Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 12:02 AM EST

PDB ID	:	6WU9
EMDB ID	:	EMD-21907
Title	:	50S subunit of 70S Ribosome Enterococcus faecalis MultiBody refinement
Authors	:	Jogl, G.; Khayat, R.
Deposited on	:	2020-05-04
Resolution	:	2.90 Å(reported)
Based on initial models	:	4YBB, 5LI0

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:

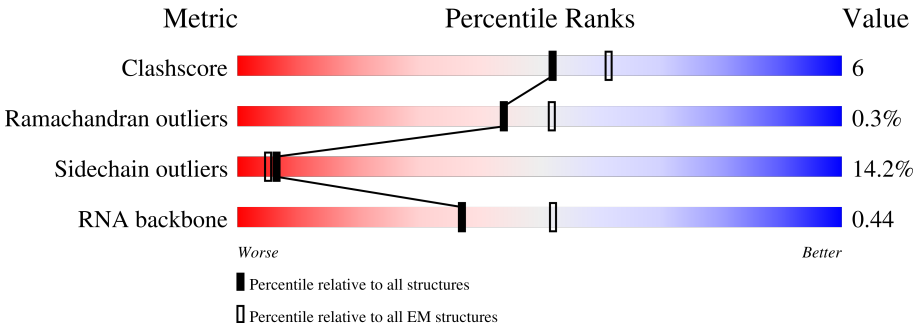
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	A	2908	60% 26% 7% • 6%
2	B	116	6% 48% 31% 19% •
3	D	207	66% 29% 5%
4	E	206	74% 21% 5%
5	F	177	55% 53% 42% 5% •
6	G	176	30% 62% 31% 7%
7	K	145	79% 17% •

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Mol	Chain	Length	Quality of chain
8	L	122	78% 20%
9	M	146	5% 81% 16%
10	N	141	10% 69% 26% 5%
11	O	124	6% 69% 26% 5%
12	P	117	14% 70% 25% 5%
13	Q	114	77% 19%
14	R	118	82% 16%
15	S	102	74% 25%
16	T	112	73% 22%
17	U	89	70% 25% 6%
18	V	101	29% 70% 23% 7%
19	X	76	70% 28%
20	Y	54	7% 74% 20% 6%
21	Z	61	10% 77% 20%
22	0	58	76% 24%
23	2	56	82% 14%
24	3	49	12% 67% 33%
25	4	44	70% 27%
26	5	64	80% 17%
27	6	38	76% 16% 8%

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 82295 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2739	58793	26244	10818	18992	2739	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	116	2480	1106	444	814	116	0	0

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	207	1579	994	292	289	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	206	1574	984	290	298	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	177	1392	887	239	260	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	176	1345	842	244	255	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	145	Total	C	N	O	S	0	0
			1130	714	205	207	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	122	Total	C	N	O	S	0	0
			922	574	176	170	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	146	Total	C	N	O	S	0	0
			1095	677	212	205	1		

- Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	141	Total	C	N	O	S	0	0
			1118	710	216	185	7		

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	124	Total	C	N	O	S	0	0
			991	612	191	185	3		

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	117	Total	C	N	O	S	0	0
			899	556	175	167	1		

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Q	114	Total	C	N	O	0	0
			924	582	185	157		

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	118	Total 950	C 602	N 184	O 160	S 4	0	0

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	102	Total 784	C 500	N 139	O 143	S 2	0	0

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	112	Total 849	C 532	N 156	O 159	S 2	0	0

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	89	Total 720	C 458	N 127	O 132	S 3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	101	Total 763	C 486	N 135	O 140	S 2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	76	Total 572	C 351	N 109	O 112	0	0

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	54	Total 425	C 265	N 86	O 72	S 2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	51	ALA	THR	conflict	UNP A0A1B4XRZ8

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			504	314	94	95	1		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	58	Total	C	N	O	S	0	0
			435	271	81	82	1		

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	56	Total	C	N	O	S	0	0
			429	262	88	73	6		

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	49	Total	C	N	O	S	0	0
			419	253	86	76	4		

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4	44	Total	C	N	O	S	0	0
			374	227	91	54	2		

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	64	Total	C	N	O	S	0	0
			522	320	122	78	2		

- Molecule 27 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	6	38	Total	C	N	O	S	0	0
			304	188	66	44	6		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

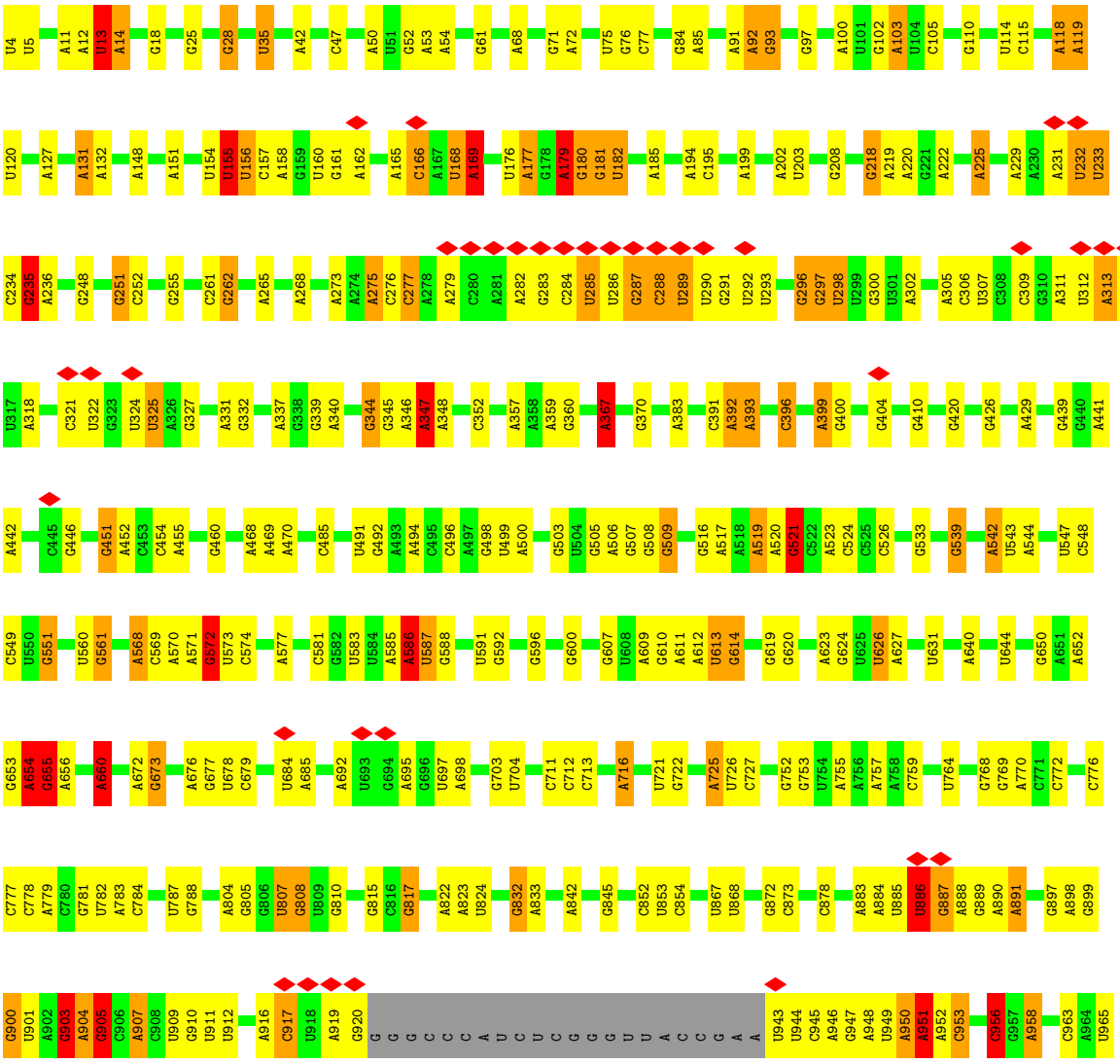
Mol	Chain	Residues	Atoms		AltConf
28	2	1	Total	Zn	0
			1	1	
28	3	1	Total	Zn	0
			1	1	
28	6	1	Total	Zn	0
			1	1	

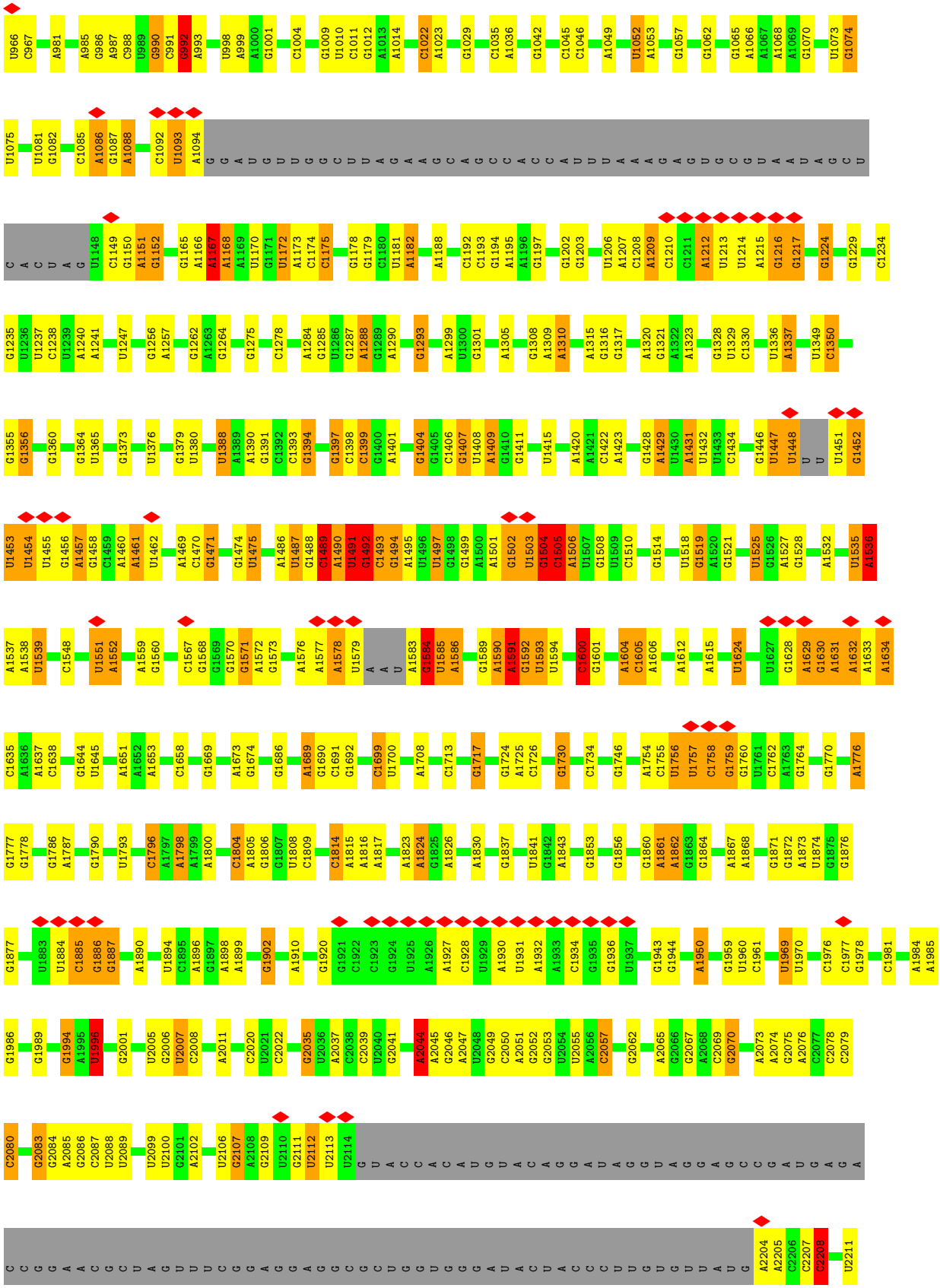
3 Residue-property plots (i)

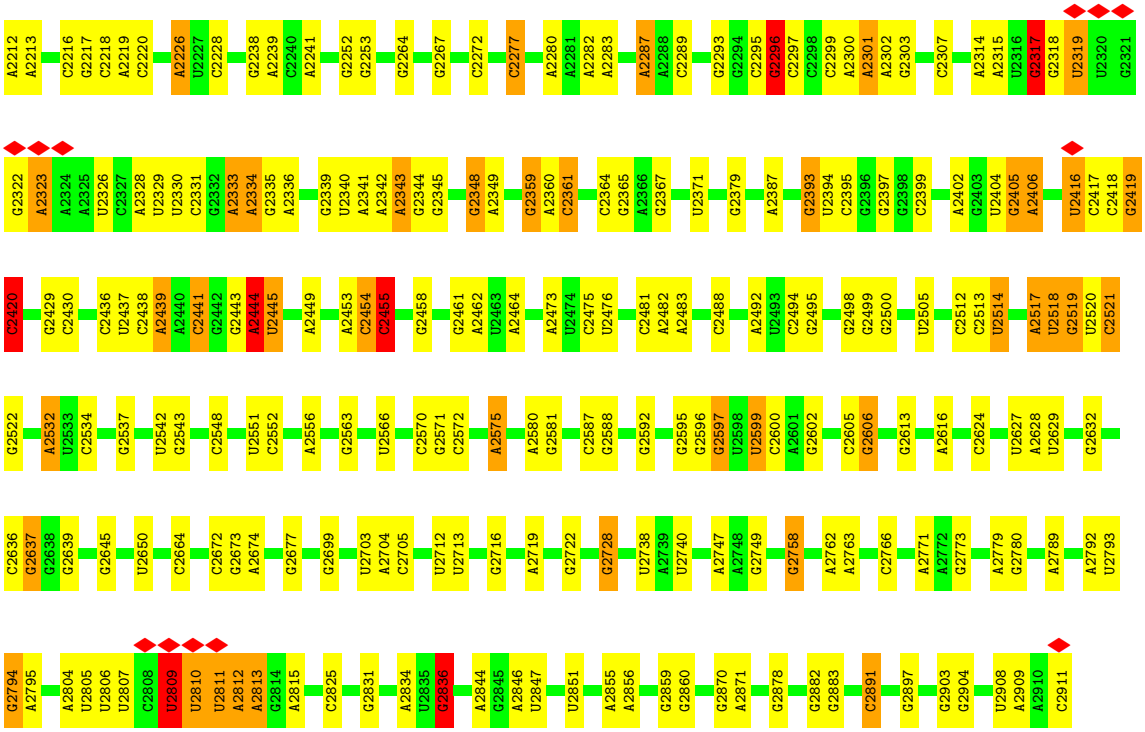
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S rRNA

Chain A:

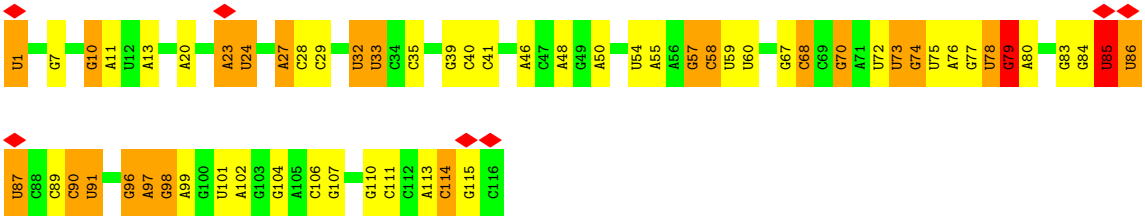






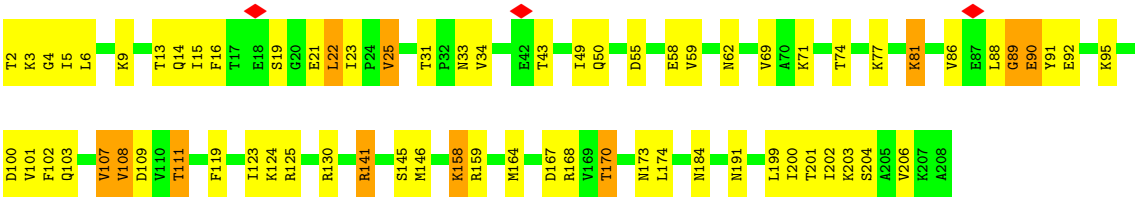
• Molecule 2: 5S rRNA

Chain B:



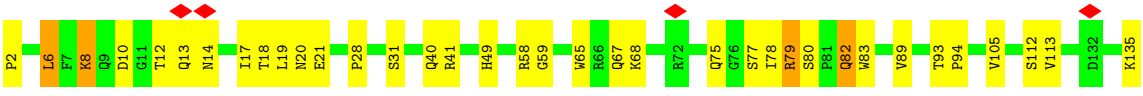
• Molecule 3: 50S ribosomal protein L3

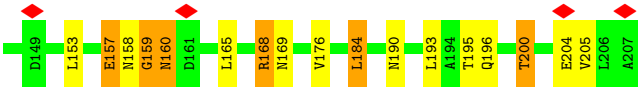
Chain D:



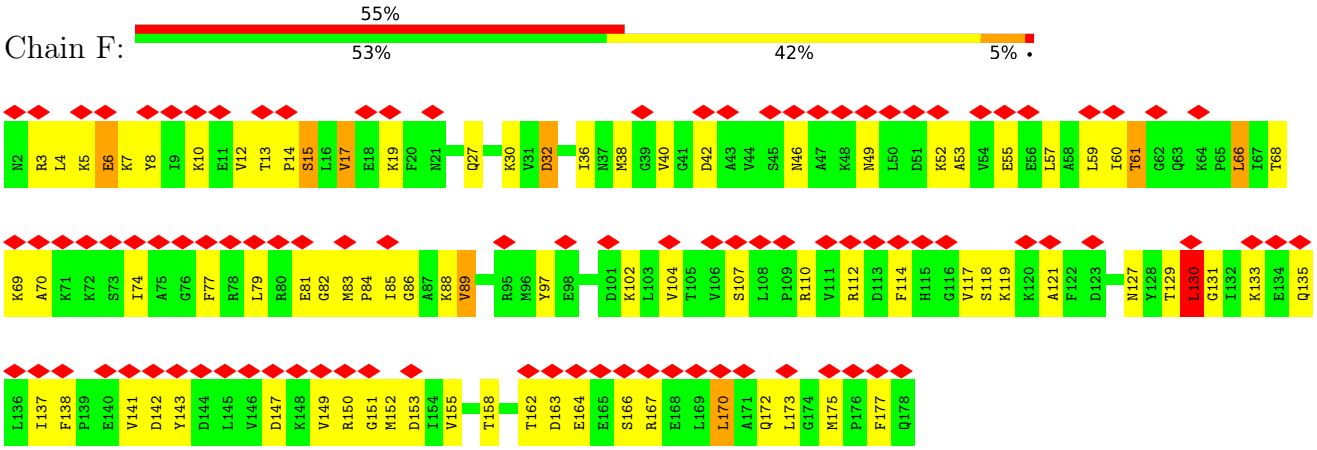
• Molecule 4: 50S ribosomal protein L4

Chain E:

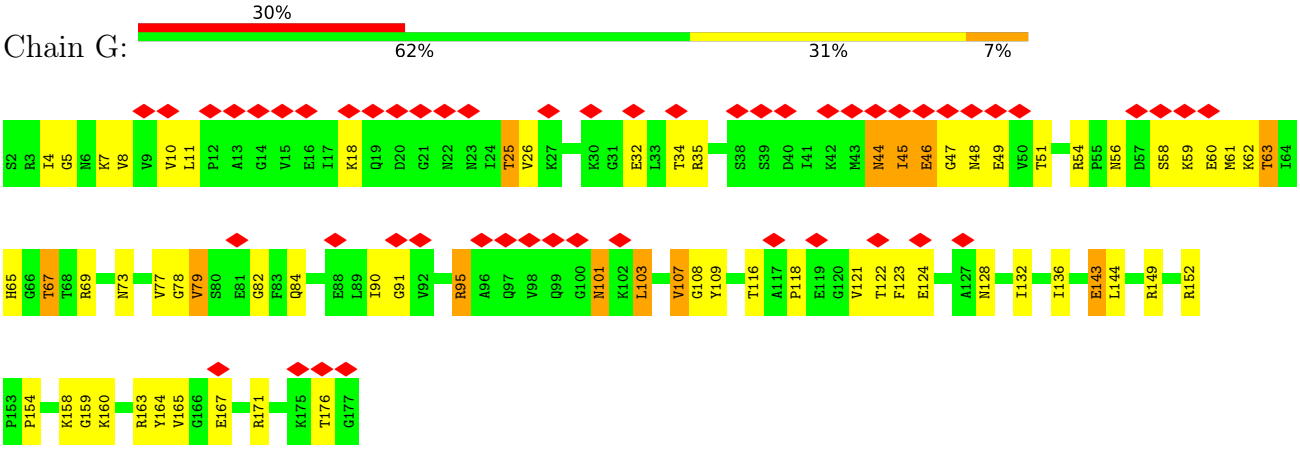




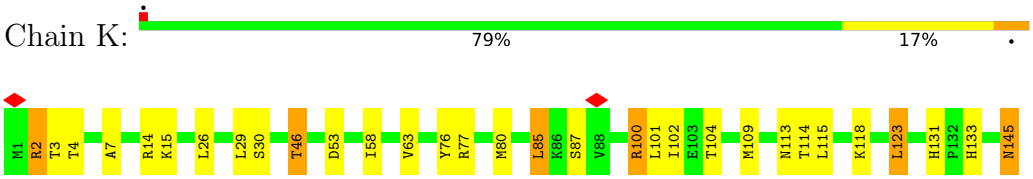
• Molecule 5: 50S ribosomal protein L5



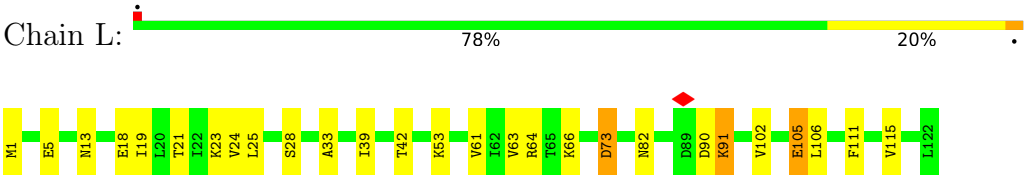
• Molecule 6: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L13

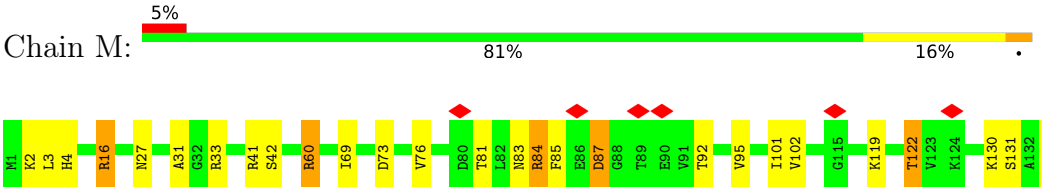


• Molecule 8: 50S ribosomal protein L14



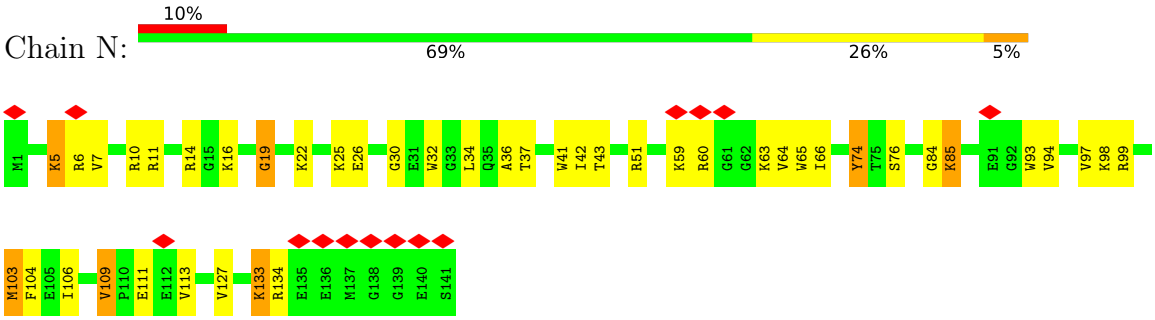
• Molecule 9: 50S ribosomal protein L15

Chain M:



