



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:13 pm GMT

PDB ID : 5MMI
EMDB ID : EMD-3531
Title : Structure of the large subunit of the chloroplast ribosome
Authors : Bieri, P.; Leibundgut, M.; Saurer, M.; Boehringer, D.; Ban, N.
Deposited on : 2016-12-10
Resolution : 3.25 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

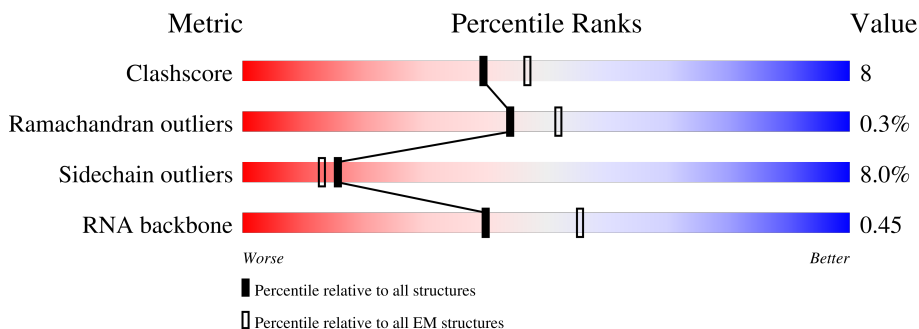
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.25 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.




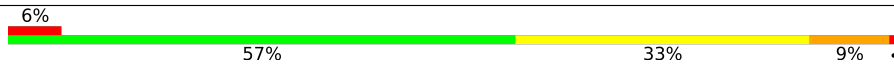

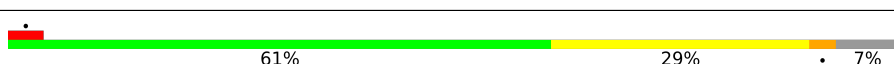



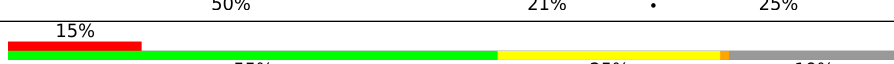


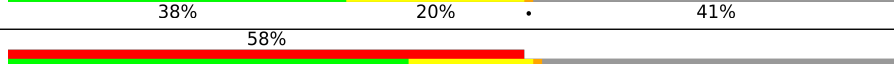
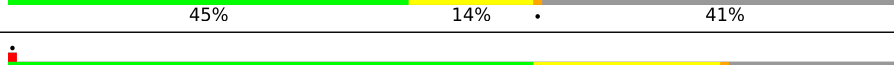





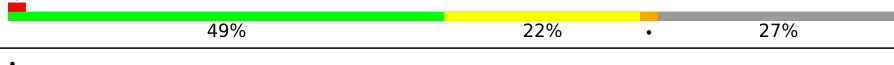
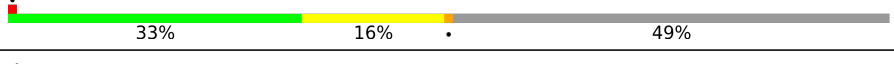
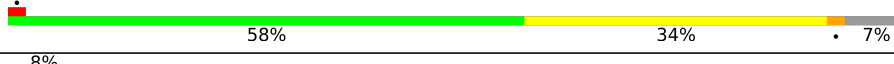





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	130	
2	1	57	
3	2	66	
4	3	152	
5	4	159	
6	5	37	
7	6	142	


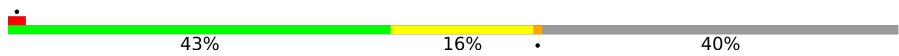

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Mol	Chain	Length	Quality of chain
8	7	116	
9	A	2810	
10	B	121	
11	C	272	
12	D	305	
13	E	293	
14	F	258	
15	G	220	
16	H	196	
17	I	232	
18	J	224	
19	K	250	
20	L	121	
21	M	271	
22	N	135	
23	O	126	
24	P	166	
25	Q	233	
26	R	128	
27	S	256	
28	T	199	
29	U	198	
30	V	192	
31	W	106	
32	X	194	

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Mol	Chain	Length	Quality of chain
33	Y	148	
34	Z	168	
35	z	2	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 95397 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	44	359	226	61	70	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	48	396	261	75	60	0	0

- Molecule 3 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	60	489	304	98	83	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	60	467	282	107	75	3	0	0

- Molecule 5 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	72	588	370	124	93	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	37	305	186	70	45	4	0	0

- Molecule 7 is a protein called plastid ribosomal protein cL37, PSRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	49	422	268	92	57	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	46	368	237	71	59	1	0	0

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	A	2798	60083	26804	11116	19365	2798	0	0

- Molecule 10 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	B	121	2584	1154	466	843	121	0	0

- Molecule 11 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	253	1952	1209	401	336	6	0	0

- Molecule 12 is a protein called plastid ribosomal protein uL3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	221	1686	1066	308	301	11	0	0

- Molecule 13 is a protein called plastid ribosomal protein uL4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	212	1676	1061	312	300	3	0	0

- Molecule 14 is a protein called plastid ribosomal protein uL5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	193	1454	923	255	268	8	0	0

- Molecule 15 is a protein called plastid ribosomal protein uL6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	178	1391	878	256	253	4	0	0

- Molecule 16 is a protein called plastid ribosomal protein bL9c.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	H	48	382	251	69	62	0	0

- Molecule 17 is a protein called plastid ribosomal protein uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	137	1106	711	186	203	6	0	0

- Molecule 18 is a protein called 50S ribosomal protein L11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	133	977	624	161	186	6	0	0

- Molecule 19 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K	203	1648	1047	307	289	5	0	0

- Molecule 20 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	121	942	588	179	170	5	0	0

- Molecule 21 is a protein called plastid ribosomal protein uL15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	185	Total	C	N	O	S	0	0
			1410	879	280	245	6		

- Molecule 22 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	135	Total	C	N	O	S	0	0
			1075	677	218	174	6		

- Molecule 23 is a protein called plastid ribosomal protein bL17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	116	Total	C	N	O	S	0	0
			944	592	193	155	4		

- Molecule 24 is a protein called plastid ribosomal protein uL18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	122	Total	C	N	O	S	0	0
			962	598	186	173	5		

- Molecule 25 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	118	Total	C	N	O	S	0	0
			953	611	186	155	1		

- Molecule 26 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	119	Total	C	N	O	S	0	0
			1029	652	213	162	2		

- Molecule 27 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	S	170	Total	C	N	O	0	0
			1310	844	227	239		

- Molecule 28 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	172	Total	C	N	O	S	0	0
			1395	892	257	237	9		

- Molecule 29 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	96	Total	C	N	O	S	0	0
			776	503	135	136	2		

- Molecule 30 is a protein called plastid ribosomal protein uL24c.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	134	Total	C	N	O	S	0	0
			1078	677	203	195	3		

- Molecule 31 is a RNA chain called 4.5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	106	Total	C	N	O	P	0	0
			2277	1017	423	731	106		

- Molecule 32 is a protein called plastid ribosomal protein bL27c.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	X	109	Total	C	N	O	0	0
			888	560	175	153		

- Molecule 33 is a protein called plastid ribosomal protein bL28c.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	77	Total	C	N	O	S	0	0
			634	402	128	103	1		

- Molecule 34 is a protein called plastid ribosomal protein uL29c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	101	Total	C	N	O	S	0	0
			846	529	167	147	3		

- Molecule 35 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	z	2	42	19	8	13	2	0	0

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
36	2	1	Total	Zn	0
			1	1	
36	5	1	Total	Zn	0
			1	1	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	4	1	Total	Mg	0
			1	1	
37	6	1	Total	Mg	0
			1	1	
37	7	1	Total	Mg	0
			1	1	
37	A	453	Total	Mg	0
			453	453	
37	B	15	Total	Mg	0
			15	15	
37	C	1	Total	Mg	0
			1	1	
37	D	2	Total	Mg	0
			2	2	
37	E	1	Total	Mg	0
			1	1	
37	H	1	Total	Mg	0
			1	1	
37	M	2	Total	Mg	0
			2	2	
37	N	1	Total	Mg	0
			1	1	
37	P	1	Total	Mg	0
			1	1	
37	R	1	Total	Mg	0
			1	1	
37	T	1	Total	Mg	0
			1	1	
37	U	1	Total	Mg	0
			1	1	

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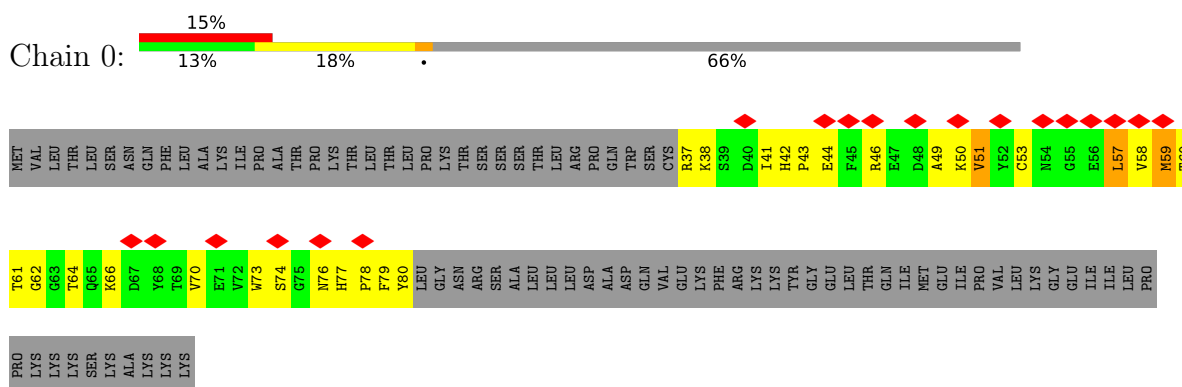
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Mol	Chain	Residues	Atoms		AltConf
37	V	2	Total 2	Mg 2	0
37	W	14	Total 14	Mg 14	0
37	X	1	Total 1	Mg 1	0
37	Y	1	Total 1	Mg 1	0

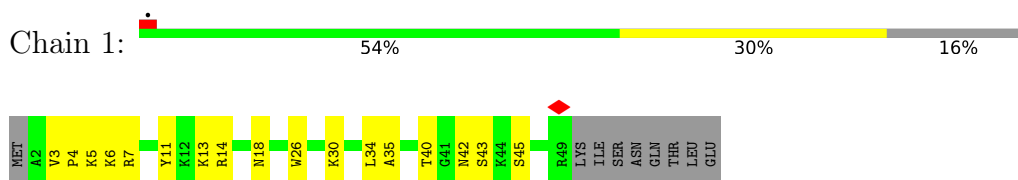
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

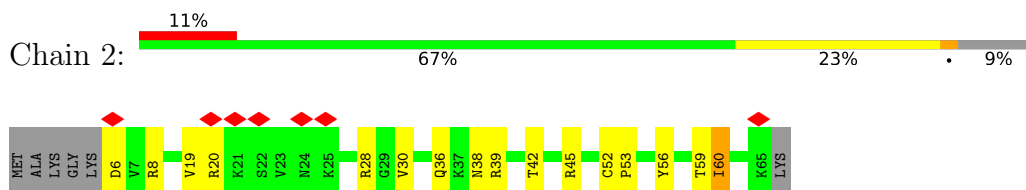
- Molecule 1: 50S ribosomal protein L31



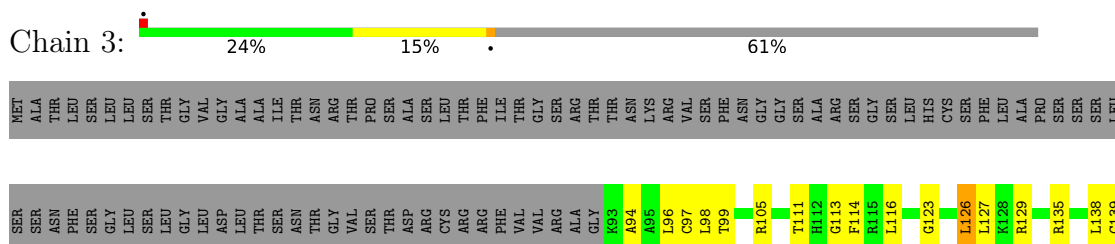
- Molecule 2: 50S ribosomal protein L32, chloroplastic

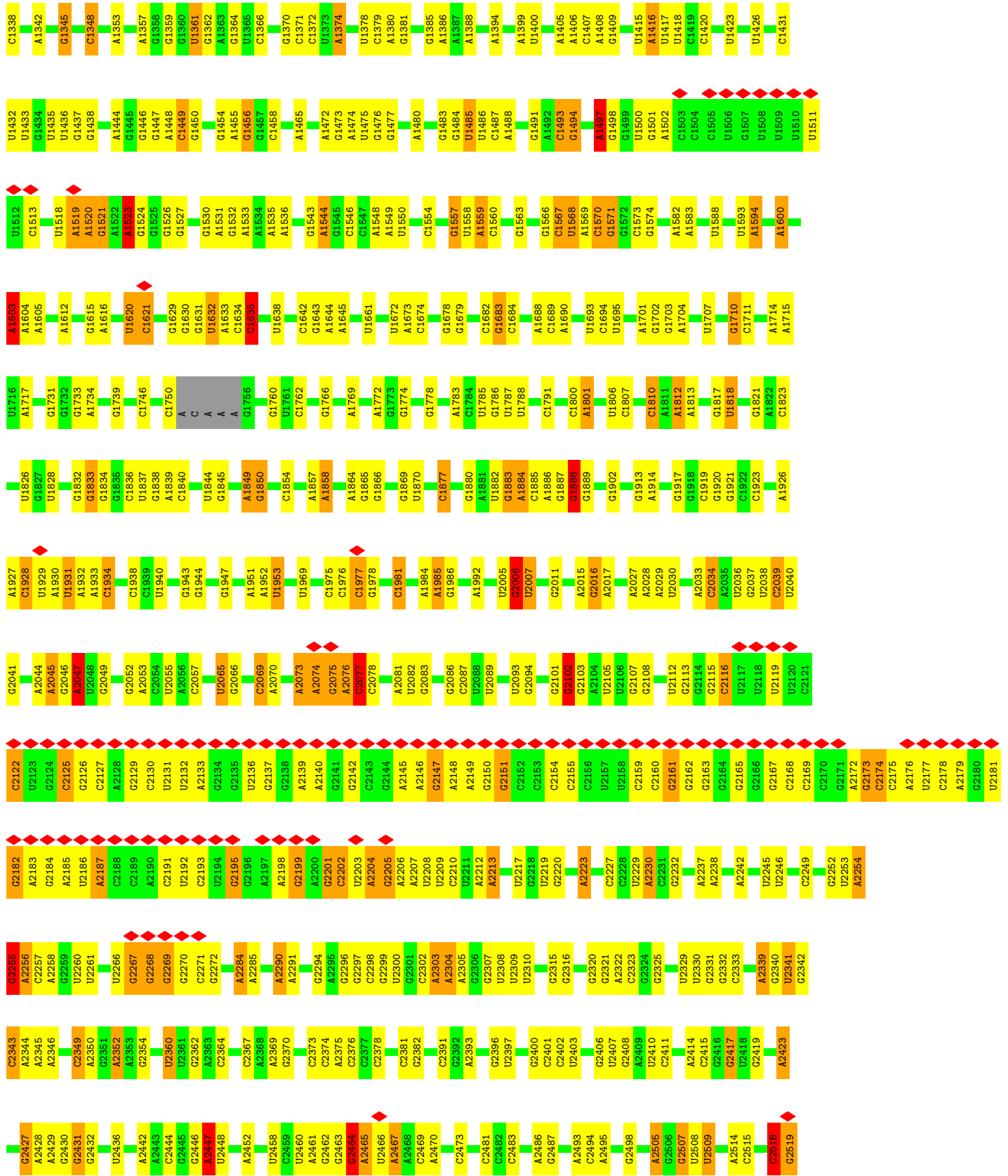


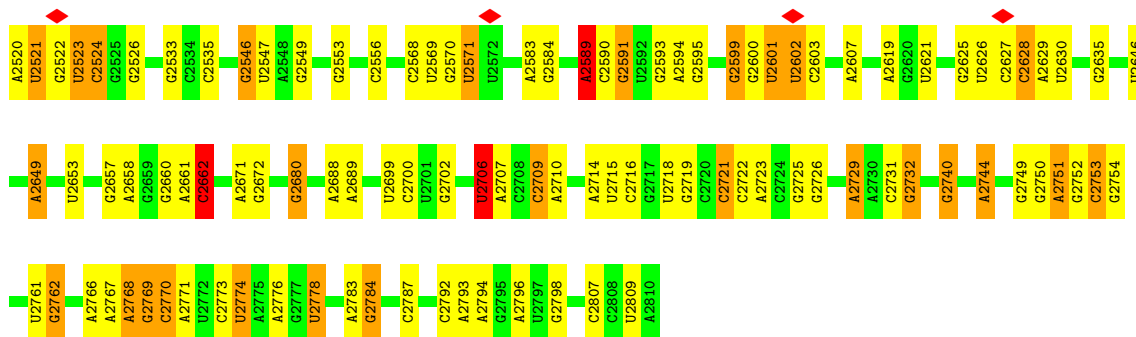
- Molecule 3: 50S ribosomal protein L33, chloroplastic



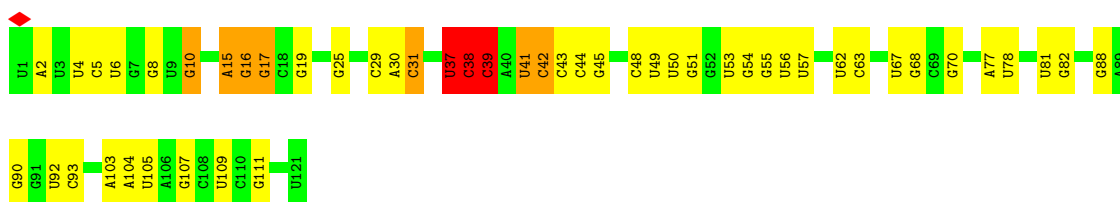
- Molecule 4: 50S ribosomal protein L34, chloroplastic



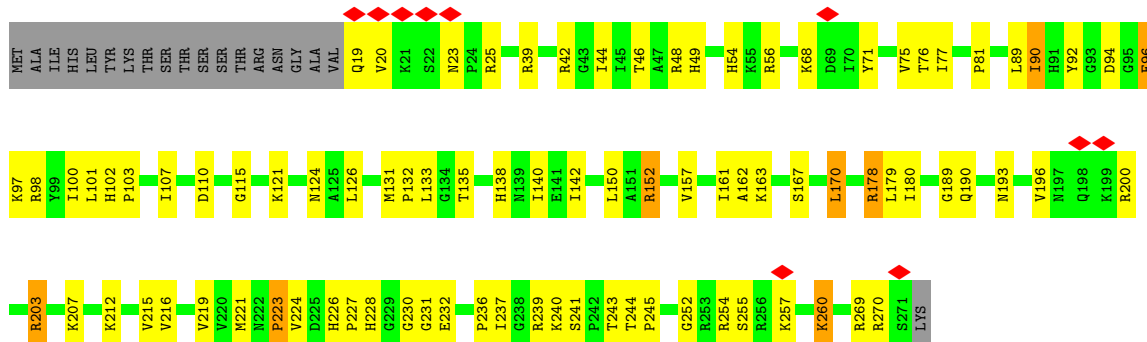




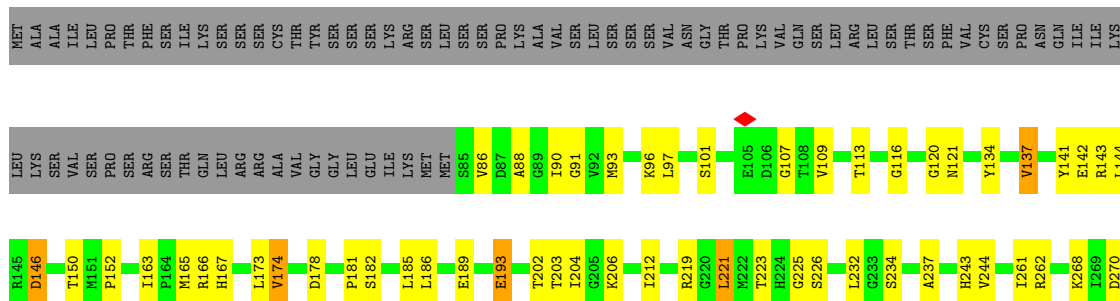
• Molecule 10: 5S ribosomal RNA

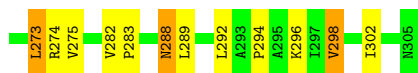


• Molecule 11: 50S ribosomal protein L2, chloroplastic

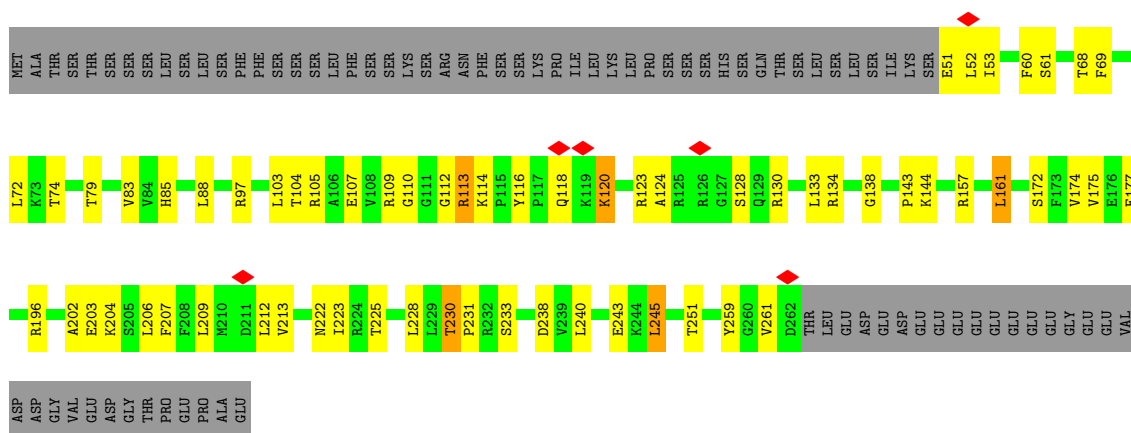


• Molecule 12: plastid ribosomal protein uL3c

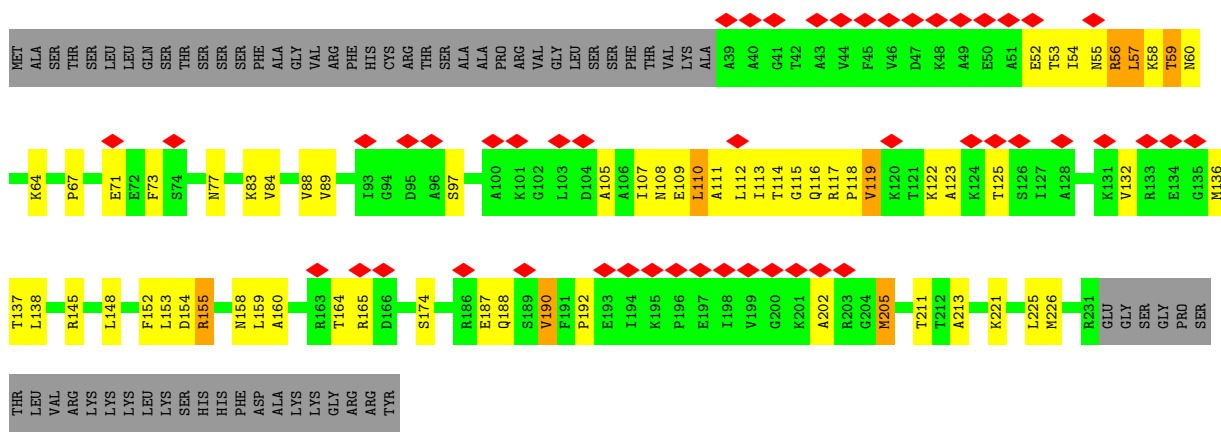




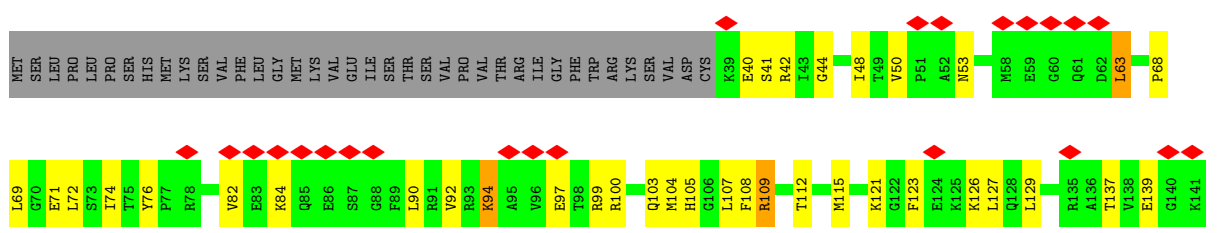
• Molecule 13: plastid ribosomal protein uL4c



• Molecule 14: plastid ribosomal protein uL5c

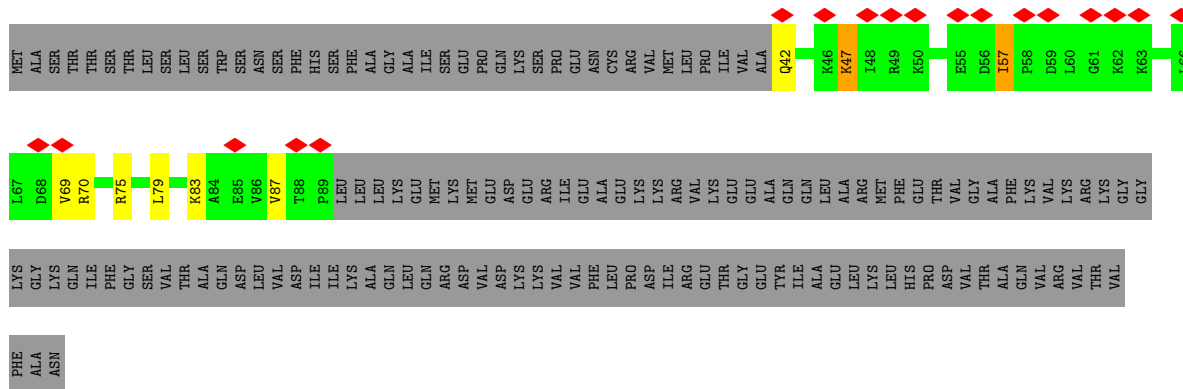


• Molecule 15: plastid ribosomal protein uL6c

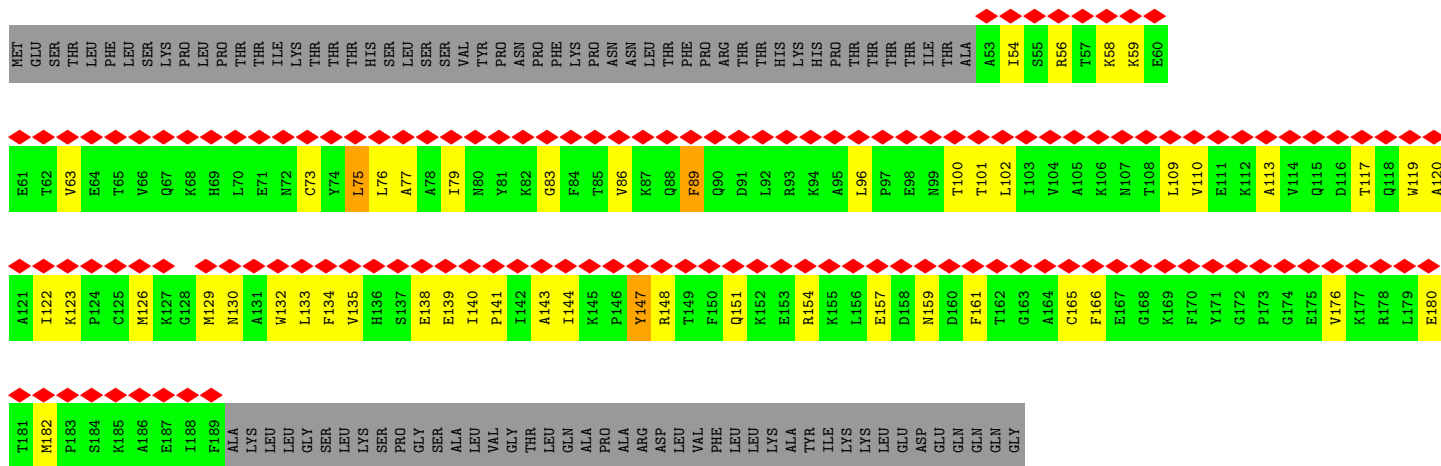
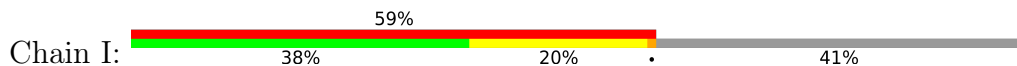




