:W:8:ASN:HD21	1.70	0.56
2:A:2855:C:H2'	2:A:2856:A:H8	1.69	0.56
24:Z:16:LEU:HB2	24:Z:19:HIS:HD2	1.71	0.56
2:A:1018:U:O2'	2:A:1120:G:N2	2.39	0.55
12:Q:86:SER:HB3	13:R:52:PRO:HD3	1.89	0.55
2:A:65:U:O2'	15:T:73:ARG:NH1	2.40	0.55
2:A:585:G:H21	2:A:1254:A:N6	2.04	0.55
2:A:1215:G:H1	2:A:1234:U:H3	1.53	0.55
1:V:12:GLN:NE2	23:B:75:G:OP1	2.39	0.55
2:A:171:U:H2'	2:A:172:A:H8	1.72	0.55
2:A:965:C:H2'	2:A:966:G:H8	1.72	0.55
2:A:2742:G:H21	6:G:152:ARG:HH12	1.55	0.55
2:A:26:G:H1'	2:A:515:A:H61	1.72	0.55
2:A:1168:G:O6	2:A:1181:U:O2	2.25	0.55
5:E:29:HIS:HD2	9:L:6:LEU:HB3	1.72	0.55
1:V:77:VAL:HG23	1:V:89:ILE:HG12	1.88	0.55
2:A:77:G:OP1	18:Y:52:ARG:NH2	2.39	0.55
6:G:120:ILE:HG13	6:G:143:VAL:HG21	1.88	0.54
1:V:21:ARG:NH1	23:B:77:U:OP1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:400:G:O6	17:X:56:ARG:NH1	2.39	0.54
2:A:2684:U:OP2	11:P:50:ARG:NH1	2.40	0.54
6:G:38:ASP:O	6:G:54:ARG:NH1	2.41	0.54
2:A:2831:G:OP2	4:D:59:ARG:NH1	2.40	0.54
3:C:144:GLU:HB3	3:C:187:CYS:HB3	1.89	0.54
18:Y:45:GLN:O	18:Y:47:ARG:N	2.41	0.54
1:V:10:LYS:HG2	1:V:11:GLU:HG3	1.90	0.53
2:A:1666:G:H4'	8:K:6:THR:HG23	1.90	0.53
10:N:83:LEU:HD23	10:N:86:ARG:HD2	1.90	0.53
3:C:143:VAL:HB	3:C:153:LEU:HB2	1.90	0.53
2:A:2023:C:H2'	2:A:2024:G:H8	1.73	0.53
5:E:182:ALA:HA	9:L:3:LEU:HD21	1.89	0.53
2:A:984:A:OP1	2:A:985:C:N4	2.41	0.53
10:N:96:ARG:NH1	10:N:116:VAL:O	2.42	0.53
2:A:1013:C:H2'	2:A:1014:A:H8	1.74	0.53
22:F:47:LYS:HA	22:F:50:ASP:HB2	1.90	0.53
2:A:629:G:N3	2:A:639:U:O2'	2.42	0.53
2:A:1333:G:H2'	2:A:1334:G:H8	1.72	0.53
2:A:460:A:OP2	20:2:41:ARG:NH1	2.42	0.53
2:A:1223:G:OP1	13:R:68:ARG:NH2	2.42	0.53
2:A:1418:G:N2	2:A:1579:A:N7	2.57	0.53
2:A:1341:G:H5'	15:T:61:LEU:HB3	1.91	0.53
2:A:2659:G:N2	2:A:2662:A:OP2	2.42	0.53
2:A:408:G:H1	2:A:419:U:H3	1.57	0.52
2:A:787:C:H5"	2:A:788:A:H5'	1.90	0.52
2:A:1779:U:OP2	2:A:1784:A:N6	2.43	0.52
17:X:59:ASP:OD2	25:H:27:ARG:NH2	2.36	0.52
2:A:2218:G:OP1	17:X:36:ARG:NH1	2.41	0.52
2:A:2743:U:OP2	2:A:2755:C:N4	2.39	0.52
2:A:9:G:O2'	2:A:2800:A:N6	2.42	0.52
2:A:531:C:O2'	12:Q:40:LYS:NZ	2.43	0.52
26:W:66:GLU:HB3	26:W:68:LYS:HE2	1.92	0.52
2:A:1992:G:O2'	2:A:1997:C:N4	2.42	0.52
2:A:1190:G:H5"	9:L:32:GLY:HA2	1.91	0.52
2:A:1816:C:N4	3:C:34:GLU:OE2	2.43	0.52
2:A:698:C:O2'	2:A:734:A:N6	2.43	0.52
22:F:62:GLN:NE2	22:F:89:THR:O	2.43	0.52
2:A:2787:C:H4'	4:D:62:LYS:HG2	1.92	0.52
2:A:272:A:H2'	2:A:273:G:H8	1.75	0.52
2:A:143:C:O2	15:T:3:ARG:NH2	2.43	0.51
2:A:1418:G:N2	2:A:1580:A:H62	2.04	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:43:ILE:HD12	8:K:56:ASP:HB3	1.91	0.51
17:X:38:TRP:H	25:H:32:PRO:HB2	1.74	0.51
2:A:626:A:H2'	9:L:78:ARG:HH22	1.74	0.51
15:T:47:VAL:HG11	15:T:85:VAL:HG11	1.92	0.51
2:A:1567:G:OP1	3:C:59:GLN:NE2	2.42	0.51
2:A:1681:G:N2	2:A:1763:G:OP2	2.43	0.51
3:C:65:ASP:OD2	3:C:101:ARG:NH1	2.42	0.51
22:F:23:SER:HB3	22:F:26:GLN:HG3	1.92	0.51
2:A:598:U:HO2'	9:L:12:SER:HG	1.58	0.51
2:A:767:U:H2'	2:A:768:G:H8	1.76	0.51
2:A:1264:A:N6	2:A:2014:A:OP2	2.43	0.51
2:A:1828:G:O6	3:C:220:ARG:NH1	2.43	0.51
2:A:2645:G:OP2	2:A:2645:G:N2	2.41	0.51
2:A:585:G:N2	2:A:1254:A:H62	2.09	0.51
2:A:2405:G:O2'	2:A:2411:A:N6	2.44	0.51
2:A:587:C:OP1	9:L:21:ARG:NH1	2.44	0.51
2:A:1794:A:HO2'	2:A:1900:A:HO2'	1.56	0.51
9:L:117:THR:HG23	9:L:118:THR:HG23	1.92	0.51
2:A:411:G:OP2	2:A:2406:A:O2'	2.28	0.51
15:T:46:ALA:O	15:T:50:LEU:HB2	2.11	0.51
2:A:300:A:H8	16:U:81:ARG:HH12	1.59	0.50
23:B:114:C:H2'	23:B:115:A:H8	1.76	0.50
9:L:90:VAL:HB	9:L:122:VAL:HA	1.93	0.50
10:N:2:ARG:NH1	10:N:5:LYS:O	2.44	0.50
2:A:335:C:O2	16:U:67:SER:OG	2.28	0.50
2:A:1316:U:H2'	2:A:1317:G:H8	1.77	0.50
2:A:1794:A:O2'	2:A:1900:A:O2'	2.28	0.50
7:J:32:LEU:HG	7:J:54:ILE:HD13	1.93	0.50
2:A:370:G:O2'	2:A:424:G:OP1	2.29	0.50
2:A:675:A:N7	2:A:803:U:N3	2.48	0.50
2:A:1222:U:H3	2:A:1227:G:H1	1.60	0.50
2:A:2822:G:O2'	2:A:2825:G:N1	2.40	0.50
2:A:1418:G:H21	2:A:1580:A:N6	2.08	0.50
2:A:2258:C:O2'	2:A:2427:C:OP2	2.30	0.50
4:D:151:THR:HG22	4:D:152:PRO:HD3	1.93	0.50
2:A:581:C:H2'	2:A:582:A:H8	1.77	0.50
2:A:1407:G:H2'	2:A:1408:G:H8	1.77	0.50
9:L:109:LYS:HG2	9:L:126:ARG:HG2	1.94	0.50
4:D:136:ASN:OD1	4:D:139:SER:OG	2.30	0.50
2:A:573:U:N3	2:A:2031:A:OP1	2.44	0.49
2:A:935:C:H2'	2:A:936:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1429:G:H2'	2:A:1430:G:H8	1.77	0.49
2:A:1992:G:N2	2:A:1996:C:O2'	2.45	0.49
2:A:1321:A:OP2	14:S:11:ARG:NH2	2.45	0.49
2:A:627:A:OP1	9:L:78:ARG:NH2	2.45	0.49
2:A:1447:C:O2'	2:A:1544:A:N3	2.40	0.49
2:A:2748:A:H5'	6:G:3:VAL:HG21	1.94	0.49
6:G:23:ILE:HG21	6:G:71:LEU:HD21	1.95	0.49
2:A:2091:C:OP1	25:H:27:ARG:NH1	2.45	0.49
2:A:1021:A:H61	2:A:1142:A:H61	1.59	0.49
2:A:2336:A:H61	26:W:39:THR:HG21	1.77	0.49
2:A:2646:C:OP2	2:A:2732:G:O2'	2.30	0.49
11:P:26:GLU:HB3	11:P:84:SER:HB3	1.95	0.49
2:A:162:U:O2	2:A:164:C:N4	2.45	0.49
2:A:1638:C:O2	2:A:2698:U:O2'	2.30	0.49
9:L:19:LEU:HD13	9:L:31:GLY:HA3	1.95	0.49
10:N:103:ARG:HG2	10:N:105:GLY:H	1.77	0.49
2:A:453:A:N3	2:A:457:A:O2'	2.45	0.49
2:A:1035:U:O2	2:A:1120:G:O6	2.30	0.49
2:A:1826:G:O2'	2:A:1971:U:OP2	2.30	0.49
2:A:1354:A:H62	2:A:1377:G:H21	1.61	0.49
26:W:67:VAL:HG22	26:W:74:LYS:HG2	1.94	0.49
2:A:95:A:H4'	18:Y:39:GLN:HA	1.95	0.49
2:A:500:G:N1	2:A:503:A:OP2	2.39	0.49
2:A:2787:C:H1'	4:D:63:PRO:HG3	1.95	0.49
4:D:4:LEU:HD21	4:D:100:LEU:HD21	1.95	0.49
10:N:63:ARG:NH1	10:N:76:VAL:O	2.45	0.49
21:O:25:ARG:NH1	23:B:8:C:O2'	2.46	0.49
2:A:373:U:H2'	2:A:374:A:H8	1.78	0.48
2:A:414:C:H2'	2:A:415:A:H8	1.76	0.48
2:A:956:G:N2	2:A:960:A:OP2	2.44	0.48
2:A:2771:C:O2'	4:D:173:GLN:NE2	2.46	0.48
2:A:2824:C:OP2	2:A:2825:G:N2	2.45	0.48
16:U:84:PHE:HE1	16:U:93:ARG:HG2	1.78	0.48
2:A:1801:A:N6	2:A:2201:G:O2'	2.38	0.48
2:A:177:G:H3'	2:A:178:G:H8	1.79	0.48
2:A:1652:A:OP1	10:N:8:ARG:NH2	2.47	0.48
2:A:2291:U:O2'	2:A:2374:C:O2	2.32	0.48
24:Z:55:LYS:NZ	24:Z:57:GLU:OE2	2.46	0.48
6:G:6:ALA:HB3	6:G:68:ARG:HE	1.78	0.48
2:A:355:U:H2'	2:A:356:G:H8	1.78	0.48
2:A:1223:G:O6	13:R:71:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1363:C:O2'	2:A:1809:A:N3	2.38	0.48
18:Y:50:VAL:HA	18:Y:53:VAL:HG12	1.95	0.48
1:V:11:GLU:OE1	1:V:19:ARG:NH2	2.44	0.48
2:A:950:G:O6	2:A:967:U:O4	2.31	0.48
2:A:1500:G:H4'	3:C:100:ARG:HH12	1.77	0.48
2:A:1668:A:N3	2:A:1670:C:N4	2.62	0.48
3:C:77:VAL:HG22	3:C:93:VAL:HG12	1.96	0.48
13:R:65:ALA:HB3	13:R:95:ASP:HB2	1.94	0.48
2:A:482:A:O2'	2:A:497:A:N1	2.45	0.48
2:A:495:G:N3	14:S:61:ASN:ND2	2.61	0.48
2:A:1528:A:N6	2:A:1543:G:O2'	2.47	0.48
2:A:2139:U:H2'	2:A:2140:G:H8	1.79	0.48
2:A:2404:U:H3	2:A:2413:G:H1	1.60	0.48
16:U:24:VAL:HG12	16:U:35:VAL:HG22	1.96	0.48
2:A:2647:U:H2'	2:A:2648:G:H8	1.79	0.48
23:B:6:G:H2'	23:B:7:G:H8	1.79	0.48
2:A:586:A:HO2'	2:A:671:C:HO2'	1.56	0.48
2:A:903:C:H2'	2:A:904:G:H8	1.79	0.48
2:A:922:C:H2'	2:A:923:G:H8	1.78	0.48
2:A:1201:U:H2'	2:A:1202:G:H8	1.78	0.48
2:A:2151:U:H2'	2:A:2152:G:H8	1.79	0.48
2:A:324:A:OP2	2:A:1205:A:N6	2.47	0.47
8:K:64:ARG:HB2	8:K:83:ALA:HB3	1.96	0.47
2:A:18:U:H4'	12:Q:22:GLY:HA2	1.96	0.47
2:A:2199:A:N1	2:A:2226:C:N4	2.62	0.47
2:A:2690:U:OP1	10:N:14:SER:OG	2.32	0.47
10:N:21:PHE:HA	10:N:24:MET:HG2	1.96	0.47
2:A:177:G:OP2	2:A:177:G:N2	2.35	0.47
2:A:739:A:H1'	2:A:740:C:H5	1.79	0.47
3:C:257:ARG:HH21	3:C:266:ILE:HD13	1.79	0.47
2:A:210:C:OP1	20:2:29:GLN:NE2	2.43	0.47
2:A:587:C:H5'	5:E:85:PHE:HE2	1.79	0.47
4:D:129:THR:OG1	4:D:140:HIS:O	2.29	0.47
5:E:2:GLU:HB3	5:E:11:ALA:HB1	1.97	0.47
2:A:633:A:O2'	2:A:2404:U:OP1	2.31	0.47
2:A:639:U:H3	2:A:649:G:H1	1.62	0.47
2:A:704:G:O2'	2:A:726:G:N2	2.46	0.47
2:A:2091:C:H5"	25:H:27:ARG:HH11	1.79	0.47
1:V:9:ARG:NH2	1:V:11:GLU:O	2.48	0.47
2:A:186:G:H2'	2:A:187:G:H8	1.80	0.47
2:A:877:A:H1'	2:A:900:A:H62	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:968:C:H2'	2:A:969:G:C8	2.50	0.47
2:A:1378:A:O2'	2:A:1380:G:OP2	2.33	0.47
11:P:90:ALA:HB2	11:P:112:ARG:HG3	1.97	0.47
1:V:2:PHE:O	1:V:62:THR:OG1	2.30	0.47
2:A:1615:C:OP2	2:A:1617:C:N4	2.45	0.47
2:A:2377:A:O2'	21:O:117:PHE:O	2.33	0.47
2:A:598:U:H2'	2:A:599:A:H8	1.79	0.47
2:A:2396:G:H2'	2:A:2397:G:H8	1.79	0.47
4:D:46:ARG:HB3	4:D:84:LEU:HD12	1.95	0.47
2:A:673:C:OP1	5:E:49:ARG:NH2	2.44	0.46
2:A:2245:U:H5"	2:A:2246:G:H5'	1.95	0.46
1:V:62:THR:HG22	1:V:71:LYS:HG2	1.97	0.46
2:A:2692:G:H2'	2:A:2693:G:H8	1.79	0.46
18:Y:45:GLN:HA	18:Y:48:ARG:HB2	1.96	0.46
2:A:107:G:H2'	2:A:108:G:H8	1.81	0.46
2:A:924:G:H2'	2:A:925:A:H8	1.80	0.46
2:A:1386:C:H2'	2:A:1387:A:C8	2.50	0.46
2:A:1386:C:H2'	2:A:1387:A:H8	1.80	0.46
3:C:131:MET:HA	3:C:134:ILE:HD12	1.96	0.46
22:F:47:LYS:O	22:F:51:ASN:ND2	2.48	0.46
2:A:923:G:H2'	2:A:924:G:H8	1.80	0.46
2:A:1727:C:H42	2:A:1733:G:H1	1.64	0.46
3:C:226:PRO:HB3	3:C:232:GLY:HA2	1.98	0.46
21:O:26:LEU:N	21:O:91:SER:O	2.48	0.46
22:F:35:LEU:HD22	22:F:60:SER:HB2	1.96	0.46
2:A:1969:A:H2'	2:A:1972:G:H21	1.81	0.46
4:D:3:GLY:HA3	4:D:204:LYS:HG2	1.97	0.46
21:O:30:ARG:NH2	23:B:48:U:OP2	2.41	0.46
2:A:1681:G:H21	2:A:1762:A:H3'	1.81	0.46
2:A:2056:G:H2'	2:A:2057:G:H8	1.81	0.46
2:A:2898:U:H2'	2:A:2899:A:H8	1.79	0.46
26:W:19:VAL:HG13	26:W:34:VAL:HG22	1.97	0.46
2:A:1929:G:OP2	2:A:1929:G:N2	2.46	0.46
2:A:2667:C:N3	6:G:109:SER:OG	2.45	0.46
22:F:132:ARG:HA	22:F:150:GLY:HA2	1.98	0.46
2:A:206:U:H2'	2:A:207:A:H8	1.81	0.46
2:A:1636:U:O2'	2:A:1760:C:O2	2.33	0.46
2:A:1744:A:H3'	2:A:1745:A:H8	1.80	0.46
2:A:2013:A:O2'	14:S:94:ASP:OD2	2.33	0.46
5:E:83:VAL:HB	5:E:86:ALA:HB2	1.97	0.46
2:A:1406:U:H2'	2:A:1407:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:797:G:OP1	5:E:55:SER:OG	2.30	0.45
2:A:1709:U:H2'	2:A:1710:G:H8	1.82	0.45
2:A:2786:U:OP1	4:D:70:LYS:NZ	2.50	0.45
7:J:72:LYS:HE3	7:J:74:TYR:HE1	1.81	0.45
21:O:67:ASN:H	21:O:70:ALA:HB3	1.81	0.45
23:B:40:U:N3	23:B:44:G:OP2	2.47	0.45
2:A:517:C:OP1	19:0:12:ARG:NH1	2.50	0.45
2:A:1315:C:O2'	2:A:1392:A:N3	2.42	0.45
7:J:34:ARG:HH22	12:Q:69:ARG:HD2	1.81	0.45
23:B:60:C:H2'	23:B:61:G:H8	1.80	0.45
2:A:2659:G:O2'	2:A:2661:G:N7	2.38	0.45
15:T:48:GLN:HE22	15:T:54:GLU:HA	1.82	0.45
2:A:1667:G:O2'	2:A:1991:U:O4	2.35	0.45
2:A:2036:C:H2'	2:A:2037:A:H8	1.82	0.45
3:C:166:ARG:HG3	3:C:171:VAL:HG12	1.98	0.45
2:A:81:G:O2'	2:A:295:G:O2'	2.34	0.45
2:A:2304:G:N1	2:A:2312:U:O4	2.49	0.45
22:F:15:LEU:HA	22:F:18:GLU:HB2	1.98	0.45
2:A:6:A:H2'	2:A:7:G:C8	2.51	0.45
2:A:48:G:N2	2:A:177:G:OP2	2.43	0.45
2:A:1170:C:H2'	2:A:1171:G:C8	2.52	0.45
2:A:1709:U:O2'	2:A:2859:G:N3	2.40	0.45