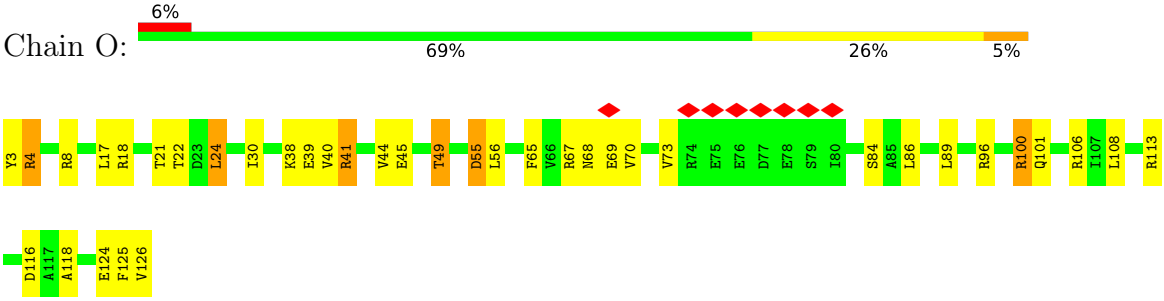
• Molecule 10: 50S ribosomal protein L16

Chain N:



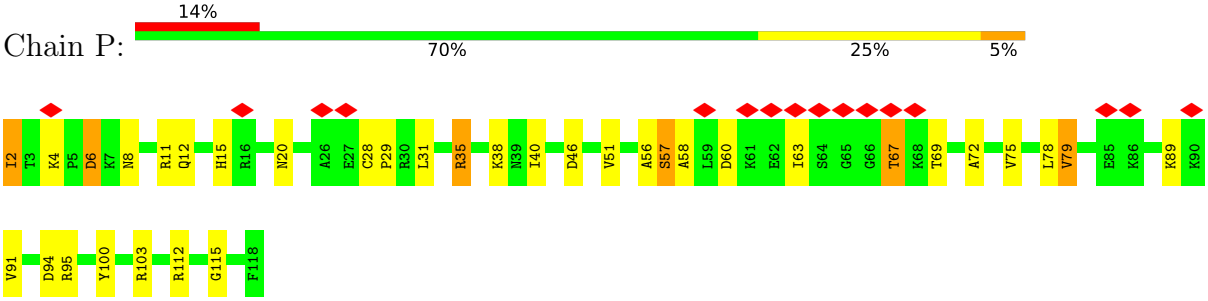
• Molecule 11: 50S ribosomal protein L17

Chain O:



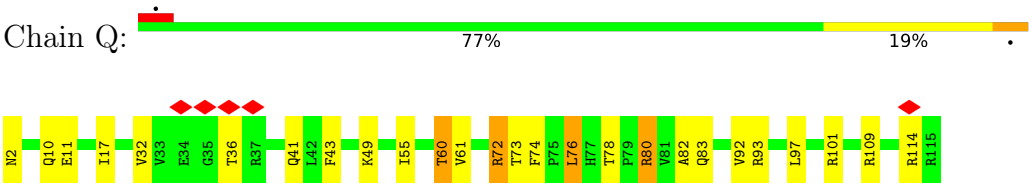
• Molecule 12: 50S ribosomal protein L18

Chain P:



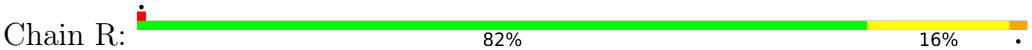
• Molecule 13: 50S ribosomal protein L19

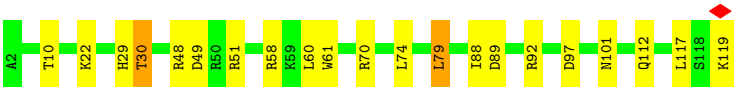
Chain Q:



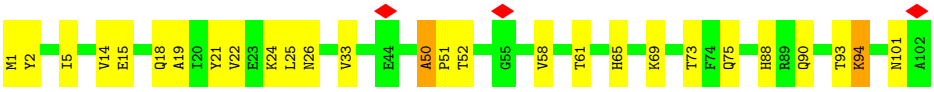
• Molecule 14: 50S ribosomal protein L20

Chain R:

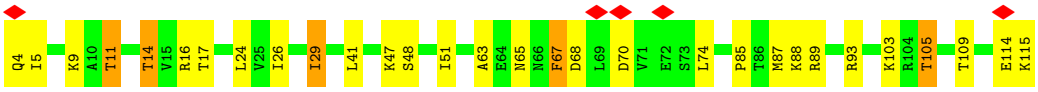




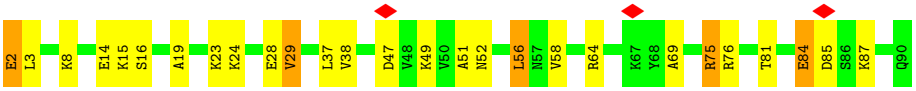
• Molecule 15: 50S ribosomal protein L21



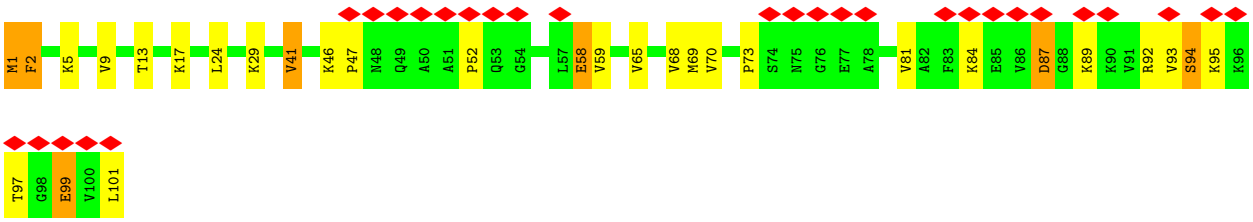
• Molecule 16: 50S ribosomal protein L22



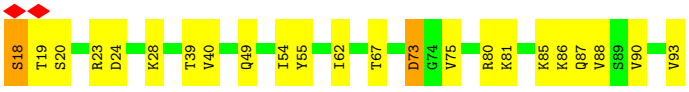
• Molecule 17: 50S ribosomal protein L23



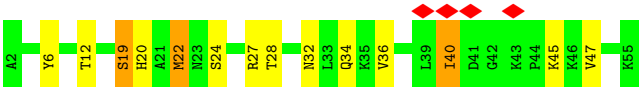
• Molecule 18: 50S ribosomal protein L24



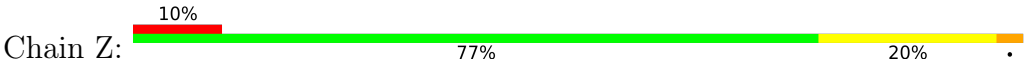
• Molecule 19: 50S ribosomal protein L27

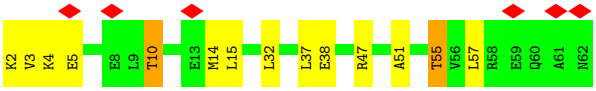


• Molecule 20: 50S ribosomal protein L28

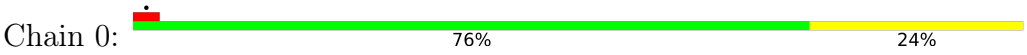


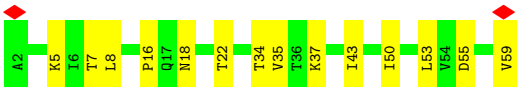
• Molecule 21: 50S ribosomal protein L29



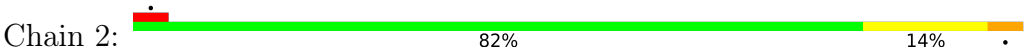


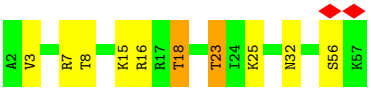
• Molecule 22: 50S ribosomal protein L30



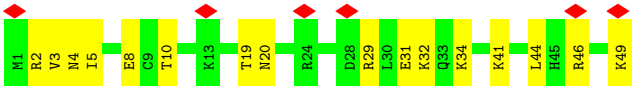


• Molecule 23: 50S ribosomal protein L32

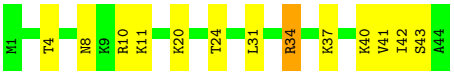




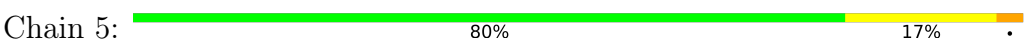
• Molecule 24: 50S ribosomal protein L33

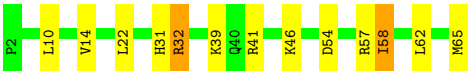


• Molecule 25: 50S ribosomal protein L34



• Molecule 26: 50S ribosomal protein L35





• Molecule 27: 50S ribosomal protein L36

Chain 6:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	335675	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.226	Depositor
Minimum map value	-0.085	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	482.68, 482.68, 482.68	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.097, 1.097, 1.097	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.21	32/65858 (0.0%)	1.30	435/102721 (0.4%)
2	B	0.97	1/2773 (0.0%)	1.23	23/4320 (0.5%)
3	D	0.54	0/1601	0.67	0/2150
4	E	0.52	0/1596	0.63	0/2159
5	F	0.36	0/1411	0.58	1/1897 (0.1%)
6	G	0.39	0/1365	0.57	0/1839
7	K	0.53	0/1151	0.68	2/1554 (0.1%)
8	L	0.51	0/929	0.65	1/1247 (0.1%)
9	M	0.52	1/1105 (0.1%)	0.64	0/1474
10	N	0.49	0/1141	0.61	0/1519
11	O	0.55	0/1000	0.71	1/1341 (0.1%)
12	P	0.47	0/908	0.64	0/1216
13	Q	0.56	0/938	0.63	0/1262
14	R	0.59	0/963	0.64	2/1280 (0.2%)
15	S	0.54	0/796	0.62	0/1068
16	T	0.49	0/858	0.64	1/1157 (0.1%)
17	U	0.50	0/727	0.65	1/972 (0.1%)
18	V	0.46	0/772	0.63	0/1035
19	X	0.56	0/578	0.61	0/773
20	Y	0.57	1/431 (0.2%)	0.60	0/574
21	Z	0.42	0/505	0.57	0/672
22	0	0.47	0/437	0.63	0/589
23	2	0.55	0/436	0.63	0/578
24	3	0.46	0/423	0.60	0/563
25	4	0.48	0/377	0.61	0/491
26	5	0.43	0/528	0.62	0/689
27	6	0.47	0/309	0.67	0/409
All	All	1.08	35/89916 (0.0%)	1.19	467/135549 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
10	N	0	2
11	O	0	2
15	S	0	1
16	T	0	1
18	V	0	1
All	All	0	8

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	903	G	C6-N1	-11.86	1.31	1.39
2	B	1	U	OP3-P	-10.45	1.48	1.61
1	A	769	G	N9-C4	-8.64	1.31	1.38
1	A	1492	G	N9-C4	-8.09	1.31	1.38
1	A	956	C	N3-C4	-7.24	1.28	1.33
1	A	2836	G	N9-C4	-7.18	1.32	1.38
20	Y	19	SER	CA-CB	-7.15	1.42	1.52
1	A	956	C	C4-N4	-7.06	1.27	1.33
9	M	60	ARG	C-N	-6.82	1.18	1.34
1	A	2444	A	N9-C4	-6.65	1.33	1.37
1	A	2044	A	N3-C4	-6.53	1.30	1.34
1	A	769	G	C2-N3	-6.40	1.27	1.32
1	A	1490	A	N9-C4	-6.38	1.34	1.37
1	A	769	G	N3-C4	-6.37	1.30	1.35
1	A	660	A	N9-C4	-6.22	1.34	1.37
1	A	660	A	N3-C4	-6.11	1.31	1.34
1	A	509	G	N9-C4	-5.91	1.33	1.38
1	A	1288	A	N3-C4	-5.89	1.31	1.34
1	A	2287	A	N3-C4	-5.86	1.31	1.34
1	A	903	G	C6-O6	-5.83	1.19	1.24
1	A	1571	G	N3-C4	-5.73	1.31	1.35
1	A	1337	A	N9-C4	-5.54	1.34	1.37
1	A	2606	G	C8-N7	-5.46	1.27	1.30
1	A	2007	U	C2-N3	-5.27	1.34	1.37
1	A	660	A	C5-C6	-5.26	1.36	1.41
1	A	2728	G	C8-N7	-5.21	1.27	1.30
1	A	539	G	N9-C4	-5.21	1.33	1.38
1	A	275	A	N9-C4	-5.18	1.34	1.37
1	A	2444	A	N3-C4	-5.18	1.31	1.34
1	A	903	G	C5-C6	-5.17	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1592	G	N9-C4	-5.13	1.33	1.38
1	A	1506	A	N9-C4	-5.11	1.34	1.37
1	A	2836	G	N3-C4	-5.08	1.31	1.35
1	A	1404	G	C6-N1	-5.07	1.36	1.39
1	A	2006	G	C8-N7	-5.00	1.27	1.30