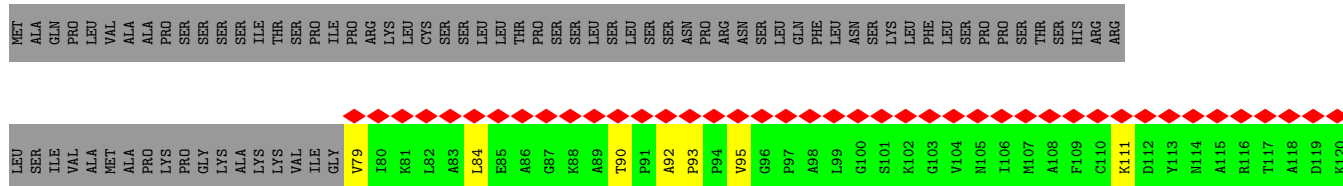
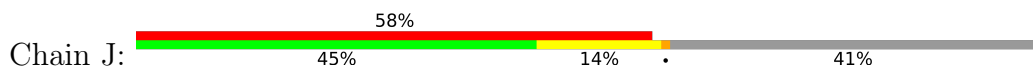
• Molecule 16: plastid ribosomal protein bL9c

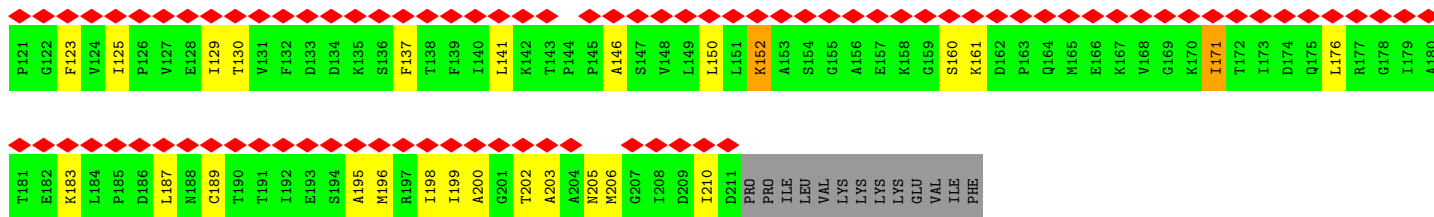


• Molecule 17: plastid ribosomal protein uL10c

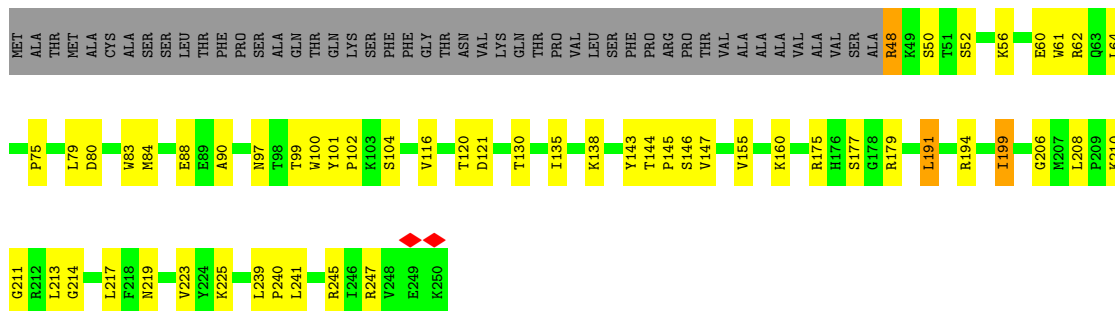


• Molecule 18: 50S ribosomal protein L11, chloroplastic

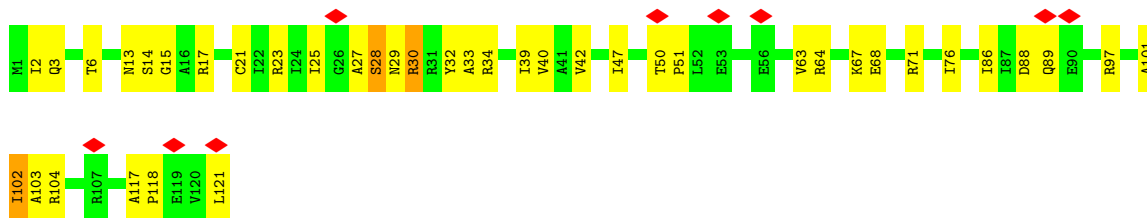




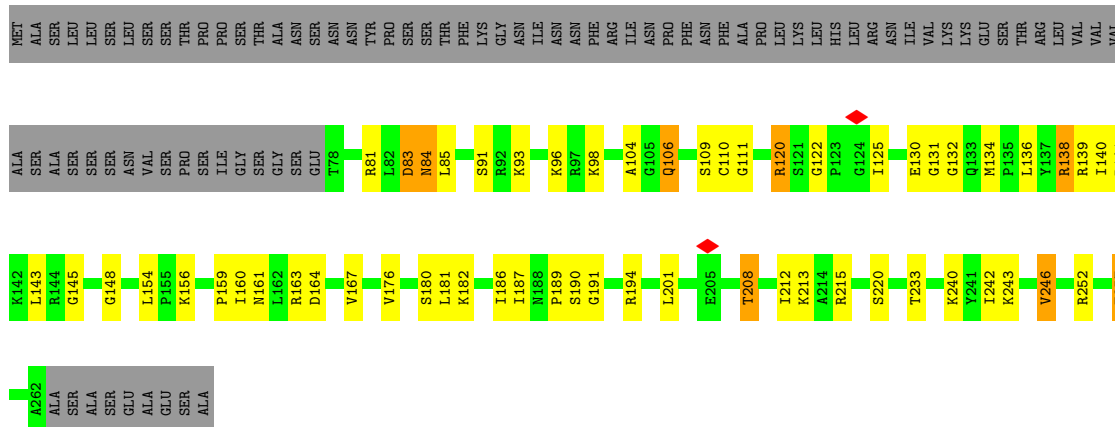
• Molecule 19: 50S ribosomal protein L13, chloroplastic



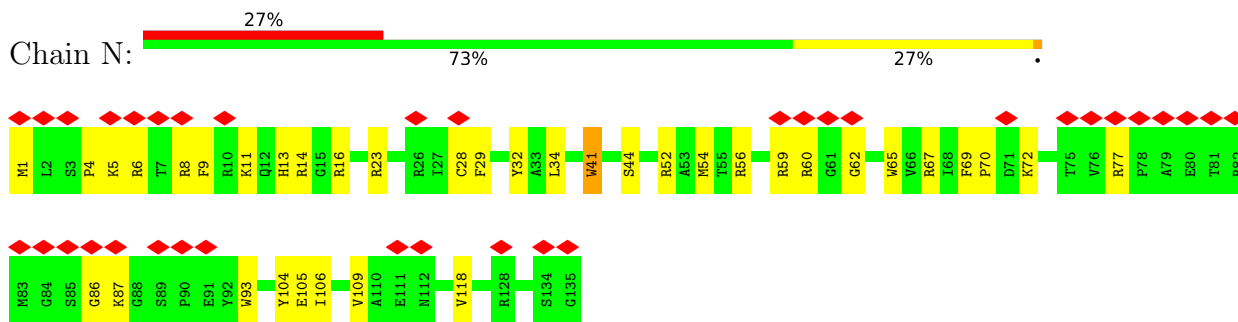
• Molecule 20: 50S ribosomal protein L14, chloroplastic



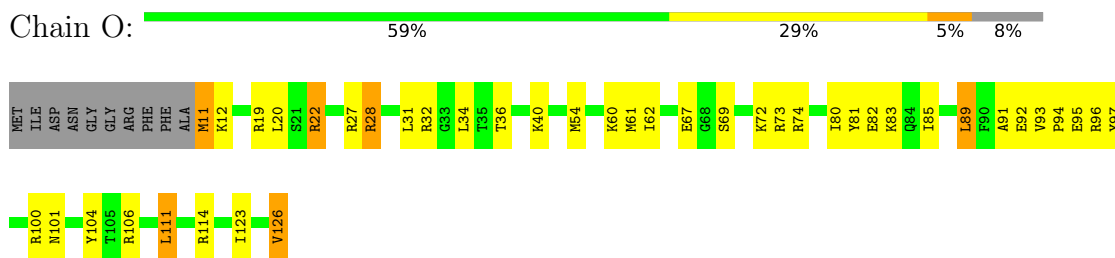
• Molecule 21: plastid ribosomal protein uL15c



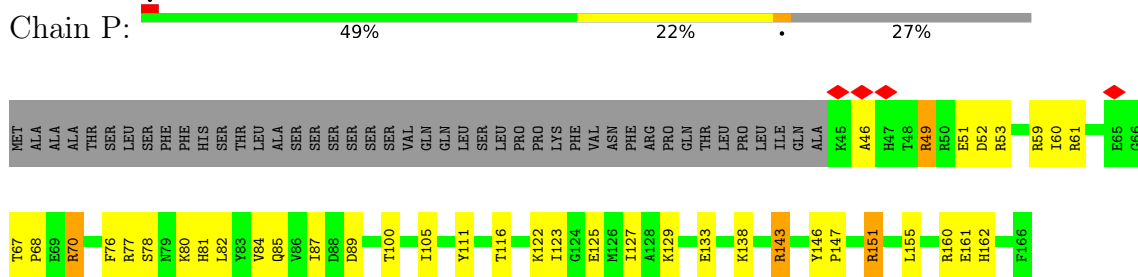
• Molecule 22: 50S ribosomal protein L16, chloroplastic



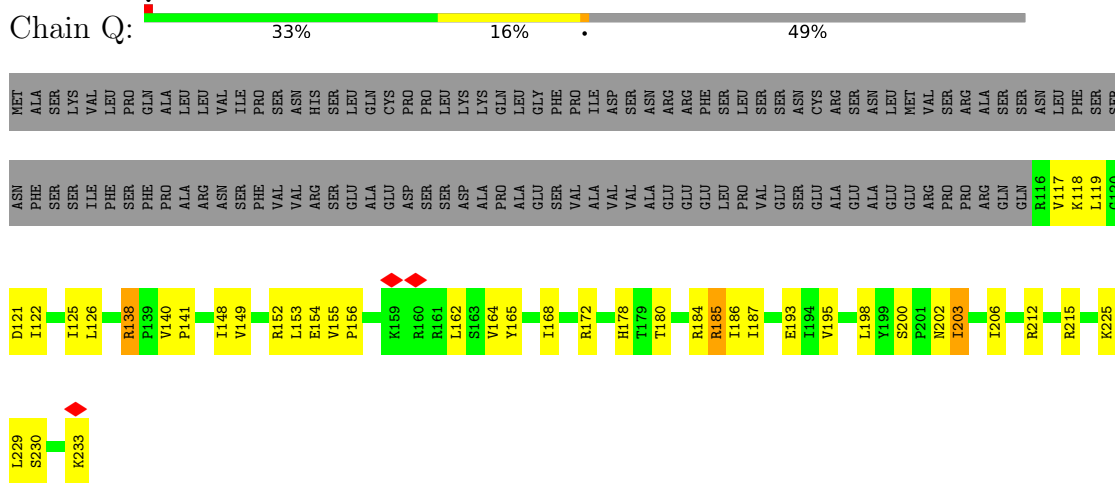
• Molecule 23: plastid ribosomal protein bL17c



• Molecule 24: plastid ribosomal protein uL18c

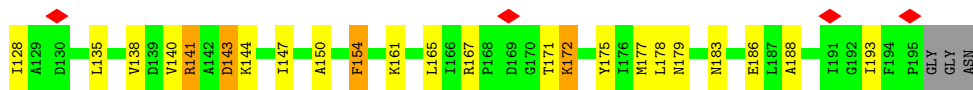


• Molecule 25: 50S ribosomal protein L19, chloroplastic

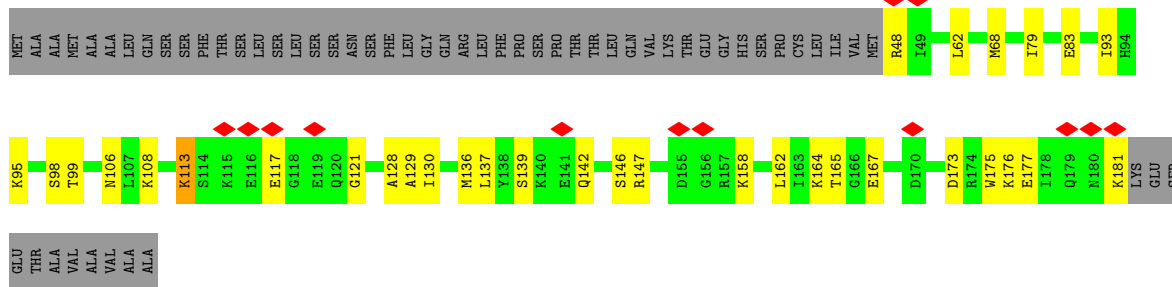


• Molecule 26: 50S ribosomal protein L20, chloroplastic

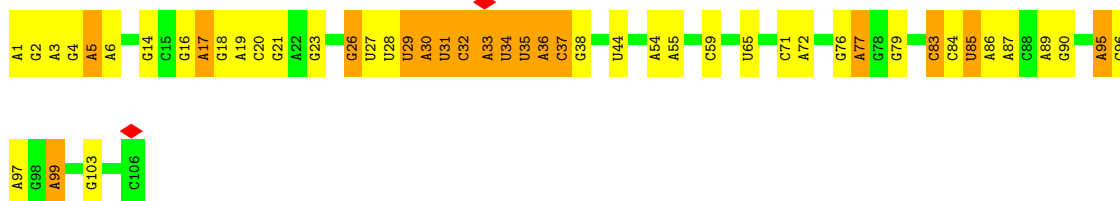




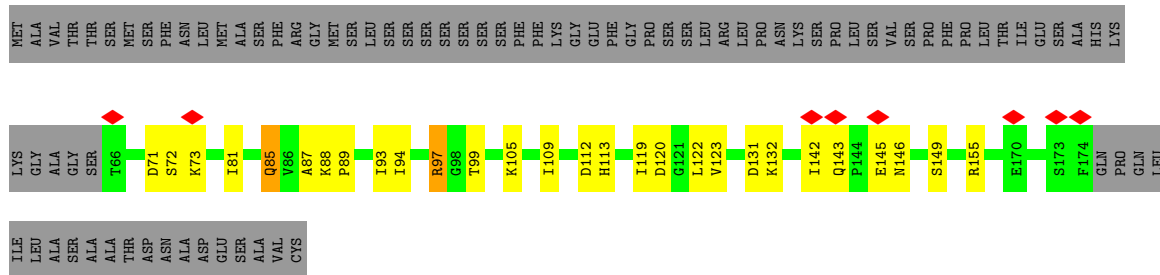
• Molecule 30: plastid ribosomal protein uL24c



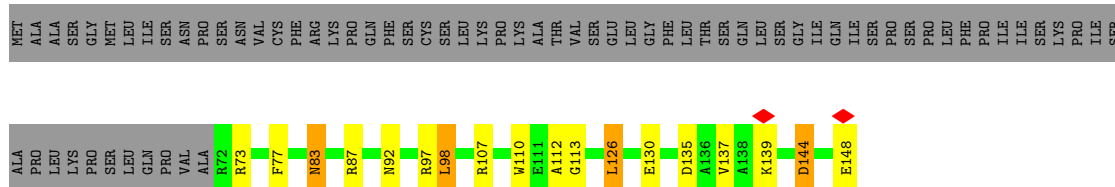
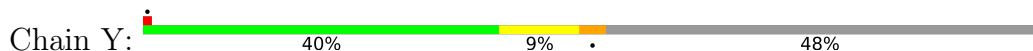
• Molecule 31: 4.5S ribosomal RNA



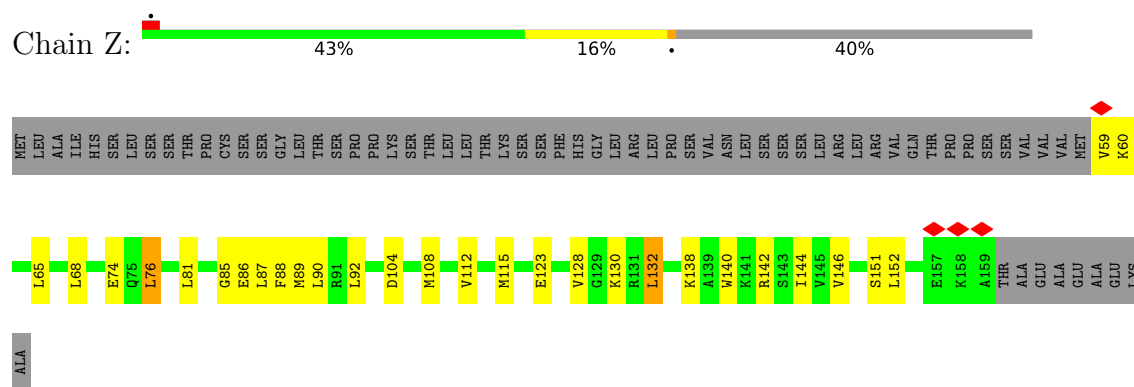
• Molecule 32: plastid ribosomal protein bL27c



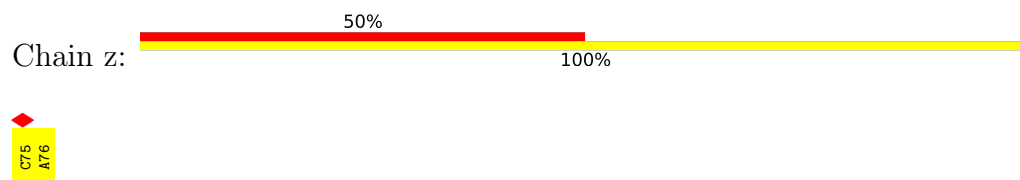
• Molecule 33: plastid ribosomal protein bL28c



- Molecule 34: plastid ribosomal protein uL29c



- Molecule 35: E-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	154332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.616	Depositor
Minimum map value	-0.270	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0	0.46	0/369	0.67	0/499
2	1	0.62	0/405	0.69	0/537
3	2	0.49	0/497	0.66	0/664
4	3	0.62	0/470	0.80	0/619
5	4	0.61	0/594	0.75	0/784
6	5	0.39	0/307	0.53	0/403
7	6	0.53	0/425	0.84	1/551 (0.2%)
8	7	0.53	0/382	0.58	0/520
9	A	0.85	39/67297 (0.1%)	1.19	236/104984 (0.2%)
10	B	0.45	1/2890 (0.0%)	1.00	5/4503 (0.1%)
11	C	0.52	0/1986	0.73	1/2666 (0.0%)
12	D	0.56	0/1713	0.72	0/2291
13	E	0.56	0/1707	0.80	1/2298 (0.0%)
14	F	0.42	0/1475	0.61	1/1990 (0.1%)
15	G	0.39	0/1412	0.60	0/1898
16	H	0.41	0/386	0.62	0/514
17	I	0.49	0/1129	0.53	0/1521
18	J	0.50	0/992	0.55	0/1343
19	K	0.51	0/1688	0.64	0/2279
20	L	0.48	0/951	0.66	0/1282
21	M	0.52	0/1430	0.71	0/1896
22	N	0.48	0/1097	0.64	1/1471 (0.1%)
23	O	0.57	0/959	0.77	0/1280
24	P	0.38	0/978	0.56	0/1311
25	Q	0.52	0/967	0.67	0/1299
26	R	0.61	0/1046	0.74	0/1395
27	S	0.51	0/1339	0.72	3/1826 (0.2%)
28	T	0.50	0/1420	0.64	0/1900
29	U	0.50	0/787	0.68	0/1056
30	V	0.43	0/1093	0.63	0/1457
31	W	0.74	0/2551	1.15	3/3977 (0.1%)
32	X	0.47	0/905	0.61	0/1204

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Y	0.51	0/644	0.64	0/856
34	Z	0.41	0/854	0.58	0/1131
35	z	0.89	0/46	1.88	2/69 (2.9%)
All	All	0.75	40/103191 (0.0%)	1.07	254/154274 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	M	0	1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	591	C	N1-C6	-7.28	1.32	1.37
9	A	1272	A	N9-C4	-7.03	1.33	1.37
9	A	1272	A	N3-C4	-6.93	1.30	1.34
9	A	1272	A	N7-C5	-6.68	1.35	1.39
9	A	810	G	C6-N1	-6.13	1.35	1.39
9	A	236	A	C5-C4	-6.09	1.34	1.38
9	A	180	A	N9-C4	-5.96	1.34	1.37
9	A	2044	A	N9-C4	-5.90	1.34	1.37
9	A	2794	A	N9-C4	-5.64	1.34	1.37
9	A	709	C	N1-C6	-5.60	1.33	1.37
9	A	2039	C	N1-C6	-5.58	1.33	1.37
9	A	1372	C	N1-C6	-5.58	1.33	1.37
9	A	999	C	N1-C6	-5.54	1.33	1.37
9	A	810	G	C5-C4	-5.52	1.34	1.38
10	B	39	C	N1-C6	-5.51	1.33	1.37
9	A	1399	A	N9-C4	-5.50	1.34	1.37
9	A	2041	G	N1-C2	-5.47	1.33	1.37
9	A	1286	A	N9-C4	-5.46	1.34	1.37
9	A	830	A	N3-C4	-5.44	1.31	1.34
9	A	2052	G	C5-C4	-5.43	1.34	1.38
9	A	590	C	N1-C6	-5.35	1.33	1.37
9	A	1272	A	C5-C6	-5.31	1.36	1.41
9	A	469	A	N9-C4	-5.30	1.34	1.37
9	A	596	A	N3-C4	-5.27	1.31	1.34
9	A	1497	A	N9-C4	5.24	1.41	1.37
9	A	2744	A	N9-C4	-5.24	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	478	A	N9-C4	-5.21	1.34	1.37
9	A	822	U	N1-C2	-5.18	1.33	1.38
9	A	790	U	C2-N3	-5.18	1.34	1.37
9	A	810	G	N7-C5	-5.17	1.36	1.39
9	A	830	A	N7-C5	-5.14	1.36	1.39
9	A	1210	A	N7-C5	-5.12	1.36	1.39
9	A	2041	G	C5-C4	-5.12	1.34	1.38
9	A	1406	A	N9-C4	-5.08	1.34	1.37
9	A	785	A	N9-C4	-5.05	1.34	1.37
9	A	1284	U	C2-N3	-5.04	1.34	1.37
9	A	785	A	N3-C4	-5.04	1.31	1.34
9	A	592	G	C6-N1	-5.02	1.36	1.39
9	A	514	A	N3-C4	-5.01	1.31	1.34
9	A	786	G	C5-C4	-5.01	1.34	1.38