2:A:2079:U:H4'	17:X:19:HIS:HB3	1.99	0.45
2:A:2194:U:H2'	2:A:2195:U:H6	1.82	0.45
2:A:2691:C:H2'	2:A:2692:G:C8	2.51	0.45
3:C:52:HIS:HA	3:C:216:ARG:HB2	1.99	0.45
25:H:1:MET:N	25:H:21:VAL:O	2.50	0.45
2:A:1141:U:O2	2:A:1142:A:N6	2.50	0.45
2:A:1997:C:H2'	2:A:1998:A:H8	1.82	0.45
2:A:2291:U:H1'	2:A:2374:C:H1'	1.99	0.45
2:A:2691:C:H2'	2:A:2692:G:H8	1.82	0.44
3:C:106:PRO:HA	3:C:194:VAL:HA	1.98	0.44
5:E:148:ILE:HB	5:E:169:VAL:HA	1.99	0.44
2:A:143:C:H2'	2:A:144:A:C8	2.52	0.44
2:A:247:G:N2	2:A:251:A:OP2	2.46	0.44
2:A:459:U:H2'	2:A:460:A:H8	1.82	0.44
2:A:630:G:N2	2:A:633:A:OP2	2.45	0.44
2:A:1420:A:O2'	2:A:2211:A:N7	2.39	0.44
2:A:2836:U:H2'	2:A:2837:A:H8	1.82	0.44
2:A:451:U:O2	2:A:453:A:N6	2.50	0.44
2:A:1592:C:H2'	2:A:1593:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2438:U:H4'	2:A:2439:A:H3'	1.99	0.44
23:B:78:A:H62	23:B:98:G:H21	1.65	0.44
2:A:57:C:H42	2:A:70:G:H1	1.65	0.44
2:A:754:U:O2'	2:A:1272:A:N1	2.49	0.44
2:A:1592:C:H2'	2:A:1593:A:H8	1.81	0.44
2:A:1999:C:O2	2:A:2687:U:O2'	2.28	0.44
5:E:176:ASP:N	5:E:176:ASP:OD1	2.51	0.44
15:T:65:GLY:N	15:T:79:ASP:OD1	2.48	0.44
19:0:37:HIS:ND1	19:0:38:LEU:O	2.43	0.44
22:F:176:PHE:HD1	22:F:176:PHE:HA	1.68	0.44
2:A:133:U:H2'	2:A:134:G:C8	2.53	0.44
2:A:1432:G:H2'	2:A:1433:A:C8	2.53	0.44
3:C:257:ARG:HH12	3:C:259:ASN:HB2	1.81	0.44
7:J:5:THR:HG23	7:J:45:THR:HG21	2.00	0.44
2:A:2114:A:H61	2:A:2119:A:H62	1.66	0.44
3:C:144:GLU:HA	3:C:151:GLY:HA2	1.98	0.44
11:P:24:THR:HB	11:P:87:ARG:HB3	2.00	0.44
1:V:44:HIS:HE1	1:V:85:LYS:HG2	1.83	0.44
2:A:1323:C:OP1	14:S:98:LYS:NZ	2.39	0.44
22:F:119:LYS:HZ3	22:F:177:ARG:HH22	1.65	0.44
23:B:77:U:O2	23:B:99:A:N7	2.51	0.44
2:A:141:G:H3'	2:A:142:A:C8	2.53	0.44
2:A:151:C:H2'	2:A:152:A:H8	1.83	0.44
2:A:1203:U:H4'	9:L:3:LEU:HG	2.00	0.44
15:T:37:ASP:O	15:T:81:LYS:NZ	2.51	0.44
2:A:36:G:N3	2:A:450:G:O2'	2.50	0.44
2:A:811:U:H3'	9:L:22:GLY:HA2	2.00	0.44
5:E:111:GLU:OE1	5:E:114:ARG:NH1	2.51	0.44
11:P:26:GLU:HB2	11:P:86:LYS:HE2	2.00	0.44
22:F:32:LYS:HB3	22:F:91:ARG:HE	1.82	0.44
2:A:645:C:H2'	2:A:647:G:C8	2.53	0.43
2:A:1300:G:N7	2:A:1626:A:O2'	2.39	0.43
2:A:1300:G:H4'	2:A:1301:A:H5"	2.00	0.43
2:A:2087:G:H2'	2:A:2088:A:H8	1.83	0.43
2:A:576:U:OP2	2:A:2055:C:N4	2.51	0.43
2:A:644:A:H2	2:A:2369:A:H1'	1.83	0.43
2:A:2692:G:H2'	2:A:2693:G:C8	2.53	0.43
2:A:2898:U:H2'	2:A:2899:A:C8	2.53	0.43
3:C:131:MET:HE1	3:C:143:VAL:HG13	2.00	0.43
2:A:2847:U:O2	2:A:2869:G:O6	2.35	0.43
17:X:35:HIS:NE2	25:H:28:ASN:OD1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1837:C:O2'	2:A:1927:A:N3	2.40	0.43
6:G:120:ILE:HD11	6:G:139:VAL:HG12	2.00	0.43
2:A:833:A:H2'	2:A:834:G:H8	1.83	0.43
2:A:18:U:H2'	2:A:19:A:H8	1.84	0.43
2:A:527:C:N4	2:A:2779:U:OP2	2.44	0.43
2:A:552:U:H2'	2:A:553:G:H8	1.84	0.43
2:A:1227:G:H2'	2:A:1228:G:H8	1.83	0.43
23:B:72:G:N2	23:B:104:A:H62	2.14	0.43
24:Z:41:PRO:HA	24:Z:44:ARG:HB3	2.00	0.43
2:A:1633:G:N7	2:A:1635:A:N6	2.66	0.43
2:A:2331:G:O3'	26:W:39:THR:OG1	2.37	0.43
4:D:148:GLN:HB3	4:D:149:ASN:H	1.65	0.43
23:B:36:C:H5"	23:B:38:C:H41	1.84	0.43
2:A:65:U:H2'	2:A:66:C:H6	1.84	0.43
2:A:226:A:H5'	2:A:257:C:H4'	2.00	0.43
12:Q:90:ASP:OD1	12:Q:90:ASP:N	2.52	0.43
15:T:74:ILE:H	15:T:74:ILE:HG13	1.72	0.43
23:B:93:C:H2'	23:B:94:A:H8	1.83	0.43
2:A:1341:G:H1'	15:T:59:ASN:HB3	2.00	0.43
2:A:2047:C:H2'	2:A:2048:G:H8	1.83	0.43
6:G:79:THR:HG22	6:G:80:GLU:HG3	2.01	0.43
22:F:157:THR:HG22	22:F:159:ALA:H	1.84	0.43
2:A:2656:U:C2	2:A:2665:A:N7	2.87	0.43
14:S:73:LYS:HB3	14:S:106:VAL:HB	1.99	0.43
16:U:32:LYS:HB3	16:U:63:ALA:HB1	2.01	0.43
2:A:84:A:H62	2:A:101:A:H2	1.67	0.42
2:A:438:G:H2'	2:A:439:A:C8	2.54	0.42
2:A:1825:U:H2'	2:A:1826:G:H8	1.84	0.42
2:A:2166:U:H3	2:A:2170:A:H62	1.67	0.42
2:A:2314:A:H1'	22:F:154:THR:HG21	2.00	0.42
14:S:84:ARG:HB2	14:S:96:ILE:HD11	2.01	0.42
2:A:18:U:H2'	2:A:19:A:C8	2.54	0.42
2:A:184:C:H2'	2:A:185:G:C8	2.54	0.42
2:A:302:C:H2'	2:A:303:G:C8	2.55	0.42
2:A:839:U:H3	2:A:939:G:H1	1.67	0.42
2:A:1830:C:H2'	2:A:1831:G:H8	1.84	0.42
2:A:2330:G:H21	26:W:38:GLY:HA2	1.84	0.42
9:L:129:LYS:HG2	9:L:132:ARG:HH22	1.84	0.42
23:B:63:C:H2'	23:B:64:G:C8	2.55	0.42
2:A:577:G:O2'	2:A:1254:A:OP1	2.38	0.42
2:A:581:C:H2'	2:A:582:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1040:A:H61	2:A:1115:G:H1	1.66	0.42
2:A:1309:G:H4'	20:2:7:PRO:HB2	2.01	0.42
22:F:104:THR:HG22	22:F:105:ILE:HG23	2.01	0.42
2:A:20:C:H2'	2:A:21:A:C8	2.54	0.42
15:T:37:ASP:OD1	15:T:37:ASP:N	2.47	0.42
16:U:12:VAL:HG21	16:U:38:ILE:HG21	2.01	0.42
2:A:45:G:H5'	2:A:46:G:H5'	2.02	0.42
2:A:1181:U:H2'	2:A:1182:G:C8	2.54	0.42
2:A:1223:G:N2	2:A:1226:A:OP2	2.40	0.42
2:A:1355:G:H2'	2:A:1356:G:H8	1.84	0.42
2:A:1664:A:H61	2:A:1996:C:H42	1.68	0.42
2:A:1997:C:H2'	2:A:1998:A:C8	2.55	0.42
2:A:2685:G:H2'	2:A:2686:G:H8	1.85	0.42
2:A:184:C:H2'	2:A:185:G:H8	1.84	0.42
2:A:607:U:H2'	2:A:608:A:H8	1.84	0.42
2:A:1932:A:H62	2:A:1968:G:H21	1.68	0.42
2:A:2827:C:H2'	2:A:2828:G:H8	1.84	0.42
18:Y:20:ASN:O	18:Y:24:GLU:HG2	2.20	0.42
2:A:573:U:O4	2:A:2029:G:O2'	2.30	0.42
2:A:2270:A:O2'	26:W:16:ARG:NH1	2.52	0.42
2:A:2746:U:H5"	6:G:137:LYS:HE2	2.01	0.42
2:A:2836:U:H2'	2:A:2837:A:C8	2.55	0.42
8:K:80:ASP:OD2	11:P:61:ARG:NH1	2.52	0.42
15:T:55:VAL:HG23	15:T:85:VAL:HG13	2.02	0.42
2:A:1252:G:H4'	12:Q:32:ARG:HH11	1.85	0.42
2:A:1428:C:N4	2:A:1570:A:OP2	2.42	0.42
2:A:2683:C:OP1	11:P:50:ARG:NH2	2.53	0.42
13:R:5:PHE:HB3	13:R:59:ILE:HD12	2.02	0.42
14:S:3:THR:OG1	14:S:62:ASP:OD2	2.35	0.42
2:A:2087:G:H2'	2:A:2088:A:C8	2.55	0.41
2:A:2368:C:H2'	2:A:2369:A:H8	1.85	0.41
5:E:176:ASP:OD1	5:E:179:SER:OG	2.30	0.41
19:0:12:ARG:HH21	19:0:16:ARG:HH12	1.68	0.41
2:A:151:C:H2'	2:A:152:A:C8	2.55	0.41
2:A:856:G:H2'	2:A:857:G:C8	2.56	0.41
2:A:1359:A:OP2	2:A:1371:G:N2	2.45	0.41
2:A:1721:G:H2'	2:A:1738:G:H22	1.86	0.41
2:A:2849:U:O4	11:P:20:ARG:NH2	2.44	0.41
4:D:105:LYS:HA	4:D:177:VAL:HG22	2.01	0.41
24:Z:8:GLN:HB2	24:Z:28:LEU:HD23	2.02	0.41
25:H:24:GLY:O	25:H:27:ARG:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:20:C:H2'	2:A:21:A:H8	1.85	0.41
2:A:1258:U:H2'	2:A:1259:G:C8	2.55	0.41
2:A:1567:G:H3'	3:C:84:PRO:HG3	2.02	0.41
2:A:1687:G:H21	2:A:1701:A:H62	1.66	0.41
2:A:1931:U:N3	2:A:1969:A:C8	2.88	0.41
2:A:2060:A:H5'	2:A:2609:U:H3	1.85	0.41
2:A:99:U:H5"	2:A:100:U:H5'	2.02	0.41
2:A:2656:U:H2'	2:A:2657:A:H8	1.85	0.41
6:G:84:LYS:HB3	6:G:132:LEU:HB2	2.02	0.41
2:A:5:A:H2'	2:A:6:A:C8	2.55	0.41
2:A:1812:U:H2'	2:A:1813:G:C8	2.56	0.41
2:A:481:G:O2'	2:A:507:A:N1	2.50	0.41
2:A:1590:A:H2'	2:A:1591:A:C8	2.56	0.41
2:A:1683:U:H2'	2:A:1684:G:H8	1.85	0.41
2:A:1710:G:H2'	2:A:1711:A:C8	2.55	0.41
2:A:2616:C:H2'	2:A:2617:U:H6	1.86	0.41
3:C:77:VAL:HG21	3:C:109:LEU:HD21	2.01	0.41
8:K:23:LYS:HB3	8:K:40:LYS:HB3	2.01	0.41
2:A:1650:A:H61	2:A:2007:U:H3	1.68	0.41
2:A:1754:A:N1	2:A:2716:C:O2'	2.52	0.41
2:A:2023:C:H2'	2:A:2024:G:C8	2.55	0.41
2:A:2679:A:H5'	4:D:170:VAL:HG11	2.02	0.41
6:G:42:VAL:HG23	6:G:51:PHE:HE1	1.85	0.41
16:U:41:VAL:HG23	16:U:60:LYS:HZ1	1.85	0.41
2:A:59:U:H1'	2:A:73:A:H2'	2.03	0.41
2:A:521:U:H2'	2:A:522:A:C8	2.56	0.41
2:A:733:G:N2	2:A:734:A:N7	2.68	0.41
2:A:1235:G:H2'	2:A:1236:G:C4	2.55	0.41
2:A:1278:C:H2'	2:A:1279:G:C8	2.55	0.41
2:A:1475:G:H1'	2:A:1476:U:H5	1.86	0.41
7:J:53:TYR:HE1	7:J:121:LYS:HG2	1.85	0.41
2:A:13:A:H61	2:A:525:U:H3'	1.86	0.41
2:A:523:C:H2'	2:A:524:G:H8	1.84	0.41
2:A:1689:A:H2'	2:A:1690:A:H8	1.85	0.41
2:A:2215:C:H2'	2:A:2216:G:H8	1.85	0.41
2:A:2385:C:H2'	2:A:2386:A:C8	2.56	0.41
5:E:143:LEU:HD13	5:E:146:VAL:HG11	2.03	0.41
11:P:50:ARG:HB3	11:P:57:ALA:HB3	2.03	0.41
14:S:8:ARG:HG3	14:S:102:HIS:HE1	1.86	0.41
14:S:34:ASP:OD2	19:0:36:LYS:NZ	2.54	0.41
15:T:15:HIS:HB3	15:T:31:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:76:C:H2'	2:A:77:G:C8	2.56	0.41
2:A:559:G:N2	12:Q:51:GLN:OE1	2.52	0.41
2:A:696:G:H2'	2:A:697:G:H8	1.86	0.41
2:A:974:G:O2'	2:A:989:G:N2	2.54	0.41
3:C:2:VAL:HG12	3:C:18:VAL:HG22	2.02	0.41
3:C:229:HIS:CD2	3:C:246:PRO:HB3	2.56	0.41
6:G:88:LEU:HG	6:G:161:VAL:HG22	2.02	0.41
2:A:16:C:H2'	2:A:17:G:H8	1.86	0.40
2:A:464:U:H1'	2:A:686:U:H5	1.86	0.40
2:A:1229:C:H2'	2:A:1230:A:C8	2.56	0.40
2:A:1568:G:OP2	3:C:62:ARG:NH1	2.53	0.40
2:A:2120:G:H2'	2:A:2121:G:C8	2.56	0.40
13:R:24:LYS:HA	13:R:94:THR:HG23	2.03	0.40
2:A:84:A:H5"	16:U:5:ARG:HG3	2.02	0.40
2:A:1015:U:H2'	2:A:1016:G:C8	2.57	0.40
3:C:70:LYS:O	3:C:117:SER:OG	2.39	0.40
2:A:591:U:H2'	2:A:592:A:H8	1.86	0.40
2:A:1142:A:H4'	7:J:27:ARG:HH22	1.85	0.40
2:A:1148:U:H2'	2:A:1149:G:C8	2.57	0.40
2:A:2070:A:H2'	2:A:2071:A:C8	2.56	0.40
22:F:2:LYS:HE2	22:F:97:GLU:HG2	2.03	0.40
23:B:111:U:H2'	23:B:112:G:H8	1.86	0.40
2:A:1431:A:H2'	2:A:1432:G:C8	2.57	0.40
2:A:2081:U:O2	2:A:2239:G:N2	2.50	0.40
17:X:63:ILE:HG21	25:H:32:PRO:HG3	2.04	0.40
2:A:1291:C:H2'	2:A:1292:G:H8	1.86	0.40
2:A:1443:U:H2'	2:A:1444:G:H8	1.86	0.40
2:A:2233:U:H2'	2:A:2234:G:H8	1.86	0.40
2:A:2626:C:H2'	2:A:2627:G:C8	2.57	0.40
2:A:2737:G:H2'	2:A:2738:A:C8	2.57	0.40
23:B:63:C:H2'	23:B:64:G:H8	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	V	92/94 (98%)	92 (100%)	0	0	100 100
3	C	269/271 (99%)	251 (93%)	18 (7%)	0	100 100
4	D	207/209 (99%)	196 (95%)	11 (5%)	0	100 100
5	E	199/201 (99%)	190 (96%)	9 (4%)	0	100 100
6	G	174/176 (99%)	166 (95%)	8 (5%)	0	100 100
7	J	140/142 (99%)	129 (92%)	11 (8%)	0	100 100
8	K	120/122 (98%)	110 (92%)	10 (8%)	0	100 100
9	L	141/143 (99%)	119 (84%)	22 (16%)	0	100 100
10	N	118/120 (98%)	109 (92%)	9 (8%)	0	100 100
11	P	112/114 (98%)	107 (96%)	5 (4%)	0	100 100
12	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100 100
13	R	101/103 (98%)	94 (93%)	7 (7%)	0	100 100
14	S	108/110 (98%)	102 (94%)	6 (6%)	0	100 100
15	T	91/93 (98%)	84 (92%)	7 (8%)	0	100 100
16	U	100/102 (98%)	84 (84%)	15 (15%)	1 (1%)	15 54
17	X	75/77 (97%)	72 (96%)	3 (4%)	0	100 100
18	Y	61/63 (97%)	54 (88%)	5 (8%)	2 (3%)	4 30
19	0	54/56 (96%)	47 (87%)	7 (13%)	0	100 100
20	2	44/46 (96%)	40 (91%)	4 (9%)	0	100 100
21	O	114/116 (98%)	104 (91%)	9 (8%)	1 (1%)	17 56
22	F	175/177 (99%)	165 (94%)	10 (6%)	0	100 100
24	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100 100
25	H	48/50 (96%)	34 (71%)	12 (25%)	2 (4%)	3 25
26	W	74/76 (97%)	74 (100%)	0	0	100 100
All	All	2788/2836 (98%)	2590 (93%)	192 (7%)	6 (0%)	50 81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	Y	46	VAL
25	H	28	ASN
18	Y	45	GLN