All (467) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	956	C	N3-C4-N4	-30.89	96.38	118.00
1	A	956	C	C5-C4-N4	25.47	138.03	120.20
1	A	903	G	N1-C6-O6	-24.12	105.42	119.90
1	A	903	G	C5-C6-O6	22.01	141.81	128.60
1	A	1591	A	N1-C6-N6	-15.79	109.12	118.60
1	A	769	G	N3-C4-N9	-14.07	117.56	126.00
1	A	769	G	N3-C4-C5	13.80	135.50	128.60
1	A	1492	G	N3-C4-C5	13.01	135.10	128.60
1	A	2287	A	N7-C8-N9	12.67	120.14	113.80
1	A	769	G	C2-N3-C4	-12.50	105.65	111.90
1	A	1492	G	N3-C4-N9	-12.02	118.79	126.00
1	A	2287	A	C8-N9-C4	-10.74	101.50	105.80
2	B	85	U	C5-C6-N1	10.49	127.94	122.70
1	A	903	G	C4-C5-N7	10.31	114.92	110.80
1	A	2836	G	N3-C4-C5	10.05	133.62	128.60
1	A	2836	G	N3-C4-N9	-9.96	120.03	126.00
1	A	903	G	C4-N9-C1'	9.85	139.30	126.50
1	A	903	G	C8-N9-C1'	-9.71	114.38	127.00
1	A	956	C	C4-C5-C6	-9.64	112.58	117.40
1	A	1591	A	C2-N3-C4	9.62	115.41	110.60
1	A	2287	A	C5-N7-C8	-9.53	99.14	103.90
1	A	2420	C	O5'-P-OP2	-9.48	97.16	105.70
1	A	769	G	N3-C2-N2	-9.29	113.40	119.90
1	A	1505	C	N3-C2-O2	-9.22	115.44	121.90
1	A	956	C	N3-C4-C5	9.19	125.58	121.90
1	A	1592	G	N3-C4-C5	9.15	133.18	128.60
1	A	1551	U	C2-N1-C1'	9.11	128.63	117.70
1	A	903	G	N9-C4-C5	-9.05	101.78	105.40
1	A	1288	A	C2-N3-C4	-8.96	106.12	110.60
1	A	1167	A	C8-N9-C4	-8.94	102.22	105.80
1	A	2836	G	C5-N7-C8	-8.90	99.85	104.30
1	A	2454	C	O4'-C1'-N1	8.86	115.29	108.20
1	A	655	G	C8-N9-C4	8.84	109.94	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	551	G	O4'-C1'-N9	8.80	115.24	108.20
1	A	2287	A	C2-N3-C4	-8.56	106.32	110.60
1	A	2836	G	C2-N3-C4	-8.49	107.66	111.90
1	A	1592	G	N3-C4-N9	-8.33	121.00	126.00
1	A	1167	A	N7-C8-N9	8.25	117.92	113.80
1	A	509	G	C5-N7-C8	-8.17	100.21	104.30
1	A	1902	G	C8-N9-C4	-8.11	103.16	106.40
1	A	1571	G	N3-C2-N2	-8.08	114.24	119.90
1	A	2836	G	N7-C8-N9	7.98	117.09	113.10
1	A	344	G	C4-N9-C1'	7.97	136.86	126.50
1	A	1394	G	C4-C5-N7	7.96	113.98	110.80
1	A	1902	G	O4'-C1'-N9	7.82	114.46	108.20
1	A	208	G	O4'-C1'-N9	7.82	114.45	108.20
1	A	1434	C	C6-N1-C2	-7.81	117.18	120.30
1	A	2287	A	N1-C2-N3	7.81	133.20	129.30
1	A	1902	G	N7-C8-N9	7.80	117.00	113.10
1	A	1591	A	C5-C6-N6	7.78	129.92	123.70
1	A	660	A	N1-C6-N6	7.76	123.26	118.60
1	A	903	G	N3-C4-N9	7.75	130.65	126.00
1	A	344	G	N7-C8-N9	7.68	116.94	113.10
2	B	77	G	C4-C5-N7	7.60	113.84	110.80
1	A	711	C	C6-N1-C2	-7.56	117.28	120.30
2	B	96	G	C4-C5-N7	7.54	113.81	110.80
1	A	509	G	N7-C8-N9	7.48	116.84	113.10
1	A	275	A	N1-C2-N3	7.48	133.04	129.30
1	A	1492	G	C2-N3-C4	-7.47	108.16	111.90
1	A	1490	A	C2-N3-C4	-7.47	106.86	110.60
1	A	1497	U	N3-C2-O2	-7.46	116.97	122.20
1	A	586	A	N1-C6-N6	-7.44	114.14	118.60
1	A	769	G	C8-N9-C1'	7.38	136.59	127.00
1	A	2287	A	O4'-C1'-N9	7.37	114.09	108.20
1	A	992	G	C8-N9-C1'	-7.34	117.45	127.00
1	A	1175	C	C6-N1-C2	-7.34	117.37	120.30
1	A	1591	A	C6-C5-N7	7.31	137.42	132.30
1	A	2044	A	N7-C8-N9	7.29	117.45	113.80
1	A	1492	G	C4-N9-C1'	-7.24	117.08	126.50
2	B	96	G	C5-N7-C8	-7.23	100.69	104.30
1	A	235	G	N7-C8-N9	7.22	116.71	113.10
1	A	716	A	C2-N3-C4	-7.21	107.00	110.60
1	A	1489	C	C6-N1-C2	-7.20	117.42	120.30
1	A	2406	A	C2-N3-C4	-7.16	107.02	110.60
1	A	344	G	C6-C5-N7	-7.15	126.11	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2556	A	C8-N9-C4	-7.14	102.94	105.80
1	A	769	G	C4-N9-C1'	-7.13	117.23	126.50
1	A	951	A	O4'-C1'-N9	7.11	113.89	108.20
1	A	2226	A	C5-N7-C8	-7.08	100.36	103.90
1	A	235	G	C8-N9-C4	-7.07	103.57	106.40
1	A	1989	G	N7-C8-N9	7.07	116.63	113.10
1	A	1699	C	C6-N1-C2	-7.06	117.47	120.30
1	A	485	C	C6-N1-C2	-7.00	117.50	120.30
2	B	96	G	C6-C5-N7	-6.97	126.22	130.40
1	A	992	G	O4'-C1'-N9	6.97	113.77	108.20
1	A	1022	C	C2-N1-C1'	6.96	126.45	118.80
2	B	77	G	C5-N7-C8	-6.94	100.83	104.30
1	A	2226	A	N7-C8-N9	6.93	117.27	113.80
1	A	344	G	C8-N9-C1'	-6.93	118.00	127.00
1	A	1489	C	N3-C2-O2	-6.92	117.05	121.90
1	A	1994	G	N3-C4-C5	-6.89	125.15	128.60
2	B	77	G	N7-C8-N9	6.89	116.55	113.10
1	A	1505	C	C6-N1-C2	-6.89	117.55	120.30
1	A	1349	U	C2-N1-C1'	6.85	125.92	117.70
1	A	1394	G	C6-C5-N7	-6.80	126.32	130.40
1	A	1989	G	C4-C5-N7	6.79	113.52	110.80
1	A	903	G	C6-C5-N7	-6.75	126.35	130.40
1	A	509	G	C2-N3-C4	-6.74	108.53	111.90
2	B	77	G	C6-C5-N7	-6.74	126.36	130.40
1	A	344	G	C5-N7-C8	-6.72	100.94	104.30
1	A	509	G	N3-C4-C5	6.71	131.96	128.60
1	A	2441	C	C6-N1-C2	-6.70	117.62	120.30
1	A	903	G	C5-N7-C8	-6.67	100.96	104.30
2	B	96	G	N7-C8-N9	6.67	116.44	113.10
1	A	619	G	N3-C4-C5	-6.64	125.28	128.60
1	A	1492	G	C8-N9-C1'	6.62	135.61	127.00
1	A	298	U	O4'-C1'-N1	6.57	113.45	108.20
5	F	130	LEU	CA-CB-CG	6.56	130.39	115.30
1	A	1551	U	N1-C2-O2	6.54	127.38	122.80
1	A	1730	G	N3-C4-N9	6.54	129.93	126.00
1	A	1989	G	C5-N7-C8	-6.53	101.03	104.30
1	A	2044	A	C8-N9-C4	-6.53	103.19	105.80
1	A	2044	A	C5-N7-C8	-6.53	100.64	103.90
1	A	1234	C	C6-N1-C2	-6.51	117.70	120.30
1	A	1591	A	C5-C6-N1	6.50	120.95	117.70
1	A	2606	G	C4-N9-C1'	6.50	134.95	126.50
1	A	1713	C	C6-N1-C2	-6.50	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	725	A	C8-N9-C4	-6.49	103.21	105.80
1	A	509	G	N3-C4-N9	-6.48	122.11	126.00
1	A	344	G	C4-C5-N7	6.47	113.39	110.80
1	A	660	A	C5-N7-C8	-6.47	100.66	103.90
1	A	953	C	C6-N1-C2	-6.47	117.71	120.30
1	A	1229	G	N3-C4-N9	6.45	129.87	126.00
1	A	2588	G	C8-N9-C4	-6.44	103.82	106.40
1	A	344	G	O4'-C1'-N9	6.44	113.35	108.20
2	B	77	G	O4'-C1'-N9	6.43	113.34	108.20
1	A	1989	G	C6-C5-N7	-6.39	126.56	130.40
1	A	169	A	O4'-C1'-N9	6.39	113.31	108.20
1	A	2272	C	C6-N1-C2	-6.39	117.75	120.30
1	A	1996	U	C2-N1-C1'	6.37	125.35	117.70
2	B	68	C	C2-N1-C1'	6.37	125.81	118.80
1	A	1504	G	O4'-C1'-N9	6.37	113.30	108.20
1	A	1360	G	C8-N9-C4	-6.37	103.85	106.40
1	A	1551	U	C6-N1-C1'	-6.36	112.30	121.20
1	A	1388	U	N3-C2-O2	-6.33	117.77	122.20
1	A	275	A	C2-N3-C4	-6.33	107.44	110.60
1	A	583	U	C5-C4-O4	-6.33	122.10	125.90
1	A	776	C	C6-N1-C2	-6.33	117.77	120.30
1	A	331	A	O4'-C1'-N9	6.32	113.25	108.20
1	A	1364	G	C8-N9-C4	-6.31	103.88	106.40
1	A	992	G	C4-N9-C1'	6.30	134.69	126.50
1	A	2277	C	C6-N1-C2	-6.29	117.78	120.30
1	A	509	G	O4'-C1'-N9	6.28	113.22	108.20
1	A	2365	G	N3-C4-N9	6.27	129.76	126.00
1	A	1397	G	N3-C4-N9	6.25	129.75	126.00
1	A	28	G	O4'-C1'-N9	6.25	113.20	108.20
1	A	2241	A	C8-N9-C4	-6.24	103.30	105.80
1	A	905	G	N3-C4-C5	-6.22	125.49	128.60
1	A	1394	G	C5-N7-C8	-6.22	101.19	104.30
1	A	1493	C	C6-N1-C2	-6.21	117.82	120.30
1	A	261	C	C6-N1-C2	-6.21	117.82	120.30
1	A	2794	G	C4-N9-C1'	6.20	134.56	126.50
1	A	367	A	C5-N7-C8	-6.18	100.81	103.90
1	A	2226	A	C8-N9-C4	-6.17	103.33	105.80
1	A	1197	G	C4-N9-C1'	6.17	134.53	126.50
1	A	2039	C	C6-N1-C2	-6.17	117.83	120.30
1	A	235	G	O4'-C1'-N9	6.17	113.14	108.20
1	A	2049	G	N1-C6-O6	-6.16	116.20	119.90
1	A	1902	G	C5-N7-C8	-6.16	101.22	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	992	G	N3-C4-N9	6.15	129.69	126.00
1	A	716	A	C5-N7-C8	-6.12	100.84	103.90
1	A	655	G	N7-C8-N9	-6.11	110.05	113.10
1	A	2628	A	C8-N9-C4	-6.11	103.36	105.80
1	A	1350	C	C2-N1-C1'	6.10	125.51	118.80
1	A	2102	A	N1-C6-N6	-6.09	114.95	118.60
1	A	2296	G	N1-C6-O6	-6.08	116.25	119.90
1	A	1321	G	N1-C6-O6	-6.06	116.26	119.90
1	A	716	A	O4'-C1'-N9	6.06	113.05	108.20
1	A	1708	A	N1-C6-N6	-6.06	114.97	118.60
1	A	2834	A	N1-C6-N6	-6.05	114.97	118.60
1	A	1429	A	O4'-C1'-N9	6.04	113.04	108.20
1	A	1814	C	C6-N1-C2	-6.04	117.89	120.30
2	B	96	G	O4'-C1'-N9	6.03	113.03	108.20
1	A	1195	A	C8-N9-C4	-6.01	103.39	105.80
1	A	1490	A	C5-C6-N1	-6.00	114.70	117.70
1	A	155	U	O4'-C1'-N1	6.00	113.00	108.20
1	A	2588	G	N7-C8-N9	5.99	116.10	113.10
1	A	1591	A	N9-C4-C5	5.99	108.19	105.80
1	A	1487	U	O5'-P-OP2	-5.99	100.31	105.70
1	A	2062	G	N3-C4-N9	5.98	129.59	126.00
2	B	79	G	N7-C8-N9	5.98	116.09	113.10
2	B	96	G	C4-N9-C1'	5.98	134.27	126.50
1	A	235	G	C4-N9-C1'	5.97	134.26	126.50
1	A	2836	G	C8-N9-C4	-5.97	104.01	106.40
1	A	2606	G	C8-N9-C1'	-5.97	119.24	127.00
1	A	1800	A	O4'-C1'-N9	5.96	112.97	108.20
1	A	1571	G	N9-C4-C5	5.96	107.78	105.40
1	A	50	A	N1-C6-N6	-5.96	115.03	118.60
1	A	1506	A	C6-N1-C2	5.96	122.17	118.60
1	A	2367	G	N3-C4-C5	-5.96	125.62	128.60
1	A	262	G	N3-C4-N9	5.95	129.57	126.00
1	A	1804	C	C6-N1-C2	-5.95	117.92	120.30
1	A	2057	C	C2-N1-C1'	5.95	125.35	118.80
1	A	1490	A	C6-N1-C2	5.95	122.17	118.60
1	A	572	G	C2-N3-C4	5.94	114.87	111.90
1	A	712	C	C6-N1-C2	-5.94	117.92	120.30
1	A	360	G	C8-N9-C4	-5.93	104.03	106.40
1	A	903	G	N7-C8-N9	5.92	116.06	113.10
1	A	1337	A	C2-N3-C4	-5.92	107.64	110.60
1	A	2599	U	N3-C2-O2	-5.92	118.06	122.20
1	A	2602	G	C8-N9-C4	-5.90	104.04	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1288	A	C5-C6-N6	5.89	128.41	123.70
1	A	1989	G	O4'-C1'-N9	5.89	112.91	108.20
1	A	370	G	N3-C4-C5	-5.89	125.66	128.60
1	A	703	G	N1-C6-O6	-5.88	116.37	119.90
1	A	2307	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1989	G	C2-N3-C4	-5.87	108.97	111.90
1	A	2809	U	C2-N1-C1'	5.87	124.74	117.70
1	A	1229	G	N3-C4-C5	-5.86	125.67	128.60
1	A	1224	G	N3-C4-N9	5.85	129.51	126.00
1	A	1011	C	C6-N1-C2	-5.83	117.97	120.30
1	A	654	A	O4'-C1'-N9	5.82	112.86	108.20
2	B	80	A	O4'-C1'-N9	5.81	112.85	108.20
16	T	24	LEU	CA-CB-CG	5.80	128.65	115.30
17	U	56	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	509	G	C8-N9-C4	-5.79	104.08	106.40
1	A	2416	U	N3-C2-O2	-5.79	118.15	122.20
1	A	103	A	N7-C8-N9	5.79	116.69	113.80
1	A	1264	G	N3-C4-N9	5.79	129.47	126.00
1	A	1288	A	N1-C2-N3	5.78	132.19	129.30
1	A	886	U	N3-C2-O2	-5.78	118.16	122.20
1	A	396	C	C2-N1-C1'	5.78	125.16	118.80
1	A	990	G	C5-N7-C8	-5.78	101.41	104.30
1	A	2645	G	N1-C6-O6	-5.77	116.44	119.90
1	A	1885	C	N1-C2-O2	5.77	122.36	118.90
1	A	781	G	C8-N9-C4	-5.76	104.10	106.40
1	A	2365	G	C4-N9-C1'	5.76	133.98	126.50
1	A	1669	G	N1-C6-O6	-5.75	116.45	119.90
1	A	2049	G	C8-N9-C4	-5.75	104.10	106.40
1	A	1042	G	N1-C6-O6	-5.75	116.45	119.90
1	A	2287	A	C6-C5-N7	-5.73	128.29	132.30
1	A	2891	C	C6-N1-C2	-5.73	118.01	120.30
1	A	777	C	C6-N1-C2	-5.73	118.01	120.30
1	A	1012	G	N3-C4-N9	5.72	129.44	126.00
1	A	1471	G	N3-C4-N9	5.72	129.43	126.00
1	A	367	A	N7-C8-N9	5.72	116.66	113.80
1	A	2859	G	O4'-C1'-N9	5.72	112.77	108.20
1	A	1379	G	C4-N9-C1'	5.71	133.93	126.50
1	A	410	G	N3-C4-C5	-5.71	125.75	128.60
1	A	620	G	N3-C4-C5	-5.71	125.75	128.60
1	A	1337	A	N3-C4-N9	-5.71	122.83	127.40
1	A	1806	G	N1-C6-O6	-5.71	116.48	119.90
2	B	85	U	C4-C5-C6	-5.71	116.28	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	29	LEU	CA-CB-CG	5.71	128.42	115.30
1	A	103	A	C5-N7-C8	-5.70	101.05	103.90
1	A	248	G	N3-C4-N9	5.69	129.41	126.00
1	A	1492	G	O4'-C1'-N9	5.68	112.75	108.20
1	A	654	A	C8-N9-C4	5.68	108.07	105.80
1	A	817	G	N3-C4-C5	-5.68	125.76	128.60
1	A	823	A	N1-C6-N6	-5.68	115.19	118.60
1	A	367	A	C8-N9-C4	-5.67	103.53	105.80
1	A	2903	G	C2-N3-C4	-5.66	109.07	111.90
1	A	1604	A	P-O3'-C3'	5.66	126.49	119.70
1	A	35	U	C2-N1-C1'	5.65	124.48	117.70
1	A	18	G	N3-C4-N9	5.64	129.39	126.00
1	A	1996	U	N1-C2-O2	5.64	126.75	122.80
1	A	1434	C	C5-C6-N1	5.63	123.82	121.00
1	A	1197	G	C8-N9-C1'	-5.63	119.68	127.00
1	A	50	A	C5-C6-N6	5.62	128.20	123.70
1	A	2051	A	C2-N3-C4	5.62	113.41	110.60
1	A	655	G	C4-N9-C1'	-5.62	119.20	126.50
1	A	1551	U	C5-C6-N1	5.61	125.50	122.70
1	A	1337	A	N3-C4-C5	5.61	130.73	126.80
1	A	1717	G	N3-C4-C5	-5.61	125.80	128.60
1	A	1591	A	C4-C5-N7	-5.60	107.90	110.70
1	A	990	G	C4-C5-N7	5.60	113.04	110.80
1	A	644	U	N3-C2-O2	-5.60	118.28	122.20
14	R	117	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	400	G	N3-C4-N9	5.57	129.34	126.00
1	A	904	A	O4'-C1'-N9	5.57	112.65	108.20
1	A	956	C	C5-C6-N1	5.56	123.78	121.00
1	A	2514	U	O4'-C1'-N1	5.56	112.65	108.20
1	A	2836	G	N3-C2-N2	-5.56	116.01	119.90
1	A	2537	G	N3-C4-N9	5.55	129.33	126.00
1	A	1717	G	C8-N9-C4	-5.55	104.18	106.40
1	A	1976	C	C6-N1-C2	-5.54	118.08	120.30
1	A	788	G	O4'-C1'-N9	5.54	112.63	108.20
1	A	1658	C	C6-N1-C2	-5.54	118.09	120.30
1	A	235	G	C5-N7-C8	-5.53	101.53	104.30
1	A	2613	G	N3-C4-C5	-5.53	125.83	128.60
1	A	2500	G	C8-N9-C4	-5.53	104.19	106.40
1	A	1397	G	C5-C6-O6	-5.53	125.28	128.60
1	A	2044	A	O4'-C1'-N9	5.53	112.62	108.20
1	A	963	C	C6-N1-C2	-5.52	118.09	120.30
1	A	2416	U	N1-C2-O2	5.52	126.66	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	222	A	C8-N9-C4	-5.51	103.60	105.80
1	A	1288	A	N3-C4-N9	-5.50	123.00	127.40
1	A	1605	C	P-O3'-C3'	5.50	126.30	119.70
1	A	905	G	N3-C4-N9	5.48	129.29	126.00
1	A	2455	C	N3-C2-O2	-5.48	118.06	121.90
1	A	769	G	C5-C6-N1	-5.47	108.77	111.50
1	A	619	G	N3-C4-N9	5.47	129.28	126.00
1	A	503	G	C6-C5-N7	5.46	133.68	130.40
1	A	1536	A	C8-N9-C4	-5.46	103.61	105.80
1	A	1996	U	N3-C2-O2	-5.46	118.38	122.20
1	A	1407	G	N1-C6-O6	-5.46	116.63	119.90
1	A	2287	A	C5-C6-N1	-5.45	114.97	117.70
1	A	1841	U	N3-C2-O2	-5.45	118.39	122.20
14	R	79	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	47	C	C6-N1-C2	-5.43	118.13	120.30
1	A	494	A	N1-C6-N6	-5.43	115.34	118.60
1	A	2365	G	C8-N9-C1'	-5.42	119.95	127.00
1	A	2825	C	C6-N1-C2	-5.42	118.13	120.30
1	A	1571	G	N3-C4-N9	-5.42	122.75	126.00
1	A	2416	U	C2-N1-C1'	5.40	124.18	117.70
1	A	768	G	N3-C4-C5	-5.40	125.90	128.60
1	A	494	A	C5-C6-N6	5.39	128.02	123.70
1	A	2705	C	C6-N1-C2	-5.39	118.14	120.30
1	A	2728	G	C5-C6-O6	5.39	131.83	128.60
1	A	1950	A	N7-C8-N9	5.38	116.49	113.80
1	A	2903	G	N3-C4-C5	5.38	131.29	128.60
1	A	1203	G	C5-C6-N1	5.38	114.19	111.50
1	A	655	G	N3-C4-C5	5.38	131.29	128.60
1	A	1065	G	C8-N9-C4	-5.38	104.25	106.40
1	A	1394	G	O4'-C1'-N9	5.37	112.49	108.20
1	A	1989	G	C4-N9-C1'	5.37	133.48	126.50
1	A	2359	G	C8-N9-C4	-5.37	104.25	106.40
1	A	2639	G	N1-C6-O6	-5.37	116.68	119.90
2	B	77	G	C4-N9-C1'	5.36	133.47	126.50
1	A	229	A	C8-N9-C4	-5.36	103.66	105.80
1	A	2637	G	N3-C4-C5	-5.36	125.92	128.60
1	A	721	U	C6-N1-C2	-5.36	117.79	121.00
1	A	781	G	N3-C4-C5	-5.35	125.92	128.60
1	A	2084	G	N3-C4-C5	-5.35	125.92	128.60
1	A	2070	G	N3-C4-N9	5.35	129.21	126.00
1	A	2067	G	N3-C4-N9	5.35	129.21	126.00
1	A	549	C	C6-N1-C2	-5.35	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	80	A	N7-C8-N9	5.35	116.47	113.80
1	A	768	G	C8-N9-C4	-5.35	104.26	106.40
2	B	79	G	C8-N9-C4	-5.34	104.26	106.40
1	A	1994	G	C2-N3-C4	5.34	114.57	111.90
1	A	1490	A	N3-C4-C5	5.33	130.53	126.80
1	A	1673	A	N9-C4-C5	5.33	107.93	105.80
1	A	772	C	C6-N1-C2	-5.33	118.17	120.30
1	A	105	C	C6-N1-C2	-5.32	118.17	120.30
1	A	400	G	C4-N9-C1'	5.32	133.41	126.50
1	A	1216	G	C8-N9-C4	-5.32	104.27	106.40
1	A	2345	G	N1-C6-O6	-5.32	116.71	119.90
1	A	1644	G	N3-C4-N9	5.31	129.18	126.00
1	A	2405	G	O4'-C1'-N9	5.31	112.44	108.20
1	A	509	G	C4-C5-N7	5.30	112.92	110.80
1	A	1592	G	C2-N3-C4	-5.30	109.25	111.90
1	A	1776	A	O4'-C1'-N9	5.29	112.43	108.20
1	A	539	G	N3-C4-N9	-5.28	122.83	126.00
1	A	2794	G	C6-C5-N7	-5.28	127.23	130.40
1	A	400	G	C8-N9-C1'	-5.28	120.14	127.00
1	A	2067	G	N3-C4-C5	-5.27	125.96	128.60
1	A	1730	G	N3-C4-C5	-5.26	125.97	128.60
1	A	1288	A	N3-C4-C5	5.25	130.48	126.80
1	A	2073	A	O4'-C1'-N9	5.25	112.40	108.20
1	A	2062	G	N3-C4-C5	-5.25	125.97	128.60
1	A	179	A	N7-C8-N9	5.24	116.42	113.80
1	A	1978	G	N3-C4-C5	-5.24	125.98	128.60
1	A	807	U	O4'-C1'-N1	5.23	112.39	108.20
1	A	716	A	N7-C8-N9	5.23	116.41	113.80
1	A	2317	G	C4-N9-C1'	5.23	133.29	126.50
1	A	13	U	P-O3'-C3'	5.22	125.97	119.70
1	A	2360	A	N1-C6-N6	-5.22	115.47	118.60
1	A	347	A	O5'-P-OP1	-5.22	101.00	105.70
1	A	1491	U	O4'-C1'-N1	5.22	112.38	108.20
1	A	2208	C	C2-N1-C1'	5.22	124.54	118.80
1	A	367	A	C4-C5-N7	5.22	113.31	110.70
1	A	1203	G	N1-C6-O6	-5.21	116.78	119.90
1	A	1950	A	O4'-C1'-N9	5.21	112.37	108.20
1	A	1959	G	N3-C4-N9	5.21	129.12	126.00
1	A	992	G	N9-C1'-C2'	-5.21	106.27	112.00
1	A	1278	C	C6-N1-C2	-5.20	118.22	120.30
1	A	1431	A	C8-N9-C4	-5.20	103.72	105.80
1	A	660	A	C2-N3-C4	-5.20	108.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	521	G	N3-C4-C5	-5.20	126.00	128.60
1	A	2289	C	C6-N1-C2	-5.20	118.22	120.30
1	A	1360	G	O4'-C1'-N9	5.20	112.36	108.20
1	A	2794	G	C4-C5-N7	5.19	112.88	110.80
1	A	181	G	C2-N3-C4	5.19	114.50	111.90
1	A	460	G	N3-C4-C5	-5.18	126.01	128.60
1	A	907	A	C6-C5-N7	-5.18	128.67	132.30
1	A	1167	A	C6-C5-N7	-5.18	128.67	132.30
1	A	1349	U	N1-C2-O2	5.18	126.43	122.80
1	A	2592	G	N1-C6-O6	-5.18	116.79	119.90
1	A	660	A	N3-C4-C5	5.18	130.43	126.80
1	A	2020	C	C6-N1-C2	-5.18	118.23	120.30
1	A	1448	U	C5-C6-N1	5.18	125.29	122.70
1	A	2022	C	C6-N1-C2	-5.18	118.23	120.30
1	A	1193	C	C6-N1-C2	-5.17	118.23	120.30
1	A	1356	G	O4'-C1'-N9	5.17	112.33	108.20
1	A	181	G	C5-C6-N1	5.16	114.08	111.50
1	A	1397	G	N3-C4-C5	-5.16	126.02	128.60
1	A	1796	C	C6-N1-C2	-5.16	118.23	120.30
1	A	103	A	C8-N9-C4	-5.16	103.74	105.80
1	A	725	A	N9-C4-C5	5.16	107.86	105.80
1	A	460	G	C8-N9-C4	-5.15	104.34	106.40
2	B	80	A	C5-N7-C8	-5.15	101.32	103.90
1	A	990	G	N7-C8-N9	5.15	115.68	113.10
1	A	1590	A	P-O3'-C3'	5.15	125.88	119.70
1	A	2728	G	N1-C6-O6	-5.14	116.82	119.90
1	A	2057	C	C6-N1-C2	-5.13	118.25	120.30
1	A	2498	G	N3-C4-C5	-5.13	126.03	128.60
1	A	1074	G	N3-C4-C5	-5.13	126.03	128.60
1	A	2575	A	C5-C6-N1	5.13	120.27	117.70
8	L	91	LYS	C-N-CA	-5.13	108.88	121.70
1	A	2228	C	C6-N1-C2	-5.12	118.25	120.30
1	A	1431	A	N7-C8-N9	5.12	116.36	113.80
1	A	2794	G	N7-C8-N9	5.12	115.66	113.10
1	A	2794	G	C5-N7-C8	-5.12	101.74	104.30
1	A	1806	G	C5-C6-O6	5.11	131.67	128.60
1	A	451	G	N3-C4-C5	-5.11	126.05	128.60
1	A	1600	C	P-O3'-C3'	5.11	125.83	119.70
1	A	1730	G	C4-N9-C1'	5.10	133.14	126.50
1	A	468	A	O5'-P-OP2	-5.10	101.11	105.70
1	A	1491	U	N3-C2-O2	-5.10	118.63	122.20
1	A	1584	G	P-O3'-C3'	5.10	125.81	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1764	G	N1-C6-O6	-5.10	116.84	119.90
1	A	1011	C	C4-C5-C6	5.09	119.95	117.40
1	A	1571	G	N1-C2-N3	5.09	126.96	123.90
2	B	79	G	C5-N7-C8	-5.09	101.75	104.30
1	A	1645	U	O4'-C1'-N1	5.09	112.27	108.20
1	A	2322	G	C5-C6-O6	-5.09	125.55	128.60
1	A	2499	G	N1-C6-O6	-5.09	116.85	119.90
1	A	2556	A	N9-C4-C5	5.09	107.83	105.80
1	A	1216	G	N7-C8-N9	5.08	115.64	113.10
2	B	96	G	C8-N9-C1'	-5.08	120.40	127.00
1	A	644	U	N1-C2-N3	5.08	117.94	114.90
1	A	1645	U	N3-C2-O2	-5.08	118.65	122.20
1	A	568	A	N7-C8-N9	5.07	116.34	113.80
1	A	2596	G	C4-N9-C1'	5.07	133.09	126.50
1	A	2365	G	N3-C4-C5	-5.07	126.06	128.60
1	A	2521	C	N3-C2-O2	-5.07	118.35	121.90
1	A	2563	G	N3-C4-C5	-5.06	126.07	128.60
1	A	114	U	C2-N1-C1'	5.06	123.77	117.70
1	A	1364	G	N7-C8-N9	5.06	115.63	113.10
1	A	1605	C	O5'-P-OP1	-5.06	101.15	105.70
1	A	2628	A	N9-C4-C5	5.06	107.82	105.80
11	O	86	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	1235	G	C2-N3-C4	5.05	114.43	111.90
1	A	2387	A	N1-C6-N6	-5.05	115.57	118.60
2	B	58	C	C2-N1-C1'	5.05	124.36	118.80
1	A	262	G	N3-C4-C5	-5.05	126.07	128.60
1	A	626	U	N3-C2-O2	-5.05	118.67	122.20
1	A	218	G	N3-C4-C5	-5.05	126.08	128.60
1	A	1022	C	C6-N1-C1'	-5.05	114.74	120.80
1	A	1505	C	N1-C2-O2	5.05	121.93	118.90
1	A	18	G	N3-C4-C5	-5.04	126.08	128.60
1	A	2722	G	C5-C6-O6	5.04	131.62	128.60
1	A	1167	A	C5-N7-C8	-5.04	101.38	103.90
1	A	25	G	C2-N3-C4	5.04	114.42	111.90
1	A	1730	G	C6-C5-N7	-5.04	127.38	130.40
1	A	2008	C	C6-N1-C2	-5.04	118.29	120.30
1	A	2041	G	C5-C6-N1	5.04	114.02	111.50
1	A	2317	G	N3-C4-N9	5.03	129.02	126.00
1	A	2794	G	C8-N9-C1'	-5.03	120.46	127.00
1	A	2632	G	N1-C6-O6	-5.03	116.88	119.90
1	A	2664	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1293	G	C4-N9-C1'	5.02	133.03	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1786	G	N1-C6-O6	-5.02	116.89	119.90
1	A	1192	C	N3-C2-O2	-5.02	118.39	121.90
1	A	963	C	C2-N1-C1'	5.02	124.32	118.80
1	A	1717	G	C2-N3-C4	5.02	114.41	111.90
1	A	832	G	C8-N9-C4	-5.02	104.39	106.40
1	A	2444	A	N3-C4-N9	-5.01	123.39	127.40
1	A	1514	G	N1-C6-O6	-5.01	116.89	119.90
1	A	1959	G	N9-C4-C5	-5.01	103.39	105.40
1	A	2087	C	C6-N1-C2	-5.01	118.30	120.30
7	K	123	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	561	G	N3-C4-N9	5.01	129.00	126.00
1	A	521	G	C5-C6-N1	5.00	114.00	111.50
1	A	905	G	N7-C8-N9	5.00	115.60	113.10
1	A	2371	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	89	GLY	Peptide
10	N	16	LYS	Peptide
10	N	19	GLY	Peptide
11	O	4	ARG	Peptide
11	O	73	VAL	Peptide
15	S	50	ALA	Peptide
16	T	67	PHE	Peptide
18	V	87	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	A	58793	0	29547	404	0
2	B	2480	0	1249	42	0
3	D	1579	0	1661	31	0
4	E	1574	0	1621	28	0
5	F	1392	0	1454	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	1345	0	1375	36	0
7	K	1130	0	1169	16	0
8	L	922	0	985	14	0
9	M	1095	0	1148	15	0
10	N	1118	0	1180	25	0
11	O	991	0	1028	21	0
12	P	899	0	932	26	0
13	Q	924	0	979	9	0
14	R	950	0	1009	11	0
15	S	784	0	826	12	0
16	T	849	0	906	13	0
17	U	720	0	772	13	0
18	V	763	0	824	15	0
19	X	572	0	580	9	0
20	Y	425	0	460	4	0
21	Z	504	0	538	5	0
22	0	435	0	472	6	0
23	2	429	0	444	3	0
24	3	419	0	435	9	0
25	4	374	0	424	9	0
26	5	522	0	576	5	0
27	6	304	0	337	6	0
28	2	1	0	0	0	0
28	3	1	0	0	0	0
28	6	1	0	0	0	0
All	All	82295	0	52931	757	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 6.