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1272	A	C2-N3-C4	-11.16	105.02	110.60
9	A	1272	A	N1-C2-N3	9.97	134.28	129.30
9	A	1272	A	C6-C5-N7	-9.58	125.60	132.30
9	A	2464	G	C8-N9-C4	9.23	110.09	106.40
9	A	2464	G	N9-C4-C5	-9.22	101.71	105.40
9	A	652	C	N3-C4-C5	8.97	125.49	121.90
9	A	2122	C	C6-N1-C2	-8.60	116.86	120.30
9	A	1272	A	C5-N7-C8	-8.58	99.61	103.90
9	A	901	C	C2-N1-C1'	8.44	128.09	118.80
9	A	1272	A	N7-C8-N9	8.42	118.01	113.80
9	A	514	A	C8-N9-C4	-8.29	102.48	105.80
9	A	652	C	C2-N3-C4	-8.07	115.86	119.90
9	A	1272	A	C4-C5-C6	7.99	121.00	117.00
9	A	540	A	C4-C5-C6	-7.88	113.06	117.00
9	A	652	C	C6-N1-C2	7.74	123.39	120.30
9	A	2706	U	N3-C2-O2	-7.55	116.92	122.20
9	A	1010	C	C6-N1-C2	7.41	123.27	120.30
9	A	2065	U	C5-C6-N1	-7.32	119.04	122.70
9	A	564	U	C5-C6-N1	-7.31	119.05	122.70
9	A	540	A	N1-C2-N3	-7.30	125.65	129.30
9	A	705	U	C5-C6-N1	-7.27	119.06	122.70
9	A	2464	G	C4-C5-N7	7.27	113.71	110.80
9	A	2635	G	C8-N9-C4	7.22	109.29	106.40
9	A	486	G	C8-N9-C4	7.16	109.26	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2102	G	C8-N9-C4	-7.13	103.55	106.40
9	A	901	C	C6-N1-C2	-7.10	117.46	120.30
9	A	641	C	C6-N1-C2	7.06	123.12	120.30
9	A	514	A	N9-C4-C5	7.04	108.62	105.80
9	A	2464	G	N3-C4-N9	7.03	130.22	126.00
9	A	2706	U	N1-C2-O2	7.02	127.72	122.80
9	A	2034	C	C6-N1-C2	7.02	123.11	120.30
9	A	2036	U	C5-C6-N1	-6.99	119.20	122.70
9	A	2391	C	C5-C6-N1	-6.96	117.52	121.00
9	A	426	C	C6-N1-C2	6.89	123.06	120.30
9	A	2360	U	C2-N1-C1'	6.82	125.89	117.70
9	A	701	U	C5-C6-N1	-6.77	119.32	122.70
9	A	2518	C	C6-N1-C2	-6.75	117.60	120.30
9	A	2102	G	N7-C8-N9	6.73	116.47	113.10
9	A	2065	U	C2-N1-C1'	-6.71	109.65	117.70
9	A	657	U	N1-C2-O2	6.68	127.48	122.80
9	A	540	A	C5-C6-N1	6.64	121.02	117.70
9	A	2122	C	C2-N1-C1'	6.64	126.10	118.80
9	A	795	U	O5'-P-OP1	-6.62	99.74	105.70
9	A	1334	U	N3-C2-O2	-6.61	117.57	122.20
9	A	970	G	N3-C4-C5	-6.61	125.29	128.60
9	A	1661	U	C5-C6-N1	-6.58	119.41	122.70
9	A	788	G	N3-C4-C5	-6.58	125.31	128.60
9	A	540	A	C8-N9-C4	6.57	108.43	105.80
9	A	311	U	C5-C6-N1	-6.55	119.42	122.70
9	A	652	C	C5-C6-N1	-6.53	117.73	121.00
9	A	2038	U	C5-C6-N1	-6.50	119.45	122.70
9	A	514	A	C6-N1-C2	-6.50	114.70	118.60
9	A	2006	G	C8-N9-C4	6.47	108.99	106.40
9	A	745	A	C8-N9-C4	6.45	108.38	105.80
9	A	1272	A	N1-C6-N6	6.45	122.47	118.60
10	B	39	C	C4-C5-C6	6.43	120.61	117.40
9	A	759	G	O4'-C1'-N9	6.43	113.34	108.20
9	A	1050	G	C6-N1-C2	-6.43	121.24	125.10
9	A	773	U	C5-C6-N1	-6.42	119.49	122.70
9	A	1272	A	C5-C6-N1	-6.42	114.49	117.70
9	A	2523	U	P-O3'-C3'	6.41	127.40	119.70
9	A	524	A	N1-C2-N3	6.40	132.50	129.30
9	A	901	C	N1-C2-O2	6.40	122.74	118.90
9	A	1281	G	C8-N9-C4	6.37	108.95	106.40
9	A	2464	G	C5-C6-O6	-6.37	124.78	128.60
9	A	1418	U	N1-C2-N3	6.37	118.72	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	802	C	N3-C4-C5	6.34	124.44	121.90
9	A	1333	U	C5-C6-N1	-6.32	119.54	122.70
9	A	1361	U	C5-C6-N1	-6.30	119.55	122.70
27	S	78	PRO	N-CA-CB	6.29	110.85	103.30
9	A	2077	C	C2-N1-C1'	6.28	125.71	118.80
9	A	548	G	C8-N9-C4	6.23	108.89	106.40
9	A	2016	G	C8-N9-C4	-6.22	103.91	106.40
7	6	131	TRP	C-N-CD	6.21	141.43	128.40
9	A	127	C	C6-N1-C2	-6.19	117.82	120.30
9	A	28	U	C5-C4-O4	-6.16	122.20	125.90
9	A	2401	C	C5-C6-N1	-6.14	117.93	121.00
9	A	761	A	C8-N9-C4	-6.11	103.36	105.80
9	A	970	G	N3-C4-N9	6.10	129.66	126.00
9	A	1264	C	C6-N1-C2	6.07	122.73	120.30
9	A	1184	G	C6-C5-N7	-6.07	126.76	130.40
9	A	788	G	C4-N9-C1'	6.07	134.39	126.50
9	A	1050	G	C5-C6-O6	-6.05	124.97	128.60
35	z	75	C	C2-N1-C1'	-6.05	112.14	118.80
35	z	75	C	C6-N1-C1'	6.05	128.06	120.80
9	A	416	C	C6-N1-C2	6.03	122.71	120.30
27	S	79	PRO	N-CA-CB	6.02	110.52	103.30
9	A	2268	G	C2-N3-C4	5.97	114.89	111.90
9	A	1010	C	C5-C6-N1	-5.96	118.02	121.00
9	A	657	U	N3-C4-C5	5.91	118.15	114.60
9	A	2649	A	N1-C2-N3	5.91	132.25	129.30
10	B	39	C	N3-C4-C5	-5.91	119.54	121.90
9	A	2065	U	N1-C2-N3	5.86	118.42	114.90
27	S	208	ARG	NE-CZ-NH1	5.86	123.23	120.30
9	A	2391	C	C6-N1-C2	5.85	122.64	120.30
9	A	2360	U	C6-N1-C1'	-5.84	113.03	121.20
9	A	1217	C	N3-C2-O2	-5.83	117.82	121.90
9	A	1688	A	C2-N3-C4	-5.83	107.69	110.60
9	A	462	G	C6-C5-N7	-5.81	126.92	130.40
9	A	514	A	N1-C6-N6	-5.81	115.12	118.60
9	A	772	A	C5-N7-C8	-5.81	101.00	103.90
9	A	1497	A	C2-N3-C4	5.80	113.50	110.60
9	A	1272	A	C8-N9-C4	-5.79	103.49	105.80
9	A	514	A	N1-C2-N3	5.78	132.19	129.30
9	A	548	G	N9-C4-C5	-5.77	103.09	105.40
9	A	2077	C	C5-C6-N1	5.76	123.88	121.00
9	A	1000	G	N3-C4-C5	-5.75	125.72	128.60
31	W	18	G	C8-N9-C4	5.74	108.69	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	585	A	C8-N9-C4	5.73	108.09	105.80
9	A	2740	G	N3-C4-C5	-5.73	125.74	128.60
9	A	773	U	C6-N1-C2	5.72	124.43	121.00
9	A	951	C	C5-C6-N1	5.72	123.86	121.00
11	C	231	GLY	N-CA-C	-5.70	98.84	113.10
9	A	25	G	N1-C6-O6	-5.70	116.48	119.90
9	A	2017	A	C6-N1-C2	-5.69	115.19	118.60
9	A	2272	G	C4-C5-N7	5.66	113.06	110.80
9	A	2721	C	C6-N1-C2	5.65	122.56	120.30
9	A	1184	G	C4-C5-N7	5.65	113.06	110.80
9	A	1016	G	C4-C5-N7	5.63	113.05	110.80
9	A	462	G	C4-C5-C6	5.63	122.18	118.80
9	A	1055	A	C8-N9-C4	5.62	108.05	105.80
9	A	1372	C	C2-N3-C4	-5.62	117.09	119.90
9	A	901	C	N3-C2-O2	-5.62	117.97	121.90
9	A	462	G	C4-N9-C1'	5.61	133.79	126.50
9	A	2034	C	C5-C6-N1	-5.61	118.19	121.00
9	A	536	C	C5-C6-N1	-5.56	118.22	121.00
9	A	1184	G	N3-C4-N9	5.55	129.33	126.00
9	A	970	G	N1-C6-O6	-5.54	116.58	119.90
9	A	1217	C	C4-C5-C6	5.54	120.17	117.40
9	A	1177	U	C5-C6-N1	-5.53	119.93	122.70
9	A	641	C	C5-C6-N1	-5.53	118.23	121.00
9	A	426	C	C5-C6-N1	-5.53	118.24	121.00
14	F	57	LEU	CA-CB-CG	-5.53	102.59	115.30
9	A	1334	U	N1-C2-O2	5.52	126.67	122.80
9	A	2568	C	C5-C6-N1	-5.52	118.24	121.00
9	A	1332	G	O4'-C1'-N9	5.51	112.61	108.20
9	A	2628	C	C6-N1-C2	-5.49	118.10	120.30
9	A	2744	A	C8-N9-C4	5.49	108.00	105.80
9	A	788	G	N3-C4-N9	5.48	129.29	126.00
9	A	2343	C	C4-C5-C6	-5.48	114.66	117.40
9	A	1272	A	C4-N9-C1'	5.48	136.16	126.30
9	A	1372	C	C5-C6-N1	-5.48	118.26	121.00
9	A	2294	G	C8-N9-C4	-5.47	104.21	106.40
9	A	1786	G	C4-N9-C1'	5.47	133.61	126.50
13	E	112	GLY	N-CA-C	-5.46	99.44	113.10
9	A	2427	G	N3-C4-N9	5.45	129.27	126.00
9	A	783	U	N3-C2-O2	-5.45	118.39	122.20
9	A	1603	A	N1-C2-N3	5.44	132.02	129.30
9	A	2794	A	C8-N9-C4	5.44	107.98	105.80
9	A	522	U	N1-C2-O2	5.43	126.60	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1947	G	C8-N9-C4	-5.42	104.23	106.40
10	B	37	U	C2-N1-C1'	5.42	124.20	117.70
9	A	1977	C	C6-N1-C2	-5.41	118.14	120.30
9	A	1272	A	C4-C5-N7	5.41	113.41	110.70
9	A	8	G	O4'-C1'-N9	5.41	112.53	108.20
9	A	232	G	C8-N9-C4	5.41	108.56	106.40
9	A	822	U	N1-C2-O2	-5.38	119.03	122.80
9	A	906	C	C6-N1-C2	-5.38	118.15	120.30
9	A	2401	C	C2-N3-C4	-5.37	117.22	119.90
9	A	901	C	C5-C6-N1	5.36	123.68	121.00
9	A	100	G	C8-N9-C4	5.36	108.54	106.40
9	A	190	G	O4'-C1'-N9	5.36	112.49	108.20
9	A	540	A	C4-N9-C1'	-5.36	116.66	126.30
9	A	1345	G	O4'-C1'-N9	5.35	112.48	108.20
9	A	2360	U	N1-C2-O2	5.35	126.55	122.80
9	A	2047	A	C6-N1-C2	-5.34	115.40	118.60
9	A	2533	G	N3-C4-N9	5.34	129.21	126.00
9	A	810	G	C6-N1-C2	-5.34	121.90	125.10
9	A	1635	C	C6-N1-C2	-5.34	118.17	120.30
9	A	1348	C	C6-N1-C2	5.33	122.43	120.30
9	A	463	C	C5-C6-N1	-5.32	118.34	121.00
9	A	1456	G	C8-N9-C4	-5.32	104.27	106.40
9	A	1600	A	C8-N9-C4	5.32	107.93	105.80
10	B	38	C	C2-N1-C1'	5.32	124.65	118.80
9	A	1211	G	C8-N9-C4	5.31	108.53	106.40
9	A	2122	C	N3-C2-O2	-5.31	118.18	121.90
9	A	901	C	C6-N1-C1'	-5.31	114.43	120.80
9	A	801	U	C5-C6-N1	-5.30	120.05	122.70
9	A	641	C	C2-N3-C4	-5.30	117.25	119.90
9	A	1299	U	C5-C6-N1	-5.28	120.06	122.70
9	A	588	A	C8-N9-C4	5.26	107.90	105.80
9	A	2065	U	C2-N3-C4	-5.26	123.84	127.00
9	A	1010	C	C2-N3-C4	-5.25	117.27	119.90
9	A	1902	G	N3-C4-C5	-5.25	125.97	128.60
9	A	2447	A	C8-N9-C4	-5.25	103.70	105.80
9	A	2349	C	C6-N1-C2	5.25	122.40	120.30
9	A	1787	U	C5-C6-N1	-5.25	120.08	122.70
9	A	2662	C	N3-C2-O2	-5.25	118.22	121.90
9	A	110	U	C5-C6-N1	-5.25	120.08	122.70
9	A	1334	U	C2-N1-C1'	5.23	123.98	117.70
9	A	2271	C	C6-N1-C2	-5.22	118.21	120.30
9	A	2784	G	C4-C5-N7	5.22	112.89	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2607	A	C8-N9-C4	5.22	107.89	105.80
9	A	2731	C	C5-C6-N1	-5.22	118.39	121.00
9	A	536	C	C4-C5-C6	5.22	120.01	117.40
10	B	37	U	N1-C2-O2	5.22	126.45	122.80
9	A	523	G	O4'-C1'-N9	5.20	112.36	108.20
9	A	701	U	C6-N1-C2	5.18	124.11	121.00
22	N	62	GLY	N-CA-C	5.18	126.04	113.10
9	A	1731	G	N3-C4-N9	5.17	129.10	126.00
9	A	1523	A	C8-N9-C4	-5.17	103.73	105.80
9	A	114	C	N1-C2-N3	5.16	122.81	119.20
9	A	1447	G	N3-C4-N9	5.14	129.08	126.00
9	A	17	C	C2-N3-C4	-5.14	117.33	119.90
9	A	2523	U	C5-C6-N1	5.14	125.27	122.70
9	A	1788	U	C5-C6-N1	-5.13	120.13	122.70
9	A	2589	A	C8-N9-C4	5.13	107.85	105.80
9	A	1050	G	C5-C6-N1	5.13	114.06	111.50
9	A	548	G	C5-C6-O6	-5.12	125.53	128.60
9	A	1012	G	C2-N3-C4	5.12	114.46	111.90
9	A	815	A	C8-N9-C4	5.11	107.84	105.80
9	A	1877	C	N1-C2-O2	5.11	121.97	118.90
9	A	2509	U	C2-N1-C1'	5.11	123.83	117.70
9	A	1309	U	C5-C4-O4	5.10	128.96	125.90
9	A	931	U	C5-C6-N1	-5.10	120.15	122.70
9	A	2505	A	C8-N9-C4	5.10	107.84	105.80
9	A	772	A	C2-N3-C4	-5.09	108.05	110.60
9	A	1370	G	C8-N9-C4	5.09	108.43	106.40
9	A	1374	A	C6-N1-C2	-5.09	115.55	118.60
9	A	1919	C	N1-C2-O2	5.08	121.95	118.90
9	A	2752	G	C8-N9-C4	5.08	108.43	106.40
9	A	478	A	C8-N9-C4	5.08	107.83	105.80
9	A	2507	G	N3-C4-C5	5.08	131.14	128.60
9	A	2635	G	N7-C8-N9	-5.08	110.56	113.10
9	A	743	C	C4-C5-C6	5.08	119.94	117.40
9	A	2391	C	C2-N3-C4	-5.07	117.36	119.90
9	A	591	C	C2-N3-C4	-5.07	117.36	119.90
31	W	18	G	N3-C4-N9	5.07	129.04	126.00
9	A	458	G	C8-N9-C4	5.07	108.43	106.40
9	A	2343	C	C5-C6-N1	5.07	123.53	121.00
9	A	596	A	N1-C6-N6	-5.07	115.56	118.60
9	A	820	G	C5-C6-N1	5.07	114.03	111.50
9	A	947	A	C8-N9-C4	-5.06	103.78	105.80
9	A	2034	C	C2-N3-C4	-5.06	117.37	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	788	G	C8-N9-C1'	-5.06	120.43	127.00
9	A	2749	G	N3-C4-C5	-5.05	126.07	128.60
9	A	564	U	C6-N1-C2	5.05	124.03	121.00
9	A	592	G	C8-N9-C4	5.04	108.42	106.40
9	A	2284	A	N1-C2-N3	5.04	131.82	129.30
9	A	1888	G	N3-C4-N9	5.04	129.02	126.00
9	A	2255	G	N1-C6-O6	-5.04	116.88	119.90
9	A	744	G	C4-C5-N7	5.03	112.81	110.80
9	A	1674	C	C2-N3-C4	-5.03	117.38	119.90
9	A	234	C	C6-N1-C2	5.03	122.31	120.30
9	A	698	C	C6-N1-C2	5.03	122.31	120.30
9	A	80	G	N3-C4-C5	-5.03	126.09	128.60
9	A	593	G	C6-C5-N7	-5.03	127.39	130.40
9	A	797	C	C6-N1-C2	5.02	122.31	120.30
9	A	2065	U	C6-N1-C1'	5.02	128.23	121.20
9	A	2401	C	C6-N1-C2	5.02	122.31	120.30
9	A	1707	U	N3-C4-O4	5.02	122.91	119.40
9	A	38	C	C6-N1-C2	-5.00	118.30	120.30
9	A	2349	C	C5-C6-N1	-5.00	118.50	121.00
31	W	18	G	N1-C2-N2	-5.00	111.70	116.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	M	104	ALA	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	0	359	0	330	26	0
2	1	396	0	437	15	0
3	2	489	0	507	10	0
4	3	467	0	526	13	0
5	4	588	0	658	12	0
6	5	305	0	344	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	6	422	0	508	16	0
8	7	368	0	386	5	0
9	A	60083	0	30260	539	0
10	B	2584	0	1305	37	0
11	C	1952	0	2038	56	0
12	D	1686	0	1772	49	0
13	E	1676	0	1737	38	0
14	F	1454	0	1488	50	0
15	G	1391	0	1458	34	0
16	H	382	0	437	5	0
17	I	1106	0	1122	40	0
18	J	977	0	1027	28	0
19	K	1648	0	1684	41	0
20	L	942	0	996	25	0
21	M	1410	0	1495	45	0
22	N	1075	0	1134	27	0
23	O	944	0	1004	31	0
24	P	962	0	984	28	0
25	Q	953	0	1050	26	0
26	R	1029	0	1092	34	0
27	S	1310	0	1315	37	0
28	T	1395	0	1482	41	0
29	U	776	0	837	23	0
30	V	1078	0	1144	23	0
31	W	2277	0	1146	27	0
32	X	888	0	923	13	0
33	Y	634	0	684	12	0
34	Z	846	0	918	17	0
35	z	42	0	23	0	0
36	2	1	0	0	0	0
36	5	1	0	0	0	0
37	4	1	0	0	0	0
37	6	1	0	0	0	0
37	7	1	0	0	0	0
37	A	453	0	0	0	0
37	B	15	0	0	0	0
37	C	1	0	0	0	0
37	D	2	0	0	0	0
37	E	1	0	0	0	0
37	H	1	0	0	0	0
37	M	2	0	0	0	0
37	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	T	1	0	0	0	0
37	U	1	0	0	0	0
37	V	2	0	0	0	0
37	W	14	0	0	0	0
37	X	1	0	0	0	0
37	Y	1	0	0	0	0
All	All	95397	0	64251	1207	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 8.