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Mol	Chain	Res	Type
21	O	88	LYS
16	U	98	ASN
25	H	32	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	V	78/78 (100%)	77 (99%)	1 (1%)	69 82
3	C	216/216 (100%)	215 (100%)	1 (0%)	88 93
4	D	164/164 (100%)	162 (99%)	2 (1%)	71 84
5	E	165/165 (100%)	162 (98%)	3 (2%)	59 77
6	G	137/137 (100%)	133 (97%)	4 (3%)	42 64
7	J	116/116 (100%)	116 (100%)	0	100 100
8	K	103/103 (100%)	100 (97%)	3 (3%)	42 64
9	L	102/102 (100%)	98 (96%)	4 (4%)	32 57
10	N	100/100 (100%)	98 (98%)	2 (2%)	55 73
11	P	99/99 (100%)	95 (96%)	4 (4%)	31 56
12	Q	89/89 (100%)	86 (97%)	3 (3%)	37 61
13	R	84/84 (100%)	82 (98%)	2 (2%)	49 69
14	S	93/93 (100%)	93 (100%)	0	100 100
15	T	80/80 (100%)	77 (96%)	3 (4%)	33 58
16	U	83/83 (100%)	81 (98%)	2 (2%)	49 69
17	X	67/67 (100%)	66 (98%)	1 (2%)	65 80
18	Y	55/55 (100%)	54 (98%)	1 (2%)	59 77
19	0	47/47 (100%)	47 (100%)	0	100 100
20	2	38/38 (100%)	37 (97%)	1 (3%)	46 67
21	O	86/86 (100%)	86 (100%)	0	100 100
22	F	148/148 (100%)	144 (97%)	4 (3%)	44 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	Z	48/48 (100%)	47 (98%)	1 (2%)	53 72
25	H	40/40 (100%)	40 (100%)	0	100 100
26	W	56/58 (97%)	56 (100%)	0	100 100
All	All	2294/2296 (100%)	2252 (98%)	42 (2%)	61 77

