



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 6, 2016 – 12:29 PM EST

PDB ID : 5LZE
EMDB ID: : EMD-4125
Title : Structure of the 70S ribosome with Sec-tRNA^{Sec} in the classical pre-translocation state (C)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2016-09-29
Resolution : 3.50 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

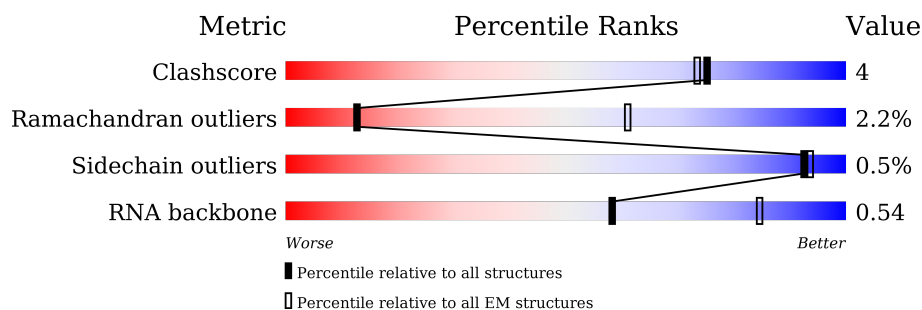
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.





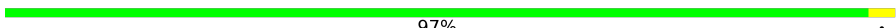
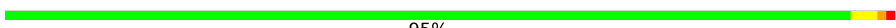









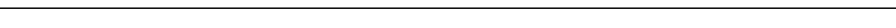











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	a	1539	69% 28% .
2	b	218	97% .
3	c	206	99% .
4	d	205	99% .
5	e	157	94% . .
6	f	100	93% 5% .
7	g	151	98% .
8	h	129	98% .













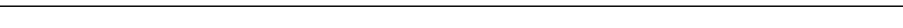
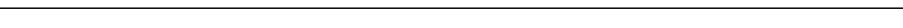


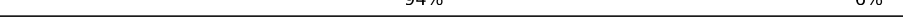







Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	i	127	 94% 5% .
10	j	98	 94% 5% .
11	k	116	 97% .
12	l	123	 95% . .
13	m	114	 93% 6% .
14	n	100	 96% .
15	o	88	 92% 7% .
16	p	82	 94% . .
17	q	80	 96% . .
18	r	65	 94% 6%
19	s	79	 96% . .
20	t	85	 100%
21	u	65	 86% 12% .
22	v	77	 65% 31% .
23	x	48	 33% 46% 21%
24	y	95	 72% 26% .
25	A	2903	 62% 29% 8% .
26	B	120	 64% 26% 9% .
27	C	271	 78% 21%
28	D	209	 90% 10%
29	E	201	 88% 11%
30	F	177	 84% 16%
31	G	176	 86% 14% .
32	I	141	 83% 16% .
33	H	149	 81% 16% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	J	142	 89% 11% .
35	K	122	 81% 17% .
36	L	143	 81% 17% ..
37	M	136	 90% 9% .
38	N	120	 88% 12%
39	O	116	 89% 11%
40	P	114	 82% 18%
41	Q	117	 90% 9% .
42	R	103	 82% 17% .
43	S	110	 86% 14%
44	T	93	 84% 16%
45	U	102	 84% 13% .
46	V	94	 82% 18%
47	W	75	 85% 13% .
48	X	77	 82% 18%
49	Y	63	 94% 6%
50	Z	58	 91% 9%
51	0	56	 89% 9% .
52	1	50	 88% 8% .
53	2	46	 83% 17%
54	3	64	 84% 16%
55	4	38	 55% 42% .
56	6	66	 64% 30% 6%
57	w	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
25	G7M	A	2069	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 148018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called tRNA^fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called fMetSec-tRNA^{Sec}.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	95	Total	C	N	O	P	0	0
			2031	907	357	672	95		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2900	Total	C	N	O	P	0	0
			62274	27787	11459	20128	2900		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	50	Total	C	N	O	S	0	0
			410	263	75	72			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 57 is a RNA chain called CCA 3' end of E-site tRNA^{Sec} (low occupancy).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