All (1207) 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)
9:A:652:C:N4	9:A:657:U:O4	1.86	1.08
9:A:2077:C:H42	9:A:2464:G:H1	1.10	0.98
20:L:15:GLY:HA3	20:L:50:THR:HG21	1.51	0.90
9:A:817:C:OP2	21:M:120:ARG:NH1	2.06	0.89
9:A:540:A:H62	9:A:2055:U:H3	1.18	0.88
9:A:550:G:H5'	19:K:104:SER:HB2	1.56	0.88
12:D:143:ARG:HD2	12:D:163:ILE:HD12	1.59	0.85
9:A:1828:U:OP2	11:C:152:ARG:NH1	2.08	0.85
19:K:75:PRO:HD2	19:K:88:GLU:HG2	1.61	0.83
12:D:93:MET:H	12:D:121:ASN:HD21	1.23	0.82
9:A:1485:U:H5'	9:A:1486:U:H5'	1.62	0.81
17:I:139:GLU:HB3	17:I:141:PRO:HD2	1.62	0.81
2:1:6:LYS:NZ	9:A:2033:A:N7	2.26	0.81
27:S:208:ARG:HG3	27:S:208:ARG:HH11	1.44	0.81
9:A:894:G:N2	9:A:901:C:O2	2.14	0.81
32:X:93:ILE:HG22	32:X:94:ILE:HG13	1.61	0.81
1:0:60:THR:HB	14:F:52:GLU:HA	1.63	0.80
9:A:2464:G:N7	9:A:2518:C:H2'	1.96	0.80
25:Q:138:ARG:HH12	25:Q:203:ILE:HB	1.47	0.80
9:A:2142:G:H1	9:A:2174:C:H42	1.29	0.80
9:A:2345:A:H2'	9:A:2346:A:C8	2.17	0.79
9:A:2125:C:O2	9:A:2161:G:N2	2.15	0.78
2:1:13:LYS:NZ	9:A:528:C:OP1	2.17	0.78
9:A:2726:G:OP1	23:O:28:ARG:NH1	2.16	0.78
10:B:8:G:H21	24:P:85:GLN:HE22	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:75:VAL:HG13	11:C:76:THR:HG22	1.65	0.77
14:F:107:ILE:HG23	14:F:118:PRO:HD2	1.67	0.77
7:6:118:ARG:NH1	9:A:1491:G:OP2	2.14	0.76
9:A:2657:G:OP2	19:K:194:ARG:NH2	2.18	0.76
13:E:128:SER:HB2	13:E:134:ARG:HH22	1.51	0.76
9:A:888:C:H3'	9:A:889:G:H8	1.49	0.76
9:A:1810:C:OP2	11:C:178:ARG:NH2	2.18	0.75
9:A:468:U:O2	9:A:471:U:O2'	2.04	0.75
3:2:6:ASP:O	3:2:39:ARG:NH2	2.20	0.75
7:6:132:PRO:O	7:6:135:LYS:N	2.16	0.75
9:A:2601:U:H5'	9:A:2602:U:H5'	1.69	0.75
9:A:2075:G:N2	9:A:2076:A:N1	2.36	0.74
10:B:44:C:O2	14:F:145:ARG:NH1	2.21	0.74
17:I:122:ILE:HD12	17:I:165:CYS:HB2	1.67	0.74
18:J:129:ILE:HD11	18:J:137:PHE:HB2	1.69	0.74
9:A:182:A:N6	9:A:2447:A:O2'	2.21	0.74
9:A:2719:G:OP1	23:O:83:LYS:NZ	2.21	0.74
9:A:2077:C:N4	9:A:2464:G:H1	1.83	0.74
28:T:164:MET:HB2	28:T:168:ARG:HB2	1.70	0.73
9:A:596:A:H62	9:A:1272:A:H2	1.37	0.73
9:A:2486:A:N6	9:A:2498:G:O2'	2.20	0.73
26:R:76:TYR:OH	26:R:84:ASP:OD2	2.07	0.73
9:A:646:G:OP2	21:M:156:LYS:NZ	2.21	0.73
20:L:88:ASP:OD1	20:L:89:GLN:N	2.20	0.73
9:A:13:A:H2'	9:A:14:A:C8	2.23	0.73
24:P:81:HIS:HD2	24:P:100:THR:HB	1.52	0.73
9:A:2767:A:H3'	9:A:2768:A:H5''	1.71	0.72
9:A:723:G:H2'	9:A:724:G:H5''	1.71	0.72
11:C:157:VAL:HB	11:C:190:GLN:HG3	1.71	0.72
9:A:2069:C:H5'	9:A:2070:A:H5''	1.71	0.72
20:L:13:ASN:HD21	20:L:97:ARG:HB3	1.53	0.72
9:A:869:G:O2'	9:A:925:G:O6	2.08	0.71
9:A:757:U:O2'	9:A:2628:C:O2'	2.08	0.71
10:B:15:A:H4'	10:B:16:G:H5''	1.72	0.71
17:I:63:VAL:HG13	17:I:113:ALA:HB2	1.71	0.71
13:E:128:SER:HB2	13:E:134:ARG:NH2	2.06	0.70
9:A:545:U:H2'	9:A:546:G:C8	2.26	0.70
17:I:77:ALA:HB3	17:I:133:LEU:HB3	1.74	0.70
27:S:192:ASP:OD1	27:S:193:ASP:N	2.25	0.70
9:A:2073:A:N6	9:A:2520:A:O5'	2.25	0.70
19:K:206:GLY:O	19:K:210:LYS:NZ	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:376:U:O2'	9:A:378:A:N1	2.24	0.70
9:A:879:G:O3'	22:N:6:ARG:NH1	2.26	0.69
14:F:55:ASN:HA	14:F:59:THR:HB	1.74	0.69
9:A:1408:A:H5'	9:A:1488:A:H1'	1.74	0.69
1:O:77:HIS:CG	1:O:78:PRO:HD2	2.28	0.69
14:F:160:ALA:HB1	14:F:190:VAL:HB	1.75	0.68
6:5:19:ARG:HG2	9:A:2774:U:H5''	1.76	0.68
13:E:230:THR:HG22	13:E:231:PRO:HD2	1.74	0.68
21:M:182:LYS:HE2	21:M:189:PRO:HG2	1.74	0.68
9:A:844:G:H1'	21:M:130:GLU:HB3	1.76	0.68
10:B:54:G:HO2'	10:B:55:G:H8	1.41	0.68
1:O:37:ARG:N	10:B:45:G:OP1	2.26	0.68
22:N:13:HIS:O	22:N:72:LYS:NZ	2.26	0.68
9:A:1531:A:N6	11:C:94:ASP:OD2	2.27	0.67
18:J:79:VAL:HG22	18:J:130:THR:HG23	1.76	0.67
9:A:1385:G:H5''	33:Y:73:ARG:HH21	1.58	0.67
10:B:10:G:O5'	24:P:61:ARG:NH1	2.28	0.67
4:3:105:ARG:NH1	4:3:149:ARG:O	2.28	0.67
13:E:103:LEU:HB3	13:E:107:GLU:HB2	1.75	0.67
9:A:1086:G:H21	18:J:198:ILE:HG12	1.60	0.67
9:A:2345:A:H2'	9:A:2346:A:H8	1.60	0.67
4:3:111:THR:O	4:3:116:LEU:HD23	1.94	0.66
9:A:2310:U:H5''	24:P:143:ARG:HH12	1.58	0.66
9:A:1978:G:O2'	9:A:1981:C:OP2	2.13	0.66
9:A:1844:U:H5''	9:A:1845:G:H5'	1.77	0.66
9:A:45:A:H2'	9:A:46:C:H5'	1.76	0.66
7:6:121:ARG:NH2	9:A:1549:A:OP1	2.29	0.66
17:I:54:ILE:HG23	17:I:58:LYS:HD3	1.78	0.66
11:C:133:LEU:HD21	11:C:163:LYS:HG2	1.78	0.66
15:G:126:LYS:HE3	15:G:205:VAL:HG11	1.78	0.66
9:A:2662:C:HO2'	9:A:2750:G:HO2'	1.37	0.66
9:A:1832:G:H2'	9:A:1833:G:H5''	1.78	0.65
7:6:121:ARG:HH22	9:A:1549:A:P	2.20	0.65
9:A:2464:G:H4'	9:A:2465:A:H5'	1.78	0.65
15:G:48:ILE:HB	15:G:90:LEU:HB2	1.79	0.65
19:K:100:TRP:H	26:R:99:GLN:HE22	1.43	0.65
11:C:167:SER:HB2	11:C:179:LEU:HG	1.77	0.65
9:A:1812:A:H2'	9:A:1813:A:C8	2.31	0.65
20:L:2:ILE:HB	20:L:33:ALA:HB3	1.78	0.65
9:A:312:C:OP1	30:V:164:LYS:NZ	2.30	0.65
9:A:1817:G:H5'	9:A:1818:U:OP2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:207:PHE:HB2	13:E:228:LEU:HD22	1.78	0.65
9:A:1091:G:O2'	18:J:160:SER:O	2.14	0.65
9:A:2078:C:C2	9:A:2464:G:N2	2.65	0.65
9:A:2105:U:OP1	16:H:47:LYS:NZ	2.18	0.65
6:5:15:ARG:NH1	9:A:2771:A:O2'	2.30	0.64
12:D:166:ARG:NH1	31:W:26:G:OP1	2.29	0.64
9:A:232:G:OP2	9:A:234:C:N4	2.30	0.64
9:A:2256:A:OP1	11:C:239:ARG:NH2	2.31	0.64
9:A:2320:G:H1	9:A:2330:U:H3	1.45	0.64
8:7:85:LEU:HD13	27:S:160:LYS:HE3	1.80	0.64
9:A:1604:A:H2'	9:A:1605:A:C8	2.32	0.64
9:A:96:C:OP1	34:Z:60:LYS:NZ	2.31	0.64
19:K:99:THR:HA	26:R:99:GLN:NE2	2.12	0.64
12:D:202:THR:HG22	12:D:288:ASN:HD21	1.63	0.64
2:1:40:THR:HG23	2:1:42:ASN:H	1.61	0.64
9:A:1769:A:HO2'	9:A:2732:G:HO2'	1.41	0.64
1:0:61:THR:HG22	1:0:62:GLY:H	1.63	0.63
29:U:108:ILE:HD13	34:Z:138:LYS:HD2	1.80	0.63
9:A:9:A:C2	31:W:99:A:H1'	2.33	0.63
13:E:104:THR:HG22	13:E:107:GLU:HG2	1.78	0.63
34:Z:90:LEU:HD21	34:Z:104:ASP:HB3	1.80	0.63
4:3:123:GLY:O	4:3:126:LEU:HB2	1.99	0.63
9:A:2089:U:OP1	11:C:239:ARG:NH1	2.31	0.63
9:A:2628:C:H5'	9:A:2629:A:OP2	1.98	0.63
9:A:1886:A:H2'	9:A:1887:G:H8	1.63	0.63
1:0:43:PRO:HG3	14:F:111:ALA:HB1	1.78	0.63
9:A:642:G:N2	9:A:645:A:OP2	2.24	0.63
9:A:2147:G:H21	9:A:2172:A:H61	1.44	0.63
11:C:207:LYS:HD2	11:C:212:LYS:HD3	1.80	0.63
15:G:76:TYR:OH	15:G:112:THR:HG21	1.99	0.63
24:P:129:LYS:O	24:P:133:GLU:HG2	1.99	0.63
9:A:176:A:H2'	9:A:177:C:C6	2.34	0.62
25:Q:186:ILE:HG12	25:Q:230:SER:HB3	1.80	0.62
9:A:495:A:O2'	30:V:121:GLY:HA3	1.99	0.62
12:D:221:LEU:O	12:D:226:SER:OG	2.17	0.62
20:L:102:ILE:HG22	20:L:103:ALA:H	1.64	0.62
21:M:159:PRO:O	21:M:160:ILE:HD13	1.99	0.62
13:E:243:GLU:OE1	21:M:81:ARG:NH2	2.32	0.62
23:O:101:ASN:OD1	31:W:44:U:O2'	2.18	0.62
28:T:113:LYS:HG3	28:T:125:ILE:HB	1.82	0.62
23:O:67:GLU:OE1	23:O:72:LYS:HE3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1090:U:H1'	18:J:205:ASN:HD21	1.64	0.62
9:A:1111:G:N1	9:A:1114:A:OP2	2.31	0.62
12:D:93:MET:H	12:D:121:ASN:ND2	1.97	0.62
9:A:98:G:H2'	30:V:175:TRP:CZ2	2.35	0.61
14:F:110:LEU:HA	14:F:113:ILE:HD12	1.82	0.61
23:O:34:LEU:HB3	23:O:54:MET:SD	2.40	0.61
2:1:5:LYS:NZ	9:A:2069:C:OP1	2.29	0.61
4:3:148:LYS:NZ	9:A:1638:U:OP2	2.30	0.61
9:A:1883:G:H2'	9:A:1884:A:O4'	2.00	0.61
20:L:76:ILE:HB	25:Q:195:VAL:HB	1.83	0.61
9:A:1082:A:H4'	17:I:83:GLY:HA2	1.82	0.61
20:L:30:ARG:HG2	20:L:32:TYR:H	1.65	0.61
13:E:116:TYR:CZ	13:E:130:ARG:HD3	2.35	0.61
19:K:121:ASP:O	19:K:247:ARG:NH1	2.34	0.61
9:A:2467:A:OP1	9:A:2514:A:O2'	2.09	0.61
17:I:100:THR:HG22	17:I:135:VAL:HG12	1.82	0.61
27:S:208:ARG:HG3	27:S:208:ARG:NH1	2.10	0.61
26:R:112:TYR:CZ	26:R:116:ILE:HD11	2.36	0.61
13:E:60:PHE:O	13:E:196:ARG:NH1	2.33	0.61
9:A:2662:C:O2'	9:A:2750:G:O2'	2.13	0.60
11:C:243:THR:HG22	11:C:244:THR:O	2.01	0.60
21:M:98:LYS:HE2	21:M:106:GLN:HG3	1.83	0.60
9:A:58:U:H1'	9:A:72:A:H2'	1.82	0.60
3:2:20:ARG:HG2	3:2:30:VAL:HG21	1.83	0.60
6:5:31:LYS:HE2	9:A:2495:A:H5'	1.83	0.60
7:6:99:LYS:O	7:6:103:LYS:HG2	2.01	0.60
15:G:94:LYS:HB2	15:G:97:GLU:OE2	2.02	0.60
27:S:208:ARG:HH11	27:S:208:ARG:CG	2.12	0.60
9:A:1473:G:H5'	9:A:1474:A:H5''	1.84	0.60
9:A:2075:G:H5''	9:A:2519:G:H4'	1.83	0.60
32:X:89:PRO:HD3	32:X:120:ASP:OD1	2.01	0.60
1:0:37:ARG:HB3	1:0:42:HIS:HD2	1.66	0.60
9:A:1345:G:OP2	28:T:113:LYS:NZ	2.34	0.60
17:I:161:PHE:HE2	17:I:176:VAL:HG11	1.67	0.60
9:A:255:A:OP2	9:A:271:G:N1	2.19	0.60
9:A:2549:G:N2	9:A:2680:G:O2'	2.35	0.60
33:Y:97:ARG:HG2	33:Y:98:LEU:N	2.16	0.60
9:A:511:G:N1	9:A:514:A:OP2	2.35	0.60
12:D:88:ALA:O	12:D:294:PRO:HG2	2.02	0.60
19:K:239:LEU:HD12	19:K:240:PRO:HD2	1.82	0.60
27:S:104:ASN:HA	27:S:107:ILE:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1689:C:O2'	23:O:19:ARG:NH2	2.35	0.60
9:A:2340:G:H2'	9:A:2341:U:H5'	1.84	0.59
9:A:984:G:N7	22:N:14:ARG:NH2	2.47	0.59
12:D:90:ILE:HD11	12:D:173:LEU:HD11	1.83	0.59
2:1:3:VAL:HG12	9:A:2029:A:C2	2.37	0.59
9:A:543:A:H2'	9:A:543:A:N3	2.17	0.59
9:A:1040:U:OP1	26:R:70:ARG:NH2	2.35	0.59
3:2:56:TYR:OH	9:A:655:C:O4'	2.18	0.59
9:A:1133:U:H2'	9:A:1134:G:H8	1.67	0.59
25:Q:138:ARG:NH1	25:Q:203:ILE:HB	2.16	0.59
9:A:2249:C:P	33:Y:97:ARG:HH22	2.26	0.59
29:U:183:ASN:HB3	29:U:186:GLU:HG3	1.85	0.59
19:K:191:LEU:HD13	19:K:199:ILE:HG13	1.84	0.59
9:A:2340:G:C2'	9:A:2341:U:H5'	2.32	0.59
18:J:171:ILE:HG12	18:J:210:ILE:HG12	1.85	0.59
29:U:119:ILE:HG21	29:U:167:ARG:HH22	1.68	0.59
9:A:411:U:H1'	16:H:42:GLN:HE21	1.68	0.58
26:R:88:ARG:HG3	26:R:115:ILE:HD12	1.84	0.58
8:7:50:ARG:NH1	9:A:1055:A:O2'	2.36	0.58
22:N:67:ARG:NH1	22:N:105:GLU:OE1	2.31	0.58
19:K:61:TRP:HZ2	28:T:157:LEU:HD23	1.67	0.58
9:A:548:G:HO2'	9:A:549:A:P	2.26	0.58
29:U:119:ILE:HG13	29:U:135:LEU:HB3	1.86	0.58
15:G:44:GLY:HA3	15:G:105:HIS:CD2	2.39	0.58
27:S:100:THR:HG22	27:S:102:GLU:H	1.68	0.58
9:A:1497:A:H2'	9:A:1497:A:N3	2.18	0.58
15:G:72:LEU:HD13	15:G:115:MET:HB2	1.86	0.58
9:A:885:G:H1	9:A:911:U:H3	1.52	0.58
12:D:143:ARG:HG2	12:D:144:LEU:H	1.68	0.58
18:J:183:LYS:HE2	18:J:187:LEU:HD21	1.85	0.57
27:S:106:ILE:HD13	28:T:162:GLY:HA3	1.85	0.57
9:A:1220:U:H1'	26:R:4:VAL:HG22	1.85	0.57
9:A:1880:G:N7	21:M:252:ARG:NH1	2.52	0.57
11:C:138:HIS:ND1	11:C:189:GLY:O	2.31	0.57
11:C:223:PRO:HD3	11:C:230:GLY:H	1.69	0.57
9:A:886:U:H3	9:A:910:A:H61	1.52	0.57
9:A:2706:U:H2'	9:A:2706:U:O2	2.05	0.57
9:A:426:C:H2'	9:A:427:A:C8	2.39	0.57
23:O:100:ARG:NH2	31:W:85:U:H5'	2.19	0.57
9:A:2761:U:OP2	9:A:2773:C:N4	2.37	0.57
18:J:189:CYS:SG	18:J:195:ALA:HB2	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:153:LEU:HD12	25:Q:165:TYR:HE2	1.69	0.57
9:A:2321:G:H22	9:A:2329:U:H3	1.50	0.57
9:A:2332:G:H2'	9:A:2333:C:C6	2.40	0.57
6:5:6:SER:HB2	9:A:2483:C:H5''	1.86	0.57
15:G:41:SER:HG	15:G:105:HIS:CE1	2.22	0.57
23:O:11:MET:SD	23:O:11:MET:N	2.78	0.57
1:0:46:ARG:CZ	1:0:66:LYS:HB2	2.35	0.57
9:A:1857:A:HO2'	9:A:1858:A:H8	1.49	0.57
12:D:274:ARG:NH1	31:W:36:A:N1	2.52	0.57
22:N:44:SER:HB3	22:N:70:PRO:HG3	1.86	0.57
28:T:70:TYR:HB2	28:T:73:CYS:SG	2.45	0.57
1:0:53:CYS:HB3	1:0:57:LEU:HB3	1.86	0.56
9:A:681:A:H5''	21:M:122:GLY:HA2	1.87	0.56
9:A:1817:G:H5''	9:A:1817:G:H8	1.70	0.56
18:J:176:LEU:HB3	18:J:196:MET:HG3	1.86	0.56
1:0:42:HIS:CE1	14:F:116:GLN:HE22	2.22	0.56
5:4:98:SER:HB2	5:4:150:LEU:HD21	1.86	0.56
9:A:474:C:O2'	13:E:118:GLN:NE2	2.38	0.56
9:A:531:A:H2'	9:A:532:A:C8	2.40	0.56
9:A:2447:A:H2'	9:A:2447:A:N3	2.19	0.56
9:A:2469:C:H2'	9:A:2470:A:C8	2.39	0.56
11:C:56:ARG:HD3	11:C:81:PRO:HB2	1.86	0.56
19:K:97:ASN:HD21	27:S:135:ILE:H	1.51	0.56
23:O:89:LEU:HD22	23:O:93:VAL:HG23	1.87	0.56
8:7:68:ALA:HB1	8:7:70:TRP:CD1	2.40	0.56
9:A:13:A:H2'	9:A:14:A:H8	1.69	0.56
9:A:1106:C:O2'	9:A:1116:A:OP1	2.17	0.56
10:B:54:G:O6	24:P:80:LYS:NZ	2.32	0.56
20:L:3:GLN:O	20:L:6:THR:OG1	2.10	0.56
24:P:84:VAL:HG21	24:P:155:LEU:HD11	1.88	0.56
5:4:107:LYS:HB2	9:A:663:A:H5'	1.87	0.56
9:A:1273:G:H1	26:R:37:GLN:HE21	1.53	0.56
4:3:99:THR:O	9:A:697:U:O2'	2.23	0.56
9:A:2206:A:H2'	9:A:2207:A:C8	2.41	0.56
18:J:200:ALA:HA	18:J:210:ILE:HD12	1.88	0.56
3:2:59:THR:HG22	3:2:60:ILE:H	1.70	0.56
9:A:1570:C:H4'	9:A:1571:G:C2	2.41	0.56
9:A:2122:C:O2	9:A:2195:G:N1	2.39	0.56
20:L:30:ARG:HD3	20:L:32:TYR:O	2.05	0.56
9:A:131:C:OP2	29:U:101:LYS:NZ	2.39	0.55
9:A:720:U:H3	9:A:733:A:H61	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1211:G:H5''	21:M:111:GLY:HA2	1.87	0.55
12:D:142:GLU:HB3	12:D:166:ARG:HB3	1.88	0.55
19:K:52:SER:HB3	31:W:1:A:O4'	2.06	0.55
9:A:635:C:H2'	9:A:636:C:C6	2.41	0.55
15:G:166:GLU:HG3	15:G:168:ASN:HB2	1.87	0.55
31:W:32:C:H2'	31:W:33:A:H2'	1.87	0.55
6:5:29:ASN:HD21	6:5:31:LYS:HB2	1.72	0.55
13:E:243:GLU:HA	21:M:81:ARG:HH21	1.71	0.55
14:F:67:PRO:O	14:F:71:GLU:HG2	2.06	0.55
20:L:25:ILE:HD11	20:L:40:VAL:HG23	1.89	0.55
9:A:2203:U:H2'	9:A:2204:A:O4'	2.07	0.55
20:L:13:ASN:ND2	20:L:97:ARG:HB3	2.19	0.55
27:S:171:TYR:CE2	27:S:232:ALA:HB2	2.42	0.55
1:0:50:LYS:HG3	1:0:58:VAL:HG13	1.88	0.55
9:A:573:G:H21	26:R:37:GLN:HE22	1.54	0.55
20:L:121:LEU:HD22	25:Q:165:TYR:HE1	1.72	0.55
9:A:2432:G:H5''	21:M:148:GLY:HA3	1.88	0.54
21:M:134:MET:O	21:M:139:ARG:NH1	2.39	0.54
9:A:704:A:O2'	9:A:1374:A:N3	2.39	0.54
28:T:62:LEU:HD22	28:T:77:PHE:CE1	2.42	0.54
32:X:143:GLN:O	32:X:145:GLU:N	2.41	0.54
9:A:1690:A:OP2	23:O:11:MET:HA	2.07	0.54
28:T:112:LYS:HB3	28:T:124:MET:HE1	1.88	0.54
29:U:135:LEU:HD21	29:U:175:TYR:CD2	2.42	0.54
9:A:1195:U:H3'	9:A:1196:A:H8	1.71	0.54
12:D:146:ASP:N	12:D:146:ASP:OD1	2.36	0.54
9:A:318:A:N3	9:A:338:G:O2'	2.41	0.54
9:A:1169:A:H5'	19:K:245:ARG:CZ	2.37	0.54
18:J:125:ILE:HG21	18:J:141:LEU:HD22	1.90	0.54
31:W:29:U:H2'	31:W:83:C:H42	1.72	0.54
9:A:1520:A:H4'	9:A:1521:G:OP1	2.08	0.54
11:C:68:LYS:HD2	11:C:115:GLY:HA2	1.89	0.54
17:I:76:LEU:HD22	17:I:134:PHE:HD1	1.73	0.54
5:4:113:ARG:HB2	21:M:141:PRO:HG2	1.89	0.54
9:A:1090:U:H1'	18:J:205:ASN:ND2	2.22	0.54
9:A:1113:A:H61	17:I:86:VAL:HG11	1.71	0.54
9:A:2047:A:O2'	9:A:2049:G:OP2	2.22	0.54
19:K:155:VAL:HB	19:K:223:VAL:HG22	1.88	0.54
29:U:138:VAL:HG21	29:U:147:ILE:HD11	1.90	0.54
9:A:1098:A:N7	9:A:1124:A:O2'	2.31	0.54
9:A:2414:A:H2'	9:A:2415:C:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:113:THR:HG21	12:D:282:VAL:HG22	1.89	0.54
28:T:146:ASP:O	28:T:150:GLU:HG2	2.07	0.54
10:B:56:U:O2'	14:F:77:ASN:ND2	2.38	0.54
15:G:82:VAL:HG22	15:G:92:VAL:HG22	1.89	0.54
19:K:130:THR:HG21	19:K:241:LEU:HD23	1.89	0.54
9:A:296:G:H2'	9:A:297:U:C5	2.43	0.53
9:A:2249:C:OP2	33:Y:97:ARG:NH2	2.38	0.53
1:O:44:GLU:O	1:O:64:THR:HG23	2.08	0.53
9:A:656:A:H2'	9:A:658:A:C8	2.44	0.53
9:A:740:G:C8	11:C:203:ARG:NH1	2.76	0.53
9:A:1088:U:O4	18:J:205:ASN:ND2	2.36	0.53
28:T:74:TYR:HB3	28:T:75:PRO:HD3	1.90	0.53
9:A:157:G:O2'	9:A:159:A:OP1	2.15	0.53
9:A:2198:A:H2'	9:A:2199:G:C8	2.43	0.53
13:E:85:HIS:HA	21:M:85:LEU:HD13	1.90	0.53
14:F:164:THR:HG22	14:F:165:ARG:H	1.72	0.53
17:I:151:GLN:HA	17:I:154:ARG:HB2	1.90	0.53
9:A:423:G:OP2	9:A:2423:A:O2'	2.26	0.53
9:A:947:A:H2'	9:A:948:U:H5''	1.90	0.53
9:A:1122:U:H1'	9:A:1125:U:H5	1.73	0.53
11:C:132:PRO:O	11:C:135:THR:OG1	2.25	0.53
24:P:61:ARG:NH2	24:P:89:ASP:OD2	2.42	0.53
28:T:114:VAL:HG22	28:T:124:MET:SD	2.49	0.53
24:P:76:PHE:CE2	24:P:78:SER:HB3	2.44	0.53
9:A:953:G:H2'	9:A:954:G:H8	1.73	0.53
9:A:1074:A:N1	17:I:63:VAL:HG21	2.23	0.53
9:A:1854:C:H5'	11:C:252:GLY:O	2.09	0.53
14:F:114:THR:HG22	14:F:152:PHE:CE1	2.44	0.53
18:J:123:PHE:HE1	18:J:152:LYS:HD2	1.73	0.53
24:P:125:GLU:HG2	24:P:162:HIS:CD2	2.44	0.53
9:A:1693:U:H2'	9:A:1694:C:H6	1.74	0.53
14:F:155:ARG:HG2	14:F:159:LEU:HD23	1.91	0.53
9:A:548:G:O2'	9:A:549:A:O5'	2.23	0.53
9:A:1837:U:H5'	9:A:1985:A:H5'	1.91	0.53
9:A:1886:A:H2'	9:A:1887:G:C8	2.44	0.53
21:M:213:LYS:HD3	21:M:233:THR:HB	1.91	0.53
6:5:3:ILE:HD13	9:A:2556:C:H4'	1.91	0.52
9:A:2767:A:H3'	9:A:2768:A:C5'	2.38	0.52
24:P:60:ILE:HD13	24:P:143:ARG:HG3	1.91	0.52
9:A:490:A:O2'	30:V:108:LYS:NZ	2.42	0.52
9:A:2307:G:H2'	9:A:2308:U:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:75:LEU:HD21	17:I:144:ILE:HD11	1.91	0.52
22:N:34:LEU:HD13	22:N:118:VAL:HG13	1.90	0.52
33:Y:77:PHE:HD2	33:Y:137:VAL:HG12	1.75	0.52
9:A:1834:G:H5''	11:C:48:ARG:HH21	1.74	0.52
13:E:240:LEU:O	21:M:81:ARG:HD3	2.09	0.52
27:S:105:ASP:OD1	27:S:106:ILE:N	2.40	0.52
1:O:79:PHE:O	1:O:80:TYR:HD2	1.92	0.52
18:J:195:ALA:O	18:J:199:ILE:HG12	2.09	0.52
28:T:186:PHE:O	28:T:190:ILE:HG13	2.09	0.52
29:U:106:ARG:HB3	29:U:143:ASP:OD2	2.09	0.52
30:V:142:GLN:NE2	30:V:165:THR:OG1	2.42	0.52
9:A:1039:A:OP1	26:R:77:ASN:HB3	2.09	0.52
9:A:1135:A:H4'	17:I:129:MET:HG2	1.91	0.52
9:A:2762:G:H1	9:A:2778:U:H3	1.58	0.52
10:B:43:C:O2'	14:F:116:GLN:NE2	2.43	0.52
28:T:91:LYS:HB3	28:T:93:PHE:CE1	2.45	0.52
28:T:141:HIS:O	28:T:142:PHE:HB2	2.08	0.52
12:D:270:ASP:HB2	12:D:275:VAL:HG22	1.92	0.52
28:T:31:GLU:OE2	28:T:176:ARG:NH2	2.43	0.52
28:T:79:LEU:HB3	28:T:134:ILE:HD11	1.92	0.52
9:A:880:U:OP1	22:N:6:ARG:HD3	2.10	0.52
9:A:1189:G:H5'	27:S:148:LYS:HE2	1.91	0.52
9:A:1273:G:OP2	26:R:13:ARG:NH2	2.41	0.52
11:C:254:ARG:NE	11:C:269:ARG:HH12	2.07	0.52
21:M:134:MET:SD	21:M:138:ARG:NH1	2.83	0.52
1:O:51:VAL:HB	1:O:59:MET:HG3	1.91	0.52
9:A:2204:A:H3'	9:A:2205:G:H8	1.75	0.52
9:A:2753:C:H5''	9:A:2753:C:H6	1.75	0.52
11:C:39:ARG:HA	11:C:44:ILE:O	2.10	0.52
9:A:576:U:H2'	9:A:577:G:O4'	2.10	0.52
9:A:2600:G:OP2	9:A:2600:G:N2	2.32	0.52
19:K:80:ASP:OD1	19:K:80:ASP:N	2.42	0.52
9:A:17:C:O2'	9:A:564:U:OP1	2.26	0.51
9:A:555:A:H61	9:A:558:A:HO2'	1.56	0.51
9:A:1291:C:H5''	9:A:1292:G:H5'	1.92	0.51
9:A:2519:G:O2'	9:A:2521:U:OP2	2.28	0.51
11:C:23:ASN:HD21	11:C:76:THR:HG21	1.75	0.51
28:T:117:ARG:HD3	28:T:123:TYR:CD1	2.46	0.51
34:Z:89:MET:HG2	34:Z:152:LEU:HB2	1.92	0.51
9:A:635:C:H2'	9:A:636:C:H6	1.74	0.51
9:A:1321:A:H4'	9:A:1322:A:H5''	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:150:THR:OG1	12:D:152:PRO:HD2	2.10	0.51
34:Z:108:MET:O	34:Z:112:VAL:HG23	2.10	0.51
9:A:144:A:N3	9:A:2223:A:O2'	2.43	0.51
9:A:297:U:C5	9:A:298:G:C8	2.99	0.51
9:A:407:C:O2'	33:Y:83:ASN:HB2	2.10	0.51
13:E:120:LYS:HG3	13:E:124:ALA:HB3	1.91	0.51
23:O:61:MET:HG3	23:O:80:ILE:HD11	1.92	0.51
1:O:57:LEU:HD21	1:O:59:MET:HG2	1.93	0.51
9:A:312:C:H2'	9:A:313:A:C8	2.45	0.51
9:A:548:G:O2'	9:A:549:A:H8	1.93	0.51
9:A:623:A:C6	13:E:233:SER:HB3	2.46	0.51
9:A:881:U:H4'	22:N:69:PHE:CE2	2.45	0.51
9:A:1269:G:OP1	26:R:2:THR:N	2.44	0.51
9:A:1530:G:H2'	9:A:1532:G:N7	2.26	0.51
9:A:2269:G:H2'	9:A:2270:G:C8	2.45	0.51
9:A:2329:U:H5'	14:F:138:LEU:HD12	1.91	0.51
14:F:108:ASN:O	14:F:112:LEU:HG	2.10	0.51
20:L:15:GLY:HA2	20:L:47:ILE:HD12	1.91	0.51
32:X:88:LYS:HB3	32:X:89:PRO:HD2	1.92	0.51
10:B:54:G:O2'	10:B:55:G:H8	1.91	0.51
23:O:100:ARG:HH21	31:W:85:U:H5'	1.74	0.51
29:U:150:ALA:O	29:U:154:PHE:HB2	2.11	0.51
9:A:1932:A:O2'	9:A:1934:C:N4	2.44	0.51
9:A:2149:A:H1'	9:A:2173:G:O2'	2.11	0.51
9:A:2432:G:C5'	21:M:148:GLY:HA3	2.41	0.51
11:C:244:THR:HG22	11:C:245:PRO:HD2	1.93	0.51
9:A:1133:U:H2'	9:A:1134:G:C8	2.43	0.51
9:A:1615:G:H2'	9:A:1616:A:C8	2.46	0.51
14:F:57:LEU:HD21	14:F:154:ASP:HB2	1.91	0.51
22:N:41:TRP:CZ2	22:N:72:LYS:HE2	2.46	0.51
28:T:123:TYR:HE2	28:T:125:ILE:HD11	1.75	0.51