All (757) 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)
1:A:1571:G:N2	1:A:1591:A:H62	1.58	1.01
1:A:275:A:H62	1:A:296:G:N2	1.67	0.93
1:A:1571:G:H22	1:A:1591:A:H62	0.94	0.92
1:A:1871:G:N2	1:A:1899:A:H62	1.69	0.91
1:A:1871:G:H21	1:A:1899:A:H62	0.92	0.90
1:A:2280:A:H62	1:A:2287:A:H2	1.19	0.86
1:A:1571:G:H22	1:A:1591:A:N6	1.73	0.85
10:N:51:ARG:HG3	10:N:66:ILE:HD11	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:C:HO2'	1:A:2287:A:H8	0.89	0.85
1:A:1871:G:H21	1:A:1899:A:N6	1.75	0.84
1:A:2704:A:N6	11:O:39:GLU:OE1	2.11	0.83
1:A:2406:A:H2	1:A:2438:C:H42	1.25	0.81
1:A:162:A:O2'	1:A:169:A:N6	2.14	0.81
1:A:500:A:H62	1:A:509:G:H8	1.28	0.81
12:P:6:ASP:OD1	12:P:6:ASP:N	2.09	0.81
6:G:44:ASN:ND2	6:G:51:THR:O	2.14	0.80
18:V:94:SER:OG	18:V:95:LYS:O	1.99	0.79
1:A:1868:A:H62	1:A:1902:G:H8	1.30	0.78
1:A:1004:C:O2'	1:A:2287:A:H8	1.67	0.78
6:G:54:ARG:NH1	6:G:56:ASN:OD1	2.17	0.78
1:A:904:A:HO2'	1:A:905:G:H8	1.31	0.77
1:A:347:A:O2'	1:A:348:A:H2'	1.85	0.77
1:A:1578:A:H2'	1:A:1579:U:C6	2.20	0.76
11:O:96:ARG:HH21	11:O:126:VAL:HG23	1.50	0.76
1:A:1151:A:H8	1:A:1152:G:H1'	1.49	0.76
5:F:40:VAL:HG12	5:F:42:ASP:H	1.49	0.76
1:A:85:A:O2'	1:A:100:A:N6	2.16	0.76
1:A:1488:G:O6	1:A:1508:G:O6	2.04	0.76
1:A:2454:C:O2'	1:A:2455:C:O5'	2.02	0.76
6:G:164:TYR:HB2	6:G:167:GLU:HG3	1.68	0.75
1:A:653:G:N1	1:A:655:G:OP2	2.19	0.74
1:A:287:G:N2	1:A:289:U:OP1	2.21	0.74
1:A:2348:G:O2'	12:P:20:ASN:ND2	2.21	0.73
1:A:84:G:H21	1:A:103:A:H2	1.34	0.73
5:F:36:ILE:HB	5:F:89:VAL:HG12	1.68	0.73
7:K:131:HIS:HD2	7:K:133:HIS:H	1.35	0.73
15:S:15:GLU:OE1	15:S:18:GLN:NE2	2.22	0.73
1:A:275:A:H62	1:A:296:G:H21	1.34	0.72
2:B:76:A:H62	2:B:96:G:H8	1.34	0.72
1:A:2811:U:H4'	1:A:2812:A:O5'	1.89	0.72
1:A:568:A:H2	1:A:2055:U:H3	1.37	0.72
1:A:716:A:H8	1:A:2083:G:H21	1.35	0.72
12:P:56:ALA:HB3	12:P:79:VAL:HG22	1.71	0.71
4:E:2:PRO:HD3	4:E:21:GLU:HG3	1.73	0.71
5:F:52:LYS:NZ	5:F:147:ASP:OD2	2.24	0.71
2:B:29:C:OP1	12:P:4:LYS:NZ	2.23	0.71
2:B:1:U:H3	2:B:115:G:H1	1.38	0.71
6:G:124:GLU:HB2	6:G:132:ILE:HB	1.71	0.71
1:A:951:A:O2'	1:A:952:A:N7	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:G:H1	25:4:37:LYS:HZ3	1.38	0.70
1:A:885:U:H2'	1:A:886:U:H4'	1.72	0.70
7:K:7:ALA:H	7:K:46:THR:HG21	1.55	0.70
1:A:2329:U:H2'	1:A:2330:U:C6	2.26	0.70
1:A:2673:G:OP2	6:G:158:LYS:NZ	2.22	0.70
1:A:2318:G:H22	1:A:2326:U:H3	1.38	0.70
13:Q:17:ILE:HD13	13:Q:76:LEU:HD22	1.72	0.70
1:A:899:G:OP2	19:X:86:LYS:NZ	2.24	0.69
1:A:2636:C:O2'	1:A:2836:G:N2	2.25	0.69
15:S:88:HIS:HE1	15:S:90:GLN:HG2	1.56	0.69
1:A:2856:A:H62	1:A:2882:G:H21	1.38	0.69
1:A:275:A:N6	1:A:296:G:H21	1.90	0.69
1:A:1756:U:O2'	1:A:1760:G:N2	2.25	0.69
3:D:123:ILE:HD12	3:D:141:ARG:HG3	1.75	0.69
2:B:78:U:H2'	2:B:79:G:H21	1.57	0.68
1:A:1629:A:H3'	1:A:1630:G:H5"	1.75	0.68
16:T:48:SER:HA	16:T:51:ILE:HD12	1.76	0.68
3:D:125:ARG:HG3	3:D:164:MET:HG3	1.76	0.68
4:E:10:ASP:OD1	4:E:10:ASP:N	2.23	0.68
2:B:97:A:O2'	2:B:98:G:OP1	2.10	0.68
5:F:130:LEU:HD13	5:F:131:GLY:H	1.58	0.67
5:F:170:LEU:HD22	5:F:175:MET:HG3	1.76	0.67
1:A:1504:G:O2'	1:A:1505:C:OP2	2.12	0.67
2:B:70:G:H8	2:B:102:A:H62	1.41	0.67
1:A:337:A:OP2	18:V:95:LYS:NZ	2.28	0.67
1:A:13:U:O2'	1:A:14:A:OP1	2.10	0.67
1:A:232:U:O2'	1:A:233:U:O5'	2.13	0.67
17:U:23:LYS:NZ	17:U:84:GLU:HA	2.10	0.67
17:U:29:VAL:HG21	17:U:38:VAL:HG22	1.78	0.66
24:3:31:GLU:HG2	24:3:46:ARG:HG2	1.77	0.66
1:A:154:U:HO2'	1:A:155:U:H6	1.41	0.66
1:A:1216:G:OP2	1:A:1217:G:N2	2.29	0.66
4:E:78:ILE:HG22	4:E:79:ARG:HD2	1.76	0.66
5:F:6:GLU:O	5:F:10:LYS:HB2	1.95	0.66
1:A:2328:A:H2'	1:A:2329:U:C6	2.30	0.66
1:A:533:G:H4'	16:T:11:THR:HG23	1.78	0.65
8:L:73:ASP:OD1	8:L:73:ASP:N	2.27	0.65
19:X:81:LYS:HB2	19:X:87:GLN:HG3	1.78	0.65
1:A:654:A:H1'	1:A:655:G:H2'	1.76	0.65
1:A:1585:U:H2'	1:A:1586:A:C8	2.32	0.65
1:A:1576:A:N1	1:A:1578:A:N6	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:6:17:ILE:HG22	27:6:18:ARG:H	1.61	0.65
1:A:1630:G:H1'	1:A:1631:A:C5	2.32	0.65
19:X:55:TYR:HE1	19:X:85:LYS:HD3	1.61	0.65
1:A:1167:A:C8	1:A:2532:A:H5"	2.33	0.64
1:A:2342:A:H2'	1:A:2343:A:C8	2.32	0.64
4:E:8:LYS:HD3	4:E:14:ASN:HD22	1.63	0.64
1:A:2453:A:H4'	1:A:2454:C:H3'	1.78	0.64
1:A:2520:U:H3	1:A:2597:G:H1	1.46	0.64
9:M:85:PHE:O	9:M:119:LYS:NZ	2.31	0.64
1:A:1216:G:H3'	1:A:1217:G:H5"	1.78	0.64
1:A:904:A:O2'	1:A:905:G:H8	1.80	0.64
1:A:623:A:H62	1:A:1288:A:H2	1.46	0.64
7:K:4:THR:HG21	14:R:61:TRP:HE1	1.62	0.64
1:A:508:G:H2'	1:A:509:G:H5'	1.80	0.63
1:A:1535:U:O2'	1:A:1536:A:OP1	2.14	0.63
1:A:1178:G:H21	7:K:109:MET:HE3	1.63	0.63
1:A:1074:G:O4'	27:6:18:ARG:NH1	2.31	0.63
18:V:97:THR:OG1	18:V:99:GLU:OE2	2.16	0.63
1:A:853:U:H2'	1:A:854:C:C6	2.34	0.63
1:A:1860:G:H2'	1:A:1861:A:C8	2.34	0.63
26:5:10:LEU:HB3	26:5:62:LEU:HD21	1.81	0.63
1:A:359:A:OP1	4:E:168:ARG:NH1	2.32	0.62
4:E:59:GLY:HA3	4:E:79:ARG:HD3	1.79	0.62
15:S:24:LYS:HA	15:S:93:THR:HG23	1.81	0.62
1:A:2333:A:H4'	1:A:2334:A:H5'	1.82	0.62
19:X:49:GLN:HE22	19:X:54:ILE:H	1.45	0.62
1:A:1570:G:H22	1:A:1592:G:H1	1.47	0.62
2:B:70:G:H8	2:B:102:A:N6	1.96	0.62
5:F:12:VAL:HG22	5:F:172:GLN:HG2	1.81	0.62
1:A:500:A:N6	1:A:509:G:H8	1.95	0.62
2:B:57:G:O2'	12:P:6:ASP:OD2	2.18	0.62
6:G:25:THR:HB	6:G:34:THR:HG22	1.82	0.62
10:N:43:THR:HG22	10:N:94:VAL:HG12	1.82	0.61
1:A:285:U:O2'	1:A:287:G:OP1	2.17	0.61
16:T:5:ILE:HD11	16:T:67:PHE:CG	2.35	0.61
1:A:539:G:N1	1:A:542:A:OP2	2.30	0.61
1:A:2280:A:N6	1:A:2287:A:H2	1.95	0.61
1:A:2329:U:H2'	1:A:2330:U:H6	1.65	0.61
1:A:2207:C:H2'	1:A:2208:C:O4'	2.00	0.61
1:A:2517:A:O2'	1:A:2519:G:OP2	2.18	0.61
1:A:891:A:O2'	22:0:22:THR:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1310:A:O2'	1:A:1689:A:N6	2.34	0.61
10:N:19:GLY:HA2	10:N:98:LYS:HD2	1.81	0.61
11:O:55:ASP:OD1	11:O:55:ASP:N	2.31	0.61
1:A:1194:G:OP2	14:R:58:ARG:NH1	2.34	0.61
1:A:626:U:H2'	1:A:627:A:H8	1.66	0.60
2:B:76:A:N6	2:B:96:G:H8	1.98	0.60
1:A:1994:G:O2'	1:A:1996:U:OP2	2.19	0.60
1:A:2514:U:O2	1:A:2518:U:N3	2.35	0.60
1:A:2771:A:N1	6:G:67:THR:HG21	2.15	0.60
1:A:1724:G:H21	1:A:1776:A:H3'	1.67	0.60
1:A:1756:U:O4	1:A:1758:C:H5"	2.01	0.60
1:A:626:U:H2'	1:A:627:A:C8	2.37	0.60
3:D:55:ASP:OD1	3:D:77:LYS:NZ	2.26	0.60
8:L:24:VAL:HG13	8:L:33:ALA:HB2	1.83	0.60
12:P:40:ILE:HD11	12:P:72:ALA:HA	1.82	0.60
14:R:97:ASP:OD1	14:R:101:ASN:ND2	2.35	0.60
1:A:1494:G:H1	1:A:1504:G:H21	1.50	0.60
5:F:166:SER:O	5:F:170:LEU:HB2	2.01	0.60
6:G:58:SER:O	6:G:61:MET:HG2	2.02	0.60
1:A:285:U:H2'	1:A:287:G:H8	1.66	0.59
7:K:63:VAL:HG21	7:K:102:ILE:HD11	1.83	0.59
1:A:262:G:H21	1:A:660:A:H8	1.51	0.59
1:A:2328:A:H2'	1:A:2329:U:H6	1.65	0.59
1:A:225:A:H62	1:A:235:G:H8	1.49	0.59
1:A:1323:A:H8	11:O:113:ARG:HD3	1.67	0.59
1:A:2341:A:H2'	1:A:2342:A:C8	2.36	0.59
10:N:41:TRP:HZ3	10:N:74:TYR:CE1	2.21	0.59
16:T:17:THR:HG22	16:T:47:LYS:HE3	1.84	0.59
21:Z:51:ALA:O	21:Z:55:THR:HG22	2.03	0.59
1:A:92:A:H2'	1:A:93:G:H5'	1.82	0.59
1:A:585:A:H4'	1:A:586:A:H5'	1.84	0.59
1:A:2810:U:C2	1:A:2811:U:H5	2.20	0.59
1:A:2758:G:N2	6:G:143:GLU:OE2	2.36	0.59
1:A:2361:C:OP1	24:3:34:LYS:NZ	2.34	0.58
1:A:2461:G:N2	1:A:2464:A:OP2	2.35	0.58
1:A:2856:A:H62	1:A:2882:G:N2	2.01	0.58
19:X:73:ASP:OD1	19:X:73:ASP:N	2.34	0.58
22:0:50:ILE:HG23	22:0:53:LEU:HD12	1.85	0.58
1:A:77:C:O2'	21:Z:55:THR:HG21	2.04	0.58
1:A:1376:U:OP1	17:U:15:LYS:NZ	2.37	0.58
1:A:1408:U:HO2'	1:A:2226:A:H8	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2454:C:HO2'	1:A:2455:C:P	2.27	0.58
1:A:1208:C:H2'	1:A:1209:A:C8	2.39	0.58
1:A:1861:A:O2'	1:A:1862:A:H8	1.87	0.58
12:P:15:HIS:HE1	12:P:94:ASP:OD2	1.87	0.58
7:K:145:ASN:OD1	7:K:145:ASN:N	2.36	0.58
1:A:586:A:O2'	1:A:587:U:H5"	2.04	0.58
5:F:53:ALA:HB2	5:F:150:ARG:HH12	1.68	0.58
6:G:4:ILE:O	6:G:69:ARG:HD3	2.04	0.58
24:3:29:ARG:NH1	24:3:49:LYS:HB2	2.19	0.58
5:F:42:ASP:O	5:F:49:ASN:ND2	2.37	0.57
19:X:55:TYR:CE1	19:X:85:LYS:HD3	2.38	0.57
5:F:38:MET:HE3	5:F:150:ARG:HH11	1.68	0.57
12:P:100:TYR:OH	12:P:112:ARG:NH2	2.37	0.57
1:A:1490:A:C2'	1:A:1491:U:H5'	2.34	0.57
1:A:607:G:H2'	1:A:2044:A:C2	2.40	0.57
12:P:40:ILE:H	12:P:58:ALA:HB2	1.69	0.57
3:D:9:LYS:HB2	3:D:200:ILE:HD11	1.86	0.57
5:F:46:ASN:O	5:F:49:ASN:ND2	2.37	0.57
25:4:34:ARG:NH1	25:4:41:VAL:O	2.37	0.57
1:A:1458:G:H1	1:A:1628:G:H21	1.53	0.57
9:M:101:ILE:HG22	9:M:102:VAL:HG23	1.85	0.57
1:A:1086:A:H2'	1:A:1086:A:N3	2.19	0.56
1:A:1585:U:H2'	1:A:1586:A:H8	1.69	0.56
15:S:50:ALA:O	15:S:52:THR:N	2.37	0.56
1:A:1633:A:O2'	1:A:1634:A:H5"	2.05	0.56
1:A:1793:U:H5	1:A:1798:A:N7	2.03	0.56
1:A:2219:A:H2'	1:A:2220:C:C6	2.41	0.56
10:N:41:TRP:HZ3	10:N:74:TYR:HE1	1.53	0.56
1:A:951:A:O2'	1:A:952:A:C8	2.56	0.56
1:A:905:G:H21	1:A:907:A:N6	2.03	0.56
1:A:160:U:H2'	1:A:161:G:O4'	2.06	0.56
1:A:2204:A:H2'	1:A:2205:A:C8	2.41	0.56
10:N:42:ILE:HD12	10:N:97:VAL:HG21	1.87	0.56
1:A:2085:A:H2'	1:A:2086:G:C8	2.41	0.56
5:F:138:PHE:HB2	5:F:141:VAL:HG23	1.88	0.56
8:L:63:VAL:HG11	8:L:102:VAL:HG22	1.88	0.56
1:A:344:G:H8	1:A:367:A:H61	1.53	0.55
1:A:916:A:H2'	1:A:917:C:O4'	2.07	0.55
1:A:1422:C:H2'	1:A:1423:A:C8	2.41	0.55
1:A:1571:G:N2	1:A:1591:A:N6	2.41	0.55
4:E:67:GLN:HG3	4:E:68:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:158:ASN:O	4:E:160:ASN:N	2.33	0.55
6:G:95:ARG:HB3	6:G:128:ASN:HB3	1.87	0.55
1:A:2444:A:HO2'	1:A:2445:U:H6	1.54	0.55
1:A:1490:A:N1	1:A:1506:A:N1	2.54	0.55
1:A:1178:G:H21	7:K:109:MET:CE	2.19	0.55
5:F:129:THR:HG22	5:F:155:VAL:HG22	1.88	0.55
15:S:5:ILE:HD11	15:S:58:VAL:HG21	1.88	0.55
1:A:391:C:O2'	1:A:392:A:O5'	2.24	0.55
1:A:234:C:O2'	1:A:235:G:O4'	2.24	0.55
1:A:1583:A:N3	1:A:1583:A:H2'	2.20	0.55
5:F:60:ILE:HG22	5:F:61:THR:HG23	1.89	0.55
17:U:64:ARG:HG3	17:U:69:ALA:HB2	1.88	0.55
1:A:151:A:H61	1:A:179:A:H2	1.54	0.55
1:A:311:A:O2'	1:A:399:A:N1	2.39	0.55
1:A:1931:U:H2'	1:A:1932:A:O4'	2.07	0.55
6:G:26:VAL:HG12	6:G:79:VAL:HG11	1.88	0.55
1:A:367:A:H2	1:A:1247:U:HO2'	1.55	0.55
1:A:1394:G:H8	1:A:1409:A:H62	1.54	0.55
1:A:275:A:N6	1:A:296:G:N2	2.44	0.54
1:A:1208:C:H2'	1:A:1209:A:H8	1.72	0.54
3:D:89:GLY:O	3:D:91:TYR:N	2.40	0.54
1:A:2482:A:HO2'	1:A:2483:A:H8	1.55	0.54
2:B:68:C:H5	2:B:104:G:H22	1.56	0.54
1:A:2860:G:OP1	13:Q:93:ARG:NH1	2.40	0.54
2:B:39:G:OP1	2:B:41:C:N4	2.40	0.54
24:3:3:VAL:HG12	24:3:4:ASN:O	2.07	0.54
1:A:883:A:H2'	1:A:884:A:C8	2.43	0.54
1:A:1151:A:C8	1:A:1152:G:H1'	2.37	0.54
10:N:85:LYS:HG2	19:X:18:SER:N	2.22	0.54
1:A:950:A:H2'	1:A:953:C:C5	2.42	0.54
1:A:508:G:C2'	1:A:509:G:H5'	2.38	0.54
5:F:119:LYS:HB3	5:F:167:ARG:NH2	2.23	0.54
18:V:84:LYS:HB2	18:V:93:VAL:HG21	1.88	0.54
1:A:313:A:H2'	1:A:314:U:O4'	2.08	0.54
11:O:100:ARG:HG3	11:O:101:GLN:O	2.08	0.54
1:A:509:G:H1	25:4:37:LYS:NZ	2.06	0.54
5:F:5:LYS:HE3	5:F:97:TYR:HE2	1.73	0.54
8:L:102:VAL:HG13	8:L:106:LEU:HD12	1.90	0.53
1:A:1081:U:H2'	1:A:1082:G:H8	1.73	0.53
1:A:285:U:H2'	1:A:287:G:C8	2.43	0.53
1:A:1754:A:H2'	1:A:1755:C:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:75:VAL:O	12:P:79:VAL:HG23	2.09	0.53
1:A:904:A:H2'	10:N:22:LYS:HE3	1.89	0.53
1:A:1591:A:H2'	1:A:1592:G:C8	2.43	0.53
2:B:68:C:H5	2:B:104:G:H1	1.55	0.53
22:0:37:LYS:HB3	22:0:43:ILE:HD13	1.89	0.53
1:A:1202:G:O3'	15:S:24:LYS:NZ	2.42	0.53
1:A:2712:U:H2'	1:A:2713:U:C6	2.43	0.53
9:M:84:ARG:HH21	9:M:101:ILE:HD11	1.74	0.53
22:0:18:ASN:O	22:0:22:THR:HG23	2.09	0.53
1:A:1631:A:C4	1:A:1632:A:H2	2.27	0.53
1:A:118:A:OP2	1:A:119:A:H5"	2.09	0.53
16:T:16:ARG:NH1	16:T:103:LYS:HD3	2.23	0.53
18:V:87:ASP:O	18:V:89:LYS:N	2.36	0.53
1:A:292:U:H2'	1:A:293:U:C6	2.44	0.53
16:T:16:ARG:HH11	16:T:103:LYS:HD3	1.74	0.53
3:D:13:THR:OG1	3:D:14:GLN:N	2.42	0.53
17:U:23:LYS:HZ1	17:U:84:GLU:HA	1.73	0.53
1:A:1310:A:HO2'	1:A:1689:A:N6	2.07	0.52
1:A:2836:G:O5'	1:A:2836:G:H8	1.91	0.52
2:B:40:C:C5	5:F:66:LEU:HG	2.44	0.52
22:0:7:THR:HB	22:0:34:THR:HG22	1.90	0.52
25:4:8:ASN:HD22	25:4:11:LYS:H	1.57	0.52
1:A:2111:G:H2'	1:A:2112:U:C6	2.44	0.52
12:P:69:THR:HG22	12:P:103:ARG:HB3	1.91	0.52
1:A:899:G:N3	1:A:2282:A:H2'	2.24	0.52
1:A:2323:A:OP1	1:A:2323:A:H8	1.92	0.52
12:P:8:ASN:O	12:P:12:GLN:HG2	2.08	0.52
2:B:86:U:H4'	2:B:87:U:H5	1.74	0.52
8:L:28:SER:O	8:L:28:SER:OG	2.24	0.52
1:A:181:G:H2'	1:A:182:U:O4'	2.10	0.52
1:A:498:G:O6	4:E:58:ARG:HD3	2.08	0.52
1:A:1758:C:H2'	1:A:1759:G:C8	2.45	0.52
1:A:1872:G:H1'	1:A:1898:A:N6	2.23	0.52
2:B:48:A:OP1	12:P:69:THR:N	2.42	0.52
1:A:943:U:H2'	1:A:944:U:C6	2.45	0.52
1:A:945:C:H2'	1:A:946:A:O4'	2.10	0.52
5:F:40:VAL:HB	5:F:85:ILE:O	2.10	0.52
13:Q:60:THR:HB	13:Q:73:THR:HG22	1.92	0.52
1:A:1451:U:O2'	1:A:1452:G:OP2	2.27	0.52
3:D:107:VAL:HG23	3:D:173:ASN:HA	1.92	0.52
10:N:32:TRP:CZ3	10:N:133:LYS:HG2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:40:VAL:O	11:O:44:VAL:HG23	2.10	0.52
1:A:678:U:H2'	1:A:679:C:C6	2.45	0.51
1:A:1212:A:HO2'	1:A:1213:U:H6	1.53	0.51
1:A:1591:A:H3'	1:A:1591:A:N3	2.25	0.51
1:A:203:U:H4'	20:Y:22:MET:HB3	1.92	0.51
27:6:36:ARG:O	27:6:36:ARG:HG3	2.10	0.51
1:A:1330:C:H5'	11:O:69:GLU:O	2.09	0.51
6:G:103:LEU:HB2	6:G:123:PHE:CE2	2.46	0.51
17:U:58:VAL:HB	17:U:75:ARG:HB2	1.91	0.51
1:A:282:A:H2'	1:A:283:G:H8	1.74	0.51
1:A:1301:G:OP1	23:2:16:ARG:NH2	2.28	0.51
1:A:1867:A:H2'	1:A:1868:A:C8	2.46	0.51
6:G:10:VAL:HG22	6:G:49:GLU:HG3	1.93	0.51
2:B:50:A:C6	12:P:38:LYS:HE2	2.45	0.51
1:A:1491:U:O2'	1:A:1492:G:C8	2.59	0.51
1:A:92:A:C2'	1:A:93:G:H5'	2.41	0.51
1:A:154:U:O2'	1:A:155:U:H6	1.93	0.51
3:D:108:VAL:HG22	3:D:203:LYS:O	2.11	0.51
4:E:75:GLN:NE2	4:E:83:TRP:HE1	2.08	0.51
10:N:7:VAL:HG11	10:N:93:TRP:HH2	1.76	0.51
1:A:288:C:HO2'	1:A:289:U:H5	1.59	0.51
1:A:2481:C:H2'	1:A:2482:A:O4'	2.08	0.51
1:A:2672:C:H5"	6:G:158:LYS:HZ2	1.75	0.51
1:A:1046:C:H1'	7:K:109:MET:HE3	1.92	0.51
1:A:1572:A:H62	1:A:1589:G:H8	1.58	0.51
1:A:1593:U:H2'	1:A:1594:U:C6	2.46	0.51
1:A:2035:G:H2'	1:A:2035:G:N3	2.26	0.51
1:A:306:C:H2'	1:A:307:U:C6	2.45	0.50
1:A:2637:G:O5'	1:A:2836:G:N2	2.44	0.50
3:D:34:VAL:HG11	3:D:74:THR:HG21	1.93	0.50
10:N:109:VAL:HG13	10:N:113:VAL:HB	1.93	0.50
18:V:70:VAL:HG11	18:V:92:ARG:HH12	1.76	0.50
1:A:179:A:O3'	1:A:180:G:H8	1.94	0.50
1:A:1872:G:H1'	1:A:1898:A:H61	1.75	0.50
27:6:17:ILE:HD12	27:6:26:ILE:HD12	1.94	0.50
1:A:991:C:H2'	1:A:992:G:H5'	1.92	0.50
1:A:1206:U:H2'	1:A:1207:A:C8	2.46	0.50
2:B:39:G:P	2:B:41:C:H41	2.33	0.50
6:G:18:LYS:HB2	6:G:25:THR:HG23	1.93	0.50
1:A:1167:A:H8	1:A:2532:A:H5"	1.76	0.50
1:A:650:G:N2	1:A:654:A:H5'	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1816:A:H2'	1:A:1817:A:C8	2.46	0.50
1:A:2044:A:C8	1:A:2513:C:H5"	2.47	0.50
2:B:72:U:C2'	2:B:73:U:H5'	2.42	0.50
1:A:161:G:H2'	1:A:162:A:N3	2.26	0.50
1:A:454:C:H2'	1:A:455:A:C8	2.47	0.50
1:A:573:U:O2'	14:R:49:ASP:OD2	2.28	0.50
21:Z:14:MET:HG3	21:Z:57:LEU:HD21	1.94	0.50
1:A:897:G:H2'	1:A:898:A:C8	2.47	0.50
17:U:51:ALA:O	17:U:81:THR:HB	2.12	0.50
1:A:1207:A:H2'	1:A:1208:C:C6	2.47	0.49
1:A:2475:C:H2'	1:A:2476:U:C6	2.46	0.49
1:A:1399:C:O2'	1:A:1823:A:N3	2.40	0.49
10:N:59:LYS:O	10:N:60:ARG:HB2	2.13	0.49
11:O:17:LEU:O	11:O:21:THR:HG23	2.12	0.49
1:A:509:G:H22	25:4:37:LYS:HZ1	1.61	0.49
1:A:653:G:H2'	1:A:654:A:H5"	1.93	0.49
1:A:943:U:H2'	1:A:944:U:H6	1.77	0.49
1:A:1537:A:N3	1:A:1624:U:O2'	2.43	0.49
1:A:1624:U:OP2	1:A:1624:U:H6	1.96	0.49
1:A:1872:G:O2'	1:A:1898:A:N6	2.46	0.49
10:N:36:ALA:HB2	10:N:103:MET:SD	2.53	0.49
27:6:22:ARG:HH11	27:6:36:ARG:HD3	1.77	0.49
5:F:8:TYR:CE1	5:F:173:LEU:HD21	2.47	0.49
14:R:29:HIS:CD2	14:R:30:THR:HG23	2.48	0.49
1:A:1757:U:H4'	1:A:1757:U:OP2	2.13	0.49
18:V:73:PRO:HD3	18:V:101:LEU:HD22	1.95	0.49
1:A:161:G:N2	1:A:168:U:H5	2.11	0.49
1:A:1206:U:H2'	1:A:1207:A:H8	1.77	0.49
1:A:1315:A:H2'	1:A:1316:G:O4'	2.13	0.49
1:A:2551:U:H2'	1:A:2552:C:C6	2.48	0.49
1:A:1502:G:H5"	1:A:1503:U:H3'	1.95	0.49
2:B:84:G:C2	2:B:85:U:C2	3.01	0.49
1:A:2738:U:OP1	3:D:124:LYS:NZ	2.30	0.49
3:D:109:ASP:OD2	3:D:206:VAL:HG23	2.13	0.49
1:A:509:G:H22	25:4:37:LYS:NZ	2.10	0.49
1:A:2011:A:OP2	3:D:130:ARG:HD3	2.13	0.49
1:A:2674:A:OP1	6:G:176:THR:HB	2.13	0.49
7:K:100:ARG:O	7:K:104:THR:HG23	2.13	0.49
9:M:122:THR:O	9:M:122:THR:OG1	2.25	0.49
16:T:14:THR:HG22	16:T:105:THR:HG21	1.95	0.49
2:B:46:A:OP1	12:P:35:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:U:H2'	2:B:79:G:N2	2.27	0.48
1:A:950:A:H2'	1:A:953:C:H5	1.77	0.48
1:A:1886:G:O2'	1:A:1887:G:OP2	2.24	0.48
1:A:1408:U:O2'	1:A:2226:A:H8	1.97	0.48
3:D:92:GLU:HG2	3:D:95:LYS:HE3	1.96	0.48
6:G:118:PRO:HD2	6:G:144:LEU:HD11	1.95	0.48
9:M:92:THR:H	9:M:95:VAL:HG12	1.78	0.48
12:P:29:PRO:HG2	12:P:91:VAL:HG12	1.94	0.48
1:A:273:A:OP2	1:A:297:G:N1	2.44	0.48
1:A:1453:U:C6	1:A:1628:G:H2'	2.48	0.48
1:A:2044:A:H8	1:A:2513:C:H5"	1.79	0.48
4:E:6:LEU:HG	4:E:17:ILE:HG13	1.95	0.48
11:O:68:ASN:O	11:O:70:VAL:N	2.40	0.48
1:A:912:U:OP1	10:N:5:LYS:N	2.44	0.48
1:A:1166:A:H8	1:A:1166:A:OP1	1.96	0.48
1:A:1256:G:OP1	14:R:22:LYS:NZ	2.47	0.48
5:F:70:ALA:HB3	5:F:82:GLY:H	1.78	0.48
16:T:87:MET:HB2	16:T:103:LYS:HB2	1.95	0.48
18:V:1:MET:SD	18:V:65:VAL:HG21	2.54	0.48
1:A:194:A:H2'	1:A:195:C:C6	2.49	0.48
11:O:45:GLU:O	11:O:49:THR:HG23	2.14	0.48
1:A:1009:G:H2'	1:A:1010:U:C6	2.49	0.48
1:A:290:U:H2'	1:A:291:G:O4'	2.14	0.47
5:F:164:GLU:HA	5:F:167:ARG:HG3	1.96	0.47
6:G:159:GLY:O	6:G:163:ARG:NH2	2.47	0.47
25:4:31:LEU:HD22	25:4:42:ILE:HD12	1.96	0.47
1:A:4:U:H2'	1:A:5:U:C6	2.49	0.47
1:A:519:A:N3	1:A:521:G:H5"	2.29	0.47
2:B:58:C:H2'	2:B:59:U:C6	2.49	0.47
5:F:3:ARG:O	5:F:7:LYS:HG3	2.14	0.47
1:A:392:A:H2'	1:A:393:A:C8	2.50	0.47
6:G:59:LYS:HG3	6:G:60:GLU:HG3	1.97	0.47