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	10	LYS
3	C	257	ARG
4	D	33	ARG
4	D	77	ARG
5	E	21	ARG
5	E	163	ASN
5	E	170	ARG
6	G	29	ASN
6	G	68	ARG
6	G	72	ASN
6	G	162	ARG
8	K	49	ARG
8	K	88	ASN
8	K	90	ASN
9	L	33	ARG
9	L	82	LEU
9	L	99	ASN
9	L	126	ARG
10	N	2	ARG
10	N	107	ASN
11	P	2	ASN
11	P	50	ARG
11	P	51	ASN
11	P	102	ARG
12	Q	49	ARG
12	Q	54	ARG
12	Q	80	ASN
13	R	10	LYS
13	R	84	ARG
15	T	1	MET
15	T	28	ASN
15	T	69	ARG
16	U	60	LYS

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Mol	Chain	Res	Type
16	U	73	ASN
17	X	26	ARG
18	Y	43	LEU
20	2	41	ARG
22	F	20	ASN
22	F	36	ASN
22	F	70	ARG
22	F	176	PHE
24	Z	53	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	44	HIS
3	C	85	ASN
3	C	196	ASN
5	E	163	ASN
6	G	29	ASN
6	G	72	ASN
8	K	88	ASN
8	K	90	ASN
9	L	54	GLN
9	L	99	ASN
10	N	3	HIS
10	N	107	ASN
11	P	2	ASN
11	P	51	ASN
12	Q	80	ASN
13	R	89	HIS
14	S	57	ASN
14	S	60	HIS
14	S	102	HIS
15	T	28	ASN
15	T	48	GLN
16	U	73	ASN
18	Y	45	GLN
22	F	20	ASN
22	F	51	ASN
26	W	8	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	2579/2904 (88%)	464 (17%)	9 (0%)
23	B	118/119 (99%)	16 (13%)	0
All	All	2697/3023 (89%)	480 (17%)	9 (0%)