33:Y:126:LEU:O	33:Y:130:GLU:HG3	2.11	0.51
9:A:2254:A:H2'	9:A:2256:A:N7	2.25	0.51
9:A:2155:C:N3	9:A:2165:G:N2	2.59	0.51
14:F:188:GLN:OE1	14:F:205:MET:HG3	2.11	0.51
15:G:99:ARG:O	15:G:103:GLN:HG3	2.11	0.51
27:S:93:PHE:CZ	27:S:95:ALA:HA	2.46	0.51
28:T:105:VAL:HG22	28:T:132:ILE:HG23	1.93	0.51
6:5:10:ILE:HG13	9:A:2494:C:N4	2.26	0.51
9:A:1408:A:H2'	9:A:1409:G:C8	2.46	0.51
9:A:1573:C:H2'	9:A:1574:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2331:G:H5'	14:F:88:VAL:HG11	1.92	0.51
21:M:176:VAL:O	21:M:180:SER:HB2	2.11	0.51
9:A:880:U:H5''	22:N:6:ARG:HG3	1.93	0.50
9:A:2066:G:H4'	12:D:237:ALA:O	2.12	0.50
10:B:42:C:C5	14:F:119:VAL:HG22	2.45	0.50
10:B:49:U:OP1	24:P:77:ARG:NH2	2.36	0.50
19:K:138:LYS:HD3	19:K:143:TYR:CE1	2.45	0.50
20:L:21:CYS:HB2	20:L:39:ILE:HD12	1.94	0.50
9:A:581:A:O2'	27:S:203:LYS:NZ	2.45	0.50
9:A:1582:A:H2'	9:A:1583:A:C8	2.46	0.50
21:M:240:LYS:HE3	21:M:242:ILE:HD11	1.92	0.50
1:O:41:ILE:HB	14:F:117:ARG:HH11	1.75	0.50
9:A:1976:C:H4'	9:A:1977:C:C5	2.45	0.50
9:A:2142:G:H1	9:A:2174:C:N4	2.04	0.50
9:A:2154:C:H42	9:A:2165:G:H1	1.60	0.50
9:A:2460:U:H2'	9:A:2461:A:C8	2.47	0.50
17:I:154:ARG:HD2	17:I:159:ASN:HB2	1.93	0.50
29:U:111:VAL:O	29:U:114:ILE:HG12	2.11	0.50
5:4:125:ASN:ND2	5:4:127:LYS:H	2.09	0.50
9:A:557:C:H5	27:S:218:ARG:HH12	1.60	0.50
9:A:1168:U:H4'	9:A:1169:A:O4'	2.12	0.50
9:A:1593:U:O2'	9:A:1594:A:OP1	2.25	0.50
14:F:73:PHE:CZ	14:F:221:LYS:HD2	2.47	0.50
25:Q:118:LYS:O	25:Q:121:ASP:HB2	2.12	0.50
9:A:1487:C:H5'	9:A:1488:A:OP1	2.12	0.50
9:A:1523:A:N3	9:A:1546:C:H4'	2.27	0.50
28:T:112:LYS:HB3	28:T:124:MET:CE	2.41	0.50
30:V:99:THR:HB	30:V:129:ALA:HB1	1.93	0.50
6:5:9:PRO:HD3	6:5:16:LEU:HD21	1.94	0.50
9:A:1394:A:H5'	9:A:2230:A:H1'	1.93	0.50
9:A:2330:U:H2'	9:A:2331:G:H8	1.77	0.50
9:A:2464:G:N2	9:A:2467:A:C6	2.80	0.50
9:A:126:C:H2'	9:A:127:C:H6	1.76	0.50
9:A:241:A:H2'	9:A:242:A:C8	2.46	0.50
9:A:1361:U:O2'	29:U:165:LEU:HD11	2.11	0.50
17:I:75:LEU:HD12	17:I:166:PHE:HB2	1.93	0.50
21:M:93:LYS:HZ3	21:M:93:LYS:HB3	1.76	0.50
24:P:46:ALA:HB1	24:P:51:GLU:OE1	2.12	0.50
9:A:1714:A:H2'	9:A:1715:A:O4'	2.12	0.50
9:A:1823:C:O2'	11:C:46:THR:OG1	2.27	0.50
11:C:121:LYS:HG2	11:C:124:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:193:GLU:OE2	12:D:268:LYS:HA	2.12	0.50
9:A:1003:A:H1'	9:A:1018:A:C2	2.47	0.50
9:A:1199:A:H3'	9:A:1200:A:H8	1.77	0.50
9:A:1535:A:H2'	9:A:1536:A:C8	2.47	0.50
11:C:75:VAL:HG11	11:C:89:LEU:HD23	1.93	0.50
9:A:37:A:H2'	9:A:38:C:C6	2.47	0.49
9:A:221:C:H2'	9:A:222:C:H6	1.77	0.49
9:A:984:G:OP2	22:N:14:ARG:NH1	2.44	0.49
9:A:1023:C:OP2	26:R:54:LYS:NZ	2.45	0.49
9:A:1074:A:O2'	17:I:59:LYS:HD2	2.12	0.49
9:A:2320:G:O2'	14:F:174:SER:O	2.29	0.49
9:A:865:A:H2'	9:A:866:G:H5''	1.94	0.49
14:F:123:ALA:HB2	14:F:138:LEU:HG	1.93	0.49
18:J:176:LEU:HD11	18:J:210:ILE:HG21	1.94	0.49
25:Q:153:LEU:HD12	25:Q:165:TYR:CE2	2.47	0.49
29:U:115:LEU:HB2	34:Z:88:PHE:HE2	1.76	0.49
9:A:1195:U:H5''	9:A:1196:A:H2'	1.93	0.49
9:A:1209:U:O2'	9:A:1210:A:H5'	2.11	0.49
9:A:1348:C:H5''	28:T:71:ARG:NH2	2.27	0.49
28:T:167:GLY:O	28:T:171:GLU:HG2	2.12	0.49
9:A:273:U:O2'	9:A:274:G:H5'	2.12	0.49
9:A:1084:G:H5''	9:A:1085:A:H5'	1.93	0.49
9:A:2729:A:N3	9:A:2729:A:H2'	2.28	0.49
12:D:90:ILE:HG22	12:D:91:GLY:O	2.12	0.49
30:V:83:GLU:CD	30:V:106:ASN:H	2.16	0.49
9:A:843:C:H2'	9:A:844:G:C8	2.48	0.49
10:B:62:U:H2'	10:B:63:C:C6	2.47	0.49
14:F:97:SER:HB3	14:F:137:THR:O	2.13	0.49
14:F:211:THR:HG22	14:F:213:ALA:H	1.77	0.49
20:L:14:SER:OG	20:L:86:ILE:HD12	2.13	0.49
28:T:93:PHE:CD2	28:T:138:ASP:HB2	2.47	0.49
30:V:68:MET:HE1	30:V:95:LYS:HA	1.95	0.49
8:7:66:LYS:O	8:7:72:ILE:HD11	2.12	0.49
9:A:296:G:H2'	9:A:297:U:C6	2.47	0.49
9:A:530:U:H2'	9:A:531:A:H8	1.78	0.49
9:A:1953:U:OP1	9:A:2621:U:O2'	2.29	0.49
13:E:72:LEU:HD22	13:E:259:TYR:HB2	1.95	0.49
15:G:155:MET:SD	15:G:188:ILE:HD13	2.53	0.49
18:J:150:LEU:HD13	18:J:203:ALA:HB2	1.95	0.49
9:A:839:G:C2	9:A:840:A:N6	2.81	0.49
9:A:1088:U:H5	18:J:202:THR:HG23	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1569:A:H2'	9:A:1569:A:N3	2.28	0.49
9:A:1693:U:H2'	9:A:1694:C:C6	2.48	0.49
12:D:273:LEU:HD13	25:Q:126:LEU:HD21	1.94	0.49
14:F:153:LEU:HD21	14:F:226:MET:HE1	1.94	0.49
17:I:154:ARG:HA	17:I:157:GLU:HB2	1.95	0.49
7:6:118:ARG:O	7:6:122:LYS:HG3	2.11	0.49
9:A:793:A:N7	11:C:216:VAL:HG21	2.27	0.49
9:A:1813:A:OP1	11:C:257:LYS:HE3	2.11	0.49
9:A:2715:U:H2'	9:A:2716:C:C6	2.48	0.49
19:K:211:GLY:O	19:K:214:GLY:N	2.46	0.49
28:T:186:PHE:CE2	28:T:190:ILE:HD11	2.48	0.49
9:A:880:U:P	22:N:6:ARG:HH11	2.35	0.49
9:A:2352:A:N7	9:A:2354:G:C5	2.81	0.49
9:A:2546:G:H5''	9:A:2547:U:H5''	1.95	0.49
14:F:89:VAL:HG21	14:F:205:MET:HE3	1.95	0.49
20:L:71:ARG:HH12	20:L:104:ARG:HH11	1.60	0.49
9:A:2268:G:H1	9:A:2467:A:H4'	1.77	0.49
30:V:79:ILE:HD11	30:V:136:MET:HB2	1.95	0.49
9:A:838:U:H4'	9:A:839:G:C8	2.48	0.48
9:A:911:U:H2'	9:A:912:C:C6	2.48	0.48
3:2:20:ARG:HD3	9:A:2417:G:OP1	2.14	0.48
9:A:673:G:O2'	21:M:93:LYS:NZ	2.41	0.48
9:A:1195:U:H3'	9:A:1196:A:C8	2.46	0.48
12:D:97:LEU:HD11	12:D:116:GLY:HA3	1.96	0.48
30:V:165:THR:HG23	30:V:167:GLU:H	1.78	0.48
34:Z:65:LEU:HD12	34:Z:68:LEU:HD12	1.94	0.48
9:A:261:U:H3	9:A:266:A:H61	1.60	0.48
9:A:2028:A:H2'	9:A:2029:A:C8	2.48	0.48
5:4:110:ILE:HG13	5:4:143:TYR:CE2	2.48	0.48
9:A:1333:U:H4'	9:A:1334:U:O5'	2.13	0.48
11:C:170:LEU:HD11	11:C:180:ILE:HD13	1.95	0.48
21:M:83:ASP:OD1	21:M:83:ASP:N	2.47	0.48
1:0:49:ALA:HA	1:0:66:LYS:O	2.13	0.48
7:6:122:LYS:NZ	9:A:1407:C:OP1	2.32	0.48
20:L:27:ALA:HB1	20:L:30:ARG:HD2	1.95	0.48
26:R:6:ARG:O	26:R:9:ILE:HG22	2.14	0.48
34:Z:140:TRP:O	34:Z:144:ILE:HG12	2.14	0.48
9:A:795:U:C5	9:A:803:G:C5	3.02	0.48
9:A:2151:G:N2	9:A:2169:C:O2	2.46	0.48
9:A:2718:U:O2'	23:O:83:LYS:HE3	2.14	0.48
10:B:29:C:H2'	10:B:30:A:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:69:LEU:HD11	15:G:121:LYS:O	2.14	0.48
15:G:71:GLU:O	15:G:176:ARG:NH1	2.45	0.48
33:Y:110:TRP:NE1	33:Y:112:ALA:HB3	2.29	0.48
9:A:1208:G:HO2'	9:A:1209:U:H6	1.62	0.48
9:A:2714:A:H2'	9:A:2715:U:O4'	2.14	0.48
11:C:107:ILE:O	11:C:110:ASP:HB2	2.13	0.48
12:D:142:GLU:O	12:D:165:MET:HA	2.13	0.48
9:A:306:G:O3'	30:V:158:LYS:NZ	2.44	0.48
9:A:555:A:N6	9:A:558:A:O2'	2.37	0.48
9:A:2154:C:N4	9:A:2165:G:H22	2.12	0.48
9:A:2524:C:C2	9:A:2599:G:N2	2.82	0.48
12:D:296:LYS:HB3	12:D:302:ILE:HD11	1.95	0.48
20:L:71:ARG:HH12	20:L:104:ARG:NH1	2.12	0.48
21:M:243:LYS:O	21:M:246:VAL:HG23	2.14	0.48
10:B:67:U:C4	10:B:109:U:C4	3.01	0.48
13:E:172:SER:HA	13:E:245:LEU:O	2.14	0.48
23:O:31:LEU:HD23	23:O:31:LEU:HA	1.57	0.48
9:A:1454:G:H2'	9:A:1455:A:C8	2.49	0.48
9:A:2393:A:O2'	24:P:160:ARG:NH1	2.39	0.48
10:B:5:C:H2'	10:B:6:U:C6	2.48	0.48
19:K:177:SER:OG	19:K:179:ARG:HG3	2.14	0.48
5:4:126:THR:HA	5:4:129:LYS:HE3	1.94	0.47
9:A:1485:U:H5'	9:A:1486:U:C5'	2.40	0.47
9:A:1701:A:H2'	9:A:1702:G:O4'	2.14	0.47
9:A:2073:A:H2'	9:A:2519:G:H21	1.78	0.47
9:A:2308:U:H2'	9:A:2309:U:C6	2.48	0.47
18:J:92:ALA:HB3	18:J:93:PRO:HD3	1.96	0.47
23:O:20:LEU:O	23:O:22:ARG:HG2	2.14	0.47
28:T:117:ARG:HD3	28:T:123:TYR:CE1	2.49	0.47
9:A:138:C:H2'	9:A:139:U:H6	1.79	0.47
9:A:753:G:H2'	9:A:754:A:C8	2.49	0.47
11:C:42:ARG:CZ	11:C:44:ILE:HD11	2.44	0.47
19:K:213:LEU:HD12	19:K:213:LEU:HA	1.75	0.47
4:3:144:PRO:HG2	4:3:149:ARG:HB2	1.97	0.47
9:A:1272:A:OP1	26:R:13:ARG:NH1	2.48	0.47
9:A:2403:U:H4'	32:X:112:ASP:HA	1.96	0.47
9:A:2463:G:H2'	9:A:2464:G:O4'	2.14	0.47
9:A:2658:A:P	19:K:175:ARG:HH12	2.37	0.47
15:G:196:PRO:HG2	15:G:197:TYR:CD2	2.49	0.47
23:O:111:LEU:HD12	23:O:111:LEU:HA	1.61	0.47
26:R:72:ARG:HA	26:R:72:ARG:HD3	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:635:C:OP2	21:M:190:SER:HB2	2.14	0.47
10:B:50:U:P	24:P:151:ARG:HE	2.37	0.47
26:R:79:SER:OG	26:R:80:LYS:N	2.47	0.47
9:A:555:A:C6	9:A:558:A:H1'	2.49	0.47
9:A:881:U:H2'	9:A:882:U:C6	2.49	0.47
9:A:1226:U:O5'	9:A:1226:U:H6	1.98	0.47
9:A:2206:A:H2'	9:A:2207:A:H8	1.78	0.47
9:A:2290:A:H2'	9:A:2291:A:C8	2.50	0.47
10:B:49:U:P	24:P:77:ARG:HH22	2.38	0.47
17:I:75:LEU:HD13	17:I:140:ILE:HB	1.96	0.47
19:K:90:ALA:O	27:S:140:ARG:HD3	2.14	0.47
31:W:5:A:H5'	31:W:6:A:OP2	2.14	0.47
9:A:947:A:H61	9:A:950:A:H61	1.61	0.47
10:B:30:A:H2'	10:B:31:C:C6	2.49	0.47
12:D:101:SER:CB	25:Q:178:HIS:HD2	2.28	0.47
15:G:177:ASP:O	15:G:181:VAL:HG12	2.13	0.47
26:R:61:TRP:O	26:R:65:ILE:HG13	2.13	0.47
9:A:646:G:H2'	9:A:647:C:C6	2.50	0.47
9:A:1494:G:H22	9:A:1550:U:H3	1.60	0.47
9:A:1567:C:H5'	9:A:1568:U:OP2	2.14	0.47
9:A:1806:U:H2'	9:A:1807:C:C6	2.50	0.47
9:A:2406:G:H5''	9:A:2407:U:O4'	2.14	0.47
15:G:63:LEU:HD21	15:G:84:LYS:HZ2	1.80	0.47
15:G:137:THR:HG22	15:G:139:GLU:HG3	1.96	0.47
17:I:161:PHE:CE2	17:I:176:VAL:HG11	2.49	0.47
23:O:36:THR:HG21	23:O:81:TYR:H	1.79	0.47
26:R:106:ASN:O	26:R:110:MET:HG3	2.15	0.47
28:T:79:LEU:HD23	28:T:79:LEU:HA	1.67	0.47
9:A:724:G:H1'	9:A:729:A:H62	1.78	0.47
9:A:1415:U:C4	9:A:1416:A:C6	3.03	0.47
15:G:112:THR:HA	15:G:115:MET:HE3	1.96	0.47
17:I:79:ILE:HG13	17:I:147:TYR:CE1	2.50	0.47
19:K:75:PRO:CD	19:K:88:GLU:HG2	2.39	0.47
26:R:49:ASP:HA	26:R:52:ARG:HB2	1.96	0.47
32:X:99:THR:HG22	32:X:113:HIS:HB3	1.97	0.47
34:Z:123:GLU:O	34:Z:128:VAL:HG22	2.13	0.47
9:A:557:C:H41	27:S:218:ARG:NH1	2.13	0.47
13:E:206:LEU:HB3	13:E:245:LEU:HD22	1.97	0.47
14:F:105:ALA:O	14:F:109:GLU:HG2	2.15	0.47
22:N:59:ARG:HG3	22:N:60:ARG:H	1.79	0.47
23:O:82:GLU:HB2	23:O:85:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:7:C:N4	9:A:8:G:C6	2.83	0.47
9:A:583:G:H5'	9:A:585:A:N7	2.30	0.47
9:A:1497:A:O2'	9:A:1498:G:H5'	2.14	0.47
17:I:79:ILE:HD11	17:I:151:GLN:NE2	2.30	0.47
17:I:120:ALA:HB1	17:I:123:LYS:HE3	1.96	0.47
29:U:140:VAL:HA	29:U:172:LYS:HB2	1.97	0.47
6:5:17:ILE:HG22	6:5:18:ARG:H	1.79	0.46
9:A:612:U:HO2'	9:A:614:G:HO2'	1.57	0.46
9:A:932:A:H2'	9:A:933:G:C8	2.50	0.46
9:A:1407:C:H2'	9:A:1408:A:C8	2.50	0.46
9:A:1864:A:H2'	9:A:1865:G:O4'	2.15	0.46
9:A:2369:A:H2'	9:A:2370:G:O4'	2.15	0.46
9:A:2725:G:H4'	23:O:32:ARG:HH12	1.78	0.46
10:B:31:C:OP1	24:P:49:ARG:HD2	2.16	0.46
14:F:54:ILE:HG23	14:F:58:LYS:HZ2	1.80	0.46
20:L:117:ALA:HA	20:L:118:PRO:HD3	1.75	0.46
29:U:161:LYS:O	29:U:177:MET:HG2	2.15	0.46
9:A:2307:G:N2	9:A:2360:U:H1'	2.29	0.46
9:A:2699:U:H2'	9:A:2700:C:H6	1.81	0.46
13:E:113:ARG:H	13:E:113:ARG:HG3	1.43	0.46
16:H:57:ILE:HD12	16:H:83:LYS:HD3	1.97	0.46
26:R:116:ILE:O	26:R:119:GLU:HG2	2.15	0.46
32:X:97:ARG:HA	32:X:97:ARG:HD3	1.51	0.46
9:A:608:U:O2'	21:M:91:SER:HB2	2.16	0.46
9:A:1225:G:P	13:E:204:LYS:HZ1	2.38	0.46
9:A:1277:G:H21	13:E:133:LEU:HB3	1.80	0.46
10:B:30:A:P	24:P:78:SER:HB2	2.55	0.46
15:G:196:PRO:O	15:G:211:ARG:HA	2.15	0.46
23:O:106:ARG:NH1	23:O:126:VAL:HG21	2.30	0.46
9:A:6:A:H2'	9:A:7:C:O4'	2.16	0.46
11:C:94:ASP:HB3	11:C:96:GLU:CD	2.36	0.46
15:G:123:PHE:O	15:G:174:SER:HA	2.16	0.46
18:J:84:LEU:HD21	18:J:95:VAL:HB	1.97	0.46
22:N:77:ARG:NH2	22:N:86:GLY:O	2.40	0.46
30:V:108:LYS:HD2	30:V:128:ALA:HB2	1.97	0.46
1:O:74:SER:HB2	14:F:158:ASN:HA	1.98	0.46
9:A:221:C:H2'	9:A:222:C:C6	2.51	0.46
9:A:1557:G:N3	9:A:1557:G:H2'	2.31	0.46
9:A:1836:C:OP1	11:C:219:VAL:HG23	2.15	0.46
9:A:2660:G:H2'	9:A:2661:A:O4'	2.14	0.46
10:B:16:G:N3	10:B:16:G:H2'	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:32:ARG:HH21	23:O:81:TYR:HE1	1.62	0.46
25:Q:138:ARG:HH22	25:Q:203:ILE:CG2	2.28	0.46
9:A:126:C:H2'	9:A:127:C:C6	2.51	0.46
9:A:564:U:C2'	9:A:565:G:H5'	2.46	0.46
9:A:1074:A:H3'	9:A:1075:G:C5'	2.45	0.46
12:D:96:LYS:HD2	12:D:282:VAL:HG23	1.96	0.46
19:K:135:ILE:HG22	19:K:217:LEU:HD22	1.98	0.46
20:L:67:LYS:HG3	20:L:68:GLU:H	1.81	0.46
27:S:105:ASP:O	27:S:109:GLN:HG2	2.16	0.46
9:A:17:C:O3'	26:R:23:SER:HA	2.15	0.46
9:A:169:C:H2'	9:A:170:U:C6	2.50	0.46
10:B:92:U:OP1	22:N:16:ARG:HG3	2.16	0.46
11:C:178:ARG:HG2	11:C:179:LEU:N	2.31	0.46
22:N:8:ARG:H	22:N:8:ARG:HD2	1.81	0.46
23:O:106:ARG:HH11	23:O:126:VAL:HG21	1.80	0.46
9:A:750:A:H1'	9:A:751:C:H5	1.80	0.46
9:A:1073:G:H4'	9:A:1074:A:H5''	1.97	0.46
2:1:45:SER:HB3	31:W:87:A:OP1	2.16	0.46
9:A:685:G:P	13:E:105:ARG:HH22	2.39	0.46
9:A:2396:G:H2'	9:A:2397:U:C6	2.51	0.46
14:F:132:VAL:HG22	14:F:136:MET:HE1	1.97	0.46
4:3:135:ARG:NH2	9:A:480:G:N7	2.61	0.46
9:A:348:U:O5'	9:A:348:U:H6	2.00	0.46
9:A:716:A:H2'	9:A:717:A:O4'	2.16	0.46
9:A:1269:G:P	13:E:143:PRO:HG3	2.56	0.46
9:A:1320:G:O5'	9:A:1320:G:H8	1.99	0.46
9:A:1632:U:O2'	9:A:1633:A:H5'	2.15	0.46
17:I:73:CYS:SG	17:I:134:PHE:HB3	2.57	0.46
27:S:124:PHE:CE1	27:S:165:GLY:HA3	2.50	0.46
27:S:230:TYR:CG	27:S:231:PRO:HD2	2.51	0.46
31:W:30:A:H2'	31:W:31:U:O4'	2.16	0.46
9:A:701:U:H2'	9:A:702:C:O4'	2.16	0.45
9:A:1309:U:O2'	9:A:1683:G:N2	2.48	0.45
9:A:1704:A:O2'	9:A:1710:G:N7	2.38	0.45
9:A:2112:U:H2'	9:A:2113:G:O4'	2.16	0.45
13:E:51:GLU:HB3	13:E:69:PHE:CD1	2.51	0.45
29:U:109:LEU:HD21	29:U:141:ARG:HB3	1.98	0.45
5:4:156:ASN:OD1	5:4:158:LYS:HD3	2.16	0.45
11:C:97:LYS:O	11:C:98:ARG:HD3	2.17	0.45
11:C:133:LEU:HD21	11:C:163:LYS:HE2	1.97	0.45
17:I:96:LEU:HD12	17:I:102:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:116:ILE:HA	26:R:119:GLU:HG2	1.99	0.45
28:T:145:TYR:HD2	28:T:172:LEU:HD23	1.82	0.45
9:A:794:A:C5	9:A:796:G:H1'	2.51	0.45
9:A:1502:A:O5'	9:A:1502:A:H8	2.00	0.45
9:A:2007:U:H5''	12:D:223:THR:OG1	2.16	0.45
9:A:2260:U:H2'	9:A:2261:U:C6	2.51	0.45
9:A:2709:C:H2'	9:A:2710:A:H8	1.81	0.45
21:M:140:ILE:HG23	21:M:141:PRO:HD2	1.99	0.45
5:4:112:ARG:HD2	21:M:140:ILE:HD13	1.97	0.45
9:A:116:A:N3	9:A:163:G:H1'	2.32	0.45
9:A:807:C:H2'	9:A:808:C:C6	2.52	0.45
9:A:1088:U:N1	9:A:1090:U:H5'	2.31	0.45
9:A:1511:U:H6	9:A:1511:U:O5'	1.98	0.45
21:M:143:LEU:HA	21:M:143:LEU:HD23	1.72	0.45
31:W:5:A:H3'	31:W:6:A:C8	2.51	0.45
9:A:457:C:O2'	9:A:458:G:H5'	2.17	0.45
9:A:1074:A:C2	17:I:109:LEU:HA	2.51	0.45
9:A:1559:A:H5'	9:A:1560:C:OP2	2.17	0.45
9:A:1801:A:OP1	11:C:207:LYS:HG3	2.16	0.45
14:F:83:LYS:O	14:F:211:THR:HG23	2.16	0.45
14:F:155:ARG:O	14:F:159:LEU:HB3	2.17	0.45
16:H:69:VAL:HG12	16:H:70:ARG:O	2.17	0.45
17:I:86:VAL:HA	17:I:89:PHE:HB2	1.99	0.45
20:L:50:THR:HG23	20:L:51:PRO:HD2	1.97	0.45
1:0:70:VAL:HG11	1:0:73:TRP:HB3	1.98	0.45
3:2:8:ARG:NH1	9:A:2302:C:OP2	2.49	0.45
25:Q:148:ILE:HD13	25:Q:168:ILE:HG13	1.98	0.45
9:A:739:G:O2'	9:A:741:U:H5''	2.16	0.45
9:A:2410:U:H2'	9:A:2411:C:C6	2.51	0.45
11:C:254:ARG:CZ	11:C:269:ARG:HH12	2.29	0.45
12:D:232:LEU:HA	12:D:232:LEU:HD12	1.70	0.45
19:K:225:LYS:HB2	19:K:225:LYS:HE3	1.55	0.45
21:M:163:ARG:O	21:M:167:VAL:HG23	2.17	0.45
22:N:11:LYS:HD3	22:N:87:LYS:HB3	1.99	0.45
22:N:54:MET:HE1	22:N:104:TYR:HB3	1.99	0.45
1:0:50:LYS:HE3	1:0:58:VAL:HG22	1.99	0.45
9:A:1559:A:H3'	9:A:1560:C:H6	1.80	0.45
20:L:28:SER:HB2	20:L:29:ASN:H	1.62	0.45
23:O:32:ARG:O	23:O:36:THR:HG23	2.17	0.45
28:T:91:LYS:HB3	28:T:93:PHE:HE1	1.82	0.45
9:A:33:A:O2'	9:A:466:A:N3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:133:A:O2'	9:A:134:A:N7	2.40	0.45
9:A:876:A:H2'	9:A:876:A:N3	2.30	0.45
14:F:164:THR:HG22	14:F:165:ARG:N	2.32	0.45
14:F:187:GLU:HG2	14:F:202:ALA:HB1	1.99	0.45
17:I:96:LEU:HD13	17:I:102:LEU:HB2	1.98	0.45
4:3:94:ALA:HB1	4:3:98:LEU:HD12	1.98	0.45
9:A:674:C:H5''	21:M:96:LYS:HG3	1.98	0.45
9:A:2792:C:H2'	9:A:2793:A:O4'	2.16	0.45
10:B:48:C:OP2	24:P:49:ARG:NH2	2.50	0.45
21:M:130:GLU:O	21:M:132:GLY:N	2.50	0.45
27:S:83:PRO:HB2	28:T:145:TYR:HE1	1.82	0.45
9:A:372:G:H2'	9:A:373:C:C6	2.53	0.44
9:A:506:G:O2'	28:T:90:ASN:ND2	2.51	0.44
9:A:591:C:H2'	9:A:592:G:C8	2.51	0.44
9:A:815:A:H2'	9:A:817:C:C4	2.52	0.44
9:A:984:G:P	22:N:87:LYS:HG3	2.57	0.44
9:A:1917:G:OP1	11:C:236:PRO:HB2	2.16	0.44
9:A:2108:G:N2	9:A:2210:C:H1'	2.33	0.44
13:E:88:LEU:HD22	21:M:85:LEU:HD12	1.98	0.44
33:Y:144:ASP:O	33:Y:148:GLU:HG3	2.18	0.44
9:A:1385:G:N2	9:A:1388:A:OP2	2.40	0.44
17:I:100:THR:HG21	17:I:143:ALA:HB2	1.99	0.44
27:S:204:LYS:HD3	27:S:204:LYS:HA	1.42	0.44
9:A:490:A:H1'	30:V:108:LYS:NZ	2.33	0.44
9:A:491:A:N3	9:A:493:G:H5''	2.32	0.44
9:A:1603:A:H2'	9:A:1604:A:C8	2.52	0.44
9:A:2284:A:H5''	9:A:2285:A:H5'	1.98	0.44
11:C:75:VAL:HG12	11:C:89:LEU:O	2.18	0.44
15:G:206:ASP:OD1	15:G:206:ASP:N	2.49	0.44
1:0:79:PHE:O	1:0:80:TYR:CD2	2.69	0.44
9:A:1921:G:N2	9:A:1938:C:H1'	2.33	0.44
9:A:2116:C:C2	9:A:2201:G:N2	2.86	0.44
12:D:86:VAL:HG11	12:D:174:VAL:HG22	2.00	0.44
14:F:73:PHE:CE2	14:F:221:LYS:HD2	2.51	0.44
23:O:96:ARG:HD3	23:O:97:TYR:CE2	2.52	0.44
24:P:67:THR:HB	24:P:68:PRO:HD2	1.99	0.44
26:R:31:LEU:O	26:R:35:ILE:HG13	2.17	0.44
29:U:124:ALA:HB2	29:U:135:LEU:HD12	1.98	0.44
9:A:645:A:H5'	21:M:156:LYS:HZ3	1.82	0.44
9:A:1055:A:C2	9:A:2505:A:H5'	2.52	0.44
9:A:1075:G:N2	9:A:1138:G:O2'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:88:G:N2	10:B:90:G:H3'	2.32	0.44
11:C:76:THR:OG1	11:C:77:ILE:N	2.51	0.44
13:E:204:LYS:HA	13:E:225:THR:HB	2.00	0.44
14:F:188:GLN:OE1	14:F:188:GLN:HA	2.16	0.44
15:G:76:TYR:HE1	15:G:108:PHE:HB3	1.82	0.44
19:K:48:ARG:HH22	31:W:1:A:H3'	1.82	0.44
24:P:105:ILE:HD13	24:P:123:ILE:HG12	1.99	0.44
25:Q:117:VAL:HG11	25:Q:125:ILE:HD12	2.00	0.44
25:Q:180:THR:HG23	25:Q:195:VAL:HG13	1.99	0.44
31:W:34:U:O3'	31:W:35:U:H4'	2.18	0.44
4:3:96:LEU:HD23	4:3:96:LEU:HA	1.78	0.44
9:A:1532:G:N1	11:C:94:ASP:OD1	2.51	0.44
9:A:2252:G:H2'	9:A:2253:U:O4'	2.18	0.44
12:D:261:ILE:HD12	12:D:283:PRO:HD3	1.99	0.44
18:J:183:LYS:HD3	18:J:199:ILE:HD11	2.00	0.44
25:Q:155:VAL:HA	25:Q:156:PRO:HD3	1.86	0.44
26:R:69:ILE:HD11	26:R:81:PHE:CD2	2.53	0.44
9:A:843:C:H2'	9:A:844:G:H8	1.82	0.44
9:A:1111:G:N2	9:A:1113:A:H3'	2.32	0.44
9:A:2237:A:H2'	9:A:2238:A:H8	1.83	0.44
9:A:2798:G:OP2	19:K:219:ASN:ND2	2.47	0.44
27:S:191:LEU:HD23	27:S:215:PRO:HA	1.99	0.44
9:A:411:U:H1'	16:H:42:GLN:NE2	2.31	0.44
9:A:1074:A:C6	17:I:63:VAL:HG21	2.53	0.44
9:A:1076:A:H62	9:A:1138:G:H21	1.64	0.44
9:A:1849:A:H5'	9:A:1850:G:OP2	2.18	0.44
9:A:2381:C:H2'	9:A:2382:G:O4'	2.18	0.44
15:G:195:GLU:HB2	15:G:196:PRO:HD2	2.00	0.44
26:R:58:ARG:HH12	26:R:94:ARG:NH1	2.15	0.44
27:S:137:ILE:HG13	27:S:140:ARG:HG3	1.99	0.44
34:Z:132:LEU:HA	34:Z:132:LEU:HD23	1.78	0.44
9:A:197:G:H2'	9:A:198:A:C8	2.52	0.44
9:A:2154:C:H42	9:A:2165:G:H22	1.65	0.44
14:F:111:ALA:O	14:F:115:GLY:N	2.50	0.44
23:O:40:LYS:HB2	23:O:85:ILE:HD13	2.00	0.44
26:R:97:LEU:HD23	26:R:97:LEU:HA	1.75	0.44
29:U:119:ILE:HD12	29:U:135:LEU:HD13	1.99	0.44
9:A:16:G:H2'	9:A:17:C:C6	2.53	0.43
9:A:349:A:H2'	9:A:350:G:O4'	2.17	0.43
9:A:879:G:H4'	22:N:8:ARG:HH21	1.83	0.43
9:A:888:C:H3'	9:A:889:G:C8	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1523:A:HO2'	9:A:1546:C:HO2'	1.63	0.43
9:A:1733:G:H4'	9:A:1992:A:H5''	1.99	0.43
9:A:2298:C:O2'	9:A:2299:G:H5'	2.18	0.43
11:C:90:ILE:HD11	11:C:92:TYR:CZ	2.53	0.43
14:F:113:ILE:O	14:F:155:ARG:NH2	2.50	0.43
14:F:117:ARG:HA	14:F:118:PRO:HD3	1.72	0.43
22:N:4:PRO:HG2	22:N:93:TRP:CZ3	2.53	0.43
24:P:82:LEU:HD12	24:P:82:LEU:HA	1.89	0.43