11:O:24:LEU:HB2	11:O:30:ILE:HD12	1.96	0.47
12:P:89:LYS:HG2	12:P:115:GLY:O	2.15	0.47
15:S:25:LEU:O	15:S:26:ASN:HB2	2.13	0.47
1:A:1535:U:HO2'	1:A:1536:A:P	2.33	0.47
1:A:2343:A:H2'	1:A:2344:G:C8	2.50	0.47
2:B:85:U:O4	2:B:86:U:N3	2.47	0.47
16:T:85:PRO:O	16:T:105:THR:OG1	2.31	0.47
1:A:900:G:O2'	1:A:901:U:OP2	2.32	0.47
2:B:59:U:H2'	2:B:60:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:100:ASP:OD1	3:D:100:ASP:N	2.36	0.47
7:K:131:HIS:CD2	7:K:133:HIS:H	2.24	0.47
1:A:727:C:H1'	25:4:4:THR:HG22	1.95	0.47
1:A:1591:A:N3	1:A:1591:A:O5'	2.48	0.47
3:D:2:THR:OG1	3:D:3:LYS:N	2.47	0.47
6:G:48:ASN:O	6:G:49:GLU:HB2	2.14	0.47
15:S:19:ALA:HB1	15:S:94:LYS:HD3	1.96	0.47
17:U:8:LYS:HB2	17:U:28:GLU:O	2.14	0.47
1:A:11:A:H2'	1:A:12:A:C8	2.50	0.47
1:A:282:A:H2'	1:A:283:G:C8	2.49	0.47
1:A:2851:U:H5"	11:O:49:THR:HG21	1.96	0.47
1:A:1085:C:O2'	1:A:1086:A:OP1	2.29	0.47
1:A:1868:A:N6	1:A:1902:G:H8	2.06	0.47
1:A:1885:C:H41	1:A:1886:G:H21	1.62	0.47
2:B:32:U:O2'	2:B:33:U:O5'	2.32	0.47
3:D:19:SER:O	13:Q:80:ARG:NH2	2.36	0.47
5:F:70:ALA:HB3	5:F:82:GLY:N	2.30	0.47
1:A:526:C:O2'	16:T:65:ASN:ND2	2.48	0.47
1:A:1457:A:N1	1:A:1630:G:H4'	2.30	0.46
8:L:111:PHE:O	8:L:115:VAL:HG23	2.14	0.46
1:A:998:U:OP2	10:N:14:ARG:NH1	2.47	0.46
2:B:89:C:OP1	10:N:99:ARG:NH2	2.34	0.46
5:F:13:THR:O	5:F:17:VAL:HB	2.14	0.46
9:M:33:ARG:NH1	9:M:41:ARG:O	2.49	0.46
9:M:133:GLN:HG3	9:M:143:ILE:HG12	1.98	0.46
15:S:21:TYR:CE2	15:S:94:LYS:HG3	2.51	0.46
16:T:63:ALA:O	16:T:68:ASP:N	2.44	0.46
3:D:13:THR:HG23	3:D:25:VAL:HG12	1.97	0.46
4:E:41:ARG:HG2	4:E:41:ARG:HH11	1.80	0.46
1:A:654:A:H4'	1:A:655:G:C8	2.50	0.46
1:A:1490:A:H2'	1:A:1491:U:H5'	1.97	0.46
3:D:5:ILE:HG13	3:D:102:PHE:HE2	1.79	0.46
5:F:135:GLN:O	5:F:141:VAL:HG21	2.16	0.46
6:G:63:THR:O	6:G:67:THR:HG23	2.16	0.46
7:K:3:THR:O	7:K:3:THR:OG1	2.32	0.46
13:Q:32:VAL:HG21	13:Q:41:GLN:HE21	1.81	0.46
15:S:65:HIS:ND1	15:S:93:THR:HG22	2.31	0.46
21:Z:10:THR:O	21:Z:14:MET:HG2	2.15	0.46
1:A:61:G:OP1	21:Z:47:ARG:NH2	2.48	0.46
1:A:1088:A:H2'	1:A:1088:A:N3	2.31	0.46
1:A:1631:A:N3	1:A:1631:A:H2'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2855:A:H2'	1:A:2856:A:C8	2.50	0.46
6:G:5:GLY:HA3	6:G:65:HIS:CD2	2.50	0.46
8:L:23:LYS:O	8:L:39:ILE:HG13	2.15	0.46
24:3:32:LYS:HA	24:3:32:LYS:HD3	1.74	0.46
1:A:492:G:C8	4:E:58:ARG:HD2	2.51	0.46
1:A:1492:G:N2	1:A:1504:G:H22	2.14	0.46
1:A:1692:G:O2'	11:O:116:ASP:OD1	2.32	0.46
2:B:90:C:HO2'	2:B:91:U:P	2.39	0.46
12:P:35:ARG:HA	12:P:40:ILE:HG22	1.97	0.46
1:A:1474:G:H2'	1:A:1475:U:C6	2.50	0.46
5:F:83:MET:O	5:F:85:ILE:HG13	2.16	0.46
18:V:47:PRO:HB3	18:V:52:PRO:O	2.15	0.46
1:A:782:U:H2'	1:A:783:A:C8	2.51	0.45
1:A:903:G:O6	1:A:956:C:N3	2.50	0.45
1:A:2314:A:H2'	1:A:2315:A:C8	2.51	0.45
5:F:4:LEU:HD22	5:F:7:LYS:HD2	1.98	0.45
5:F:55:GLU:O	5:F:59:LEU:HG	2.16	0.45
5:F:104:VAL:HG22	5:F:175:MET:H	1.80	0.45
1:A:1447:U:H2'	1:A:1448:U:O4'	2.16	0.45
1:A:469:A:H2'	1:A:470:A:C8	2.52	0.45
1:A:2763:A:H4'	6:G:62:LYS:HB2	1.97	0.45
24:3:41:LYS:HD3	24:3:41:LYS:HA	1.73	0.45
1:A:1167:A:N3	1:A:1167:A:H2'	2.31	0.45
1:A:2809:U:OP2	1:A:2810:U:N3	2.49	0.45
3:D:146:MET:HA	3:D:158:LYS:HE2	1.97	0.45
5:F:66:LEU:HD23	5:F:66:LEU:HA	1.73	0.45
15:S:88:HIS:CE1	15:S:90:GLN:HG2	2.44	0.45
1:A:251:G:O5'	1:A:252:C:H5"	2.17	0.45
1:A:1804:C:H2'	1:A:1805:A:C5	2.51	0.45
1:A:1861:A:H8	1:A:1861:A:OP2	1.99	0.45
1:A:2439:A:H5"	1:A:2441:C:O4'	2.17	0.45
1:A:2908:U:H2'	1:A:2909:A:O4'	2.15	0.45
5:F:117:VAL:HG12	5:F:118:SER:O	2.16	0.45
11:O:22:THR:HG21	11:O:67:ARG:HB2	1.99	0.45
5:F:68:THR:N	5:F:86:GLY:O	2.42	0.45
1:A:523:A:H5"	18:V:46:LYS:HG2	1.98	0.45
1:A:697:U:H2'	1:A:698:A:C8	2.52	0.45
1:A:2812:A:O2'	1:A:2813:A:OP1	2.20	0.45
11:O:96:ARG:HH21	11:O:126:VAL:CG2	2.25	0.45
15:S:69:LYS:HB3	15:S:69:LYS:HE2	1.67	0.45
26:5:32:ARG:H	26:5:32:ARG:HG3	1.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:U:H2'	1:A:325:U:O4'	2.17	0.45
1:A:613:U:H2'	1:A:614:G:C8	2.52	0.45
1:A:1390:A:H2'	1:A:1391:G:O4'	2.17	0.45
1:A:2264:G:N2	10:N:84:GLY:HA2	2.32	0.45
1:A:2359:G:N3	1:A:2395:C:H2'	2.31	0.45
9:M:83:ASN:O	9:M:119:LYS:NZ	2.47	0.45
17:U:19:ALA:HB1	17:U:24:LYS:HB2	1.99	0.45
1:A:1052:U:OP2	14:R:70:ARG:NH2	2.44	0.45
1:A:1453:U:H4'	1:A:1454:U:C6	2.52	0.45
5:F:117:VAL:HB	5:F:177:PHE:HD1	1.81	0.45
6:G:154:PRO:HA	6:G:160:LYS:O	2.17	0.45
9:M:2:LYS:HD3	9:M:4:HIS:CE1	2.52	0.45
1:A:1328:G:H2'	1:A:1329:U:C6	2.52	0.45
1:A:2458:G:OP2	4:E:68:LYS:NZ	2.38	0.45
18:V:41:VAL:O	18:V:58:GLU:HA	2.17	0.45
1:A:1451:U:P	1:A:1630:G:H22	2.40	0.44
1:A:2342:A:H2'	1:A:2343:A:H8	1.82	0.44
4:E:12:THR:O	4:E:14:ASN:N	2.50	0.44
6:G:10:VAL:HG13	6:G:48:ASN:O	2.17	0.44
12:P:40:ILE:O	12:P:58:ALA:HB2	2.18	0.44
23:2:23:THR:HG21	23:2:25:LYS:HE3	1.99	0.44
1:A:1499:G:H22	1:A:2716:G:H22	1.66	0.44
11:O:38:LYS:O	11:O:41:ARG:HG2	2.18	0.44
1:A:885:U:N3	1:A:886:U:H1'	2.32	0.44
1:A:1960:U:H2'	1:A:1961:C:C6	2.52	0.44
1:A:2078:C:H2'	1:A:2079:C:C6	2.53	0.44
1:A:2595:G:H2'	1:A:2595:G:N3	2.32	0.44
18:V:24:LEU:HD23	18:V:24:LEU:HA	1.66	0.44
1:A:900:G:N2	1:A:958:A:OP2	2.30	0.44
1:A:2494:C:H2'	1:A:2495:G:H5'	2.00	0.44
4:E:6:LEU:HD23	4:E:6:LEU:HA	1.74	0.44
1:A:1489:C:H3'	1:A:1490:A:C8	2.53	0.44
1:A:1584:G:H1'	1:A:1585:U:OP2	2.18	0.44
1:A:2605:C:H2'	1:A:2606:G:C8	2.52	0.44
4:E:28:PRO:HA	4:E:112:SER:HB2	1.98	0.44
5:F:69:LYS:HA	5:F:84:PRO:HA	1.98	0.44
6:G:90:ILE:HG22	6:G:91:GLY:H	1.82	0.44
1:A:2299:C:OP2	24:3:2:ARG:NH1	2.50	0.44
3:D:6:LEU:HD11	3:D:81:LYS:HB2	2.00	0.44
8:L:61:VAL:HG21	8:L:111:PHE:CE2	2.53	0.44
1:A:1240:A:H2'	1:A:1241:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:U:O2'	2:B:74:G:H8	2.00	0.44
3:D:33:ASN:N	3:D:33:ASN:HD22	2.16	0.44
5:F:14:PRO:O	5:F:17:VAL:HG12	2.18	0.44
1:A:283:G:N2	1:A:288:C:O2	2.37	0.44
2:B:27:A:H2'	2:B:28:C:C6	2.53	0.44
3:D:31:THR:HG22	3:D:184:ASN:HD22	1.83	0.44
6:G:45:ILE:HG22	6:G:46:GLU:H	1.82	0.44
1:A:162:A:N6	1:A:166:C:OP2	2.47	0.44
1:A:339:G:H2'	1:A:340:A:C8	2.53	0.44
1:A:516:G:N1	1:A:519:A:OP2	2.51	0.44
1:A:1823:A:H2'	1:A:1824:A:C8	2.52	0.44
1:A:2393:G:H2'	1:A:2394:U:C6	2.53	0.44
5:F:119:LYS:HB3	5:F:167:ARG:HH21	1.83	0.43
10:N:133:LYS:H	10:N:133:LYS:HG3	1.73	0.43
1:A:276:C:C2'	1:A:277:C:H5'	2.49	0.43
1:A:1068:A:N6	1:A:1165:G:H2'	2.32	0.43
5:F:102:LYS:O	5:F:107:SER:OG	2.24	0.43
6:G:7:LYS:HE3	6:G:7:LYS:HB2	1.85	0.43
13:Q:92:VAL:HG11	13:Q:97:LEU:HD21	2.01	0.43
18:V:1:MET:O	18:V:2:PHE:HD1	2.01	0.43
1:A:519:A:HO2'	1:A:521:G:H8	1.66	0.43
1:A:1393:C:H2'	1:A:1394:G:O4'	2.17	0.43
2:B:46:A:P	12:P:35:ARG:HH22	2.41	0.43
7:K:2:ARG:HD2	7:K:3:THR:HG23	1.99	0.43
1:A:499:U:H5"	25:4:40:LYS:HD3	2.00	0.43
1:A:1035:C:O2	7:K:4:THR:HG23	2.19	0.43
1:A:2571:G:H2'	1:A:2572:C:C6	2.53	0.43
1:A:1088:A:N1	1:A:1152:G:O2'	2.47	0.43
1:A:1167:A:O2'	1:A:1168:A:H5"	2.19	0.43
10:N:30:GLY:O	10:N:134:ARG:NH1	2.51	0.43
1:A:872:G:H2'	1:A:873:C:C6	2.53	0.43
4:E:135:LYS:HE2	4:E:135:LYS:HB2	1.79	0.43
16:T:74:LEU:HD23	16:T:114:GLU:HA	2.01	0.43
2:B:10:G:OP2	19:X:80:ARG:NH1	2.52	0.43
3:D:4:GLY:HA2	3:D:202:ILE:O	2.19	0.43
4:E:200:THR:O	4:E:204:GLU:HG3	2.19	0.43
6:G:149:ARG:O	6:G:149:ARG:HG2	2.18	0.43
9:M:73:ASP:OD1	9:M:73:ASP:N	2.51	0.43
3:D:107:VAL:HA	3:D:174:LEU:O	2.18	0.43
13:Q:43:PHE:HE2	13:Q:61:VAL:HB	1.84	0.43
1:A:1525:U:O2	1:A:1552:A:N6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1725:A:H2'	1:A:1726:C:C6	2.53	0.43
2:B:1:U:O2	2:B:115:G:N2	2.39	0.43
3:D:111:THR:HG22	3:D:170:THR:HB	2.01	0.43
16:T:29:ILE:HD11	16:T:41:LEU:HG	1.99	0.43
17:U:29:VAL:HG21	17:U:38:VAL:CG2	2.47	0.43
1:A:345:G:H2'	1:A:346:A:C8	2.53	0.42
1:A:357:A:N3	4:E:169:ASN:ND2	2.66	0.42
1:A:854:C:H1'	1:A:1262:G:N2	2.34	0.42
1:A:2106:U:H4'	1:A:2107:G:H5"	2.00	0.42
1:A:2295:C:O2'	1:A:2296:G:H5'	2.19	0.42
1:A:2454:C:O2'	1:A:2455:C:O4'	2.37	0.42
3:D:123:ILE:HD13	3:D:130:ARG:HG3	2.01	0.42
3:D:159:ARG:HE	3:D:159:ARG:HB2	1.67	0.42
9:M:84:ARG:NH2	9:M:101:ILE:HD11	2.33	0.42
24:3:5:ILE:HG22	24:3:19:THR:HG23	2.01	0.42
26:5:54:ASP:O	26:5:58:ILE:HB	2.19	0.42
1:A:505:G:H2'	1:A:506:A:C8	2.54	0.42
1:A:1212:A:O2'	1:A:1213:U:H6	2.01	0.42
1:A:1216:G:N3	1:A:1216:G:H2'	2.34	0.42
5:F:15:SER:O	5:F:19:LYS:HG3	2.19	0.42
1:A:339:G:H2'	1:A:340:A:H8	1.85	0.42
1:A:1872:G:HO2'	1:A:1873:A:H8	1.65	0.42
1:A:2052:G:H2'	1:A:2053:G:O4'	2.19	0.42
1:A:2085:A:H2'	1:A:2086:G:H8	1.80	0.42
1:A:2855:A:H2'	1:A:2856:A:H8	1.84	0.42
5:F:74:ILE:O	5:F:79:LEU:HB2	2.18	0.42
17:U:2:GLU:CD	17:U:2:GLU:N	2.72	0.42
1:A:1447:U:N3	1:A:1448:U:C4	2.87	0.42
1:A:1489:C:H2'	1:A:1490:A:C8	2.54	0.42
1:A:1755:C:H2'	1:A:1756:U:H4'	2.01	0.42
1:A:2079:C:H2'	1:A:2080:C:H6	1.84	0.42
1:A:2099:U:H2'	1:A:2100:U:C6	2.54	0.42
12:P:67:THR:O	12:P:67:THR:OG1	2.32	0.42
14:R:119:LYS:HA	14:R:119:LYS:HD3	1.85	0.42
23:2:15:LYS:O	23:2:18:THR:HG23	2.19	0.42
1:A:1093:U:H2'	1:A:1094:A:O4'	2.20	0.42
1:A:1172:U:H5'	7:K:85:LEU:HD11	2.01	0.42
1:A:2317:G:O2'	5:F:121:ALA:HA	2.19	0.42
2:B:50:A:N6	12:P:38:LYS:HG2	2.35	0.42
2:B:97:A:HO2'	2:B:98:G:P	2.37	0.42
24:3:19:THR:OG1	24:3:20:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:A:H2'	1:A:132:A:C8	2.55	0.42
1:A:572:G:H2'	1:A:573:U:C6	2.54	0.42
1:A:672:A:H5"	1:A:673:G:OP2	2.19	0.42
1:A:1757:U:H2'	1:A:1758:C:C2	2.54	0.42
8:L:66:LYS:HE3	8:L:66:LYS:HB3	1.91	0.42
19:X:75:VAL:O	19:X:90:VAL:HA	2.20	0.42
20:Y:40:ILE:HD11	20:Y:45:LYS:HB2	2.01	0.42
1:A:156:U:H2'	1:A:157:C:C6	2.54	0.42
1:A:987:A:H2'	1:A:988:C:C6	2.54	0.42
1:A:1409:A:H5'	1:A:2226:A:O4'	2.20	0.42
1:A:2219:A:H2'	1:A:2220:C:H6	1.83	0.42
2:B:89:C:P	10:N:99:ARG:HH22	2.42	0.42
3:D:2:THR:OG1	3:D:204:SER:OG	2.37	0.42
4:E:2:PRO:HD2	4:E:19:LEU:O	2.20	0.42
4:E:59:GLY:HA2	4:E:79:ARG:HH11	1.84	0.42
10:N:64:VAL:HG22	10:N:106:ILE:HG12	2.02	0.42
14:R:48:ARG:HE	14:R:48:ARG:HB3	1.66	0.42
1:A:2319:U:N3	5:F:151:GLY:O	2.44	0.42
3:D:16:PHE:CE1	3:D:22:LEU:HG	2.55	0.42
10:N:66:ILE:HG12	10:N:104:PHE:CE1	2.55	0.42
1:A:454:C:H2'	1:A:455:A:H8	1.85	0.42
1:A:1699:C:H2'	1:A:1700:U:H6	1.85	0.42
8:L:91:LYS:HB3	8:L:111:PHE:CD2	2.55	0.42
12:P:57:SER:HB2	12:P:60:ASP:HB2	2.00	0.42
18:V:81:VAL:HG13	18:V:92:ARG:HB3	2.01	0.42
1:A:288:C:H1'	1:A:289:U:H5	1.85	0.42
1:A:1394:G:N1	1:A:1407:G:N7	2.68	0.42
1:A:2911:C:H6	1:A:2911:C:O5'	2.02	0.42
2:B:70:G:N3	2:B:70:G:O4'	2.52	0.42
2:B:72:U:H2'	2:B:73:U:H5'	2.02	0.42
11:O:18:ARG:HD3	11:O:65:PHE:HA	2.01	0.42
1:A:2429:G:H2'	1:A:2430:C:C6	2.55	0.41
1:A:312:U:O5'	1:A:312:U:H6	2.02	0.41
1:A:697:U:H2'	1:A:698:A:H8	1.85	0.41
1:A:1323:A:C8	11:O:113:ARG:HD3	2.51	0.41
1:A:1355:G:O2'	1:A:1356:G:H5'	2.20	0.41
1:A:1461:A:N3	1:A:1461:A:H2'	2.36	0.41
1:A:1808:U:H2'	1:A:1809:C:C6	2.55	0.41
1:A:2453:A:H4'	1:A:2454:C:C3'	2.47	0.41
5:F:32:ASP:OD2	12:P:2:ILE:HD12	2.21	0.41
7:K:76:TYR:CE1	7:K:87:SER:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:C:HO2'	1:A:127:A:HO2'	1.59	0.41
1:A:154:U:O2'	1:A:155:U:H5'	2.20	0.41
1:A:1181:U:H4'	1:A:1182:A:O4'	2.20	0.41
1:A:2088:U:H2'	1:A:2089:U:C6	2.55	0.41
1:A:2420:C:C4	9:M:69:ILE:HD12	2.55	0.41
4:E:158:ASN:HB3	4:E:159:GLY:H	1.74	0.41
5:F:104:VAL:CG2	5:F:175:MET:H	2.33	0.41
6:G:18:LYS:HB2	6:G:25:THR:CG2	2.50	0.41
14:R:88:ILE:HD11	14:R:112:GLN:OE1	2.20	0.41
1:A:911:U:H5"	10:N:6:ARG:O	2.20	0.41
1:A:2419:G:O2'	1:A:2420:C:OP2	2.34	0.41
2:B:50:A:N1	12:P:38:LYS:HE2	2.35	0.41
4:E:157:GLU:H	4:E:157:GLU:HG3	1.56	0.41
5:F:163:ASP:O	5:F:167:ARG:HG3	2.21	0.41
6:G:107:VAL:O	6:G:109:TYR:N	2.54	0.41
12:P:63:ILE:HD11	12:P:78:LEU:HD12	2.01	0.41
14:R:70:ARG:HA	14:R:74:LEU:O	2.20	0.41
1:A:11:A:H2'	1:A:12:A:H8	1.86	0.41
1:A:1489:C:H3'	1:A:1490:A:H8	1.85	0.41
3:D:88:LEU:O	3:D:89:GLY:C	2.59	0.41
6:G:73:ASN:O	6:G:77:VAL:HG23	2.21	0.41
6:G:101:ASN:O	6:G:116:THR:HA	2.20	0.41
1:A:591:U:H2'	1:A:592:G:O4'	2.21	0.41
1:A:1492:G:H22	1:A:1504:G:N2	2.19	0.41
2:B:113:A:H2'	2:B:114:C:C6	2.55	0.41
4:E:40:GLN:OE1	4:E:184:LEU:HB2	2.20	0.41
10:N:32:TRP:CZ2	10:N:111:GLU:HG2	2.54	0.41
18:V:81:VAL:CG1	18:V:92:ARG:HB3	2.50	0.41
22:0:5:LYS:HB3	22:0:5:LYS:HE3	1.86	0.41
1:A:441:A:H2'	1:A:442:A:C8	2.56	0.41
1:A:853:U:H2'	1:A:854:C:H6	1.82	0.41
1:A:1518:U:O2'	1:A:1519:G:C8	2.73	0.41
1:A:1600:C:H6	1:A:1600:C:H2'	1.57	0.41
1:A:1699:C:H2'	1:A:1700:U:C6	2.56	0.41
5:F:40:VAL:HG22	5:F:150:ARG:NH1	2.35	0.41
5:F:164:GLU:HA	5:F:167:ARG:CG	2.50	0.41
10:N:63:LYS:HD2	10:N:65:TRP:CZ2	2.56	0.41
17:U:23:LYS:HZ3	17:U:84:GLU:HA	1.84	0.41
1:A:84:G:N2	1:A:103:A:H2	2.10	0.41
1:A:91:A:OP1	1:A:91:A:H8	2.04	0.41
6:G:163:ARG:HG3	6:G:164:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:15:LYS:O	7:K:53:ASP:HB3	2.20	0.41
9:M:130:LYS:HB2	9:M:130:LYS:HE2	1.88	0.41
27:6:11:CYS:SG	27:6:12:GLU:N	2.94	0.41
1:A:234:C:O2'	1:A:235:G:N3	2.46	0.41
1:A:716:A:H2	1:A:842:A:H61	1.69	0.41
1:A:1237:U:H2'	1:A:1238:C:C6	2.55	0.41
1:A:1518:U:O2'	1:A:1519:G:OP2	2.30	0.41
1:A:1538:A:H5"	1:A:1539:U:OP1	2.20	0.41
1:A:2379:G:N7	26:5:39:LYS:NZ	2.68	0.41
1:A:2575:A:O2'	8:L:23:LYS:HG3	2.20	0.41
1:A:2806:U:H2'	1:A:2807:U:C6	2.56	0.41
1:A:2809:U:O2	1:A:2809:U:H2'	2.20	0.41
3:D:5:ILE:HD11	3:D:101:VAL:HB	2.02	0.41
4:E:196:GLN:O	4:E:200:THR:HG23	2.21	0.41
9:M:27:ASN:O	9:M:31:ALA:HA	2.21	0.41
11:O:113:ARG:HD2	11:O:116:ASP:HB2	2.02	0.41
11:O:116:ASP:HB3	11:O:118:ALA:H	1.85	0.41
20:Y:6:TYR:CD2	20:Y:47:VAL:HG21	2.55	0.41
20:Y:19:SER:O	20:Y:19:SER:OG	2.33	0.41
1:A:807:U:O2'	1:A:808:G:OP2	2.38	0.41
1:A:2300:A:H4'	1:A:2301:A:O4'	2.20	0.41
2:B:23:A:H2'	2:B:24:U:C6	2.56	0.41
2:B:32:U:HO2'	2:B:33:U:P	2.44	0.41
1:A:176:U:H2'	1:A:177:A:C8	2.57	0.40
1:A:297:G:H5"	1:A:305:A:OP1	2.21	0.40
1:A:1824:A:H8	1:A:1824:A:O5'	2.04	0.40
1:A:1969:U:C4	1:A:2566:U:H1'	2.57	0.40
1:A:2318:G:O2'	5:F:153:ASP:OD1	2.33	0.40
1:A:53:A:H2'	1:A:54:A:C8	2.56	0.40
1:A:713:C:H4'	4:E:82:GLN:HE22	1.85	0.40
1:A:1631:A:N9	1:A:1632:A:H2	2.19	0.40
8:L:64:ARG:O	8:L:82:ASN:HA	2.21	0.40
11:O:4:ARG:HB2	11:O:39:GLU:OE2	2.21	0.40
1:A:288:C:H1'	1:A:289:U:C5	2.56	0.40
1:A:887:G:H5"	1:A:888:A:OP1	2.22	0.40
1:A:1213:U:H2'	1:A:1214:U:O4'	2.21	0.40
1:A:1492:G:N2	1:A:1504:G:N2	2.69	0.40
2:B:110:G:H2'	2:B:111:C:H6	1.87	0.40
8:L:63:VAL:HG22	8:L:106:LEU:HD11	2.03	0.40
8:L:105:GLU:H	8:L:105:GLU:HG2	1.64	0.40
1:A:897:G:H2'	1:A:898:A:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1960:U:H2'	1:A:1961:C:H6	1.86	0.40
1:A:2454:C:H6	1:A:2454:C:H2'	1.70	0.40
4:E:158:ASN:C	4:E:160:ASN:H	2.23	0.40
6:G:78:GLY:HA2	6:G:82:GLY:H	1.87	0.40
9:M:87:ASP:OD1	9:M:119:LYS:HA	2.22	0.40
13:Q:72:ARG:HD3	13:Q:74:PHE:CZ	2.57	0.40
1:A:573:U:H2'	1:A:574:C:C6	2.56	0.40
5:F:30:LYS:O	5:F:158:THR:HB	2.22	0.40
13:Q:82:ALA:O	13:Q:83:GLN:HG2	2.21	0.40
17:U:23:LYS:HE2	17:U:85:ASP:H	1.87	0.40
26:5:14:VAL:HG13	26:5:22:LEU:HD22	2.03	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	
3	D	205/207 (99%)	188 (92%)	16 (8%)	1 (0%)	29	61
4	E	204/206 (99%)	181 (89%)	21 (10%)	2 (1%)	15	45
5	F	175/177 (99%)	148 (85%)	27 (15%)	0	100	100
6	G	174/176 (99%)	145 (83%)	27 (16%)	2 (1%)	14	42
7	K	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
8	L	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	19	51
9	M	144/146 (99%)	118 (82%)	25 (17%)	1 (1%)	22	54
10	N	139/141 (99%)	119 (86%)	20 (14%)	0	100	100
11	O	122/124 (98%)	102 (84%)	20 (16%)	0	100	100
12	P	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
13	Q	112/114 (98%)	104 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
15	S	100/102 (98%)	91 (91%)	8 (8%)	1 (1%)	15 45
16	T	110/112 (98%)	103 (94%)	7 (6%)	0	100 100
17	U	87/89 (98%)	73 (84%)	14 (16%)	0	100 100
18	V	99/101 (98%)	81 (82%)	18 (18%)	0	100 100
19	X	74/76 (97%)	70 (95%)	4 (5%)	0	100 100
20	Y	52/54 (96%)	43 (83%)	8 (15%)	1 (2%)	8 28
21	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100 100
22	0	56/58 (97%)	54 (96%)	2 (4%)	0	100 100
23	2	54/56 (96%)	46 (85%)	8 (15%)	0	100 100
24	3	47/49 (96%)	43 (92%)	4 (8%)	0	100 100
25	4	42/44 (96%)	42 (100%)	0	0	100 100
26	5	62/64 (97%)	59 (95%)	3 (5%)	0	100 100
27	6	36/38 (95%)	32 (89%)	4 (11%)	0	100 100
All	All	2647/2697 (98%)	2354 (89%)	284 (11%)	9 (0%)	44 71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	90	GLU
9	M	16	ARG
4	E	13	GLN
8	L	25	LEU
20	Y	20	HIS
6	G	47	GLY
4	E	159	GLY
6	G	108	GLY
15	S	51	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
3	D	170/170 (100%)	140 (82%)	30 (18%)	2 5
4	E	172/172 (100%)	144 (84%)	28 (16%)	2 7
5	F	154/154 (100%)	129 (84%)	25 (16%)	2 7
6	G	146/146 (100%)	123 (84%)	23 (16%)	2 8
7	K	122/122 (100%)	105 (86%)	17 (14%)	3 10
8	L	98/98 (100%)	87 (89%)	11 (11%)	6 18
9	M	112/112 (100%)	102 (91%)	10 (9%)	9 29
10	N	112/112 (100%)	98 (88%)	14 (12%)	4 14
11	O	106/106 (100%)	92 (87%)	14 (13%)	4 12
12	P	91/91 (100%)	79 (87%)	12 (13%)	4 12
13	Q	97/97 (100%)	83 (86%)	14 (14%)	3 9
14	R	94/94 (100%)	87 (93%)	7 (7%)	13 38
15	S	83/83 (100%)	73 (88%)	10 (12%)	5 15
16	T	95/95 (100%)	82 (86%)	13 (14%)	3 11
17	U	80/80 (100%)	66 (82%)	14 (18%)	2 6
18	V	85/85 (100%)	71 (84%)	14 (16%)	2 7
19	X	61/61 (100%)	48 (79%)	13 (21%)	1 3
20	Y	47/47 (100%)	38 (81%)	9 (19%)	1 4
21	Z	55/55 (100%)	45 (82%)	10 (18%)	1 5
22	0	49/49 (100%)	44 (90%)	5 (10%)	7 22
23	2	46/46 (100%)	39 (85%)	7 (15%)	3 8
24	3	49/49 (100%)	46 (94%)	3 (6%)	18 48
25	4	39/39 (100%)	34 (87%)	5 (13%)	4 13
26	5	51/51 (100%)	44 (86%)	7 (14%)	3 11
27	6	35/35 (100%)	30 (86%)	5 (14%)	3 10
All	All	2249/2249 (100%)	1929 (86%)	320 (14%)	6 10

