



## Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 06:24 pm GMT

PDB ID : 6GZQ  
EMDB ID : EMD-0101  
Title : T. thermophilus hibernating 70S ribosome  
Authors : Flygaard, R.K.; Jenner, L.B.  
Deposited on : 2018-07-04  
Resolution : 3.28 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

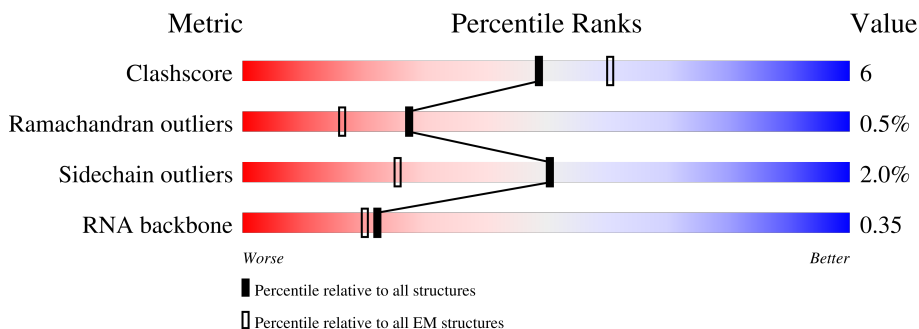
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.28 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.









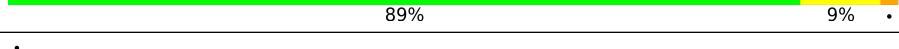
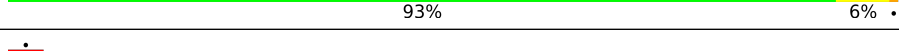
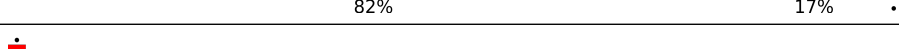
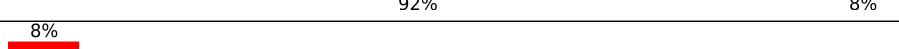
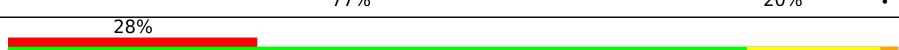

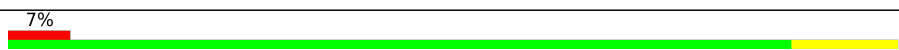

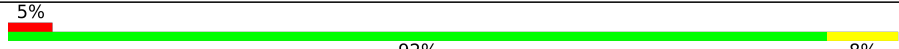



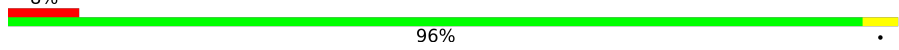


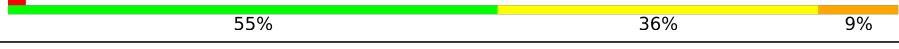
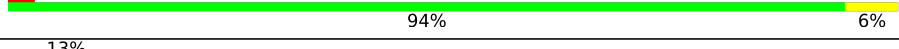


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	C1	272	
2	D1	205	
3	E1	208	
4	F1	181	
5	G1	170	
6	H1	50	
7	I1	138	



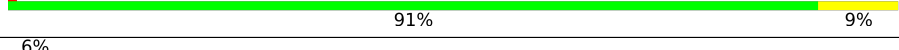
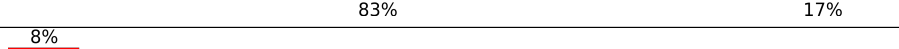
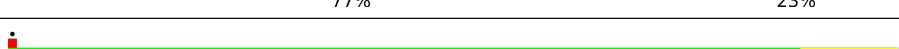
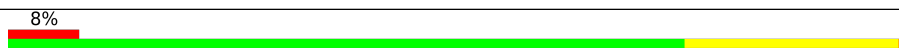
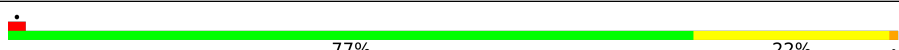



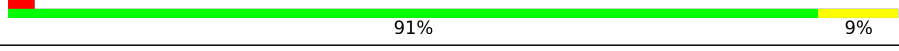
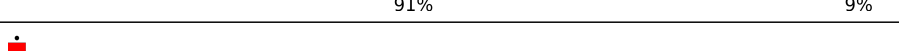
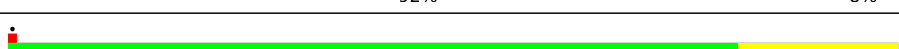
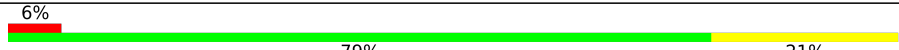




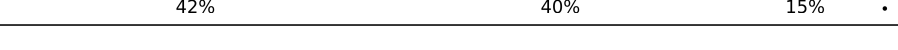


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Mol	Chain	Length	Quality of chain
8	J1	122	
9	K1	150	
10	L1	141	
11	M1	117	
12	N1	111	
13	O1	137	
14	P1	117	
15	Q1	101	
16	R1	113	
17	S1	92	
18	T1	102	
19	U1	179	
20	V1	77	
21	W1	97	
22	X1	69	
23	Y1	59	
24	Z1	63	
25	a1	59	
26	b1	45	
27	c1	49	
28	d1	61	
29	A1	2912	
30	B1	122	
31	e1	36	
32	B2	237	

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Mol	Chain	Length	Quality of chain
33	C2	206	
34	D2	208	
35	E2	151	
36	F2	101	
37	G2	155	
38	H2	138	
39	I2	127	
40	J2	99	
41	K2	118	
42	L2	125	
43	M2	117	
44	N2	60	
45	O2	88	
46	P2	84	
47	Q2	100	
48	R2	62	
49	S2	78	
50	T2	99	
51	U2	25	
52	V2	121	
53	A2	1506	

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 144138 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 L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	272	Total	C	N	O	S	0	0
			2116	1335	420	358	3		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D1	205	Total	C	N	O	S	0	0
			1569	991	300	272	6		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E1	208	Total	C	N	O	S	0	0
			1628	1037	304	284	3		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F1	181	Total	C	N	O	S	0	0
			1474	942	268	260	4		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G1	170	Total	C	N	O	S	0	0
			1308	829	245	233	1		

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H1	50	Total	C	N	O	S	0	0
			383	245	66	71	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I1	138	Total	C	N	O	S	0	0
			1105	712	206	183	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J1	122	Total	C	N	O	S	0	0
			933	588	171	170	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K1	150	Total	C	N	O	S	0	0
			1145	712	232	198	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L1	141	Total	C	N	O	S	0	0
			1122	715	212	188	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M1	117	Total	C	N	O	0	0
			960	599	202	159		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	N1	111	Total	C	N	O	0	0
			882	556	176	150		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O1	137	Total	C	N	O	S	0	0
			1142	710	234	197	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P1	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q1	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R1	113	Total	C	N	O	S	0	0
			900	566	177	155	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	S1	92	Total	C	N	O	0	0
			726	471	131	124		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T1	102	Total	C	N	O	S	0	0
			786	505	150	126	5		

- Molecule 19 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U1	179	Total	C	N	O	S	0	0
			1429	911	255	260	3		

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V1	77	Total	C	N	O	S	0	0
			613	379	129	104	1		

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W1	97	Total	C	N	O	S	0	0
			763	481	150	131	1		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X1	69	Total	C	N	O	S	0	0
			581	358	118	104	1		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Y1	59	Total	C	N	O	0	0
			469	298	90	81		

- Molecule 24 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z1	63	Total	C	N	O	S	0	0
			516	326	93	92	5		

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a1	59	Total	C	N	O	S	0	0
			459	288	90	76	5		

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b1	45	Total	C	N	O	S	0	0
			390	241	79	66	4		

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c1	49	Total	C	N	O	S	0	0
			430	263	108	57	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	d1	61	Total	C	N	O	S	0	0
			489	312	99	76	2		

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A1	2912	Total	C	N	O	P	0	0
			62707	27911	11722	20163	2911		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	156	U	UNK	conflict	GB 55771382
A1	682	A	G	conflict	GB 55771382
A1	686	C	G	conflict	GB 55771382
A1	697	G	C	conflict	GB 55771382
A1	701	A	C	conflict	GB 55771382
A1	1106	U	G	conflict	GB 55771382
A1	1128	A	C	conflict	GB 55771382

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B1	122	Total	C	N	O	P	0	0
			2617	1166	486	844	121		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	36	Total	C	N	O	S	0	0
			299	183	67	46	3		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B2	237	Total	C	N	O	S	0	0
			1925	1228	344	348	5		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	C2	206	Total	C	N	O	S	0	0
			1613	1016	314	282	1		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D2	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E2	151	Total	C	N	O	S	0	0
			1156	729	218	205	4		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	F2	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	G2	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	H2	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	I2	127	Total	C	N	O	0	0
			1010	639	197	174		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	J2	99	Total	C	N	O	S	0	0
			802	504	157	140	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	K2	118	Total	C	N	O	S	0	0
			879	546	167	163	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L2	125	Total	C	N	O	S	0	0
			976	614	196	165	1		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M2	117	Total	C	N	O	S	0	0
			934	577	192	163	2		

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N2	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	O2	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	P2	84	Total	C	N	O	S	0	0
			706	446	140	119	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Q2	100	Total	C	N	O	S	0	0
			835	534	155	144	2		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	R2	62	Total	C	N	O	0	0
			515	328	101	86		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S2	78	Total	C	N	O	S	0	0
			625	398	115	110	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	T2	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 51 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	U2	25	Total	C	N	O	0	0
			218	134	52	32		

- Molecule 52 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	V2	121	Total	C	N	O	S	0	0
			983	615	185	182	1		

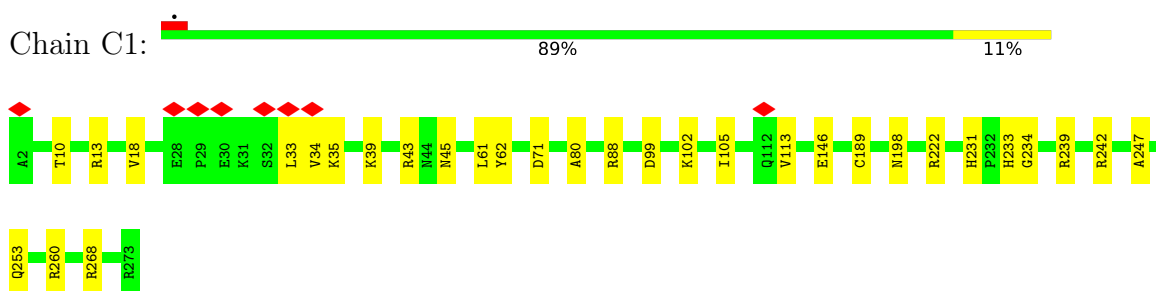
- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A2	1506	Total	C	N	O	P	0	0
			32369	14408	5997	10459	1505		

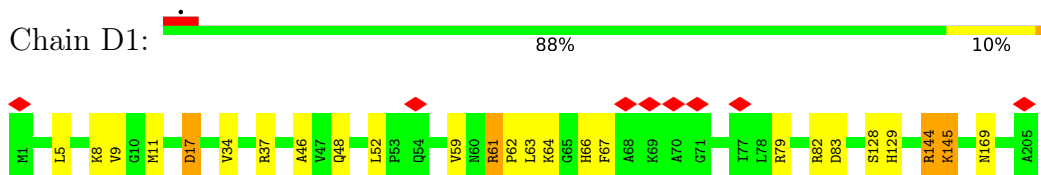
### 3 Residue-property plots [i](#)

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.

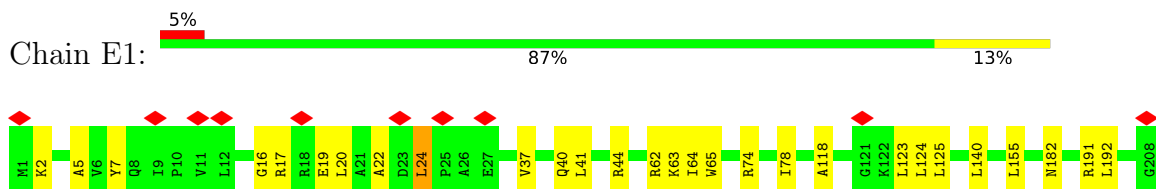
- Molecule 1: 50S ribosomal protein L2



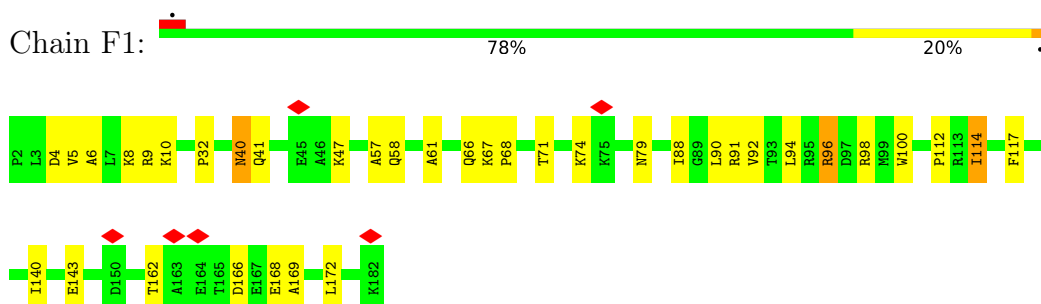
- Molecule 2: 50S ribosomal protein L3



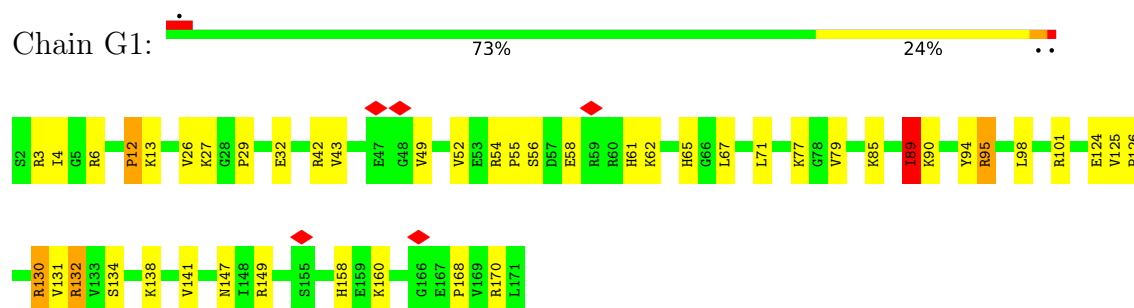
- Molecule 3: 50S ribosomal protein L4



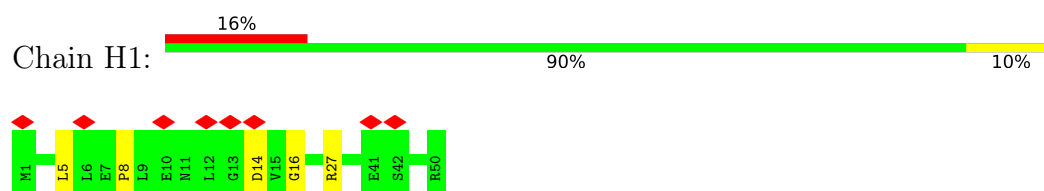
- Molecule 4: 50S ribosomal protein L5



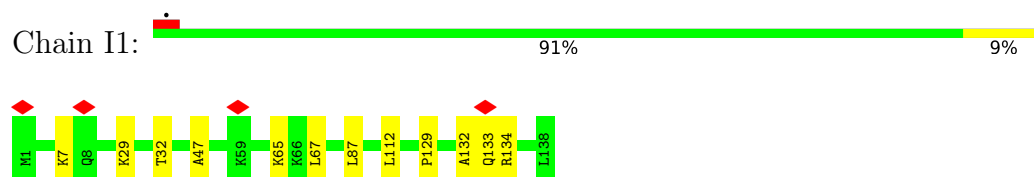
- Molecule 5: 50S ribosomal protein L6



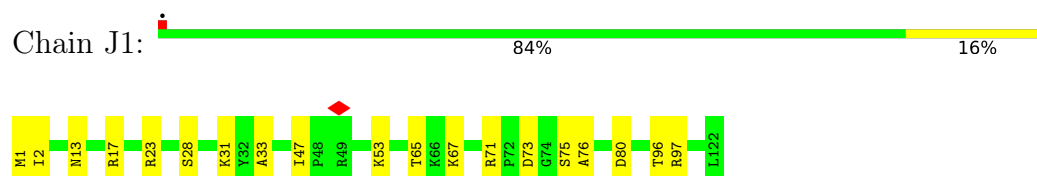
- Molecule 6: 50S ribosomal protein L9



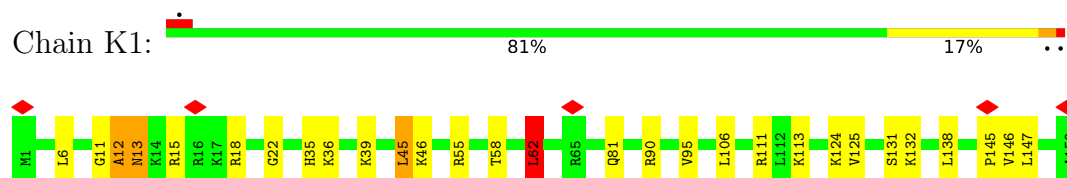
- Molecule 7: 50S ribosomal protein L13



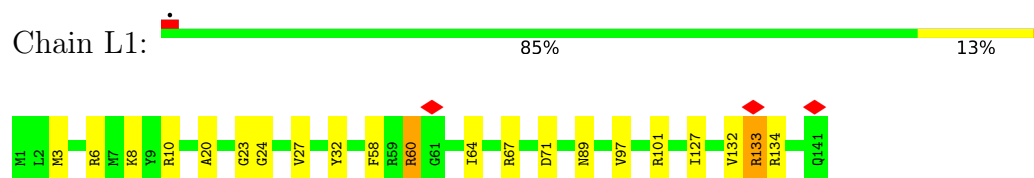
- Molecule 8: 50S ribosomal protein L14



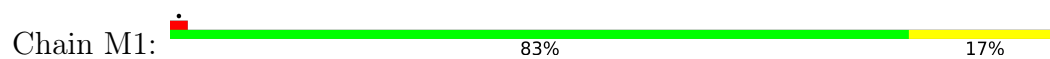
- Molecule 9: 50S ribosomal protein L15



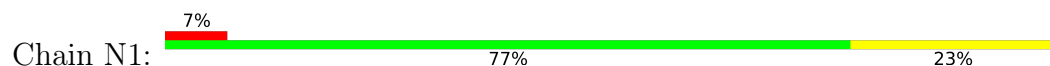
- Molecule 10: 50S ribosomal protein L16



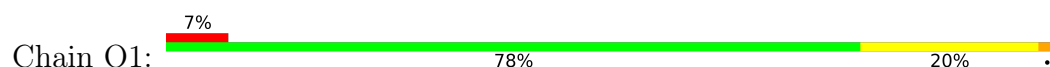
- Molecule 11: 50S ribosomal protein L17



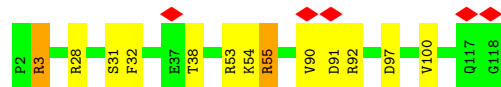
- Molecule 12: 50S ribosomal protein L18



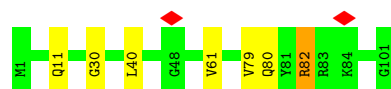
- Molecule 13: 50S ribosomal protein L19



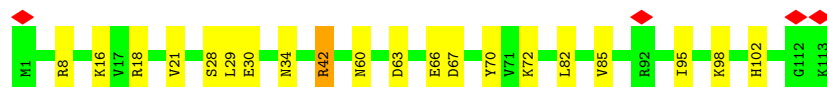
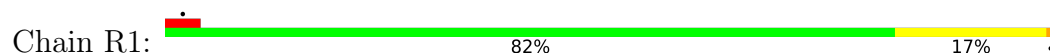
- Molecule 14: 50S ribosomal protein L20



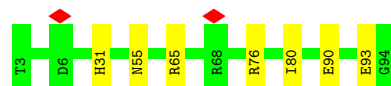
- Molecule 15: 50S ribosomal protein L21



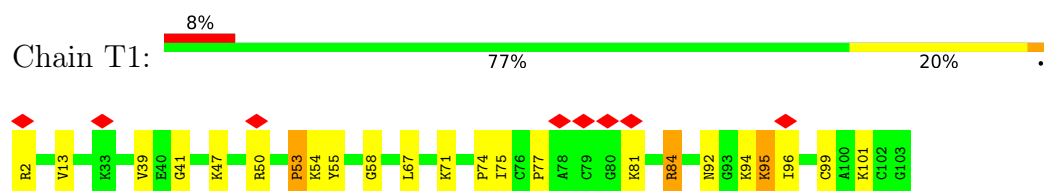
- Molecule 16: 50S ribosomal protein L22



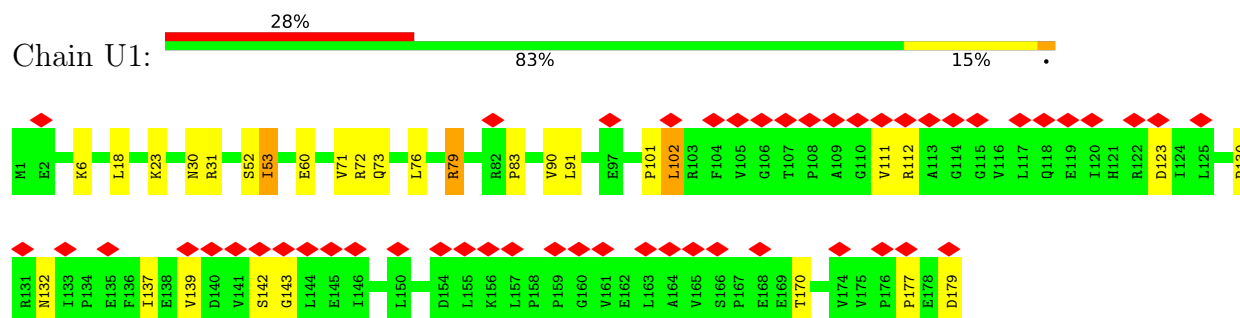
- Molecule 17: 50S ribosomal protein L23



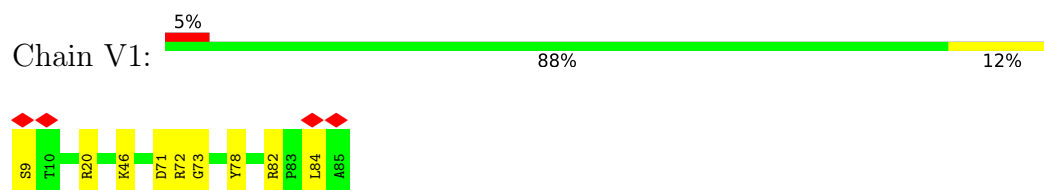
- Molecule 18: 50S ribosomal protein L24



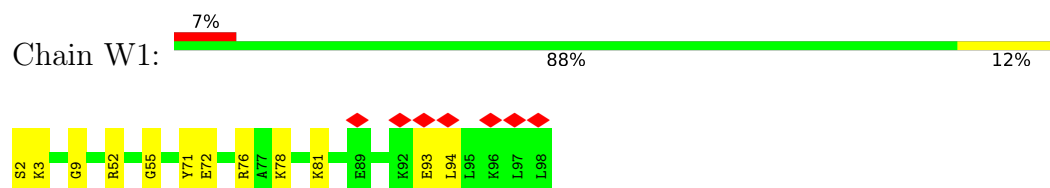
- Molecule 19: 50S ribosomal protein L25



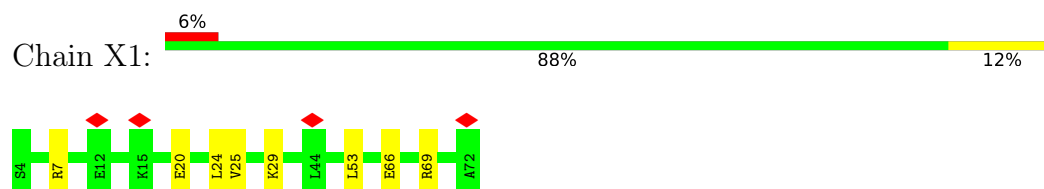
- Molecule 20: 50S ribosomal protein L27



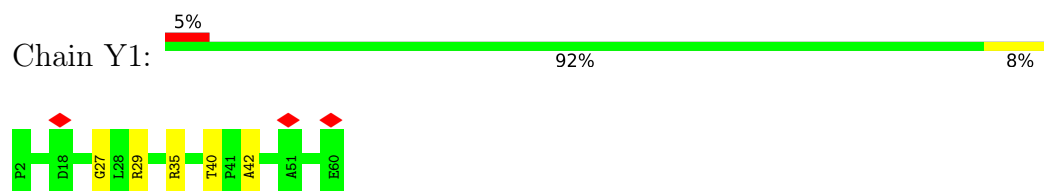
- Molecule 21: 50S ribosomal protein L28



- Molecule 22: 50S ribosomal protein L29



- Molecule 23: 50S ribosomal protein L30

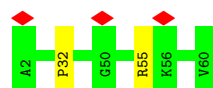


- Molecule 24: 50S ribosomal protein L31

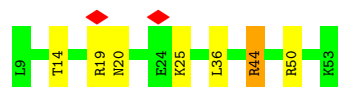
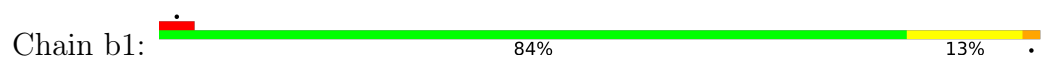




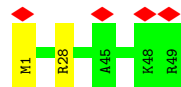
- Molecule 25: 50S ribosomal protein L32



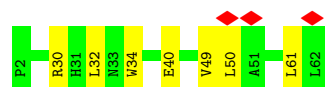
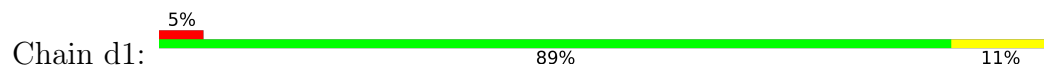
- Molecule 26: 50S ribosomal protein L33



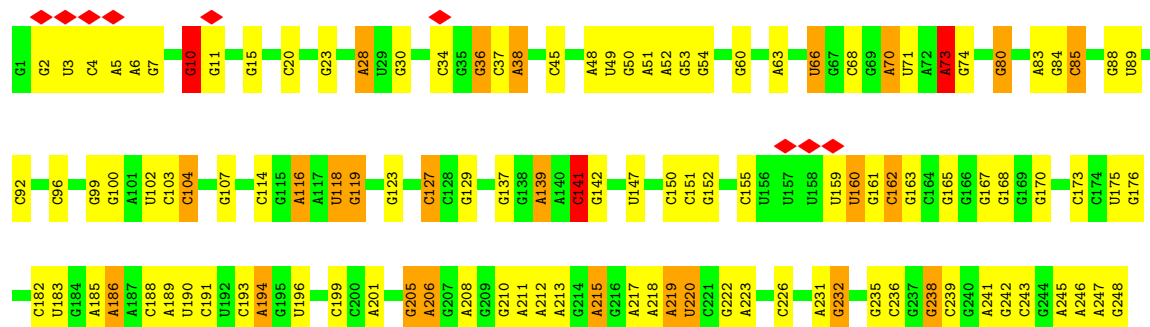
- Molecule 27: 50S ribosomal protein L34

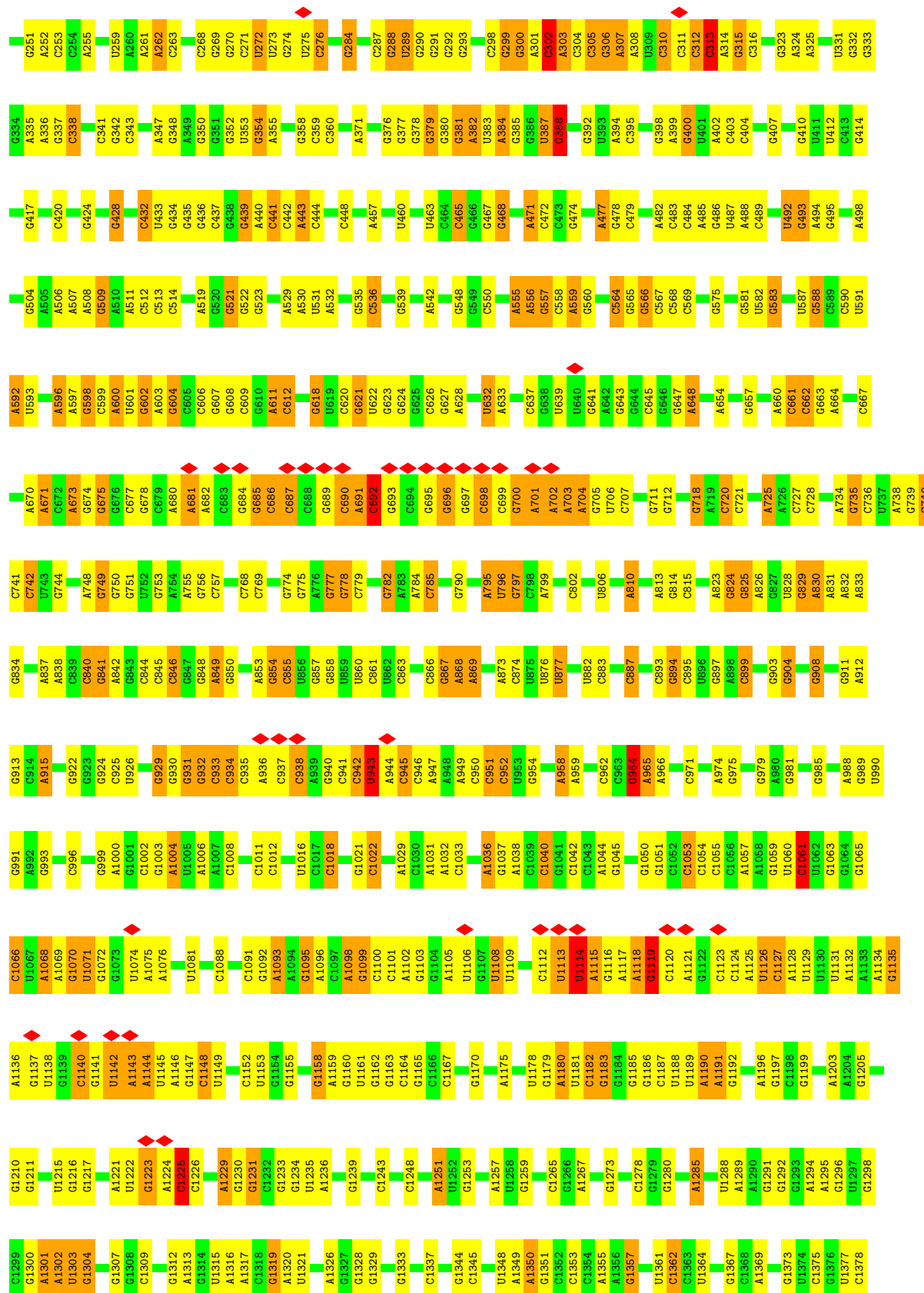


- Molecule 28: 50S ribosomal protein L35

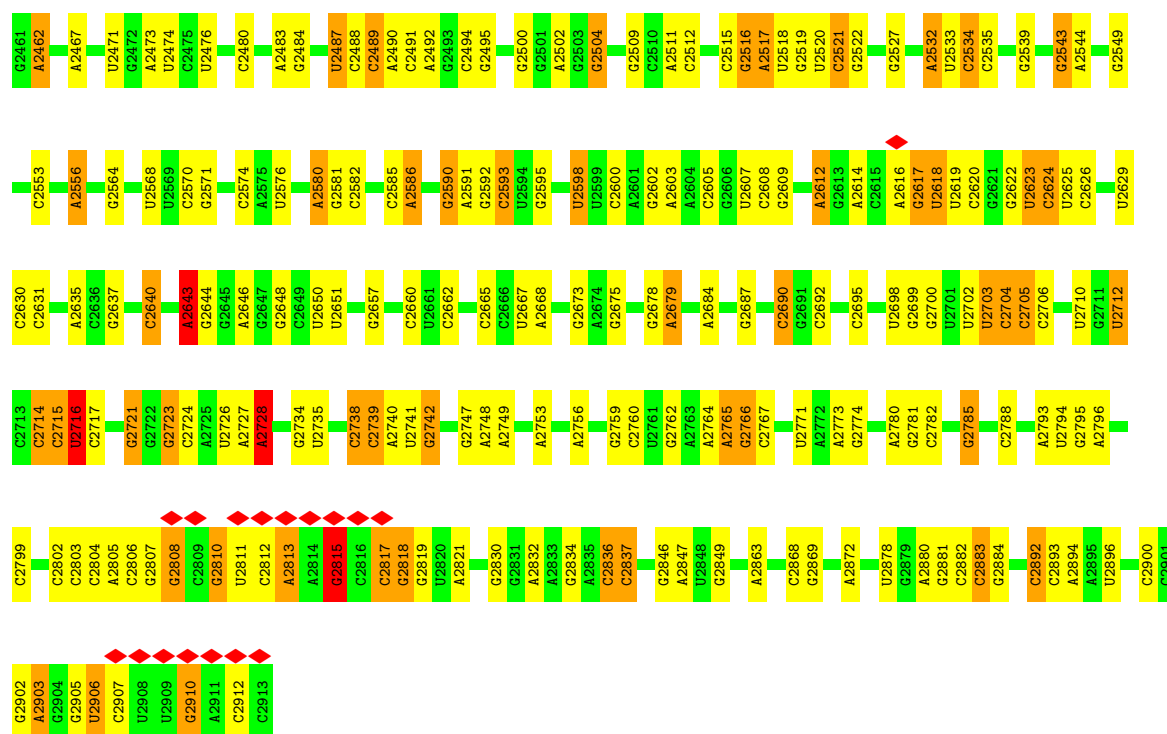


- Molecule 29: 23S ribosomal RNA

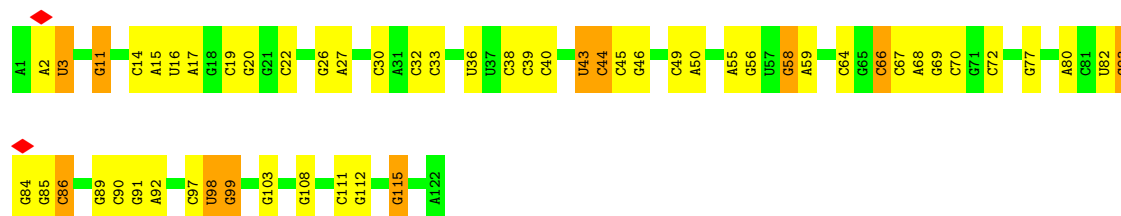




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U2271	A2193	U2271	A2193	G2136	G2059	C1982	G1907	A1836	G1765	C1662	U1595	A1516	A1441	A1442
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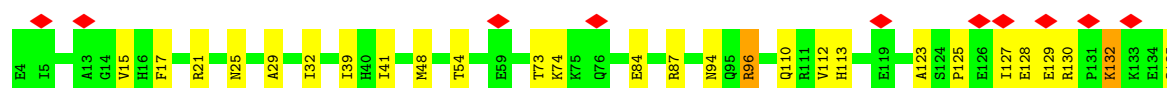
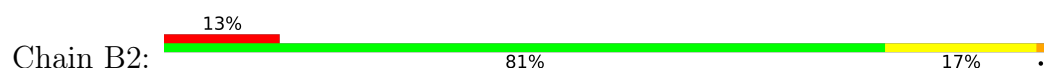
• Molecule 30: 5S ribosomal RNA

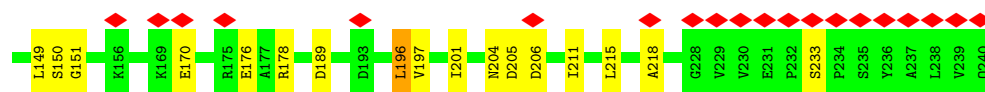


• Molecule 31: 50S ribosomal protein L36

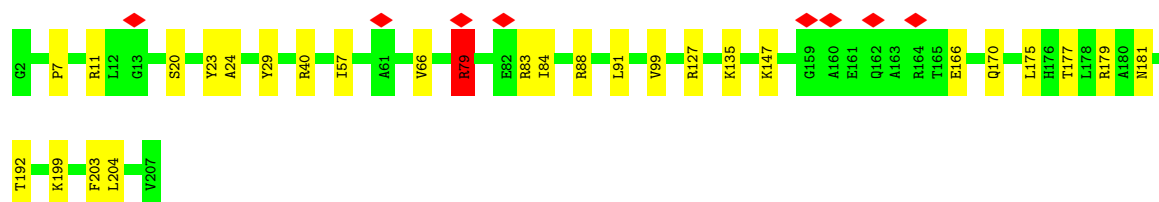


• Molecule 32: 30S ribosomal protein S2

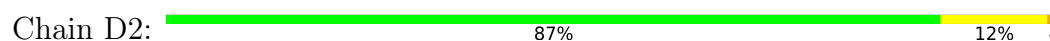




- Molecule 33: 30S ribosomal protein S3



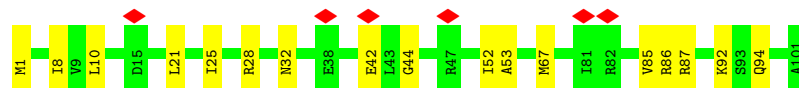
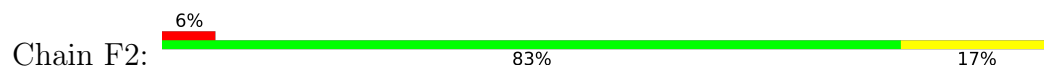
- Molecule 34: 30S ribosomal protein S4



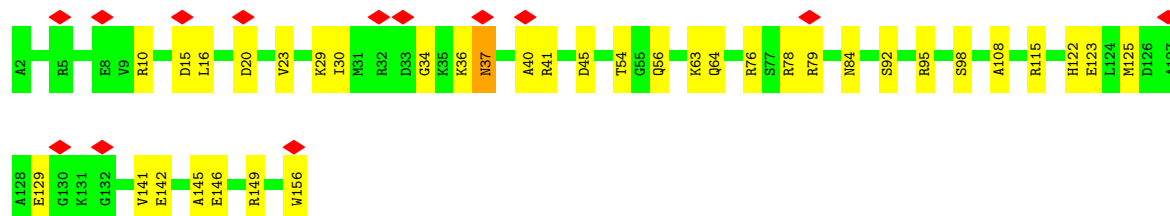
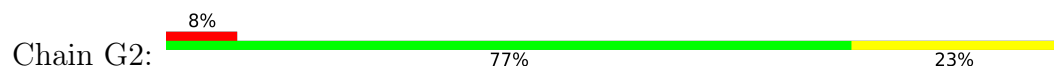
- Molecule 35: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S6



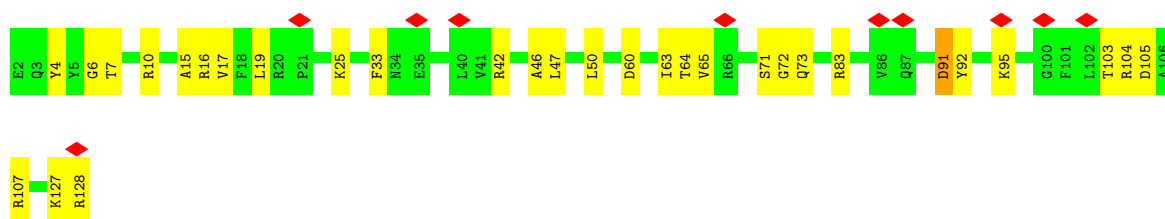
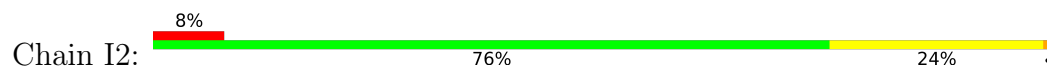
- Molecule 37: 30S ribosomal protein S7



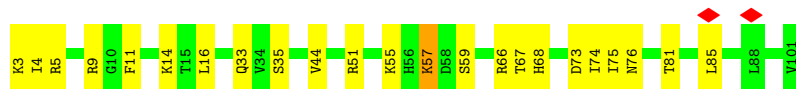
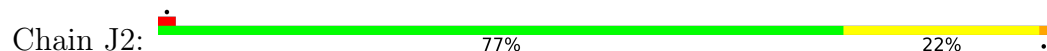
- Molecule 38: 30S ribosomal protein S8



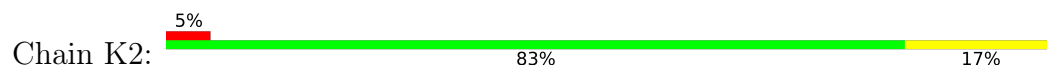
- Molecule 39: 30S ribosomal protein S9



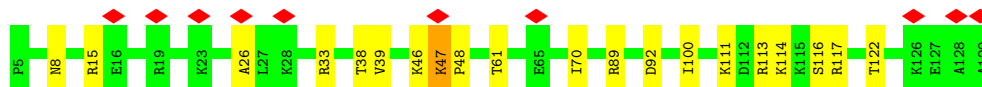
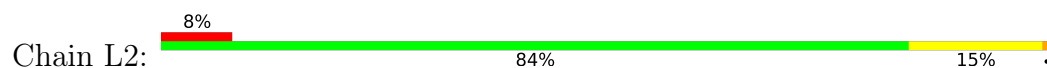
- Molecule 40: 30S ribosomal protein S10



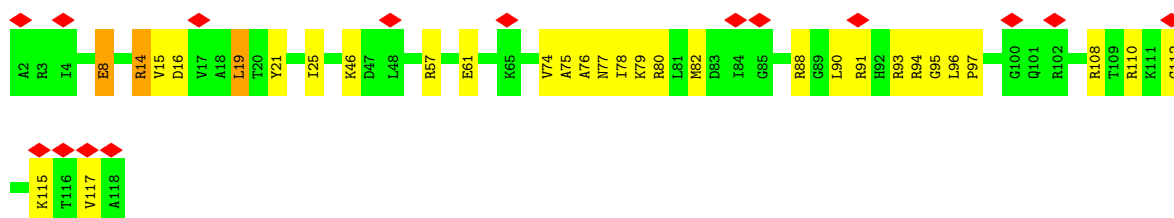
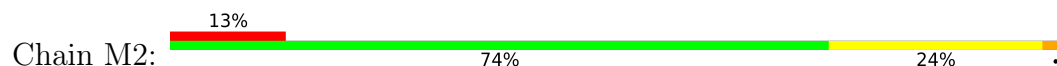
- Molecule 41: 30S ribosomal protein S11




- Molecule 42: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S14 type Z

Chain N2:  88% 12%



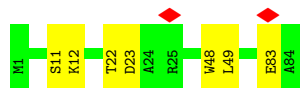
- Molecule 45: 30S ribosomal protein S15

Chain O2:  91% 9%




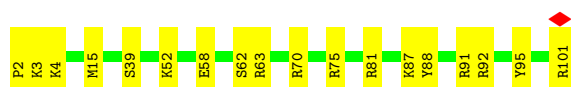
- Molecule 46: 30S ribosomal protein S16

Chain P2:  92% 8%




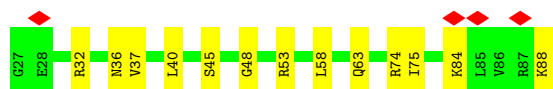
- Molecule 47: 30S ribosomal protein S17

Chain Q2:  82% 18%




- Molecule 48: 30S ribosomal protein S18

Chain R2:  79% 21% 6%



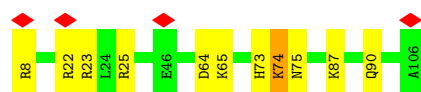
- Molecule 49: 30S ribosomal protein S19

Chain S2:  77% 18% 5% 9%

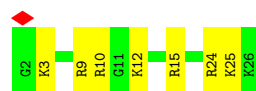
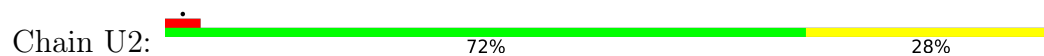


- Molecule 50: 30S ribosomal protein S20

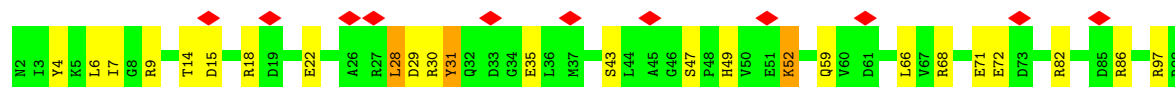
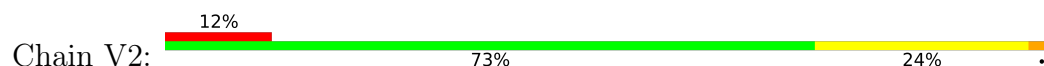
Chain T2:  89% 10%



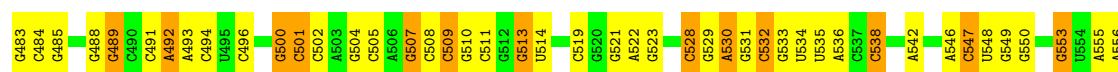
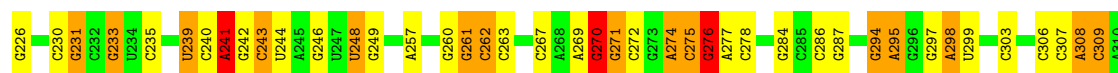
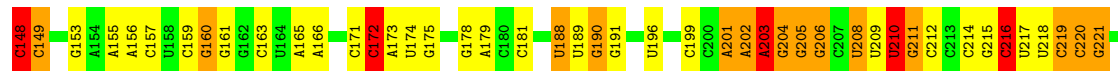
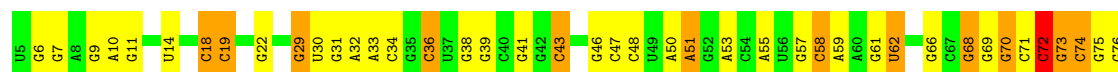
- Molecule 51: 30S ribosomal protein Thx