All (480) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	10	A
2	A	12	U
2	A	23	G
2	A	27	G
2	A	35	G
2	A	46	G
2	A	51	G
2	A	63	A
2	A	71	A
2	A	73	A
2	A	74	A
2	A	75	G
2	A	84	A
2	A	96	C
2	A	103	A
2	A	118	A
2	A	119	A
2	A	120	U
2	A	125	A
2	A	134	G
2	A	138	U
2	A	139	U
2	A	140	C
2	A	141	G
2	A	142	A
2	A	143	C
2	A	147	C
2	A	163	C
2	A	181	A
2	A	190	A
2	A	196	A
2	A	199	A
2	A	215	G
2	A	216	A
2	A	221	A
2	A	222	A

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Mol	Chain	Res	Type
2	A	223	A
2	A	228	C
2	A	230	G
2	A	241	A
2	A	248	G
2	A	255	A
2	A	265	A
2	A	266	G
2	A	267	C
2	A	271	G
2	A	272	A
2	A	273	G
2	A	278	A
2	A	302	C
2	A	311	A
2	A	317	G
2	A	329	G
2	A	330	A
2	A	353	C
2	A	361	G
2	A	367	G
2	A	371	A
2	A	372	G
2	A	373	U
2	A	384	A
2	A	386	G
2	A	396	G
2	A	399	U
2	A	405	U
2	A	406	G
2	A	411	G
2	A	424	G
2	A	430	A
2	A	448	U
2	A	451	U
2	A	454	A
2	A	455	C
2	A	467	G
2	A	475	C
2	A	477	A
2	A	480	A
2	A	481	G

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Mol	Chain	Res	Type
2	A	490	C
2	A	491	G
2	A	504	A
2	A	505	A
2	A	508	A
2	A	510	C
2	A	518	G
2	A	531	C
2	A	532	A
2	A	546	U
2	A	547	A
2	A	548	G
2	A	549	G
2	A	550	C
2	A	563	A
2	A	573	U
2	A	586	A
2	A	588	U
2	A	603	A
2	A	607	U
2	A	613	A
2	A	614	A
2	A	615	U
2	A	627	A
2	A	637	A
2	A	645	C
2	A	646	U
2	A	647	G
2	A	654	A
2	A	655	A
2	A	659	G
2	A	668	A
2	A	669	G
2	A	675	A
2	A	686	U
2	A	705	A
2	A	726	G
2	A	729	G
2	A	730	A
2	A	747	U
2	A	748	G
2	A	763	G

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Mol	Chain	Res	Type
2	A	765	C
2	A	775	G
2	A	776	G
2	A	782	A
2	A	784	G
2	A	785	G
2	A	789	A
2	A	791	C
2	A	792	A
2	A	805	G
2	A	812	C
2	A	819	A
2	A	827	U
2	A	828	U
2	A	830	G
2	A	845	A
2	A	846	U
2	A	847	U
2	A	856	G
2	A	858	G
2	A	878	A
2	A	887	U
2	A	890	C
2	A	896	A
2	A	910	A
2	A	914	G
2	A	932	U
2	A	933	A
2	A	934	U
2	A	945	A
2	A	953	G
2	A	957	C
2	A	959	A
2	A	961	C
2	A	973	A
2	A	980	A
2	A	983	A
2	A	985	C
2	A	995	C
2	A	996	A
2	A	1009	A
2	A	1012	U

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Mol	Chain	Res	Type
2	A	1013	C
2	A	1022	G
2	A	1026	G
2	A	1033	U
2	A	1116	G
2	A	1132	U
2	A	1133	A
2	A	1135	C
2	A	1136	G
2	A	1139	G
2	A	1142	A
2	A	1151	A
2	A	1171	G
2	A	1172	C
2	A	1173	U
2	A	1174	U
2	A	1175	A
2	A	1180	U
2	A	1181	U
2	A	1182	G
2	A	1186	G
2	A	1204	A
2	A	1205	A
2	A	1206	G
2	A	1212	G
2	A	1236	G
2	A	1238	G
2	A	1249	U
2	A	1253	A
2	A	1256	G
2	A	1262	A
2	A	1266	G
2	A	1271	G
2	A	1272	A
2	A	1300	G
2	A	1301	A
2	A	1302	A
2	A	1306	C
2	A	1314	C
2	A	1321	A
2	A	1329	U
2	A	1341	G

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Mol	Chain	Res	Type
2	A	1345	C
2	A	1347	A
2	A	1360	G
2	A	1365	A
2	A	1368	G
2	A	1374	G
2	A	1378	A
2	A	1379	U
2	A	1383	A
2	A	1416	G
2	A	1419	A
2	A	1420	A
2	A	1428	C
2	A	1452	G
2	A	1453	A
2	A	1458	U
2	A	1482	G
2	A	1493	C
2	A	1504	A
2	A	1508	A
2	A	1509	A
2	A	1510	G
2	A	1515	A
2	A	1523	U
2	A	1524	G
2	A	1530	G
2	A	1533	C
2	A	1535	A
2	A	1554	U
2	A	1555	G
2	A	1558	C
2	A	1560	G
2	A	1566	A
2	A	1569	A
2	A	1578	U
2	A	1583	A
2	A	1584	U
2	A	1585	C
2	A	1598	A
2	A	1603	A
2	A	1607	C
2	A	1608	A

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Mol	Chain	Res	Type
2	A	1613	G
2	A	1618	A
2	A	1634	A
2	A	1646	C
2	A	1647	U
2	A	1648	U
2	A	1654	A
2	A	1674	G
2	A	1714	U
2	A	1715	G
2	A	1729	U
2	A	1730	C
2	A	1732	C
2	A	1733	G
2	A	1738	G
2	A	1750	G
2	A	1754	A
2	A	1756	G
2	A	1764	C
2	A	1773	A
2	A	1800	C
2	A	1801	A
2	A	1807	G
2	A	1808	A
2	A	1816	C
2	A	1819	A
2	A	1829	A
2	A	1833	C
2	A	1835	G
2	A	1909	C
2	A	1912	A
2	A	1913	A
2	A	1914	C
2	A	1919	A
2	A	1925	C
2	A	1926	U
2	A	1930	G
2	A	1931	U
2	A	1970	A
2	A	1971	U
2	A	1972	G
2	A	1991	U

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Mol	Chain	Res	Type
2	A	1992	G
2	A	1993	U
2	A	1997	C
2	A	2021	C
2	A	2022	U
2	A	2023	C
2	A	2025	C
2	A	2030	A
2	A	2031	A
2	A	2032	G
2	A	2033	A
2	A	2043	C
2	A	2052	A
2	A	2055	C
2	A	2056	G
2	A	2060	A
2	A	2061	G
2	A	2062	A
2	A	2064	C
2	A	2066	C
2	A	2069	G
2	A	2076	U
2	A	2077	A
2	A	2078	C
2	A	2081	U
2	A	2092	U
2	A	2093	G
2	A	2094	A
2	A	2096	C
2	A	2097	A
2	A	2102	G
2	A	2105	U
2	A	2107	G
2	A	2108	A
2	A	2110	G
2	A	2111	U
2	A	2112	G
2	A	2113	U
2	A	2116	G
2	A	2117	A
2	A	2118	U
2	A	2119	A