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	15	ILE
3	D	21	GLU
3	D	22	LEU
3	D	23	ILE

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Mol	Chain	Res	Type
3	D	25	VAL
3	D	43	THR
3	D	49	ILE
3	D	50	GLN
3	D	58	GLU
3	D	59	VAL
3	D	62	ASN
3	D	69	VAL
3	D	71	LYS
3	D	81	LYS
3	D	86	VAL
3	D	90	GLU
3	D	103	GLN
3	D	107	VAL
3	D	108	VAL
3	D	111	THR
3	D	119	PHE
3	D	141	ARG
3	D	145	SER
3	D	158	LYS
3	D	167	ASP
3	D	168	ARG
3	D	170	THR
3	D	191	ASN
3	D	199	LEU
3	D	201	THR
4	E	6	LEU
4	E	8	LYS
4	E	18	THR
4	E	20	ASN
4	E	31	SER
4	E	49	HIS
4	E	65	TRP
4	E	77	SER
4	E	79	ARG
4	E	80	SER
4	E	82	GLN
4	E	89	VAL
4	E	93	THR
4	E	94	PRO
4	E	105	VAL
4	E	113	VAL

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Mol	Chain	Res	Type
4	E	153	LEU
4	E	157	GLU
4	E	160	ASN
4	E	165	LEU
4	E	168	ARG
4	E	176	VAL
4	E	184	LEU
4	E	190	ASN
4	E	193	LEU
4	E	195	THR
4	E	200	THR
4	E	205	VAL
5	F	6	GLU
5	F	15	SER
5	F	17	VAL
5	F	27	GLN
5	F	32	ASP
5	F	57	LEU
5	F	61	THR
5	F	66	LEU
5	F	77	PHE
5	F	81	GLU
5	F	88	LYS
5	F	89	VAL
5	F	110	ARG
5	F	112	ARG
5	F	114	PHE
5	F	127	ASN
5	F	130	LEU
5	F	133	LYS
5	F	137	ILE
5	F	142	ASP
5	F	143	TYR
5	F	149	VAL
5	F	152	MET
5	F	162	THR
5	F	170	LEU
6	G	8	VAL
6	G	11	LEU
6	G	25	THR
6	G	32	GLU
6	G	35	ARG

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Mol	Chain	Res	Type
6	G	44	ASN
6	G	45	ILE
6	G	46	GLU
6	G	63	THR
6	G	67	THR
6	G	79	VAL
6	G	84	GLN
6	G	95	ARG
6	G	101	ASN
6	G	103	LEU
6	G	107	VAL
6	G	121	VAL
6	G	122	THR
6	G	136	ILE
6	G	143	GLU
6	G	152	ARG
6	G	165	VAL
6	G	171	ARG
7	K	2	ARG
7	K	14	ARG
7	K	26	LEU
7	K	30	SER
7	K	46	THR
7	K	58	ILE
7	K	77	ARG
7	K	80	MET
7	K	85	LEU
7	K	100	ARG
7	K	101	LEU
7	K	113	ASN
7	K	114	THR
7	K	115	LEU
7	K	118	LYS
7	K	123	LEU
7	K	145	ASN
8	L	1	MET
8	L	5	GLU
8	L	13	ASN
8	L	18	GLU
8	L	19	ILE
8	L	21	THR
8	L	42	THR