25:Q:118:LYS:HB2	25:Q:121:ASP:OD2	2.18	0.43
9:A:495:A:OP1	30:V:113:LYS:NZ	2.41	0.43
9:A:2769:G:C4	15:G:42:ARG:HD3	2.53	0.43
9:A:2770:C:H2'	9:A:2771:A:O4'	2.18	0.43
12:D:107:GLY:HA3	25:Q:202:ASN:ND2	2.33	0.43
22:N:1:MET:HG2	22:N:44:SER:HB2	2.00	0.43
30:V:137:LEU:HD23	30:V:137:LEU:HA	1.80	0.43
9:A:14:A:H5'	9:A:15:G:OP2	2.18	0.43
9:A:530:U:H2'	9:A:531:A:C8	2.53	0.43
9:A:1092:C:H4'	18:J:161:LYS:HG2	2.01	0.43
9:A:1142:G:O2'	9:A:1143:C:H5'	2.18	0.43
9:A:2245:U:H2'	9:A:2246:U:C6	2.53	0.43
12:D:223:THR:O	12:D:225:GLY:N	2.52	0.43
13:E:144:LYS:HA	13:E:144:LYS:HD3	1.73	0.43
21:M:81:ARG:H	21:M:84:ASN:ND2	2.17	0.43
21:M:187:ILE:O	21:M:189:PRO:HD3	2.18	0.43
22:N:29:PHE:CD2	22:N:67:ARG:HD3	2.53	0.43
34:Z:86:GLU:HB3	34:Z:108:MET:HE1	1.99	0.43
3:2:8:ARG:NH1	3:2:38:ASN:HB2	2.34	0.43
9:A:254:U:C5	9:A:272:U:C4	3.07	0.43
9:A:640:G:H2'	9:A:641:C:C6	2.53	0.43
9:A:1087:G:H1'	18:J:198:ILE:HG23	2.00	0.43
10:B:81:U:H2'	10:B:82:G:C8	2.54	0.43
7:6:115:ARG:HA	7:6:118:ARG:HD2	2.00	0.43
9:A:1620:U:O2'	9:A:1621:C:H4'	2.19	0.43
9:A:1635:C:OP1	29:U:144:LYS:HB2	2.17	0.43
9:A:2201:G:N2	9:A:2202:C:N3	2.66	0.43
9:A:2373:C:H2'	9:A:2374:C:O4'	2.19	0.43
9:A:2410:U:H2'	9:A:2411:C:H6	1.84	0.43
15:G:147:LEU:HA	15:G:147:LEU:HD23	1.76	0.43
15:G:184:PHE:O	15:G:188:ILE:HG12	2.19	0.43
17:I:141:PRO:HB3	17:I:182:MET:HB3	2.00	0.43
1:0:38:LYS:HD2	1:0:41:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:556:C:H4'	9:A:557:C:OP1	2.15	0.43
11:C:257:LYS:HB2	11:C:260:LYS:HG3	1.99	0.43
13:E:202:ALA:O	13:E:225:THR:HG21	2.18	0.43
17:I:110:VAL:HG21	17:I:132:TRP:HE1	1.84	0.43
19:K:48:ARG:N	31:W:95:A:OP1	2.51	0.43
25:Q:154:GLU:HA	25:Q:162:LEU:HD22	2.01	0.43
26:R:26:GLY:O	26:R:30:ARG:NH1	2.52	0.43
27:S:100:THR:O	27:S:103:TYR:HB3	2.19	0.43
27:S:128:VAL:HG22	27:S:133:GLN:HG2	2.01	0.43
28:T:117:ARG:HA	28:T:117:ARG:HD2	1.38	0.43
7:6:121:ARG:HH12	9:A:1549:A:H5'	1.84	0.43
9:A:598:U:H2'	9:A:599:C:C6	2.53	0.43
9:A:888:C:H5	9:A:908:A:H2	1.66	0.43
9:A:2257:C:O2'	9:A:2258:A:H5'	2.19	0.43
10:B:37:U:OP1	10:B:37:U:H6	2.01	0.43
11:C:100:ILE:HD12	11:C:101:LEU:O	2.17	0.43
12:D:90:ILE:HD13	12:D:173:LEU:HD21	2.00	0.43
12:D:181:PRO:O	12:D:182:SER:HB3	2.19	0.43
24:P:70:ARG:HH11	24:P:138:LYS:HE3	1.84	0.43
25:Q:225:LYS:HB3	25:Q:229:LEU:HD12	2.00	0.43
27:S:116:PRO:HA	27:S:117:PRO:HD3	1.89	0.43
1:0:53:CYS:HG	1:0:73:TRP:HE1	1.63	0.43
5:4:132:LEU:HD23	5:4:132:LEU:HA	1.84	0.43
9:A:169:C:H2'	9:A:170:U:H6	1.83	0.43
9:A:1926:A:H62	9:A:1931:U:H3	1.67	0.43
9:A:2722:C:H2'	9:A:2723:A:O4'	2.19	0.43
11:C:161:ILE:HG13	11:C:162:ALA:N	2.33	0.43
17:I:76:LEU:HD22	17:I:134:PHE:CD1	2.53	0.43
19:K:99:THR:HA	26:R:99:GLN:HE22	1.83	0.43
27:S:137:ILE:CG1	27:S:140:ARG:HG3	2.49	0.43
31:W:1:A:H2'	31:W:2:G:H8	1.83	0.43
34:Z:74:GLU:H	34:Z:74:GLU:HG3	1.44	0.43
34:Z:85:GLY:O	34:Z:88:PHE:HB3	2.19	0.43
13:E:203:GLU:O	13:E:204:LYS:HB2	2.19	0.43
14:F:221:LYS:O	14:F:225:LEU:HG	2.19	0.43
15:G:92:VAL:HG21	15:G:109:ARG:HB2	2.01	0.43
29:U:101:LYS:HG2	29:U:102:LEU:HD12	2.01	0.43
32:X:85:GLN:O	32:X:122:LEU:HA	2.18	0.43
2:1:35:ALA:HB2	28:T:67:LEU:HD12	2.00	0.43
7:6:115:ARG:NH1	9:A:1491:G:OP1	2.52	0.43
9:A:211:A:H2'	9:A:212:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:891:G:C2	9:A:906:C:C2	3.07	0.43
12:D:120:GLY:HA3	12:D:141:TYR:O	2.19	0.43
20:L:63:VAL:HG23	20:L:64:ARG:HG3	2.00	0.43
32:X:87:ALA:O	32:X:120:ASP:HA	2.18	0.43
34:Z:92:LEU:HD23	34:Z:92:LEU:HA	1.86	0.43
1:O:76:ASN:O	1:O:76:ASN:ND2	2.52	0.42
4:3:138:LEU:HD23	4:3:138:LEU:HA	1.77	0.42
7:6:137:LYS:HE2	7:6:137:LYS:HB3	1.66	0.42
9:A:844:G:H2'	9:A:845:C:C6	2.54	0.42
9:A:1448:A:H4'	9:A:1449:C:O4'	2.19	0.42
9:A:2430:G:H2'	9:A:2431:G:O4'	2.18	0.42
10:B:41:U:H3'	10:B:42:C:C5'	2.48	0.42
12:D:90:ILE:HD11	12:D:137:VAL:HG11	2.01	0.42
13:E:109:ARG:HG2	13:E:110:GLY:N	2.33	0.42
19:K:144:THR:HG22	19:K:146:SER:H	1.84	0.42
21:M:161:ASN:HA	21:M:201:LEU:O	2.18	0.42
28:T:152:LEU:HD22	28:T:156:LYS:HB3	2.01	0.42
34:Z:76:LEU:HD22	34:Z:115:MET:CE	2.49	0.42
9:A:636:C:O2'	9:A:668:U:H5''	2.18	0.42
9:A:1689:C:H3'	23:O:12:LYS:HG2	2.00	0.42
9:A:2039:C:H2'	9:A:2040:U:O4'	2.18	0.42
9:A:2066:G:N3	12:D:243:HIS:HA	2.34	0.42
9:A:2139:A:O2'	9:A:2187:A:N6	2.52	0.42
11:C:193:ASN:OD1	11:C:196:VAL:HG23	2.19	0.42
17:I:154:ARG:HG2	17:I:157:GLU:OE1	2.20	0.42
29:U:114:ILE:HG13	29:U:115:LEU:HG	2.00	0.42
9:A:295:C:N4	9:A:296:G:O6	2.52	0.42
9:A:583:G:N1	9:A:2045:A:OP1	2.32	0.42
9:A:1840:C:OP1	11:C:200:ARG:NH2	2.52	0.42
9:A:1887:G:H2'	9:A:1888:G:H8	1.84	0.42
12:D:166:ARG:HG2	12:D:167:HIS:NE2	2.35	0.42
14:F:60:ASN:ND2	14:F:64:LYS:HD2	2.34	0.42
15:G:74:ILE:HG12	15:G:115:MET:SD	2.59	0.42
9:A:1559:A:H3'	9:A:1560:C:C6	2.54	0.42
9:A:1703:G:N2	9:A:2006:G:OP2	2.32	0.42
9:A:2204:A:H3'	9:A:2205:G:C8	2.54	0.42
11:C:102:HIS:HA	11:C:103:PRO:HD3	1.89	0.42
12:D:203:THR:HG22	12:D:204:ILE:N	2.34	0.42
14:F:56:ARG:O	14:F:60:ASN:HB3	2.19	0.42
17:I:140:ILE:O	17:I:144:ILE:HG12	2.20	0.42
19:K:101:TYR:HA	19:K:102:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:M:257:PHE:CD1	21:M:257:PHE:N	2.86	0.42
25:Q:119:LEU:O	25:Q:122:ILE:HB	2.19	0.42
30:V:175:TRP:CZ3	30:V:176:LYS:HG3	2.54	0.42
2:1:26:TRP:O	2:1:30:LYS:HG2	2.19	0.42
4:3:113:GLY:HA2	4:3:141:LYS:O	2.20	0.42
9:A:1116:A:N6	18:J:205:ASN:HB2	2.35	0.42
9:A:1192:A:H2'	9:A:1193:U:C6	2.54	0.42
10:B:4:U:H2'	10:B:5:C:C6	2.55	0.42
13:E:51:GLU:HG3	13:E:53:ILE:H	1.85	0.42
19:K:144:THR:HA	19:K:145:PRO:HD3	1.84	0.42
25:Q:185:ARG:HG3	25:Q:187:ILE:HG13	2.01	0.42
26:R:28:HIS:O	26:R:35:ILE:HG12	2.20	0.42
1:0:53:CYS:SG	1:0:73:TRP:NE1	2.92	0.42
9:A:262:G:C2	9:A:264:A:H5''	2.54	0.42
9:A:331:A:OP2	13:E:222:ASN:HB2	2.20	0.42
9:A:712:G:N2	9:A:743:C:C2	2.88	0.42
9:A:1543:G:H5'	9:A:1544:A:OP2	2.20	0.42
12:D:90:ILE:HD13	12:D:90:ILE:HA	1.65	0.42
2:1:43:SER:OG	31:W:89:A:H1'	2.19	0.42
7:6:96:LEU:O	7:6:100:LEU:HG	2.20	0.42
9:A:483:A:H2'	9:A:484:G:C8	2.54	0.42
9:A:1088:U:C2	9:A:1090:U:H5'	2.54	0.42
9:A:1114:A:H4'	9:A:1131:A:C2	2.54	0.42
9:A:1337:U:H2'	9:A:1338:C:H6	1.85	0.42
9:A:1364:G:N2	9:A:1426:U:C2	2.88	0.42
9:A:1632:U:C2'	9:A:1633:A:H5'	2.50	0.42
13:E:175:VAL:HG12	13:E:177:GLU:H	1.83	0.42
14:F:159:LEU:HD21	14:F:192:PRO:CG	2.49	0.42
15:G:53:ASN:HB3	15:G:68:PRO:HG3	2.01	0.42
22:N:32:TYR:HB2	22:N:106:ILE:HG23	2.02	0.42
22:N:65:TRP:HB2	22:N:105:GLU:HB2	2.02	0.42
23:O:62:ILE:HG21	23:O:104:TYR:CD2	2.55	0.42
25:Q:152:ARG:HG2	25:Q:164:VAL:HG22	2.02	0.42
28:T:173:LEU:HD23	28:T:173:LEU:HA	1.87	0.42
30:V:98:SER:O	30:V:98:SER:OG	2.35	0.42
31:W:36:A:O2'	31:W:37:C:OP1	2.34	0.42
9:A:844:G:C6	9:A:845:C:N4	2.88	0.42
9:A:1317:C:H2'	9:A:1318:C:H6	1.85	0.42
9:A:2255:G:N3	9:A:2255:G:H2'	2.34	0.42
11:C:237:ILE:HD13	11:C:237:ILE:HG21	1.85	0.42
20:L:101:ALA:C	20:L:102:ILE:HG12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:185:ARG:NH2	25:Q:233:LYS:HD3	2.34	0.42
26:R:88:ARG:HE	26:R:118:LYS:HG3	1.85	0.42
33:Y:110:TRP:CE3	33:Y:113:GLY:HA3	2.55	0.42
1:O:77:HIS:HD2	1:O:79:PHE:CD1	2.38	0.42
3:2:36:GLN:HE21	9:A:2302:C:N4	2.17	0.42
9:A:1196:A:H61	9:A:1201:A:H61	1.67	0.42
9:A:1289:A:C2	9:A:2027:A:C4	3.07	0.42
9:A:1548:A:O2'	9:A:1549:A:O5'	2.37	0.42
9:A:2142:G:H21	9:A:2187:A:H4'	1.84	0.42
9:A:2167:G:H2'	9:A:2168:C:O4'	2.20	0.42
9:A:2464:G:H8	9:A:2464:G:H5''	1.84	0.42
17:I:148:ARG:HD2	17:I:180:GLU:OE2	2.19	0.42
23:O:92:GLU:O	23:O:95:GLU:HB3	2.20	0.42
31:W:17:A:H1'	31:W:23:G:C2	2.55	0.42
1:O:46:ARG:NH1	1:O:66:LYS:HB2	2.35	0.42
9:A:166:A:H2'	9:A:167:A:C8	2.55	0.42
9:A:1913:G:N3	9:A:1913:G:H2'	2.34	0.42
13:E:123:ARG:O	13:E:124:ALA:HB2	2.20	0.42
14:F:54:ILE:H	14:F:54:ILE:HG13	1.57	0.42
19:K:120:THR:HA	19:K:160:LYS:HB2	2.02	0.42
24:P:80:LYS:O	24:P:111:TYR:OH	2.30	0.42
29:U:125:ILE:O	29:U:128:ILE:HB	2.20	0.42
32:X:131:ASP:OD1	32:X:132:LYS:N	2.51	0.42
7:6:131:TRP:HA	7:6:131:TRP:CE3	2.55	0.41
9:A:115:G:C6	9:A:117:A:N6	2.88	0.41
9:A:628:A:H2'	9:A:629:C:O4'	2.19	0.41
9:A:754:A:O2'	9:A:1695:U:OP1	2.34	0.41
9:A:1082:A:H4'	17:I:83:GLY:CA	2.47	0.41
9:A:2303:A:H4'	9:A:2304:A:O4'	2.20	0.41
9:A:2589:A:OP1	9:A:2591:G:H4'	2.20	0.41
9:A:2595:G:N7	12:D:234:SER:HB2	2.35	0.41
10:B:53:U:C4	10:B:54:G:C2	3.09	0.41
11:C:226:HIS:HA	11:C:227:PRO:HD3	1.82	0.41
13:E:212:LEU:HD23	13:E:212:LEU:HA	1.91	0.41
15:G:160:GLU:OE2	15:G:176:ARG:HG3	2.20	0.41
17:I:126:MET:HA	17:I:130:ASN:ND2	2.35	0.41
18:J:206:MET:HB2	18:J:206:MET:HE3	1.93	0.41
27:S:102:GLU:H	27:S:102:GLU:HG3	1.66	0.41
29:U:188:ALA:HB1	29:U:193:ILE:O	2.20	0.41
32:X:71:ASP:OD1	32:X:72:SER:N	2.50	0.41
4:3:114:PHE:HA	4:3:139:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1837:U:H2'	9:A:1838:G:O4'	2.19	0.41
10:B:51:G:OP1	24:P:116:THR:HG23	2.19	0.41
27:S:146:ARG:HA	27:S:217:THR:OG1	2.20	0.41
27:S:161:VAL:O	27:S:177:VAL:HG23	2.20	0.41
28:T:126:LYS:O	28:T:128:PRO:HD3	2.20	0.41
30:V:175:TRP:CH2	30:V:176:LYS:HG3	2.55	0.41
34:Z:81:LEU:HD11	34:Z:144:ILE:HD12	2.02	0.41
4:3:146:SER:HA	4:3:150:ALA:HB2	2.01	0.41
5:4:95:HIS:NE2	9:A:236:A:OP1	2.48	0.41
7:6:130:ALA:HB1	7:6:136:MET:CG	2.51	0.41
9:A:585:A:H2'	9:A:586:U:H6	1.85	0.41
9:A:1518:U:C5	9:A:1519:A:H2	2.38	0.41
9:A:1678:G:H2'	9:A:1679:G:O4'	2.20	0.41
9:A:2086:G:H2'	9:A:2087:C:O4'	2.21	0.41
9:A:2093:U:H2'	9:A:2094:G:O4'	2.20	0.41
9:A:2374:C:H2'	9:A:2376:C:OP2	2.20	0.41
13:E:79:THR:O	13:E:83:VAL:HG23	2.20	0.41
24:P:76:PHE:HE2	24:P:78:SER:HB3	1.86	0.41
27:S:121:GLU:HB3	27:S:123:ILE:HG22	2.02	0.41
28:T:30:ASP:HB3	28:T:137:ARG:HG3	2.02	0.41
28:T:68:MET:HA	28:T:69:PRO:HD3	1.89	0.41
30:V:139:SER:HB2	30:V:162:LEU:CD1	2.50	0.41
31:W:32:C:H5'	31:W:33:A:OP2	2.20	0.41
2:1:4:PRO:HG2	9:A:2030:U:O2	2.21	0.41
7:6:131:TRP:O	7:6:132:PRO:C	2.57	0.41
9:A:1928:C:H2'	9:A:1929:U:C6	2.56	0.41
9:A:2595:G:H4'	9:A:2595:G:OP2	2.20	0.41
12:D:90:ILE:HD12	12:D:90:ILE:HG23	1.84	0.41
23:O:91:ALA:O	23:O:94:PRO:HD2	2.21	0.41
2:1:18:ASN:ND2	9:A:14:A:O3'	2.54	0.41
3:2:8:ARG:NH2	9:A:2302:C:C5	2.89	0.41
9:A:1099:G:O2'	9:A:1117:G:OP2	2.38	0.41
9:A:1141:C:H2'	9:A:1142:G:H8	1.85	0.41
9:A:1883:G:C2	21:M:257:PHE:CE1	3.09	0.41
9:A:2078:C:O2	9:A:2464:G:N2	2.53	0.41
9:A:2653:U:O2'	12:D:134:TYR:OH	2.28	0.41
11:C:239:ARG:C	11:C:241:SER:H	2.24	0.41
12:D:185:LEU:O	12:D:186:LEU:HD23	2.20	0.41
13:E:161:LEU:HA	13:E:161:LEU:HD23	1.71	0.41
17:I:56:ARG:HA	17:I:59:LYS:HE2	2.02	0.41
21:M:191:GLY:O	21:M:194:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:236:A:H8	9:A:236:A:O5'	2.04	0.41
9:A:368:U:H4'	9:A:368:U:OP1	2.20	0.41
9:A:988:A:H5''	9:A:989:G:OP1	2.20	0.41
9:A:2213:A:OP1	33:Y:107:ARG:NH2	2.54	0.41
9:A:2267:G:H8	9:A:2268:G:H5''	1.86	0.41
9:A:2339:A:C6	9:A:2350:A:N6	2.89	0.41
11:C:221:MET:H	11:C:221:MET:HG3	1.63	0.41
12:D:186:LEU:HB2	12:D:189:GLU:HG3	2.02	0.41
19:K:208:LEU:HA	19:K:208:LEU:HD23	1.70	0.41
21:M:181:LEU:HB3	21:M:187:ILE:HD12	2.02	0.41
27:S:108:ASN:ND2	27:S:113:LYS:HE3	2.35	0.41
2:1:13:LYS:HG2	2:1:14:ARG:N	2.35	0.41
8:7:54:LYS:HE2	9:A:2473:C:O3'	2.21	0.41
9:A:842:G:C6	9:A:843:C:C4	3.08	0.41
9:A:2074:A:H4'	9:A:2075:G:OP1	2.20	0.41
9:A:2354:G:H2'	9:A:2354:G:N3	2.36	0.41
19:K:83:TRP:CG	19:K:84:MET:N	2.89	0.41
24:P:146:TYR:HA	24:P:147:PRO:HD3	1.97	0.41
27:S:166:THR:HG22	27:S:168:ALA:H	1.85	0.41
27:S:234:THR:HB	27:S:236:GLU:HG3	2.03	0.41
30:V:62:LEU:HD23	30:V:62:LEU:HA	1.84	0.41
30:V:177:GLU:HG2	30:V:181:LYS:HE3	2.02	0.41
2:1:3:VAL:HG12	9:A:2029:A:N3	2.35	0.41
2:1:34:LEU:HD12	2:1:34:LEU:HA	1.87	0.41
3:2:52:CYS:HA	3:2:53:PRO:HD3	1.87	0.41
9:A:311:U:OP2	30:V:147:ARG:NH2	2.54	0.41
9:A:644:A:H2'	9:A:645:A:C8	2.55	0.41
9:A:722:G:C2	9:A:732:A:C6	3.09	0.41
9:A:1672:U:H2'	9:A:1673:A:C8	2.55	0.41
9:A:1702:G:O3'	20:L:6:THR:HG23	2.20	0.41
9:A:2751:A:H1'	12:D:298:VAL:HG13	2.03	0.41
19:K:100:TRP:CE3	26:R:102:ILE:HD13	2.55	0.41
27:S:127:VAL:HG12	27:S:161:VAL:HG22	2.02	0.41
28:T:145:TYR:O	28:T:149:LEU:HG	2.20	0.41
9:A:116:A:OP2	9:A:117:A:H2'	2.21	0.41
9:A:531:A:H2'	9:A:532:A:H8	1.83	0.41
9:A:1075:G:H8	9:A:1075:G:OP2	2.04	0.41
9:A:1142:G:C6	9:A:1143:C:N4	2.88	0.41
9:A:2045:A:C6	9:A:2515:C:H1'	2.56	0.41
9:A:2136:U:OP1	9:A:2182:G:N2	2.53	0.41
9:A:2699:U:H2'	9:A:2700:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:131:MET:HA	11:C:132:PRO:HD3	1.81	0.41
12:D:166:ARG:HH12	31:W:26:G:P	2.43	0.41
13:E:105:ARG:HA	13:E:138:GLY:HA3	2.02	0.41
14:F:148:LEU:HD12	14:F:148:LEU:HA	1.84	0.41
14:F:159:LEU:HD21	14:F:192:PRO:HG3	2.02	0.41
15:G:63:LEU:HD11	15:G:84:LYS:NZ	2.36	0.41
18:J:146:ALA:HB3	18:J:202:THR:HG21	2.01	0.41
19:K:48:ARG:NH2	31:W:1:A:H3'	2.34	0.41
21:M:109:SER:O	21:M:110:CYS:HB2	2.20	0.41
23:O:89:LEU:HD22	23:O:93:VAL:CG2	2.50	0.41
30:V:68:MET:SD	30:V:93:ILE:HD11	2.60	0.41
5:4:136:ILE:HD13	5:4:136:ILE:HA	1.85	0.41
9:A:295:C:N4	9:A:296:G:C6	2.89	0.41
9:A:767:A:H2'	9:A:768:G:O4'	2.21	0.41
9:A:1146:U:H2'	9:A:1147:U:C6	2.55	0.41
9:A:1570:C:H5''	9:A:1571:G:OP1	2.20	0.41
9:A:1717:A:N3	9:A:1772:A:H2'	2.36	0.41
9:A:2075:G:H5''	9:A:2520:A:OP1	2.21	0.41
12:D:101:SER:HB3	25:Q:178:HIS:HD2	1.86	0.41
15:G:104:MET:O	15:G:107:LEU:HB3	2.21	0.41
15:G:214:GLY:O	15:G:215:LYS:HB2	2.20	0.41
22:N:23:ARG:HG3	22:N:23:ARG:HH11	1.86	0.41
25:Q:140:VAL:HA	25:Q:141:PRO:HD3	1.79	0.41
32:X:146:ASN:HB2	32:X:149:SER:OG	2.21	0.41
2:1:6:LYS:HD3	2:1:6:LYS:HA	1.82	0.40
9:A:424:A:N6	9:A:2429:A:O4'	2.54	0.40
9:A:643:A:O2'	21:M:145:GLY:HA3	2.20	0.40
9:A:887:G:O2'	9:A:909:A:N6	2.54	0.40
12:D:166:ARG:HG2	12:D:167:HIS:CD2	2.56	0.40
23:O:69:SER:OG	23:O:72:LYS:HG2	2.20	0.40
32:X:119:ILE:HG22	32:X:120:ASP:O	2.21	0.40
9:A:1378:U:H2'	9:A:1379:C:O4'	2.21	0.40
9:A:1493:C:H5'	9:A:1494:G:OP2	2.21	0.40
9:A:2073:A:O2'	9:A:2074:A:P	2.78	0.40
9:A:2570:G:H2'	9:A:2571:U:O4'	2.22	0.40
14:F:116:GLN:NE2	14:F:117:ARG:O	2.54	0.40
17:I:138:GLU:HG3	17:I:139:GLU:H	1.86	0.40
18:J:111:LYS:HA	18:J:111:LYS:HD2	1.85	0.40
19:K:50:SER:HA	31:W:1:A:N7	2.35	0.40
22:N:41:TRP:HZ2	22:N:72:LYS:HE2	1.84	0.40
25:Q:184:ARG:NH2	25:Q:193:GLU:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:105:PRO:HD2	34:Z:142:ARG:HG2	2.03	0.40
31:W:76:G:H5''	31:W:77:A:OP1	2.22	0.40
9:A:311:U:H3	9:A:325:A:H61	1.68	0.40
9:A:758:U:H4'	28:T:121:ARG:HH21	1.87	0.40
9:A:2101:G:C3'	9:A:2102:G:H5''	2.52	0.40
9:A:2208:U:H2'	9:A:2209:U:O4'	2.22	0.40
10:B:29:C:C2	10:B:30:A:C8	3.09	0.40
10:B:77:A:H2'	10:B:78:U:C6	2.57	0.40
11:C:140:ILE:HB	11:C:150:LEU:HB2	2.02	0.40
12:D:282:VAL:HB	12:D:283:PRO:HD2	2.03	0.40
18:J:152:LYS:HE3	18:J:152:LYS:HB2	1.94	0.40
19:K:56:LYS:O	19:K:60:GLU:HG3	2.21	0.40
19:K:100:TRP:N	26:R:99:GLN:HE22	2.16	0.40
19:K:239:LEU:HD12	19:K:239:LEU:HA	1.95	0.40
24:P:122:LYS:HD2	24:P:122:LYS:HA	1.79	0.40
27:S:93:PHE:CG	28:T:163:LEU:HD22	2.55	0.40
7:6:138:LYS:HB3	7:6:138:LYS:HE2	1.82	0.40
9:A:266:A:OP2	33:Y:139:LYS:NZ	2.46	0.40
9:A:1063:U:OP1	15:G:99:ARG:NH2	2.54	0.40
10:B:17:G:N2	10:B:70:G:H1'	2.36	0.40
10:B:54:G:H8	10:B:54:G:O5'	2.05	0.40
10:B:103:A:H2'	10:B:104:A:O4'	2.22	0.40
12:D:288:ASN:ND2	12:D:289:LEU:H	2.19	0.40
26:R:112:TYR:OH	26:R:116:ILE:HD11	2.21	0.40
5:4:125:ASN:OD1	5:4:127:LYS:HB3	2.22	0.40
9:A:1800:C:H5''	9:A:1801:A:OP1	2.21	0.40
9:A:2628:C:H3'	9:A:2629:A:C8	2.56	0.40
10:B:38:C:OP2	10:B:39:C:H5	2.04	0.40
11:C:49:HIS:CD2	11:C:215:VAL:HG22	2.57	0.40
14:F:113:ILE:HG22	14:F:152:PHE:HE1	1.86	0.40
21:M:136:LEU:HG	21:M:140:ILE:HD12	2.03	0.40
28:T:33:THR:HG23	28:T:135:VAL:HG22	2.03	0.40
31:W:35:U:H6	31:W:35:U:H2'	1.68	0.40
31:W:54:A:H2'	31:W:55:A:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	42/130 (32%)	39 (93%)	3 (7%)	0	100	100
2	1	46/57 (81%)	44 (96%)	2 (4%)	0	100	100
3	2	58/66 (88%)	53 (91%)	5 (9%)	0	100	100
4	3	58/152 (38%)	54 (93%)	4 (7%)	0	100	100
5	4	70/159 (44%)	66 (94%)	4 (6%)	0	100	100
6	5	35/37 (95%)	35 (100%)	0	0	100	100
7	6	47/142 (33%)	46 (98%)	0	1 (2%)	7	32
8	7	44/116 (38%)	40 (91%)	3 (7%)	1 (2%)	6	29
11	C	251/272 (92%)	238 (95%)	12 (5%)	1 (0%)	34	67
12	D	219/305 (72%)	205 (94%)	13 (6%)	1 (0%)	29	62
13	E	210/293 (72%)	193 (92%)	17 (8%)	0	100	100
14	F	191/258 (74%)	178 (93%)	13 (7%)	0	100	100
15	G	176/220 (80%)	167 (95%)	9 (5%)	0	100	100
16	H	46/196 (24%)	43 (94%)	3 (6%)	0	100	100
17	I	135/232 (58%)	132 (98%)	3 (2%)	0	100	100
18	J	131/224 (58%)	126 (96%)	5 (4%)	0	100	100
19	K	201/250 (80%)	194 (96%)	7 (4%)	0	100	100
20	L	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
21	M	183/271 (68%)	169 (92%)	12 (7%)	2 (1%)	14	46
22	N	133/135 (98%)	122 (92%)	11 (8%)	0	100	100
23	O	114/126 (90%)	110 (96%)	4 (4%)	0	100	100
24	P	120/166 (72%)	114 (95%)	6 (5%)	0	100	100
25	Q	116/233 (50%)	114 (98%)	2 (2%)	0	100	100
26	R	117/128 (91%)	110 (94%)	7 (6%)	0	100	100
27	S	168/256 (66%)	157 (94%)	9 (5%)	2 (1%)	13	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	T	170/199 (85%)	161 (95%)	8 (5%)	1 (1%)	25	59
29	U	94/198 (48%)	89 (95%)	5 (5%)	0	100	100
30	V	132/192 (69%)	121 (92%)	10 (8%)	1 (1%)	19	52
32	X	107/194 (55%)	95 (89%)	12 (11%)	0	100	100
33	Y	75/148 (51%)	74 (99%)	1 (1%)	0	100	100
34	Z	99/168 (59%)	95 (96%)	3 (3%)	1 (1%)	15	47
All	All	3707/5644 (66%)	3499 (94%)	197 (5%)	11 (0%)	44	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	C	232	GLU
21	M	131	GLY
27	S	78	PRO
34	Z	151	SER
7	6	131	TRP
8	7	88	GLU
21	M	208	THR
27	S	79	PRO
28	T	146	ASP
30	V	117	GLU
12	D	212	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	39/117 (33%)	36 (92%)	3 (8%)	13	38
2	1	41/50 (82%)	39 (95%)	2 (5%)	25	55
3	2	56/60 (93%)	51 (91%)	5 (9%)	9	32
4	3	50/125 (40%)	45 (90%)	5 (10%)	7	27
5	4	62/140 (44%)	55 (89%)	7 (11%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5	34/34 (100%)	30 (88%)	4 (12%)	5	21
7	6	46/124 (37%)	44 (96%)	2 (4%)	29	59
8	7	40/96 (42%)	35 (88%)	5 (12%)	4	19
11	C	201/217 (93%)	181 (90%)	20 (10%)	7	27
12	D	182/259 (70%)	167 (92%)	15 (8%)	11	36
13	E	179/255 (70%)	160 (89%)	19 (11%)	6	25
14	F	152/214 (71%)	141 (93%)	11 (7%)	14	41
15	G	151/190 (80%)	141 (93%)	10 (7%)	16	45
16	H	42/170 (25%)	37 (88%)	5 (12%)	5	20
17	I	119/204 (58%)	113 (95%)	6 (5%)	24	55
18	J	106/189 (56%)	103 (97%)	3 (3%)	43	69
19	K	176/213 (83%)	168 (96%)	8 (4%)	27	58
20	L	101/101 (100%)	94 (93%)	7 (7%)	15	43
21	M	141/215 (66%)	126 (89%)	15 (11%)	6	25
22	N	108/108 (100%)	101 (94%)	7 (6%)	17	46
23	O	96/103 (93%)	84 (88%)	12 (12%)	4	19
24	P	100/139 (72%)	90 (90%)	10 (10%)	7	27
25	Q	104/207 (50%)	94 (90%)	10 (10%)	8	29
26	R	106/115 (92%)	98 (92%)	8 (8%)	13	39
27	S	137/223 (61%)	134 (98%)	3 (2%)	52	74
28	T	152/176 (86%)	138 (91%)	14 (9%)	9	31
29	U	85/171 (50%)	74 (87%)	11 (13%)	4	18
30	V	121/169 (72%)	116 (96%)	5 (4%)	30	60
32	X	92/163 (56%)	83 (90%)	9 (10%)	8	29
33	Y	67/130 (52%)	60 (90%)	7 (10%)	7	25
34	Z	93/153 (61%)	87 (94%)	6 (6%)	17	46
All	All	3179/4830 (66%)	2925 (92%)	254 (8%)	16	37