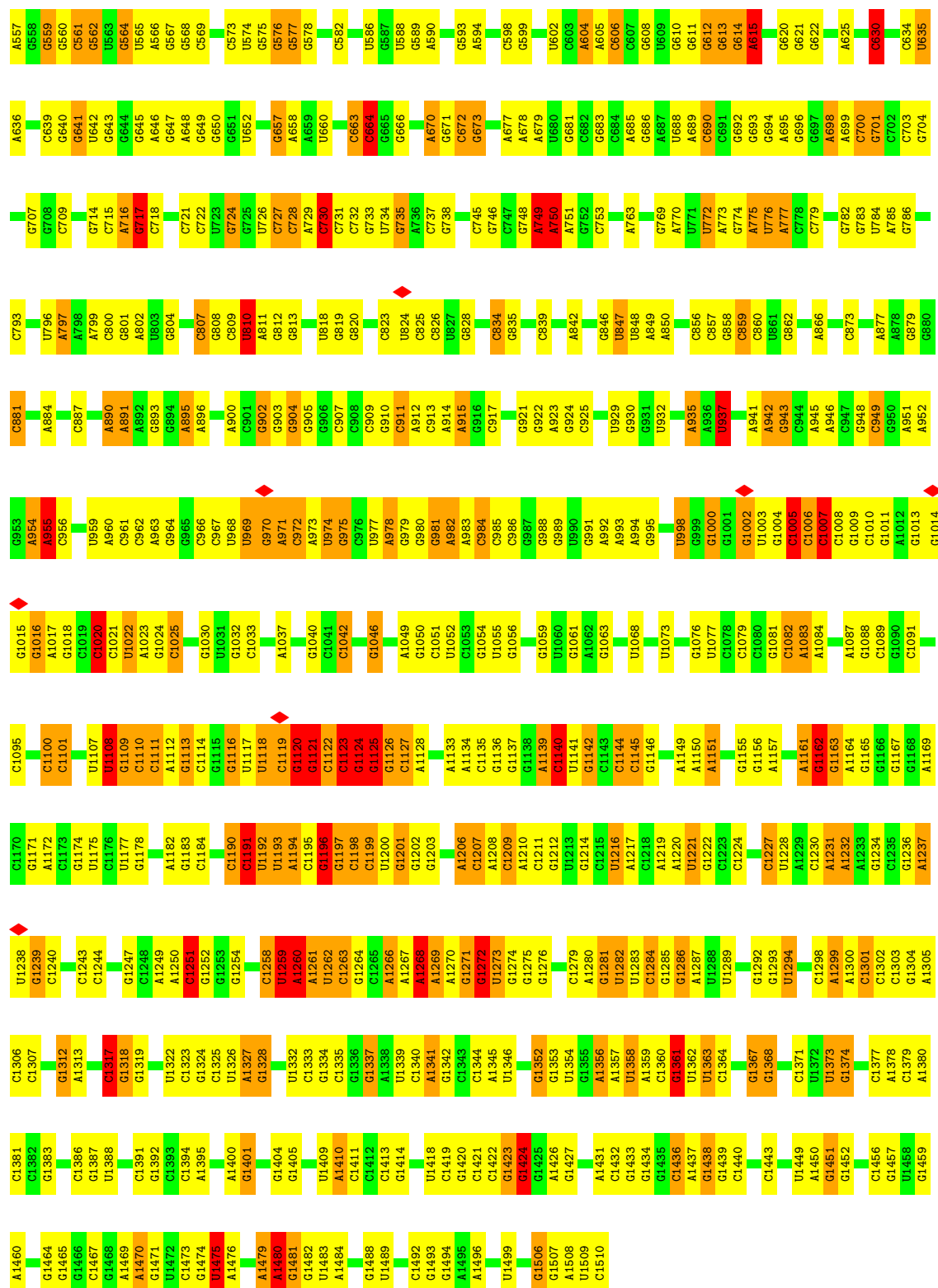
- Molecule 52: Ribosome hibernation promoting factor



- Molecule 53: 16S ribosomal RNA







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45422	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 ( $e^-/\text{\AA}^2$ )	1.06	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	35.207	Depositor
Minimum map value	-15.042	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.439	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	770.0, 770.0, 770.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	C1	0.77	1/2166 (0.0%)	0.76	0/2919
2	D1	0.71	0/1602	0.77	1/2160 (0.0%)
3	E1	0.72	0/1663	0.69	0/2249
4	F1	0.53	0/1499	0.66	0/2016
5	G1	0.52	0/1333	0.73	1/1802 (0.1%)
6	H1	0.49	0/387	0.71	0/523
7	I1	0.68	0/1132	0.68	0/1525
8	J1	0.70	0/943	0.69	0/1269
9	K1	0.61	0/1162	0.84	1/1544 (0.1%)
10	L1	0.65	0/1143	0.70	0/1527
11	M1	0.66	0/974	0.79	0/1302
12	N1	0.58	0/892	0.72	0/1187
13	O1	0.62	0/1156	0.67	0/1542
14	P1	0.77	0/982	0.68	0/1306
15	Q1	0.61	0/790	0.67	0/1057
16	R1	0.64	0/911	0.75	3/1220 (0.2%)
17	S1	0.68	0/740	0.72	0/993
18	T1	0.55	0/799	0.69	0/1064
19	U1	0.52	0/1461	0.66	1/1982 (0.1%)
20	V1	0.69	0/621	0.69	0/827
21	W1	0.66	0/770	0.74	0/1022
22	X1	0.52	0/583	0.69	0/771
23	Y1	0.65	0/474	0.68	0/635
24	Z1	0.48	0/528	0.78	0/709
25	a1	0.75	1/473 (0.2%)	0.71	0/639
26	b1	0.66	0/397	0.95	1/529 (0.2%)
27	c1	0.78	0/438	0.75	0/575
28	d1	0.74	0/495	0.99	3/649 (0.5%)
29	A1	1.64	325/70233 (0.5%)	1.41	861/109643 (0.8%)
30	B1	1.26	2/2928 (0.1%)	1.37	34/4568 (0.7%)
31	e1	0.71	0/302	0.69	0/397
32	B2	0.55	0/1960	0.68	0/2642
33	C2	0.61	0/1637	0.70	0/2205
34	D2	0.67	0/1733	0.76	0/2318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	E2	0.66	0/1172	0.71	0/1576
36	F2	0.55	0/856	0.64	0/1154
37	G2	0.51	0/1276	0.66	1/1709 (0.1%)
38	H2	0.70	0/1136	0.68	0/1527
39	I2	0.54	0/1029	0.72	0/1379
40	J2	0.50	0/815	0.65	1/1095 (0.1%)
41	K2	0.58	0/894	0.68	0/1205
42	L2	0.68	0/992	0.72	0/1327
43	M2	0.43	0/944	0.71	0/1265
44	N2	0.62	0/501	0.69	0/664
45	O2	0.59	0/745	0.70	0/992
46	P2	0.71	0/722	0.69	0/970
47	Q2	0.66	0/848	0.66	0/1131
48	R2	0.55	0/520	0.73	0/690
49	S2	0.44	0/639	0.72	0/860
50	T2	0.49	0/765	0.69	0/1007
51	U2	0.54	0/222	0.67	0/288
52	V2	0.59	0/997	0.84	1/1341 (0.1%)
53	A2	3.30	114/36234 (0.3%)	1.91	551/56554 (1.0%)
All	All	1.97	443/156614 (0.3%)	1.41	1460/234050 (0.6%)

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
1	C1	0	1
2	D1	0	1
3	E1	0	1
4	F1	0	1
5	G1	0	1
9	K1	0	2
14	P1	0	1
15	Q1	0	1
17	S1	0	1
18	T1	0	2
19	U1	0	1
24	Z1	0	1
26	b1	0	2
28	d1	0	2
32	B2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	C2	0	2
34	D2	0	3
37	G2	0	2
39	I2	0	1
40	J2	0	1
42	L2	0	2
43	M2	0	2
49	S2	0	1
51	U2	0	1
52	V2	0	2
All	All	0	37

All (443) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A2	700	C	N1-C6	189.65	2.50	1.37
53	A2	717	G	C6-N1	170.78	2.59	1.39
53	A2	717	G	N3-C4	146.04	2.37	1.35
53	A2	136	G	C2-N2	143.97	2.78	1.34
53	A2	1121	G	C2-N2	142.36	2.77	1.34
53	A2	717	G	N1-C2	138.85	2.48	1.37
53	A2	700	C	N3-C4	128.10	2.23	1.33
53	A2	216	C	N3-C4	126.72	2.22	1.33
53	A2	1110	C	N3-C4	125.93	2.22	1.33
53	A2	717	G	C2-N3	125.28	2.33	1.32
53	A2	717	G	C5-C4	119.04	2.21	1.38
53	A2	216	C	C2-N3	114.65	2.27	1.35
53	A2	1110	C	C2-N3	112.60	2.25	1.35
53	A2	1110	C	N1-C6	108.09	2.02	1.37
53	A2	216	C	N1-C6	105.72	2.00	1.37
53	A2	717	G	C5-C6	91.24	2.33	1.42
53	A2	1110	C	C4-C5	79.68	2.06	1.43
53	A2	216	C	C4-C5	75.82	2.03	1.43
53	A2	1110	C	C5-C6	73.20	1.93	1.34
53	A2	216	C	C5-C6	69.32	1.89	1.34
53	A2	1110	C	N1-C2	69.32	2.09	1.40
53	A2	216	C	N1-C2	65.35	2.05	1.40
53	A2	700	C	C2-N3	28.83	1.58	1.35
53	A2	700	C	C4-N4	25.84	1.57	1.33
53	A2	700	C	C1'-N1	12.29	1.67	1.48
53	A2	700	C	N1-C2	-10.02	1.30	1.40
29	A1	555	A	N9-C4	-9.54	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	832	A	N9-C4	-9.26	1.32	1.37
29	A1	1714	A	N9-C4	-8.71	1.32	1.37
53	A2	1374	G	N7-C5	-8.52	1.34	1.39
29	A1	1726	A	N9-C4	-8.48	1.32	1.37
29	A1	1824	A	N9-C4	-8.27	1.32	1.37
29	A1	542	A	N9-C4	-8.15	1.32	1.37
29	A1	832	A	N7-C5	-8.05	1.34	1.39
29	A1	867	G	N7-C5	-8.05	1.34	1.39
29	A1	1686	A	N9-C4	-7.96	1.33	1.37
53	A2	717	G	C8-N7	7.95	1.35	1.30
29	A1	2078	A	N9-C4	-7.92	1.33	1.37
29	A1	1036	A	N9-C4	-7.73	1.33	1.37
29	A1	849	A	N9-C4	-7.34	1.33	1.37
29	A1	73	A	N9-C4	-7.29	1.33	1.37
25	a1	32	PRO	C-N	-7.23	1.17	1.34
29	A1	206	A	N9-C4	-7.22	1.33	1.37
29	A1	832	A	C5-C6	-7.16	1.34	1.41
53	A2	1268	A	N7-C5	-7.15	1.34	1.39
29	A1	2044	A	N9-C4	-7.14	1.33	1.37
53	A2	1457	G	N7-C5	-6.95	1.35	1.39
53	A2	1121	G	N1-C2	6.89	1.43	1.37
29	A1	1819	A	N7-C5	-6.80	1.35	1.39
29	A1	632	U	C2-N3	-6.80	1.32	1.37
29	A1	185	A	N9-C4	-6.79	1.33	1.37
53	A2	1121	G	C5-C4	-6.78	1.33	1.38
1	C1	239	ARG	C-N	-6.77	1.18	1.34
29	A1	823	A	C5-C6	-6.77	1.34	1.41
53	A2	750	A	N7-C5	-6.76	1.35	1.39
53	A2	802	A	N9-C4	-6.76	1.33	1.37
29	A1	2457	C	N1-C6	-6.73	1.33	1.37
29	A1	1793	A	N9-C4	-6.72	1.33	1.37
29	A1	611	A	N9-C4	-6.62	1.33	1.37
29	A1	1923	G	N9-C4	-6.59	1.32	1.38
29	A1	2075	A	N9-C4	-6.59	1.33	1.37
29	A1	2301	A	N9-C4	-6.58	1.33	1.37
53	A2	635	U	C4-O4	-6.55	1.18	1.23
29	A1	965	A	N7-C5	-6.52	1.35	1.39
53	A2	557	A	N9-C4	-6.52	1.33	1.37
29	A1	842	A	N7-C5	-6.51	1.35	1.39
53	A2	810	U	C2-N3	-6.48	1.33	1.37
53	A2	679	A	N7-C5	-6.45	1.35	1.39
29	A1	2441	C	N1-C6	-6.42	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A2	277	A	N9-C4	-6.42	1.33	1.37
29	A1	2614	A	N9-C4	-6.42	1.33	1.37
29	A1	2444	A	N9-C4	-6.41	1.34	1.37
29	A1	2002	A	N9-C4	-6.40	1.34	1.37
29	A1	1997	G	N7-C5	-6.40	1.35	1.39
29	A1	782	G	N1-C2	-6.39	1.32	1.37
29	A1	2096	G	N7-C5	-6.37	1.35	1.39
29	A1	1615	A	N9-C4	-6.37	1.34	1.37
29	A1	1403	G	N7-C5	-6.37	1.35	1.39
29	A1	738	A	N9-C4	-6.35	1.34	1.37
29	A1	1833	C	N1-C6	-6.33	1.33	1.37
29	A1	1714	A	C5-C6	-6.30	1.35	1.41
29	A1	648	A	N9-C4	-6.29	1.34	1.37
29	A1	2467	A	N7-C5	-6.28	1.35	1.39
29	A1	116	A	N7-C5	-6.27	1.35	1.39
29	A1	1714	A	N7-C5	-6.26	1.35	1.39
29	A1	823	A	N9-C4	-6.25	1.34	1.37
53	A2	635	U	C2-N3	-6.25	1.33	1.37
29	A1	1824	A	N3-C4	-6.21	1.31	1.34
29	A1	2102	C	N1-C6	-6.21	1.33	1.37
53	A2	1479	A	N7-C5	-6.20	1.35	1.39
29	A1	1824	A	N7-C5	-6.18	1.35	1.39
29	A1	1234	G	N7-C5	-6.18	1.35	1.39
29	A1	795	A	N9-C4	-6.18	1.34	1.37
29	A1	592	A	N7-C5	-6.17	1.35	1.39
29	A1	1807	C	N3-C4	-6.16	1.29	1.33
29	A1	823	A	N7-C5	-6.14	1.35	1.39
29	A1	1072	G	N7-C5	-6.09	1.35	1.39
29	A1	2024	G	N7-C5	-6.09	1.35	1.39
29	A1	1824	A	C5-C4	-6.08	1.34	1.38
29	A1	1725	A	N9-C4	-6.07	1.34	1.37
53	A2	605	A	N9-C4	-6.06	1.34	1.37
29	A1	529	A	N9-C4	-6.05	1.34	1.37
29	A1	832	A	N3-C4	-6.05	1.31	1.34
29	A1	1180	A	N9-C4	-6.05	1.34	1.37
29	A1	70	A	N9-C4	-6.04	1.34	1.37
53	A2	276	G	N7-C5	-6.03	1.35	1.39
29	A1	2603	A	N3-C4	-6.02	1.31	1.34
29	A1	2001	A	N9-C4	-6.00	1.34	1.37
29	A1	1711	C	N1-C6	-5.99	1.33	1.37
29	A1	1809	G	N7-C5	-5.98	1.35	1.39
29	A1	725	A	N7-C5	-5.97	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	1832	G	C6-N1	-5.96	1.35	1.39
29	A1	2391	A	N9-C4	-5.95	1.34	1.37
29	A1	853	A	N9-C4	-5.94	1.34	1.37
29	A1	1823	C	N1-C6	-5.94	1.33	1.37
29	A1	2728	A	N9-C4	-5.93	1.34	1.37
29	A1	611	A	N3-C4	-5.93	1.31	1.34
53	A2	770	A	N9-C4	-5.93	1.34	1.37
53	A2	136	G	C2-N3	5.91	1.37	1.32
29	A1	1719	C	N1-C6	-5.91	1.33	1.37
29	A1	2612	A	N7-C5	-5.91	1.35	1.39
29	A1	2025	A	N9-C4	-5.91	1.34	1.37
29	A1	555	A	N3-C4	-5.89	1.31	1.34
29	A1	1852	A	N7-C5	-5.89	1.35	1.39
29	A1	2586	A	N9-C4	-5.88	1.34	1.37
53	A2	1460	A	N9-C4	-5.86	1.34	1.37
29	A1	2702	U	C2-N3	-5.85	1.33	1.37
29	A1	736	C	N1-C6	-5.85	1.33	1.37
29	A1	840	C	N1-C6	-5.84	1.33	1.37
29	A1	965	A	C5-C6	-5.84	1.35	1.41
29	A1	725	A	C5-C6	-5.84	1.35	1.41
29	A1	2440	A	N9-C4	-5.84	1.34	1.37
29	A1	654	A	N9-C4	-5.82	1.34	1.37
29	A1	848	G	N7-C5	-5.82	1.35	1.39
53	A2	749	A	C5-C6	-5.81	1.35	1.41
29	A1	648	A	N7-C5	-5.81	1.35	1.39
29	A1	1824	A	C5-C6	-5.80	1.35	1.41
29	A1	1923	G	N3-C4	-5.80	1.31	1.35
53	A2	657	G	N3-C4	-5.79	1.31	1.35
29	A1	858	G	C5-C4	-5.79	1.34	1.38
29	A1	2057	A	N9-C4	-5.79	1.34	1.37
53	A2	446	A	N9-C4	-5.77	1.34	1.37
29	A1	488	A	N9-C4	-5.76	1.34	1.37
29	A1	2366	A	N9-C4	-5.76	1.34	1.37
29	A1	2740	A	N3-C4	-5.76	1.31	1.34
29	A1	2450	G	C6-N1	-5.74	1.35	1.39
29	A1	1858	A	N9-C4	-5.74	1.34	1.37
53	A2	955	A	C5-C6	-5.72	1.35	1.41
29	A1	1425	G	N7-C5	-5.70	1.35	1.39
53	A2	709	C	N3-C4	-5.70	1.29	1.33
29	A1	612	C	N1-C6	-5.69	1.33	1.37
29	A1	748	A	N9-C4	-5.69	1.34	1.37
29	A1	810	A	N9-C4	-5.68	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	2580	A	N3-C4	-5.68	1.31	1.34
53	A2	1481	G	C5-C4	-5.67	1.34	1.38
29	A1	1076	A	N9-C4	-5.67	1.34	1.37
29	A1	823	A	N3-C4	-5.66	1.31	1.34
29	A1	2522	G	C5-C4	-5.66	1.34	1.38
29	A1	2018	C	N1-C6	-5.66	1.33	1.37
29	A1	2010	A	N7-C5	-5.66	1.35	1.39
29	A1	1003	G	N7-C5	-5.65	1.35	1.39
29	A1	2740	A	C5-C4	-5.65	1.34	1.38
29	A1	2344	G	N7-C5	-5.64	1.35	1.39
29	A1	241	A	N7-C5	-5.63	1.35	1.39
29	A1	1983	G	C6-N1	-5.63	1.35	1.39
53	A2	657	G	N9-C4	-5.63	1.33	1.38
53	A2	717	G	N9-C8	5.63	1.41	1.37
29	A1	1747	A	N9-C4	-5.62	1.34	1.37
29	A1	2700	G	N7-C5	-5.62	1.35	1.39
53	A2	1327	A	N9-C4	-5.62	1.34	1.37
53	A2	641	G	N7-C5	-5.60	1.35	1.39
29	A1	2556	A	N9-C4	-5.60	1.34	1.37
53	A2	327	G	C5-C4	-5.60	1.34	1.38
29	A1	494	A	N9-C4	-5.60	1.34	1.37
29	A1	633	A	N9-C4	-5.59	1.34	1.37
29	A1	1836	A	N9-C4	-5.58	1.34	1.37
29	A1	2406	A	N9-C4	-5.58	1.34	1.37
29	A1	1929	C	N1-C6	-5.57	1.33	1.37
29	A1	2447	A	N9-C4	-5.57	1.34	1.37
53	A2	1169	A	N9-C4	-5.56	1.34	1.37
29	A1	2402	A	N3-C4	-5.56	1.31	1.34
53	A2	751	A	N9-C4	-5.56	1.34	1.37
53	A2	716	A	N7-C5	-5.55	1.35	1.39
29	A1	206	A	C5-C4	-5.53	1.34	1.38
29	A1	471	A	C5-C6	-5.52	1.36	1.41
29	A1	725	A	N9-C4	-5.52	1.34	1.37
53	A2	810	U	N3-C4	-5.52	1.33	1.38
53	A2	797	A	N7-C5	-5.52	1.35	1.39
29	A1	194	A	C5-C4	-5.52	1.34	1.38
29	A1	2078	A	N7-C5	-5.52	1.35	1.39
53	A2	750	A	C5-C6	-5.52	1.36	1.41
29	A1	2029	A	N7-C5	-5.52	1.35	1.39
29	A1	493	G	N7-C5	-5.49	1.35	1.39
53	A2	113	A	N9-C4	-5.49	1.34	1.37
29	A1	2586	A	N7-C5	-5.49	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	602	G	N3-C4	-5.48	1.31	1.35
29	A1	2450	G	N1-C2	-5.48	1.33	1.37
29	A1	2248	G	N7-C5	-5.47	1.35	1.39
53	A2	902	G	N9-C4	-5.47	1.33	1.38
29	A1	830	A	C5-C4	-5.47	1.34	1.38
29	A1	478	G	N7-C5	-5.47	1.35	1.39
53	A2	699	A	C5-C6	-5.47	1.36	1.41
29	A1	748	A	N3-C4	-5.46	1.31	1.34
29	A1	1068	A	N9-C4	-5.45	1.34	1.37
29	A1	600	A	N7-C5	-5.45	1.35	1.39
29	A1	1818	A	N9-C4	-5.45	1.34	1.37
53	A2	566	A	N9-C4	-5.45	1.34	1.37
29	A1	846	C	C4-C5	-5.44	1.38	1.43
29	A1	2467	A	N9-C4	-5.44	1.34	1.37
53	A2	33	A	N7-C5	-5.44	1.35	1.39
53	A2	1450	A	N9-C4	-5.44	1.34	1.37
29	A1	1992	G	C5-C4	-5.43	1.34	1.38
29	A1	530	A	N9-C4	-5.42	1.34	1.37
29	A1	2090	C	N1-C6	-5.42	1.33	1.37
29	A1	1718	A	N7-C5	-5.42	1.35	1.39
29	A1	711	G	N7-C5	-5.42	1.35	1.39
29	A1	778	G	N7-C5	-5.42	1.35	1.39
53	A2	746	G	N7-C5	-5.42	1.35	1.39
29	A1	1714	A	N3-C4	-5.41	1.31	1.34
29	A1	2462	A	N9-C4	-5.41	1.34	1.37
29	A1	958	A	N9-C4	-5.41	1.34	1.37
53	A2	891	A	C5-C4	-5.41	1.34	1.38
29	A1	186	A	C5-C4	-5.41	1.34	1.38
29	A1	1257	A	N9-C4	-5.41	1.34	1.37
29	A1	2064	C	N1-C6	-5.41	1.33	1.37
29	A1	607	G	C6-N1	-5.39	1.35	1.39
29	A1	778	G	C5-C4	-5.38	1.34	1.38
29	A1	1718	A	N3-C4	-5.38	1.31	1.34
29	A1	868	A	C5-C4	-5.38	1.34	1.38
53	A2	31	G	N9-C4	-5.38	1.33	1.38
29	A1	2033	G	C5-C4	-5.38	1.34	1.38
53	A2	1374	G	C5-C6	-5.38	1.36	1.42
29	A1	854	G	C5-C4	-5.37	1.34	1.38
29	A1	2096	G	C5-C4	-5.37	1.34	1.38
29	A1	841	G	C6-N1	-5.37	1.35	1.39
29	A1	2586	A	C5-C4	-5.37	1.34	1.38
29	A1	837	A	N7-C5	-5.36	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	988	A	N9-C4	-5.36	1.34	1.37
29	A1	2345	G	N7-C5	-5.35	1.36	1.39
29	A1	261	A	N7-C5	-5.35	1.36	1.39
29	A1	2091	G	C5-C4	-5.35	1.34	1.38
29	A1	2712	U	C2-N3	-5.35	1.34	1.37
29	A1	1697	C	N1-C6	-5.35	1.33	1.37
29	A1	1716	G	C6-N1	-5.35	1.35	1.39
29	A1	867	G	C8-N7	-5.35	1.27	1.30
29	A1	28	A	N7-C5	-5.35	1.36	1.39
29	A1	2292	A	N9-C4	-5.34	1.34	1.37
53	A2	679	A	C5-C6	-5.34	1.36	1.41
29	A1	2051	G	C6-N1	-5.34	1.35	1.39
29	A1	2500	G	N7-C5	-5.34	1.36	1.39
53	A2	1481	G	N1-C2	-5.34	1.33	1.37
29	A1	559	A	N3-C4	-5.33	1.31	1.34
53	A2	698	A	N9-C4	-5.33	1.34	1.37
29	A1	1687	C	N1-C6	-5.33	1.33	1.37
29	A1	252	A	N9-C4	-5.32	1.34	1.37
29	A1	1823	C	N1-C2	-5.32	1.34	1.40
29	A1	2080	G	C6-N1	-5.32	1.35	1.39
29	A1	2460	G	C5-C4	-5.32	1.34	1.38
29	A1	506	A	N9-C4	-5.31	1.34	1.37
29	A1	1403	G	N9-C8	-5.31	1.34	1.37
29	A1	1312	G	N7-C5	-5.31	1.36	1.39
29	A1	712	G	N7-C5	-5.31	1.36	1.39
29	A1	2443	G	C6-N1	-5.31	1.35	1.39
29	A1	588	G	C5-C4	-5.30	1.34	1.38
29	A1	2252	G	N7-C5	-5.30	1.36	1.39
29	A1	185	A	N3-C4	-5.30	1.31	1.34
53	A2	1050	G	N7-C5	-5.30	1.36	1.39
29	A1	2273	G	N7-C5	-5.29	1.36	1.39
53	A2	955	A	N7-C5	-5.29	1.36	1.39
53	A2	1460	A	C5-C4	-5.29	1.35	1.38
29	A1	2241	A	N9-C4	-5.28	1.34	1.37
29	A1	2276	U	C2-N3	-5.28	1.34	1.37
53	A2	575	G	N9-C4	-5.28	1.33	1.38
53	A2	1395	A	N9-C4	-5.27	1.34	1.37
29	A1	1057	A	N7-C5	-5.27	1.36	1.39
53	A2	492	A	N7-C5	-5.27	1.36	1.39
53	A2	257	A	N7-C5	-5.27	1.36	1.39
29	A1	2631	C	N1-C6	-5.26	1.33	1.37
29	A1	2695	C	N1-C6	-5.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	206	A	N3-C4	-5.26	1.31	1.34
29	A1	869	A	N7-C5	-5.26	1.36	1.39
29	A1	1848	A	N7-C5	-5.26	1.36	1.39
53	A2	1480	A	N9-C4	-5.26	1.34	1.37
53	A2	1059	G	N9-C4	-5.25	1.33	1.38
29	A1	2350	A	N7-C5	-5.25	1.36	1.39
29	A1	894	G	N9-C4	-5.25	1.33	1.38
29	A1	2635	A	N9-C4	-5.25	1.34	1.37
29	A1	2586	A	N3-C4	-5.25	1.31	1.34
29	A1	603	A	C5-C4	-5.24	1.35	1.38
29	A1	721	C	N1-C6	-5.24	1.34	1.37
53	A2	858	G	C6-N1	-5.24	1.35	1.39
29	A1	1805	G	N7-C5	-5.24	1.36	1.39
53	A2	109	A	N7-C5	-5.23	1.36	1.39
29	A1	1818	A	N7-C5	-5.23	1.36	1.39
29	A1	824	G	N7-C5	-5.23	1.36	1.39
53	A2	699	A	N9-C4	-5.23	1.34	1.37
29	A1	1806	A	N9-C4	-5.23	1.34	1.37
53	A2	1460	A	N3-C4	-5.23	1.31	1.34
29	A1	1860	C	N1-C6	-5.23	1.34	1.37
29	A1	2038	A	N7-C5	-5.22	1.36	1.39
29	A1	592	A	N9-C4	-5.22	1.34	1.37
29	A1	1969	G	N7-C5	-5.22	1.36	1.39
29	A1	2447	A	N3-C4	-5.22	1.31	1.34
53	A2	900	A	N7-C5	-5.22	1.36	1.39
53	A2	308	A	N9-C4	-5.22	1.34	1.37
29	A1	596	A	N7-C5	-5.21	1.36	1.39
29	A1	1656	A	N9-C4	-5.21	1.34	1.37
29	A1	2282	A	N7-C5	-5.21	1.36	1.39
53	A2	849	A	N7-C5	-5.21	1.36	1.39
29	A1	873	A	N3-C4	-5.20	1.31	1.34
29	A1	734	A	N7-C5	-5.20	1.36	1.39
29	A1	1069	A	N9-C4	-5.19	1.34	1.37
29	A1	1191	A	N9-C4	-5.18	1.34	1.37
29	A1	1826	C	N1-C6	-5.18	1.34	1.37
29	A1	744	G	N7-C5	-5.18	1.36	1.39
53	A2	751	A	C5-C4	-5.18	1.35	1.38
29	A1	1716	G	N7-C5	-5.17	1.36	1.39
29	A1	999	G	C5-C4	-5.17	1.34	1.38
29	A1	2460	G	N1-C2	-5.17	1.33	1.37
30	B1	80	A	N9-C4	-5.17	1.34	1.37
29	A1	2112	G	N7-C5	-5.17	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	778	G	N9-C8	-5.16	1.34	1.37
29	A1	83	A	N9-C4	-5.16	1.34	1.37
29	A1	188	C	N1-C6	-5.16	1.34	1.37
29	A1	471	A	N9-C4	-5.16	1.34	1.37
29	A1	2847	A	N9-C4	-5.16	1.34	1.37
29	A1	248	G	N7-C5	-5.15	1.36	1.39
29	A1	707	C	N1-C6	-5.15	1.34	1.37
29	A1	1806	A	C5-C4	-5.15	1.35	1.38
29	A1	236	C	N1-C6	-5.15	1.34	1.37
29	A1	559	A	N9-C4	-5.15	1.34	1.37
29	A1	2402	A	C5-C4	-5.15	1.35	1.38
29	A1	2017	U	C2-N3	-5.14	1.34	1.37
29	A1	1298	G	N9-C4	-5.14	1.33	1.38
29	A1	1676	G	N7-C5	-5.14	1.36	1.39
29	A1	648	A	N3-C4	-5.14	1.31	1.34
29	A1	2301	A	N3-C4	-5.14	1.31	1.34
29	A1	2452	U	N1-C2	-5.14	1.33	1.38
29	A1	2556	A	C5-C6	-5.14	1.36	1.41
53	A2	274	A	N9-C4	-5.14	1.34	1.37
29	A1	1236	A	N7-C5	-5.13	1.36	1.39
29	A1	1982	C	N1-C6	-5.13	1.34	1.37
53	A2	763	A	N9-C4	-5.13	1.34	1.37
53	A2	1261	A	N9-C4	-5.13	1.34	1.37
29	A1	858	G	N9-C8	-5.13	1.34	1.37
53	A2	1459	G	N7-C5	-5.13	1.36	1.39
53	A2	295	A	N7-C5	-5.13	1.36	1.39
29	A1	911	G	N7-C5	-5.13	1.36	1.39
29	A1	2059	G	C5-C4	-5.13	1.34	1.38
29	A1	1205	G	N7-C5	-5.12	1.36	1.39
29	A1	1350	A	N3-C4	-5.12	1.31	1.34
29	A1	671	A	N7-C5	-5.12	1.36	1.39
53	A2	1506	G	N7-C5	-5.12	1.36	1.39
29	A1	677	C	C4-C5	-5.12	1.38	1.43
29	A1	1667	G	N7-C5	-5.12	1.36	1.39
53	A2	206	G	C6-N1	-5.12	1.35	1.39
53	A2	1378	A	N9-C4	-5.11	1.34	1.37
29	A1	1620	A	N7-C5	-5.11	1.36	1.39
29	A1	1616	A	N9-C4	-5.11	1.34	1.37
29	A1	1622	G	C5-C4	-5.11	1.34	1.38
53	A2	536	A	N7-C5	-5.11	1.36	1.39
29	A1	2054	A	N9-C8	-5.11	1.33	1.37
53	A2	359	A	N7-C5	-5.10	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	1190	A	N9-C4	-5.10	1.34	1.37
29	A1	2043	A	N3-C4	-5.10	1.31	1.34
29	A1	1018	C	C4-C5	-5.10	1.38	1.43
29	A1	2602	G	N7-C5	-5.10	1.36	1.39
29	A1	2739	C	N1-C6	-5.10	1.34	1.37
29	A1	1273	G	C5-C4	-5.09	1.34	1.38
29	A1	2740	A	N7-C5	-5.09	1.36	1.39
29	A1	1045	G	N7-C5	-5.09	1.36	1.39
29	A1	474	G	N7-C5	-5.09	1.36	1.39
29	A1	2880	A	N7-C5	-5.09	1.36	1.39
29	A1	211	A	N9-C4	-5.09	1.34	1.37
30	B1	99	G	N9-C4	-5.09	1.33	1.38
29	A1	235	G	C6-N1	-5.08	1.35	1.39
29	A1	725	A	N3-C4	-5.08	1.31	1.34
29	A1	2104	G	N7-C5	-5.08	1.36	1.39
53	A2	1049	A	N9-C4	-5.08	1.34	1.37
29	A1	188	C	N3-C4	-5.08	1.30	1.33
29	A1	194	A	N9-C4	-5.08	1.34	1.37
29	A1	720	C	N3-C4	-5.08	1.30	1.33
29	A1	1345	C	N3-C4	-5.08	1.30	1.33
29	A1	1032	A	N7-C5	-5.08	1.36	1.39
29	A1	30	G	C5-C4	-5.07	1.34	1.38
29	A1	815	C	N3-C4	-5.07	1.30	1.33
29	A1	2459	G	N7-C5	-5.07	1.36	1.39
29	A1	959	A	N7-C5	-5.07	1.36	1.39
29	A1	1844	G	N7-C5	-5.07	1.36	1.39
29	A1	2246	U	N1-C2	-5.06	1.33	1.38
29	A1	738	A	C6-N1	-5.06	1.32	1.35
29	A1	1861	G	N7-C5	-5.06	1.36	1.39
29	A1	1956	A	C5-C6	-5.06	1.36	1.41
29	A1	2027	G	C5-C4	-5.06	1.34	1.38
53	A2	51	A	N9-C4	-5.06	1.34	1.37
29	A1	810	A	C5-C6	-5.05	1.36	1.41
29	A1	2564	G	N7-C5	-5.05	1.36	1.39
29	A1	477	A	N7-C5	-5.05	1.36	1.39
29	A1	602	G	N9-C4	-5.05	1.33	1.38
29	A1	2511	A	C5-C4	-5.05	1.35	1.38
29	A1	1652	C	N3-C4	-5.05	1.30	1.33
29	A1	1792	A	N3-C4	-5.05	1.31	1.34
29	A1	1802	G	N7-C5	-5.05	1.36	1.39
29	A1	1301	A	N9-C4	-5.04	1.34	1.37
29	A1	829	G	C5-C4	-5.04	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A2	557	A	N3-C4	-5.04	1.31	1.34
29	A1	196	U	C2-N3	-5.04	1.34	1.37
29	A1	232	G	N9-C8	-5.04	1.34	1.37
29	A1	1474	G	N7-C5	-5.04	1.36	1.39
29	A1	2406	A	N7-C5	-5.04	1.36	1.39
53	A2	769	G	N7-C5	-5.04	1.36	1.39
29	A1	1656	A	N3-C4	-5.04	1.31	1.34
29	A1	1846	G	N9-C8	-5.03	1.34	1.37
53	A2	298	A	N9-C4	-5.03	1.34	1.37
53	A2	358	A	N9-C4	-5.03	1.34	1.37
29	A1	494	A	N3-C4	-5.03	1.31	1.34
29	A1	828	U	C2-N3	-5.03	1.34	1.37
29	A1	1858	A	N7-C5	-5.03	1.36	1.39
53	A2	99	C	N1-C6	-5.02	1.34	1.37
29	A1	2695	C	N3-C4	-5.02	1.30	1.33
53	A2	1400	A	N7-C5	-5.02	1.36	1.39
53	A2	604	A	N7-C5	-5.02	1.36	1.39
29	A1	2027	G	N7-C5	-5.01	1.36	1.39
29	A1	2593	C	N1-C6	-5.01	1.34	1.37
29	A1	1830	C	C4-C5	-5.01	1.39	1.43
29	A1	2274	C	N1-C6	-5.01	1.34	1.37
29	A1	784	A	N7-C5	-5.01	1.36	1.39
53	A2	1481	G	C6-N1	-5.01	1.36	1.39
29	A1	215	A	N7-C5	-5.01	1.36	1.39
29	A1	1285	A	N3-C4	-5.01	1.31	1.34
29	A1	1319	G	N7-C5	-5.01	1.36	1.39
29	A1	1956	A	N7-C5	-5.01	1.36	1.39
29	A1	2512	C	N3-C4	-5.01	1.30	1.33
29	A1	1004	A	N9-C4	-5.01	1.34	1.37
29	A1	611	A	C5-C4	-5.01	1.35	1.38
29	A1	2522	G	N3-C4	-5.00	1.31	1.35
29	A1	583	G	C5-C4	-5.00	1.34	1.38
29	A1	1749	A	N9-C4	-5.00	1.34	1.37
29	A1	2098	U	N1-C2	-5.00	1.34	1.38
29	A1	2290	G	N7-C5	-5.00	1.36	1.39
29	A1	2617	G	C5-C4	-5.00	1.34	1.38
29	A1	2756	A	N7-C5	-5.00	1.36	1.39
53	A2	423	G	N9-C4	-5.00	1.33	1.38