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Mol	Chain	Res	Type
8	L	53	LYS
8	L	73	ASP
8	L	90	ASP
8	L	105	GLU
9	M	3	LEU
9	M	16	ARG
9	M	42	SER
9	M	60	ARG
9	M	76	VAL
9	M	81	THR
9	M	84	ARG
9	M	87	ASP
9	M	122	THR
9	M	131	SER
10	N	5	LYS
10	N	10	ARG
10	N	11	ARG
10	N	25	LYS
10	N	26	GLU
10	N	34	LEU
10	N	37	THR
10	N	74	TYR
10	N	76	SER
10	N	85	LYS
10	N	103	MET
10	N	109	VAL
10	N	127	VAL
10	N	133	LYS
11	O	3	TYR
11	O	8	ARG
11	O	24	LEU
11	O	41	ARG
11	O	49	THR
11	O	55	ASP
11	O	56	LEU
11	O	84	SER
11	O	89	LEU
11	O	100	ARG
11	O	106	ARG
11	O	108	LEU
11	O	124	GLU
11	O	125	PHE

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Mol	Chain	Res	Type
12	P	2	ILE
12	P	6	ASP
12	P	11	ARG
12	P	28	CYS
12	P	31	LEU
12	P	35	ARG
12	P	46	ASP
12	P	51	VAL
12	P	57	SER
12	P	67	THR
12	P	79	VAL
12	P	95	ARG
13	Q	2	ASN
13	Q	10	GLN
13	Q	11	GLU
13	Q	36	THR
13	Q	49	LYS
13	Q	55	ILE
13	Q	60	THR
13	Q	72	ARG
13	Q	76	LEU
13	Q	78	THR
13	Q	80	ARG
13	Q	101	ARG
13	Q	109	ARG
13	Q	114	ARG
14	R	10	THR
14	R	30	THR
14	R	51	ARG
14	R	60	LEU
14	R	79	LEU
14	R	89	ASP
14	R	92	ARG
15	S	1	MET
15	S	2	TYR
15	S	14	VAL
15	S	22	VAL
15	S	33	VAL
15	S	61	THR
15	S	73	THR
15	S	75	GLN
15	S	94	LYS

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Mol	Chain	Res	Type
15	S	101	ASN
16	T	4	GLN
16	T	9	LYS
16	T	11	THR
16	T	14	THR
16	T	26	ILE
16	T	29	ILE
16	T	70	ASP
16	T	88	LYS
16	T	89	ARG
16	T	93	ARG
16	T	105	THR
16	T	109	THR
16	T	115	LYS
17	U	2	GLU
17	U	3	LEU
17	U	14	GLU
17	U	16	SER
17	U	29	VAL
17	U	37	LEU
17	U	47	ASP
17	U	49	LYS
17	U	52	ASN
17	U	56	LEU
17	U	75	ARG
17	U	76	ARG
17	U	84	GLU
17	U	87	LYS
18	V	1	MET
18	V	2	PHE
18	V	5	LYS
18	V	9	VAL
18	V	13	THR
18	V	17	LYS
18	V	29	LYS
18	V	41	VAL
18	V	58	GLU
18	V	59	VAL
18	V	68	VAL
18	V	69	MET
18	V	94	SER
18	V	99	GLU

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Mol	Chain	Res	Type
19	X	18	SER
19	X	19	THR
19	X	20	SER
19	X	23	ARG
19	X	24	ASP
19	X	28	LYS
19	X	39	THR
19	X	40	VAL
19	X	62	ILE
19	X	67	THR
19	X	73	ASP
19	X	88	VAL
19	X	93	VAL
20	Y	12	THR
20	Y	22	MET
20	Y	24	SER
20	Y	27	ARG
20	Y	28	THR
20	Y	32	ASN
20	Y	34	GLN
20	Y	36	VAL
20	Y	40	ILE
21	Z	2	LYS
21	Z	3	VAL
21	Z	4	LYS
21	Z	5	GLU
21	Z	10	THR
21	Z	15	LEU
21	Z	32	LEU
21	Z	37	LEU
21	Z	38	GLU
21	Z	55	THR
22	0	8	LEU
22	0	16	PRO
22	0	35	VAL
22	0	55	ASP
22	0	59	VAL
23	2	3	VAL
23	2	7	ARG
23	2	8	THR
23	2	18	THR
23	2	23	THR

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Mol	Chain	Res	Type
23	2	32	ASN
23	2	56	SER
24	3	8	GLU
24	3	10	THR
24	3	44	LEU
25	4	10	ARG
25	4	20	LYS
25	4	24	THR
25	4	34	ARG
25	4	43	SER
26	5	31	HIS
26	5	32	ARG
26	5	41	ARG
26	5	46	LYS
26	5	57	ARG
26	5	58	ILE
26	5	65	MET
27	6	4	ARG
27	6	11	CYS
27	6	15	LYS
27	6	26	ILE
27	6	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	37	GLN
3	D	62	ASN
3	D	68	HIS
4	E	13	GLN
4	E	14	ASN
4	E	49	HIS
4	E	75	GLN
4	E	82	GLN
4	E	141	GLN
4	E	196	GLN
5	F	37	ASN
5	F	49	ASN
7	K	48	HIS
7	K	59	ASN
7	K	113	ASN
7	K	131	HIS

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Mol	Chain	Res	Type
9	M	4	HIS
9	M	38	GLN
9	M	54	GLN
9	M	133	GLN
12	P	12	GLN
12	P	15	HIS
12	P	20	ASN
12	P	114	ASN
13	Q	41	GLN
14	R	101	ASN
15	S	18	GLN
15	S	83	HIS
15	S	86	GLN
15	S	88	HIS
16	T	4	GLN
16	T	46	ASN
16	T	65	ASN
19	X	49	GLN
20	Y	17	ASN
20	Y	23	ASN
20	Y	32	ASN
20	Y	34	GLN
21	Z	36	GLN
21	Z	48	GLN
22	0	40	ASN
23	2	40	HIS
25	4	8	ASN
26	5	4	GLN
26	5	31	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2733/2908 (93%)	536 (19%)	24 (0%)
2	B	115/116 (99%)	32 (27%)	3 (2%)
All	All	2848/3024 (94%)	568 (19%)	27 (0%)

All (568) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	U

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Mol	Chain	Res	Type
1	A	14	A
1	A	28	G
1	A	35	U
1	A	42	A
1	A	52	G
1	A	68	A
1	A	71	G
1	A	72	A
1	A	75	U
1	A	76	G
1	A	92	A
1	A	93	G
1	A	97	G
1	A	102	G
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	131	A
1	A	148	A
1	A	155	U
1	A	156	U
1	A	158	A
1	A	165	A
1	A	166	C
1	A	168	U
1	A	169	A
1	A	177	A
1	A	180	G
1	A	182	U
1	A	185	A
1	A	199	A
1	A	202	A
1	A	218	G
1	A	219	A
1	A	220	A
1	A	225	A
1	A	231	A
1	A	232	U
1	A	233	U
1	A	235	G
1	A	236	A

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Mol	Chain	Res	Type
1	A	251	G
1	A	255	G
1	A	265	A
1	A	268	A
1	A	277	C
1	A	279	A
1	A	284	C
1	A	285	U
1	A	286	U
1	A	287	G
1	A	288	C
1	A	289	U
1	A	296	G
1	A	297	G
1	A	298	U
1	A	300	G
1	A	302	A
1	A	309	C
1	A	313	A
1	A	315	G
1	A	316	G
1	A	318	A
1	A	321	C
1	A	322	U
1	A	325	U
1	A	327	G
1	A	332	G
1	A	347	A
1	A	352	C
1	A	367	A
1	A	383	A
1	A	392	A
1	A	393	A
1	A	396	C
1	A	399	A
1	A	404	G
1	A	420	G
1	A	426	G
1	A	429	A
1	A	439	G
1	A	446	G
1	A	451	G

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Mol	Chain	Res	Type
1	A	452	A
1	A	491	U
1	A	496	C
1	A	507	G
1	A	517	A
1	A	520	A
1	A	521	G
1	A	524	C
1	A	542	A
1	A	543	U
1	A	544	A
1	A	547	U
1	A	548	C
1	A	551	G
1	A	560	U
1	A	561	G
1	A	569	C
1	A	570	A
1	A	571	A
1	A	572	G
1	A	577	A
1	A	581	C
1	A	586	A
1	A	587	U
1	A	588	G
1	A	596	G
1	A	600	G
1	A	609	A
1	A	610	G
1	A	611	A
1	A	612	A
1	A	613	U
1	A	614	G
1	A	624	G
1	A	631	U
1	A	640	A
1	A	652	A
1	A	654	A
1	A	655	G
1	A	656	A
1	A	660	A
1	A	673	G

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Mol	Chain	Res	Type
1	A	676	A
1	A	677	G
1	A	684	U
1	A	685	A
1	A	692	A
1	A	695	A
1	A	704	U
1	A	722	G
1	A	726	U
1	A	752	G
1	A	753	G
1	A	755	A
1	A	757	A
1	A	759	C
1	A	764	U
1	A	770	A
1	A	778	C
1	A	779	A
1	A	784	C
1	A	787	U
1	A	804	A
1	A	805	G
1	A	808	G
1	A	810	G
1	A	815	G
1	A	817	G
1	A	822	A
1	A	824	U
1	A	832	G
1	A	833	A
1	A	845	G
1	A	852	C
1	A	867	U
1	A	868	U
1	A	878	C
1	A	886	U
1	A	887	G
1	A	889	G
1	A	890	A
1	A	891	A
1	A	900	G
1	A	903	G

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Mol	Chain	Res	Type
1	A	905	G
1	A	909	U
1	A	910	G
1	A	917	C
1	A	919	A
1	A	920	G
1	A	947	G
1	A	948	A
1	A	950	A
1	A	951	A
1	A	956	C
1	A	958	A
1	A	965	U
1	A	966	U
1	A	967	C
1	A	981	A
1	A	985	A
1	A	986	G
1	A	990	G
1	A	992	G
1	A	993	A
1	A	999	A
1	A	1001	G
1	A	1014	A
1	A	1023	A
1	A	1029	G
1	A	1036	A
1	A	1045	C
1	A	1049	A
1	A	1052	U
1	A	1053	A
1	A	1057	G
1	A	1062	G
1	A	1066	A
1	A	1070	G
1	A	1073	U
1	A	1075	U
1	A	1086	A
1	A	1087	G
1	A	1088	A
1	A	1092	C
1	A	1093	U

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Mol	Chain	Res	Type
1	A	1149	C
1	A	1150	G
1	A	1151	A
1	A	1152	G
1	A	1167	A
1	A	1168	A
1	A	1170	U
1	A	1172	U
1	A	1173	A
1	A	1174	C
1	A	1175	C
1	A	1179	G
1	A	1182	A
1	A	1188	A
1	A	1209	A
1	A	1210	C
1	A	1212	A
1	A	1215	A
1	A	1217	G
1	A	1224	G
1	A	1257	A
1	A	1275	G
1	A	1284	A
1	A	1285	G
1	A	1287	G
1	A	1290	A
1	A	1293	G
1	A	1299	A
1	A	1305	A
1	A	1308	G
1	A	1309	A
1	A	1310	A
1	A	1317	G
1	A	1320	A
1	A	1336	U
1	A	1337	A
1	A	1350	C
1	A	1365	U
1	A	1373	G
1	A	1380	U
1	A	1388	U
1	A	1397	G

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Mol	Chain	Res	Type
1	A	1398	C
1	A	1399	C
1	A	1401	A
1	A	1404	G
1	A	1406	C
1	A	1409	A
1	A	1411	G
1	A	1415	U
1	A	1420	A
1	A	1428	G
1	A	1429	A
1	A	1431	A
1	A	1432	U
1	A	1446	G
1	A	1447	U
1	A	1452	G
1	A	1453	U
1	A	1454	U
1	A	1455	U
1	A	1456	G
1	A	1457	A
1	A	1460	A
1	A	1461	A
1	A	1462	U
1	A	1469	A
1	A	1470	C
1	A	1471	G
1	A	1475	U
1	A	1487	U
1	A	1489	C
1	A	1491	U
1	A	1492	G
1	A	1493	C
1	A	1494	G
1	A	1495	A
1	A	1497	U
1	A	1501	A
1	A	1502	G
1	A	1503	U
1	A	1504	G
1	A	1505	C
1	A	1510	C

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Mol	Chain	Res	Type
1	A	1519	G
1	A	1521	G
1	A	1525	U
1	A	1527	A
1	A	1528	G
1	A	1532	A
1	A	1535	U
1	A	1536	A
1	A	1539	U
1	A	1548	C
1	A	1551	U
1	A	1552	A
1	A	1559	A
1	A	1560	G
1	A	1567	C
1	A	1568	G
1	A	1573	G
1	A	1577	A
1	A	1578	A
1	A	1584	G
1	A	1585	U
1	A	1586	A
1	A	1591	A
1	A	1593	U
1	A	1601	G
1	A	1605	C
1	A	1606	A
1	A	1612	A
1	A	1615	A
1	A	1624	U
1	A	1629	A
1	A	1630	G
1	A	1631	A
1	A	1632	A
1	A	1634	A
1	A	1635	C
1	A	1637	A
1	A	1638	C
1	A	1651	A
1	A	1653	A
1	A	1674	G
1	A	1686	G

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Mol	Chain	Res	Type
1	A	1689	A
1	A	1690	G
1	A	1691	C
1	A	1717	G
1	A	1730	G
1	A	1734	C
1	A	1746	G
1	A	1756	U
1	A	1757	U
1	A	1758	C
1	A	1759	G
1	A	1762	C
1	A	1770	G
1	A	1777	G
1	A	1778	G
1	A	1787	A
1	A	1790	G
1	A	1796	C
1	A	1798	A
1	A	1814	C
1	A	1815	A
1	A	1824	A
1	A	1826	A
1	A	1830	A
1	A	1837	G
1	A	1843	A
1	A	1853	G
1	A	1856	G
1	A	1861	A
1	A	1862	A
1	A	1864	G
1	A	1874	U
1	A	1876	G
1	A	1877	G
1	A	1884	U
1	A	1886	G
1	A	1887	G
1	A	1890	A
1	A	1894	U
1	A	1896	A
1	A	1910	A
1	A	1920	G

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Mol	Chain	Res	Type
1	A	1927	A
1	A	1928	C
1	A	1930	A
1	A	1934	C
1	A	1936	G
1	A	1943	G
1	A	1944	G
1	A	1950	A
1	A	1969	U
1	A	1970	U
1	A	1977	C
1	A	1981	C
1	A	1984	A
1	A	1985	A
1	A	1986	G
1	A	1996	U
1	A	2001	G
1	A	2005	U
1	A	2007	U
1	A	2035	G
1	A	2037	A
1	A	2044	A
1	A	2045	A
1	A	2046	G
1	A	2047	A
1	A	2050	C
1	A	2057	C
1	A	2065	A
1	A	2069	C
1	A	2070	G
1	A	2074	A
1	A	2075	G
1	A	2076	A
1	A	2080	C
1	A	2083	G
1	A	2107	G
1	A	2109	G
1	A	2112	U
1	A	2113	U
1	A	2208	C
1	A	2211	U
1	A	2212	A

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Mol	Chain	Res	Type
1	A	2213	A
1	A	2216	C
1	A	2217	G
1	A	2218	C
1	A	2238	G
1	A	2239	A
1	A	2252	G
1	A	2253	G
1	A	2267	G
1	A	2277	C
1	A	2283	A
1	A	2293	G
1	A	2296	G
1	A	2297	C
1	A	2301	A
1	A	2302	A
1	A	2303	G
1	A	2317	G
1	A	2319	U
1	A	2323	A
1	A	2331	C
1	A	2333	A
1	A	2334	A
1	A	2335	G
1	A	2336	A
1	A	2339	G
1	A	2340	U
1	A	2343	A
1	A	2348	G
1	A	2349	A
1	A	2361	C
1	A	2364	C
1	A	2393	G
1	A	2397	G
1	A	2399	C
1	A	2402	A
1	A	2404	U
1	A	2405	G
1	A	2416	U
1	A	2417	C
1	A	2418	C
1	A	2420	C

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Mol	Chain	Res	Type
1	A	2436	C
1	A	2437	U
1	A	2439	A
1	A	2443	G
1	A	2445	U
1	A	2449	A
1	A	2455	C
1	A	2462	A
1	A	2473	A
1	A	2488	C
1	A	2492	A
1	A	2505	U
1	A	2512	C
1	A	2517	A
1	A	2518	U
1	A	2519	G
1	A	2521	C
1	A	2522	G
1	A	2532	A
1	A	2534	C
1	A	2542	U
1	A	2543	G
1	A	2548	C
1	A	2570	C
1	A	2580	A
1	A	2581	G
1	A	2587	C
1	A	2597	G
1	A	2599	U
1	A	2600	C
1	A	2616	A
1	A	2624	C
1	A	2627	U
1	A	2629	U
1	A	2650	U
1	A	2677	G
1	A	2699	G
1	A	2703	U
1	A	2719	A
1	A	2728	G
1	A	2740	U
1	A	2747	A

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Mol	Chain	Res	Type
1	A	2749	G
1	A	2758	G
1	A	2762	A
1	A	2766	C
1	A	2773	G
1	A	2779	A
1	A	2780	G
1	A	2789	A
1	A	2792	A
1	A	2793	U
1	A	2794	G
1	A	2795	A
1	A	2804	A
1	A	2805	U
1	A	2809	U
1	A	2810	U
1	A	2812	A
1	A	2813	A
1	A	2815	A
1	A	2831	G
1	A	2836	G
1	A	2844	A
1	A	2846	A
1	A	2847	U
1	A	2870	G
1	A	2871	A
1	A	2878	G
1	A	2883	G
1	A	2891	C
1	A	2897	G
1	A	2904	G
2	B	7	G
2	B	10	G
2	B	11	A
2	B	13	A
2	B	20	A
2	B	23	A
2	B	24	U
2	B	27	A
2	B	33	U
2	B	35	C
2	B	54	U

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Mol	Chain	Res	Type
2	B	55	A
2	B	57	G
2	B	67	G
2	B	70	G
2	B	73	U
2	B	74	G
2	B	75	U
2	B	78	U
2	B	79	G
2	B	83	G
2	B	85	U
2	B	86	U
2	B	87	U
2	B	91	U
2	B	97	A
2	B	98	G
2	B	99	A
2	B	101	U
2	B	106	C
2	B	107	G
2	B	114	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	13	U
1	A	179	A
1	A	519	A
1	A	655	G
1	A	725	A
1	A	890	A
1	A	947	G
1	A	949	U
1	A	1022	C
1	A	1167	A
1	A	1431	A
1	A	1486	A
1	A	1584	G
1	A	1585	U
1	A	1590	A
1	A	1600	C
1	A	1604	A

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Mol	Chain	Res	Type
1	A	1605	C
1	A	1861	A
1	A	2419	G
1	A	2444	A
1	A	2532	A
1	A	2811	U
1	A	2812	A
2	B	32	U
2	B	90	C
2	B	97	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
9	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	60:ARG	C	61:LEU	N	1.18

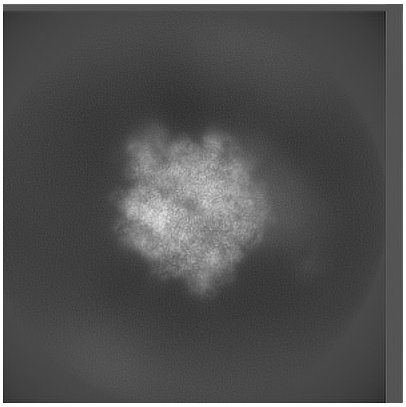
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21907. These allow visual inspection of the internal detail of the map and identification of artifacts.

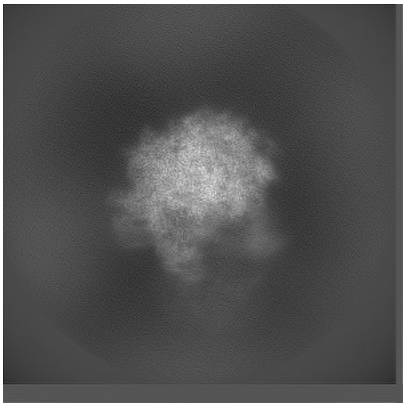
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

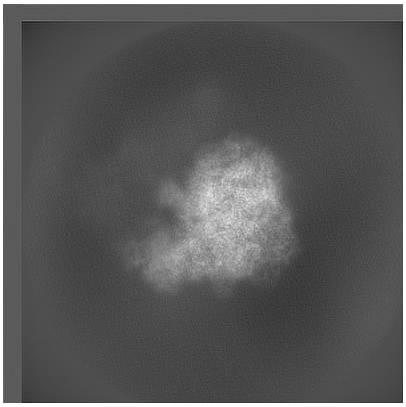
6.1.1 Primary map



X



Y

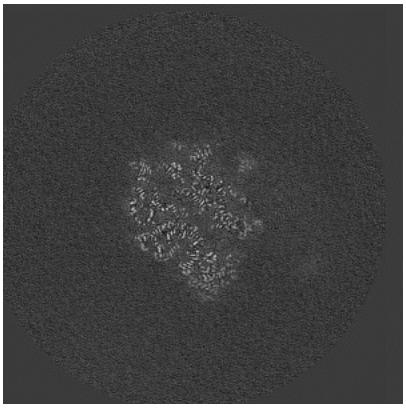


Z

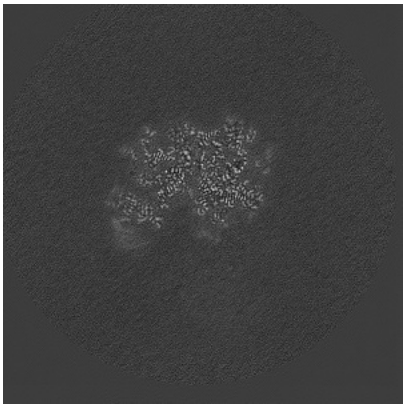
The images above show the map projected in three orthogonal directions.