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Mol	Chain	Res	Type
2	A	2120	G
2	A	2122	U
2	A	2123	G
2	A	2124	G
2	A	2126	A
2	A	2127	G
2	A	2128	G
2	A	2132	U
2	A	2133	G
2	A	2136	G
2	A	2139	U
2	A	2146	C
2	A	2147	A
2	A	2148	G
2	A	2157	G
2	A	2158	A
2	A	2161	C
2	A	2162	G
2	A	2164	C
2	A	2165	C
2	A	2167	U
2	A	2170	A
2	A	2171	A
2	A	2172	U
2	A	2173	A
2	A	2178	C
2	A	2187	U
2	A	2197	U
2	A	2198	A
2	A	2203	U
2	A	2204	G
2	A	2211	A
2	A	2212	A
2	A	2214	C
2	A	2218	G
2	A	2223	G
2	A	2225	A
2	A	2238	G
2	A	2239	G
2	A	2248	C
2	A	2250	G
2	A	2251	G

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Mol	Chain	Res	Type
2	A	2252	G
2	A	2253	G
2	A	2254	C
2	A	2255	G
2	A	2266	A
2	A	2275	C
2	A	2283	C
2	A	2287	A
2	A	2288	A
2	A	2297	A
2	A	2305	U
2	A	2307	G
2	A	2309	A
2	A	2311	A
2	A	2314	A
2	A	2321	U
2	A	2322	A
2	A	2325	G
2	A	2333	A
2	A	2336	A
2	A	2350	C
2	A	2357	G
2	A	2376	A
2	A	2383	G
2	A	2385	C
2	A	2391	G
2	A	2402	U
2	A	2406	A
2	A	2425	A
2	A	2426	A
2	A	2428	G
2	A	2429	G
2	A	2430	A
2	A	2433	A
2	A	2434	A
2	A	2436	G
2	A	2438	U
2	A	2439	A
2	A	2441	U
2	A	2443	C
2	A	2609	U
2	A	2610	C

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Mol	Chain	Res	Type
2	A	2614	A
2	A	2629	U
2	A	2630	G
2	A	2634	A
2	A	2636	C
2	A	2639	A
2	A	2646	C
2	A	2654	A
2	A	2656	U
2	A	2658	C
2	A	2682	A
2	A	2689	U
2	A	2690	U
2	A	2714	G
2	A	2716	C
2	A	2718	G
2	A	2725	A
2	A	2728	U
2	A	2729	G
2	A	2731	G
2	A	2732	G
2	A	2733	A
2	A	2739	U
2	A	2744	G
2	A	2748	A
2	A	2757	A
2	A	2765	A
2	A	2769	U
2	A	2778	A
2	A	2791	G
2	A	2798	U
2	A	2801	G
2	A	2818	U
2	A	2820	A
2	A	2825	G
2	A	2835	A
2	A	2848	G
2	A	2849	U
2	A	2850	A
2	A	2867	G
2	A	2872	A
2	A	2873	A

Continued on next page...

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Mol	Chain	Res	Type
2	A	2879	A
2	A	2880	C
2	A	2884	U
2	A	2885	G
2	A	2886	A
2	A	2887	A
2	A	2893	A
2	A	2903	U
23	B	13	G
23	B	15	A
23	B	16	G
23	B	24	G
23	B	25	U
23	B	35	C
23	B	36	C
23	B	37	C
23	B	41	G
23	B	56	G
23	B	87	U
23	B	89	U
23	B	90	C
23	B	91	C
23	B	99	A
23	B	109	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	271	G
2	A	404	A
2	A	479	A
2	A	1378	A
2	A	1606	C
2	A	2092	U
2	A	2252	G
2	A	2425	A
2	A	2756	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2243:U	O3'	2244:U	P	7.41
1	A	973:A	O3'	974:G	P	3.29

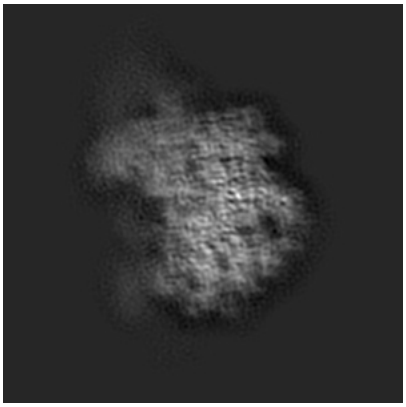
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4380. These allow visual inspection of the internal detail of the map and identification of artifacts.

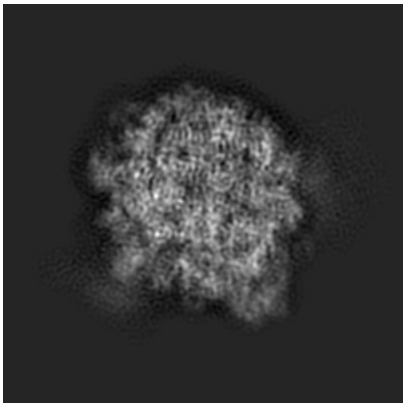
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

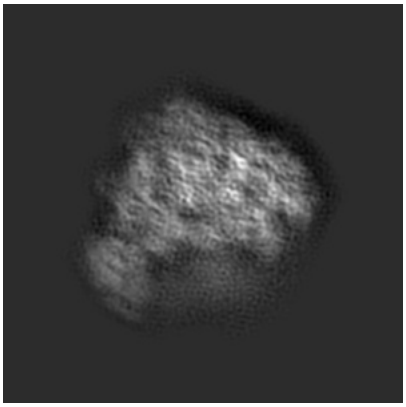
6.1.1 Primary map



X



Y

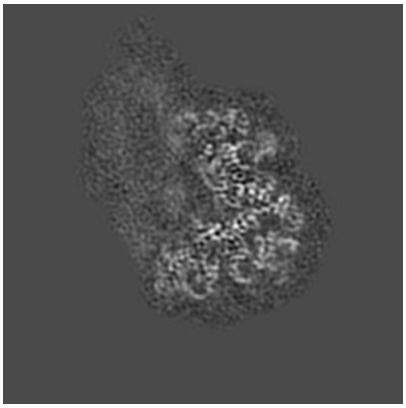


Z

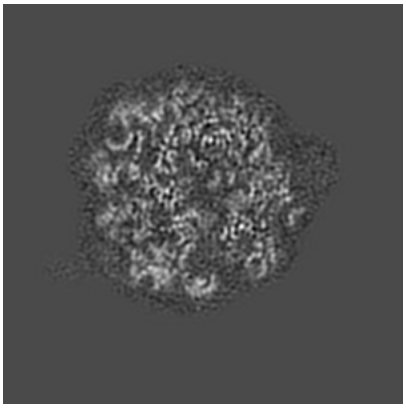
The images above show the map projected in three orthogonal directions.

6.2 Central slices

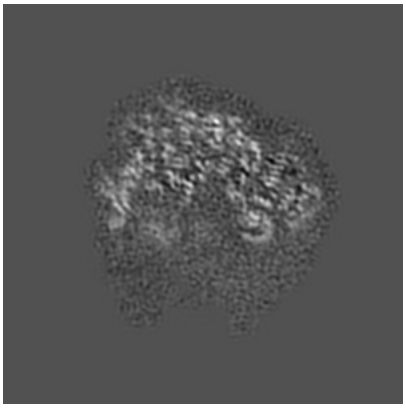
6.2.1 Primary map



X Index: 135



Y Index: 135

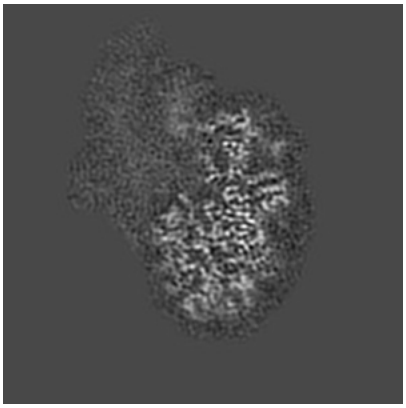


Z Index: 135

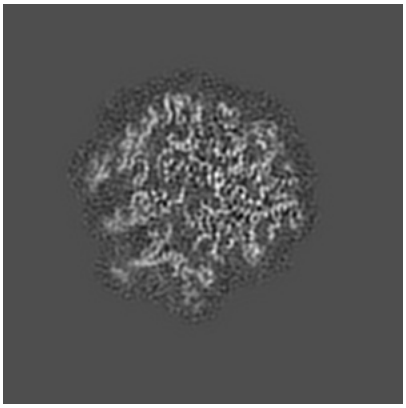
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

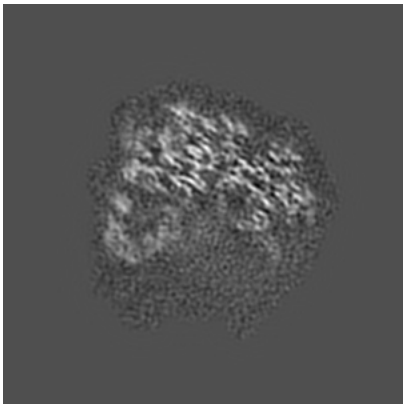
6.3.1 Primary map



X Index: 159



Y Index: 154



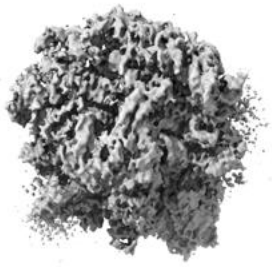
Z Index: 140

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 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