All (1460) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	700	C	C4-C5-C6	-192.11	21.34	117.40
53	A2	700	C	N1-C2-N3	-133.89	25.48	119.20
53	A2	700	C	C2-N3-C4	86.94	163.37	119.90
53	A2	700	C	C5-C6-N1	59.60	150.80	121.00
53	A2	700	C	C6-N1-C2	49.66	140.16	120.30
53	A2	700	C	C2-N1-C1'	-46.13	68.06	118.80
53	A2	700	C	N1-C2-O2	41.20	143.62	118.90
53	A2	717	G	C4-C5-N7	-37.36	95.86	110.80
53	A2	1121	G	N1-C2-N3	-37.16	101.60	123.90
53	A2	1121	G	C2-N3-C4	30.24	127.02	111.90
53	A2	717	G	N7-C8-N9	28.78	127.49	113.10
53	A2	717	G	N3-C4-N9	26.94	142.16	126.00
53	A2	700	C	C5-C4-N4	-26.16	101.89	120.20
53	A2	216	C	N3-C4-C5	-25.73	111.61	121.90
53	A2	700	C	C6-N1-C1'	25.59	151.51	120.80
53	A2	1110	C	N3-C4-C5	-25.29	111.79	121.90
53	A2	717	G	N9-C4-C5	-25.06	95.38	105.40
53	A2	717	G	C2-N3-C4	24.44	124.12	111.90
53	A2	216	C	C6-N1-C2	23.16	129.56	120.30
53	A2	1110	C	N1-C2-N3	-22.45	103.48	119.20
53	A2	216	C	N1-C2-N3	-22.27	103.61	119.20
53	A2	1110	C	C6-N1-C2	21.76	129.00	120.30
53	A2	136	G	N3-C2-N2	20.86	134.50	119.90
53	A2	717	G	N1-C2-N3	-20.00	111.90	123.90
53	A2	1121	G	C6-N1-C2	18.36	136.12	125.10
53	A2	1110	C	C2-N3-C4	18.30	129.05	119.90
53	A2	700	C	N3-C4-C5	17.98	129.09	121.90
53	A2	810	U	N3-C2-O2	-16.37	110.74	122.20
53	A2	136	G	N1-C2-N3	-16.14	114.21	123.90
53	A2	216	C	N3-C2-O2	15.43	132.70	121.90
53	A2	700	C	N3-C4-N4	15.41	128.79	118.00
53	A2	216	C	C2-N3-C4	15.26	127.53	119.90
53	A2	1121	G	N1-C2-N2	14.61	129.35	116.20
53	A2	810	U	N1-C2-O2	13.98	132.59	122.80
53	A2	717	G	C6-C5-N7	13.81	138.69	130.40
53	A2	1121	G	N3-C2-N2	13.07	129.05	119.90
53	A2	231	G	N1-C6-O6	-12.82	112.21	119.90
53	A2	1110	C	N1-C2-O2	12.57	126.44	118.90
53	A2	717	G	N3-C4-C5	-12.52	122.34	128.60
53	A2	717	G	C8-N9-C4	12.30	111.32	106.40
29	A1	159	U	N1-C2-O2	12.26	131.38	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	159	U	C2-N1-C1'	12.05	132.16	117.70
53	A2	700	C	O4'-C1'-N1	11.72	117.58	108.20
53	A2	216	C	C4-C5-C6	11.65	123.23	117.40
53	A2	1360	C	C5-C6-N1	11.63	126.81	121.00
29	A1	832	A	C5-N7-C8	-11.52	98.14	103.90
29	A1	188	C	N1-C2-O2	11.45	125.77	118.90
53	A2	1110	C	N3-C2-O2	11.44	129.91	121.90
29	A1	159	U	N3-C2-O2	-11.37	114.24	122.20
29	A1	1114	U	N1-C2-O2	11.27	130.69	122.80
53	A2	1284	C	N1-C2-O2	11.24	125.64	118.90
53	A2	1140	C	N1-C2-O2	11.12	125.57	118.90
29	A1	1592	C	N1-C2-O2	11.06	125.53	118.90
53	A2	717	G	C5-N7-C8	10.97	109.78	104.30
53	A2	1140	C	C2-N1-C1'	10.79	130.67	118.80
53	A2	717	G	C4-C5-C6	10.77	125.26	118.80
29	A1	832	A	C4-C5-N7	10.61	116.00	110.70
29	A1	677	C	C5-C6-N1	10.60	126.30	121.00
53	A2	700	C	N1-C1'-C2'	10.54	127.70	114.00
29	A1	1114	U	C2-N1-C1'	10.53	130.33	117.70
29	A1	1841	U	C2-N1-C1'	10.49	130.29	117.70
53	A2	136	G	C6-N1-C2	10.40	131.34	125.10
53	A2	717	G	N3-C2-N2	10.37	127.16	119.90
29	A1	1114	U	N3-C2-O2	-10.34	114.96	122.20
29	A1	2738	C	C6-N1-C2	-10.32	116.17	120.30
53	A2	810	U	C2-N1-C1'	10.29	130.05	117.70
29	A1	1841	U	N3-C2-O2	-10.29	115.00	122.20
53	A2	231	G	C5-C6-O6	10.28	134.77	128.60
53	A2	824	U	C2-N1-C1'	10.27	130.02	117.70
29	A1	1018	C	C6-N1-C2	-10.22	116.21	120.30
53	A2	824	U	N1-C2-O2	10.22	129.95	122.80
53	A2	231	G	C4-C5-N7	-10.18	106.73	110.80
53	A2	750	A	N1-C6-N6	10.07	124.64	118.60
29	A1	188	C	N3-C2-O2	-10.06	114.86	121.90
29	A1	1958	C	C6-N1-C2	-10.03	116.29	120.30
29	A1	1958	C	N1-C2-O2	9.98	124.89	118.90
53	A2	932	U	N3-C2-O2	-9.89	115.27	122.20
29	A1	1841	U	N1-C2-O2	9.82	129.67	122.80
29	A1	1958	C	N3-C2-O2	-9.75	115.08	121.90
53	A2	1284	C	N3-C2-O2	-9.74	115.08	121.90
29	A1	1624	C	C2-N1-C1'	9.73	129.50	118.80
53	A2	528	C	C6-N1-C2	-9.72	116.41	120.30
53	A2	443	C	C2-N1-C1'	9.66	129.43	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2521	C	N1-C2-O2	9.66	124.69	118.90
29	A1	1592	C	N3-C2-O2	-9.64	115.15	121.90
29	A1	671	A	C8-N9-C4	-9.63	101.95	105.80
29	A1	2702	U	N3-C2-O2	-9.62	115.47	122.20
53	A2	1140	C	N3-C2-O2	-9.59	115.19	121.90
29	A1	815	C	N3-C2-O2	-9.58	115.19	121.90
29	A1	359	C	C6-N1-C2	-9.54	116.48	120.30
53	A2	1110	C	C4-C5-C6	9.51	122.15	117.40
53	A2	1110	C	C5-C4-N4	9.51	126.86	120.20
29	A1	1673	C	C6-N1-C2	-9.36	116.56	120.30
53	A2	1360	C	C6-N1-C2	-9.34	116.56	120.30
29	A1	867	G	C6-C5-N7	-9.33	124.80	130.40
29	A1	2063	C	C6-N1-C2	-9.31	116.58	120.30
29	A1	1624	C	N1-C2-O2	9.28	124.47	118.90
53	A2	276	G	C6-C5-N7	-9.27	124.84	130.40
29	A1	2521	C	N3-C2-O2	-9.27	115.41	121.90
53	A2	721	C	C6-N1-C2	-9.23	116.61	120.30
53	A2	772	U	N3-C2-O2	-9.22	115.74	122.20
29	A1	104	C	C6-N1-C2	-9.19	116.62	120.30
53	A2	1121	G	C6-C5-N7	9.15	135.89	130.40
53	A2	276	G	C4-C5-N7	8.97	114.39	110.80
29	A1	1974	G	C6-C5-N7	-8.96	125.03	130.40
29	A1	1923	G	C2-N3-C4	-8.89	107.45	111.90
29	A1	1459	C	N1-C2-O2	8.86	124.22	118.90
29	A1	444	C	N1-C2-O2	8.85	124.21	118.90
29	A1	2799	C	N1-C2-O2	8.84	124.21	118.90
53	A2	34	C	C6-N1-C2	-8.82	116.77	120.30
53	A2	19	C	C6-N1-C2	-8.82	116.77	120.30
53	A2	1289	U	N1-C2-O2	8.79	128.95	122.80
29	A1	1974	G	C4-C5-N7	8.73	114.29	110.80
29	A1	2630	C	N1-C2-O2	8.70	124.12	118.90
53	A2	824	U	N3-C2-O2	-8.66	116.14	122.20
29	A1	1923	G	N3-C4-N9	-8.66	120.80	126.00
29	A1	2512	C	C6-N1-C2	-8.66	116.84	120.30
53	A2	136	G	N9-C4-C5	-8.65	101.94	105.40
29	A1	823	A	C5-N7-C8	-8.64	99.58	103.90
53	A2	136	G	C4-C5-N7	8.63	114.25	110.80
53	A2	1121	G	C4-C5-C6	-8.62	113.63	118.80
29	A1	671	A	O5'-P-OP1	-8.62	97.94	105.70
29	A1	815	C	N1-C2-O2	8.62	124.07	118.90
29	A1	2704	C	N1-C2-O2	8.62	124.07	118.90
53	A2	635	U	N3-C4-O4	-8.59	113.39	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	1394	C	N1-C2-O2	8.57	124.04	118.90
29	A1	1361	U	N3-C2-O2	-8.54	116.22	122.20
53	A2	932	U	N1-C2-O2	8.53	128.77	122.80
53	A2	749	A	OP1-P-O3'	8.51	123.92	105.20
53	A2	1451	G	C8-N9-C4	-8.51	103.00	106.40
29	A1	1877	C	C6-N1-C2	-8.50	116.90	120.30
30	B1	86	C	N1-C2-O2	8.49	124.00	118.90
29	A1	2063	C	C2-N1-C1'	8.45	128.10	118.80
29	A1	160	U	C2-N1-C1'	8.43	127.82	117.70
53	A2	216	C	C5-C4-N4	8.41	126.09	120.20
29	A1	1911	C	C6-N1-C2	-8.40	116.94	120.30
53	A2	949	C	N3-C2-O2	-8.40	116.02	121.90
53	A2	1299	A	N7-C8-N9	8.39	118.00	113.80
29	A1	2224	C	C6-N1-C2	-8.39	116.94	120.30
29	A1	1624	C	N3-C2-O2	-8.37	116.04	121.90
29	A1	785	C	C6-N1-C2	-8.35	116.96	120.30
29	A1	1234	G	C8-N9-C4	-8.33	103.07	106.40
29	A1	1923	G	N3-C4-C5	8.31	132.76	128.60
29	A1	1938	C	N1-C2-O2	8.30	123.88	118.90
53	A2	276	G	C5-N7-C8	-8.28	100.16	104.30
53	A2	1007	C	C5-C6-N1	8.26	125.13	121.00
53	A2	36	C	C6-N1-C2	-8.26	117.00	120.30
29	A1	846	C	C6-N1-C2	-8.25	117.00	120.30
29	A1	311	C	C6-N1-C2	-8.24	117.00	120.30
29	A1	2063	C	N1-C2-O2	8.23	123.84	118.90
29	A1	1148	C	C6-N1-C2	-8.22	117.01	120.30
53	A2	749	A	N1-C2-N3	-8.21	125.19	129.30
53	A2	210	U	C2-N1-C1'	8.21	127.55	117.70
29	A1	1234	G	C6-C5-N7	-8.20	125.48	130.40
29	A1	1867	U	N3-C2-O2	-8.17	116.48	122.20
29	A1	2311	C	C6-N1-C2	-8.16	117.03	120.30
29	A1	2704	C	C2-N1-C1'	8.16	127.78	118.80
53	A2	749	A	P-O3'-C3'	8.15	129.49	119.70
29	A1	1867	U	N1-C2-O2	8.15	128.50	122.80
29	A1	564	C	C5-C6-N1	8.13	125.07	121.00
29	A1	1018	C	C5-C6-N1	8.11	125.06	121.00
53	A2	985	C	N1-C2-O2	8.11	123.77	118.90
29	A1	1362	C	C5-C6-N1	8.10	125.05	121.00
53	A2	276	G	N7-C8-N9	8.10	117.15	113.10
29	A1	2741	U	N3-C2-O2	-8.07	116.55	122.20
53	A2	722	C	C6-N1-C2	-8.07	117.07	120.30
53	A2	955	A	C4-C5-N7	8.07	114.74	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2335	G	C4-N9-C1'	8.06	136.98	126.50
29	A1	2213	U	N1-C2-O2	8.05	128.44	122.80
29	A1	2063	C	N3-C2-O2	-8.05	116.27	121.90
53	A2	1123	C	C6-N1-C2	-8.04	117.08	120.30
29	A1	2213	U	C2-N1-C1'	8.03	127.33	117.70
29	A1	1958	C	C2-N1-C1'	8.03	127.63	118.80
53	A2	932	U	C2-N1-C1'	8.02	127.32	117.70
53	A2	443	C	N1-C2-O2	8.01	123.70	118.90
53	A2	772	U	N1-C2-O2	8.00	128.40	122.80
29	A1	1362	C	C6-N1-C2	-7.99	117.10	120.30
53	A2	217	U	C2-N1-C1'	7.97	127.27	117.70
29	A1	2735	U	C5-C4-O4	-7.93	121.14	125.90
29	A1	832	A	N7-C8-N9	7.92	117.76	113.80
29	A1	159	U	C6-N1-C1'	-7.92	110.11	121.20
29	A1	1819	A	N7-C8-N9	7.92	117.76	113.80
29	A1	1917	C	N1-C2-O2	7.91	123.65	118.90
29	A1	1819	A	C5-N7-C8	-7.91	99.94	103.90
53	A2	717	G	C4-N9-C1'	-7.91	116.22	126.50
53	A2	235	C	C6-N1-C2	-7.89	117.14	120.30
53	A2	612	G	C6-C5-N7	-7.87	125.68	130.40
29	A1	1659	C	N1-C2-O2	7.86	123.61	118.90
53	A2	350	C	N3-C2-O2	-7.86	116.40	121.90
53	A2	136	G	C2-N3-C4	7.85	115.83	111.90
29	A1	2521	C	C6-N1-C2	-7.83	117.17	120.30
29	A1	1234	G	N7-C8-N9	7.82	117.01	113.10
53	A2	276	G	N1-C6-O6	7.82	124.59	119.90
29	A1	2088	C	C6-N1-C2	-7.81	117.17	120.30
29	A1	782	G	N3-C2-N2	7.81	125.37	119.90
53	A2	727	C	C6-N1-C2	-7.81	117.18	120.30
29	A1	1732	C	C5-C6-N1	7.80	124.90	121.00
29	A1	1398	C	N3-C2-O2	-7.80	116.44	121.90
29	A1	823	A	C4-C5-N7	7.79	114.60	110.70
29	A1	1917	C	N3-C2-O2	-7.79	116.45	121.90
29	A1	662	C	N1-C2-O2	7.79	123.57	118.90
53	A2	750	A	C5-N7-C8	-7.78	100.01	103.90
30	B1	86	C	C6-N1-C2	-7.75	117.20	120.30
29	A1	1585	C	C6-N1-C2	-7.75	117.20	120.30
29	A1	550	C	C6-N1-C2	-7.75	117.20	120.30
29	A1	1182	C	C2-N1-C1'	7.73	127.31	118.80
53	A2	130	C	C6-N1-C2	-7.70	117.22	120.30
29	A1	1685	C	C6-N1-C2	-7.68	117.23	120.30
53	A2	834	C	N1-C2-O2	7.68	123.51	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	955	A	N9-C4-C5	-7.67	102.73	105.80
29	A1	2702	U	N1-C2-O2	7.66	128.16	122.80
29	A1	2808	G	C4-N9-C1'	7.64	136.43	126.50
53	A2	528	C	C2-N1-C1'	7.64	127.21	118.80
53	A2	635	U	N3-C4-C5	7.64	119.19	114.60
29	A1	1398	C	N1-C2-O2	7.64	123.48	118.90
29	A1	815	C	C6-N1-C2	-7.62	117.25	120.30
29	A1	1592	C	C2-N1-C1'	7.62	127.19	118.80
53	A2	528	C	C5-C6-N1	7.62	124.81	121.00
29	A1	2016	G	P-O3'-C3'	7.62	128.85	119.70
53	A2	1374	G	N7-C8-N9	7.62	116.91	113.10
53	A2	1140	C	C6-N1-C1'	-7.62	111.66	120.80
53	A2	984	C	N1-C2-O2	7.61	123.47	118.90
29	A1	782	G	C4-C5-N7	7.61	113.84	110.80
29	A1	1607	A	P-O3'-C3'	7.61	128.83	119.70
29	A1	1821	C	C6-N1-C2	-7.61	117.26	120.30
29	A1	2406	A	C5-N7-C8	-7.61	100.09	103.90
53	A2	859	C	C6-N1-C2	-7.61	117.26	120.30
29	A1	1944	C	C5-C6-N1	7.61	124.80	121.00
53	A2	1475	U	P-O3'-C3'	7.59	128.81	119.70
53	A2	350	C	N1-C2-O2	7.59	123.45	118.90
29	A1	2274	C	C5-C6-N1	7.58	124.79	121.00
29	A1	1465	C	N3-C2-O2	-7.58	116.59	121.90
29	A1	2153	C	C6-N1-C2	-7.55	117.28	120.30
29	A1	943	U	C2-N1-C1'	7.54	126.74	117.70
53	A2	262	C	C6-N1-C2	-7.53	117.29	120.30
29	A1	1814	C	N3-C2-O2	-7.53	116.63	121.90
29	A1	2504	G	C4-N9-C1'	7.52	136.28	126.50
53	A2	1394	C	N3-C2-O2	-7.52	116.64	121.90
29	A1	104	C	C5-C6-N1	7.52	124.76	121.00
30	B1	86	C	N3-C2-O2	-7.51	116.64	121.90
29	A1	1419	G	C6-C5-N7	-7.51	125.89	130.40
53	A2	231	G	C6-C5-N7	7.46	134.88	130.40
53	A2	856	C	C6-N1-C2	-7.46	117.32	120.30
53	A2	664	C	O5'-P-OP1	7.45	119.64	110.70
53	A2	36	C	C5-C6-N1	7.44	124.72	121.00
29	A1	795	A	C8-N9-C4	7.43	108.77	105.80
53	A2	1289	U	N3-C2-O2	-7.43	117.00	122.20
29	A1	1624	C	C6-N1-C1'	-7.41	111.90	120.80
29	A1	1423	C	N1-C2-O2	7.41	123.35	118.90
29	A1	2741	U	N1-C2-O2	7.39	127.97	122.80
53	A2	1196	G	C5-C6-O6	-7.38	124.17	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	1814	C	N1-C2-O2	7.38	123.33	118.90
29	A1	810	A	C4-C5-N7	7.37	114.39	110.70
53	A2	19	C	C5-C6-N1	7.37	124.69	121.00
29	A1	769	C	N1-C2-O2	7.37	123.32	118.90
29	A1	118	U	N3-C2-O2	-7.35	117.05	122.20
29	A1	1764	G	N3-C4-N9	7.35	130.41	126.00
29	A1	2406	A	C4-C5-N7	7.34	114.37	110.70
29	A1	1702	G	OP2-P-O3'	7.34	121.36	105.20
29	A1	810	A	C5-N7-C8	-7.33	100.23	103.90
29	A1	677	C	C6-N1-C2	-7.33	117.37	120.30
29	A1	1585	C	O4'-C1'-N1	7.33	114.06	108.20
29	A1	448	C	C6-N1-C2	-7.32	117.37	120.30
53	A2	1423	G	C4-N9-C1'	7.32	136.02	126.50
29	A1	823	A	N1-C6-N6	7.31	122.99	118.60
53	A2	1184	C	N1-C2-O2	7.31	123.29	118.90
29	A1	2799	C	C5-C6-N1	7.30	124.65	121.00
53	A2	513	G	C8-N9-C4	-7.30	103.48	106.40
29	A1	381	G	N3-C4-N9	-7.29	121.62	126.00
53	A2	657	G	N3-C4-N9	-7.29	121.63	126.00
29	A1	403	C	C6-N1-C2	-7.29	117.39	120.30
29	A1	557	G	C8-N9-C4	-7.28	103.49	106.40
30	B1	70	C	C6-N1-C2	-7.28	117.39	120.30
53	A2	34	C	N1-C2-O2	7.28	123.27	118.90
53	A2	309	C	N1-C2-O2	7.27	123.26	118.90
53	A2	750	A	C4-C5-N7	7.27	114.34	110.70
29	A1	2213	U	N3-C2-O2	-7.27	117.11	122.20
29	A1	127	C	N1-C2-O2	7.25	123.25	118.90
29	A1	677	C	N1-C2-O2	7.25	123.25	118.90
29	A1	785	C	C5-C6-N1	7.25	124.62	121.00
29	A1	1541	C	O5'-P-OP2	-7.25	99.18	105.70
29	A1	1494	C	C6-N1-C2	-7.24	117.40	120.30
53	A2	443	C	N3-C2-O2	-7.24	116.83	121.90
29	A1	1108	U	P-O3'-C3'	7.22	128.37	119.70
53	A2	1005	C	P-O3'-C3'	7.22	128.37	119.70
29	A1	1182	C	N1-C2-O2	7.21	123.23	118.90
29	A1	1911	C	C5-C6-N1	7.21	124.60	121.00
29	A1	2167	C	C5-C6-N1	7.21	124.60	121.00
29	A1	1243	C	C6-N1-C2	-7.20	117.42	120.30
30	B1	70	C	C5-C6-N1	7.20	124.60	121.00
53	A2	1374	G	C8-N9-C4	-7.20	103.52	106.40
29	A1	10	G	C8-N9-C4	7.18	109.27	106.40
29	A1	1319	G	C8-N9-C4	-7.17	103.53	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2186	G	N3-C4-C5	-7.17	125.02	128.60
30	B1	86	C	C2-N1-C1'	7.17	126.69	118.80
29	A1	220	U	N1-C2-O2	7.16	127.81	122.80
53	A2	810	U	C6-N1-C1'	-7.15	111.19	121.20
28	d1	61	LEU	CA-CB-CG	7.15	131.75	115.30
29	A1	1764	G	C4-N9-C1'	7.15	135.80	126.50
53	A2	949	C	N1-C2-O2	7.15	123.19	118.90
53	A2	241	A	P-O3'-C3'	7.14	128.27	119.70
53	A2	231	G	N9-C4-C5	7.14	108.25	105.40
53	A2	216	C	N1-C2-O2	7.14	123.18	118.90
53	A2	856	C	C5-C6-N1	7.13	124.57	121.00
53	A2	513	G	N7-C8-N9	7.13	116.67	113.10
29	A1	671	A	N7-C8-N9	7.12	117.36	113.80
29	A1	1714	A	C5-N7-C8	-7.12	100.34	103.90
29	A1	690	C	C2-N1-C1'	7.12	126.63	118.80
29	A1	2274	C	C6-N1-C2	-7.12	117.45	120.30
53	A2	519	C	C6-N1-C2	-7.11	117.46	120.30
29	A1	167	G	C4-N9-C1'	7.11	135.74	126.50
29	A1	2409	C	C5-C6-N1	7.10	124.55	121.00
29	A1	677	C	C4-C5-C6	-7.09	113.85	117.40
29	A1	943	U	N1-C2-O2	7.09	127.77	122.80
53	A2	750	A	N7-C8-N9	7.09	117.35	113.80
29	A1	167	G	N3-C4-C5	-7.09	125.06	128.60
29	A1	2704	C	N3-C2-O2	-7.09	116.94	121.90
53	A2	34	C	N3-C2-O2	-7.08	116.94	121.90
53	A2	1374	G	C5-N7-C8	-7.07	100.76	104.30
53	A2	149	C	O5'-P-OP1	7.07	119.19	110.70
29	A1	2443	G	O5'-P-OP2	-7.07	99.34	105.70
53	A2	793	C	N1-C2-O2	7.07	123.14	118.90
29	A1	2521	C	C2-N1-C1'	7.07	126.57	118.80
29	A1	188	C	C2-N1-C1'	7.06	126.57	118.80
29	A1	846	C	C5-C6-N1	7.06	124.53	121.00
53	A2	217	U	N3-C2-O2	-7.06	117.26	122.20
29	A1	127	C	C6-N1-C2	-7.05	117.48	120.30
29	A1	432	C	P-O3'-C3'	7.04	128.15	119.70
53	A2	243	C	N3-C2-O2	-7.03	116.98	121.90
53	A2	276	G	O4'-C1'-N9	7.03	113.83	108.20
29	A1	1114	U	C6-N1-C1'	-7.02	111.38	121.20
29	A1	883	C	C6-N1-C2	-7.00	117.50	120.30
53	A2	824	U	C6-N1-C1'	-7.00	111.40	121.20
53	A2	243	C	C6-N1-C2	-7.00	117.50	120.30
53	A2	423	G	C8-N9-C1'	6.99	136.08	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2741	U	C2-N1-C1'	6.99	126.08	117.70
53	A2	101	G	C4-C5-N7	6.98	113.59	110.80
29	A1	1465	C	N1-C2-O2	6.98	123.09	118.90
29	A1	444	C	N3-C2-O2	-6.98	117.01	121.90
29	A1	677	C	C2-N3-C4	6.98	123.39	119.90
29	A1	2665	C	N1-C2-O2	6.98	123.09	118.90
53	A2	468	G	P-O3'-C3'	6.98	128.08	119.70
29	A1	2595	G	C4-N9-C1'	6.98	135.57	126.50
53	A2	1306	C	C6-N1-C2	-6.97	117.51	120.30
53	A2	750	A	C6-C5-N7	-6.97	127.42	132.30
29	A1	1877	C	C5-C6-N1	6.97	124.48	121.00
29	A1	1673	C	C5-C6-N1	6.96	124.48	121.00
29	A1	1814	C	C2-N1-C1'	6.96	126.46	118.80
29	A1	2063	C	C5-C6-N1	6.96	124.48	121.00
29	A1	167	G	C8-N9-C4	-6.95	103.62	106.40
53	A2	423	G	C4-N9-C1'	-6.94	117.47	126.50
29	A1	769	C	N3-C2-O2	-6.93	117.05	121.90
53	A2	276	G	C2-N3-C4	-6.93	108.43	111.90
29	A1	564	C	N1-C2-O2	6.93	123.06	118.90
29	A1	2504	G	C6-C5-N7	-6.93	126.24	130.40
53	A2	528	C	N3-C2-O2	-6.92	117.06	121.90
30	B1	90	C	C2-N1-C1'	6.91	126.40	118.80
29	A1	727	C	C6-N1-C2	-6.91	117.54	120.30
29	A1	718	G	C4-N9-C1'	6.91	135.48	126.50
29	A1	2692	C	C5-C6-N1	6.90	124.45	121.00
29	A1	219	A	P-O3'-C3'	6.90	127.98	119.70
53	A2	408	G	C4-N9-C1'	6.90	135.47	126.50
53	A2	612	G	N3-C4-N9	6.89	130.13	126.00
53	A2	1423	G	C8-N9-C1'	-6.89	118.04	127.00
29	A1	2900	C	N1-C2-O2	6.89	123.03	118.90
29	A1	965	A	C4-C5-N7	6.89	114.14	110.70
53	A2	519	C	C5-C6-N1	6.88	124.44	121.00
29	A1	119	G	C4-N9-C1'	6.88	135.44	126.50
29	A1	127	C	N3-C2-O2	-6.87	117.09	121.90
29	A1	1676	G	C6-C5-N7	-6.87	126.28	130.40
29	A1	2201	C	C6-N1-C2	-6.87	117.55	120.30
53	A2	915	A	N1-C6-N6	-6.87	114.48	118.60
16	R1	67	ASP	CB-CG-OD1	6.86	124.48	118.30
29	A1	2799	C	C6-N1-C2	-6.84	117.56	120.30
53	A2	839	C	N3-C2-O2	-6.84	117.11	121.90
53	A2	985	C	N3-C2-O2	-6.84	117.11	121.90
29	A1	316	C	N1-C2-O2	6.84	123.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	952	C	N1-C2-O2	6.84	123.00	118.90
29	A1	220	U	N3-C2-O2	-6.81	117.43	122.20
53	A2	1272	G	C8-N9-C4	-6.81	103.67	106.40
53	A2	262	C	C5-C6-N1	6.81	124.41	121.00
29	A1	899	C	C6-N1-C2	-6.81	117.58	120.30
53	A2	890	A	P-O3'-C3'	6.81	127.87	119.70
29	A1	1841	U	C6-N1-C1'	-6.80	111.67	121.20
53	A2	1282	U	C2-N1-C1'	6.80	125.86	117.70
29	A1	1419	G	C4-C5-N7	6.79	113.52	110.80
29	A1	1592	C	C6-N1-C2	-6.79	117.58	120.30
53	A2	210	U	N1-C2-O2	6.79	127.55	122.80
29	A1	2574	C	C5-C6-N1	6.78	124.39	121.00
29	A1	1459	C	N3-C2-O2	-6.78	117.16	121.90
29	A1	159	U	C5-C6-N1	6.77	126.08	122.70
29	A1	289	U	N3-C2-O2	-6.77	117.46	122.20
53	A2	132	G	C6-N1-C2	6.77	129.16	125.10
29	A1	1659	C	N3-C2-O2	-6.76	117.16	121.90
29	A1	1070	G	P-O3'-C3'	6.76	127.81	119.70
29	A1	1938	C	N3-C2-O2	-6.76	117.17	121.90
53	A2	657	G	N3-C2-N2	-6.76	115.17	119.90
30	B1	72	C	N3-C2-O2	-6.76	117.17	121.90
29	A1	1423	C	N3-C2-O2	-6.75	117.17	121.90
53	A2	136	G	C8-N9-C1'	-6.75	118.22	127.00
53	A2	243	C	N1-C2-O2	6.75	122.95	118.90
29	A1	388	G	N7-C8-N9	6.75	116.48	113.10
29	A1	1743	C	P-O3'-C3'	6.75	127.80	119.70
53	A2	171	C	N1-C2-O2	6.75	122.95	118.90
53	A2	1410	A	O4'-C1'-N9	6.75	113.60	108.20
29	A1	119	G	C8-N9-C1'	-6.75	118.22	127.00
29	A1	824	G	C4-C5-N7	6.75	113.50	110.80
29	A1	867	G	C4-C5-N7	6.75	113.50	110.80
53	A2	34	C	C2-N1-C1'	6.75	126.22	118.80
53	A2	443	C	C6-N1-C1'	-6.75	112.70	120.80
29	A1	2311	C	C5-C6-N1	6.75	124.37	121.00
29	A1	316	C	C6-N1-C2	-6.74	117.60	120.30
29	A1	711	G	C6-C5-N7	-6.74	126.36	130.40
53	A2	276	G	C4-N9-C1'	6.74	135.26	126.50
29	A1	1764	G	C8-N9-C1'	-6.74	118.24	127.00
29	A1	832	A	C6-C5-N7	-6.73	127.59	132.30
29	A1	1807	C	N1-C2-O2	6.73	122.94	118.90
29	A1	489	C	C5-C6-N1	6.73	124.37	121.00
53	A2	834	C	N3-C2-O2	-6.73	117.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2054	A	N1-C6-N6	-6.72	114.56	118.60
29	A1	2799	C	N3-C2-O2	-6.72	117.19	121.90
29	A1	2630	C	N3-C2-O2	-6.70	117.21	121.90
53	A2	839	C	N1-C2-O2	6.69	122.92	118.90
53	A2	728	C	O5'-P-OP2	-6.68	99.68	105.70
29	A1	2535	C	C2-N1-C1'	6.68	126.15	118.80
53	A2	58	C	C6-N1-C2	-6.68	117.63	120.30
53	A2	1284	C	C2-N1-C1'	6.68	126.15	118.80
53	A2	1337	G	C6-C5-N7	-6.67	126.40	130.40
29	A1	725	A	C2-N3-C4	-6.67	107.27	110.60
53	A2	1451	G	N9-C4-C5	6.66	108.06	105.40
29	A1	1944	C	C6-N1-C2	-6.65	117.64	120.30
29	A1	2705	C	C6-N1-C2	-6.65	117.64	120.30
29	A1	2799	C	C2-N1-C1'	6.65	126.11	118.80
29	A1	2087	C	N3-C2-O2	-6.64	117.25	121.90
29	A1	186	A	C5-C6-N1	6.64	121.02	117.70
29	A1	2335	G	C8-N9-C4	-6.63	103.75	106.40
29	A1	2087	C	N1-C2-O2	6.63	122.88	118.90
29	A1	381	G	N3-C4-C5	6.63	131.91	128.60
29	A1	1807	C	N3-C2-O2	-6.63	117.26	121.90
53	A2	1299	A	C5-N7-C8	-6.62	100.59	103.90
29	A1	1182	C	N3-C2-O2	-6.62	117.27	121.90
29	A1	1747	A	O4'-C1'-N9	6.62	113.49	108.20
30	B1	3	U	N1-C2-O2	6.62	127.43	122.80
53	A2	528	C	N1-C2-O2	6.62	122.87	118.90
53	A2	750	A	C5-C6-N6	-6.61	118.41	123.70
53	A2	793	C	N3-C2-O2	-6.61	117.27	121.90
53	A2	1140	C	C6-N1-C2	-6.60	117.66	120.30
29	A1	2837	C	C6-N1-C2	-6.60	117.66	120.30
29	A1	1539	G	N3-C4-N9	6.60	129.96	126.00
29	A1	2716	U	C5-C6-N1	6.59	126.00	122.70
29	A1	289	U	N1-C2-O2	6.59	127.41	122.80
53	A2	1193	U	C2-N1-C1'	6.59	125.61	117.70
53	A2	34	C	C5-C6-N1	6.59	124.29	121.00
29	A1	2892	C	N1-C2-O2	6.59	122.85	118.90
29	A1	400	G	O4'-C1'-N9	6.59	113.47	108.20
53	A2	408	G	C8-N9-C1'	-6.59	118.44	127.00
30	B1	3	U	C2-N1-C1'	6.58	125.60	117.70
53	A2	1198	C	C6-N1-C2	-6.58	117.67	120.30
29	A1	1057	A	O5'-P-OP2	-6.57	99.78	105.70
37	G2	34	GLY	N-CA-C	-6.57	96.67	113.10
29	A1	678	G	N3-C4-C5	-6.57	125.32	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	624	G	C6-C5-N7	-6.55	126.47	130.40
53	A2	673	G	C4-N9-C1'	6.55	135.02	126.50
29	A1	2595	G	C8-N9-C1'	-6.55	118.48	127.00
30	B1	115	G	C4-N9-C1'	6.54	135.01	126.50
53	A2	606	C	C6-N1-C2	-6.54	117.68	120.30
53	A2	670	A	P-O3'-C3'	6.54	127.54	119.70
29	A1	555	A	C2-N3-C4	-6.53	107.33	110.60
53	A2	1377	C	C6-N1-C2	-6.53	117.69	120.30
29	A1	1091	C	C6-N1-C2	-6.53	117.69	120.30
29	A1	1912	G	C4-C5-N7	6.53	113.41	110.80
29	A1	1969	G	C6-C5-N7	-6.53	126.48	130.40
29	A1	1697	C	C6-N1-C2	-6.52	117.69	120.30
29	A1	1965	C	N1-C2-O2	6.51	122.81	118.90
53	A2	690	C	N3-C2-O2	-6.51	117.34	121.90
53	A2	1227	C	C6-N1-C2	-6.51	117.70	120.30
53	A2	1184	C	N3-C2-O2	-6.51	117.35	121.90
29	A1	2079	C	N3-C4-C5	6.50	124.50	121.90
53	A2	330	C	N3-C2-O2	-6.50	117.35	121.90
29	A1	938	C	C2-N1-C1'	6.49	125.94	118.80
53	A2	217	U	C6-N1-C2	-6.49	117.11	121.00
29	A1	692	C	C6-N1-C2	-6.49	117.70	120.30
29	A1	1744	G	C4-C5-N7	6.49	113.40	110.80
53	A2	690	C	N1-C2-O2	6.49	122.79	118.90
53	A2	955	A	C4-N9-C1'	6.49	137.98	126.30
29	A1	444	C	C2-N1-C1'	6.49	125.93	118.80
29	A1	531	U	C2-N1-C1'	6.48	125.48	117.70
53	A2	132	G	N3-C4-N9	-6.48	122.11	126.00
53	A2	72	C	C5-C6-N1	6.48	124.24	121.00
53	A2	188	U	C2-N1-C1'	6.47	125.47	117.70
53	A2	217	U	N1-C2-O2	6.47	127.33	122.80
29	A1	2704	C	C6-N1-C2	-6.47	117.71	120.30
53	A2	577	G	C8-N9-C4	-6.47	103.81	106.40
29	A1	1991	C	C2-N1-C1'	6.45	125.90	118.80
29	A1	2788	C	C6-N1-C2	-6.45	117.72	120.30
53	A2	172	C	N1-C2-O2	6.45	122.77	118.90
29	A1	1756	G	O4'-C1'-N9	6.44	113.35	108.20
53	A2	309	C	C6-N1-C2	-6.44	117.72	120.30
29	A1	243	C	C2-N1-C1'	6.44	125.88	118.80
29	A1	1676	G	N3-C4-N9	6.44	129.87	126.00
29	A1	2167	C	C6-N1-C2	-6.44	117.72	120.30
53	A2	1114	C	C5-C6-N1	6.43	124.22	121.00
29	A1	316	C	C2-N1-C1'	6.43	125.88	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	891	A	O5'-P-OP1	-6.43	99.91	105.70
29	A1	2504	G	C8-N9-C1'	-6.43	118.64	127.00
29	A1	1234	G	C4-N9-C1'	6.43	134.85	126.50
29	A1	73	A	C2-N3-C4	-6.42	107.39	110.60
29	A1	80	G	C6-C5-N7	-6.42	126.55	130.40
29	A1	1540	G	N3-C4-C5	-6.42	125.39	128.60
53	A2	673	G	C6-C5-N7	-6.42	126.55	130.40
29	A1	388	G	C6-C5-N7	-6.42	126.55	130.40
29	A1	1709	C	C6-N1-C2	-6.42	117.73	120.30
53	A2	1333	C	N1-C2-O2	6.41	122.75	118.90
29	A1	742	C	C6-N1-C2	-6.41	117.73	120.30
30	B1	64	C	N3-C2-O2	-6.41	117.41	121.90
53	A2	1251	C	C5-C6-N1	6.41	124.20	121.00
53	A2	1272	G	N7-C8-N9	6.41	116.30	113.10
29	A1	1832	G	P-O3'-C3'	6.41	127.39	119.70
29	A1	832	A	N1-C6-N6	6.40	122.44	118.60
53	A2	1275	G	N3-C2-N2	-6.40	115.42	119.90
29	A1	1112	C	C5-C6-N1	6.40	124.20	121.00
29	A1	2258	U	N1-C2-O2	6.39	127.27	122.80
53	A2	217	U	C5-C6-N1	6.39	125.89	122.70
29	A1	1234	G	C4-C5-C6	6.38	122.63	118.80
53	A2	148	C	C2-N1-C1'	6.38	125.82	118.80
53	A2	955	A	C8-N9-C1'	-6.38	116.21	127.70
29	A1	1955	U	N3-C2-O2	-6.38	117.73	122.20
29	A1	1148	C	C5-C6-N1	6.38	124.19	121.00
29	A1	2598	U	C2-N1-C1'	6.38	125.35	117.70
29	A1	2605	C	N3-C4-C5	6.36	124.45	121.90
53	A2	1374	G	C6-C5-N7	-6.36	126.58	130.40
29	A1	531	U	N1-C2-O2	6.35	127.25	122.80
29	A1	1022	C	N1-C2-O2	6.35	122.71	118.90
53	A2	101	G	C6-C5-N7	-6.35	126.59	130.40
29	A1	855	C	C6-N1-C2	-6.34	117.76	120.30
53	A2	1337	G	C4-N9-C1'	6.34	134.75	126.50
29	A1	2574	C	C6-N1-C2	-6.34	117.76	120.30
29	A1	1319	G	C6-C5-N7	-6.34	126.60	130.40
53	A2	18	C	C5-C6-N1	6.33	124.17	121.00
29	A1	1873	G	C4-N9-C1'	6.33	134.72	126.50
29	A1	2640	C	N1-C2-O2	6.33	122.69	118.90
53	A2	241	A	N1-C6-N6	-6.32	114.81	118.60
53	A2	772	U	C2-N1-C1'	6.31	125.27	117.70
53	A2	1110	C	C5-C6-N1	6.31	124.15	121.00
29	A1	2580	A	P-O3'-C3'	6.31	127.27	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2812	C	N1-C2-O2	6.31	122.68	118.90
53	A2	615	A	N7-C8-N9	6.30	116.95	113.80
29	A1	531	U	N3-C2-O2	-6.30	117.79	122.20
29	A1	2467	A	C5-N7-C8	-6.30	100.75	103.90
53	A2	62	U	N3-C2-O2	-6.30	117.79	122.20
53	A2	1456	C	C6-N1-C2	-6.30	117.78	120.30
53	A2	136	G	C6-C5-N7	-6.30	126.62	130.40
53	A2	969	U	P-O3'-C3'	6.30	127.26	119.70
29	A1	2892	C	N3-C2-O2	-6.29	117.49	121.90
29	A1	1142	U	N3-C2-O2	-6.29	117.80	122.20
29	A1	2361	C	O5'-P-OP2	-6.29	100.04	105.70
29	A1	950	C	N1-C2-O2	6.29	122.67	118.90
29	A1	312	C	C6-N1-C2	6.29	122.81	120.30
29	A1	1126	U	N1-C2-O2	6.28	127.20	122.80
29	A1	1459	C	C5-C6-N1	6.28	124.14	121.00
29	A1	1965	C	N3-C2-O2	-6.28	117.50	121.90
29	A1	2089	C	C6-N1-C2	-6.28	117.79	120.30
29	A1	1819	A	C4-C5-N7	6.28	113.84	110.70
29	A1	2900	C	C2-N1-C1'	6.28	125.71	118.80
53	A2	1341	A	P-O3'-C3'	6.28	127.23	119.70
29	A1	648	A	C5-N7-C8	-6.27	100.76	103.90
53	A2	136	G	N1-C2-N2	-6.27	110.56	116.20
28	d1	50	LEU	CA-CB-CG	6.26	129.71	115.30
30	B1	86	C	C5-C6-N1	6.26	124.13	121.00
29	A1	1088	C	N1-C2-O2	6.26	122.66	118.90
29	A1	160	U	N1-C2-O2	6.25	127.18	122.80
53	A2	1126	G	N7-C8-N9	6.25	116.22	113.10
29	A1	673	A	C5-N7-C8	-6.24	100.78	103.90
53	A2	839	C	C6-N1-C2	-6.24	117.80	120.30
53	A2	144	C	C6-N1-C2	-6.24	117.81	120.30
53	A2	1457	G	N1-C6-O6	6.24	123.64	119.90
53	A2	203	A	C5-N7-C8	-6.24	100.78	103.90
29	A1	673	A	C4-C5-N7	6.23	113.82	110.70
53	A2	270	G	C4-N9-C1'	6.23	134.60	126.50
29	A1	662	C	N3-C2-O2	-6.23	117.54	121.90
53	A2	309	C	C2-N1-C1'	6.23	125.66	118.80
53	A2	513	G	C6-C5-N7	-6.23	126.66	130.40
53	A2	575	G	N3-C4-N9	-6.23	122.26	126.00
29	A1	2892	C	C2-N1-C1'	6.23	125.65	118.80
53	A2	1299	A	C8-N9-C4	-6.23	103.31	105.80
53	A2	1479	A	C4-N9-C1'	6.23	137.51	126.30
53	A2	423	G	N3-C4-N9	-6.22	122.27	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	439	G	O5'-P-OP2	-6.22	100.10	105.70
29	A1	1319	G	N7-C8-N9	6.22	116.21	113.10
53	A2	1190	C	P-O3'-C3'	6.22	127.16	119.70
29	A1	690	C	N1-C2-O2	6.21	122.63	118.90
29	A1	2738	C	C5-C6-N1	6.21	124.11	121.00
29	A1	1617	G	C4-C5-N7	6.21	113.28	110.80
29	A1	823	A	N7-C8-N9	6.21	116.91	113.80
29	A1	2512	C	N3-C2-O2	-6.21	117.55	121.90
29	A1	2808	G	C8-N9-C1'	-6.21	118.93	127.00
53	A2	577	G	N3-C4-C5	-6.20	125.50	128.60
29	A1	248	G	C6-C5-N7	-6.20	126.68	130.40
53	A2	210	U	C6-N1-C1'	-6.20	112.53	121.20
29	A1	782	G	N1-C2-N2	-6.19	110.63	116.20
53	A2	206	G	N1-C2-N2	-6.19	110.63	116.20
53	A2	881	C	C5-C6-N1	6.18	124.09	121.00
29	A1	951	C	N3-C2-O2	-6.18	117.57	121.90
29	A1	2003	C	C6-N1-C2	-6.18	117.83	120.30
29	A1	1697	C	C5-C6-N1	6.17	124.09	121.00
29	A1	2618	U	N3-C2-O2	-6.17	117.88	122.20
29	A1	127	C	C2-N1-C1'	6.17	125.59	118.80
53	A2	443	C	C6-N1-C2	-6.17	117.83	120.30
29	A1	741	C	N3-C2-O2	-6.17	117.58	121.90
29	A1	828	U	N3-C2-O2	-6.17	117.88	122.20
53	A2	376	C	N1-C2-O2	6.16	122.60	118.90
30	B1	30	C	N1-C2-O2	6.16	122.60	118.90
29	A1	1112	C	C6-N1-C2	-6.16	117.83	120.30
29	A1	2409	C	C6-N1-C2	-6.16	117.84	120.30
29	A1	1714	A	C4-C5-N7	6.16	113.78	110.70
29	A1	1736	G	C6-C5-N7	-6.16	126.71	130.40
53	A2	955	A	C5-N7-C8	-6.16	100.82	103.90
53	A2	1499	U	C6-N1-C2	-6.15	117.31	121.00
29	A1	877	U	N3-C2-O2	-6.15	117.90	122.20
53	A2	1184	C	C2-N1-C1'	6.15	125.56	118.80
29	A1	2582	C	C6-N1-C2	-6.14	117.84	120.30
29	A1	718	G	C8-N9-C1'	-6.13	119.03	127.00
29	A1	1819	A	C4-N9-C1'	6.13	137.34	126.30
29	A1	2679	A	C5-N7-C8	-6.13	100.83	103.90
16	R1	66	GLU	C-N-CA	6.13	137.02	121.70
29	A1	844	C	C6-N1-C2	-6.12	117.85	120.30
29	A1	1819	A	C8-N9-C4	-6.12	103.35	105.80
29	A1	1542	A	C5-C6-N1	6.12	120.76	117.70
26	b1	36	LEU	CA-CB-CG	6.12	129.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	1540	G	N3-C4-N9	6.12	129.67	126.00
29	A1	1660	C	C5-C6-N1	6.12	124.06	121.00
29	A1	1974	G	O4'-C1'-N9	6.12	113.09	108.20
53	A2	93	C	C5-C6-N1	6.12	124.06	121.00
29	A1	2335	G	N3-C4-C5	-6.12	125.54	128.60
53	A2	559	G	C6-C5-N7	-6.12	126.73	130.40
29	A1	448	C	N3-C2-O2	-6.11	117.62	121.90
29	A1	951	C	N1-C2-O2	6.11	122.56	118.90
29	A1	1660	C	C6-N1-C2	-6.10	117.86	120.30
30	B1	30	C	N3-C2-O2	-6.10	117.63	121.90
53	A2	136	G	N3-C4-N9	6.10	129.66	126.00
29	A1	199	C	N1-C2-O2	6.10	122.56	118.90
29	A1	139	A	N7-C8-N9	6.10	116.85	113.80
53	A2	606	C	C5-C6-N1	6.10	124.05	121.00
30	B1	72	C	N1-C2-O2	6.09	122.56	118.90
9	K1	62	LEU	CB-CG-CD1	6.09	121.36	111.00
29	A1	824	G	C6-C5-N7	-6.09	126.75	130.40
29	A1	1459	C	C6-N1-C2	-6.09	117.86	120.30
29	A1	1958	C	C5-C6-N1	6.09	124.04	121.00
29	A1	2364	C	N3-C2-O2	-6.08	117.64	121.90
53	A2	1353	G	C4-N9-C1'	6.08	134.40	126.50
29	A1	2453	A	P-O3'-C3'	6.07	126.98	119.70
53	A2	132	G	C5-C6-N1	-6.07	108.47	111.50
53	A2	181	C	C6-N1-C2	-6.07	117.87	120.30
53	A2	231	G	C4-N9-C1'	-6.07	118.61	126.50
29	A1	1702	G	P-O3'-C3'	6.07	126.98	119.70
29	A1	1955	U	N1-C2-O2	6.07	127.05	122.80
53	A2	1450	A	O4'-C1'-N9	6.06	113.05	108.20
53	A2	206	G	C2-N3-C4	-6.06	108.87	111.90
29	A1	1187	C	C6-N1-C2	-6.05	117.88	120.30
53	A2	206	G	N3-C2-N2	6.05	124.14	119.90
29	A1	550	C	C5-C6-N1	6.05	124.03	121.00
53	A2	922	G	N9-C4-C5	-6.05	102.98	105.40
29	A1	1974	G	N9-C4-C5	-6.05	102.98	105.40
53	A2	36	C	C2-N1-C1'	6.05	125.45	118.80
29	A1	2710	U	C5-C6-N1	6.05	125.72	122.70
53	A2	1227	C	C5-C6-N1	6.05	124.02	121.00
53	A2	1201	G	N1-C6-O6	-6.04	116.27	119.90
29	A1	1152	C	C6-N1-C2	-6.04	117.88	120.30
29	A1	1912	G	C5-N7-C8	-6.04	101.28	104.30
29	A1	2582	C	C5-C6-N1	6.04	124.02	121.00
29	A1	2088	C	C5-C6-N1	6.04	124.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	612	G	C4-C5-N7	6.04	113.21	110.80
53	A2	1360	C	C6-N1-C1'	6.04	128.04	120.80
29	A1	1869	C	N1-C2-O2	6.03	122.52	118.90
53	A2	1251	C	C6-N1-C2	-6.03	117.89	120.30
29	A1	1991	C	C5-C6-N1	6.03	124.02	121.00
29	A1	1494	C	N3-C2-O2	-6.03	117.68	121.90
29	A1	1629	A	O4'-C1'-N9	6.03	113.02	108.20
29	A1	316	C	C5-C6-N1	6.02	124.01	121.00
29	A1	310	C	C6-N1-C2	-6.02	117.89	120.30
29	A1	1469	G	C6-C5-N7	-6.02	126.79	130.40
29	A1	2345	G	C4-C5-N7	6.02	113.21	110.80
53	A2	407	A	P-O3'-C3'	6.02	126.92	119.70
29	A1	2345	G	C6-C5-N7	-6.01	126.79	130.40
29	A1	2700	G	C4-C5-N7	6.01	113.21	110.80
29	A1	606	C	C6-N1-C2	-6.01	117.89	120.30
53	A2	1114	C	C6-N1-C2	-6.01	117.90	120.30
29	A1	727	C	N3-C2-O2	-6.00	117.70	121.90
29	A1	867	G	N3-C4-N9	6.00	129.60	126.00
29	A1	2127	C	C6-N1-C2	-6.00	117.90	120.30
29	A1	403	C	C5-C6-N1	5.99	124.00	121.00
53	A2	716	A	C5-N7-C8	-5.99	100.90	103.90
29	A1	2700	G	C6-C5-N7	-5.99	126.81	130.40
29	A1	160	U	C6-N1-C1'	-5.99	112.82	121.20
53	A2	559	G	C4-N9-C1'	5.99	134.28	126.50
29	A1	150	C	C6-N1-C2	-5.98	117.91	120.30
53	A2	408	G	C6-C5-N7	-5.98	126.81	130.40
53	A2	955	A	C6-C5-N7	-5.98	128.12	132.30
29	A1	564	C	C4-C5-C6	-5.97	114.41	117.40
29	A1	1126	U	N3-C2-O2	-5.97	118.02	122.20
29	A1	1912	G	O4'-C1'-N9	5.97	112.98	108.20
53	A2	985	C	C2-N1-C1'	5.97	125.37	118.80
29	A1	1304	G	N3-C4-N9	5.97	129.58	126.00
29	A1	2454	C	N3-C4-C5	5.97	124.29	121.90
29	A1	2068	C	C6-N1-C2	-5.96	117.92	120.30
29	A1	2335	G	C8-N9-C1'	-5.96	119.25	127.00
29	A1	606	C	N3-C2-O2	-5.96	117.73	121.90
29	A1	1664	A	C4-C5-N7	5.96	113.68	110.70
29	A1	1003	G	C6-C5-N7	-5.96	126.83	130.40
29	A1	310	C	C5-C6-N1	5.95	123.97	121.00
53	A2	1198	C	C5-C6-N1	5.94	123.97	121.00
29	A1	2705	C	C5-C6-N1	5.94	123.97	121.00
53	A2	972	C	C5-C6-N1	5.94	123.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2679	A	O4'-C1'-N9	5.93	112.95	108.20
29	A1	316	C	N3-C2-O2	-5.93	117.75	121.90
29	A1	1545	U	C5-C6-N1	5.93	125.67	122.70
29	A1	1546	C	N3-C4-C5	5.93	124.27	121.90
53	A2	1122	C	N1-C2-O2	5.93	122.45	118.90
29	A1	1127	C	C6-N1-C2	-5.92	117.93	120.30
29	A1	1895	G	C4-N9-C1'	5.92	134.20	126.50
29	A1	1925	A	C5-C6-N1	5.92	120.66	117.70
53	A2	219	C	N1-C2-O2	5.92	122.45	118.90
29	A1	2198	C	C6-N1-C2	-5.92	117.93	120.30
29	A1	661	C	C5-C6-N1	5.92	123.96	121.00
29	A1	1459	C	C2-N1-C1'	5.92	125.31	118.80
30	B1	49	C	C5-C6-N1	5.92	123.96	121.00
29	A1	690	C	N3-C2-O2	-5.91	117.76	121.90
53	A2	239	U	P-O3'-C3'	5.91	126.80	119.70
53	A2	309	C	C5-C6-N1	5.91	123.96	121.00
30	B1	58	G	C4-N9-C1'	5.91	134.19	126.50
30	B1	72	C	C2-N1-C1'	5.91	125.30	118.80