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	51	VAL
1	0	57	LEU

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Mol	Chain	Res	Type
1	0	59	MET
2	1	7	ARG
2	1	11	TYR
3	2	19	VAL
3	2	28	ARG
3	2	42	THR
3	2	45	ARG
3	2	60	ILE
4	3	97	CYS
4	3	126	LEU
4	3	127	LEU
4	3	129	ARG
4	3	142	THR
5	4	91	LYS
5	4	104	VAL
5	4	109	LYS
5	4	118	GLN
5	4	119	HIS
5	4	125	ASN
5	4	143	TYR
6	5	1	MET
6	5	4	ARG
6	5	29	ASN
6	5	36	GLN
7	6	118	ARG
7	6	138	LYS
8	7	50	ARG
8	7	54	LYS
8	7	66	LYS
8	7	74	ARG
8	7	88	GLU
11	C	19	GLN
11	C	20	VAL
11	C	25	ARG
11	C	54	HIS
11	C	71	TYR
11	C	90	ILE
11	C	96	GLU
11	C	126	LEU
11	C	142	ILE
11	C	152	ARG
11	C	170	LEU

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Mol	Chain	Res	Type
11	C	178	ARG
11	C	203	ARG
11	C	223	PRO
11	C	224	VAL
11	C	228	HIS
11	C	240	LYS
11	C	255	SER
11	C	260	LYS
11	C	270	ARG
12	D	109	VAL
12	D	137	VAL
12	D	146	ASP
12	D	174	VAL
12	D	178	ASP
12	D	193	GLU
12	D	206	LYS
12	D	219	ARG
12	D	221	LEU
12	D	244	VAL
12	D	262	ARG
12	D	273	LEU
12	D	288	ASN
12	D	292	LEU
12	D	298	VAL
13	E	52	LEU
13	E	61	SER
13	E	68	THR
13	E	74	THR
13	E	97	ARG
13	E	113	ARG
13	E	114	LYS
13	E	120	LYS
13	E	157	ARG
13	E	161	LEU
13	E	174	VAL
13	E	209	LEU
13	E	213	VAL
13	E	223	ILE
13	E	230	THR
13	E	238	ASP
13	E	245	LEU
13	E	251	THR

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Mol	Chain	Res	Type
13	E	261	VAL
14	F	53	THR
14	F	56	ARG
14	F	59	THR
14	F	84	VAL
14	F	110	LEU
14	F	119	VAL
14	F	122	LYS
14	F	125	THR
14	F	155	ARG
14	F	190	VAL
14	F	205	MET
15	G	40	GLU
15	G	50	VAL
15	G	63	LEU
15	G	94	LYS
15	G	100	ARG
15	G	109	ARG
15	G	127	LEU
15	G	129	LEU
15	G	169	THR
15	G	213	GLU
16	H	47	LYS
16	H	57	ILE
16	H	75	ARG
16	H	79	LEU
16	H	87	VAL
17	I	75	LEU
17	I	89	PHE
17	I	101	THR
17	I	117	THR
17	I	119	TRP
17	I	147	TYR
18	J	90	THR
18	J	152	LYS
18	J	171	ILE
19	K	48	ARG
19	K	62	ARG
19	K	64	LEU
19	K	79	LEU
19	K	116	VAL
19	K	147	VAL

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Mol	Chain	Res	Type
19	K	191	LEU
19	K	199	ILE
20	L	17	ARG
20	L	23	ARG
20	L	28	SER
20	L	30	ARG
20	L	34	ARG
20	L	42	VAL
20	L	102	ILE
21	M	83	ASP
21	M	84	ASN
21	M	106	GLN
21	M	120	ARG
21	M	125	ILE
21	M	138	ARG
21	M	154	LEU
21	M	164	ASP
21	M	186	ILE
21	M	208	THR
21	M	212	ILE
21	M	215	ARG
21	M	220	SER
21	M	246	VAL
21	M	257	PHE
22	N	5	LYS
22	N	9	PHE
22	N	28	CYS
22	N	41	TRP
22	N	52	ARG
22	N	56	ARG
22	N	109	VAL
23	O	11	MET
23	O	22	ARG
23	O	27	ARG
23	O	28	ARG
23	O	60	LYS
23	O	73	ARG
23	O	74	ARG
23	O	89	LEU
23	O	111	LEU
23	O	114	ARG
23	O	123	ILE

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Mol	Chain	Res	Type
23	O	126	VAL
24	P	49	ARG
24	P	52	ASP
24	P	53	ARG
24	P	59	ARG
24	P	70	ARG
24	P	87	ILE
24	P	127	ILE
24	P	143	ARG
24	P	151	ARG
24	P	161	GLU
25	Q	138	ARG
25	Q	149	VAL
25	Q	172	ARG
25	Q	185	ARG
25	Q	198	LEU
25	Q	200	SER
25	Q	203	ILE
25	Q	206	ILE
25	Q	212	ARG
25	Q	215	ARG
26	R	11	ARG
26	R	23	SER
26	R	33	ARG
26	R	48	ARG
26	R	76	TYR
26	R	85	LEU
26	R	108	ILE
26	R	113	ASN
27	S	202	LYS
27	S	208	ARG
27	S	216	ILE
28	T	35	ARG
28	T	38	SER
28	T	43	VAL
28	T	47	ARG
28	T	100	ILE
28	T	117	ARG
28	T	127	ARG
28	T	134	ILE
28	T	139	ILE
28	T	153	THR

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Mol	Chain	Res	Type
28	T	160	LEU
28	T	163	LEU
28	T	174	CYS
28	T	183	ILE
29	U	102	LEU
29	U	103	LYS
29	U	111	VAL
29	U	119	ILE
29	U	141	ARG
29	U	143	ASP
29	U	154	PHE
29	U	171	THR
29	U	172	LYS
29	U	178	LEU
29	U	179	ASN
30	V	48	ARG
30	V	113	LYS
30	V	130	ILE
30	V	146	SER
30	V	173	ASP
32	X	73	LYS
32	X	81	ILE
32	X	85	GLN
32	X	97	ARG
32	X	105	LYS
32	X	109	ILE
32	X	123	VAL
32	X	142	ILE
32	X	155	ARG
33	Y	83	ASN
33	Y	87	ARG
33	Y	92	ASN
33	Y	98	LEU
33	Y	126	LEU
33	Y	135	ASP
33	Y	144	ASP
34	Z	59	VAL
34	Z	76	LEU
34	Z	87	LEU
34	Z	130	LYS
34	Z	132	LEU
34	Z	146	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	42	HIS
1	0	77	HIS
3	2	36	GLN
4	3	143	ASN
7	6	102	GLN
11	C	23	ASN
12	D	121	ASN
12	D	288	ASN
13	E	91	HIS
13	E	118	GLN
13	E	171	ASN
14	F	60	ASN
15	G	114	ASN
15	G	183	GLN
16	H	42	GLN
17	I	90	GLN
17	I	130	ASN
19	K	97	ASN
20	L	73	ASN
20	L	92	ASN
21	M	84	ASN
21	M	133	GLN
21	M	161	ASN
23	O	18	HIS
23	O	75	GLN
23	O	87	HIS
24	P	81	HIS
24	P	85	GLN
24	P	108	ASN
24	P	162	HIS
25	Q	178	HIS
25	Q	202	ASN
26	R	37	GLN
26	R	83	HIS
26	R	99	GLN
26	R	113	ASN
27	S	108	ASN
27	S	189	GLN
28	T	90	ASN
28	T	97	ASN
29	U	153	ASN

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Mol	Chain	Res	Type
30	V	142	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	120/121 (99%)	19 (15%)	0
31	W	105/106 (99%)	38 (36%)	0
35	z	1/2 (50%)	1 (100%)	0
9	A	2794/2810 (99%)	642 (22%)	8 (0%)
All	All	3020/3039 (99%)	700 (23%)	8 (0%)

All (700) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	9	A
9	A	10	G
9	A	12	A
9	A	13	A
9	A	14	A
9	A	31	C
9	A	33	A
9	A	34	G
9	A	39	C
9	A	45	A
9	A	46	C
9	A	54	G
9	A	57	G
9	A	66	G
9	A	70	A
9	A	73	U
9	A	74	G
9	A	82	G
9	A	84	G
9	A	90	A
9	A	94	A
9	A	97	A
9	A	98	G
9	A	99	A
9	A	100	G
9	A	116	A
9	A	117	A

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Mol	Chain	Res	Type
9	A	118	U
9	A	123	C
9	A	130	U
9	A	131	C
9	A	143	G
9	A	144	A
9	A	149	A
9	A	158	C
9	A	159	A
9	A	160	A
9	A	181	A
9	A	184	A
9	A	200	G
9	A	201	A
9	A	206	A
9	A	207	A
9	A	208	A
9	A	216	C
9	A	218	A
9	A	224	G
9	A	226	A
9	A	233	G
9	A	249	C
9	A	250	A
9	A	251	G
9	A	252	C
9	A	266	A
9	A	267	C
9	A	275	U
9	A	276	G
9	A	282	G
9	A	284	A
9	A	286	U
9	A	287	A
9	A	288	C
9	A	289	A
9	A	294	U
9	A	297	U
9	A	298	G
9	A	299	C
9	A	304	A
9	A	311	U

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Mol	Chain	Res	Type
9	A	316	G
9	A	317	G
9	A	320	U
9	A	326	A
9	A	332	G
9	A	333	A
9	A	338	G
9	A	339	A
9	A	340	A
9	A	344	C
9	A	362	A
9	A	363	C
9	A	364	U
9	A	368	U
9	A	370	A
9	A	377	G
9	A	379	C
9	A	383	A
9	A	384	G
9	A	398	G
9	A	400	G
9	A	415	U
9	A	416	C
9	A	417	A
9	A	418	G
9	A	423	G
9	A	424	A
9	A	436	G
9	A	437	G
9	A	448	C
9	A	451	G
9	A	452	G
9	A	453	U
9	A	454	G
9	A	466	A
9	A	467	G
9	A	468	U
9	A	469	A
9	A	471	U
9	A	479	G
9	A	492	A
9	A	493	G

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Mol	Chain	Res	Type
9	A	502	U
9	A	507	G
9	A	519	A
9	A	520	C
9	A	529	G
9	A	539	A
9	A	541	G
9	A	542	C
9	A	543	A
9	A	544	G
9	A	549	A
9	A	554	G
9	A	556	C
9	A	557	C
9	A	558	A
9	A	559	G
9	A	560	A
9	A	561	C
9	A	562	C
9	A	565	G
9	A	573	G
9	A	582	A
9	A	583	G
9	A	585	A
9	A	593	G
9	A	597	C
9	A	608	U
9	A	609	G
9	A	610	G
9	A	612	U
9	A	613	U
9	A	614	G
9	A	623	A
9	A	630	C
9	A	632	G
9	A	633	A
9	A	635	C
9	A	639	A
9	A	643	A
9	A	645	A
9	A	649	A
9	A	657	U

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Mol	Chain	Res	Type
9	A	658	A
9	A	665	U
9	A	667	G
9	A	680	G
9	A	681	A
9	A	696	A
9	A	697	U
9	A	701	U
9	A	705	U
9	A	712	G
9	A	713	A
9	A	724	G
9	A	727	A
9	A	728	A
9	A	729	A
9	A	730	C
9	A	731	U
9	A	734	G
9	A	740	G
9	A	741	U
9	A	749	G
9	A	758	U
9	A	759	G
9	A	760	A
9	A	768	G
9	A	775	A
9	A	776	G
9	A	782	G
9	A	786	G
9	A	787	G
9	A	788	G
9	A	793	A
9	A	795	U
9	A	796	G
9	A	803	G
9	A	816	G
9	A	817	C
9	A	823	C
9	A	838	U
9	A	839	G
9	A	853	G
9	A	856	U

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Mol	Chain	Res	Type
9	A	857	G
9	A	858	G
9	A	859	A
9	A	866	G
9	A	869	G
9	A	879	G
9	A	880	U
9	A	888	C
9	A	890	G
9	A	893	C
9	A	895	C
9	A	902	G
9	A	904	U
9	A	905	A
9	A	906	C
9	A	907	C
9	A	910	A
9	A	913	G
9	A	916	G
9	A	919	A
9	A	923	C
9	A	924	U
9	A	937	U
9	A	938	G
9	A	939	A
9	A	943	C
9	A	946	A
9	A	947	A
9	A	948	U
9	A	965	G
9	A	974	G
9	A	981	G
9	A	989	G
9	A	1002	G
9	A	1007	A
9	A	1011	A
9	A	1017	G
9	A	1018	A
9	A	1024	A
9	A	1039	A
9	A	1040	U
9	A	1041	G

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Mol	Chain	Res	Type
9	A	1045	G
9	A	1050	G
9	A	1051	U
9	A	1052	G
9	A	1053	A
9	A	1054	U
9	A	1055	A
9	A	1061	G
9	A	1062	G
9	A	1065	G
9	A	1071	C
9	A	1072	A
9	A	1075	G
9	A	1098	A
9	A	1099	G
9	A	1116	A
9	A	1118	U
9	A	1140	G
9	A	1143	C
9	A	1144	U
9	A	1147	U
9	A	1148	G
9	A	1155	A
9	A	1158	U
9	A	1160	A
9	A	1162	C
9	A	1163	G
9	A	1169	A
9	A	1170	A
9	A	1173	G
9	A	1184	G
9	A	1190	G
9	A	1196	A
9	A	1197	A
9	A	1198	A
9	A	1199	A
9	A	1202	A
9	A	1226	U
9	A	1227	U
9	A	1231	G
9	A	1239	C
9	A	1241	U

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Mol	Chain	Res	Type
9	A	1248	G
9	A	1253	G
9	A	1254	U
9	A	1255	U
9	A	1257	G
9	A	1259	C
9	A	1261	A
9	A	1274	A
9	A	1277	G
9	A	1289	A
9	A	1292	G
9	A	1293	C
9	A	1295	A
9	A	1296	A
9	A	1310	C
9	A	1315	G
9	A	1321	A
9	A	1322	A
9	A	1327	U
9	A	1333	U
9	A	1342	A
9	A	1353	A
9	A	1357	A
9	A	1359	G
9	A	1362	G
9	A	1366	C
9	A	1371	C
9	A	1380	A
9	A	1381	G
9	A	1386	A
9	A	1400	U
9	A	1405	A
9	A	1416	A
9	A	1417	U
9	A	1420	C
9	A	1423	U
9	A	1431	C
9	A	1432	U
9	A	1433	U
9	A	1435	U
9	A	1436	U
9	A	1437	G

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Mol	Chain	Res	Type
9	A	1438	G
9	A	1444	A
9	A	1446	G
9	A	1449	C
9	A	1450	G
9	A	1456	G
9	A	1458	C
9	A	1465	A
9	A	1472	A
9	A	1475	U
9	A	1476	G
9	A	1477	G
9	A	1480	A
9	A	1483	G
9	A	1484	G
9	A	1485	U
9	A	1493	C
9	A	1494	G
9	A	1497	A
9	A	1500	U
9	A	1501	G
9	A	1513	C
9	A	1519	A
9	A	1520	A
9	A	1521	G
9	A	1523	A
9	A	1524	G
9	A	1526	G
9	A	1527	G
9	A	1533	A
9	A	1544	A
9	A	1554	C
9	A	1557	G
9	A	1558	U
9	A	1559	A
9	A	1563	G
9	A	1566	G
9	A	1567	C
9	A	1568	U
9	A	1570	C
9	A	1571	G
9	A	1588	U

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Mol	Chain	Res	Type
9	A	1594	A
9	A	1600	A
9	A	1603	A
9	A	1612	A
9	A	1620	U
9	A	1621	C
9	A	1629	G
9	A	1630	G
9	A	1631	G
9	A	1632	U
9	A	1634	C
9	A	1635	C
9	A	1642	C
9	A	1643	G
9	A	1644	A
9	A	1645	A
9	A	1682	C
9	A	1683	G
9	A	1684	C
9	A	1710	G
9	A	1711	C
9	A	1734	A
9	A	1739	G
9	A	1746	C
9	A	1750	C
9	A	1760	G
9	A	1762	C
9	A	1766	G
9	A	1774	G
9	A	1778	G
9	A	1783	A
9	A	1785	U
9	A	1791	C
9	A	1801	A
9	A	1810	C
9	A	1812	A
9	A	1818	U
9	A	1821	G
9	A	1826	U
9	A	1833	G
9	A	1839	A
9	A	1849	A

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Mol	Chain	Res	Type
9	A	1850	G
9	A	1858	A
9	A	1866	G
9	A	1869	G
9	A	1870	U
9	A	1877	C
9	A	1882	U
9	A	1883	G
9	A	1884	A
9	A	1885	C
9	A	1888	G
9	A	1889	G
9	A	1914	A
9	A	1920	G
9	A	1923	C
9	A	1927	A
9	A	1928	C
9	A	1930	A
9	A	1931	U
9	A	1933	A
9	A	1934	C
9	A	1940	U
9	A	1943	G
9	A	1944	G
9	A	1951	A
9	A	1952	A
9	A	1953	U
9	A	1969	U
9	A	1975	C
9	A	1981	C
9	A	1984	A
9	A	1985	A
9	A	1986	G
9	A	2005	U
9	A	2006	G
9	A	2007	U
9	A	2011	G
9	A	2015	A
9	A	2016	G
9	A	2034	C
9	A	2037	G
9	A	2045	A

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Mol	Chain	Res	Type
9	A	2046	G
9	A	2047	A
9	A	2053	A
9	A	2057	C
9	A	2065	U
9	A	2069	C
9	A	2073	A
9	A	2074	A
9	A	2075	G
9	A	2076	A
9	A	2077	C
9	A	2081	A
9	A	2082	U
9	A	2083	G
9	A	2102	G
9	A	2103	G
9	A	2107	G
9	A	2115	G
9	A	2116	C
9	A	2119	U
9	A	2125	C
9	A	2126	G
9	A	2127	C
9	A	2129	G
9	A	2130	C
9	A	2131	U
9	A	2132	U
9	A	2133	A
9	A	2137	G
9	A	2140	A
9	A	2145	A
9	A	2146	A
9	A	2147	G
9	A	2148	A
9	A	2150	G
9	A	2151	G
9	A	2159	C
9	A	2160	C
9	A	2161	G
9	A	2162	G
9	A	2163	G
9	A	2173	G

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Mol	Chain	Res	Type
9	A	2174	C
9	A	2175	C
9	A	2176	A
9	A	2177	U
9	A	2178	C
9	A	2179	A
9	A	2181	U
9	A	2182	G
9	A	2183	A
9	A	2184	G
9	A	2185	A
9	A	2186	U
9	A	2187	A
9	A	2191	C
9	A	2192	U
9	A	2193	C
9	A	2195	G
9	A	2199	G
9	A	2201	G
9	A	2202	C
9	A	2204	A
9	A	2205	G
9	A	2212	A
9	A	2213	A
9	A	2217	U
9	A	2219	U
9	A	2220	G
9	A	2223	A
9	A	2227	C
9	A	2229	U
9	A	2230	A
9	A	2232	G
9	A	2242	A
9	A	2254	A
9	A	2255	G
9	A	2256	A
9	A	2266	U
9	A	2267	G
9	A	2269	G
9	A	2290	A
9	A	2296	G
9	A	2297	G

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Mol	Chain	Res	Type
9	A	2300	U
9	A	2303	A
9	A	2304	A
9	A	2305	A
9	A	2315	G
9	A	2316	G
9	A	2322	A
9	A	2323	C
9	A	2325	G
9	A	2339	A
9	A	2341	U
9	A	2342	G
9	A	2343	C
9	A	2344	A
9	A	2349	C
9	A	2352	A
9	A	2362	G
9	A	2364	C
9	A	2367	C
9	A	2375	A
9	A	2378	C
9	A	2400	G
9	A	2402	C
9	A	2408	G
9	A	2417	G
9	A	2419	G
9	A	2423	A
9	A	2427	G
9	A	2428	A
9	A	2431	G
9	A	2436	U
9	A	2442	A
9	A	2444	C
9	A	2446	G
9	A	2447	A
9	A	2448	U
9	A	2452	A
9	A	2458	U
9	A	2462	G
9	A	2464	G
9	A	2465	A
9	A	2466	U

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Mol	Chain	Res	Type
9	A	2467	A
9	A	2481	C
9	A	2487	G
9	A	2493	A
9	A	2507	G
9	A	2508	U
9	A	2509	U
9	A	2518	C
9	A	2519	G
9	A	2521	U
9	A	2522	G
9	A	2523	U
9	A	2524	C
9	A	2526	G
9	A	2535	C
9	A	2546	G
9	A	2553	G
9	A	2569	U
9	A	2571	U
9	A	2583	A
9	A	2584	G
9	A	2589	A
9	A	2590	C
9	A	2591	G
9	A	2593	G
9	A	2594	A
9	A	2599	G
9	A	2601	U
9	A	2602	U
9	A	2603	C
9	A	2619	A
9	A	2625	G
9	A	2626	U
9	A	2627	C
9	A	2630	U
9	A	2646	U
9	A	2649	A
9	A	2662	C
9	A	2671	A
9	A	2672	G
9	A	2680	G
9	A	2688	A

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Mol	Chain	Res	Type
9	A	2689	A
9	A	2702	G
9	A	2706	U
9	A	2707	A
9	A	2709	C
9	A	2721	C
9	A	2729	A
9	A	2732	G
9	A	2740	G
9	A	2744	A
9	A	2751	A
9	A	2753	C
9	A	2754	G
9	A	2762	G
9	A	2766	A
9	A	2768	A
9	A	2769	G
9	A	2770	C
9	A	2774	U
9	A	2776	A
9	A	2778	U
9	A	2783	A
9	A	2784	G
9	A	2787	C
9	A	2796	A
9	A	2807	C
9	A	2809	U
10	B	2	A
10	B	10	G
10	B	15	A
10	B	16	G
10	B	17	G
10	B	19	G
10	B	25	G
10	B	31	C
10	B	37	U
10	B	38	C
10	B	39	C
10	B	41	U
10	B	42	C
10	B	57	U
10	B	68	G

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Mol	Chain	Res	Type
10	B	93	C
10	B	105	U
10	B	107	G
10	B	111	G
31	W	3	A
31	W	4	G
31	W	5	A
31	W	14	G
31	W	16	G
31	W	17	A
31	W	19	A
31	W	20	C
31	W	21	G
31	W	26	G
31	W	27	U
31	W	28	U
31	W	29	U
31	W	30	A
31	W	31	U
31	W	32	C
31	W	33	A
31	W	34	U
31	W	35	U
31	W	36	A
31	W	37	C
31	W	38	G
31	W	59	C
31	W	65	U
31	W	71	C
31	W	72	A
31	W	77	A
31	W	79	G
31	W	83	C
31	W	84	C
31	W	85	U
31	W	86	A
31	W	90	G
31	W	95	A
31	W	96	C
31	W	97	A
31	W	99	A
31	W	103	G

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Mol	Chain	Res	Type
35	z	76	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	548	G
9	A	556	C
9	A	680	G
9	A	795	U
9	A	1520	A
9	A	2447	A
9	A	2518	C
9	A	2753	C

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 503 ligands modelled in this entry, 503 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

There are no chain breaks in this entry.

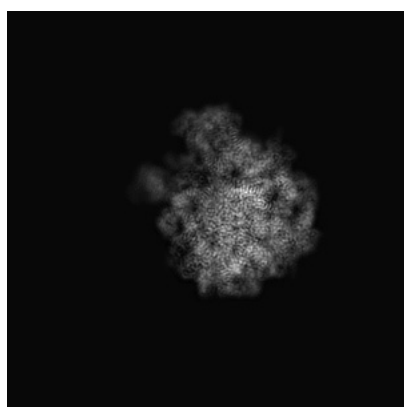
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3531. These allow visual inspection of the internal detail of the map and identification of artifacts.