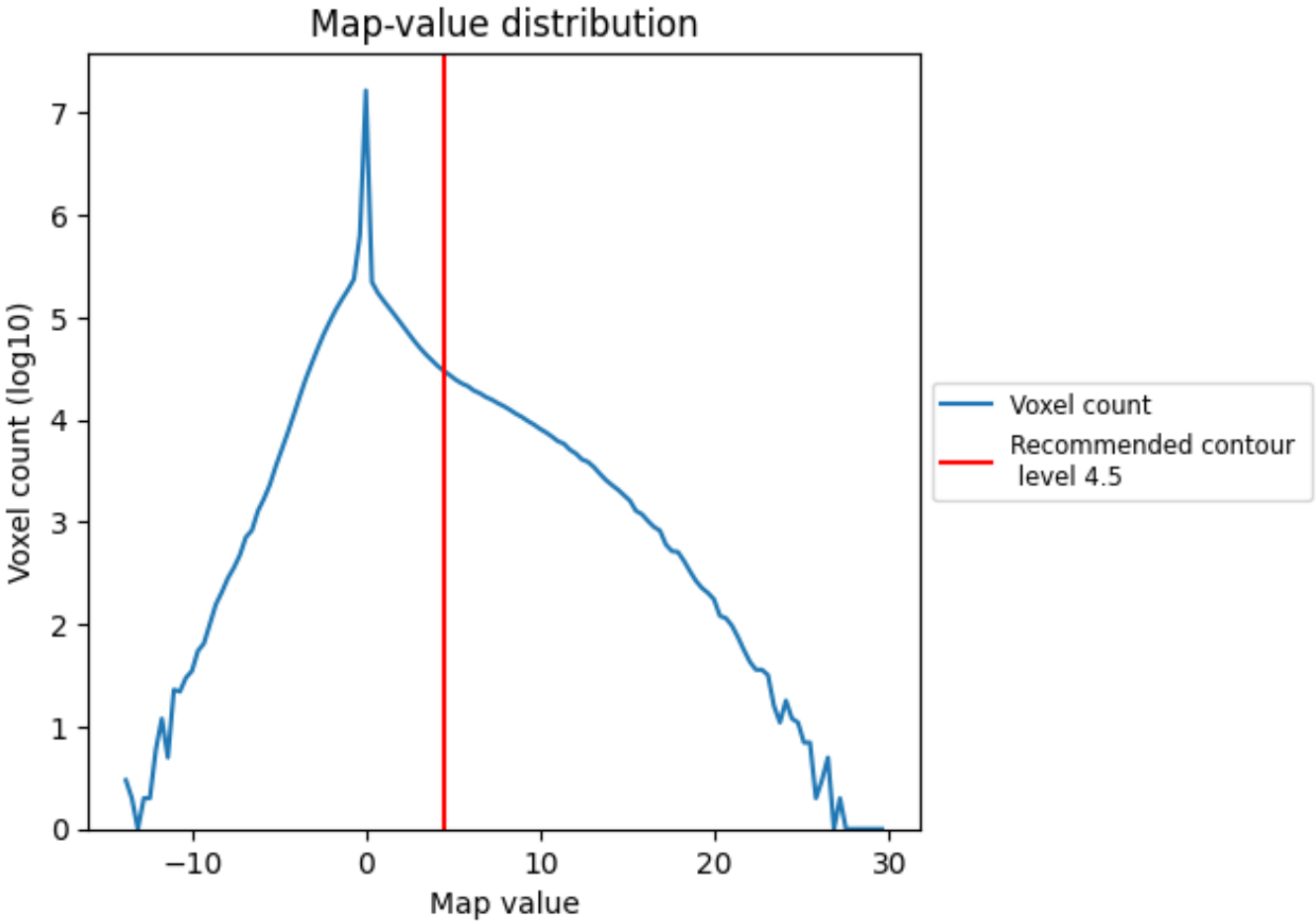
6.5 Mask visualisation (i)

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

7 Map analysis

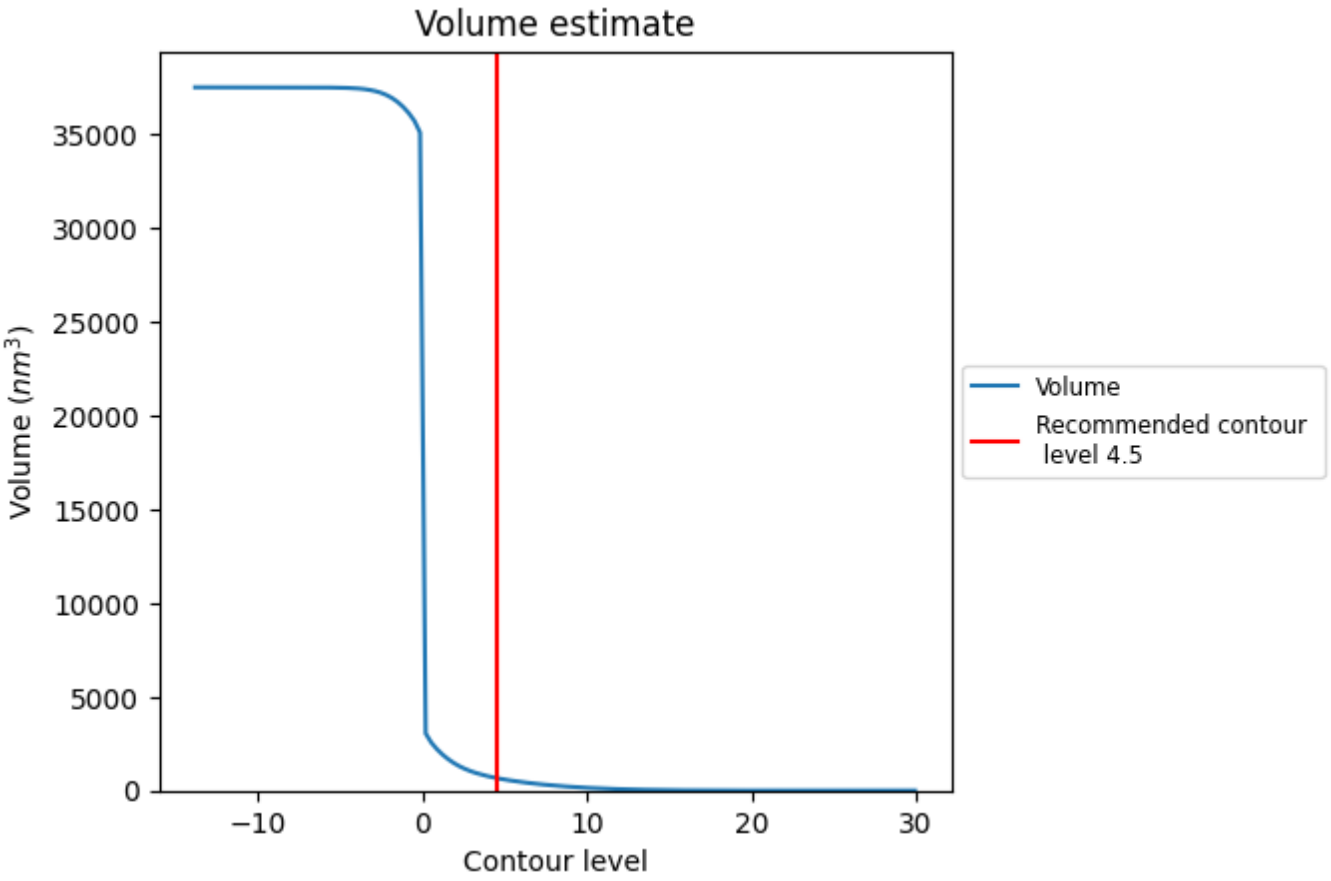
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

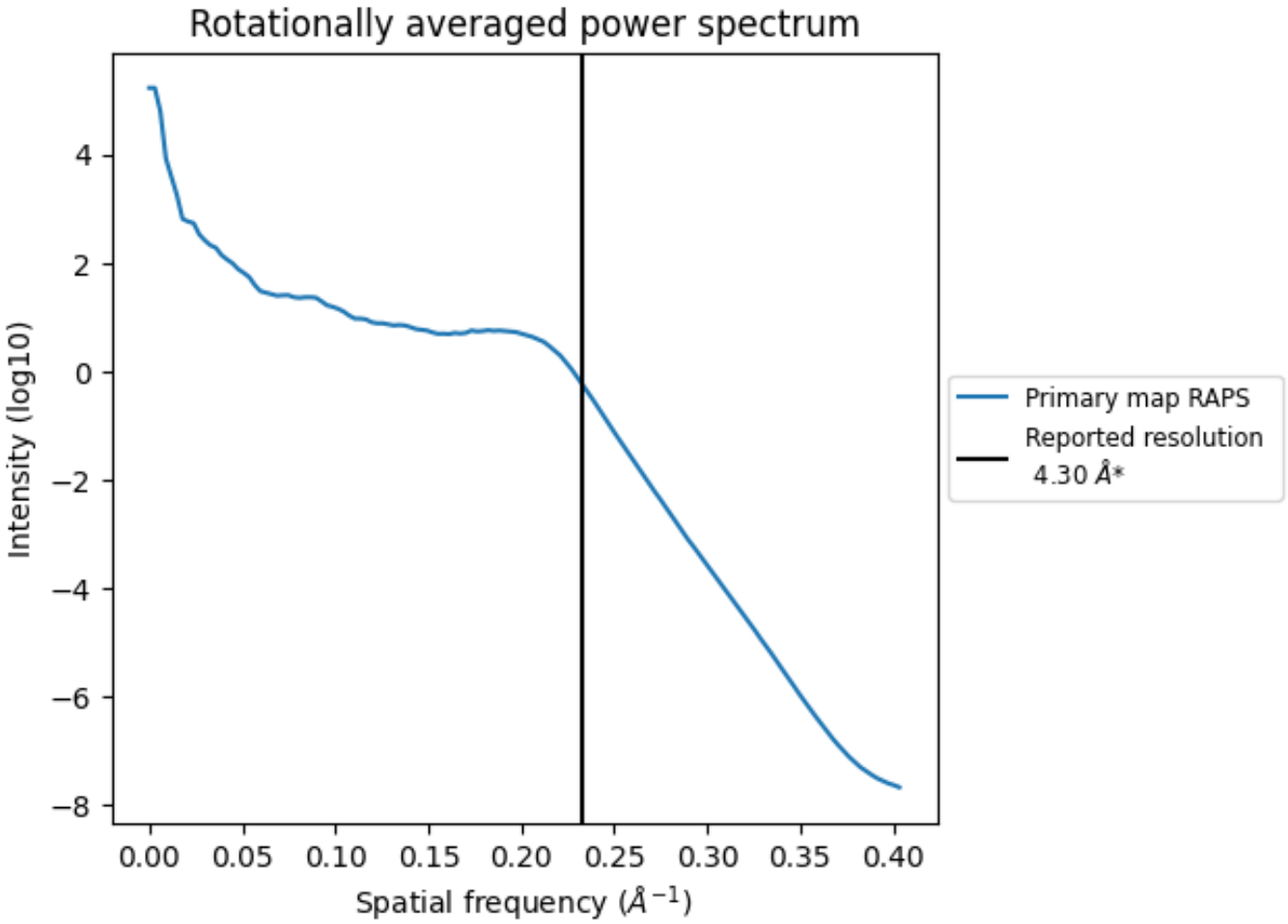
7.2 Volume estimate



The volume at the recommended contour level is 670 nm^3; this corresponds to an approximate mass of 605 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 0.233 Å^{-1}