29	A1	735	G	C4-N9-C1'	5.91	134.18	126.50
29	A1	1539	G	C6-C5-N7	-5.91	126.86	130.40
29	A1	2356	C	C6-N1-C2	-5.91	117.94	120.30
53	A2	1360	C	C4-C5-C6	-5.91	114.45	117.40
29	A1	828	U	N1-C2-O2	5.90	126.93	122.80
29	A1	1673	C	C2-N1-C1'	5.90	125.29	118.80
53	A2	202	A	C8-N9-C4	-5.90	103.44	105.80
29	A1	2016	G	OP2-P-O3'	5.90	118.18	105.20
29	A1	965	A	C6-C5-N7	-5.90	128.17	132.30
29	A1	1676	G	C4-C5-N7	5.90	113.16	110.80
53	A2	231	G	C8-N9-C1'	5.89	134.66	127.00
53	A2	108	G	P-O3'-C3'	5.89	126.77	119.70
29	A1	1685	C	C5-C6-N1	5.89	123.94	121.00
29	A1	492	U	C5-C6-N1	5.89	125.64	122.70
29	A1	569	C	N1-C2-O2	5.88	122.43	118.90
29	A1	2630	C	C2-N1-C1'	5.88	125.27	118.80
53	A2	917	C	C6-N1-C2	-5.88	117.95	120.30
29	A1	1745	G	C6-C5-N7	-5.88	126.87	130.40
29	A1	2774	G	C4-N9-C1'	5.88	134.14	126.50
29	A1	2808	G	N3-C4-N9	5.87	129.53	126.00
29	A1	1061	C	C6-N1-C2	-5.87	117.95	120.30
29	A1	1809	G	C4-C5-N7	5.87	113.15	110.80
29	A1	2258	U	N3-C2-O2	-5.87	118.09	122.20
29	A1	2665	C	N3-C2-O2	-5.87	117.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	1756	G	C4-C5-N7	5.86	113.14	110.80
53	A2	241	A	C5-C6-N1	5.86	120.63	117.70
29	A1	162	C	C6-N1-C2	-5.86	117.96	120.30
29	A1	802	C	C2-N1-C1'	5.86	125.25	118.80
53	A2	673	G	C8-N9-C1'	-5.86	119.38	127.00
53	A2	1124	G	C4-N9-C1'	5.86	134.11	126.50
53	A2	1289	U	C2-N1-C1'	5.86	124.73	117.70
53	A2	203	A	N7-C8-N9	5.85	116.73	113.80
53	A2	1184	C	C6-N1-C2	-5.85	117.96	120.30
29	A1	1475	A	P-O3'-C3'	5.85	126.72	119.70
29	A1	1974	G	C4-N9-C1'	5.85	134.10	126.50
29	A1	1115	A	O4'-C1'-N9	5.85	112.88	108.20
29	A1	1539	G	C4-N9-C1'	5.85	134.10	126.50
53	A2	203	A	O4'-C1'-N9	5.84	112.87	108.20
53	A2	932	U	O4'-C1'-N1	5.84	112.87	108.20
30	B1	83	G	O4'-C1'-N9	5.84	112.87	108.20
29	A1	539	G	N1-C6-O6	-5.84	116.40	119.90
29	A1	1727	G	C4-C5-N7	5.84	113.14	110.80
30	B1	39	C	N1-C2-O2	5.83	122.40	118.90
29	A1	243	C	N1-C2-O2	5.83	122.40	118.90
53	A2	716	A	N7-C8-N9	5.83	116.71	113.80
29	A1	1718	A	C4-N9-C1'	5.83	136.79	126.30
53	A2	630	C	N3-C4-C5	5.82	124.23	121.90
29	A1	706	U	N3-C2-O2	-5.82	118.13	122.20
29	A1	2364	C	N1-C2-O2	5.82	122.39	118.90
29	A1	2161	C	C6-N1-C2	-5.82	117.97	120.30
29	A1	388	G	C4-C5-N7	5.82	113.13	110.80
53	A2	231	G	C5-N7-C8	5.82	107.21	104.30
29	A1	1732	C	C6-N1-C2	-5.81	117.97	120.30
53	A2	297	G	C4-C5-N7	5.81	113.12	110.80
29	A1	80	G	N1-C2-N2	-5.81	110.97	116.20
29	A1	381	G	C4-N9-C1'	-5.81	118.95	126.50
53	A2	336	C	C5-C6-N1	5.81	123.90	121.00
29	A1	2276	U	N3-C2-O2	-5.80	118.14	122.20
29	A1	311	C	C5-C6-N1	5.80	123.90	121.00
29	A1	1142	U	N1-C2-O2	5.80	126.86	122.80
53	A2	737	C	N3-C2-O2	-5.80	117.84	121.90
29	A1	1453	U	N3-C2-O2	-5.80	118.14	122.20
53	A2	360	U	O4'-C1'-N1	5.79	112.83	108.20
29	A1	2012	C	N1-C2-O2	5.79	122.38	118.90
53	A2	233	G	C6-C5-N7	-5.79	126.93	130.40
29	A1	965	A	N1-C6-N6	5.79	122.07	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	1727	G	C2-N3-C4	-5.79	109.01	111.90
53	A2	1227	C	N1-C2-O2	5.78	122.37	118.90
29	A1	1018	C	C2-N1-C1'	5.78	125.16	118.80
29	A1	2356	C	C5-C6-N1	5.78	123.89	121.00
53	A2	297	G	C6-C5-N7	-5.78	126.93	130.40
53	A2	672	C	C6-N1-C2	-5.78	117.99	120.30
53	A2	1259	U	N1-C2-O2	5.78	126.84	122.80
29	A1	2373	C	C6-N1-C2	-5.78	117.99	120.30
53	A2	881	C	C4-C5-C6	-5.77	114.51	117.40
53	A2	1377	C	C2-N1-C1'	5.77	125.15	118.80
29	A1	2728	A	C5-N7-C8	-5.77	101.02	103.90
29	A1	802	C	C6-N1-C2	-5.77	117.99	120.30
29	A1	1112	C	N1-C2-O2	5.77	122.36	118.90
29	A1	1453	U	N1-C2-O2	5.76	126.84	122.80
53	A2	216	C	C5-C6-N1	5.76	123.88	121.00
29	A1	20	C	C6-N1-C2	-5.76	118.00	120.30
29	A1	1756	G	N7-C8-N9	5.76	115.98	113.10
29	A1	741	C	C6-N1-C2	-5.76	118.00	120.30
29	A1	604	G	C4-N9-C1'	5.76	133.99	126.50
29	A1	323	G	C4-C5-N7	5.76	113.10	110.80
29	A1	1633	C	C6-N1-C2	-5.76	118.00	120.30
29	A1	1807	C	C6-N1-C2	-5.76	118.00	120.30
53	A2	31	G	N3-C4-C5	5.76	131.48	128.60
29	A1	1072	G	C8-N9-C4	-5.75	104.10	106.40
53	A2	1193	U	N1-C2-O2	5.75	126.83	122.80
29	A1	248	G	N7-C8-N9	5.75	115.98	113.10
29	A1	1304	G	C4-N9-C1'	5.75	133.98	126.50
30	B1	3	U	N3-C2-O2	-5.75	118.18	122.20
29	A1	1494	C	N1-C2-O2	5.75	122.35	118.90
53	A2	513	G	C5-N7-C8	-5.74	101.43	104.30
53	A2	716	A	C4-C5-N7	5.74	113.57	110.70
53	A2	969	U	C5-C6-N1	-5.74	119.83	122.70
29	A1	388	G	C8-N9-C4	-5.74	104.10	106.40
53	A2	31	G	O5'-P-OP2	-5.74	100.53	105.70
53	A2	577	G	N7-C8-N9	5.74	115.97	113.10
29	A1	1054	C	N3-C2-O2	-5.74	117.89	121.90
29	A1	555	A	N3-C4-C5	5.73	130.81	126.80
29	A1	567	C	N3-C2-O2	-5.73	117.89	121.90
29	A1	2129	C	C6-N1-C2	-5.73	118.01	120.30
53	A2	509	C	N3-C4-C5	5.73	124.19	121.90
53	A2	824	U	C5-C6-N1	5.73	125.56	122.70
19	U1	102	LEU	CA-CB-CG	5.73	128.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	1361	U	N1-C2-O2	5.73	126.81	122.80
29	A1	1819	A	C6-C5-N7	-5.73	128.29	132.30
29	A1	2224	C	C5-C6-N1	5.73	123.86	121.00
53	A2	749	A	C4-C5-N7	5.73	113.56	110.70
29	A1	210	G	C6-C5-N7	-5.72	126.97	130.40
29	A1	2068	C	N3-C2-O2	-5.72	117.89	121.90
29	A1	1583	U	C2-N1-C1'	5.72	124.57	117.70
53	A2	1374	G	N1-C6-O6	5.72	123.33	119.90
53	A2	309	C	N3-C2-O2	-5.72	117.90	121.90
53	A2	679	A	C5-N7-C8	-5.72	101.04	103.90
29	A1	96	C	C6-N1-C2	-5.71	118.01	120.30
29	A1	1189	U	C5-C6-N1	5.71	125.56	122.70
29	A1	2535	C	C5-C6-N1	5.71	123.86	121.00
53	A2	750	A	N1-C2-N3	-5.71	126.45	129.30
53	A2	202	A	N7-C8-N9	5.70	116.65	113.80
53	A2	1479	A	C8-N9-C1'	-5.70	117.43	127.70
29	A1	569	C	N3-C2-O2	-5.70	117.91	121.90
29	A1	1022	C	N3-C2-O2	-5.70	117.91	121.90
53	A2	244	U	N3-C2-O2	-5.70	118.21	122.20
29	A1	2068	C	N1-C2-O2	5.70	122.32	118.90
29	A1	741	C	N1-C2-O2	5.70	122.32	118.90
29	A1	1539	G	C4-C5-N7	5.69	113.08	110.80
29	A1	2186	G	N3-C4-N9	5.69	129.41	126.00
29	A1	2868	C	C6-N1-C2	-5.69	118.03	120.30
53	A2	1335	C	C6-N1-C2	-5.69	118.03	120.30
29	A1	2590	G	C4-N9-C1'	5.69	133.89	126.50
53	A2	1282	U	N1-C2-O2	5.69	126.78	122.80
29	A1	1974	G	C5-N7-C8	-5.68	101.46	104.30
53	A2	211	G	C8-N9-C4	5.68	108.67	106.40
29	A1	2612	A	C8-N9-C4	-5.68	103.53	105.80
30	B1	115	G	C8-N9-C1'	-5.68	119.62	127.00
29	A1	188	C	C6-N1-C2	-5.67	118.03	120.30
29	A1	1126	U	C2-N1-C1'	5.67	124.50	117.70
29	A1	778	G	C8-N9-C1'	-5.67	119.64	127.00
29	A1	1974	G	C8-N9-C1'	-5.66	119.64	127.00
29	A1	381	G	C8-N9-C1'	5.66	134.36	127.00
53	A2	132	G	C2-N3-C4	-5.66	109.07	111.90
29	A1	2742	G	C6-C5-N7	-5.66	127.01	130.40
29	A1	2016	G	O4'-C1'-N9	-5.65	103.68	108.20
29	A1	1659	C	C2-N1-C1'	5.65	125.01	118.80
29	A1	1225	C	P-O3'-C3'	5.64	126.47	119.70
53	A2	132	G	N3-C4-C5	5.64	131.42	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	1401	G	C4-C5-N7	5.64	113.06	110.80
53	A2	43	C	N1-C2-O2	5.64	122.28	118.90
29	A1	2607	U	N3-C4-O4	5.64	123.35	119.40
30	B1	16	U	N3-C2-O2	-5.64	118.25	122.20
29	A1	137	G	C4-N9-C1'	5.63	133.82	126.50
29	A1	624	G	C4-C5-N7	5.63	113.05	110.80
29	A1	2812	C	N3-C2-O2	-5.63	117.95	121.90
53	A2	1237	A	C8-N9-C4	5.63	108.05	105.80
53	A2	1353	G	C8-N9-C1'	-5.63	119.68	127.00
29	A1	2467	A	C4-C5-N7	5.63	113.52	110.70
29	A1	1070	G	C4-N9-C1'	5.63	133.82	126.50
29	A1	1736	G	C4-C5-N7	5.63	113.05	110.80
29	A1	236	C	C6-N1-C2	-5.63	118.05	120.30
29	A1	1718	A	C8-N9-C1'	-5.63	117.57	127.70
30	B1	72	C	C6-N1-C2	-5.63	118.05	120.30
29	A1	1071	U	N1-C2-O2	5.62	126.74	122.80
53	A2	1374	G	C4-C5-N7	5.62	113.05	110.80
29	A1	725	A	C5-N7-C8	-5.62	101.09	103.90
53	A2	1243	C	N1-C2-O2	5.62	122.27	118.90
30	B1	83	G	C4-N9-C1'	5.62	133.81	126.50
29	A1	1251	A	C4-C5-N7	5.61	113.51	110.70
29	A1	1727	G	C5-N7-C8	-5.61	101.49	104.30
29	A1	2700	G	C4-N9-C1'	5.61	133.80	126.50
29	A1	692	C	C5-C6-N1	5.61	123.81	121.00
53	A2	149	C	C5-C4-N4	-5.61	116.27	120.20
29	A1	1574	G	C8-N9-C4	-5.61	104.16	106.40
29	A1	675	G	C6-C5-N7	-5.61	127.04	130.40
53	A2	1258	C	N3-C2-O2	-5.61	117.98	121.90
53	A2	1479	A	C4-C5-N7	5.61	113.50	110.70
30	B1	11	G	C6-C5-N7	-5.60	127.04	130.40
29	A1	670	A	P-O3'-C3'	-5.60	112.98	119.70
53	A2	244	U	N1-C2-O2	5.60	126.72	122.80
53	A2	1410	A	C5-N7-C8	-5.60	101.10	103.90
53	A2	31	G	C4-C5-N7	5.60	113.04	110.80
29	A1	1809	G	C6-C5-N7	-5.59	127.04	130.40
53	A2	125	C	N3-C2-O2	-5.59	117.98	121.90
53	A2	746	G	N1-C2-N3	5.59	127.26	123.90
29	A1	1756	G	C5-N7-C8	-5.59	101.50	104.30
29	A1	2643	A	C8-N9-C4	5.59	108.04	105.80
53	A2	635	U	C4-C5-C6	-5.59	116.34	119.70
29	A1	1869	C	N3-C2-O2	-5.59	117.99	121.90
29	A1	1516	C	C6-N1-C2	-5.59	118.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2406	A	N9-C4-C5	-5.59	103.56	105.80
53	A2	664	C	O5'-P-OP2	-5.59	100.67	105.70
53	A2	737	C	C2-N1-C1'	5.59	124.95	118.80
53	A2	330	C	N1-C2-O2	5.59	122.25	118.90
53	A2	1108	U	P-O3'-C3'	5.59	126.41	119.70
29	A1	2301	A	C2-N3-C4	-5.58	107.81	110.60
29	A1	2322	G	N3-C4-N9	5.58	129.35	126.00
53	A2	1423	G	C6-C5-N7	-5.58	127.05	130.40
29	A1	73	A	O4'-C1'-N9	-5.58	103.74	108.20
29	A1	302	C	N1-C2-O2	5.58	122.25	118.90
29	A1	692	C	N1-C2-O2	5.58	122.25	118.90
29	A1	1923	G	C4-N9-C1'	-5.58	119.25	126.50
53	A2	565	U	N3-C2-O2	-5.58	118.30	122.20
29	A1	1591	A	N9-C4-C5	-5.58	103.57	105.80
29	A1	1718	A	C4-C5-N7	5.57	113.49	110.70
29	A1	1541	C	C6-N1-C2	5.57	122.53	120.30
53	A2	483	G	C4-N9-C1'	5.57	133.74	126.50
53	A2	1198	C	C2-N1-C1'	5.57	124.92	118.80
29	A1	2079	C	C2-N1-C1'	-5.56	112.68	118.80
29	A1	2162	C	C6-N1-C2	-5.56	118.08	120.30
29	A1	2782	C	C6-N1-C2	-5.56	118.08	120.30
53	A2	159	C	C5-C6-N1	5.56	123.78	121.00
29	A1	2049	C	C5-C6-N1	5.56	123.78	121.00
29	A1	2186	G	C2-N3-C4	5.56	114.68	111.90
29	A1	305	C	C6-N1-C2	-5.56	118.08	120.30
29	A1	1123	C	C6-N1-C2	-5.55	118.08	120.30
29	A1	2334	A	C4-N9-C1'	5.55	136.29	126.30
29	A1	1040	C	C6-N1-C2	-5.55	118.08	120.30
29	A1	1925	A	C2-N3-C4	5.55	113.38	110.60
29	A1	2640	C	C6-N1-C2	-5.55	118.08	120.30
29	A1	248	G	C4-N9-C1'	5.55	133.72	126.50
29	A1	417	G	C4-C5-N7	5.55	113.02	110.80
29	A1	489	C	C6-N1-C2	-5.55	118.08	120.30
29	A1	938	C	N1-C2-O2	5.55	122.23	118.90
53	A2	331	C	C6-N1-C2	-5.55	118.08	120.30
29	A1	1927	G	C4-N9-C1'	5.54	133.71	126.50
53	A2	846	G	C4-C5-N7	5.54	113.02	110.80
29	A1	824	G	N9-C4-C5	-5.54	103.18	105.40
29	A1	950	C	N3-C2-O2	-5.54	118.02	121.90
53	A2	205	G	P-O3'-C3'	5.54	126.35	119.70
53	A2	612	G	C4-N9-C1'	5.54	133.71	126.50
53	A2	1356	A	C5-N7-C8	-5.54	101.13	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2679	A	C4-C5-N7	5.54	113.47	110.70
29	A1	10	G	N7-C8-N9	-5.54	110.33	113.10
29	A1	2022	G	C6-C5-N7	-5.54	127.08	130.40
29	A1	1703	A	C5-C6-N1	5.54	120.47	117.70
52	V2	6	LEU	CA-CB-CG	5.54	128.03	115.30
53	A2	149	C	C6-N1-C2	-5.53	118.09	120.30
53	A2	220	C	C6-N1-C2	-5.53	118.09	120.30
53	A2	472	C	C6-N1-C2	-5.53	118.09	120.30
29	A1	1091	C	C5-C6-N1	5.53	123.77	121.00
53	A2	1289	U	C5-C6-N1	5.53	125.47	122.70
16	R1	63	ASP	CB-CG-OD1	5.53	123.27	118.30
29	A1	20	C	C2-N1-C1'	5.53	124.88	118.80
29	A1	1375	C	C6-N1-C2	-5.53	118.09	120.30
29	A1	1923	G	P-O3'-C3'	5.52	126.33	119.70
29	A1	1022	C	C2-N1-C1'	5.52	124.87	118.80
29	A1	1596	C	N3-C2-O2	-5.52	118.04	121.90
2	D1	17	ASP	CB-CG-OD1	5.52	123.27	118.30
29	A1	602	G	N3-C4-N9	-5.52	122.69	126.00
29	A1	823	A	C5-C6-N6	-5.52	119.29	123.70
29	A1	1991	C	C6-N1-C2	-5.52	118.09	120.30
29	A1	1745	G	C8-N9-C1'	-5.51	119.83	127.00
29	A1	1574	G	N7-C8-N9	5.51	115.86	113.10
53	A2	93	C	C6-N1-C2	-5.51	118.10	120.30
53	A2	272	C	C6-N1-C2	-5.51	118.09	120.30
29	A1	358	G	C4-N9-C1'	5.51	133.66	126.50
29	A1	2774	G	N3-C4-N9	5.51	129.31	126.00
53	A2	575	G	N3-C4-C5	5.51	131.35	128.60
29	A1	1764	G	N3-C4-C5	-5.51	125.85	128.60
29	A1	159	U	C6-N1-C2	-5.51	117.70	121.00
53	A2	14	U	C6-N1-C2	-5.51	117.70	121.00
53	A2	160	G	C6-C5-N7	-5.50	127.10	130.40
28	d1	61	LEU	CB-CG-CD1	-5.50	101.65	111.00
29	A1	1812	U	C2-N1-C1'	5.50	124.30	117.70
29	A1	2624	C	P-O3'-C3'	5.50	126.30	119.70
29	A1	2335	G	N7-C8-N9	5.50	115.85	113.10
53	A2	984	C	N3-C2-O2	-5.50	118.05	121.90
29	A1	288	G	P-O3'-C3'	5.50	126.30	119.70
29	A1	1744	G	C6-C5-N7	-5.50	127.10	130.40
53	A2	1421	C	C6-N1-C2	-5.50	118.10	120.30
29	A1	952	C	N3-C2-O2	-5.49	118.06	121.90
29	A1	2348	G	N7-C8-N9	5.49	115.84	113.10
29	A1	740	C	C6-N1-C2	-5.49	118.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	1868	G	C4-N9-C1'	5.49	133.63	126.50
53	A2	730	C	C5-C4-N4	-5.49	116.36	120.20
29	A1	337	G	C4-C5-N7	5.49	112.99	110.80
29	A1	1319	G	N3-C4-C5	-5.48	125.86	128.60
29	A1	1319	G	C4-C5-N7	5.48	112.99	110.80
53	A2	1470	A	C2-N3-C4	5.48	113.34	110.60
29	A1	118	U	N1-C2-O2	5.48	126.64	122.80
29	A1	618	G	C4-C5-N7	5.48	112.99	110.80
29	A1	2121	C	N1-C2-O2	5.48	122.19	118.90
29	A1	1873	G	N3-C4-C5	-5.48	125.86	128.60
29	A1	2153	C	C5-C6-N1	5.48	123.74	121.00
29	A1	1917	C	C2-N1-C1'	5.47	124.82	118.80
53	A2	902	G	C4-C5-N7	5.47	112.99	110.80
29	A1	2417	C	C6-N1-C2	-5.47	118.11	120.30
30	B1	16	U	N1-C2-O2	5.47	126.63	122.80
53	A2	810	U	N3-C4-O4	-5.47	115.57	119.40
53	A2	235	C	C5-C6-N1	5.47	123.74	121.00
29	A1	1525	C	C6-N1-C2	-5.47	118.11	120.30
53	A2	160	G	C4-C5-N7	5.47	112.99	110.80
53	A2	1373	U	N1-C2-N3	5.47	118.18	114.90
53	A2	261	G	N3-C4-C5	5.46	131.33	128.60
53	A2	900	A	C5-N7-C8	-5.46	101.17	103.90
53	A2	172	C	N3-C2-O2	-5.46	118.08	121.90
29	A1	1088	C	C2-N1-C1'	5.46	124.81	118.80
29	A1	1768	G	C6-C5-N7	-5.46	127.12	130.40
29	A1	2535	C	N1-C2-O2	5.46	122.17	118.90
53	A2	29	G	C4-N9-C1'	5.46	133.60	126.50
29	A1	272	U	C5-C6-N1	5.46	125.43	122.70
29	A1	1066	C	C6-N1-C2	-5.46	118.12	120.30
29	A1	127	C	C5-C6-N1	5.45	123.73	121.00
29	A1	742	C	C5-C6-N1	5.45	123.73	121.00
29	A1	1345	C	C6-N1-C2	-5.45	118.12	120.30
53	A2	985	C	C6-N1-C2	-5.45	118.12	120.30
29	A1	1182	C	C6-N1-C1'	-5.45	114.27	120.80
29	A1	1002	C	C5-C6-N1	5.44	123.72	121.00
29	A1	1764	G	C6-C5-N7	-5.44	127.13	130.40
40	J2	16	LEU	CB-CG-CD2	-5.44	101.75	111.00
53	A2	149	C	C5-C6-N1	5.44	123.72	121.00
29	A1	444	C	C5-C6-N1	5.44	123.72	121.00
29	A1	276	C	N1-C2-O2	5.43	122.16	118.90
29	A1	564	C	C6-N1-C2	-5.43	118.13	120.30
29	A1	1867	U	C2-N1-C1'	5.43	124.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	255	A	C5-N7-C8	-5.43	101.19	103.90
29	A1	1119	G	C4-N9-C1'	5.43	133.56	126.50
29	A1	1455	C	N3-C2-O2	-5.43	118.10	121.90
29	A1	337	G	C5-C6-O6	-5.42	125.35	128.60
53	A2	18	C	C4-C5-C6	-5.42	114.69	117.40
53	A2	349	G	C4-N9-C1'	5.42	133.54	126.50
53	A2	1122	C	N3-C2-O2	-5.42	118.11	121.90
29	A1	662	C	C2-N1-C1'	5.42	124.76	118.80
29	A1	1756	G	C4-N9-C1'	5.42	133.54	126.50
29	A1	313	C	C5-C6-N1	5.41	123.71	121.00
29	A1	529	A	C4-C5-N7	5.41	113.41	110.70
53	A2	1499	U	C5-C6-N1	5.41	125.41	122.70
29	A1	2704	C	C5-C6-N1	5.41	123.71	121.00
29	A1	1933	C	C6-N1-C2	-5.41	118.14	120.30
29	A1	1969	G	C4-N9-C1'	5.41	133.53	126.50
53	A2	970	G	O5'-P-OP2	-5.41	100.83	105.70
29	A1	757	C	N3-C2-O2	-5.40	118.12	121.90
29	A1	1591	A	C4-C5-N7	5.40	113.40	110.70
29	A1	465	C	N1-C2-O2	5.40	122.14	118.90
53	A2	248	U	N3-C2-O2	-5.40	118.42	122.20
29	A1	1499	G	P-O3'-C3'	5.40	126.18	119.70
29	A1	2590	G	C8-N9-C1'	-5.40	119.98	127.00
53	A2	323	C	N3-C2-O2	-5.40	118.12	121.90
53	A2	1488	G	C8-N9-C1'	-5.40	119.98	127.00
29	A1	474	G	N3-C4-N9	5.40	129.24	126.00
29	A1	2640	C	N3-C2-O2	-5.39	118.12	121.90
53	A2	188	U	C6-N1-C1'	-5.39	113.65	121.20
29	A1	1804	C	C6-N1-C2	-5.39	118.14	120.30
29	A1	778	G	C4-N9-C1'	5.39	133.51	126.50
29	A1	2766	G	N3-C4-C5	5.39	131.29	128.60
30	B1	56	G	C4-N9-C1'	5.39	133.51	126.50
29	A1	1950	U	O4'-C1'-N1	5.39	112.51	108.20
29	A1	139	A	C5-N7-C8	-5.38	101.21	103.90
29	A1	866	C	C6-N1-C2	-5.38	118.15	120.30
53	A2	216	C	N3-C4-N4	5.38	121.77	118.00
53	A2	561	C	C6-N1-C2	-5.38	118.15	120.30
29	A1	951	C	C6-N1-C2	-5.38	118.15	120.30
53	A2	136	G	C4-N9-C1'	5.38	133.49	126.50
53	A2	190	G	O4'-C1'-N9	5.38	112.50	108.20
29	A1	2900	C	N3-C2-O2	-5.38	118.14	121.90
53	A2	1125	G	C4-N9-C1'	5.38	133.49	126.50
29	A1	1069	A	C5-N7-C8	-5.38	101.21	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	181	C	C5-C6-N1	5.38	123.69	121.00
29	A1	897	G	C4-N9-C1'	5.37	133.49	126.50
29	A1	965	A	C5-N7-C8	-5.37	101.21	103.90
29	A1	2815	G	C4-C5-N7	5.37	112.95	110.80
53	A2	1479	A	C6-C5-N7	-5.37	128.54	132.30
53	A2	62	U	N1-C2-O2	5.36	126.56	122.80
29	A1	1821	C	C5-C6-N1	5.36	123.68	121.00
29	A1	1231	G	C4-N9-C1'	5.36	133.47	126.50
53	A2	700	C	N3-C2-O2	-5.36	118.15	121.90
29	A1	407	G	N1-C6-O6	-5.36	116.69	119.90
29	A1	1018	C	N3-C2-O2	-5.36	118.15	121.90
29	A1	2716	U	N1-C2-O2	5.36	126.55	122.80
29	A1	248	G	C4-C5-N7	5.36	112.94	110.80
29	A1	1033	C	O5'-P-OP1	-5.36	100.88	105.70
29	A1	2418	C	C6-N1-C2	-5.36	118.16	120.30
53	A2	1352	G	C6-C5-N7	-5.36	127.19	130.40
29	A1	1022	C	C6-N1-C2	-5.35	118.16	120.30
29	A1	1617	G	C5-C6-O6	-5.35	125.39	128.60
53	A2	347	C	C5-C6-N1	5.35	123.67	121.00
29	A1	1119	G	N3-C4-N9	5.35	129.21	126.00
29	A1	1304	G	N3-C4-C5	-5.35	125.93	128.60
53	A2	679	A	C4-C5-N7	5.35	113.37	110.70
29	A1	850	G	C4-C5-N7	5.35	112.94	110.80
29	A1	199	C	N3-C2-O2	-5.34	118.16	121.90
29	A1	647	G	C6-C5-N7	-5.34	127.19	130.40
53	A2	364	C	N3-C2-O2	-5.34	118.16	121.90
29	A1	609	C	C6-N1-C2	-5.34	118.16	120.30
29	A1	1726	A	C5-N7-C8	-5.34	101.23	103.90
29	A1	2012	C	N3-C2-O2	-5.34	118.16	121.90
29	A1	2136	G	C4-N9-C1'	5.34	133.44	126.50
53	A2	559	G	C8-N9-C1'	-5.34	120.06	127.00
53	A2	1459	G	C4-C5-N7	5.34	112.94	110.80
29	A1	782	G	C5-N7-C8	-5.34	101.63	104.30
29	A1	471	A	C4-C5-N7	5.33	113.37	110.70
53	A2	295	A	C5-N7-C8	-5.33	101.23	103.90
29	A1	941	C	C5-C6-N1	5.33	123.67	121.00
53	A2	716	A	C4-N9-C1'	5.33	135.90	126.30
29	A1	66	U	N3-C2-O2	-5.33	118.47	122.20
29	A1	10	G	C4-N9-C1'	-5.33	119.57	126.50
29	A1	2882	C	C6-N1-C2	-5.33	118.17	120.30
29	A1	338	C	C6-N1-C2	-5.33	118.17	120.30
29	A1	841	G	C4-N9-C1'	5.33	133.43	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	2702	U	C2-N1-C1'	5.33	124.09	117.70
53	A2	575	G	C4-N9-C1'	-5.33	119.57	126.50
53	A2	1298	C	N1-C2-O2	5.33	122.10	118.90
29	A1	2089	C	C5-C6-N1	5.33	123.66	121.00
30	B1	22	C	N1-C2-O2	5.32	122.09	118.90
53	A2	261	G	O4'-C1'-N9	-5.32	103.94	108.20
29	A1	1718	A	C5-C6-N1	5.32	120.36	117.70
53	A2	748	G	OP2-P-O3'	5.32	116.89	105.20
53	A2	1228	U	C2-N1-C1'	5.32	124.08	117.70
53	A2	972	C	C6-N1-C2	-5.31	118.17	120.30
29	A1	1743	C	OP2-P-O3'	5.31	116.89	105.20
29	A1	2364	C	C6-N1-C2	-5.31	118.17	120.30
53	A2	1506	G	C8-N9-C4	-5.31	104.28	106.40
29	A1	782	G	C5-C6-N1	5.31	114.16	111.50
30	B1	83	G	C6-C5-N7	-5.31	127.21	130.40
29	A1	226	C	N1-C2-O2	5.31	122.09	118.90
29	A1	1711	C	C2-N1-C1'	5.31	124.64	118.80
53	A2	1394	C	C2-N1-C1'	5.31	124.64	118.80
29	A1	943	U	C6-N1-C1'	-5.31	113.77	121.20
53	A2	332	C	C6-N1-C2	-5.31	118.18	120.30
53	A2	582	C	N1-C2-O2	5.31	122.08	118.90
29	A1	877	U	C2-N1-C1'	5.30	124.06	117.70
29	A1	2692	C	C6-N1-C2	-5.30	118.18	120.30
29	A1	1534	A	C5-C6-N1	5.30	120.35	117.70
53	A2	642	U	N3-C4-C5	5.30	117.78	114.60
53	A2	1317	C	P-O3'-C3'	5.30	126.06	119.70
29	A1	1361	U	C2-N1-C1'	5.29	124.05	117.70
53	A2	807	C	C5-C6-N1	5.29	123.65	121.00
29	A1	437	C	C6-N1-C2	-5.29	118.18	120.30
29	A1	2487	U	N1-C2-O2	5.29	126.50	122.80
29	A1	66	U	N1-C2-O2	5.29	126.50	122.80
53	A2	1423	G	O4'-C1'-N9	-5.28	103.97	108.20
53	A2	276	G	C8-N9-C4	-5.28	104.29	106.40
29	A1	1814	C	C6-N1-C1'	-5.28	114.47	120.80
53	A2	100	G	C5-C6-N1	5.27	114.14	111.50
29	A1	2271	U	N3-C2-O2	-5.27	118.51	122.20
30	B1	64	C	N1-C2-O2	5.27	122.06	118.90
29	A1	1362	C	C2-N1-C1'	5.27	124.60	118.80
53	A2	507	G	C4-N9-C1'	5.27	133.35	126.50
29	A1	238	G	OP1-P-O3'	5.27	116.79	105.20
29	A1	1248	C	C2-N1-C1'	5.27	124.59	118.80
29	A1	1315	U	N1-C2-O2	5.27	126.49	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	907	C	C6-N1-C2	-5.27	118.19	120.30
29	A1	2704	C	C6-N1-C1'	-5.27	114.48	120.80
29	A1	1745	G	C4-N9-C1'	5.26	133.34	126.50
29	A1	2057	A	O5'-P-OP2	-5.26	100.96	105.70
53	A2	271	G	O4'-C1'-N9	5.26	112.41	108.20
53	A2	534	U	C5-C6-N1	5.26	125.33	122.70
53	A2	717	G	N1-C2-N2	5.26	120.94	116.20
53	A2	1193	U	C6-N1-C1'	-5.26	113.83	121.20
29	A1	474	G	C6-C5-N7	-5.26	127.24	130.40
29	A1	823	A	C6-C5-N7	-5.26	128.62	132.30
29	A1	1676	G	C8-N9-C1'	-5.26	120.17	127.00
53	A2	1424	G	C4-N9-C1'	-5.26	119.67	126.50
53	A2	941	A	C4-C5-N7	5.25	113.33	110.70
53	A2	1118	U	C5-C6-N1	5.25	125.33	122.70
53	A2	483	G	C8-N9-C1'	-5.25	120.17	127.00
29	A1	162	C	C5-C6-N1	5.25	123.62	121.00
29	A1	444	C	C6-N1-C2	-5.25	118.20	120.30
29	A1	1873	G	N3-C4-N9	5.25	129.15	126.00
53	A2	479	A	O4'-C1'-N9	-5.25	104.00	108.20
29	A1	943	U	N3-C2-O2	-5.25	118.53	122.20
29	A1	598	G	C6-C5-N7	-5.25	127.25	130.40
29	A1	1234	G	N1-C6-O6	5.25	123.05	119.90
29	A1	639	U	C2-N1-C1'	5.24	123.99	117.70
29	A1	2213	U	C6-N1-C1'	-5.24	113.86	121.20
53	A2	575	G	C8-N9-C1'	5.24	133.81	127.00
29	A1	1676	G	C4-N9-C1'	5.24	133.31	126.50
29	A1	1598	C	C6-N1-C2	-5.24	118.21	120.30
29	A1	1673	C	N3-C2-O2	-5.24	118.23	121.90
29	A1	2350	A	C5-N7-C8	-5.24	101.28	103.90
53	A2	1025	C	C6-N1-C2	-5.24	118.21	120.30
29	A1	2406	A	O4'-C1'-N9	5.23	112.39	108.20
29	A1	1677	U	C6-N1-C2	-5.23	117.86	121.00
29	A1	1923	G	C8-N9-C1'	5.23	133.80	127.00
53	A2	620	G	N9-C4-C5	-5.23	103.31	105.40
53	A2	1333	C	N3-C2-O2	-5.23	118.24	121.90
29	A1	1979	U	N3-C2-O2	-5.23	118.54	122.20
29	A1	1905	C	N1-C2-O2	5.23	122.04	118.90
53	A2	1079	C	N1-C2-O2	5.23	122.04	118.90
29	A1	2335	G	C6-C5-N7	-5.23	127.26	130.40
29	A1	167	G	N3-C4-N9	5.22	129.13	126.00
29	A1	479	C	N3-C4-C5	5.22	123.99	121.90
29	A1	1445	U	N3-C2-O2	-5.22	118.54	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	1777	C	C6-N1-C2	-5.22	118.21	120.30
29	A1	2794	U	N3-C2-O2	-5.22	118.54	122.20
53	A2	1306	C	C5-C6-N1	5.22	123.61	121.00
29	A1	2532	A	C5-N7-C8	-5.22	101.29	103.90
53	A2	307	C	N1-C2-O2	5.22	122.03	118.90
53	A2	511	C	C6-N1-C2	-5.22	118.21	120.30
29	A1	1727	G	N1-C6-O6	5.22	123.03	119.90
29	A1	1873	G	C8-N9-C1'	-5.22	120.22	127.00
53	A2	219	C	N3-C2-O2	-5.22	118.25	121.90
53	A2	937	U	N3-C2-O2	-5.22	118.55	122.20
53	A2	608	G	C6-C5-N7	-5.22	127.27	130.40
53	A2	1470	A	O4'-C1'-N9	5.22	112.37	108.20
29	A1	2213	U	C5-C6-N1	5.22	125.31	122.70
53	A2	1352	G	N9-C4-C5	-5.22	103.31	105.40
53	A2	472	C	C5-C6-N1	5.21	123.61	121.00
5	G1	98	LEU	CA-CB-CG	5.21	127.29	115.30
29	A1	965	A	N9-C4-C5	-5.21	103.72	105.80
29	A1	1187	C	C2-N1-C1'	5.21	124.53	118.80
29	A1	1673	C	N1-C2-O2	5.21	122.03	118.90
29	A1	2710	U	C2-N1-C1'	5.21	123.95	117.70
29	A1	841	G	N3-C4-N9	5.21	129.13	126.00
29	A1	1852	A	P-O3'-C3'	5.21	125.95	119.70
29	A1	2703	U	P-O3'-C3'	5.21	125.95	119.70
29	A1	2301	A	N3-C4-C5	5.20	130.44	126.80
53	A2	406	A	O5'-P-OP2	-5.20	101.02	105.70
53	A2	1091	C	N3-C2-O2	-5.20	118.26	121.90
29	A1	675	G	C4-C5-N7	5.20	112.88	110.80
29	A1	841	G	N3-C4-C5	-5.20	126.00	128.60
29	A1	1251	A	O4'-C1'-N9	5.20	112.36	108.20
29	A1	1592	C	C5-C6-N1	5.20	123.60	121.00
29	A1	1648	C	C2-N1-C1'	5.20	124.52	118.80
29	A1	2808	G	N7-C8-N9	5.20	115.70	113.10
53	A2	1162	G	O4'-C1'-N9	5.20	112.36	108.20
29	A1	826	A	N1-C6-N6	-5.20	115.48	118.60
29	A1	2812	C	C2-N1-C1'	5.20	124.52	118.80
53	A2	1260	A	N1-C6-N6	-5.20	115.48	118.60
29	A1	1919	C	N1-C2-O2	5.19	122.02	118.90
53	A2	483	G	C6-C5-N7	-5.19	127.28	130.40
53	A2	483	G	N3-C4-N9	5.19	129.12	126.00
29	A1	2054	A	O4'-C1'-N9	5.19	112.35	108.20
29	A1	2487	U	N3-C2-O2	-5.19	118.57	122.20
53	A2	1020	C	C6-N1-C2	-5.19	118.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	37	C	C6-N1-C2	-5.19	118.22	120.30
53	A2	248	U	N1-C2-O2	5.19	126.43	122.80
29	A1	513	C	C6-N1-C2	-5.19	118.23	120.30
53	A2	131	C	C6-N1-C2	-5.19	118.22	120.30
53	A2	138	G	N1-C6-O6	-5.18	116.79	119.90
53	A2	1360	C	C2-N3-C4	5.18	122.49	119.90
29	A1	1912	G	C4-N9-C1'	5.18	133.23	126.50
29	A1	2216	G	C8-N9-C1'	-5.18	120.27	127.00
29	A1	568	C	C5-C6-N1	5.17	123.59	121.00
29	A1	2322	G	C4-N9-C1'	5.17	133.22	126.50
53	A2	355	A	N1-C6-N6	5.17	121.70	118.60
53	A2	1360	C	N3-C2-O2	5.17	125.52	121.90
29	A1	2715	C	P-O3'-C3'	5.17	125.90	119.70
29	A1	2012	C	C6-N1-C2	-5.17	118.23	120.30
29	A1	2142	U	N1-C2-O2	5.17	126.42	122.80
53	A2	679	A	N7-C8-N9	5.17	116.38	113.80
53	A2	749	A	C5-C6-N6	-5.17	119.56	123.70
53	A2	1361	G	N1-C2-N2	-5.17	111.55	116.20
29	A1	556	A	C4-N9-C1'	5.17	135.60	126.30
53	A2	562	G	C4-N9-C1'	-5.17	119.79	126.50
53	A2	907	C	N3-C2-O2	-5.16	118.29	121.90
29	A1	36	G	C6-C5-N7	-5.16	127.30	130.40
29	A1	1167	C	N1-C2-O2	5.16	122.00	118.90
53	A2	267	C	N1-C2-O2	5.16	122.00	118.90
53	A2	519	C	C2-N1-C1'	5.16	124.48	118.80
53	A2	922	G	C4-C5-N7	5.16	112.86	110.80
29	A1	272	U	C2-N1-C1'	5.16	123.89	117.70
29	A1	1923	G	N3-C2-N2	-5.16	116.29	119.90
53	A2	1413	C	N1-C2-O2	5.16	121.99	118.90
29	A1	964	G	C5-C6-O6	-5.15	125.51	128.60
53	A2	243	C	C2-N1-C1'	5.15	124.47	118.80
53	A2	1352	G	N3-C4-N9	5.15	129.09	126.00
29	A1	259	U	N1-C2-O2	5.15	126.41	122.80
29	A1	826	A	C2-N3-C4	5.15	113.18	110.60
29	A1	1825	G	C2-N3-C4	-5.15	109.32	111.90
53	A2	535	U	C6-N1-C2	-5.15	117.91	121.00
53	A2	1005	C	OP1-P-O3'	5.15	116.53	105.20
53	A2	1386	C	C6-N1-C2	-5.15	118.24	120.30
29	A1	2728	A	C4-C5-N7	5.15	113.27	110.70
53	A2	1191	C	C6-N1-C2	-5.15	118.24	120.30
29	A1	2491	C	C6-N1-C2	-5.15	118.24	120.30
53	A2	270	G	C8-N9-C1'	-5.15	120.31	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	612	G	C8-N9-C1'	-5.15	120.31	127.00
29	A1	1114	U	C5-C6-N1	5.14	125.27	122.70
29	A1	1251	A	C5-N7-C8	-5.14	101.33	103.90
29	A1	1539	G	N3-C4-C5	-5.14	126.03	128.60
29	A1	1112	C	C2-N1-C1'	5.14	124.46	118.80
29	A1	938	C	C6-N1-C2	-5.14	118.24	120.30
53	A2	746	G	N1-C2-N2	-5.14	111.58	116.20
53	A2	859	C	C5-C6-N1	5.14	123.57	121.00
29	A1	1494	C	C2-N1-C1'	5.14	124.45	118.80
30	B1	39	C	N3-C2-O2	-5.14	118.30	121.90
29	A1	2250	C	N1-C2-O2	5.14	121.98	118.90
29	A1	137	G	C8-N9-C1'	-5.13	120.33	127.00
29	A1	648	A	C4-C5-N7	5.13	113.27	110.70
53	A2	1114	C	C2-N1-C1'	5.13	124.45	118.80
29	A1	813	A	O4'-C1'-N9	5.13	112.31	108.20
53	A2	408	G	N3-C4-N9	5.13	129.08	126.00
29	A1	1045	G	C6-C5-N7	-5.13	127.32	130.40
29	A1	2393	G	C4-N9-C1'	5.13	133.17	126.50
53	A2	172	C	C2-N1-C1'	5.13	124.44	118.80
29	A1	661	C	C6-N1-C2	-5.13	118.25	120.30
53	A2	1509	U	C5-C6-N1	5.13	125.26	122.70
29	A1	1676	G	N9-C4-C5	-5.13	103.35	105.40
29	A1	2207	C	N1-C2-O2	5.12	121.97	118.90
53	A2	263	C	N3-C2-O2	-5.12	118.31	121.90
53	A2	753	C	N3-C2-O2	-5.12	118.31	121.90
53	A2	501	C	C5-C6-N1	5.12	123.56	121.00
53	A2	562	G	C4-C5-N7	-5.12	108.75	110.80
53	A2	1020	C	C5-C6-N1	5.12	123.56	121.00
29	A1	2742	G	C4-N9-C1'	5.12	133.15	126.50
53	A2	101	G	C5-N7-C8	-5.12	101.74	104.30
53	A2	376	C	N3-C2-O2	-5.12	118.32	121.90
29	A1	2154	U	O4'-C1'-N1	5.11	112.29	108.20
29	A1	2252	G	C4-N9-C1'	5.11	133.15	126.50
53	A2	1227	C	N3-C2-O2	-5.11	118.32	121.90
29	A1	474	G	C4-N9-C1'	5.11	133.14	126.50
29	A1	678	G	C4-C5-N7	-5.11	108.76	110.80
29	A1	1278	C	C6-N1-C2	-5.11	118.26	120.30
29	A1	1917	C	C6-N1-C2	-5.11	118.26	120.30
29	A1	323	G	C5-N7-C8	-5.11	101.75	104.30
53	A2	29	G	C8-N9-C4	-5.11	104.36	106.40
53	A2	1368	G	C6-C5-N7	-5.11	127.34	130.40
29	A1	96	C	N3-C2-O2	-5.11	118.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	493	G	C6-C5-N7	-5.10	127.34	130.40
29	A1	661	C	C2-N1-C1'	5.10	124.41	118.80
29	A1	2812	C	C6-N1-C2	-5.10	118.26	120.30
29	A1	796	U	O5'-P-OP2	-5.10	101.11	105.70
53	A2	214	C	N1-C2-O2	5.10	121.96	118.90
29	A1	2377	C	C6-N1-C2	-5.10	118.26	120.30
53	A2	1410	A	C4-C5-N7	5.10	113.25	110.70
53	A2	29	G	N7-C8-N9	5.09	115.65	113.10
53	A2	261	G	P-O3'-C3'	5.09	125.81	119.70
29	A1	2001	A	C5-N7-C8	-5.09	101.36	103.90
29	A1	2580	A	OP2-P-O3'	5.09	116.39	105.20
29	A1	2774	G	C8-N9-C1'	-5.09	120.39	127.00
29	A1	1718	A	O4'-C1'-N9	5.09	112.27	108.20
53	A2	210	U	C5-C6-N1	5.09	125.24	122.70
29	A1	141	C	N3-C2-O2	-5.08	118.34	121.90
29	A1	671	A	OP1-P-OP2	5.08	127.23	119.60
29	A1	1345	C	N3-C2-O2	-5.08	118.34	121.90
29	A1	1725	A	C5-N7-C8	-5.08	101.36	103.90
53	A2	721	C	C5-C6-N1	5.08	123.54	121.00
53	A2	1422	C	N1-C2-O2	5.08	121.95	118.90
29	A1	210	G	N3-C4-N9	5.08	129.05	126.00
29	A1	2662	C	C6-N1-C2	-5.08	118.27	120.30
29	A1	769	C	C6-N1-C2	-5.08	118.27	120.30
53	A2	323	C	N1-C2-O2	5.08	121.95	118.90
29	A1	268	C	C6-N1-C2	-5.08	118.27	120.30
29	A1	1243	C	C5-C6-N1	5.08	123.54	121.00
53	A2	276	G	C8-N9-C1'	-5.08	120.40	127.00
53	A2	860	C	N3-C2-O2	-5.08	118.35	121.90
29	A1	690	C	C6-N1-C2	-5.08	118.27	120.30
29	A1	1540	G	O4'-C1'-N9	5.08	112.26	108.20
29	A1	1987	U	C5-C6-N1	5.08	125.24	122.70
29	A1	2640	C	C5-C6-N1	5.07	123.54	121.00
53	A2	1373	U	C6-N1-C1'	5.07	128.30	121.20
53	A2	1438	G	N3-C4-C5	5.07	131.13	128.60
53	A2	1492	C	N1-C2-O2	5.07	121.94	118.90
53	A2	323	C	C2-N1-C1'	5.07	124.38	118.80
29	A1	119	G	N3-C4-N9	5.07	129.04	126.00
29	A1	1912	G	N7-C8-N9	5.07	115.63	113.10
29	A1	2017	U	O5'-P-OP1	-5.07	101.14	105.70
29	A1	2316	G	C4-C5-N7	5.07	112.83	110.80
29	A1	2406	A	C6-C5-N7	-5.07	128.75	132.30
29	A1	2598	U	N3-C2-O2	-5.07	118.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	408	G	P-O3'-C3'	5.07	125.78	119.70
53	A2	1042	C	N1-C2-O2	5.07	121.94	118.90
29	A1	670	A	O3'-P-O5'	5.06	113.62	104.00
29	A1	1233	G	C8-N9-C4	-5.06	104.38	106.40
29	A1	1702	G	N9-C4-C5	-5.06	103.38	105.40
29	A1	248	G	C8-N9-C4	-5.06	104.38	106.40
29	A1	618	G	C6-C5-N7	-5.06	127.36	130.40
29	A1	2350	A	C6-C5-N7	-5.06	128.76	132.30
29	A1	1777	C	N3-C2-O2	-5.06	118.36	121.90
29	A1	2067	C	C5-C6-N1	5.06	123.53	121.00
53	A2	307	C	N3-C2-O2	-5.06	118.36	121.90
29	A1	379	G	N3-C4-C5	-5.05	126.07	128.60
29	A1	474	G	C8-N9-C1'	-5.05	120.43	127.00
29	A1	536	C	C6-N1-C2	5.05	122.32	120.30
29	A1	2282	A	C8-N9-C4	-5.05	103.78	105.80
53	A2	148	C	O4'-C1'-N1	5.05	112.24	108.20
29	A1	1265	C	C6-N1-C2	-5.05	118.28	120.30
53	A2	1364	C	N1-C2-O2	5.05	121.93	118.90
53	A2	1089	C	N3-C2-O2	-5.05	118.37	121.90
53	A2	1124	G	N3-C4-C5	-5.05	126.08	128.60
29	A1	2166	C	C6-N1-C2	-5.05	118.28	120.30
29	A1	2249	G	C4-N9-C1'	5.05	133.06	126.50
29	A1	104	C	N3-C2-O2	-5.04	118.37	121.90
29	A1	479	C	C2-N3-C4	-5.04	117.38	119.90
29	A1	1053	C	C6-N1-C2	-5.04	118.28	120.30
29	A1	1540	G	N9-C1'-C2'	-5.04	106.45	112.00
29	A1	1608	G	O4'-C1'-N9	5.04	112.23	108.20
30	B1	66	C	N3-C2-O2	-5.04	118.37	121.90
53	A2	1450	A	C5-N7-C8	-5.04	101.38	103.90
53	A2	808	G	C8-N9-C4	5.04	108.42	106.40
53	A2	1363	U	N1-C2-O2	5.04	126.33	122.80
29	A1	186	A	C2-N3-C4	5.04	113.12	110.60
29	A1	1841	U	C5-C6-N1	5.04	125.22	122.70
29	A1	287	C	C2-N1-C1'	5.04	124.34	118.80
29	A1	2417	C	N1-C2-O2	5.04	121.92	118.90
53	A2	1144	C	P-O3'-C3'	5.04	125.75	119.70
29	A1	2637	G	C4-C5-N7	5.04	112.81	110.80
29	A1	691	A	C2-N3-C4	5.04	113.12	110.60
29	A1	621	G	N3-C4-N9	5.03	129.02	126.00
29	A1	288	G	OP2-P-O3'	5.03	116.27	105.20
29	A1	877	U	N1-C2-O2	5.03	126.32	122.80
29	A1	1684	G	C4-N9-C1'	5.03	133.04	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	1357	G	C8-N9-C4	-5.03	104.39	106.40
29	A1	448	C	N1-C2-O2	5.03	121.92	118.90
29	A1	637	C	N3-C2-O2	-5.03	118.38	121.90
53	A2	1091	C	N1-C2-O2	5.03	121.92	118.90
29	A1	73	A	N3-C4-C5	5.03	130.32	126.80
29	A1	1119	G	C8-N9-C1'	-5.03	120.47	127.00
29	A1	1769	A	C2-N3-C4	5.03	113.11	110.60
29	A1	2494	C	C5-C6-N1	5.03	123.51	121.00
53	A2	807	C	C6-N1-C2	-5.03	118.29	120.30
29	A1	2335	G	N3-C4-N9	5.02	129.01	126.00
53	A2	513	G	C4-C5-N7	5.02	112.81	110.80
53	A2	1457	G	C8-N9-C4	-5.02	104.39	106.40
29	A1	883	C	C5-C6-N1	5.02	123.51	121.00
53	A2	1120	G	O4'-C1'-N9	5.02	112.22	108.20
29	A1	1393	C	C5-C6-N1	5.02	123.51	121.00
29	A1	2808	G	N3-C4-C5	-5.02	126.09	128.60
53	A2	440	G	C6-C5-N7	-5.02	127.39	130.40
53	A2	1110	C	C2-N1-C1'	-5.02	113.28	118.80
29	A1	1445	U	N1-C2-O2	5.02	126.31	122.80
29	A1	1280	G	C4-C5-N7	5.01	112.81	110.80
29	A1	1756	G	C6-C5-N7	-5.01	127.39	130.40
53	A2	262	C	O5'-P-OP1	-5.01	101.19	105.70
29	A1	92	C	C6-N1-C2	-5.01	118.30	120.30
53	A2	615	A	C5-N7-C8	-5.01	101.39	103.90
53	A2	974	U	C6-N1-C2	-5.01	117.99	121.00
53	A2	663	C	P-O3'-C3'	5.01	125.71	119.70
29	A1	899	C	N3-C2-O2	-5.00	118.40	121.90
29	A1	637	C	N1-C2-O2	5.00	121.90	118.90
29	A1	2406	A	N7-C8-N9	5.00	116.30	113.80
29	A1	2476	U	N1-C2-O2	5.00	126.30	122.80
29	A1	2607	U	C6-N1-C2	-5.00	118.00	121.00
53	A2	1358	U	N3-C2-O2	-5.00	118.70	122.20
29	A1	1632	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	B2	123	ALA	Peptide
32	B2	94	ASN	Peptide
1	C1	33	LEU	Peptide
33	C2	166	GLU	Peptide