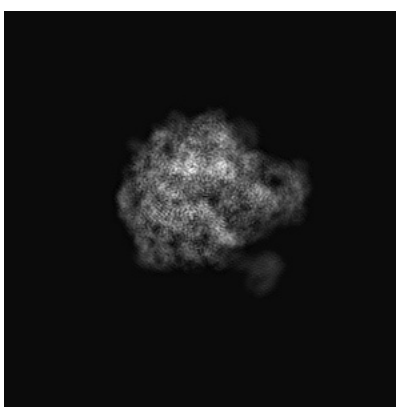
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

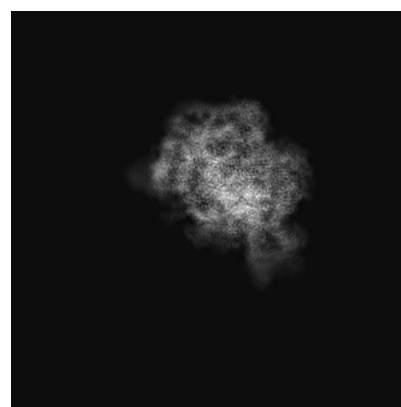
6.1.1 Primary map



X



Y

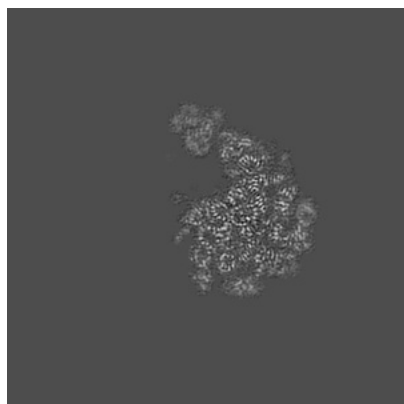


Z

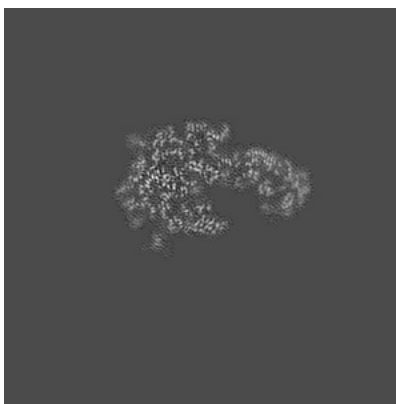
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

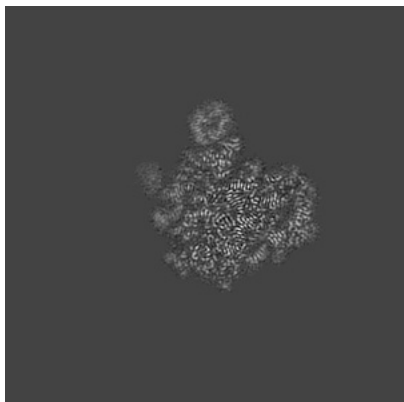


Z Index: 160

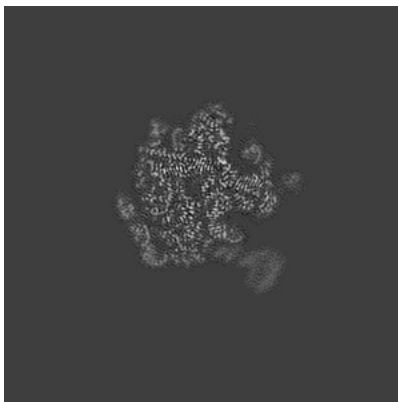
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

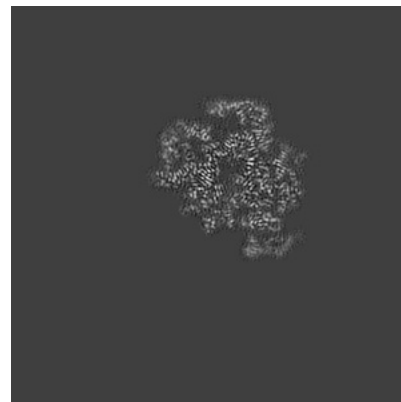
6.3.1 Primary map



X Index: 190



Y Index: 187



Z Index: 149

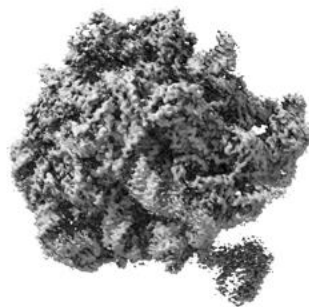
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

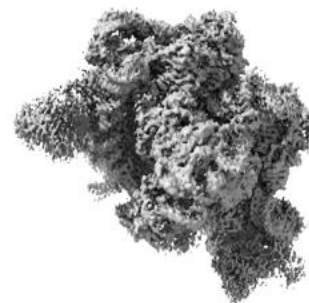
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

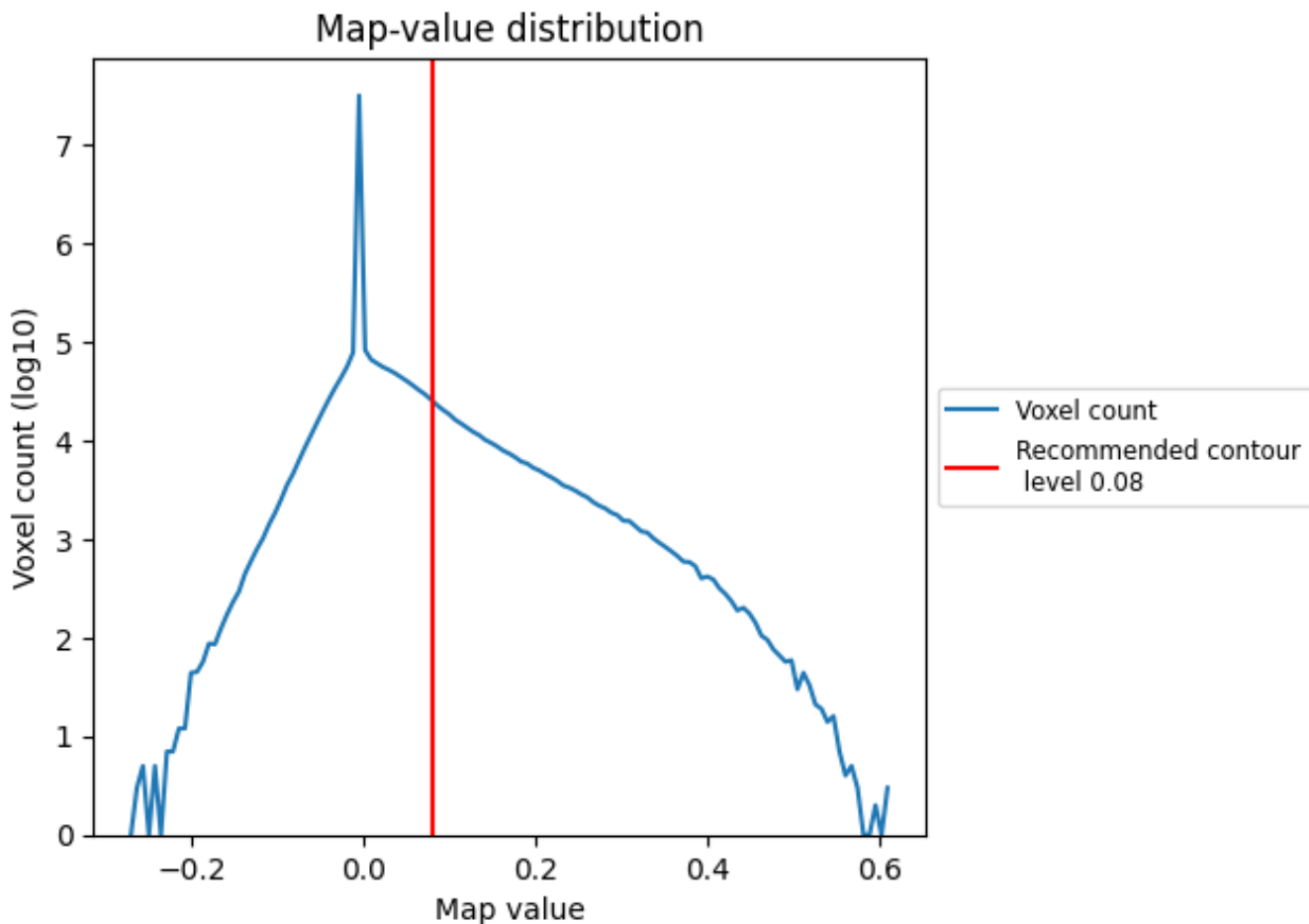
6.5 Mask visualisation

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

7 Map analysis [i](#)

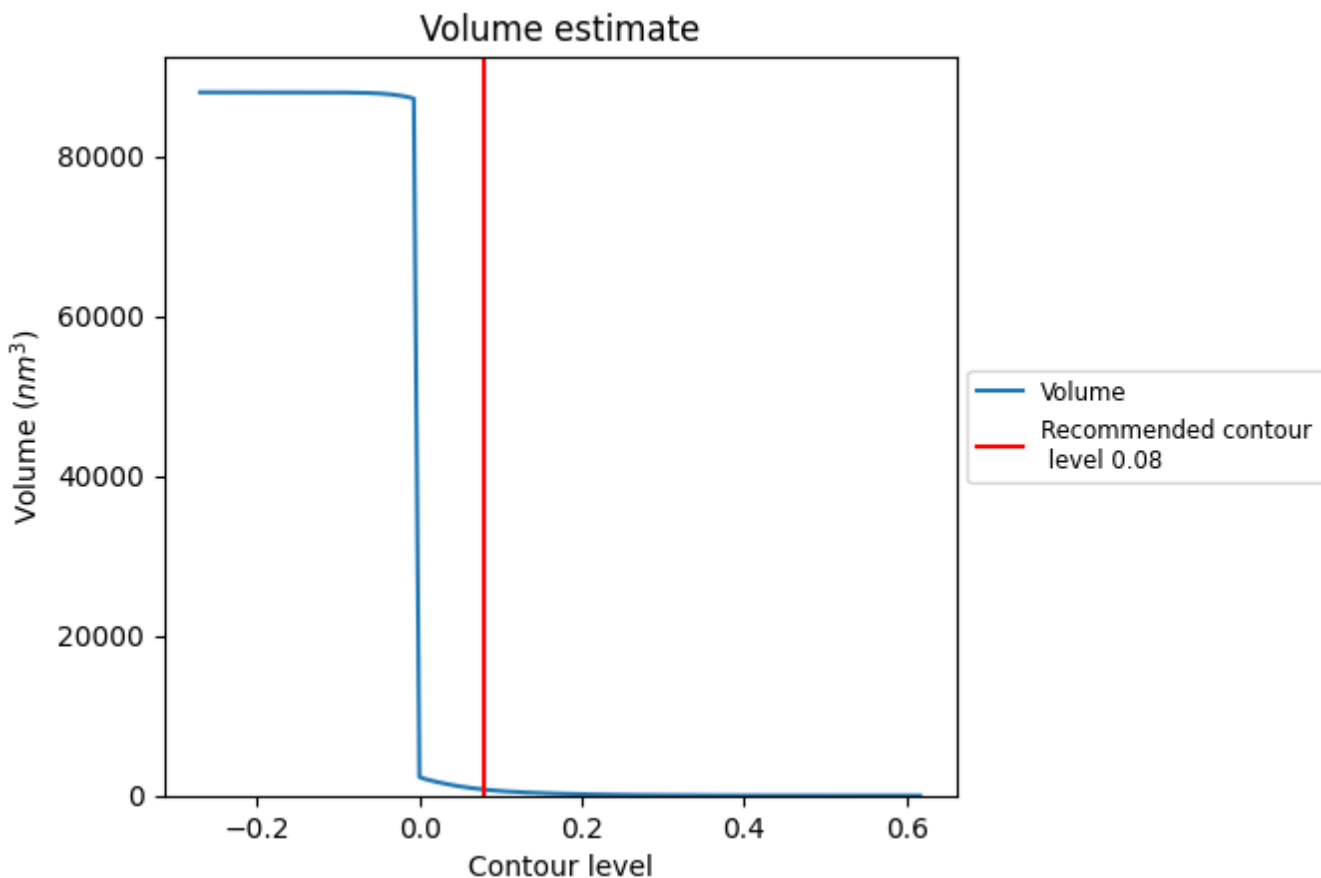
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

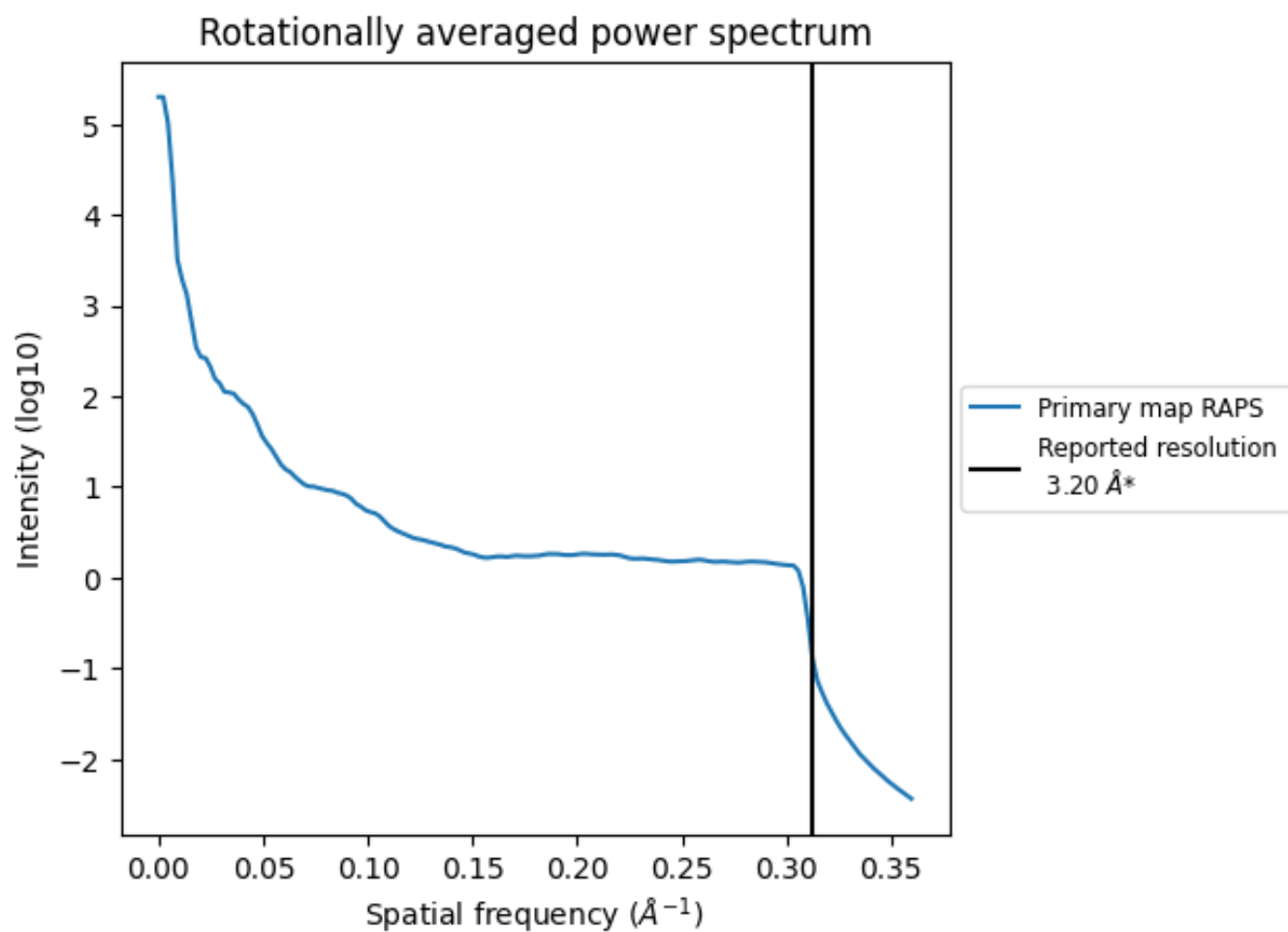
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 750 nm³; this corresponds to an approximate mass of 678 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

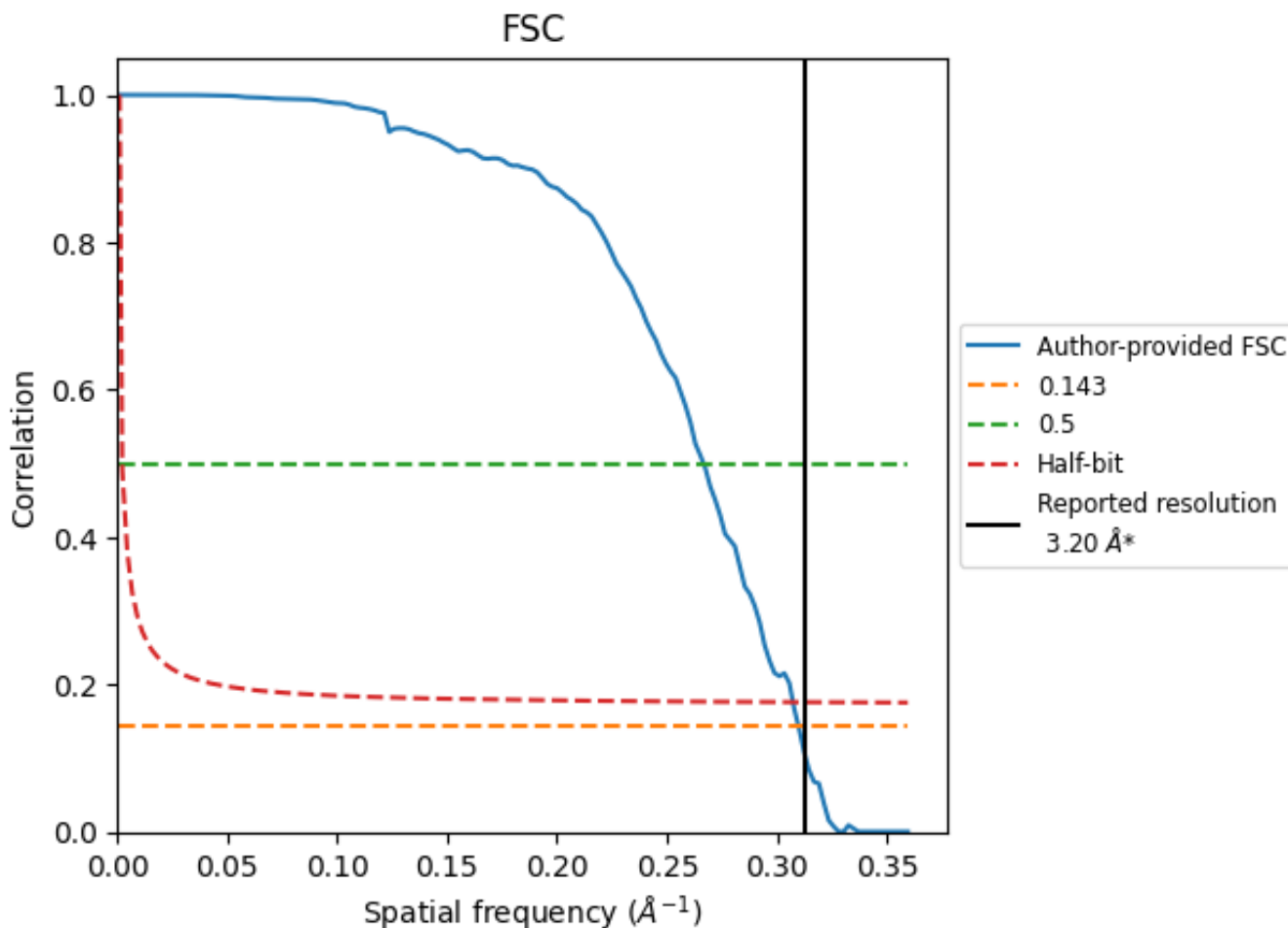


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

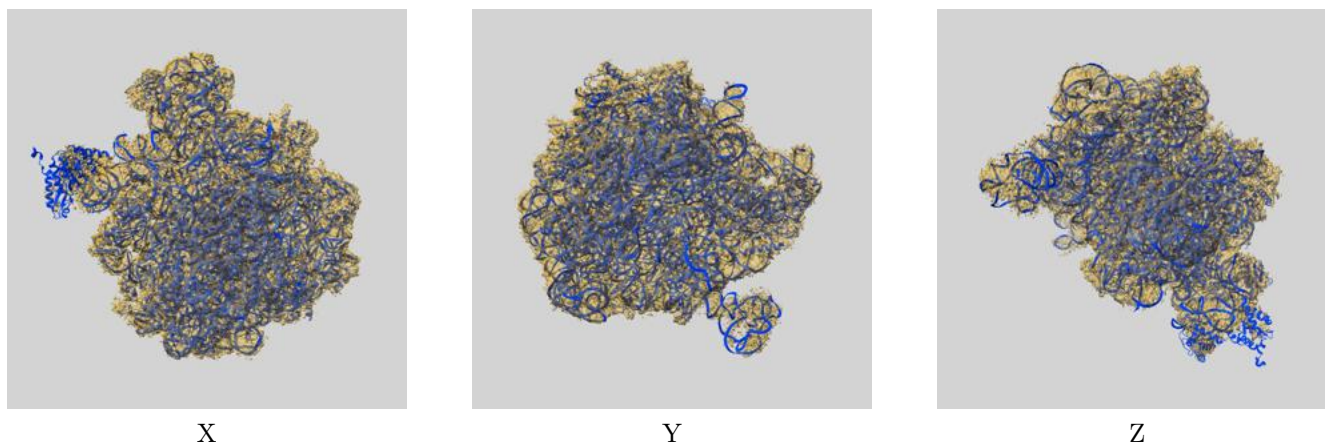
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.75	3.25
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

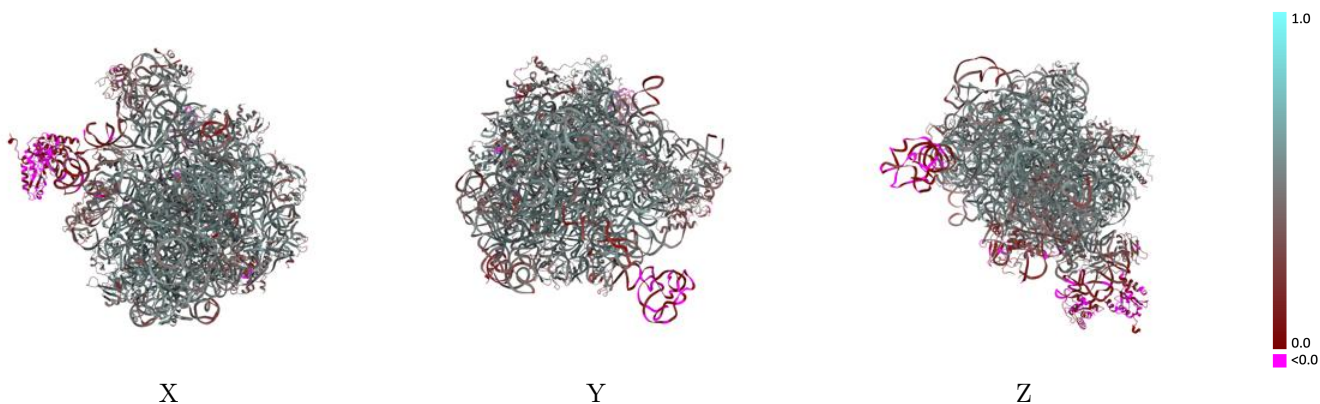
This section contains information regarding the fit between EMDB map EMD-3531 and PDB model 5MMI. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



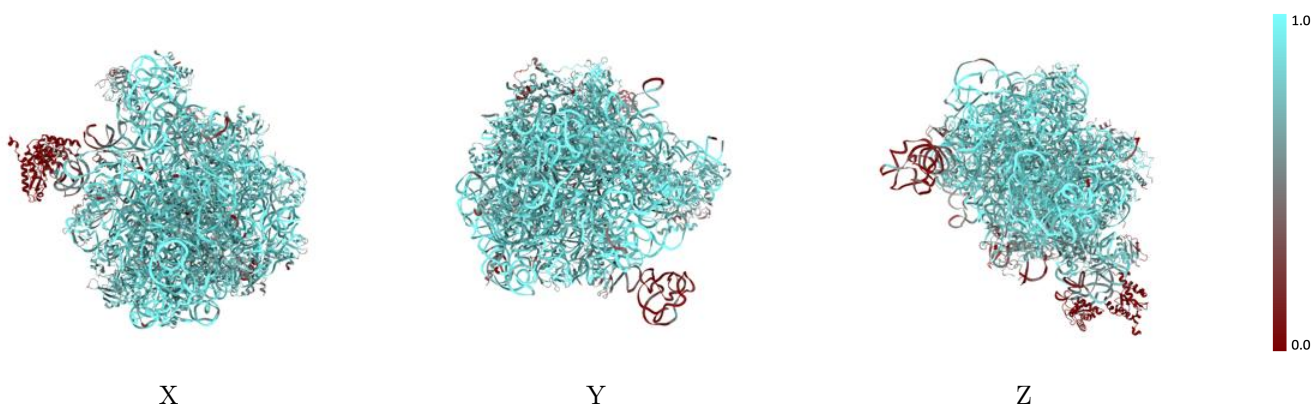
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



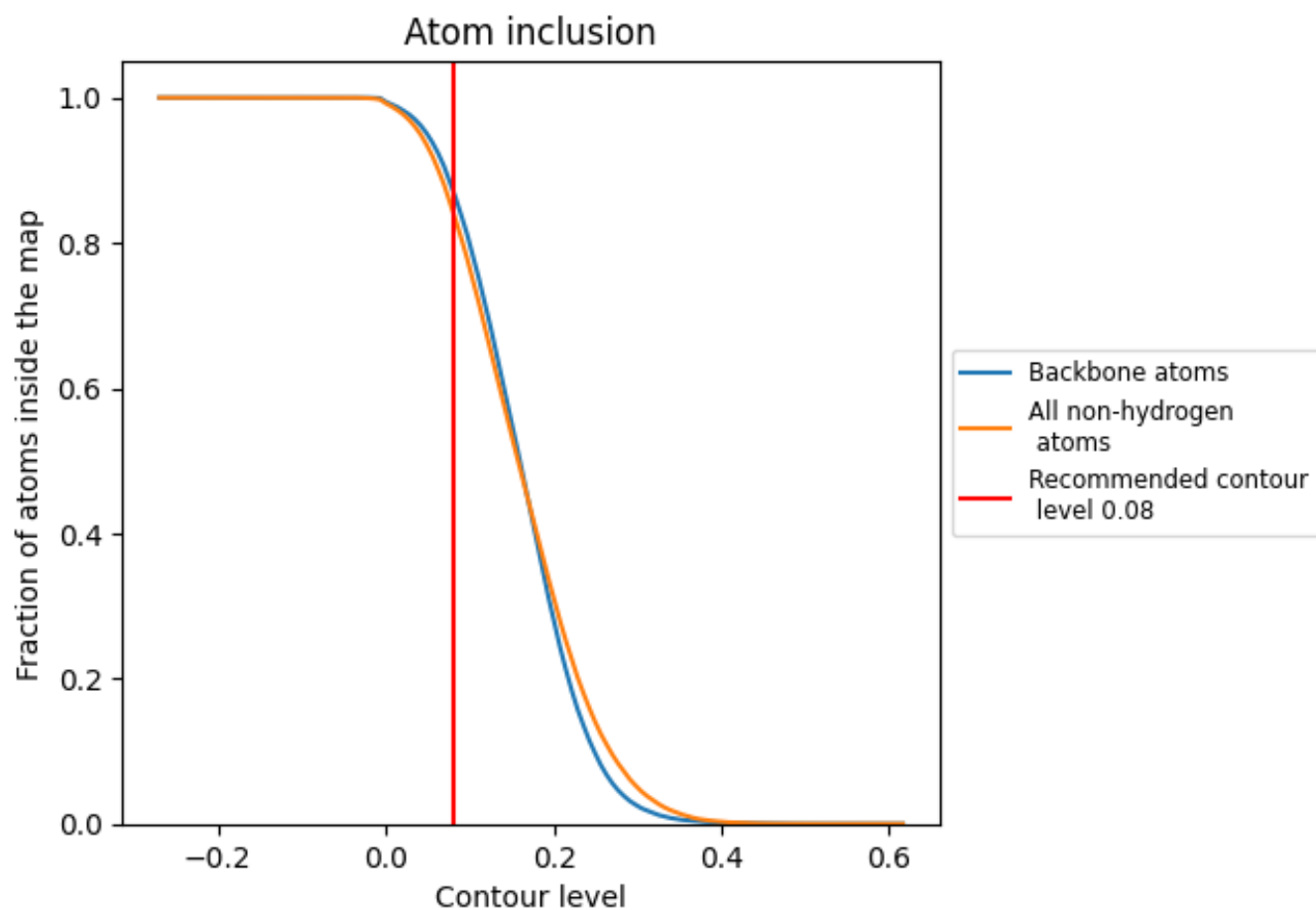
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8434	 0.4690
0	 0.4416	 0.2120
1	 0.8359	 0.5280
2	 0.7611	 0.4720
3	 0.8600	 0.5580
4	 0.8310	 0.5360
5	 0.7552	 0.4690
6	 0.7266	 0.4260
7	 0.8268	 0.4900
A	 0.8993	 0.4880
B	 0.9396	 0.4510
C	 0.7868	 0.4900
D	 0.8463	 0.5130
E	 0.8082	 0.4880
F	 0.5710	 0.3020
G	 0.6578	 0.3450
H	 0.4828	 0.3860
I	 0.0376	 0.0180
J	 0.0701	 0.0320
K	 0.8322	 0.4980
L	 0.7309	 0.4880
M	 0.8287	 0.4810
N	 0.5414	 0.4030
O	 0.8497	 0.5190
P	 0.8053	 0.4350
Q	 0.7780	 0.4790
R	 0.8712	 0.5220
S	 0.7603	 0.4590
T	 0.7688	 0.4630
U	 0.7464	 0.4570
V	 0.7458	 0.4450
W	 0.9459	 0.5100
X	 0.8174	 0.4850
Y	 0.8068	 0.5030
Z	 0.7466	 0.4290
z	 0.4048	 0.4000