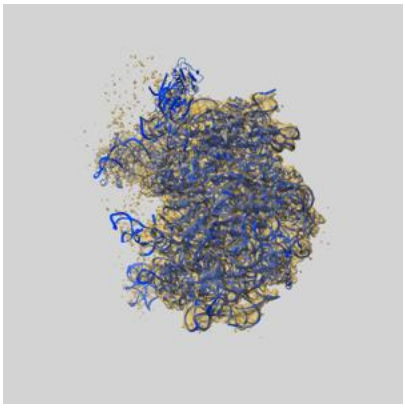
8 Fourier-Shell correlation

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

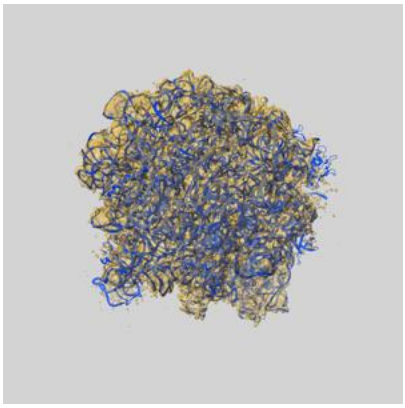
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4380 and PDB model 6GC4. Per-residue inclusion information can be found in section 3 on page 8.

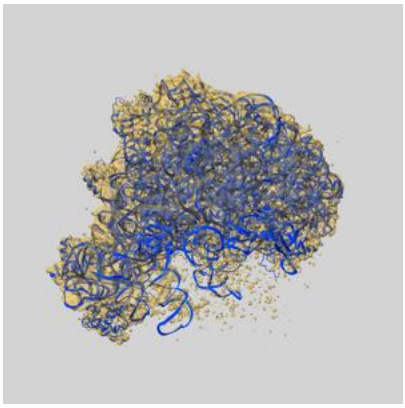
9.1 Map-model overlay



X



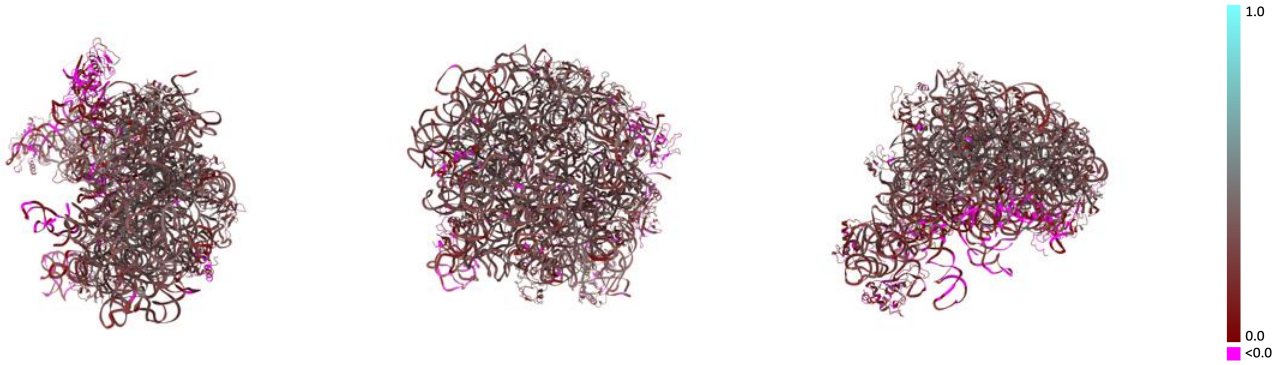
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 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.

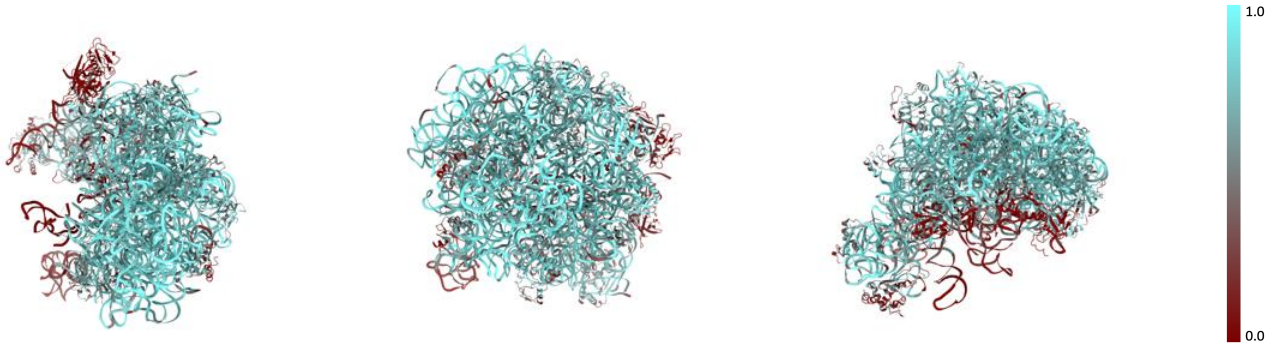
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

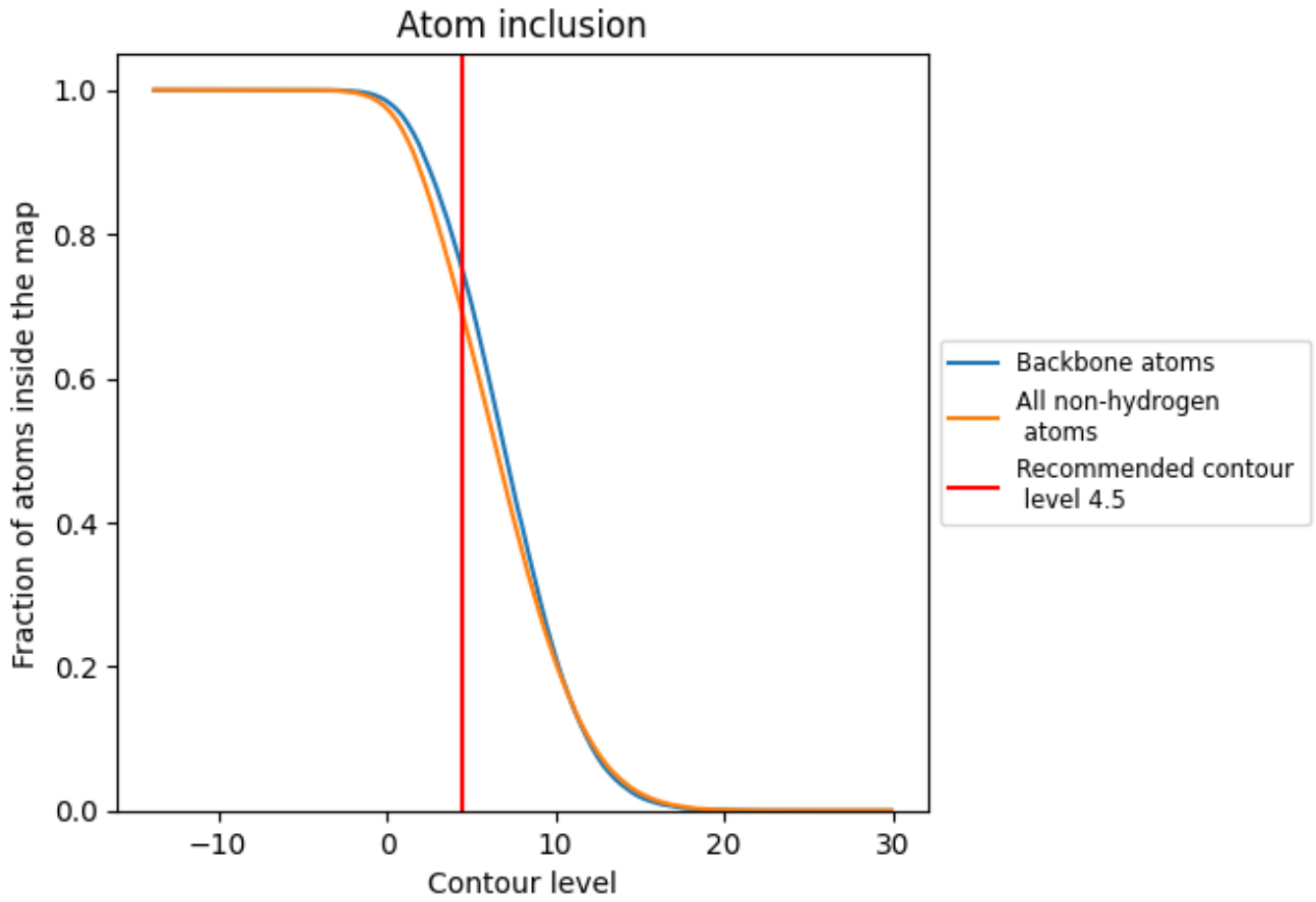
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 69% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6892	0.2620
0	0.6869	0.3170
2	0.6901	0.3230
A	0.7510	0.2740
B	0.7611	0.2280
C	0.5622	0.2830
D	0.6079	0.2720
E	0.5711	0.2450
F	0.3253	0.1090
G	0.0285	0.0130
H	0.1346	0.0940
J	0.6691	0.3000
K	0.5591	0.2470
L	0.4734	0.2180
N	0.6956	0.3130
O	0.5944	0.2070
P	0.6295	0.2760
Q	0.7026	0.3140
R	0.6524	0.2890
S	0.6507	0.2880
T	0.6542	0.2810
U	0.6003	0.2550
V	0.0759	0.1330
W	0.5474	0.2900
X	0.5458	0.2540
Y	0.3119	0.1190
Z	0.5721	0.2860