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Mol	Chain	Res	Type	Group
33	C2	79	ARG	Peptide
2	D1	61	ARG	Peptide
34	D2	150	GLU	Peptide
34	D2	208	SER	Peptide
34	D2	31	CYS	Peptide
3	E1	24	LEU	Peptide
4	F1	114	ILE	Peptide
5	G1	89	ILE	Peptide
37	G2	142	GLU	Peptide
37	G2	15	ASP	Peptide
39	I2	91	ASP	Peptide
40	J2	57	LYS	Peptide
9	K1	12	ALA	Peptide
9	K1	35	HIS	Peptide
42	L2	26	ALA	Peptide
42	L2	47	LYS	Peptide
43	M2	19	LEU	Peptide
43	M2	8	GLU	Peptide
14	P1	91	ASP	Peptide
15	Q1	79	VAL	Peptide
17	S1	31	HIS	Peptide
49	S2	68	GLY	Peptide
18	T1	94	LYS	Peptide
18	T1	95	LYS	Peptide
19	U1	52	SER	Peptide
51	U2	24	ARG	Peptide
52	V2	35	GLU	Peptide
52	V2	52	LYS	Peptide
24	Z1	43	TYR	Peptide
26	b1	14	THR	Peptide
26	b1	44	ARG	Peptide
28	d1	34	TRP	Peptide
28	d1	40	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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	C1	2116	0	2194	20	0
2	D1	1569	0	1634	14	0
3	E1	1628	0	1680	17	0
4	F1	1474	0	1535	30	0
5	G1	1308	0	1382	29	0
6	H1	383	0	410	4	0
7	I1	1105	0	1180	8	0
8	J1	933	0	996	14	0
9	K1	1145	0	1228	17	0
10	L1	1122	0	1179	11	0
11	M1	960	0	1021	12	0
12	N1	882	0	943	17	0
13	O1	1142	0	1202	20	0
14	P1	964	0	1022	8	0
15	Q1	779	0	852	4	0
16	R1	900	0	964	10	0
17	S1	726	0	778	2	0
18	T1	786	0	878	15	0
19	U1	1429	0	1454	18	0
20	V1	613	0	633	6	0
21	W1	763	0	848	6	0
22	X1	581	0	629	5	0
23	Y1	469	0	518	2	0
24	Z1	516	0	514	15	0
25	a1	459	0	479	0	0
26	b1	390	0	404	0	0
27	c1	430	0	480	0	0
28	d1	489	0	560	0	0
29	A1	62707	0	31613	271	0
30	B1	2617	0	1328	12	0
31	e1	299	0	326	0	0
32	B2	1925	0	1975	27	0
33	C2	1613	0	1677	15	0
34	D2	1703	0	1765	19	0
35	E2	1156	0	1213	9	0
36	F2	843	0	857	12	0
37	G2	1257	0	1296	22	0
38	H2	1116	0	1177	10	0
39	I2	1010	0	1037	24	0
40	J2	802	0	849	13	0
41	K2	879	0	899	13	0
42	L2	976	0	1062	13	0
43	M2	934	0	992	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	N2	492	0	533	5	0
45	O2	734	0	771	6	0
46	P2	706	0	725	4	0
47	Q2	835	0	904	14	0
48	R2	515	0	568	8	0
49	S2	625	0	636	12	0
50	T2	763	0	861	7	0
51	U2	218	0	234	5	0
52	V2	983	0	1008	27	0
53	A2	32369	0	16339	365	0
All	All	144138	0	98242	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1080) 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)
53:A2:1110:C:C5	53:A2:1110:C:C6	1.92	1.57
53:A2:216:C:C6	53:A2:216:C:C5	1.89	1.55
53:A2:216:C:C5	53:A2:216:C:C4	2.03	1.47
53:A2:1110:C:C5	53:A2:1110:C:C4	2.06	1.41
53:A2:136:G:N2	53:A2:216:C:N3	1.78	1.32
53:A2:775:A:O2'	53:A2:776:U:C5'	1.77	1.29
53:A2:216:C:C6	53:A2:216:C:N1	2.00	1.28
53:A2:1110:C:N3	53:A2:1121:G:N2	1.79	1.28
53:A2:717:G:C4	53:A2:717:G:C5	2.21	1.27
53:A2:1110:C:C6	53:A2:1110:C:N1	2.02	1.27
53:A2:700:C:N3	53:A2:700:C:C6	2.02	1.26
53:A2:216:C:N1	53:A2:216:C:C2	2.05	1.24
53:A2:1110:C:N1	53:A2:1110:C:C2	2.09	1.20
53:A2:717:G:C5	53:A2:717:G:C6	2.33	1.15
53:A2:700:C:N3	53:A2:717:G:N1	1.95	1.12
53:A2:775:A:O2'	53:A2:776:U:H5''	0.93	1.11
53:A2:1110:C:C4	53:A2:1110:C:N3	2.22	1.08
53:A2:216:C:C4	53:A2:216:C:N3	2.22	1.07
53:A2:700:C:N3	53:A2:700:C:C4	2.23	1.06
53:A2:1110:C:N3	53:A2:1110:C:C2	2.25	1.04
53:A2:216:C:N3	53:A2:216:C:C2	2.27	1.02
52:V2:99:TYR:CD1	52:V2:103:ARG:NH1	2.32	0.98
53:A2:1110:C:C2	53:A2:1121:G:N2	2.32	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A2:136:G:N2	53:A2:216:C:C2	2.33	0.97
53:A2:717:G:N3	53:A2:717:G:C2	2.33	0.96
53:A2:1110:C:C4	53:A2:1121:G:N2	2.36	0.94
53:A2:717:G:C4	53:A2:717:G:N3	2.37	0.93
53:A2:136:G:N2	53:A2:216:C:C4	2.37	0.92
53:A2:700:C:N3	53:A2:717:G:C6	2.41	0.88
53:A2:775:A:C2'	53:A2:776:U:C5'	2.52	0.87
53:A2:775:A:C2'	53:A2:776:U:H5''	2.05	0.86
53:A2:700:C:N3	53:A2:717:G:C2	2.44	0.85
53:A2:136:G:C2	53:A2:216:C:N3	2.45	0.84
53:A2:136:G:C2	53:A2:216:C:C2	2.66	0.84
53:A2:1110:C:N3	53:A2:1121:G:C2	2.48	0.81
53:A2:717:G:N1	53:A2:717:G:C2	2.48	0.81
53:A2:775:A:HO2'	53:A2:776:U:H5''	0.99	0.80
39:I2:7:THR:H	39:I2:83:ARG:HG3	1.45	0.79
53:A2:700:C:C6	53:A2:717:G:C4	2.71	0.79
53:A2:1110:C:C2	53:A2:1121:G:C2	2.72	0.78
52:V2:99:TYR:HD1	52:V2:103:ARG:HH11	1.33	0.76
52:V2:99:TYR:CE1	52:V2:103:ARG:NH1	2.53	0.75
53:A2:136:G:C2	53:A2:216:C:C4	2.76	0.74
32:B2:84:GLU:HG2	32:B2:87:ARG:HH21	1.50	0.74
53:A2:700:C:C4	53:A2:717:G:N1	2.56	0.73
53:A2:700:C:N1	53:A2:717:G:C4	2.56	0.73
53:A2:700:C:C6	53:A2:717:G:C2	2.77	0.73
52:V2:31:TYR:CD1	52:V2:31:TYR:N	2.56	0.72
52:V2:31:TYR:N	52:V2:31:TYR:HD1	1.87	0.72
53:A2:700:C:C4	53:A2:717:G:C6	2.78	0.72
53:A2:1110:C:C4	53:A2:1121:G:C2	2.77	0.72
53:A2:1387:G:H1	53:A2:1473:C:H42	1.38	0.72
53:A2:38:G:H22	53:A2:392:A:H5''	1.55	0.71
53:A2:717:G:C6	53:A2:717:G:N1	2.59	0.71
53:A2:641:G:H1	53:A2:730:C:H42	1.38	0.70
34:D2:35:ARG:NH2	53:A2:408:G:N7	2.40	0.69
34:D2:122:ARG:NH1	53:A2:399:U:OP1	2.25	0.69
29:A1:1893:G:H1	29:A1:1906:C:H42	1.41	0.69
53:A2:700:C:C6	53:A2:717:G:N3	2.61	0.68
53:A2:1110:C:N1	53:A2:1121:G:N2	2.40	0.68
13:O1:51:ARG:NH2	29:A1:2699:G:OP2	2.27	0.68
53:A2:136:G:N2	53:A2:216:C:N1	2.41	0.68
19:U1:72:ARG:HG3	19:U1:73:GLN:HG3	1.76	0.68
53:A2:136:G:N1	53:A2:216:C:N3	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A2:576:G:N7	53:A2:630:C:N4	2.41	0.67
19:U1:76:LEU:HA	19:U1:83:PRO:HA	1.76	0.67
29:A1:1628:A:OP2	29:A1:1630:G:N2	2.27	0.67
29:A1:1824:A:N6	29:A1:1861:G:O2'	2.28	0.67
53:A2:1110:C:C6	53:A2:1121:G:N2	2.63	0.67
53:A2:700:C:N3	53:A2:717:G:C5	2.63	0.67
53:A2:1110:C:C5	53:A2:1121:G:N2	2.63	0.67
32:B2:21:ARG:HE	32:B2:39:ILE:HG12	1.58	0.67
52:V2:30:ARG:HB2	52:V2:31:TYR:CE1	2.29	0.67
16:R1:42:ARG:HB2	29:A1:2034:G:H5''	1.76	0.66
29:A1:313:C:OP2	29:A1:380:G:N2	2.27	0.66
53:A2:700:C:N1	53:A2:717:G:C2	2.63	0.66
53:A2:216:C:C6	53:A2:216:C:H2'	2.31	0.66
53:A2:136:G:N2	53:A2:216:C:C5	2.64	0.66
18:T1:47:LYS:NZ	29:A1:509:G:OP2	2.28	0.66
45:O2:23:GLY:HA3	53:A2:733:G:H21	1.60	0.66
11:M1:12:ARG:O	11:M1:17:ARG:NH1	2.29	0.65
53:A2:136:G:N2	53:A2:216:C:C6	2.64	0.65
23:Y1:40:THR:HG22	23:Y1:42:ALA:H	1.61	0.65
29:A1:10:G:H2'	29:A1:11:G:H8	1.62	0.65
13:O1:6:LEU:H	13:O1:9:LEU:HB2	1.62	0.65
29:A1:2715:C:H3'	29:A1:2716:U:H5''	1.79	0.65
32:B2:128:GLU:HG2	32:B2:129:GLU:HG2	1.78	0.65
53:A2:1110:C:C6	53:A2:1121:G:C2	2.85	0.65
53:A2:1007:C:N3	53:A2:1014:G:N1	2.44	0.64
4:F1:68:PRO:HB3	4:F1:92:VAL:HB	1.79	0.64
18:T1:81:LYS:HB2	18:T1:96:ILE:HG22	1.78	0.64
53:A2:982:A:N7	53:A2:1005:C:N4	2.43	0.64
53:A2:700:C:C6	53:A2:717:G:C5	2.85	0.64
53:A2:1005:C:N3	53:A2:1018:G:N2	2.45	0.64
8:J1:1:MET:N	29:A1:1714:A:O2'	2.31	0.64
53:A2:136:G:C2	53:A2:216:C:N1	2.66	0.64
4:F1:41:GLN:HE21	4:F1:90:LEU:HD12	1.63	0.64
15:Q1:80:GLN:O	15:Q1:82:ARG:NH1	2.31	0.64
53:A2:975:G:O2'	53:A2:1025:C:O2	2.16	0.64
29:A1:931:G:N2	29:A1:933:C:O2	2.31	0.63
43:M2:79:LYS:HA	43:M2:82:MET:HB2	1.81	0.63
29:A1:682:A:N6	29:A1:700:G:OP1	2.31	0.63
29:A1:1068:A:N1	29:A1:1188:U:O2'	2.32	0.63
53:A2:136:G:C2	53:A2:216:C:C6	2.86	0.63
9:K1:55:ARG:HH12	29:A1:2372:G:H1	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A2:1006:C:H42	53:A2:1015:G:H1	1.46	0.63
9:K1:62:LEU:H	29:A1:2407:A:H4'	1.64	0.63
21:W1:72:GLU:O	21:W1:76:ARG:NH1	2.32	0.63
53:A2:700:C:N1	53:A2:717:G:N3	2.47	0.63
12:N1:15:ARG:NH1	30:B1:11:G:OP1	2.32	0.63
34:D2:49:ARG:NH2	53:A2:492:A:OP2	2.32	0.63
1:C1:99:ASP:O	29:A1:1548:G:N2	2.32	0.62
2:D1:8:LYS:O	13:O1:2:ASN:ND2	2.32	0.62
19:U1:18:LEU:HB3	19:U1:23:LYS:HB2	1.79	0.62
37:G2:115:ARG:NH1	53:A2:1220:A:O2'	2.32	0.62
53:A2:1110:C:N1	53:A2:1121:G:C2	2.67	0.62
53:A2:700:C:C2	53:A2:717:G:N1	2.67	0.62
1:C1:13:ARG:HH21	29:A1:777:G:H4'	1.63	0.62
7:I1:7:LYS:NZ	29:A1:566:G:OP1	2.32	0.62
36:F2:92:LYS:O	36:F2:94:GLN:NE2	2.33	0.62
13:O1:85:LYS:NZ	13:O1:87:ASP:OD2	2.28	0.62
29:A1:314:A:N6	29:A1:376:G:O2'	2.32	0.62
53:A2:80:U:OP2	53:A2:84:C:N4	2.33	0.62
36:F2:94:GLN:OE1	48:R2:32:ARG:NH2	2.32	0.62
39:I2:128:ARG:HH11	52:V2:4:TYR:HE2	1.47	0.62
53:A2:86:C:N4	53:A2:92:U:O4	2.33	0.62
53:A2:203:A:H8	53:A2:204:G:H1'	1.65	0.62
34:D2:73:ARG:NH2	53:A2:530:A:OP1	2.33	0.62
53:A2:749:A:O2'	53:A2:750:A:N7	2.32	0.62
53:A2:924:G:N2	53:A2:1216:U:O2	2.33	0.62
4:F1:40:ASN:ND2	4:F1:90:LEU:O	2.32	0.61
12:N1:23:ARG:NH1	12:N1:85:VAL:O	2.32	0.61
47:Q2:81:ARG:NH2	53:A2:630:C:OP1	2.33	0.61
53:A2:700:C:H1'	53:A2:717:G:N3	2.16	0.61
29:A1:2157:G:H1'	29:A1:2181:G:H1	1.65	0.61
39:I2:17:VAL:HG22	39:I2:63:ILE:HG12	1.81	0.61
1:C1:35:LYS:NZ	1:C1:102:LYS:O	2.33	0.61
18:T1:92:ASN:HB2	18:T1:95:LYS:HZ3	1.66	0.61
43:M2:76:ALA:HA	43:M2:79:LYS:HB2	1.82	0.61
1:C1:45:ASN:OD1	1:C1:45:ASN:N	2.33	0.61
13:O1:62:THR:HG22	13:O1:75:ILE:HG12	1.82	0.61
1:C1:88:ARG:NH2	29:A1:1850:G:OP1	2.34	0.61
3:E1:63:LYS:NZ	3:E1:65:TRP:O	2.33	0.61
29:A1:38:A:N6	29:A1:468:G:O6	2.33	0.61
34:D2:13:ARG:NH1	34:D2:38:TYR:O	2.34	0.61
16:R1:70:TYR:OH	16:R1:72:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G1:54:ARG:NH1	5:G1:56:SER:O	2.34	0.60
18:T1:81:LYS:HB3	18:T1:84:ARG:HH12	1.65	0.60
29:A1:2213:U:N3	29:A1:2214:G:N7	2.50	0.60
1:C1:146:GLU:HB2	1:C1:189:CYS:HB3	1.83	0.60
21:W1:52:ARG:HH21	21:W1:55:GLY:HA2	1.65	0.60
53:A2:700:C:C2	53:A2:717:G:C6	2.89	0.60
29:A1:1120:C:O2	29:A1:1140:C:N4	2.34	0.60
53:A2:986:C:N4	53:A2:1000:G:N3	2.42	0.60
19:U1:112:ARG:HB3	19:U1:177:PRO:HD3	1.83	0.60
52:V2:68:ARG:NH1	53:A2:943:G:N7	2.50	0.60
8:J1:23:ARG:NH1	29:A1:2576:U:O2	2.35	0.60
29:A1:2149:G:O2'	29:A1:2186:G:N2	2.34	0.60
32:B2:127:ILE:HG23	32:B2:135:GLN:HA	1.84	0.60
53:A2:136:G:C2	53:A2:216:C:C5	2.90	0.60
29:A1:151:C:H42	29:A1:165:G:H1	1.49	0.60
29:A1:1632:A:O2'	29:A1:1634:A:N1	2.35	0.60
42:L2:117:ARG:NH2	53:A2:484:C:OP1	2.35	0.60
29:A1:175:U:H3	29:A1:201:A:H61	1.50	0.59
29:A1:2145:G:O6	29:A1:2199:C:N4	2.35	0.59
43:M2:78:ILE:O	43:M2:82:MET:N	2.30	0.59
51:U2:12:LYS:NZ	53:A2:1307:C:OP1	2.33	0.59
53:A2:94:A:H2'	53:A2:95:G:H8	1.68	0.59
13:O1:107:ASP:N	13:O1:107:ASP:OD1	2.32	0.59
29:A1:504:G:N1	29:A1:507:A:OP2	2.35	0.59
29:A1:1845:A:H2'	29:A1:1846:G:H8	1.66	0.59
32:B2:15:VAL:O	32:B2:204:ASN:ND2	2.36	0.59
47:Q2:91:ARG:HH12	53:A2:275:C:H41	1.51	0.59
53:A2:1247:G:N2	53:A2:1250:A:OP2	2.36	0.59
24:Z1:28:LYS:HG2	24:Z1:31:ILE:HD11	1.84	0.59
32:B2:48:MET:SD	32:B2:48:MET:N	2.76	0.59
53:A2:1119:C:O2'	53:A2:1120:G:N2	2.33	0.59
53:A2:664:C:N4	53:A2:692:G:O6	2.36	0.59
53:A2:1237:A:H62	53:A2:1258:C:H3'	1.67	0.59
53:A2:700:C:N1	53:A2:717:G:C5	2.70	0.59
32:B2:110:GLN:HA	32:B2:113:HIS:HD2	1.68	0.58
32:B2:130:ARG:O	32:B2:135:GLN:NE2	2.33	0.58
29:A1:931:G:H21	29:A1:932:G:H1	1.50	0.58
29:A1:2088:C:O2'	29:A1:2265:G:N2	2.36	0.58
30:B1:85:G:N2	30:B1:98:U:OP1	2.36	0.58
53:A2:967:C:H5	53:A2:1197:G:H21	1.49	0.58
53:A2:1110:C:C5	53:A2:1121:G:C2	2.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A2:1139:A:O4'	53:A2:1162:G:N2	2.35	0.58
42:L2:114:LYS:HB2	53:A2:521:G:H5'	1.84	0.58
53:A2:1117:U:H2'	53:A2:1119:C:H1'	1.85	0.58
29:A1:1465:C:H41	29:A1:1630:G:H21	1.50	0.58
3:E1:41:LEU:O	29:A1:471:A:N6	2.36	0.58
29:A1:1102:A:H2'	29:A1:1103:G:H8	1.68	0.58
29:A1:1695:C:H5''	29:A1:1696:G:H5''	1.85	0.58
53:A2:1054:G:O6	53:A2:1084:A:N6	2.35	0.58
8:J1:2:ILE:HB	8:J1:33:ALA:HB3	1.86	0.58
29:A1:1137:G:N2	29:A1:1138:U:O4	2.37	0.58
29:A1:1222:U:O2	29:A1:1225:C:N4	2.36	0.58
37:G2:76:ARG:NH2	37:G2:156:TRP:O	2.36	0.58
53:A2:153:G:N2	53:A2:156:A:OP2	2.37	0.58
53:A2:1203:G:OP2	53:A2:1303:C:N4	2.37	0.58
29:A1:682:A:O2'	29:A1:701:A:N6	2.37	0.58
29:A1:1576:A:OP2	29:A1:1591:A:N6	2.35	0.58
43:M2:76:ALA:O	43:M2:80:ARG:N	2.36	0.58
33:C2:57:ILE:HG12	33:C2:66:VAL:HG22	1.85	0.58
33:C2:177:THR:HG22	33:C2:179:ARG:H	1.69	0.58
8:J1:97:ARG:NH1	53:A2:334:C:OP2	2.36	0.57
53:A2:74:C:H2'	53:A2:75:G:H8	1.69	0.57
21:W1:2:SER:OG	21:W1:3:LYS:N	2.37	0.57
37:G2:30:ILE:O	53:A2:1221:U:N3	2.37	0.57
53:A2:700:C:C6	53:A2:717:G:N1	2.70	0.57
7:I1:129:PRO:O	7:I1:134:ARG:NH2	2.36	0.57
29:A1:1870:C:N4	29:A1:1923:G:N7	2.53	0.57
53:A2:338:U:O2'	53:A2:341:G:O6	2.19	0.57
53:A2:553:G:O6	53:A2:842:A:N6	2.37	0.57
53:A2:1197:G:O2'	53:A2:1199:C:OP2	2.22	0.57
9:K1:124:LYS:HD2	9:K1:145:PRO:HD3	1.85	0.57
29:A1:302:C:OP2	29:A1:387:U:N3	2.38	0.57
33:C2:20:SER:OG	33:C2:40:ARG:NH2	2.33	0.57
53:A2:672:C:HO2'	53:A2:688:U:HO2'	1.47	0.57
14:P1:3:ARG:NH1	29:A1:477:A:O2'	2.38	0.57
53:A2:408:G:H2'	53:A2:423:G:H22	1.70	0.57
29:A1:930:G:N2	29:A1:945:C:O4'	2.38	0.57
53:A2:1109:G:H1	53:A2:1127:C:H42	1.52	0.57
1:C1:13:ARG:NH2	29:A1:778:G:OP2	2.37	0.57
2:D1:128:SER:OG	2:D1:129:HIS:N	2.37	0.57
24:Z1:16:CYS:HB3	24:Z1:36:CYS:HA	1.87	0.57
49:S2:32:LYS:HG2	49:S2:50:ALA:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:U2:10:ARG:NH2	53:A2:1224:C:OP2	2.36	0.57
53:A2:612:G:HO2'	53:A2:614:G:H1	1.52	0.57
24:Z1:34:GLU:HB2	43:M2:57:ARG:HH22	1.69	0.56
29:A1:1098:A:N6	29:A1:2766:G:O6	2.38	0.56
47:Q2:70:ARG:NH1	53:A2:230:C:OP1	2.37	0.56
50:T2:22:ARG:HH11	50:T2:25:ARG:HE	1.53	0.56
53:A2:812:G:N7	53:A2:835:G:N2	2.52	0.56
1:C1:39:LYS:HE3	1:C1:62:TYR:HB2	1.87	0.56
13:O1:92:GLY:HA2	13:O1:116:ALA:HA	1.87	0.56
16:R1:16:LYS:NZ	29:A1:2035:U:OP2	2.35	0.56
47:Q2:101:ARG:NE	53:A2:873:C:OP1	2.37	0.56
49:S2:55:LYS:HD2	53:A2:935:A:H1'	1.87	0.56
53:A2:988:G:H2'	53:A2:989:G:H8	1.70	0.56
12:N1:5:THR:HG22	12:N1:7:TYR:H	1.71	0.56
29:A1:929:G:N2	29:A1:946:C:O2'	2.38	0.56
34:D2:165:MET:HA	34:D2:168:ARG:HE	1.70	0.56
18:T1:39:VAL:HG23	18:T1:41:GLY:H	1.69	0.56
47:Q2:3:LYS:NZ	53:A2:121:G:O2'	2.37	0.56
29:A1:307:A:N6	29:A1:382:A:N7	2.53	0.56
53:A2:647:G:H22	53:A2:724:G:H1	1.52	0.56
29:A1:2135:C:N4	29:A1:2173:G:O2'	2.38	0.56
52:V2:71:GLU:OE1	52:V2:86:ARG:NH2	2.39	0.56
53:A2:172:C:N4	53:A2:199:C:OP1	2.38	0.56
14:P1:31:SER:OG	14:P1:32:PHE:N	2.36	0.56
18:T1:13:VAL:HG22	18:T1:74:PRO:HA	1.88	0.56
53:A2:1015:G:O2'	53:A2:1017:A:OP1	2.18	0.56
29:A1:590:C:N4	29:A1:601:U:O4	2.38	0.56
29:A1:2590:G:O2'	29:A1:2593:C:OP2	2.24	0.56
43:M2:75:ALA:O	43:M2:79:LYS:N	2.37	0.56
53:A2:216:C:C6	53:A2:216:C:C2'	2.89	0.56
53:A2:438:C:H2'	53:A2:439:G:H8	1.70	0.56
32:B2:125:PRO:HA	32:B2:128:GLU:HB3	1.88	0.55
53:A2:818:U:H3	53:A2:828:G:H1	1.54	0.55
15:Q1:30:GLY:H	15:Q1:61:VAL:HG13	1.71	0.55
32:B2:112:VAL:HG22	32:B2:149:LEU:HD13	1.88	0.55
18:T1:2:ARG:HH22	29:A1:80:G:H21	1.55	0.55
53:A2:415:U:O2'	53:A2:418:G:O6	2.20	0.55
34:D2:25:ARG:NH2	53:A2:406:A:OP2	2.40	0.55
37:G2:10:ARG:NH1	53:A2:1358:U:O4	2.34	0.55
53:A2:339:A:H5''	53:A2:340:C:H5	1.71	0.55
53:A2:904:G:O2'	53:A2:1480:A:N7	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G1:29:PRO:HD2	5:G1:79:VAL:HB	1.88	0.55
16:R1:8:ARG:HG2	16:R1:102:HIS:HD2	1.72	0.55
16:R1:60:ASN:ND2	29:A1:514:C:O2'	2.38	0.55
29:A1:51:A:H2'	29:A1:52:A:H8	1.72	0.55
49:S2:46:GLY:H	49:S2:62:ILE:HB	1.70	0.55
53:A2:734:U:O2'	53:A2:735:G:O4'	2.25	0.55
53:A2:1015:G:H21	53:A2:1016:G:H2'	1.72	0.55
53:A2:1271:G:H3'	53:A2:1272:G:H8	1.71	0.55
4:F1:5:VAL:HG12	4:F1:8:LYS:H	1.71	0.55
5:G1:43:VAL:HG12	5:G1:52:VAL:HG22	1.89	0.55
29:A1:627:G:N2	29:A1:704:A:OP2	2.35	0.55
37:G2:92:SER:HB2	37:G2:95:ARG:HB2	1.87	0.55
43:M2:74:VAL:O	43:M2:78:ILE:N	2.39	0.55
11:M1:96:ARG:HH21	11:M1:117:VAL:HG23	1.72	0.55
52:V2:102:LYS:O	52:V2:103:ARG:HB2	2.06	0.55
11:M1:97:VAL:HG22	11:M1:114:VAL:HG22	1.89	0.55
29:A1:685:G:N2	29:A1:700:G:O2'	2.39	0.55
29:A1:1891:G:H1'	29:A1:1908:A:H61	1.72	0.55
4:F1:58:GLN:OE1	4:F1:67:LYS:NZ	2.40	0.55
53:A2:351:A:N3	53:A2:363:U:O2'	2.39	0.55
29:A1:2714:C:N4	29:A1:2721:G:O6	2.39	0.55
53:A2:90:G:O2'	53:A2:91:G:N2	2.39	0.55
8:J1:80:ASP:OD2	13:O1:64:ARG:NH2	2.36	0.54
18:T1:58:GLY:O	29:A1:511:A:O2'	2.22	0.54
53:A2:902:G:O6	53:A2:1374:G:N1	2.40	0.54
9:K1:146:VAL:HG22	9:K1:147:LEU:HG	1.88	0.54
19:U1:30:ASN:ND2	19:U1:90:VAL:O	2.40	0.54
29:A1:2212:C:H2'	29:A1:2213:U:H4'	1.89	0.54
41:K2:55:LYS:HE3	53:A2:673:G:H22	1.72	0.54
41:K2:85:ARG:NH1	53:A2:690:C:OP1	2.35	0.54
52:V2:28:LEU:HD23	52:V2:29:ASP:H	1.71	0.54
29:A1:933:C:H2'	29:A1:940:G:H1	1.73	0.54
29:A1:1765:G:H1	29:A1:1775:C:H42	1.55	0.54
43:M2:90:LEU:HD23	43:M2:93:ARG:HH21	1.72	0.54
53:A2:660:U:H3	53:A2:696:G:H22	1.53	0.54
11:M1:96:ARG:NH1	29:A1:2894:A:OP1	2.41	0.54
33:C2:199:LYS:NZ	53:A2:1040:G:OP1	2.41	0.54
40:J2:44:VAL:HG22	40:J2:66:ARG:HG2	1.89	0.54
53:A2:1236:G:N1	53:A2:1260:A:N7	2.55	0.54
5:G1:4:ILE:HD12	5:G1:6:ARG:HB2	1.88	0.54
29:A1:1055:C:N4	29:A1:1183:G:O6	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:F2:28:ARG:O	36:F2:32:ASN:ND2	2.40	0.54
40:J2:51:ARG:HB2	40:J2:59:SER:HB3	1.89	0.54
3:E1:5:ALA:O	3:E1:17:ARG:NH2	2.41	0.54
16:R1:82:LEU:HB2	16:R1:98:LYS:HB2	1.88	0.54
29:A1:305:C:N4	29:A1:306:G:N7	2.55	0.54
32:B2:96:ARG:NH1	53:A2:1082:C:OP2	2.41	0.54
53:A2:904:G:N1	53:A2:1373:U:O2	2.41	0.54
43:M2:91:ARG:HH21	43:M2:97:PRO:HG2	1.72	0.54
9:K1:18:ARG:NH2	29:A1:1239:G:OP2	2.37	0.54
29:A1:1815:C:H1'	29:A1:2623:U:H5''	1.90	0.54
34:D2:31:CYS:O	34:D2:33:MET:N	2.41	0.54
35:E2:97:GLY:N	35:E2:117:ASP:OD2	2.40	0.54
38:H2:69:ARG:NE	38:H2:73:ASP:O	2.40	0.54
41:K2:112:THR:O	48:R2:84:LYS:NZ	2.35	0.54
53:A2:1251:C:O2'	53:A2:1294:U:O2'	2.23	0.54
8:J1:65:THR:HG22	8:J1:67:LYS:H	1.72	0.54
29:A1:302:C:N4	29:A1:303:A:N3	2.56	0.54
29:A1:1738:A:H62	29:A1:1747:A:H2	1.56	0.54
29:A1:2172:G:C2	29:A1:2173:G:H1'	2.43	0.54
53:A2:612:G:N7	53:A2:613:G:N2	2.56	0.54
3:E1:7:TYR:HD2	3:E1:16:GLY:H	1.55	0.54
53:A2:70:G:OP1	53:A2:70:G:N2	2.36	0.54
5:G1:125:VAL:O	5:G1:130:ARG:NH1	2.41	0.53
18:T1:54:LYS:HB2	18:T1:55:TYR:HD1	1.73	0.53
29:A1:442:C:O2'	29:A1:1897:U:O2'	2.19	0.53
29:A1:590:C:O2	29:A1:602:G:N1	2.40	0.53
29:A1:2341:A:N7	29:A1:2402:A:N6	2.55	0.53
53:A2:1237:A:N6	53:A2:1259:U:OP2	2.41	0.53
36:F2:52:ILE:HG13	36:F2:87:ARG:HH21	1.73	0.53
39:I2:105:ASP:N	39:I2:105:ASP:OD1	2.36	0.53
53:A2:241:A:H62	53:A2:276:G:H8	1.57	0.53
53:A2:1121:G:N2	53:A2:1121:G:C2	2.76	0.53
2:D1:37:ARG:HD2	2:D1:46:ALA:HB3	1.91	0.53
53:A2:775:A:C2'	53:A2:776:U:O5'	2.56	0.53
32:B2:176:GLU:OE2	53:A2:1083:A:N6	2.42	0.53
53:A2:452:C:H2'	53:A2:453:G:H8	1.73	0.53
53:A2:1101:C:O2	53:A2:1137:G:N2	2.42	0.53
53:A2:1220:A:H62	53:A2:1280:A:H62	1.57	0.53
9:K1:113:LYS:NZ	29:A1:663:G:N7	2.52	0.53
12:N1:83:LYS:HD2	12:N1:108:GLY:HA2	1.91	0.53
13:O1:41:ARG:NH2	53:A2:341:G:OP1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W1:93:GLU:HG3	21:W1:94:LEU:HG	1.90	0.53
29:A1:298:C:O3'	29:A1:299:G:N2	2.41	0.53
53:A2:962:C:N3	53:A2:963:A:N6	2.56	0.53
10:L1:67:ARG:NH1	29:A1:954:G:O2'	2.42	0.53
53:A2:72:C:O2'	53:A2:73:G:O4'	2.27	0.53
53:A2:983:A:H4'	53:A2:1020:C:H1'	1.89	0.53
47:Q2:62:SER:OG	47:Q2:63:ARG:N	2.40	0.53
51:U2:3:LYS:NZ	53:A2:1217:A:OP2	2.33	0.53
14:P1:90:VAL:HG11	15:Q1:40:LEU:HB2	1.91	0.53
11:M1:82:GLU:HG3	11:M1:83:ILE:HG12	1.91	0.53
12:N1:110:LEU:HD12	12:N1:112:PHE:H	1.74	0.53
53:A2:1493:G:N2	53:A2:1496:A:OP2	2.42	0.53
1:C1:80:ALA:HA	1:C1:113:VAL:HG13	1.90	0.52
9:K1:95:VAL:HG22	9:K1:125:VAL:HA	1.91	0.52
29:A1:1498:A:O2'	29:A1:1578:G:N2	2.40	0.52
29:A1:2471:U:O2	29:A1:2509:G:N2	2.42	0.52
49:S2:36:ARG:HH12	49:S2:53:ASN:HA	1.74	0.52
53:A2:1251:C:HO2'	53:A2:1294:U:HO2'	1.54	0.52
7:I1:133:GLN:NE2	29:A1:2910:G:OP2	2.42	0.52
32:B2:87:ARG:NH2	32:B2:233:SER:OG	2.42	0.52
53:A2:979:G:H21	53:A2:1022:U:H3'	1.75	0.52
53:A2:980:G:O2'	53:A2:1022:U:O4	2.27	0.52
53:A2:1236:G:H1	53:A2:1263:C:H42	1.55	0.52
29:A1:2834:G:N2	29:A1:2836:C:OP1	2.42	0.52
4:F1:32:PRO:HG2	4:F1:172:LEU:HD13	1.91	0.52
29:A1:1215:U:H3	29:A1:1229:A:H61	1.56	0.52
29:A1:2128:G:O6	29:A1:2209:C:O2'	2.27	0.52
29:A1:2232:U:H5''	29:A1:2233:G:H8	1.74	0.52
1:C1:10:THR:O	1:C1:13:ARG:N	2.39	0.52
5:G1:168:PRO:HG2	5:G1:170:ARG:HH12	1.74	0.52
53:A2:104:G:O6	53:A2:325:C:N4	2.42	0.52
53:A2:1423:G:O2'	53:A2:1437:A:N6	2.42	0.52
10:L1:32:TYR:HE1	10:L1:133:ARG:HG3	1.74	0.52
39:I2:16:ARG:N	39:I2:64:THR:O	2.42	0.52
40:J2:33:GLN:HG2	40:J2:76:ASN:HD21	1.74	0.52
2:D1:11:MET:H	13:O1:8:LYS:HZ1	1.58	0.52
39:I2:104:ARG:NH2	53:A2:1100:C:O2'	2.42	0.52
42:L2:46:LYS:HE2	42:L2:47:LYS:HG3	1.91	0.52
52:V2:30:ARG:N	52:V2:31:TYR:HD1	2.07	0.52
12:N1:61:ASN:HD22	12:N1:62:LYS:H	1.58	0.52
37:G2:63:LYS:HG3	37:G2:64:GLN:HE21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:50:ALA:HB1	49:S2:57:HIS:HB3	1.92	0.52
53:A2:500:G:N2	53:A2:513:G:OP1	2.42	0.52
3:E1:64:ILE:HD11	3:E1:78:ILE:HG23	1.92	0.52
4:F1:91:ARG:NH2	30:B1:43:U:O4	2.42	0.52
5:G1:124:GLU:HB2	5:G1:132:ARG:HD2	1.92	0.52
29:A1:667:C:H42	29:A1:675:G:H1	1.58	0.52
40:J2:3:LYS:HG3	40:J2:75:ILE:HG22	1.90	0.52
53:A2:1420:G:N2	53:A2:1440:C:O2	2.40	0.52
16:R1:85:VAL:HG22	16:R1:95:ILE:HG22	1.92	0.51
33:C2:79:ARG:HH12	33:C2:83:ARG:HD3	1.75	0.51
53:A2:700:C:C6	53:A2:700:C:N1	2.50	0.51
20:V1:20:ARG:NE	29:A1:2371:U:OP1	2.43	0.51
53:A2:546:A:O2'	53:A2:549:G:O2'	2.25	0.51
53:A2:775:A:N6	53:A2:777:A:C6	2.79	0.51
29:A1:686:C:OP2	29:A1:687:C:N4	2.43	0.51
29:A1:1367:G:O6	29:A1:1381:C:N4	2.42	0.51
44:N2:31:ARG:NH1	53:A2:954:A:OP1	2.44	0.51
53:A2:937:U:O4	53:A2:1206:A:O2'	2.27	0.51
53:A2:992:A:N7	53:A2:993:A:N6	2.59	0.51
5:G1:58:GLU:HB2	5:G1:61:HIS:HD2	1.76	0.51
6:H1:5:LEU:H	6:H1:16:GLY:HA2	1.75	0.51
6:H1:8:PRO:HG3	6:H1:14:ASP:HA	1.91	0.51
6:H1:27:ARG:NH2	29:A1:2116:U:OP2	2.33	0.51
8:J1:73:ASP:N	8:J1:73:ASP:OD1	2.41	0.51
19:U1:170:THR:HG21	29:A1:924:G:H4'	1.90	0.51
53:A2:1202:G:OP1	53:A2:1301:C:N4	2.44	0.51
4:F1:57:ALA:O	4:F1:61:ALA:N	2.42	0.51
53:A2:136:G:N2	53:A2:136:G:C2	2.78	0.51
53:A2:522:A:H2'	53:A2:523:G:H8	1.76	0.51
53:A2:1117:U:O2	53:A2:1119:C:O2'	2.26	0.51
18:T1:50:ARG:HB2	18:T1:53:PRO:HG3	1.92	0.51
29:A1:1116:G:N2	29:A1:1143:A:OP2	2.43	0.51
42:L2:113:ARG:HH21	42:L2:116:SER:HB2	1.75	0.51
44:N2:45:ARG:NH2	53:A2:1042:C:OP1	2.44	0.51
4:F1:74:LYS:NZ	29:A1:2327:C:OP2	2.39	0.51
29:A1:2726:U:H5	29:A1:2728:A:H2'	1.75	0.51
39:I2:25:LYS:H	39:I2:60:ASP:HA	1.76	0.51
53:A2:208:U:N3	53:A2:210:U:OP2	2.43	0.51
29:A1:627:G:H1	29:A1:703:A:H3'	1.75	0.51
38:H2:26:VAL:HG23	38:H2:59:LEU:HB2	1.93	0.51
53:A2:1194:A:O2'	53:A2:1197:G:OP2	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J1:76:ALA:HB3	13:O1:75:ILE:HD12	1.93	0.51
29:A1:441:C:HO2'	29:A1:1904:C:HO2'	1.55	0.51
29:A1:696:G:N2	29:A1:697:G:O6	2.44	0.51
53:A2:598:C:H2'	53:A2:599:G:H8	1.76	0.51
53:A2:1304:G:H2'	53:A2:1305:A:H8	1.75	0.51
22:X1:66:GLU:HG2	22:X1:69:ARG:HH21	1.76	0.51
29:A1:2186:G:H4'	29:A1:2196:U:H3'	1.92	0.51
37:G2:79:ARG:NH2	53:A2:1363:U:O4	2.44	0.51
39:I2:6:GLY:N	39:I2:17:VAL:O	2.44	0.51
43:M2:77:ASN:HA	43:M2:80:ARG:HG2	1.93	0.51
53:A2:119:G:N1	53:A2:231:G:N7	2.59	0.51
12:N1:70:GLY:HA3	12:N1:104:GLY:HA3	1.93	0.50
29:A1:5:A:H3'	29:A1:6:A:H8	1.75	0.50
50:T2:87:LYS:HA	50:T2:90:GLN:HB2	1.93	0.50
14:P1:55:ARG:NH1	29:A1:1203:A:O3'	2.44	0.50
29:A1:1464:G:N2	29:A1:1632:A:O4'	2.42	0.50
43:M2:16:ASP:N	43:M2:16:ASP:OD1	2.43	0.50
4:F1:71:THR:OG1	4:F1:88:ILE:O	2.26	0.50
20:V1:73:GLY:HA3	30:B1:14:C:H2'	1.92	0.50
29:A1:1095:G:OP2	29:A1:1158:G:N1	2.38	0.50
29:A1:2260:G:H2'	29:A1:2261:A:H8	1.76	0.50
52:V2:30:ARG:HB2	52:V2:31:TYR:CD1	2.46	0.50
53:A2:1286:G:H21	53:A2:1312:G:H2'	1.76	0.50
3:E1:17:ARG:NH1	3:E1:19:GLU:OE1	2.45	0.50
29:A1:2303:G:N2	29:A1:2358:U:O2	2.44	0.50
53:A2:929:U:H3	53:A2:1210:A:H61	1.58	0.50
4:F1:168:GLU:O	4:F1:172:LEU:N	2.44	0.50
16:R1:30:GLU:O	16:R1:34:ASN:ND2	2.44	0.50
37:G2:98:SER:OG	53:A2:1358:U:OP1	2.28	0.50
39:I2:107:ARG:HG2	53:A2:1328:G:C8	2.46	0.50
53:A2:133:G:N2	53:A2:220:C:O2	2.44	0.50
20:V1:9:SER:HG	29:A1:2270:G:HO2'	1.57	0.50
29:A1:66:U:H3	29:A1:73:A:H2	1.57	0.50
29:A1:304:C:H42	29:A1:385:G:H22	1.60	0.50
41:K2:116:HIS:HB2	53:A2:717:G:H21	1.76	0.50
42:L2:8:ASN:ND2	53:A2:568:G:O2'	2.45	0.50
4:F1:136:ARG:NH1	29:A1:2319:A:O2'	2.44	0.50
29:A1:908:G:O2'	29:A1:964:G:O6	2.21	0.50
41:K2:15:ALA:HB1	41:K2:78:GLN:HB2	1.93	0.50
53:A2:589:G:O2'	53:A2:615:A:N6	2.45	0.50
14:P1:28:ARG:NH1	14:P1:38:THR:OG1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A1:869:A:N3	29:A1:990:U:O2'	2.43	0.50
29:A1:2230:G:OP2	29:A1:2231:A:N6	2.44	0.50
29:A1:2803:C:O2'	29:A1:2821:A:N3	2.43	0.50
34:D2:49:ARG:NH2	53:A2:493:A:OP2	2.27	0.50
43:M2:14:ARG:H	43:M2:14:ARG:HD3	1.76	0.50
53:A2:460:G:H2'	53:A2:461:G:H8	1.77	0.50
53:A2:775:A:H2'	53:A2:776:U:C5'	2.38	0.50
38:H2:15:ASN:ND2	53:A2:809:C:O2	2.45	0.50
29:A1:2487:U:OP1	29:A1:2543:G:N2	2.45	0.49
43:M2:19:LEU:HD22	43:M2:25:ILE:HG21	1.93	0.49
52:V2:14:THR:OG1	52:V2:15:ASP:N	2.45	0.49
5:G1:13:LYS:HZ3	5:G1:77:LYS:HA	1.77	0.49
29:A1:325:A:O2'	29:A1:343:C:O2'	2.26	0.49
49:S2:39:THR:HA	49:S2:70:LYS:HA	1.93	0.49
53:A2:1206:A:H4'	53:A2:1207:C:H5'	1.94	0.49
3:E1:41:LEU:HD22	3:E1:44:ARG:HH21	1.76	0.49
13:O1:100:TYR:HE1	13:O1:103:ARG:HH21	1.60	0.49
29:A1:1470:G:O2'	29:A1:1540:G:O2'	2.28	0.49
37:G2:29:LYS:HE3	53:A2:1357:A:H4'	1.94	0.49
37:G2:78:ARG:HD2	37:G2:156:TRP:HB2	1.94	0.49
45:O2:65:ARG:NH2	53:A2:564:G:OP1	2.44	0.49
48:R2:74:ARG:NH1	53:A2:701:G:O6	2.45	0.49
19:U1:142:SER:OG	19:U1:143:GLY:N	2.46	0.49
32:B2:17:PHE:HB3	32:B2:41:ILE:HG23	1.94	0.49
52:V2:71:GLU:HG2	52:V2:82:ARG:HB2	1.94	0.49
53:A2:208:U:H2'	53:A2:209:U:H2'	1.95	0.49
1:C1:247:ALA:HA	1:C1:253:GLN:HA	1.94	0.49
5:G1:6:ARG:HB3	5:G1:65:HIS:CD2	2.48	0.49
29:A1:681:A:H2'	29:A1:682:A:H8	1.76	0.49
29:A1:1119:G:N2	29:A1:1138:U:O4	2.45	0.49
29:A1:2158:A:N6	29:A1:2181:G:O2'	2.45	0.49
29:A1:2643:A:N6	29:A1:2906:U:H3	2.10	0.49
43:M2:88:ARG:NH2	53:A2:1302:C:OP1	2.45	0.49
50:T2:8:ARG:NH1	53:A2:157:C:O5'	2.39	0.49
30:B1:82:U:H2'	30:B1:83:G:H21	1.77	0.49
34:D2:65:ARG:HH21	34:D2:71:SER:HA	1.78	0.49
36:F2:53:ALA:HB3	36:F2:86:ARG:HH11	1.76	0.49
37:G2:122:HIS:ND1	37:G2:125:MET:SD	2.84	0.49
19:U1:91:LEU:HD22	19:U1:130:PRO:HB3	1.95	0.49
29:A1:1302:A:H5''	29:A1:1303:U:H5'	1.95	0.49
4:F1:94:LEU:HD22	4:F1:98:ARG:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U1:6:LYS:HA	19:U1:60:GLU:HB3	1.94	0.49
29:A1:674:G:N2	29:A1:2364:C:O2'	2.42	0.49
29:A1:799:A:OP1	29:A1:1663:C:N4	2.44	0.49
45:O2:6:GLU:O	45:O2:10:LYS:N	2.46	0.49
53:A2:1317:C:O2	53:A2:1318:G:N1	2.46	0.49
29:A1:681:A:OP1	29:A1:698:C:N4	2.40	0.49
34:D2:10:ARG:NH1	53:A2:423:G:OP2	2.46	0.49
35:E2:120:THR:O	53:A2:7:G:O2'	2.30	0.49
23:Y1:27:GLY:O	23:Y1:35:ARG:NH1	2.46	0.49
29:A1:1542:A:H1'	29:A1:1544:A:H61	1.77	0.49
29:A1:1573:G:HO2'	29:A1:1574:G:H8	1.61	0.49
41:K2:13:GLN:HE21	41:K2:75:TYR:HB3	1.78	0.49
53:A2:106:G:O6	53:A2:308:A:N6	2.45	0.49
29:A1:2257:U:H2'	29:A1:2258:U:H6	1.78	0.48
36:F2:52:ILE:O	36:F2:86:ARG:NH1	2.46	0.48
39:I2:71:SER:HB3	53:A2:1354:U:H5''	1.94	0.48
49:S2:55:LYS:HG3	53:A2:963:A:H4'	1.93	0.48
53:A2:1328:G:N2	53:A2:1356:A:OP2	2.38	0.48
29:A1:1578:G:O6	29:A1:1590:G:N2	2.47	0.48
53:A2:1268:A:H2'	53:A2:1269:A:C8	2.47	0.48
2:D1:5:LEU:HD21	2:D1:79:ARG:HB2	1.94	0.48
19:U1:132:ASN:OD1	19:U1:132:ASN:N	2.42	0.48
29:A1:893:C:H42	29:A1:981:G:H1	1.61	0.48
29:A1:2260:G:H2'	29:A1:2261:A:C8	2.47	0.48
32:B2:178:ARG:HB3	38:H2:72:PRO:HA	1.95	0.48
53:A2:406:A:H2'	53:A2:408:G:C8	2.48	0.48
53:A2:1224:C:O2	53:A2:1276:G:N2	2.46	0.48
11:M1:77:ARG:HH21	29:A1:1503:U:P	2.37	0.48
29:A1:2869:G:N2	29:A1:2872:A:OP2	2.37	0.48
45:O2:33:THR:O	45:O2:37:ASN:ND2	2.46	0.48
53:A2:1410:A:H62	53:A2:1449:U:H3	1.61	0.48
29:A1:2389:G:N2	29:A1:2392:A:OP2	2.44	0.48
52:V2:9:ARG:HD3	52:V2:43:SER:HB3	1.95	0.48
29:A1:1975:U:N3	29:A1:1978:G:OP2	2.41	0.48
32:B2:205:ASP:HA	32:B2:211:ILE:HD11	1.95	0.48
40:J2:11:PHE:O	40:J2:68:HIS:ND1	2.43	0.48
29:A1:934:C:OP1	29:A1:940:G:N2	2.41	0.48
29:A1:1135:G:O6	29:A1:1137:G:N2	2.42	0.48
49:S2:36:ARG:NH1	49:S2:52:TYR:O	2.46	0.48
51:U2:15:ARG:NH1	53:A2:1346:U:OP1	2.47	0.48
53:A2:612:G:O2'	53:A2:614:G:N1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T1:2:ARG:HH22	29:A1:80:G:N2	2.12	0.48
19:U1:111:VAL:HG22	19:U1:112:ARG:HG2	1.95	0.48
29:A1:725:A:H8	29:A1:2093:G:H21	1.61	0.48
34:D2:36:ARG:HH12	53:A2:408:G:H1	1.62	0.48
53:A2:650:G:OP1	53:A2:715:C:O2'	2.30	0.48
1:C1:231:HIS:HE1	1:C1:233:HIS:CD2	2.32	0.48
8:J1:75:SER:HG	13:O1:32:TYR:HH	1.56	0.48
42:L2:33:ARG:NH2	42:L2:61:THR:OG1	2.47	0.48
47:Q2:58:GLU:OE2	47:Q2:75:ARG:NH2	2.47	0.48
29:A1:1390:A:O2'	29:A1:1392:G:OP2	2.32	0.48
44:N2:29:ARG:NH2	53:A2:951:A:OP1	2.47	0.48
47:Q2:95:TYR:OH	53:A2:274:A:OP2	2.29	0.48
53:A2:610:G:H2'	53:A2:611:G:C8	2.49	0.48
53:A2:750:A:N6	53:A2:796:U:O2	2.45	0.48
8:J1:17:ARG:HE	8:J1:47:ILE:HD13	1.79	0.47
32:B2:196:LEU:HD12	32:B2:197:VAL:HG13	1.96	0.47
53:A2:216:C:C2	53:A2:216:C:C1'	2.94	0.47
29:A1:313:C:H1'	29:A1:379:G:H1	1.79	0.47
29:A1:2810:G:O4'	29:A1:2815:G:N2	2.46	0.47
38:H2:12:ARG:NH1	38:H2:25:ASP:O	2.47	0.47
29:A1:262:A:N7	29:A1:284:G:N2	2.62	0.47
29:A1:2906:U:H2'	29:A1:2907:C:H6	1.79	0.47
53:A2:402:G:O6	53:A2:430:C:N4	2.47	0.47
29:A1:170:G:N2	29:A1:205:G:O6	2.47	0.47
40:J2:81:THR:HA	40:J2:85:LEU:HD12	1.95	0.47
35:E2:79:GLU:OE2	38:H2:105:ARG:NH1	2.47	0.47
35:E2:148:VAL:HG21	38:H2:107:LEU:HD22	1.95	0.47
36:F2:21:LEU:O	36:F2:25:ILE:N	2.47	0.47
39:I2:33:PHE:HZ	39:I2:46:ALA:HB3	1.79	0.47
42:L2:70:ILE:HG12	42:L2:100:ILE:HD12	1.95	0.47
4:F1:126:ASP:OD1	4:F1:129:GLY:N	2.47	0.47
12:N1:33:LYS:HG3	12:N1:34:HIS:CD2	2.50	0.47
29:A1:1573:G:O2'	29:A1:1574:G:O4'	2.32	0.47
37:G2:41:ARG:O	37:G2:45:ASP:N	2.47	0.47
41:K2:30:VAL:HG21	41:K2:68:ALA:HB2	1.97	0.47
9:K1:15:ARG:HH21	29:A1:1294:A:P	2.37	0.47
12:N1:5:THR:HB	12:N1:8:GLU:HG2	1.96	0.47
29:A1:1210:G:H2'	29:A1:1211:G:H8	1.80	0.47
29:A1:1222:U:H4'	29:A1:1223:G:H4'	1.95	0.47
29:A1:2366:A:H62	29:A1:2379:G:H21	1.63	0.47
42:L2:46:LYS:HE2	42:L2:47:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A2:1285:G:N1	53:A2:1313:A:OP2	2.38	0.47
53:A2:1304:G:H2'	53:A2:1305:A:C8	2.49	0.47
7:I1:47:ALA:HB2	7:I1:112:LEU:HD11	1.96	0.47
29:A1:1566:C:H2'	29:A1:1567:G:H8	1.80	0.47
29:A1:2134:G:N3	29:A1:2204:U:N3	2.62	0.47
32:B2:204:ASN:HB3	32:B2:206:ASP:H	1.78	0.47
38:H2:82:HIS:HE1	38:H2:84:ARG:HD3	1.80	0.47
5:G1:132:ARG:NE	5:G1:134:SER:HB3	2.30	0.47
29:A1:304:C:H41	29:A1:385:G:H1	1.62	0.47
53:A2:978:A:H2'	53:A2:979:G:C8	2.50	0.47
53:A2:1249:A:H2'	53:A2:1250:A:C8	2.49	0.47
5:G1:27:LYS:N	5:G1:32:GLU:OE1	2.46	0.47
29:A1:1466:G:H21	29:A1:1629:A:H2	1.64	0.47
53:A2:640:G:N7	53:A2:641:G:N1	2.64	0.47
53:A2:672:C:O2'	53:A2:688:U:O2'	2.23	0.47
3:E1:20:LEU:HG	3:E1:22:ALA:H	1.79	0.46
5:G1:138:LYS:HA	5:G1:141:VAL:HB	1.97	0.46
22:X1:66:GLU:HG2	22:X1:69:ARG:NH2	2.30	0.46
35:E2:74:GLY:O	35:E2:116:THR:OG1	2.33	0.46
39:I2:127:LYS:HD3	52:V2:66:LEU:HD22	1.97	0.46
53:A2:119:G:OP1	53:A2:588:U:O2'	2.21	0.46
53:A2:1002:G:N2	53:A2:1014:G:OP1	2.48	0.46
3:E1:124:LEU:HD22	3:E1:191:ARG:HH21	1.79	0.46
12:N1:83:LYS:O	12:N1:109:GLY:N	2.48	0.46
32:B2:74:LYS:HE3	32:B2:205:ASP:HB2	1.97	0.46
1:C1:71:ASP:N	1:C1:71:ASP:OD1	2.48	0.46
29:A1:1175:A:N7	29:A1:2502:A:O2'	2.48	0.46
29:A1:1329:G:H1	29:A1:1337:C:H42	1.63	0.46
42:L2:33:ARG:NH1	53:A2:358:A:OP1	2.49	0.46
43:M2:91:ARG:HA	43:M2:96:LEU:HD12	1.97	0.46
53:A2:160:G:H2'	53:A2:161:G:H8	1.80	0.46
53:A2:921:G:N1	53:A2:1319:G:OP2	2.48	0.46
3:E1:7:TYR:HD1	3:E1:125:LEU:HB2	1.80	0.46
12:N1:24:LEU:HG	12:N1:41:ASP:HA	1.98	0.46
29:A1:306:G:H1	29:A1:383:U:H5	1.62	0.46
32:B2:132:LYS:HA	32:B2:135:GLN:HB2	1.97	0.46
53:A2:914:A:O2'	53:A2:1361:G:O6	2.27	0.46
13:O1:93:ARG:HG2	13:O1:117:ASP:HB2	1.97	0.46
18:T1:75:ILE:HG13	18:T1:77:PRO:HD3	1.97	0.46
29:A1:7:G:H1	29:A1:2907:C:H42	1.64	0.46
29:A1:2608:C:N4	29:A1:2609:G:O6	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A2:639:C:N3	53:A2:640:G:N1	2.64	0.46
53:A2:775:A:HO2'	53:A2:776:U:C5'	1.92	0.46
4:F1:4:ASP:HB3	4:F1:9:ARG:HH12	1.81	0.46
4:F1:96:ARG:NH2	30:B1:46:G:O2'	2.48	0.46
5:G1:3:ARG:HB2	29:A1:2766:G:C6	2.51	0.46
10:L1:23:GLY:HA2	10:L1:24:GLY:HA3	1.64	0.46
29:A1:333:G:H21	29:A1:354:G:H21	1.63	0.46
39:I2:47:LEU:HB3	39:I2:50:LEU:HD12	1.98	0.46
53:A2:10:A:H2'	53:A2:11:G:H8	1.81	0.46
53:A2:775:A:N6	53:A2:777:A:N1	2.63	0.46
29:A1:622:U:H2'	29:A1:623:G:C8	2.51	0.46
32:B2:73:THR:HG21	32:B2:170:GLU:HB2	1.98	0.46
32:B2:215:LEU:HA	32:B2:218:ALA:HB3	1.98	0.46
53:A2:1323:C:H2'	53:A2:1324:G:C8	2.51	0.46
9:K1:81:GLN:HG2	9:K1:106:LEU:HD12	1.98	0.46
24:Z1:18:CYS:H	24:Z1:19:GLY:HA2	1.80	0.46
29:A1:604:G:H1	29:A1:1309:C:H42	1.64	0.46
29:A1:825:G:N1	29:A1:2096:G:OP1	2.44	0.46
29:A1:2644:G:H21	29:A1:2903:A:H1'	1.81	0.46
37:G2:79:ARG:O	37:G2:84:ASN:ND2	2.46	0.46
52:V2:18:ARG:O	52:V2:22:GLU:N	2.48	0.46
53:A2:700:C:N3	53:A2:717:G:C4	2.78	0.46
4:F1:32:PRO:HB2	4:F1:172:LEU:HD22	1.97	0.46
53:A2:147:C:O2'	53:A2:148:C:O5'	2.33	0.46
53:A2:1192:U:O2'	53:A2:1194:A:O5'	2.28	0.46
3:E1:37:VAL:HG21	9:K1:6:LEU:HD21	1.98	0.46
4:F1:166:ASP:HA	4:F1:169:ALA:HB3	1.97	0.46
29:A1:627:G:H3'	29:A1:703:A:H61	1.79	0.46
29:A1:2807:G:N1	29:A1:2815:G:O6	2.49	0.46
43:M2:8:GLU:HB3	43:M2:15:VAL:HG21	1.97	0.46
52:V2:52:LYS:HG2	52:V2:72:GLU:HG2	1.96	0.46
29:A1:2171:G:N7	29:A1:2172:G:O2'	2.49	0.45
53:A2:392:A:N7	53:A2:530:A:O2'	2.47	0.45
53:A2:749:A:N6	53:A2:797:A:N1	2.48	0.45
53:A2:775:A:H62	53:A2:777:A:N6	2.13	0.45
53:A2:1110:C:C2	53:A2:1121:G:N1	2.84	0.45
53:A2:1211:C:H2'	53:A2:1212:G:C8	2.51	0.45
10:L1:127:ILE:H	10:L1:127:ILE:HG13	1.60	0.45
24:Z1:14:ILE:HB	24:Z1:24:THR:HG23	1.98	0.45
39:I2:107:ARG:HG3	53:A2:1328:G:H5''	1.98	0.45
43:M2:95:GLY:HA2	43:M2:110:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Q2:39:SER:OG	53:A2:275:C:N4	2.47	0.45
53:A2:1108:U:OP1	53:A2:1262:U:O2'	2.29	0.45
9:K1:125:VAL:HG11	9:K1:138:LEU:HD13	1.99	0.45
10:L1:132:VAL:HG12	10:L1:134:ARG:H	1.82	0.45
29:A1:867:G:HO2'	29:A1:887:C:HO2'	1.63	0.45
29:A1:2052:U:H2'	29:A1:2053:G:C8	2.51	0.45
29:A1:2074:C:N4	29:A1:2075:A:N1	2.64	0.45
29:A1:2818:G:H2'	29:A1:2819:G:C8	2.52	0.45
45:O2:20:GLY:O	53:A2:733:G:O2'	2.28	0.45
53:A2:59:A:H61	53:A2:347:C:H41	1.64	0.45
53:A2:610:G:H2'	53:A2:611:G:H8	1.81	0.45
4:F1:5:VAL:HG11	4:F1:100:TRP:HB3	1.97	0.45
29:A1:795:A:H1'	29:A1:797:G:H21	1.80	0.45
53:A2:1392:G:N2	53:A2:1467:C:O2	2.35	0.45
4:F1:66:GLN:NE2	30:B1:44:C:O2'	2.49	0.45
4:F1:114:ILE:HD11	4:F1:140:ILE:HD13	1.98	0.45
5:G1:67:LEU:O	5:G1:71:LEU:N	2.42	0.45
19:U1:18:LEU:HD22	19:U1:23:LYS:HG3	1.97	0.45
33:C2:24:ALA:HB3	33:C2:29:TYR:HD1	1.81	0.45
48:R2:37:VAL:HA	48:R2:40:LEU:HD12	1.99	0.45
53:A2:967:C:N4	53:A2:1197:G:O4'	2.49	0.45
29:A1:80:G:H1	29:A1:103:C:H42	1.65	0.45
29:A1:1164:C:H2'	29:A1:1165:G:H8	1.81	0.45
29:A1:2141:A:N6	29:A1:2186:G:OP1	2.49	0.45
32:B2:54:THR:HG21	32:B2:201:ILE:HD11	1.98	0.45
36:F2:8:ILE:HG23	36:F2:85:VAL:HG13	1.99	0.45
53:A2:1051:C:H42	53:A2:1088:G:H1	1.64	0.45
53:A2:1162:G:N7	53:A2:1163:G:N1	2.65	0.45
2:D1:34:VAL:HB	2:D1:48:GLN:HB2	1.98	0.45
8:J1:13:ASN:HD21	8:J1:96:THR:HG1	1.59	0.45
13:O1:133:GLU:O	13:O1:137:LYS:NZ	2.41	0.45
29:A1:332:G:N1	29:A1:335:A:OP2	2.50	0.45
37:G2:146:GLU:OE1	37:G2:149:ARG:NH2	2.40	0.45
53:A2:489:G:N2	53:A2:509:C:O2	2.50	0.45
53:A2:964:G:O6	53:A2:1199:C:N4	2.49	0.45
2:D1:62:PRO:O	2:D1:64:LYS:N	2.50	0.45
13:O1:53:ARG:NH2	13:O1:55:ASN:OD1	2.50	0.45
18:T1:67:LEU:HD11	18:T1:71:LYS:HD2	1.98	0.45
29:A1:622:U:H2'	29:A1:623:G:H8	1.81	0.45
29:A1:2516:G:H5''	29:A1:2517:A:H5''	1.98	0.45
41:K2:62:GLN:HG2	41:K2:97:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Q2:88:TYR:OH	47:Q2:92:ARG:NH2	2.50	0.45
53:A2:368:A:N6	53:A2:386:G:H21	2.15	0.45
5:G1:58:GLU:HB2	5:G1:61:HIS:CD2	2.52	0.45
19:U1:101:PRO:HA	19:U1:123:ASP:HA	1.99	0.45
21:W1:78:LYS:HB3	21:W1:94:LEU:HD11	1.99	0.45
24:Z1:43:TYR:H	24:Z1:47:GLN:HB2	1.82	0.45
29:A1:2135:C:H2'	29:A1:2142:U:H5''	1.98	0.45
50:T2:65:LYS:NZ	53:A2:201:A:OP1	2.38	0.45
35:E2:36:ASP:OD1	35:E2:36:ASP:N	2.50	0.45
40:J2:57:LYS:HD2	40:J2:57:LYS:HA	1.78	0.45
47:Q2:87:LYS:NZ	53:A2:567:G:OP2	2.50	0.45
50:T2:64:ASP:OD2	53:A2:199:C:O2'	2.29	0.45
52:V2:9:ARG:NH2	53:A2:942:A:OP2	2.38	0.45
53:A2:298:A:O2'	53:A2:538:C:O2'	2.26	0.45
53:A2:1424:G:OP2	53:A2:1436:C:N4	2.49	0.45
4:F1:66:GLN:HA	24:Z1:6:HIS:HD2	1.82	0.44
19:U1:102:LEU:HD23	19:U1:137:ILE:HG23	1.98	0.44
29:A1:2705:C:O2'	29:A1:2883:C:O2'	2.28	0.44
39:I2:72:GLY:N	53:A2:1354:U:OP1	2.45	0.44
42:L2:113:ARG:HB2	42:L2:122:THR:HG21	1.98	0.44
4:F1:6:ALA:O	4:F1:10:LYS:N	2.50	0.44
5:G1:58:GLU:O	5:G1:62:LYS:N	2.41	0.44
24:Z1:14:ILE:N	24:Z1:24:THR:OG1	2.50	0.44
29:A1:2247:U:H2'	29:A1:2248:G:C8	2.53	0.44
34:D2:145:GLU:HB2	34:D2:182:LYS:HB2	1.98	0.44
47:Q2:2:PRO:N	53:A2:120:G:HO2'	2.15	0.44
53:A2:645:G:H2'	53:A2:646:A:H8	1.82	0.44
10:L1:27:VAL:O	10:L1:134:ARG:NH1	2.50	0.44
29:A1:1961:A:H62	29:A1:1964:U:H5	1.65	0.44
53:A2:220:C:N3	53:A2:221:G:N1	2.65	0.44
53:A2:1438:G:H2'	53:A2:1439:G:H8	1.81	0.44
13:O1:1:MET:HB3	13:O1:2:ASN:H	1.64	0.44
22:X1:53:LEU:HD23	22:X1:53:LEU:HA	1.83	0.44
33:C2:23:TYR:HA	40:J2:11:PHE:HE2	1.82	0.44
35:E2:84:PHE:HB3	35:E2:134:ALA:HB2	2.00	0.44
36:F2:42:GLU:HG2	36:F2:44:GLY:H	1.82	0.44
37:G2:141:VAL:O	37:G2:145:ALA:N	2.51	0.44
39:I2:10:ARG:NH2	53:A2:1328:G:O6	2.48	0.44
24:Z1:36:CYS:SG	24:Z1:40:HIS:N	2.79	0.44
29:A1:681:A:H61	29:A1:699:C:H3'	1.82	0.44
52:V2:7:ILE:HG22	53:A2:930:G:H4'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:V2:114:VAL:O	52:V2:115:ARG:NE	2.51	0.44
53:A2:700:C:N3	53:A2:717:G:N3	2.65	0.44
11:M1:36:THR:O	11:M1:112:ALA:N	2.50	0.44
12:N1:61:ASN:HB3	12:N1:64:GLU:HB2	1.98	0.44
12:N1:110:LEU:HB2	12:N1:112:PHE:CE1	2.52	0.44
29:A1:1521:A:H62	29:A1:1569:G:H21	1.65	0.44
49:S2:37:ARG:NH1	53:A2:1201:G:OP1	2.51	0.44
53:A2:1194:A:H1'	53:A2:1196:G:H5''	1.99	0.44
2:D1:59:VAL:HG12	2:D1:62:PRO:HD2	2.00	0.44
48:R2:53:ARG:HG2	48:R2:63:GLN:HE21	1.81	0.44
7:I1:67:LEU:HD23	7:I1:87:LEU:HD23	1.99	0.44
29:A1:1344:G:OP1	29:A1:2723:G:O2'	2.30	0.44
52:V2:47:SER:O	52:V2:49:HIS:ND1	2.39	0.44
4:F1:66:GLN:HA	24:Z1:6:HIS:CD2	2.53	0.44
5:G1:4:ILE:HG21	5:G1:6:ARG:HH21	1.82	0.44
29:A1:1963:U:OP1	29:A1:2618:U:O2'	2.33	0.44
32:B2:189:ASP:N	32:B2:189:ASP:OD1	2.51	0.44
35:E2:92:LYS:HA	35:E2:93:PRO:HD3	1.88	0.44
43:M2:108:ARG:O	43:M2:112:GLY:N	2.46	0.44
46:P2:83:GLU:O	53:A2:457:A:O2'	2.36	0.44
53:A2:1123:C:H2'	53:A2:1124:G:H2'	1.99	0.44
2:D1:82:ARG:NH1	29:A1:2651:U:OP1	2.51	0.43
3:E1:155:LEU:HB3	3:E1:192:LEU:HD23	2.00	0.43
30:B1:19:C:H2'	30:B1:20:G:H8	1.83	0.43
39:I2:92:TYR:HD1	39:I2:95:LYS:HB2	1.83	0.43
53:A2:1155:G:H2'	53:A2:1156:G:C8	2.54	0.43
29:A1:657:G:N2	29:A1:660:A:OP2	2.46	0.43
29:A1:2169:C:H2'	29:A1:2171:G:H22	1.84	0.43
32:B2:29:ALA:HA	32:B2:32:ILE:HG12	1.99	0.43
36:F2:1:MET:N	36:F2:67:MET:O	2.39	0.43
46:P2:22:THR:OG1	46:P2:23:ASP:N	2.50	0.43
53:A2:1464:G:H2'	53:A2:1465:G:H8	1.83	0.43
9:K1:36:LYS:HD3	9:K1:39:LYS:HB3	2.00	0.43
10:L1:58:PHE:HE2	10:L1:64:ILE:HD11	1.83	0.43
20:V1:46:LYS:HD2	20:V1:78:TYR:HE1	1.82	0.43
29:A1:383:U:H3'	29:A1:384:A:H8	1.82	0.43
53:A2:923:A:H2'	53:A2:924:G:H8	1.84	0.43
4:F1:112:PRO:HB3	24:Z1:35:VAL:HG11	2.01	0.43
12:N1:30:ARG:NH2	30:B1:50:A:OP1	2.51	0.43
30:B1:67:C:N4	30:B1:111:C:O2'	2.44	0.43
39:I2:73:GLN:NE2	53:A2:1230:C:O2'	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F1:166:ASP:OD1	4:F1:166:ASP:N	2.38	0.43
9:K1:36:LYS:HZ3	29:A1:990:U:P	2.42	0.43
14:P1:54:LYS:NZ	29:A1:1042:C:OP2	2.41	0.43
47:Q2:15:MET:HB2	53:A2:270:G:C6	2.54	0.43
53:A2:613:G:OP1	53:A2:614:G:N2	2.52	0.43
2:D1:66:HIS:HA	2:D1:67:PHE:HA	1.74	0.43
10:L1:97:VAL:HG13	10:L1:101:ARG:HG2	2.01	0.43
29:A1:1619:A:H2'	29:A1:1620:A:C8	2.54	0.43
29:A1:2132:C:O2'	29:A1:2165:G:N1	2.46	0.43
43:M2:94:ARG:HH12	49:S2:81:ARG:HA	1.83	0.43
53:A2:294:G:N2	53:A2:548:U:O2	2.51	0.43
53:A2:1046:G:O2'	53:A2:1171:G:N2	2.51	0.43
53:A2:1140:C:O2'	53:A2:1142:G:OP1	2.30	0.43
29:A1:51:A:H2'	29:A1:52:A:C8	2.51	0.43
29:A1:141:C:H2'	29:A1:142:G:C8	2.54	0.43
29:A1:1725:A:N6	29:A1:1726:A:N1	2.66	0.43
32:B2:150:SER:OG	32:B2:151:GLY:N	2.52	0.43
34:D2:70:ILE:HD11	34:D2:75:PHE:HD1	1.83	0.43
53:A2:1110:C:C2	53:A2:1110:C:C1'	2.99	0.43
33:C2:84:ILE:HG23	33:C2:88:ARG:HH12	1.84	0.43
34:D2:94:LEU:O	34:D2:191:ARG:NH2	2.51	0.43
37:G2:36:LYS:HE2	39:I2:42:ARG:HH22	1.83	0.43
43:M2:117:VAL:HG21	53:A2:1209:C:H5'	2.00	0.43
46:P2:11:SER:OG	46:P2:12:LYS:N	2.50	0.43
53:A2:573:C:N4	53:A2:574:U:O4	2.52	0.43
8:J1:23:ARG:NH2	8:J1:28:SER:O	2.52	0.43
29:A1:300:G:N2	29:A1:388:G:N7	2.66	0.43
33:C2:91:LEU:HD23	33:C2:99:VAL:HB	2.00	0.43
53:A2:55:A:H62	53:A2:352:G:H21	1.67	0.43
53:A2:70:G:H2'	53:A2:71:C:C2	2.53	0.43
53:A2:1007:C:H4'	53:A2:1017:A:H61	1.84	0.43
2:D1:9:VAL:HA	13:O1:2:ASN:HD21	1.84	0.43
2:D1:144:ARG:HB3	2:D1:145:LYS:H	1.55	0.43
29:A1:5:A:H3'	29:A1:6:A:C8	2.54	0.43
29:A1:232:G:N2	29:A1:245:A:OP2	2.35	0.43
29:A1:314:A:H8	29:A1:315:G:C8	2.37	0.43
29:A1:1780:G:H2'	29:A1:1781:G:H8	1.83	0.43
29:A1:2591:A:H5''	29:A1:2592:G:H5'	2.01	0.43
30:B1:36:U:O2	30:B1:38:C:N4	2.52	0.43
37:G2:108:ALA:HB2	37:G2:123:GLU:HG2	2.01	0.43
53:A2:1281:G:N2	53:A2:1282:U:O4	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:233:HIS:HA	1:C1:234:GLY:HA2	1.80	0.42
4:F1:79:ASN:HD22	29:A1:2324:A:H2	1.66	0.42
29:A1:304:C:N4	29:A1:385:G:H22	2.15	0.42
29:A1:2817:C:H2'	29:A1:2818:G:C8	2.54	0.42
36:F2:87:ARG:NH1	48:R2:75:ILE:O	2.52	0.42
51:U2:25:LYS:NZ	53:A2:1266:A:OP2	2.36	0.42
53:A2:377:A:H2'	53:A2:378:A:H8	1.84	0.42
53:A2:988:G:H22	53:A2:998:U:H1'	1.85	0.42
5:G1:26:VAL:N	5:G1:32:GLU:OE1	2.36	0.42
9:K1:11:GLY:HA3	29:A1:623:G:H4'	2.00	0.42
29:A1:246:A:H2'	29:A1:247:A:C8	2.54	0.42
29:A1:1687:C:O2	29:A1:2712:U:O2'	2.37	0.42
33:C2:135:LYS:NZ	33:C2:170:GLN:HE21	2.16	0.42
45:O2:57:LEU:HD23	45:O2:57:LEU:HA	1.82	0.42
52:V2:30:ARG:C	52:V2:31:TYR:CD1	2.92	0.42
5:G1:27:LYS:H	5:G1:32:GLU:HB3	1.85	0.42
11:M1:34:ILE:HD11	29:A1:1326:A:H4'	2.01	0.42
16:R1:18:ARG:HA	16:R1:21:VAL:HG12	2.00	0.42
29:A1:292:G:H2'	29:A1:293:G:H8	1.84	0.42
29:A1:1142:U:O2'	29:A1:1144:A:OP1	2.32	0.42
33:C2:127:ARG:HH21	33:C2:192:THR:HG21	1.84	0.42
53:A2:74:C:N3	53:A2:89:U:N3	2.68	0.42
53:A2:114:C:N4	53:A2:231:G:OP2	2.38	0.42
4:F1:143:GLU:HA	24:Z1:31:ILE:HG13	2.00	0.42
18:T1:84:ARG:HB2	18:T1:95:LYS:HD2	2.02	0.42
29:A1:739:G:O2'	29:A1:829:G:OP1	2.33	0.42
29:A1:1216:G:H2'	29:A1:1217:G:C8	2.55	0.42
38:H2:119:LEU:HD11	38:H2:127:LEU:HD12	2.01	0.42
53:A2:451:C:N3	53:A2:452:C:N4	2.68	0.42
9:K1:22:GLY:HA3	29:A1:860:U:H3'	2.01	0.42
14:P1:92:ARG:NH2	15:Q1:11:GLN:HB2	2.35	0.42
14:P1:97:ASP:HA	14:P1:100:VAL:HG12	2.02	0.42
17:S1:55:ASN:HB2	17:S1:80:ILE:HG12	1.99	0.42
20:V1:82:ARG:HH12	20:V1:84:LEU:HB2	1.83	0.42
29:A1:1113:U:H6	29:A1:1113:U:H2'	1.72	0.42
29:A1:1162:G:H2'	29:A1:1163:G:H8	1.84	0.42
29:A1:1179:G:N2	29:A1:1180:A:N3	2.68	0.42
3:E1:62:ARG:NH2	29:A1:845:C:O3'	2.48	0.42
4:F1:32:PRO:HA	4:F1:162:THR:HB	2.01	0.42
6:H1:27:ARG:HD2	21:W1:71:TYR:HE2	1.84	0.42
9:K1:131:SER:OG	9:K1:132:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L1:71:ASP:N	10:L1:71:ASP:OD1	2.53	0.42
29:A1:521:G:H2'	29:A1:522:G:H8	1.84	0.42
29:A1:1092:G:N2	29:A1:1093:A:N7	2.68	0.42
29:A1:2764:A:H3'	29:A1:2765:A:H2'	2.02	0.42
33:C2:204:LEU:HD13	33:C2:204:LEU:HA	1.88	0.42
37:G2:37:ASN:HA	37:G2:40:ALA:HB3	2.01	0.42
47:Q2:4:LYS:HD2	53:A2:231:G:H21	1.84	0.42
53:A2:589:G:H22	53:A2:614:G:H4'	1.85	0.42
53:A2:1149:A:H2'	53:A2:1150:A:C8	2.55	0.42
53:A2:1271:G:H3'	53:A2:1272:G:C8	2.54	0.42
1:C1:18:VAL:HG21	29:A1:1614:C:H5''	2.01	0.42
7:I1:132:ALA:H	7:I1:134:ARG:NH1	2.17	0.42
29:A1:1162:G:H2'	29:A1:1163:G:C8	2.55	0.42
29:A1:2406:A:OP2	29:A1:2436:A:N6	2.48	0.42
33:C2:7:PRO:O	33:C2:11:ARG:NH1	2.52	0.42
41:K2:98:LEU:HD23	41:K2:98:LEU:HA	1.90	0.42
52:V2:30:ARG:C	52:V2:31:TYR:HD1	2.21	0.42
53:A2:594:A:H61	53:A2:612:G:H1	1.67	0.42
39:I2:103:THR:OG1	53:A2:1161:A:OP1	2.25	0.42
39:I2:104:ARG:HE	53:A2:1100:C:H4'	1.85	0.42
40:J2:35:SER:HB2	40:J2:73:ASP:HB2	2.01	0.42
44:N2:53:LEU:HD23	44:N2:53:LEU:HA	1.89	0.42
53:A2:1273:U:H2'	53:A2:1274:G:H8	1.85	0.42
11:M1:36:THR:OG1	11:M1:37:THR:N	2.53	0.42
13:O1:60:THR:HG22	13:O1:77:PRO:HA	2.02	0.42
20:V1:71:ASP:OD1	20:V1:72:ARG:N	2.52	0.42
29:A1:402:A:H62	29:A1:428:G:H21	1.67	0.42
29:A1:749:G:O6	29:A1:782:G:N2	2.53	0.42
29:A1:2092:U:H3	29:A1:2444:A:H2	1.67	0.42
29:A1:2487:U:OP1	29:A1:2489:C:N4	2.51	0.42
29:A1:2527:G:H1	29:A1:2585:C:H42	1.66	0.42
40:J2:9:ARG:HH21	40:J2:67:THR:HG21	1.84	0.42
53:A2:810:U:O2'	53:A2:847:U:O4	2.24	0.42
53:A2:1110:C:H41	53:A2:1122:C:H5	1.68	0.42
1:C1:35:LYS:HE2	1:C1:35:LYS:HB3	1.67	0.42
3:E1:118:ALA:HB2	3:E1:123:LEU:HD22	2.02	0.42
11:M1:13:HIS:CE1	11:M1:15:SER:HB2	2.55	0.42
12:N1:24:LEU:HB2	12:N1:85:VAL:HG12	2.02	0.42
24:Z1:19:GLY:O	24:Z1:38:LYS:NZ	2.53	0.42
29:A1:312:C:H2'	29:A1:380:G:N3	2.35	0.42
29:A1:1857:G:H2'	29:A1:1858:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A1:2301:A:H62	29:A1:2358:U:H3	1.67	0.42
37:G2:129:GLU:N	37:G2:129:GLU:OE1	2.53	0.42
41:K2:27:ASN:OD1	41:K2:28:THR:N	2.52	0.42
53:A2:216:C:C6	53:A2:216:C:C1'	2.95	0.42
53:A2:441:G:C5	53:A2:469:G:H8	2.37	0.42
53:A2:484:C:O2	53:A2:532:C:O2'	2.35	0.42
53:A2:981:G:N2	53:A2:1021:C:O4'	2.53	0.42
53:A2:1231:A:H2'	53:A2:1232:A:O4'	2.19	0.42
53:A2:1250:A:H2	53:A2:1293:G:H21	1.67	0.42
5:G1:85:LYS:HA	5:G1:85:LYS:HD3	1.92	0.41
11:M1:14:SER:HA	11:M1:17:ARG:HG2	2.01	0.41
29:A1:903:G:H2'	29:A1:904:G:C8	2.55	0.41
42:L2:15:ARG:HH21	53:A2:547:C:P	2.42	0.41
53:A2:484:C:H2'	53:A2:485:G:C8	2.55	0.41
53:A2:1150:A:H2'	53:A2:1151:A:C8	2.55	0.41
4:F1:117:PHE:HB3	24:Z1:42:PHE:O	2.20	0.41
5:G1:3:ARG:NH2	29:A1:1160:G:OP1	2.53	0.41
5:G1:12:PRO:HD3	5:G1:49:VAL:HG22	2.01	0.41
24:Z1:58:ARG:NH2	24:Z1:62:ARG:HE	2.18	0.41
29:A1:1114:U:N3	29:A1:1118:A:N7	2.67	0.41
29:A1:2328:C:H2'	29:A1:2329:G:H8	1.85	0.41
38:H2:119:LEU:HB3	38:H2:123:GLU:HG3	2.01	0.41
39:I2:15:ALA:HA	39:I2:65:VAL:HA	2.01	0.41
39:I2:91:ASP:HB2	39:I2:92:TYR:CE2	2.55	0.41
52:V2:120:LEU:HA	52:V2:121:ARG:HA	1.81	0.41
53:A2:772:U:O2'	53:A2:774:G:N7	2.41	0.41
53:A2:1030:G:N1	53:A2:1191:C:N3	2.68	0.41
3:E1:40:GLN:HE22	3:E1:182:ASN:HB2	1.84	0.41
29:A1:2178:G:N1	29:A1:2179:G:O6	2.54	0.41
34:D2:102:ASP:OD1	34:D2:102:ASP:N	2.52	0.41
40:J2:14:LYS:NZ	53:A2:1135:C:OP1	2.46	0.41
53:A2:72:C:O2'	53:A2:73:G:O5'	2.38	0.41
53:A2:693:G:H2'	53:A2:694:G:C8	2.56	0.41
53:A2:775:A:H2'	53:A2:776:U:O5'	2.20	0.41
5:G1:126:PRO:HA	5:G1:131:VAL:HG22	2.02	0.41
8:J1:71:ARG:HH22	13:O1:74:ARG:NE	2.18	0.41
29:A1:162:C:H2'	29:A1:163:G:C8	2.55	0.41
29:A1:926:U:O4	29:A1:946:C:N4	2.49	0.41
37:G2:20:ASP:HB3	37:G2:23:VAL:HG23	2.01	0.41
43:M2:79:LYS:HD2	43:M2:82:MET:HB2	2.02	0.41
3:E1:24:LEU:HD23	3:E1:24:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S1:90:GLU:HA	17:S1:93:GLU:HB2	2.03	0.41
29:A1:1061:C:H42	29:A1:1197:G:H1	1.68	0.41
29:A1:2287:A:H2'	29:A1:2288:A:C8	2.55	0.41
37:G2:54:THR:O	37:G2:56:GLN:N	2.53	0.41
53:A2:178:G:H2'	53:A2:179:A:H8	1.86	0.41
1:C1:222:ARG:NH1	29:A1:1860:C:OP2	2.48	0.41
5:G1:132:ARG:HE	5:G1:134:SER:HB3	1.85	0.41
16:R1:28:SER:OG	16:R1:29:LEU:N	2.54	0.41
29:A1:582:U:H2'	29:A1:583:G:H8	1.85	0.41
29:A1:2023:C:H2'	29:A1:2024:G:H8	1.85	0.41
29:A1:2328:C:H2'	29:A1:2329:G:C8	2.56	0.41
34:D2:162:LEU:HD23	34:D2:162:LEU:HA	1.90	0.41
53:A2:700:C:C4	53:A2:717:G:C5	2.98	0.41
53:A2:955:A:O2'	53:A2:1303:C:N3	2.41	0.41
53:A2:1149:A:H2'	53:A2:1150:A:H8	1.85	0.41
1:C1:105:ILE:HD13	1:C1:105:ILE:HA	1.85	0.41
2:D1:61:ARG:HA	2:D1:63:LEU:HG	2.02	0.41
5:G1:95:ARG:H	5:G1:95:ARG:HD3	1.84	0.41
33:C2:175:LEU:HD23	33:C2:175:LEU:HA	1.89	0.41
50:T2:73:HIS:O	50:T2:75:ASN:N	2.54	0.41
53:A2:46:G:N1	53:A2:361:C:O2	2.53	0.41
53:A2:774:G:N1	53:A2:1475:U:OP1	2.47	0.41
53:A2:1116:G:N7	53:A2:1124:G:N1	2.67	0.41
53:A2:1239:G:H2'	53:A2:1240:C:C6	2.55	0.41
11:M1:80:PHE:HA	11:M1:84:ALA:HB3	2.03	0.41
12:N1:80:LEU:HD23	12:N1:80:LEU:HA	1.92	0.41
29:A1:604:G:O2'	29:A1:2043:A:OP1	2.39	0.41
33:C2:147:LYS:HB2	33:C2:203:PHE:HD2	1.85	0.41
35:E2:118:ILE:HD12	35:E2:118:ILE:HA	1.95	0.41
49:S2:12:ASP:HB3	49:S2:13:ASP:H	1.60	0.41
53:A2:10:A:H2'	53:A2:11:G:C8	2.55	0.41
53:A2:461:G:H2'	53:A2:462:A:C8	2.56	0.41
53:A2:783:G:N2	53:A2:784:U:O4	2.53	0.41
53:A2:1110:C:N4	53:A2:1122:C:H41	2.19	0.41
1:C1:260:ARG:NH1	29:A1:1832:G:OP1	2.49	0.41
3:E1:140:LEU:HD23	3:E1:140:LEU:HA	1.84	0.41
7:I1:65:LYS:HB2	7:I1:65:LYS:HE2	1.89	0.41
10:L1:20:ALA:HB2	19:U1:79:ARG:HH21	1.86	0.41
29:A1:1523:C:H2'	29:A1:1524:G:C8	2.56	0.41
34:D2:22:LYS:NZ	53:A2:425:A:OP2	2.52	0.41
39:I2:4:TYR:HB2	39:I2:19:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:K2:53:SER:OG	53:A2:678:A:OP2	2.33	0.41
41:K2:95:ILE:HG21	48:R2:88:LYS:HE3	2.03	0.41
43:M2:21:TYR:HE1	53:A2:1312:G:H8	1.69	0.41
53:A2:138:G:N2	53:A2:173:A:N3	2.69	0.41
53:A2:567:G:H2'	53:A2:568:G:H8	1.86	0.41
53:A2:910:G:N2	53:A2:1367:G:N3	2.68	0.41
53:A2:1111:C:O2'	53:A2:1113:G:OP2	2.26	0.41
53:A2:1409:U:H3	53:A2:1451:G:H1	1.69	0.41
8:J1:31:LYS:NZ	29:A1:2690:C:OP2	2.37	0.41
10:L1:60:ARG:NE	19:U1:179:ASP:O	2.54	0.41
12:N1:35:ILE:H	12:N1:53:SER:HB2	1.85	0.41
19:U1:102:LEU:HD22	19:U1:139:VAL:HG12	2.02	0.41
29:A1:1142:U:H2'	29:A1:1144:A:H5''	2.03	0.41
29:A1:1483:G:H21	29:A1:1527:G:H5'	1.86	0.41
29:A1:2810:G:O2'	29:A1:2813:A:N7	2.41	0.41
48:R2:45:SER:OG	48:R2:48:GLY:N	2.54	0.41
53:A2:971:A:N6	53:A2:1196:G:O2'	2.50	0.41
53:A2:1145:C:N4	53:A2:1146:G:O6	2.54	0.41
18:T1:99:CYS:SG	18:T1:101:LYS:NZ	2.94	0.40
29:A1:702:A:C8	29:A1:703:A:H4'	2.56	0.40
29:A1:1874:U:H2'	29:A1:1875:G:H8	1.86	0.40
29:A1:2483:A:N6	29:A1:2495:G:O2'	2.54	0.40
30:B1:89:G:N2	30:B1:92:A:OP2	2.53	0.40
42:L2:47:LYS:NZ	42:L2:92:ASP:O	2.52	0.40
43:M2:15:VAL:HG12	43:M2:19:LEU:HG	2.04	0.40
43:M2:21:TYR:HE1	53:A2:1312:G:C8	2.39	0.40
49:S2:15:LEU:HG	49:S2:38:SER:HB2	2.03	0.40
50:T2:74:LYS:HE2	50:T2:74:LYS:HB2	1.94	0.40
53:A2:1124:G:H8	53:A2:1125:G:C5	2.39	0.40
7:I1:29:LYS:O	7:I1:32:THR:OG1	2.37	0.40
9:K1:45:LEU:HD13	9:K1:46:LYS:H	1.86	0.40
22:X1:25:VAL:O	22:X1:29:LYS:HG2	2.20	0.40
29:A1:1098:A:H2	29:A1:1099:G:C8	2.39	0.40
29:A1:1216:G:H2'	29:A1:1217:G:H8	1.85	0.40
29:A1:1874:U:H2'	29:A1:1875:G:C8	2.56	0.40
29:A1:1878:G:N2	29:A1:1920:G:N3	2.69	0.40
29:A1:2202:C:H2'	29:A1:2203:C:C6	2.56	0.40
29:A1:2749:A:H62	29:A1:2785:G:H21	1.69	0.40
40:J2:4:ILE:N	40:J2:74:ILE:O	2.46	0.40
42:L2:38:THR:HG22	42:L2:39:VAL:HG23	2.02	0.40
44:N2:50:LYS:HE3	44:N2:50:LYS:HB2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A2:611:G:H2'	53:A2:612:G:H8	1.86	0.40
5:G1:89:ILE:HG21	5:G1:94:TYR:HB2	2.03	0.40
19:U1:53:ILE:HG12	19:U1:71:VAL:HG13	2.02	0.40
29:A1:943:U:H4'	29:A1:944:A:H2'	2.04	0.40
34:D2:151:LYS:HB2	34:D2:151:LYS:HE2	1.88	0.40
40:J2:55:LYS:HE2	40:J2:55:LYS:HB2	1.92	0.40
43:M2:110:ARG:HA	43:M2:110:ARG:HD2	1.92	0.40
46:P2:48:TRP:CE3	46:P2:49:LEU:HB2	2.56	0.40
53:A2:1054:G:H2'	53:A2:1055:U:O4'	2.21	0.40
1:C1:61:LEU:HD12	1:C1:61:LEU:HA	1.83	0.40
2:D1:52:LEU:HA	2:D1:52:LEU:HD23	1.76	0.40
22:X1:20:GLU:O	22:X1:24:LEU:N	2.49	0.40
29:A1:85:C:HO2'	29:A1:102:U:HO2'	1.55	0.40
29:A1:913:G:H21	29:A1:915:A:H61	1.70	0.40
29:A1:2057:A:O2'	29:A1:2059:G:OP2	2.38	0.40
32:B2:205:ASP:N	32:B2:205:ASP:OD1	2.52	0.40
37:G2:16:LEU:HD23	37:G2:16:LEU:HA	1.91	0.40
53:A2:842:A:N3	53:A2:895:A:O2'	2.54	0.40
53:A2:1423:G:H4'	53:A2:1424:G:C4	2.56	0.40
5:G1:125:VAL:HB	5:G1:130:ARG:NH1	2.36	0.40
5:G1:158:HIS:HE1	5:G1:160:LYS:NZ	2.20	0.40
29:A1:443:A:N6	29:A1:2422:U:O4	2.42	0.40
29:A1:692:C:H6	29:A1:692:C:H2'	1.70	0.40
29:A1:930:G:O6	29:A1:942:C:N4	2.54	0.40
29:A1:1842:A:N6	29:A1:1843:A:N1	2.70	0.40
29:A1:2533:U:H1'	29:A1:2534:C:H5	1.87	0.40
36:F2:10:LEU:HD23	36:F2:10:LEU:HA	1.90	0.40
41:K2:79:SER:OG	41:K2:106:LYS:NZ	2.53	0.40
52:V2:30:ARG:N	52:V2:31:TYR:CD1	2.89	0.40
53:A2:68:G:H2'	53:A2:70:G:H22	1.87	0.40
53:A2:212:C:H6	53:A2:212:C:H2'	1.73	0.40
53:A2:911:C:H42	53:A2:915:A:H61	1.68	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	C1	270/272 (99%)	237 (88%)	32 (12%)	1 (0%)	30	61
2	D1	203/205 (99%)	164 (81%)	35 (17%)	4 (2%)	6	28
3	E1	206/208 (99%)	180 (87%)	26 (13%)	0	100	100
4	F1	179/181 (99%)	157 (88%)	22 (12%)	0	100	100
5	G1	168/170 (99%)	136 (81%)	28 (17%)	4 (2%)	5	24
6	H1	48/50 (96%)	38 (79%)	10 (21%)	0	100	100
7	I1	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
8	J1	120/122 (98%)	97 (81%)	23 (19%)	0	100	100
9	K1	148/150 (99%)	107 (72%)	38 (26%)	3 (2%)	6	28
10	L1	139/141 (99%)	117 (84%)	20 (14%)	2 (1%)	9	34
11	M1	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
12	N1	109/111 (98%)	94 (86%)	15 (14%)	0	100	100
13	O1	135/137 (98%)	114 (84%)	20 (15%)	1 (1%)	19	49
14	P1	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
15	Q1	99/101 (98%)	83 (84%)	16 (16%)	0	100	100
16	R1	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
17	S1	90/92 (98%)	77 (86%)	13 (14%)	0	100	100
18	T1	100/102 (98%)	77 (77%)	22 (22%)	1 (1%)	13	42
19	U1	177/179 (99%)	134 (76%)	42 (24%)	1 (1%)	22	52
20	V1	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
21	W1	95/97 (98%)	81 (85%)	13 (14%)	1 (1%)	12	40
22	X1	67/69 (97%)	60 (90%)	7 (10%)	0	100	100
23	Y1	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
24	Z1	61/63 (97%)	41 (67%)	17 (28%)	3 (5%)	2	12
25	a1	57/59 (97%)	47 (82%)	10 (18%)	0	100	100
26	b1	43/45 (96%)	29 (67%)	14 (33%)	0	100	100
27	c1	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
28	d1	59/61 (97%)	48 (81%)	10 (17%)	1 (2%)	7	31
31	e1	34/36 (94%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B2	235/237 (99%)	197 (84%)	38 (16%)	0	100	100
33	C2	204/206 (99%)	180 (88%)	24 (12%)	0	100	100
34	D2	206/208 (99%)	178 (86%)	27 (13%)	1 (0%)	25	56
35	E2	149/151 (99%)	134 (90%)	15 (10%)	0	100	100
36	F2	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
37	G2	153/155 (99%)	126 (82%)	27 (18%)	0	100	100
38	H2	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
39	I2	125/127 (98%)	100 (80%)	25 (20%)	0	100	100
40	J2	97/99 (98%)	84 (87%)	13 (13%)	0	100	100
41	K2	116/118 (98%)	97 (84%)	19 (16%)	0	100	100
42	L2	123/125 (98%)	97 (79%)	25 (20%)	1 (1%)	16	45
43	M2	115/117 (98%)	96 (84%)	18 (16%)	1 (1%)	14	44
44	N2	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
45	O2	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
46	P2	82/84 (98%)	74 (90%)	8 (10%)	0	100	100
47	Q2	98/100 (98%)	84 (86%)	14 (14%)	0	100	100
48	R2	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
49	S2	76/78 (97%)	53 (70%)	23 (30%)	0	100	100
50	T2	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	13	42
51	U2	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
52	V2	119/121 (98%)	92 (77%)	26 (22%)	1 (1%)	16	45
All	All	5720/5820 (98%)	4828 (84%)	865 (15%)	27 (0%)	27	56