6.2 Central slices

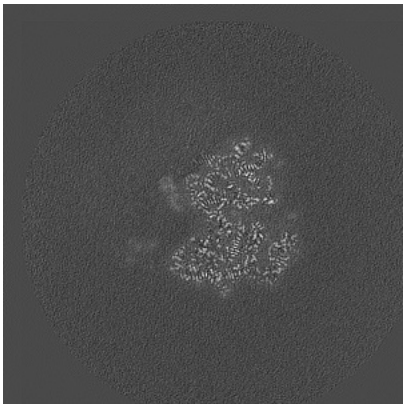
6.2.1 Primary map



X Index: 220



Y Index: 220

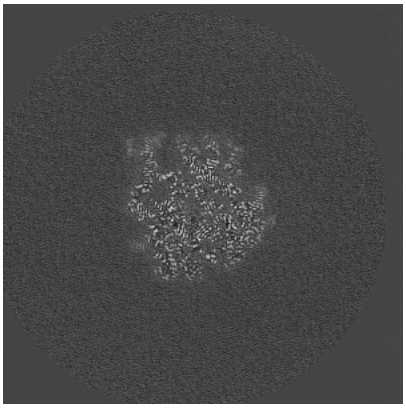


Z Index: 220

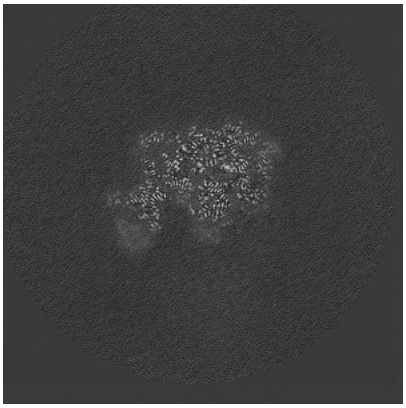
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

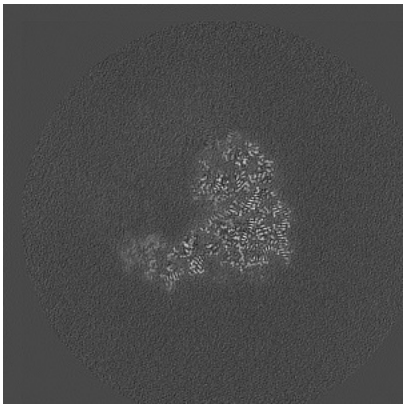
6.3.1 Primary map



X Index: 258



Y Index: 228

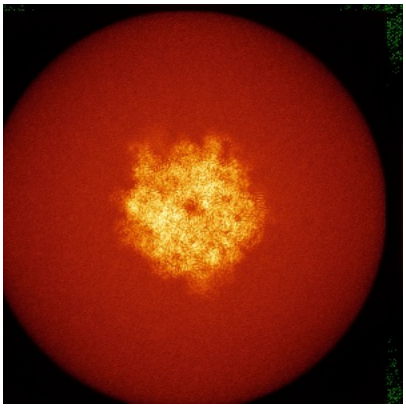


Z Index: 204

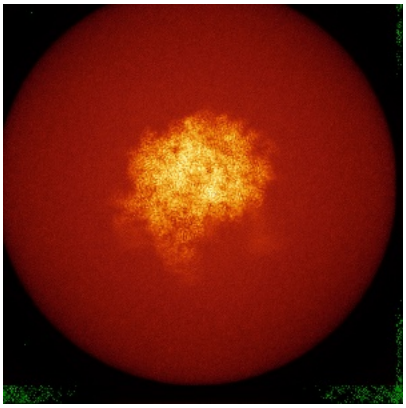
The images above show the largest variance slices of the map in three orthogonal directions.

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

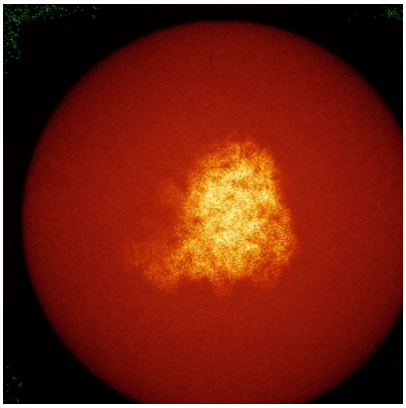
6.4.1 Primary map



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

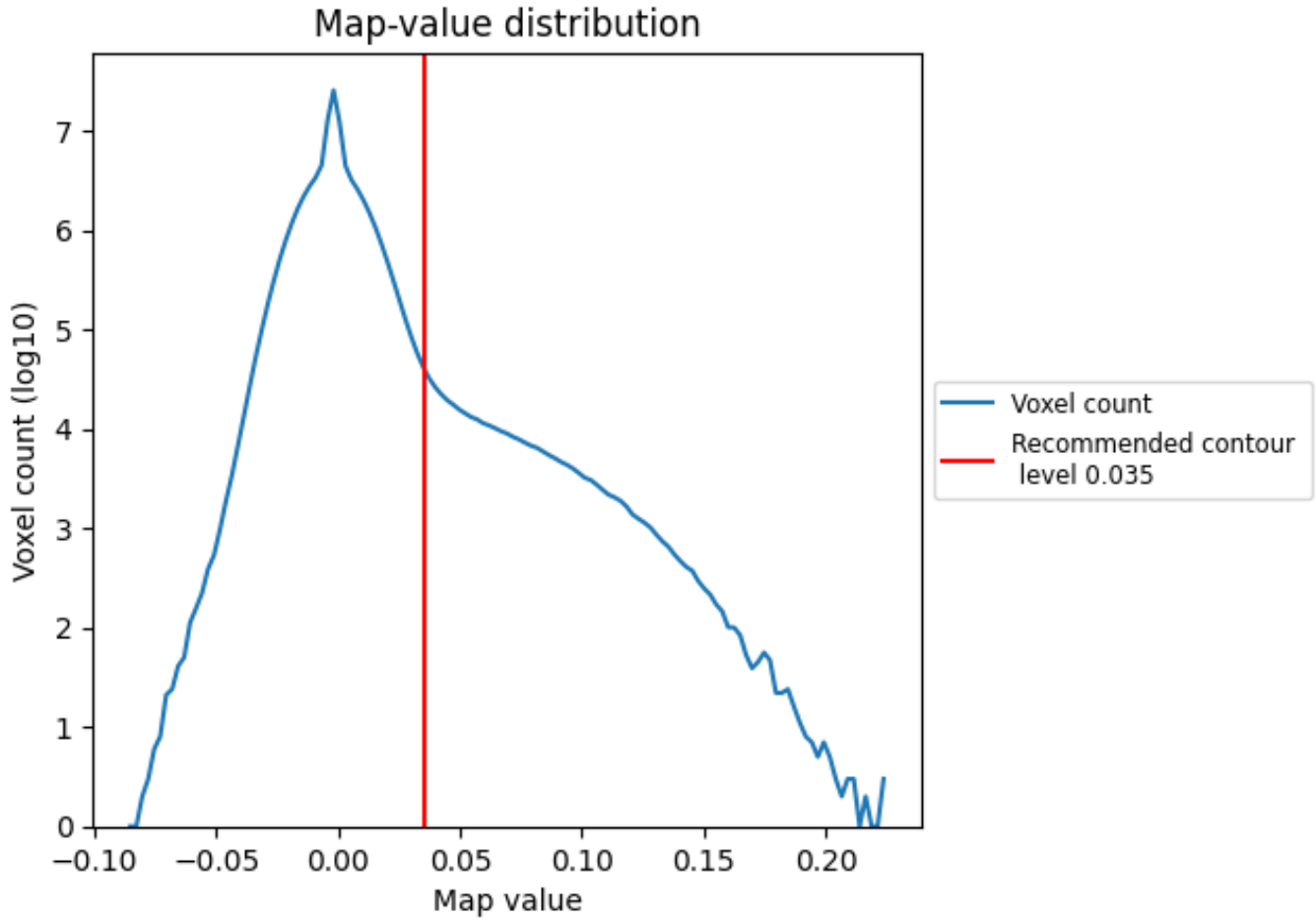
6.6 Mask visualisation (i)

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

7 Map analysis

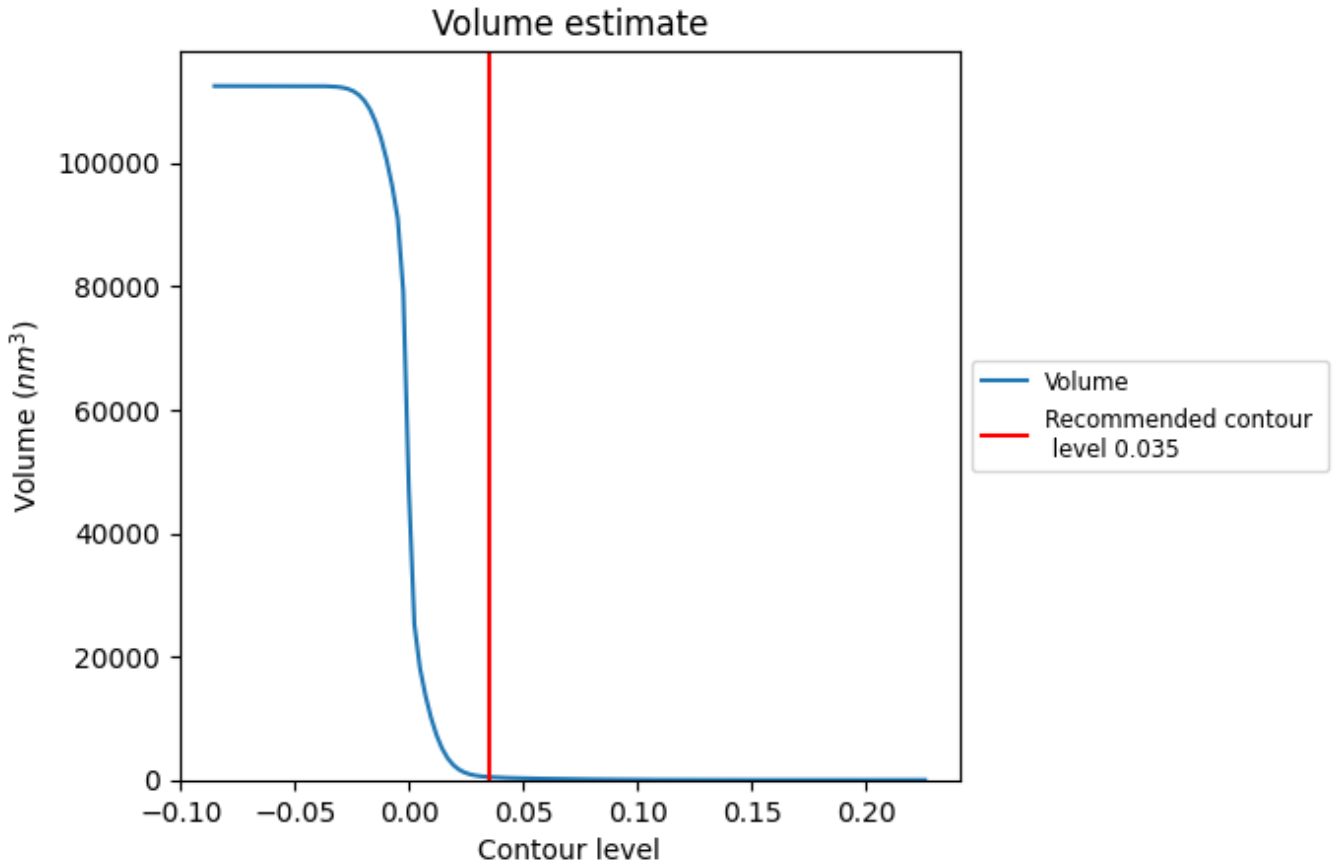
This section contains the results of statistical analysis of the map.

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.

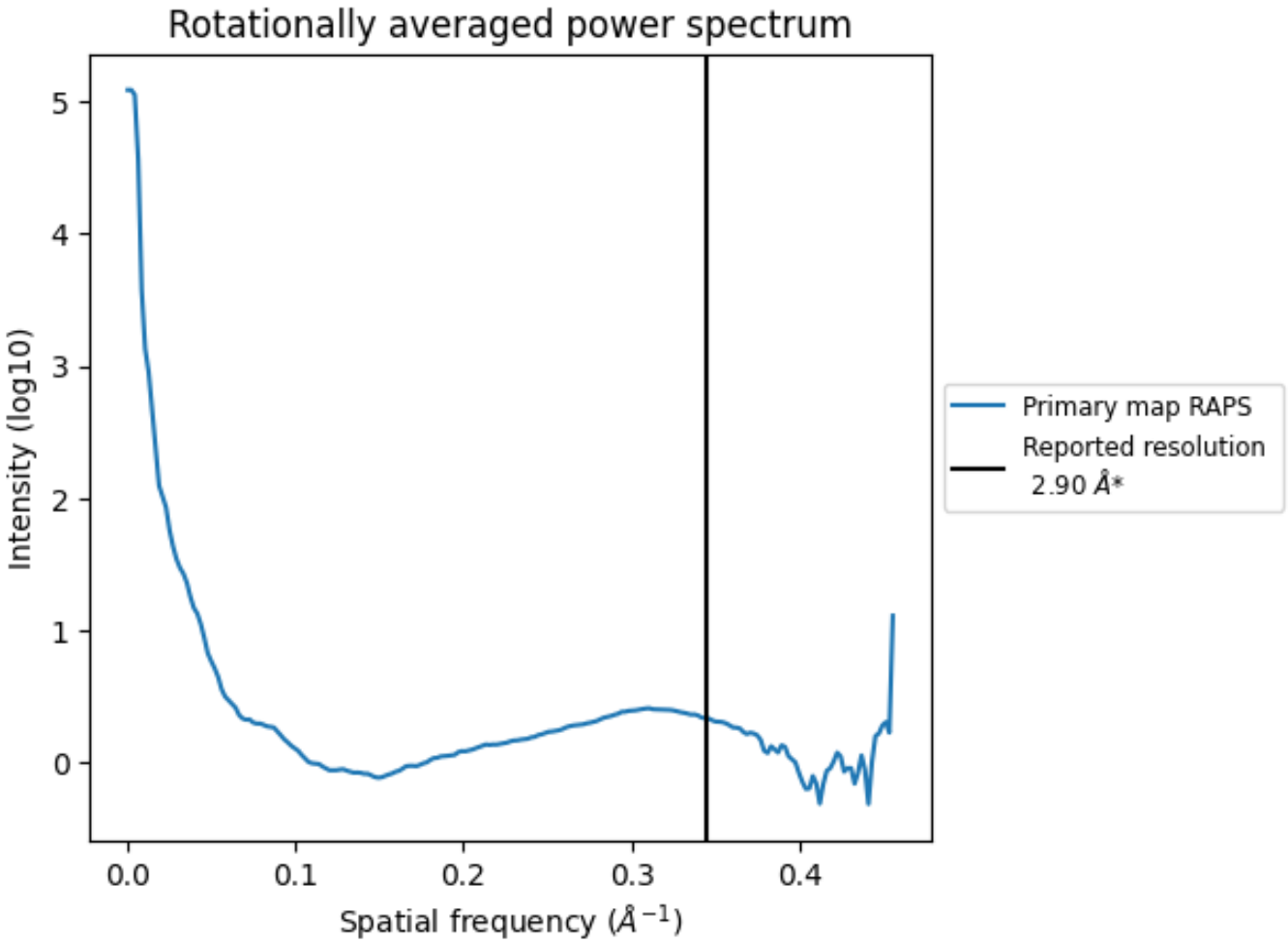
7.2 Volume estimate



The volume at the recommended contour level is 483 nm^3; this corresponds to an approximate mass of 437 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 0.345 $Å^{-1}$

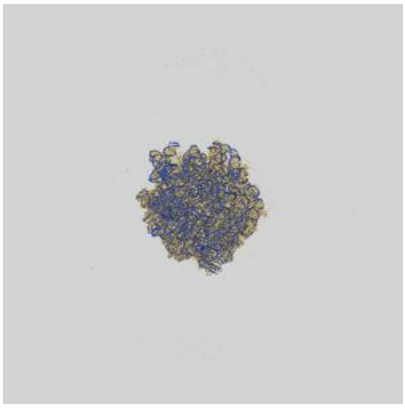
8 Fourier-Shell correlation (i)

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

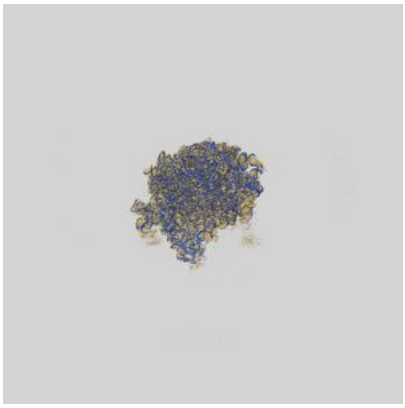
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21907 and PDB model 6WU9. Per-residue inclusion information can be found in section 3 on page 9.

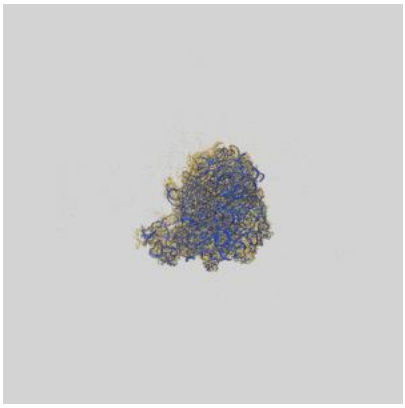
9.1 Map-model overlay



X



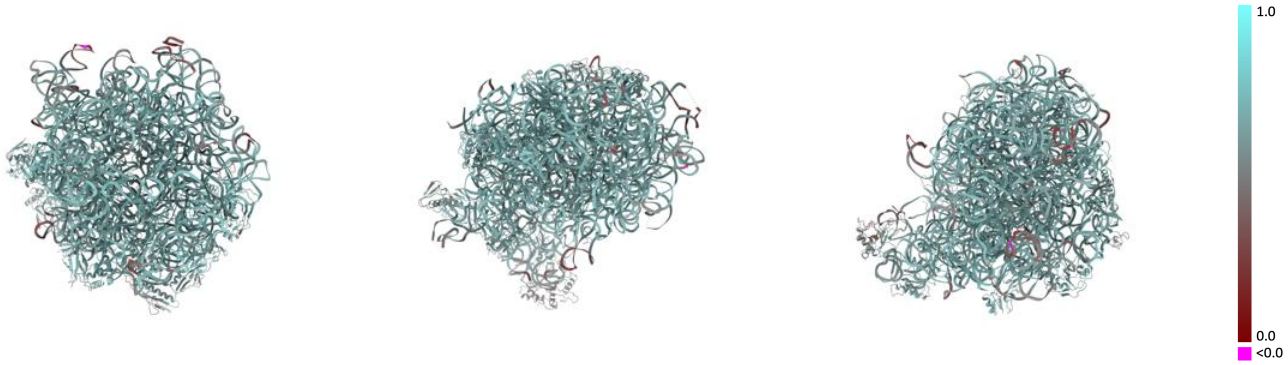
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

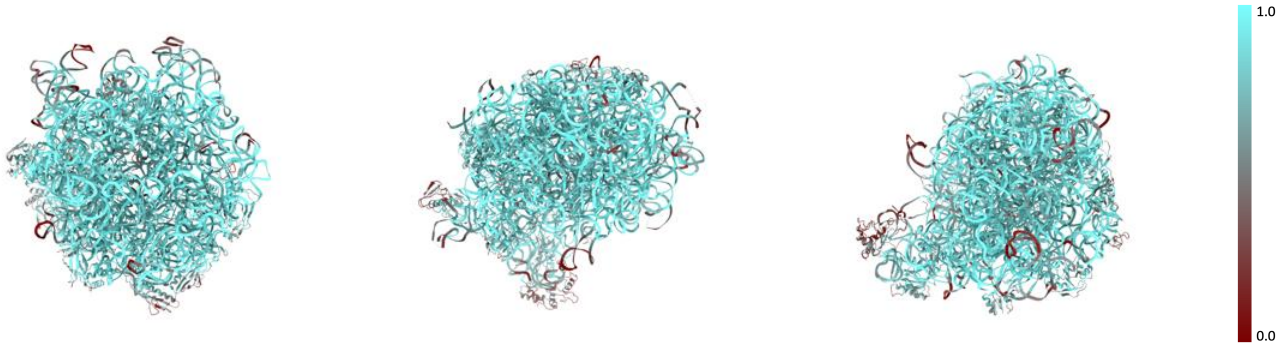
9.2 Q-score mapped to coordinate model (i)



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.

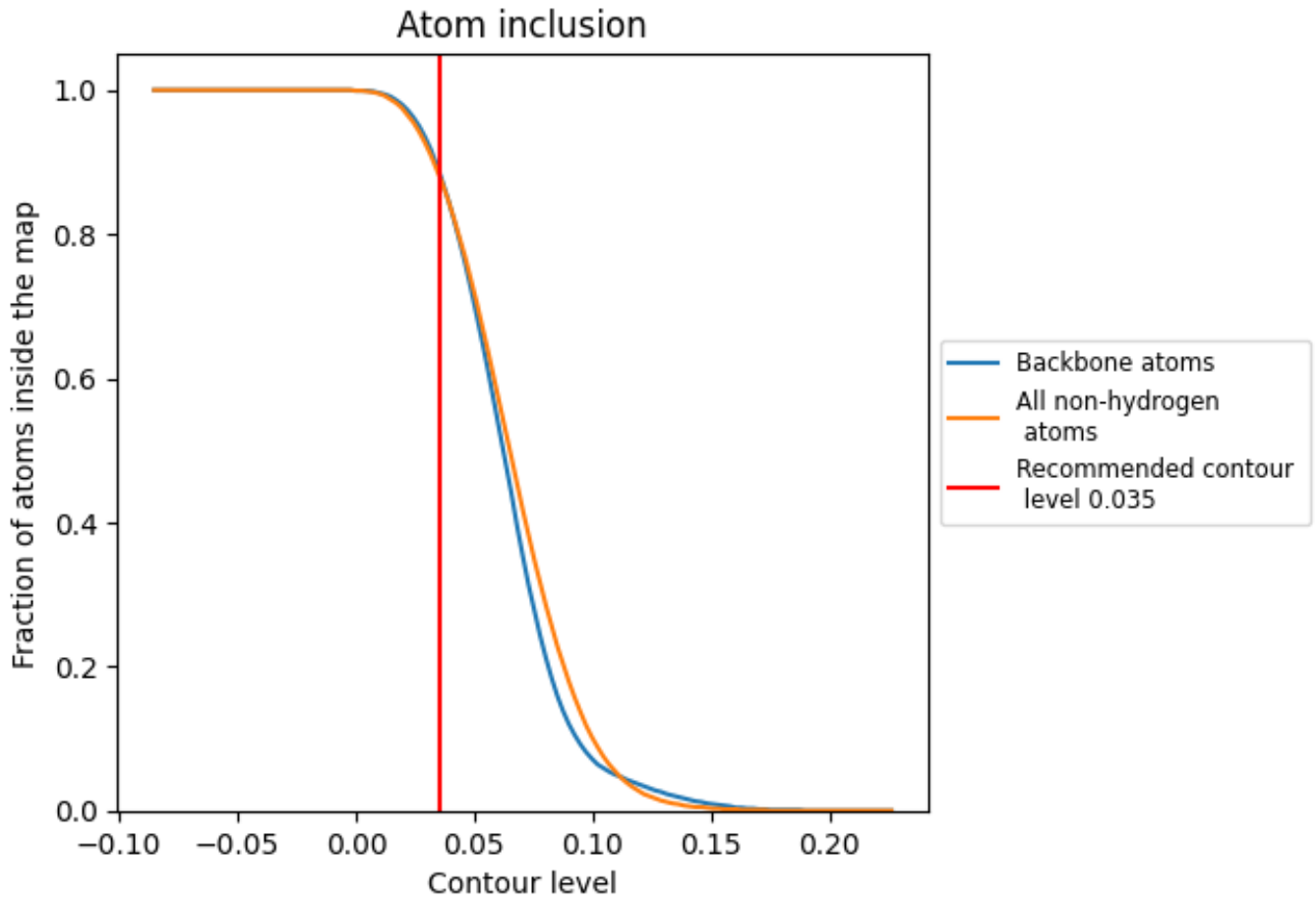
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.6370
0	0.8280	0.6310
2	0.8900	0.6670
3	0.7400	0.6430
4	0.9540	0.6850
5	0.9360	0.6810
6	0.9220	0.6540
A	0.9200	0.6420
B	0.8020	0.5860
D	0.8990	0.6690
E	0.8420	0.6430
F	0.3580	0.4920
G	0.5620	0.5590
K	0.9020	0.6560
L	0.8730	0.6520
M	0.8030	0.6400
N	0.7880	0.6200
O	0.8650	0.6380
P	0.7160	0.6030
Q	0.8590	0.6450
R	0.9220	0.6720
S	0.8120	0.6380
T	0.8750	0.6550
U	0.8240	0.6310
V	0.6190	0.5810
X	0.9080	0.6680
Y	0.7650	0.6270
Z	0.7070	0.6050