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G1	90	LYS
50	T2	74	LYS
9	K1	58	THR
19	U1	53	ILE
24	Z1	25	TYR
28	d1	49	VAL
34	D2	32	ALA
52	V2	103	ARG
2	D1	17	ASP

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Mol	Chain	Res	Type
2	D1	145	LYS
9	K1	12	ALA
43	M2	61	GLU
1	C1	34	VAL
9	K1	13	ASN
10	L1	8	LYS
2	D1	83	ASP
2	D1	144	ARG
10	L1	6	ARG
24	Z1	3	GLU
24	Z1	57	GLU
42	L2	48	PRO
5	G1	12	PRO
5	G1	89	ILE
13	O1	56	GLY
18	T1	53	PRO
21	W1	9	GLY
5	G1	55	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C1	214/214 (100%)	210 (98%)	4 (2%)	52	72
2	D1	165/165 (100%)	164 (99%)	1 (1%)	84	90
3	E1	165/165 (100%)	163 (99%)	2 (1%)	67	81
4	F1	155/155 (100%)	152 (98%)	3 (2%)	52	72
5	G1	142/142 (100%)	135 (95%)	7 (5%)	21	49
6	H1	41/41 (100%)	41 (100%)	0	100	100
7	I1	117/117 (100%)	117 (100%)	0	100	100
8	J1	100/100 (100%)	99 (99%)	1 (1%)	73	84
9	K1	116/116 (100%)	111 (96%)	5 (4%)	25	52
10	L1	111/111 (100%)	106 (96%)	5 (4%)	23	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M1	100/100 (100%)	98 (98%)	2 (2%)	50	71
12	N1	87/87 (100%)	84 (97%)	3 (3%)	32	58
13	O1	120/120 (100%)	115 (96%)	5 (4%)	25	53
14	P1	93/93 (100%)	90 (97%)	3 (3%)	34	60
15	Q1	82/82 (100%)	81 (99%)	1 (1%)	67	81
16	R1	92/92 (100%)	91 (99%)	1 (1%)	70	82
17	S1	74/74 (100%)	72 (97%)	2 (3%)	40	65
18	T1	85/85 (100%)	84 (99%)	1 (1%)	67	81
19	U1	158/158 (100%)	156 (99%)	2 (1%)	65	79
20	V1	62/62 (100%)	62 (100%)	0	100	100
21	W1	82/82 (100%)	81 (99%)	1 (1%)	67	81
22	X1	64/64 (100%)	63 (98%)	1 (2%)	58	75
23	Y1	51/51 (100%)	50 (98%)	1 (2%)	50	71
24	Z1	57/57 (100%)	55 (96%)	2 (4%)	31	57
25	a1	51/51 (100%)	50 (98%)	1 (2%)	50	71
26	b1	44/44 (100%)	39 (89%)	5 (11%)	4	19
27	c1	42/42 (100%)	40 (95%)	2 (5%)	21	50
28	d1	51/51 (100%)	49 (96%)	2 (4%)	27	55
31	e1	33/33 (100%)	31 (94%)	2 (6%)	15	42
32	B2	205/205 (100%)	201 (98%)	4 (2%)	50	71
33	C2	160/160 (100%)	158 (99%)	2 (1%)	65	79
34	D2	180/180 (100%)	179 (99%)	1 (1%)	84	90
35	E2	116/116 (100%)	115 (99%)	1 (1%)	75	85
36	F2	90/90 (100%)	90 (100%)	0	100	100
37	G2	126/126 (100%)	125 (99%)	1 (1%)	79	87
38	H2	119/119 (100%)	119 (100%)	0	100	100
39	I2	98/98 (100%)	98 (100%)	0	100	100
40	J2	89/89 (100%)	88 (99%)	1 (1%)	70	82
41	K2	89/89 (100%)	88 (99%)	1 (1%)	70	82
42	L2	104/104 (100%)	102 (98%)	2 (2%)	52	72
43	M2	94/94 (100%)	91 (97%)	3 (3%)	34	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	N2	49/49 (100%)	47 (96%)	2 (4%)	26	54
45	O2	79/79 (100%)	79 (100%)	0	100	100
46	P2	72/72 (100%)	72 (100%)	0	100	100
47	Q2	95/95 (100%)	94 (99%)	1 (1%)	70	82
48	R2	55/55 (100%)	53 (96%)	2 (4%)	30	57
49	S2	67/67 (100%)	63 (94%)	4 (6%)	16	42
50	T2	76/76 (100%)	75 (99%)	1 (1%)	65	79
51	U2	20/20 (100%)	19 (95%)	1 (5%)	20	48
52	V2	103/103 (100%)	98 (95%)	5 (5%)	21	49
All	All	4840/4840 (100%)	4743 (98%)	97 (2%)	50	71

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C1	43	ARG
1	C1	198	ASN
1	C1	242	ARG
1	C1	268	ARG
2	D1	169	ASN
3	E1	2	LYS
3	E1	74	ARG
4	F1	40	ASN
4	F1	47	LYS
4	F1	96	ARG
5	G1	42	ARG
5	G1	95	ARG
5	G1	101	ARG
5	G1	130	ARG
5	G1	132	ARG
5	G1	147	ASN
5	G1	149	ARG
8	J1	53	LYS
9	K1	13	ASN
9	K1	45	LEU
9	K1	62	LEU
9	K1	90	ARG
9	K1	111	ARG
10	L1	3	MET
10	L1	10	ARG

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Mol	Chain	Res	Type
10	L1	60	ARG
10	L1	89	ASN
10	L1	133	ARG
11	M1	9	LYS
11	M1	67	LEU
12	N1	57	LYS
12	N1	61	ASN
12	N1	106	ARG
13	O1	13	ARG
13	O1	41	ARG
13	O1	85	LYS
13	O1	107	ASP
13	O1	108	ARG
14	P1	3	ARG
14	P1	53	ARG
14	P1	55	ARG
15	Q1	82	ARG
16	R1	42	ARG
17	S1	65	ARG
17	S1	76	ARG
18	T1	84	ARG
19	U1	31	ARG
19	U1	79	ARG
21	W1	81	LYS
22	X1	7	ARG
23	Y1	29	ARG
24	Z1	38	LYS
24	Z1	55	ARG
25	a1	55	ARG
26	b1	19	ARG
26	b1	20	ASN
26	b1	25	LYS
26	b1	44	ARG
26	b1	50	ARG
27	c1	1	MET
27	c1	28	ARG
28	d1	30	ARG
28	d1	32	LEU
31	e1	9	ARG
31	e1	22	ARG
32	B2	25	ASN
32	B2	96	ARG

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Mol	Chain	Res	Type
32	B2	132	LYS
32	B2	196	LEU
33	C2	79	ARG
33	C2	181	ASN
34	D2	49	ARG
35	E2	15	ARG
37	G2	37	ASN
40	J2	5	ARG
41	K2	18	ARG
42	L2	89	ARG
42	L2	111	LYS
43	M2	14	ARG
43	M2	46	LYS
43	M2	115	LYS
44	N2	44	LEU
44	N2	57	ARG
47	Q2	52	LYS
48	R2	36	ASN
48	R2	58	LEU
49	S2	37	ARG
49	S2	53	ASN
49	S2	70	LYS
49	S2	81	ARG
50	T2	23	ARG
51	U2	9	ARG
52	V2	28	LEU
52	V2	31	TYR
52	V2	59	GLN
52	V2	97	ARG
52	V2	122	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	C1	198	ASN
1	C1	233	HIS
2	D1	85	ASN
2	D1	135	HIS
2	D1	169	ASN
3	E1	69	HIS
4	F1	40	ASN
4	F1	41	GLN

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Mol	Chain	Res	Type
4	F1	66	GLN
4	F1	79	ASN
5	G1	61	HIS
5	G1	65	HIS
5	G1	147	ASN
5	G1	158	HIS
9	K1	13	ASN
9	K1	68	GLN
10	L1	89	ASN
11	M1	11	ASN
12	N1	34	HIS
12	N1	61	ASN
14	P1	49	HIS
14	P1	117	GLN
16	R1	34	ASN
16	R1	60	ASN
16	R1	102	HIS
19	U1	30	ASN
19	U1	34	ASN
19	U1	73	GLN
22	X1	47	ASN
25	a1	23	HIS
26	b1	26	ASN
26	b1	49	HIS
28	d1	31	HIS
32	B2	25	ASN
32	B2	95	GLN
32	B2	113	HIS
33	C2	181	ASN
34	D2	103	ASN
36	F2	32	ASN
37	G2	64	GLN
38	H2	78	GLN
38	H2	82	HIS
39	I2	73	GLN
40	J2	62	HIS
40	J2	76	ASN
41	K2	13	GLN
42	L2	8	ASN
45	O2	37	ASN
45	O2	46	HIS
48	R2	36	ASN

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Mol	Chain	Res	Type
48	R2	63	GLN
49	S2	23	ASN
49	S2	57	HIS
50	T2	26	ASN
52	V2	2	ASN
52	V2	107	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	A1	2911/2912 (99%)	950 (32%)	25 (0%)
30	B1	121/122 (99%)	29 (23%)	0
53	A2	1505/1506 (99%)	522 (34%)	23 (1%)
All	All	4537/4540 (99%)	1501 (33%)	48 (1%)

All (1501) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	A1	2	G
29	A1	3	U
29	A1	4	C
29	A1	10	G
29	A1	15	G
29	A1	23	G
29	A1	28	A
29	A1	34	C
29	A1	36	G
29	A1	38	A
29	A1	45	C
29	A1	48	A
29	A1	49	U
29	A1	50	G
29	A1	53	G
29	A1	54	G
29	A1	60	G
29	A1	63	A
29	A1	68	C
29	A1	70	A
29	A1	71	U
29	A1	73	A
29	A1	74	G

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Mol	Chain	Res	Type
29	A1	84	G
29	A1	85	C
29	A1	88	G
29	A1	89	U
29	A1	99	G
29	A1	100	G
29	A1	104	C
29	A1	107	G
29	A1	114	C
29	A1	116	A
29	A1	118	U
29	A1	119	G
29	A1	123	G
29	A1	127	C
29	A1	129	G
29	A1	139	A
29	A1	141	C
29	A1	147	U
29	A1	152	G
29	A1	155	C
29	A1	160	U
29	A1	161	G
29	A1	168	G
29	A1	173	C
29	A1	176	G
29	A1	182	C
29	A1	183	U
29	A1	186	A
29	A1	189	A
29	A1	190	U
29	A1	191	C
29	A1	193	C
29	A1	194	A
29	A1	205	G
29	A1	206	A
29	A1	208	A
29	A1	212	A
29	A1	213	A
29	A1	215	A
29	A1	217	A
29	A1	218	A
29	A1	219	A

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Mol	Chain	Res	Type
29	A1	220	U
29	A1	222	G
29	A1	223	A
29	A1	231	A
29	A1	238	G
29	A1	239	C
29	A1	242	G
29	A1	251	G
29	A1	253	C
29	A1	262	A
29	A1	263	C
29	A1	269	G
29	A1	270	G
29	A1	271	C
29	A1	272	U
29	A1	273	U
29	A1	274	G
29	A1	275	U
29	A1	276	C
29	A1	284	G
29	A1	289	U
29	A1	290	G
29	A1	291	G
29	A1	299	G
29	A1	300	G
29	A1	301	A
29	A1	302	C
29	A1	303	A
29	A1	306	G
29	A1	307	A
29	A1	308	A
29	A1	310	C
29	A1	313	C
29	A1	315	G
29	A1	324	A
29	A1	331	U
29	A1	336	A
29	A1	338	C
29	A1	341	C
29	A1	342	G
29	A1	347	A
29	A1	348	G

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Mol	Chain	Res	Type
29	A1	350	G
29	A1	352	G
29	A1	353	U
29	A1	354	G
29	A1	355	A
29	A1	360	C
29	A1	371	A
29	A1	377	G
29	A1	378	G
29	A1	381	G
29	A1	382	A
29	A1	384	A
29	A1	387	U
29	A1	388	G
29	A1	392	G
29	A1	394	A
29	A1	395	C
29	A1	398	G
29	A1	399	A
29	A1	400	G
29	A1	404	C
29	A1	410	G
29	A1	412	U
29	A1	414	G
29	A1	420	C
29	A1	424	G
29	A1	428	G
29	A1	433	U
29	A1	434	G
29	A1	435	G
29	A1	436	G
29	A1	439	G
29	A1	440	A
29	A1	441	C
29	A1	443	A
29	A1	457	A
29	A1	460	U
29	A1	463	U
29	A1	465	C
29	A1	467	G
29	A1	468	G
29	A1	472	C

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Mol	Chain	Res	Type
29	A1	482	A
29	A1	483	C
29	A1	484	C
29	A1	485	A
29	A1	486	G
29	A1	487	U
29	A1	492	U
29	A1	493	G
29	A1	495	G
29	A1	498	A
29	A1	508	A
29	A1	509	G
29	A1	512	C
29	A1	519	A
29	A1	521	G
29	A1	523	G
29	A1	532	A
29	A1	535	G
29	A1	536	C
29	A1	548	G
29	A1	555	A
29	A1	556	A
29	A1	557	G
29	A1	558	C
29	A1	559	A
29	A1	560	G
29	A1	564	C
29	A1	565	G
29	A1	566	G
29	A1	575	G
29	A1	581	G
29	A1	587	U
29	A1	588	G
29	A1	591	U
29	A1	592	A
29	A1	593	U
29	A1	596	A
29	A1	597	A
29	A1	598	G
29	A1	599	C
29	A1	600	A
29	A1	608	G

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Mol	Chain	Res	Type
29	A1	611	A
29	A1	612	C
29	A1	618	G
29	A1	620	C
29	A1	621	G
29	A1	626	C
29	A1	628	A
29	A1	632	U
29	A1	641	G
29	A1	643	G
29	A1	645	C
29	A1	648	A
29	A1	661	C
29	A1	662	C
29	A1	664	A
29	A1	671	A
29	A1	673	A
29	A1	680	A
29	A1	681	A
29	A1	684	G
29	A1	685	G
29	A1	686	C
29	A1	687	C
29	A1	689	G
29	A1	690	C
29	A1	691	A
29	A1	692	C
29	A1	693	G
29	A1	695	G
29	A1	696	G
29	A1	698	C
29	A1	700	G
29	A1	701	A
29	A1	702	A
29	A1	703	A
29	A1	704	A
29	A1	705	G
29	A1	718	G
29	A1	720	C
29	A1	728	C
29	A1	735	G
29	A1	740	C

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Mol	Chain	Res	Type
29	A1	742	C
29	A1	749	G
29	A1	750	G
29	A1	751	G
29	A1	753	G
29	A1	755	A
29	A1	756	G
29	A1	768	C
29	A1	774	G
29	A1	775	G
29	A1	777	G
29	A1	779	C
29	A1	785	C
29	A1	790	G
29	A1	796	U
29	A1	797	G
29	A1	806	U
29	A1	810	A
29	A1	814	G
29	A1	824	G
29	A1	825	G
29	A1	830	A
29	A1	831	A
29	A1	833	A
29	A1	834	G
29	A1	838	A
29	A1	840	C
29	A1	841	G
29	A1	846	C
29	A1	849	A
29	A1	854	G
29	A1	855	C
29	A1	857	G
29	A1	861	C
29	A1	863	C
29	A1	868	A
29	A1	874	C
29	A1	876	U
29	A1	877	U
29	A1	882	U
29	A1	887	C
29	A1	894	G

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Mol	Chain	Res	Type
29	A1	895	C
29	A1	899	C
29	A1	904	G
29	A1	908	G
29	A1	912	A
29	A1	915	A
29	A1	922	G
29	A1	925	C
29	A1	929	G
29	A1	931	G
29	A1	932	G
29	A1	933	C
29	A1	934	C
29	A1	935	C
29	A1	936	A
29	A1	937	C
29	A1	938	C
29	A1	942	C
29	A1	943	U
29	A1	945	C
29	A1	947	A
29	A1	949	A
29	A1	952	C
29	A1	958	A
29	A1	962	C
29	A1	964	G
29	A1	965	A
29	A1	966	A
29	A1	971	C
29	A1	974	A
29	A1	975	G
29	A1	979	G
29	A1	985	G
29	A1	989	G
29	A1	991	G
29	A1	993	G
29	A1	996	C
29	A1	1000	A
29	A1	1004	A
29	A1	1006	A
29	A1	1008	C
29	A1	1011	C

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Mol	Chain	Res	Type
29	A1	1012	C
29	A1	1016	U
29	A1	1018	C
29	A1	1021	G
29	A1	1022	C
29	A1	1029	A
29	A1	1031	A
29	A1	1036	A
29	A1	1037	G
29	A1	1038	A
29	A1	1040	C
29	A1	1044	A
29	A1	1050	G
29	A1	1051	G
29	A1	1053	C
29	A1	1059	G
29	A1	1060	U
29	A1	1061	C
29	A1	1063	G
29	A1	1065	G
29	A1	1066	C
29	A1	1070	G
29	A1	1071	U
29	A1	1074	U
29	A1	1075	A
29	A1	1081	U
29	A1	1093	A
29	A1	1095	G
29	A1	1096	A
29	A1	1098	A
29	A1	1099	G
29	A1	1100	C
29	A1	1101	C
29	A1	1105	A
29	A1	1106	U
29	A1	1108	U
29	A1	1109	U
29	A1	1113	U
29	A1	1114	U
29	A1	1115	A
29	A1	1117	A
29	A1	1118	A

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Mol	Chain	Res	Type
29	A1	1119	G
29	A1	1121	A
29	A1	1124	C
29	A1	1125	A
29	A1	1126	U
29	A1	1127	C
29	A1	1128	A
29	A1	1129	U
29	A1	1131	U
29	A1	1132	A
29	A1	1134	A
29	A1	1135	G
29	A1	1136	A
29	A1	1140	C
29	A1	1141	G
29	A1	1143	A
29	A1	1144	A
29	A1	1145	U
29	A1	1146	A
29	A1	1147	G
29	A1	1148	C
29	A1	1149	U
29	A1	1153	U
29	A1	1155	G
29	A1	1158	G
29	A1	1159	A
29	A1	1161	U
29	A1	1170	G
29	A1	1178	U
29	A1	1181	U
29	A1	1182	C
29	A1	1183	G
29	A1	1185	G
29	A1	1186	G
29	A1	1190	A
29	A1	1191	A
29	A1	1192	G
29	A1	1196	A
29	A1	1199	G
29	A1	1221	A
29	A1	1223	G
29	A1	1224	A

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Mol	Chain	Res	Type
29	A1	1226	C
29	A1	1229	A
29	A1	1230	G
29	A1	1231	G
29	A1	1235	U
29	A1	1251	A
29	A1	1253	G
29	A1	1259	G
29	A1	1267	A
29	A1	1285	A
29	A1	1288	U
29	A1	1289	A
29	A1	1291	G
29	A1	1292	G
29	A1	1295	A
29	A1	1296	G
29	A1	1300	G
29	A1	1301	A
29	A1	1302	A
29	A1	1303	U
29	A1	1304	G
29	A1	1307	G
29	A1	1313	A
29	A1	1316	A
29	A1	1317	A
29	A1	1319	G
29	A1	1320	A
29	A1	1321	U
29	A1	1328	G
29	A1	1333	G
29	A1	1348	U
29	A1	1349	A
29	A1	1350	A
29	A1	1351	G
29	A1	1353	C
29	A1	1355	A
29	A1	1357	G
29	A1	1362	C
29	A1	1364	U
29	A1	1369	A
29	A1	1373	G
29	A1	1377	U

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Mol	Chain	Res	Type
29	A1	1378	C
29	A1	1380	G
29	A1	1382	G
29	A1	1389	U
29	A1	1390	A
29	A1	1392	G
29	A1	1397	A
29	A1	1398	C
29	A1	1400	U
29	A1	1403	G
29	A1	1405	U
29	A1	1407	A
29	A1	1408	A
29	A1	1409	G
29	A1	1411	C
29	A1	1413	A
29	A1	1414	A
29	A1	1416	G
29	A1	1422	G
29	A1	1424	C
29	A1	1429	G
29	A1	1432	A
29	A1	1433	G
29	A1	1434	C
29	A1	1443	A
29	A1	1454	U
29	A1	1459	C
29	A1	1462	G
29	A1	1463	U
29	A1	1464	G
29	A1	1467	A
29	A1	1468	U
29	A1	1469	G
29	A1	1471	G
29	A1	1476	C
29	A1	1478	C
29	A1	1480	C
29	A1	1483	G
29	A1	1485	C
29	A1	1488	G
29	A1	1490	G
29	A1	1493	A

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Mol	Chain	Res	Type
29	A1	1498	A
29	A1	1499	G
29	A1	1500	C
29	A1	1504	G
29	A1	1509	A
29	A1	1512	C
29	A1	1516	C
29	A1	1520	A
29	A1	1524	G
29	A1	1531	G
29	A1	1535	G
29	A1	1537	U
29	A1	1538	A
29	A1	1539	G
29	A1	1540	G
29	A1	1541	C
29	A1	1542	A
29	A1	1543	A
29	A1	1545	U
29	A1	1546	C
29	A1	1549	C
29	A1	1551	U
29	A1	1552	C
29	A1	1557	C
29	A1	1558	A
29	A1	1559	A
29	A1	1560	G
29	A1	1562	U
29	A1	1565	G
29	A1	1571	U
29	A1	1574	G
29	A1	1581	C
29	A1	1584	A
29	A1	1585	C
29	A1	1586	G
29	A1	1587	G
29	A1	1589	U
29	A1	1591	A
29	A1	1592	C
29	A1	1593	A
29	A1	1595	C
29	A1	1596	C

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Mol	Chain	Res	Type
29	A1	1599	C
29	A1	1607	A
29	A1	1608	G
29	A1	1609	G
29	A1	1615	A
29	A1	1616	A
29	A1	1618	A
29	A1	1619	A
29	A1	1620	A
29	A1	1627	U
29	A1	1630	G
29	A1	1631	C
29	A1	1632	A
29	A1	1633	C
29	A1	1635	A
29	A1	1639	G
29	A1	1644	A
29	A1	1646	C
29	A1	1655	C
29	A1	1656	A
29	A1	1658	A
29	A1	1660	C
29	A1	1663	C
29	A1	1664	A
29	A1	1665	C
29	A1	1667	G
29	A1	1683	A
29	A1	1687	C
29	A1	1688	U
29	A1	1695	C
29	A1	1697	C
29	A1	1701	A
29	A1	1703	A
29	A1	1718	A
29	A1	1722	U
29	A1	1723	G
29	A1	1726	A
29	A1	1732	C
29	A1	1736	G
29	A1	1740	C
29	A1	1744	G
29	A1	1747	A

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Mol	Chain	Res	Type
29	A1	1748	G
29	A1	1749	A
29	A1	1750	A
29	A1	1761	C
29	A1	1764	G
29	A1	1765	G
29	A1	1769	A
29	A1	1770	U
29	A1	1771	G
29	A1	1777	C
29	A1	1778	G
29	A1	1782	A
29	A1	1783	G
29	A1	1784	C
29	A1	1788	A
29	A1	1789	G
29	A1	1796	G
29	A1	1797	G
29	A1	1805	G
29	A1	1806	A
29	A1	1809	G
29	A1	1813	A
29	A1	1814	C
29	A1	1817	A
29	A1	1820	A
29	A1	1824	A
29	A1	1827	U
29	A1	1832	G
29	A1	1833	C
29	A1	1834	G
29	A1	1835	A
29	A1	1840	G
29	A1	1842	A
29	A1	1844	G
29	A1	1848	A
29	A1	1849	G
29	A1	1853	U
29	A1	1854	A
29	A1	1861	G
29	A1	1862	A
29	A1	1880	A
29	A1	1881	A

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Mol	Chain	Res	Type
29	A1	1885	C
29	A1	1886	A
29	A1	1888	G
29	A1	1891	G
29	A1	1898	G
29	A1	1902	G
29	A1	1904	C
29	A1	1905	C
29	A1	1906	C
29	A1	1907	G
29	A1	1911	C
29	A1	1912	G
29	A1	1914	A
29	A1	1920	G
29	A1	1921	G
29	A1	1924	A
29	A1	1927	G
29	A1	1930	G
29	A1	1936	A
29	A1	1937	A
29	A1	1938	C
29	A1	1940	A
29	A1	1943	A
29	A1	1944	C
29	A1	1952	A
29	A1	1953	G
29	A1	1954	G
29	A1	1955	U
29	A1	1958	C
29	A1	1962	A
29	A1	1964	U
29	A1	1967	U
29	A1	1968	U
29	A1	1977	A
29	A1	1979	U
29	A1	1987	U
29	A1	1991	C
29	A1	1993	A
29	A1	1994	A
29	A1	1995	A
29	A1	1996	A
29	A1	2001	A

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Mol	Chain	Res	Type
29	A1	2006	C
29	A1	2012	C
29	A1	2016	G
29	A1	2017	U
29	A1	2020	C
29	A1	2033	G
29	A1	2044	A
29	A1	2047	G
29	A1	2049	C
29	A1	2052	U
29	A1	2055	A
29	A1	2057	A
29	A1	2058	U
29	A1	2063	C
29	A1	2065	U
29	A1	2067	C
29	A1	2076	G
29	A1	2079	C
29	A1	2080	G
29	A1	2084	A
29	A1	2085	G
29	A1	2086	A
29	A1	2089	C
29	A1	2093	G
29	A1	2094	G
29	A1	2098	U
29	A1	2109	C
29	A1	2117	G
29	A1	2118	G
29	A1	2123	U
29	A1	2127	C
29	A1	2128	G
29	A1	2129	C
29	A1	2130	G
29	A1	2131	C
29	A1	2132	C
29	A1	2133	U
29	A1	2135	C
29	A1	2136	G
29	A1	2137	U
29	A1	2138	A
29	A1	2139	G

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Mol	Chain	Res	Type
29	A1	2140	G
29	A1	2141	A
29	A1	2142	U
29	A1	2143	A
29	A1	2147	G
29	A1	2150	A
29	A1	2151	G
29	A1	2152	C
29	A1	2153	C
29	A1	2155	G
29	A1	2156	U
29	A1	2157	G
29	A1	2158	A
29	A1	2159	A
29	A1	2160	C
29	A1	2161	C
29	A1	2163	C
29	A1	2165	G
29	A1	2168	U
29	A1	2170	C
29	A1	2171	G
29	A1	2172	G
29	A1	2173	G
29	A1	2174	U
29	A1	2178	G
29	A1	2179	G
29	A1	2183	G
29	A1	2184	G
29	A1	2185	C
29	A1	2187	C
29	A1	2188	C
29	A1	2189	G
29	A1	2190	G
29	A1	2192	G
29	A1	2193	A
29	A1	2194	A
29	A1	2195	A
29	A1	2196	U
29	A1	2198	C
29	A1	2201	C
29	A1	2202	C
29	A1	2208	G

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Mol	Chain	Res	Type
29	A1	2209	C
29	A1	2210	G
29	A1	2213	U
29	A1	2216	G
29	A1	2217	G
29	A1	2222	A
29	A1	2223	A
29	A1	2229	G
29	A1	2230	G
29	A1	2231	A
29	A1	2232	U
29	A1	2233	G
29	A1	2239	A
29	A1	2241	A
29	A1	2243	C
29	A1	2248	G
29	A1	2249	G
29	A1	2250	C
29	A1	2252	G
29	A1	2253	G
29	A1	2257	U
29	A1	2263	U
29	A1	2265	G
29	A1	2266	G
29	A1	2267	G
29	A1	2268	C
29	A1	2270	G
29	A1	2271	U
29	A1	2280	A
29	A1	2282	A
29	A1	2289	C
29	A1	2293	G
29	A1	2297	C
29	A1	2298	C
29	A1	2300	A
29	A1	2301	A
29	A1	2302	A
29	A1	2305	U
29	A1	2308	C
29	A1	2309	C
29	A1	2315	C
29	A1	2319	A

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Mol	Chain	Res	Type
29	A1	2321	G
29	A1	2322	G
29	A1	2323	A
29	A1	2327	C
29	A1	2328	C
29	A1	2332	G
29	A1	2333	G
29	A1	2334	A
29	A1	2336	A
29	A1	2339	G
29	A1	2341	A
29	A1	2343	G
29	A1	2344	G
29	A1	2345	G
29	A1	2347	A
29	A1	2348	G
29	A1	2350	A
29	A1	2356	C
29	A1	2358	U
29	A1	2360	A
29	A1	2361	C
29	A1	2364	C
29	A1	2365	G
29	A1	2367	G
29	A1	2368	G
29	A1	2371	U
29	A1	2372	G
29	A1	2378	C
29	A1	2396	G
29	A1	2397	G
29	A1	2398	G
29	A1	2399	C
29	A1	2402	A
29	A1	2407	A
29	A1	2410	G
29	A1	2413	G
29	A1	2416	C
29	A1	2417	C
29	A1	2425	A
29	A1	2427	G
29	A1	2437	U
29	A1	2439	A

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Mol	Chain	Res	Type
29	A1	2443	G
29	A1	2444	A
29	A1	2453	A
29	A1	2454	C
29	A1	2455	C
29	A1	2457	C
29	A1	2459	G
29	A1	2462	A
29	A1	2473	A
29	A1	2474	U
29	A1	2480	C
29	A1	2484	G
29	A1	2488	C
29	A1	2489	C
29	A1	2490	A
29	A1	2492	A
29	A1	2504	G
29	A1	2515	C
29	A1	2516	G
29	A1	2517	A
29	A1	2518	U
29	A1	2519	G
29	A1	2520	U
29	A1	2521	C
29	A1	2532	A
29	A1	2534	C
29	A1	2539	G
29	A1	2543	G
29	A1	2544	A
29	A1	2549	G
29	A1	2553	C
29	A1	2556	A
29	A1	2568	U
29	A1	2570	C
29	A1	2571	G
29	A1	2581	G
29	A1	2586	A
29	A1	2598	U
29	A1	2600	C
29	A1	2612	A
29	A1	2616	A
29	A1	2617	G

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Mol	Chain	Res	Type
29	A1	2619	U
29	A1	2620	C
29	A1	2622	G
29	A1	2623	U
29	A1	2624	C
29	A1	2625	U
29	A1	2626	C
29	A1	2629	U
29	A1	2640	C
29	A1	2643	A
29	A1	2646	A
29	A1	2648	G
29	A1	2650	U
29	A1	2657	G
29	A1	2660	C
29	A1	2667	U
29	A1	2668	A
29	A1	2673	G
29	A1	2675	G
29	A1	2678	G
29	A1	2679	A
29	A1	2684	A
29	A1	2687	G
29	A1	2690	C
29	A1	2698	U
29	A1	2703	U
29	A1	2704	C
29	A1	2706	C
29	A1	2714	C
29	A1	2716	U
29	A1	2717	C
29	A1	2721	G
29	A1	2723	G
29	A1	2724	C
29	A1	2727	A
29	A1	2728	A
29	A1	2734	G
29	A1	2738	C
29	A1	2739	C
29	A1	2742	G
29	A1	2747	G
29	A1	2748	A

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Mol	Chain	Res	Type
29	A1	2753	A
29	A1	2759	G
29	A1	2760	C
29	A1	2762	G
29	A1	2765	A
29	A1	2767	C
29	A1	2771	U
29	A1	2773	A
29	A1	2780	A
29	A1	2781	G
29	A1	2785	G
29	A1	2793	A
29	A1	2795	G
29	A1	2796	A
29	A1	2802	C
29	A1	2804	C
29	A1	2805	A
29	A1	2806	C
29	A1	2808	G
29	A1	2810	G
29	A1	2811	U
29	A1	2813	A
29	A1	2815	G
29	A1	2817	C
29	A1	2818	G
29	A1	2830	G
29	A1	2832	A
29	A1	2836	C
29	A1	2837	C
29	A1	2846	G
29	A1	2849	G
29	A1	2863	A
29	A1	2878	U
29	A1	2881	G
29	A1	2883	C
29	A1	2884	G
29	A1	2892	C
29	A1	2893	C
29	A1	2896	U
29	A1	2902	G
29	A1	2903	A
29	A1	2905	G

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Mol	Chain	Res	Type
29	A1	2906	U
29	A1	2910	G
29	A1	2912	C
30	B1	2	A
30	B1	3	U
30	B1	15	A
30	B1	17	A
30	B1	26	G
30	B1	27	A
30	B1	32	C
30	B1	33	C
30	B1	40	C
30	B1	43	U
30	B1	44	C
30	B1	45	C
30	B1	55	A
30	B1	58	G
30	B1	59	A
30	B1	66	C
30	B1	68	A
30	B1	69	G
30	B1	77	G
30	B1	84	G
30	B1	86	C
30	B1	91	G
30	B1	97	C
30	B1	98	U
30	B1	99	G
30	B1	103	G
30	B1	108	G
30	B1	112	G
30	B1	115	G
53	A2	6	G
53	A2	9	G
53	A2	18	C
53	A2	19	C
53	A2	22	G
53	A2	29	G
53	A2	30	U
53	A2	32	A
53	A2	36	C
53	A2	39	G

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Mol	Chain	Res	Type
53	A2	41	G
53	A2	43	C
53	A2	47	C
53	A2	48	C
53	A2	50	A
53	A2	51	A
53	A2	53	A
53	A2	57	G
53	A2	58	C
53	A2	61	G
53	A2	62	U
53	A2	66	G
53	A2	68	G
53	A2	69	G
53	A2	70	G
53	A2	72	C
53	A2	73	G
53	A2	74	C
53	A2	76	G
53	A2	77	G
53	A2	79	U
53	A2	80	U
53	A2	83	A
53	A2	84	C
53	A2	85	U
53	A2	86	C
53	A2	89	U
53	A2	90	G
53	A2	91	G
53	A2	92	U
53	A2	94	A
53	A2	100	G
53	A2	109	A
53	A2	113	A
53	A2	114	C
53	A2	121	G
53	A2	123	G
53	A2	125	C
53	A2	126	C
53	A2	128	A
53	A2	131	C
53	A2	132	G

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Mol	Chain	Res	Type
53	A2	135	A
53	A2	136	G
53	A2	137	A
53	A2	138	G
53	A2	140	G
53	A2	145	A
53	A2	148	C
53	A2	149	C
53	A2	155	A
53	A2	163	C
53	A2	165	A
53	A2	166	A
53	A2	172	C
53	A2	174	U
53	A2	175	G
53	A2	188	U
53	A2	189	U
53	A2	190	G
53	A2	191	G
53	A2	196	U
53	A2	201	A
53	A2	202	A
53	A2	203	A
53	A2	204	G
53	A2	205	G
53	A2	206	G
53	A2	208	U
53	A2	210	U
53	A2	211	G
53	A2	215	G
53	A2	216	C
53	A2	218	U
53	A2	219	C
53	A2	221	G
53	A2	226	G
53	A2	233	G
53	A2	240	C
53	A2	242	G
53	A2	243	C
53	A2	246	G
53	A2	248	U
53	A2	249	G

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Mol	Chain	Res	Type
53	A2	260	G
53	A2	261	G
53	A2	262	C
53	A2	269	A
53	A2	270	G
53	A2	271	G
53	A2	275	C
53	A2	276	G
53	A2	278	C
53	A2	284	G
53	A2	286	C
53	A2	287	G
53	A2	294	G
53	A2	295	A
53	A2	299	U
53	A2	303	C
53	A2	306	C
53	A2	309	C
53	A2	311	G
53	A2	316	A
53	A2	323	C
53	A2	324	A
53	A2	327	G
53	A2	336	C
53	A2	337	C
53	A2	346	G
53	A2	347	C
53	A2	348	A
53	A2	349	G
53	A2	360	U
53	A2	362	U
53	A2	367	C
53	A2	379	G
53	A2	381	C
53	A2	383	G
53	A2	385	C
53	A2	387	G
53	A2	392	A
53	A2	393	C
53	A2	394	G
53	A2	395	C
53	A2	401	G

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Mol	Chain	Res	Type
53	A2	405	G
53	A2	407	A
53	A2	408	G
53	A2	409	A
53	A2	414	C
53	A2	417	C
53	A2	419	G
53	A2	423	G
53	A2	424	U
53	A2	429	U
53	A2	430	C
53	A2	431	C
53	A2	438	C
53	A2	452	C
53	A2	455	C
53	A2	456	G
53	A2	469	G
53	A2	470	U
53	A2	471	A
53	A2	472	C
53	A2	473	C
53	A2	479	A
53	A2	480	A
53	A2	481	U
53	A2	488	G
53	A2	489	G
53	A2	491	C
53	A2	494	C
53	A2	496	C
53	A2	500	G
53	A2	501	C
53	A2	502	C
53	A2	504	G
53	A2	505	C
53	A2	507	G
53	A2	508	C
53	A2	510	G
53	A2	514	U
53	A2	528	C
53	A2	529	G
53	A2	530	A
53	A2	531	G

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Mol	Chain	Res	Type
53	A2	532	C
53	A2	533	G
53	A2	538	C
53	A2	542	A
53	A2	547	C
53	A2	550	G
53	A2	553	G
53	A2	555	A
53	A2	556	A
53	A2	559	G
53	A2	560	G
53	A2	561	C
53	A2	564	G
53	A2	569	C
53	A2	576	G
53	A2	577	G
53	A2	578	G
53	A2	586	U
53	A2	590	A
53	A2	593	G
53	A2	602	U
53	A2	604	A
53	A2	606	C
53	A2	613	G
53	A2	614	G
53	A2	615	A
53	A2	621	G
53	A2	622	G
53	A2	625	A
53	A2	630	C
53	A2	634	C
53	A2	635	U
53	A2	636	A
53	A2	643	G
53	A2	648	A
53	A2	649	G
53	A2	652	U
53	A2	657	G
53	A2	658	A
53	A2	663	C
53	A2	664	C
53	A2	666	G

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Mol	Chain	Res	Type
53	A2	670	A
53	A2	671	G
53	A2	677	A
53	A2	681	G
53	A2	683	G
53	A2	685	A
53	A2	686	G
53	A2	689	A
53	A2	695	A
53	A2	698	A
53	A2	701	G
53	A2	703	C
53	A2	704	G
53	A2	707	G
53	A2	714	G
53	A2	716	A
53	A2	717	G
53	A2	718	C
53	A2	724	G
53	A2	726	U
53	A2	727	C
53	A2	728	C
53	A2	729	A
53	A2	730	C
53	A2	731	C
53	A2	732	C
53	A2	735	G
53	A2	738	G
53	A2	745	C
53	A2	749	A
53	A2	750	A
53	A2	773	A
53	A2	775	A
53	A2	776	U
53	A2	777	A
53	A2	779	C
53	A2	782	G
53	A2	785	A
53	A2	786	G
53	A2	799	A
53	A2	800	C
53	A2	801	G

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Mol	Chain	Res	Type
53	A2	804	G
53	A2	807	C
53	A2	810	U
53	A2	811	A
53	A2	813	G
53	A2	819	G
53	A2	820	G
53	A2	823	C
53	A2	825	C
53	A2	826	C
53	A2	834	C
53	A2	847	U
53	A2	848	U
53	A2	850	A
53	A2	857	C
53	A2	859	C
53	A2	862	G
53	A2	866	A
53	A2	877	A
53	A2	879	G
53	A2	881	C
53	A2	884	A
53	A2	887	C
53	A2	891	A
53	A2	893	G
53	A2	895	A
53	A2	896	A
53	A2	903	G
53	A2	904	G
53	A2	905	G
53	A2	909	C
53	A2	911	C
53	A2	912	A
53	A2	913	C
53	A2	925	C
53	A2	935	A
53	A2	937	U
53	A2	942	A
53	A2	943	G
53	A2	945	A
53	A2	946	A
53	A2	948	G

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Mol	Chain	Res	Type
53	A2	949	C
53	A2	952	A
53	A2	954	A
53	A2	955	A
53	A2	956	C
53	A2	960	A
53	A2	961	C
53	A2	966	C
53	A2	968	U
53	A2	969	U
53	A2	970	G
53	A2	971	A
53	A2	972	C
53	A2	973	A
53	A2	974	U
53	A2	975	G
53	A2	977	U
53	A2	978	A
53	A2	981	G
53	A2	982	A
53	A2	984	C
53	A2	991	G
53	A2	994	A
53	A2	995	G
53	A2	998	U
53	A2	1000	G
53	A2	1002	G
53	A2	1003	U
53	A2	1004	G
53	A2	1005	C
53	A2	1006	C
53	A2	1007	C
53	A2	1008	C
53	A2	1009	G
53	A2	1010	C
53	A2	1011	G
53	A2	1013	G
53	A2	1016	G
53	A2	1020	C
53	A2	1022	U
53	A2	1023	A
53	A2	1024	G

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Mol	Chain	Res	Type
53	A2	1032	G
53	A2	1033	C
53	A2	1037	A
53	A2	1046	G
53	A2	1052	U
53	A2	1056	G
53	A2	1061	G
53	A2	1063	G
53	A2	1068	U
53	A2	1073	U
53	A2	1076	G
53	A2	1077	U
53	A2	1081	G
53	A2	1082	C
53	A2	1083	A
53	A2	1087	A
53	A2	1095	C
53	A2	1100	C
53	A2	1101	C
53	A2	1107	U
53	A2	1108	U
53	A2	1109	G
53	A2	1111	C
53	A2	1112	A
53	A2	1113	G
53	A2	1116	G
53	A2	1118	U
53	A2	1119	C
53	A2	1120	G
53	A2	1121	G
53	A2	1123	C
53	A2	1124	G
53	A2	1125	G
53	A2	1126	G
53	A2	1127	C
53	A2	1128	A
53	A2	1133	A
53	A2	1134	A
53	A2	1136	G
53	A2	1139	A
53	A2	1140	C
53	A2	1141	U

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Mol	Chain	Res	Type
53	A2	1142	G
53	A2	1145	C
53	A2	1151	A
53	A2	1157	A
53	A2	1161	A
53	A2	1162	G
53	A2	1163	G
53	A2	1164	A
53	A2	1165	G
53	A2	1167	G
53	A2	1172	A
53	A2	1174	G
53	A2	1175	U
53	A2	1177	U
53	A2	1178	G
53	A2	1182	A
53	A2	1183	G
53	A2	1191	C
53	A2	1192	U
53	A2	1193	U
53	A2	1194	A
53	A2	1195	C
53	A2	1196	G
53	A2	1197	G
53	A2	1198	C
53	A2	1199	C
53	A2	1200	U
53	A2	1206	A
53	A2	1207	C
53	A2	1208	A
53	A2	1209	C
53	A2	1214	G
53	A2	1216	U
53	A2	1219	A
53	A2	1221	U
53	A2	1222	G
53	A2	1227	C
53	A2	1231	A
53	A2	1232	A
53	A2	1234	G
53	A2	1238	U
53	A2	1239	G

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Mol	Chain	Res	Type
53	A2	1244	C
53	A2	1251	C
53	A2	1252	G
53	A2	1254	G
53	A2	1259	U
53	A2	1260	A
53	A2	1261	A
53	A2	1262	U
53	A2	1263	C
53	A2	1264	G
53	A2	1266	A
53	A2	1267	A
53	A2	1268	A
53	A2	1269	A
53	A2	1270	A
53	A2	1271	G
53	A2	1272	G
53	A2	1273	U
53	A2	1279	C
53	A2	1281	G
53	A2	1283	U
53	A2	1284	C
53	A2	1286	G
53	A2	1287	A
53	A2	1292	G
53	A2	1294	U
53	A2	1299	A
53	A2	1300	A
53	A2	1301	C
53	A2	1312	G
53	A2	1317	C
53	A2	1318	G
53	A2	1322	U
53	A2	1325	C
53	A2	1326	U
53	A2	1327	A
53	A2	1328	G
53	A2	1332	U
53	A2	1334	G
53	A2	1337	G
53	A2	1339	U
53	A2	1340	C

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Mol	Chain	Res	Type
53	A2	1342	G
53	A2	1344	C
53	A2	1345	A
53	A2	1352	G
53	A2	1359	A
53	A2	1361	G
53	A2	1362	U
53	A2	1367	G
53	A2	1368	G
53	A2	1371	C
53	A2	1379	C
53	A2	1380	A
53	A2	1381	C
53	A2	1383	G
53	A2	1388	U
53	A2	1391	C
53	A2	1401	G
53	A2	1404	G
53	A2	1405	G
53	A2	1411	C
53	A2	1414	G
53	A2	1418	U
53	A2	1419	C
53	A2	1424	G
53	A2	1426	A
53	A2	1427	G
53	A2	1431	A
53	A2	1432	C
53	A2	1433	G
53	A2	1434	G
53	A2	1436	C
53	A2	1443	C
53	A2	1452	G
53	A2	1469	A
53	A2	1470	A
53	A2	1471	G
53	A2	1474	G
53	A2	1476	A
53	A2	1479	A
53	A2	1480	A
53	A2	1481	G
53	A2	1482	G

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Mol	Chain	Res	Type
53	A2	1483	U
53	A2	1484	A
53	A2	1489	U
53	A2	1494	G
53	A2	1506	G
53	A2	1507	G
53	A2	1508	A
53	A2	1510	C

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	A1	219	A
29	A1	288	G
29	A1	432	C
29	A1	951	C
29	A1	1070	G
29	A1	1108	U
29	A1	1225	C
29	A1	1475	A
29	A1	1499	G
29	A1	1607	A
29	A1	1663	C
29	A1	1702	G
29	A1	1743	C
29	A1	1832	G
29	A1	1852	A
29	A1	1890	G
29	A1	1923	G
29	A1	2016	G
29	A1	2084	A
29	A1	2360	A
29	A1	2453	A
29	A1	2580	A
29	A1	2616	A
29	A1	2624	C
29	A1	2703	U
53	A2	108	G
53	A2	205	G
53	A2	239	U
53	A2	241	A
53	A2	261	G

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Mol	Chain	Res	Type
53	A2	407	A
53	A2	468	G
53	A2	562	G
53	A2	670	A
53	A2	749	A
53	A2	890	A
53	A2	955	A
53	A2	959	U
53	A2	969	U
53	A2	1005	C
53	A2	1108	U
53	A2	1144	C
53	A2	1190	C
53	A2	1207	C
53	A2	1272	G
53	A2	1317	C
53	A2	1341	A
53	A2	1475	U

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C1	1
25	a1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C1	239:ARG	C	240:ALA	N	1.18
1	a1	32:PRO	C	33:CYS	N	1.17

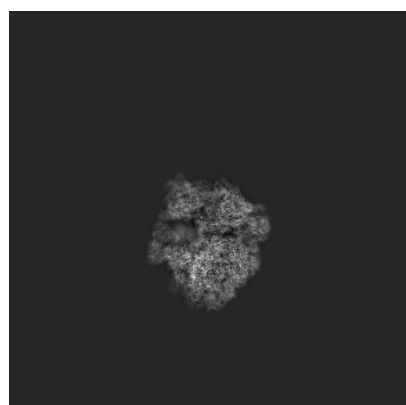
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0101. These allow visual inspection of the internal detail of the map and identification of artifacts.

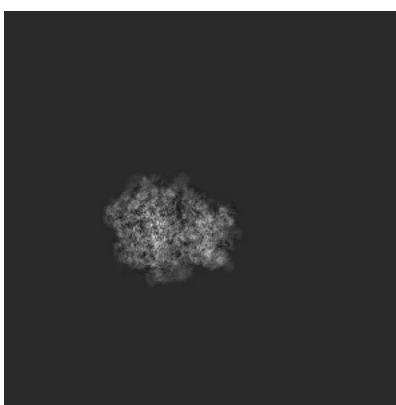
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

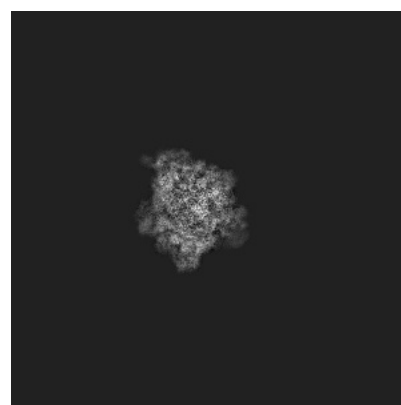
#### 6.1.1 Primary map



X



Y

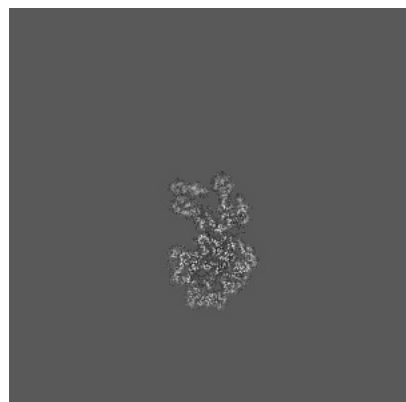


Z

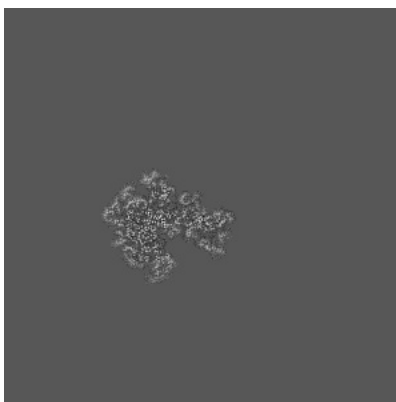
The images above show the map projected in three orthogonal directions.

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

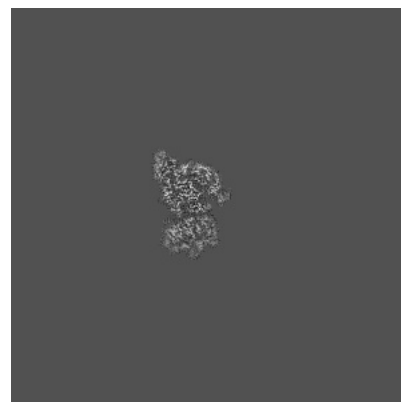
#### 6.2.1 Primary map



X Index: 350



Y Index: 350

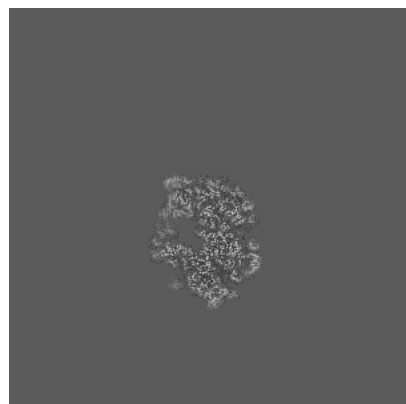


Z Index: 350

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

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

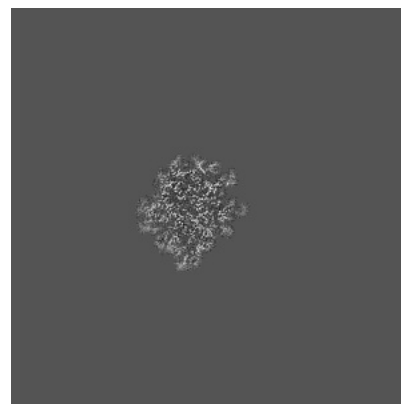
### 6.3.1 Primary map



X Index: 328



Y Index: 372

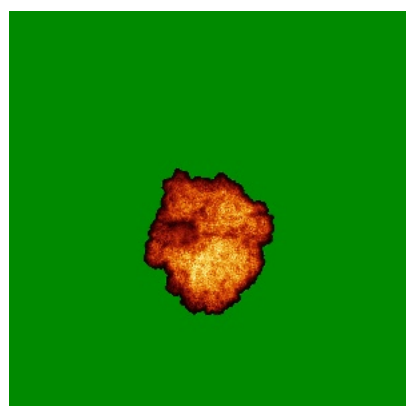


Z Index: 268

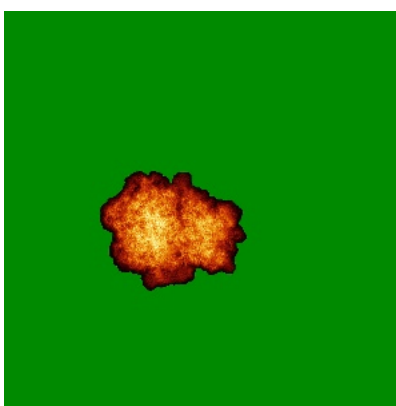
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

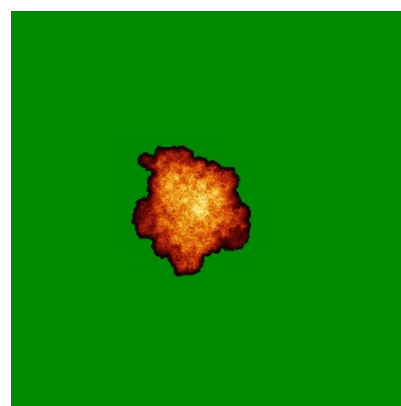
### 6.4.1 Primary map



X



Y



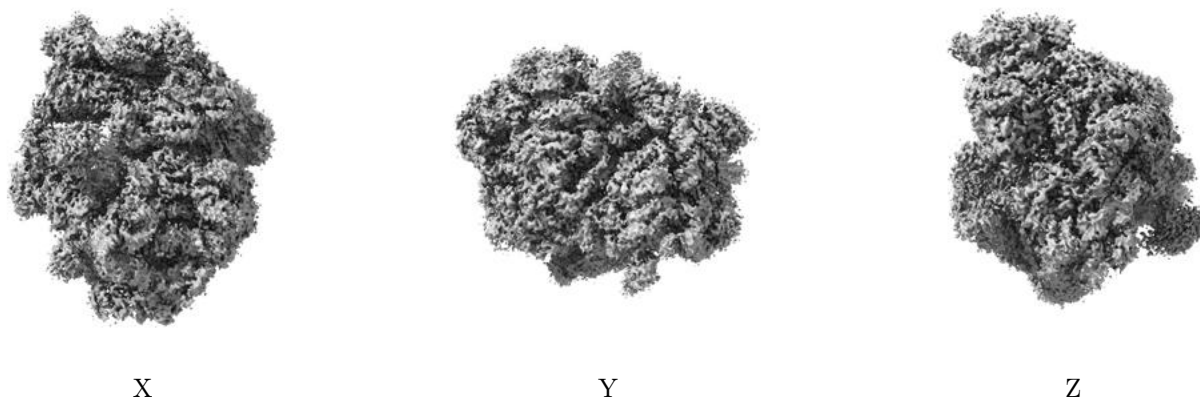
Z

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



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

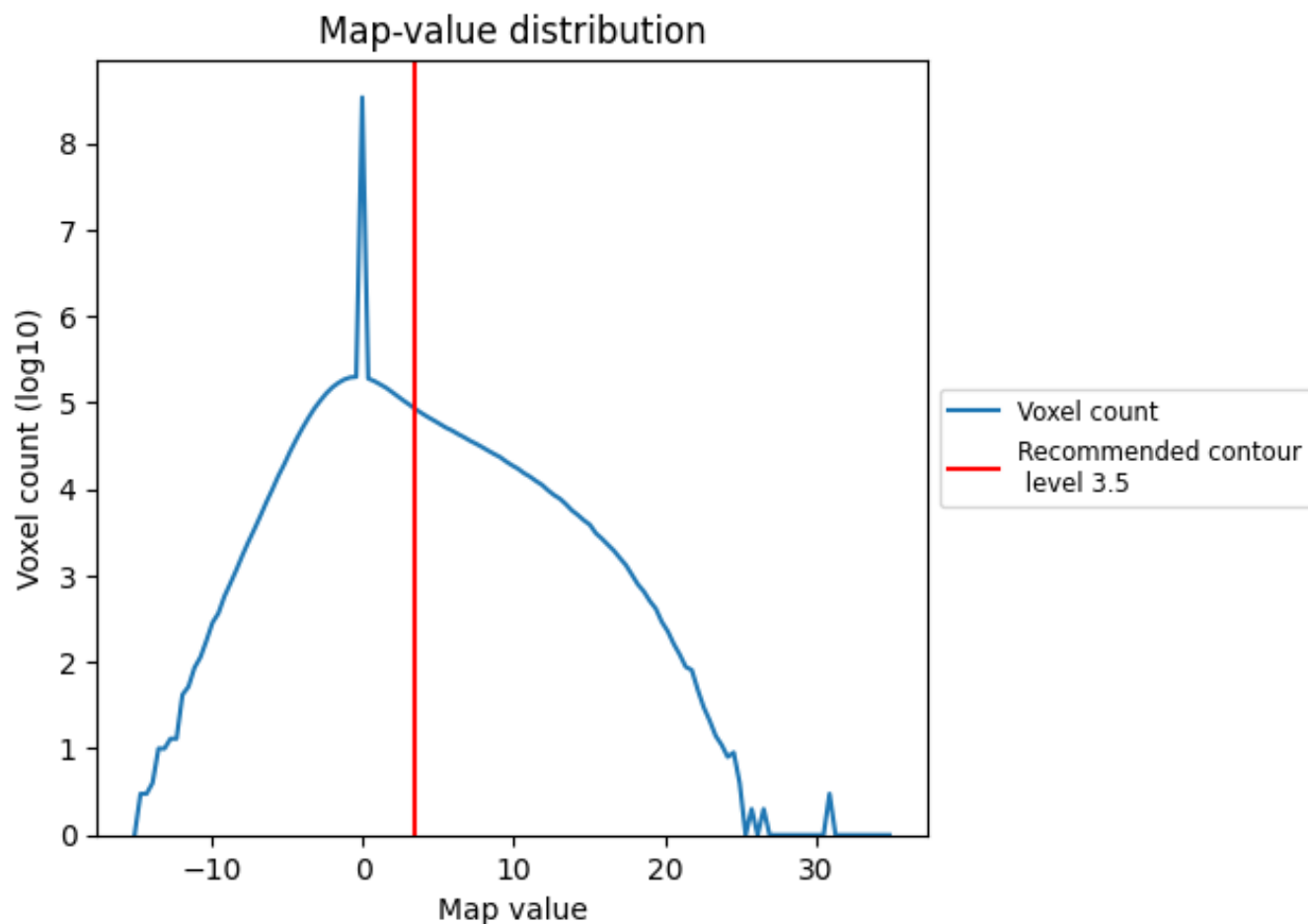
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

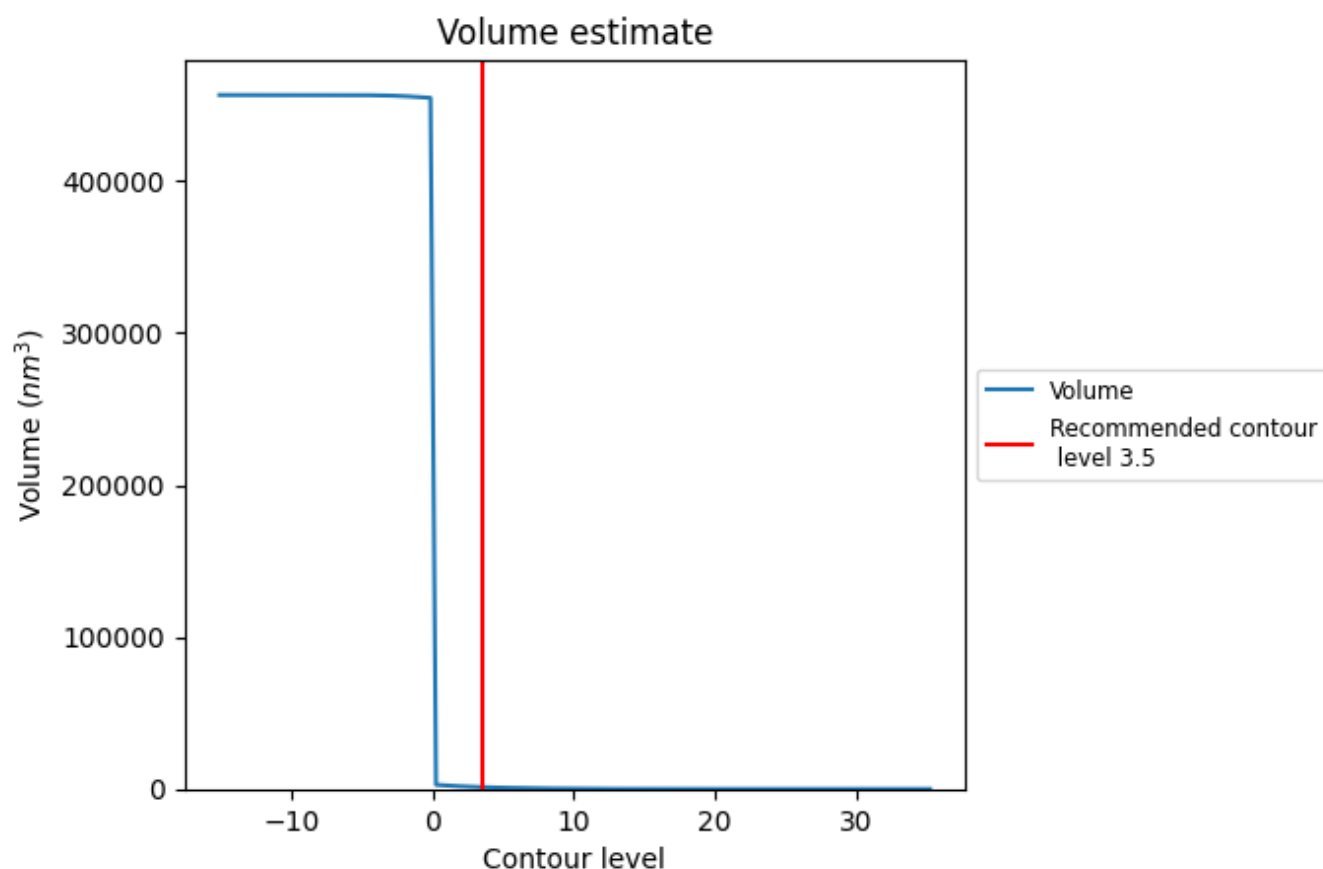
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

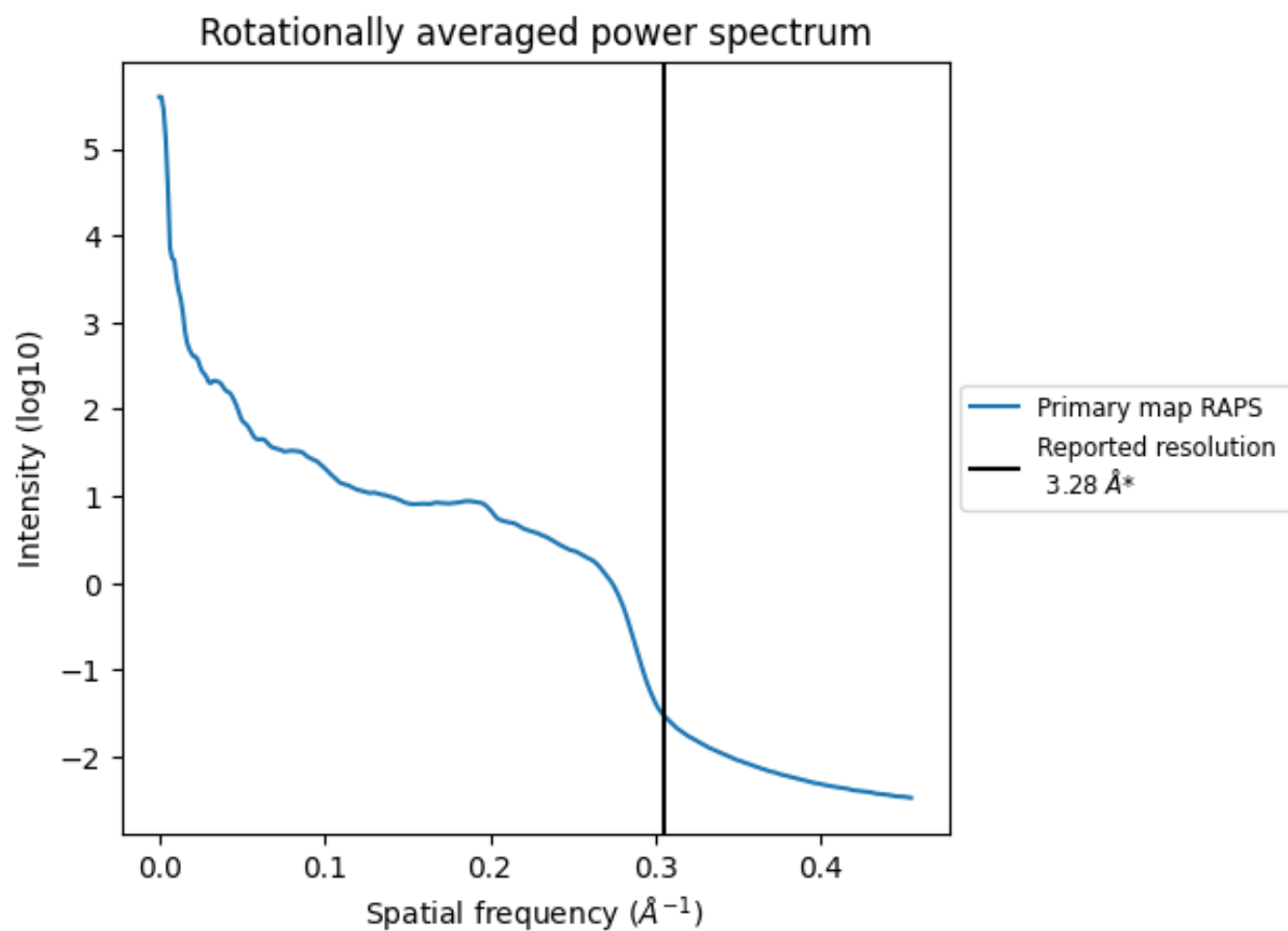
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1192  $\text{nm}^3$ ; this corresponds to an approximate mass of 1077 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.305  $\text{\AA}^{-1}$

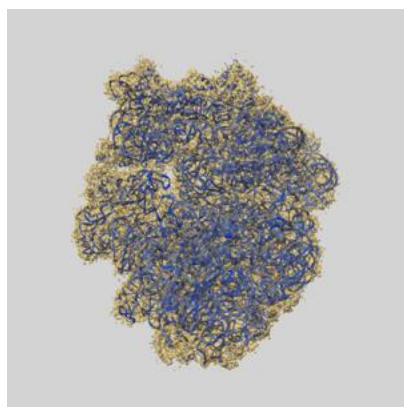
## 8 Fourier-Shell correlation

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

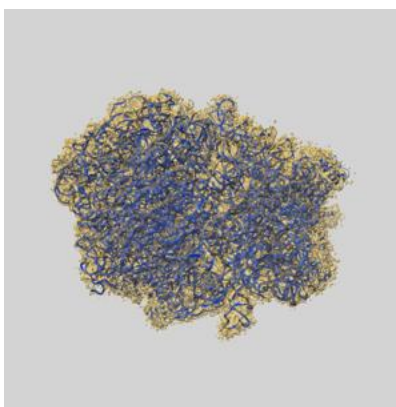
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0101 and PDB model 6GZQ. Per-residue inclusion information can be found in section 3 on page 13.

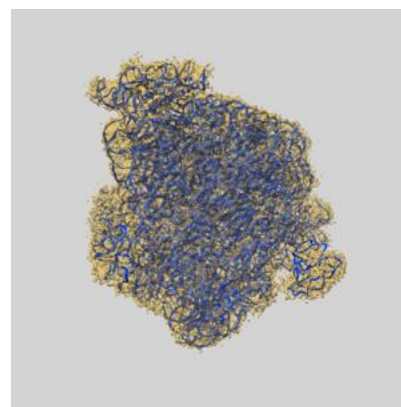
### 9.1 Map-model overlay [i](#)



X



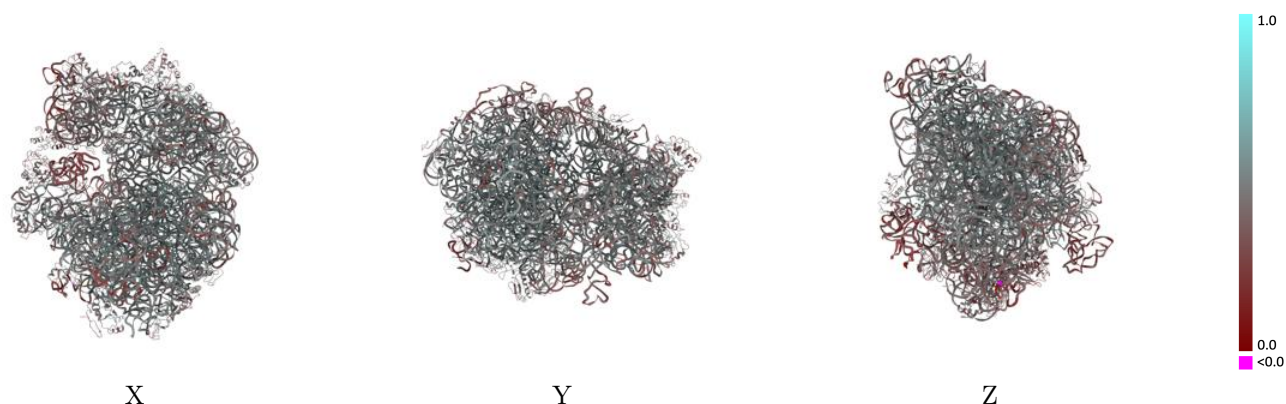
Y



Z

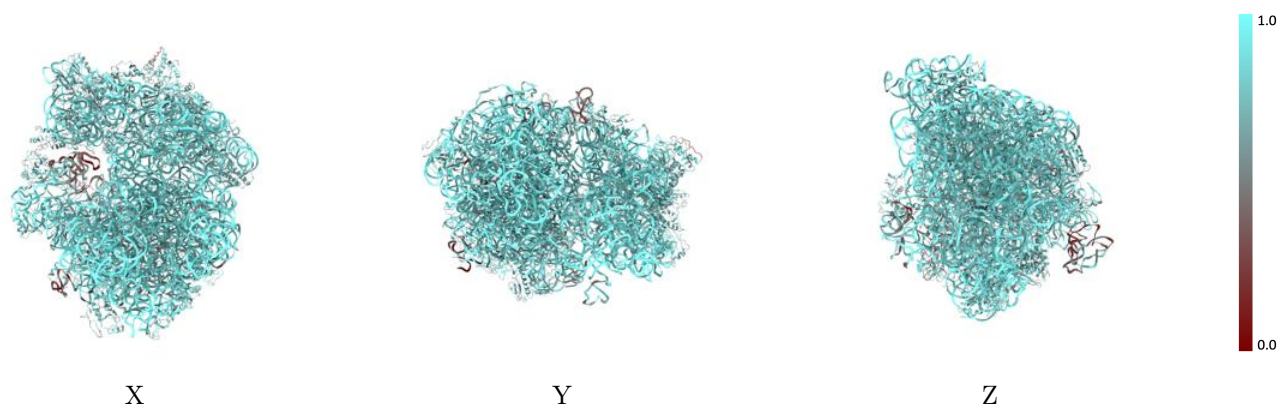
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



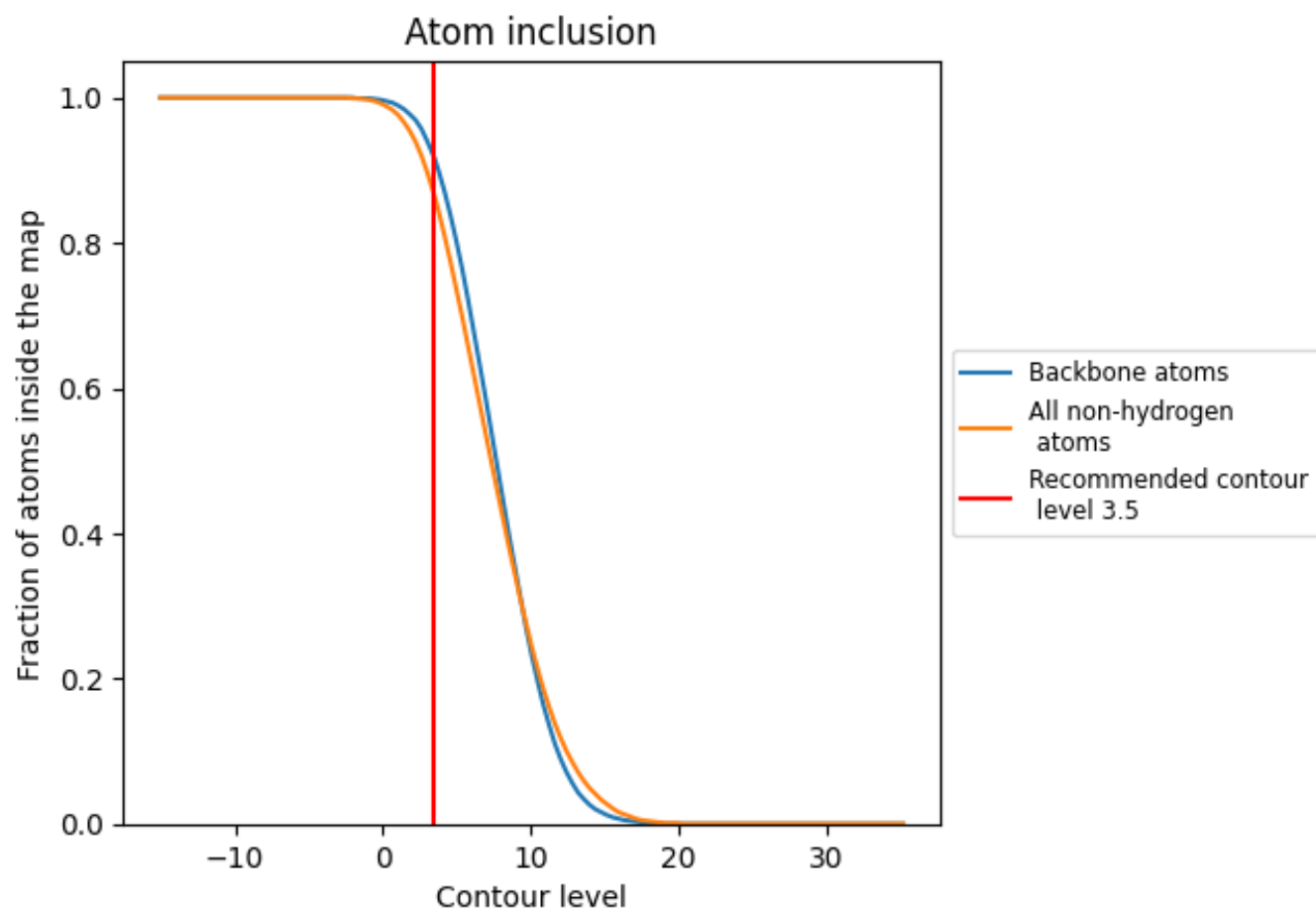
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 92% of all backbone atoms, 86% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8650	 0.4640
A1	 0.9050	 0.4790
A2	 0.9270	 0.4550
B1	 0.9300	 0.4520
B2	 0.6970	 0.4040
C1	 0.8140	 0.5040
C2	 0.7500	 0.4450
D1	 0.8050	 0.4980
D2	 0.8100	 0.4570
E1	 0.7650	 0.4720
E2	 0.7790	 0.4800
F1	 0.7490	 0.4030
F2	 0.7380	 0.4110
G1	 0.7460	 0.4010
G2	 0.7120	 0.3950
H1	 0.6590	 0.4060
H2	 0.8220	 0.4730
I1	 0.7820	 0.4870
I2	 0.6850	 0.3770
J1	 0.7680	 0.4970
J2	 0.7200	 0.4080
K1	 0.7660	 0.4600
K2	 0.7970	 0.4540
L1	 0.7770	 0.4840
L2	 0.7710	 0.4770
M1	 0.8110	 0.5090
M2	 0.6890	 0.3530
N1	 0.8210	 0.4530
N2	 0.7770	 0.4590
O1	 0.7550	 0.4570
O2	 0.7950	 0.4560
P1	 0.8310	 0.4940
P2	 0.8320	 0.4910
Q1	 0.7790	 0.4640
Q2	 0.7910	 0.4740



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Chain	Atom inclusion	Q-score
R1	 0.7820	 0.4920
R2	 0.7390	 0.4300
S1	 0.8070	 0.4910
S2	 0.7230	 0.3600
T1	 0.7460	 0.4220
T2	 0.7590	 0.4450
U1	 0.5790	 0.4000
U2	 0.7460	 0.3720
V1	 0.8260	 0.5000
V2	 0.6810	 0.4230
W1	 0.7370	 0.4740
X1	 0.7630	 0.4220
Y1	 0.7670	 0.4790
Z1	 0.6420	 0.3110
a1	 0.7850	 0.4540
b1	 0.7520	 0.3760
c1	 0.7790	 0.5200
d1	 0.7550	 0.4690
e1	 0.8180	 0.5080