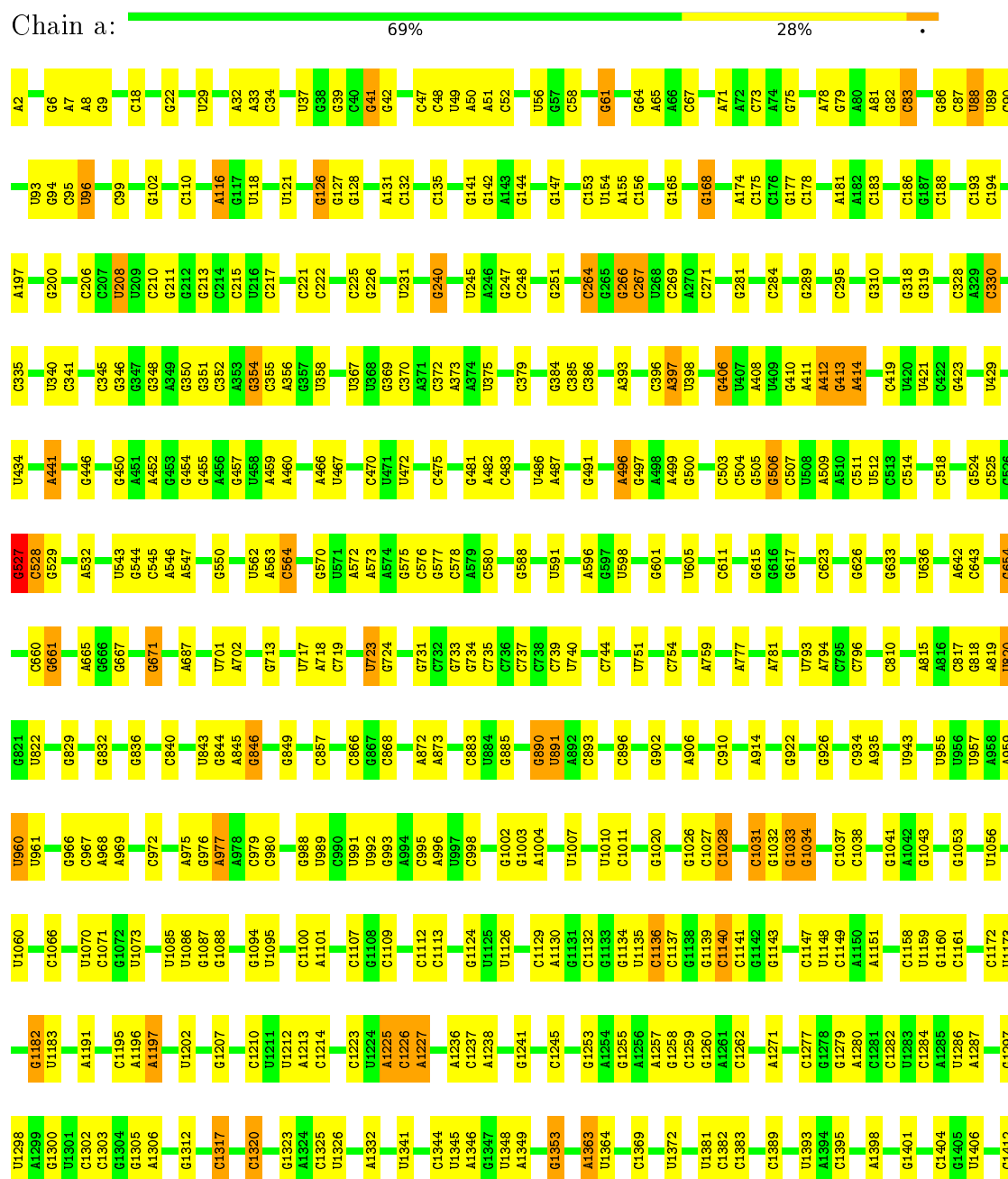
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

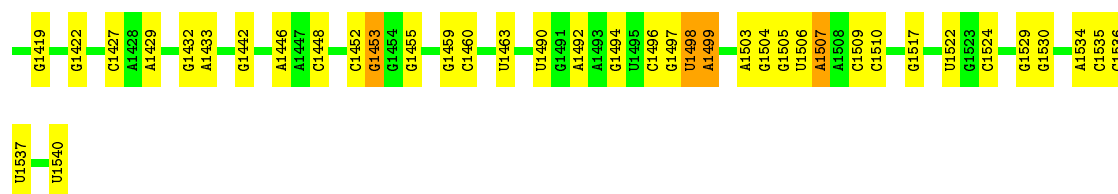
Mol	Chain	Residues	Atoms		AltConf
58	4	1	Total	Zn	0
			1	1	
58	6	1	Total	Zn	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 16S ribosomal RNA





- Molecule 2: 30S ribosomal protein S2

Chain b: 97%



- Molecule 3: 30S ribosomal protein S3

Chain c: 99%



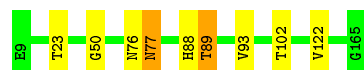
- Molecule 4: 30S ribosomal protein S4

Chain d: 99%



- Molecule 5: 30S ribosomal protein S5

Chain e: 94%



- Molecule 6: 30S ribosomal protein S6

Chain f: 93% 5%



- Molecule 7: 30S ribosomal protein S7

Chain g: 98%



- Molecule 8: 30S ribosomal protein S8

Chain h:  98% .



- Molecule 9: 30S ribosomal protein S9

Chain i:  94% 5% .



- Molecule 10: 30S ribosomal protein S10

Chain j:  94% 5% .



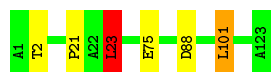
- Molecule 11: 30S ribosomal protein S11

Chain k:  97% .



- Molecule 12: 30S ribosomal protein S12

Chain l:  95% . .



- Molecule 13: 30S ribosomal protein S13

Chain m:  93% 6% .



- Molecule 14: 30S ribosomal protein S14

Chain n:  96% .



- Molecule 15: 30S ribosomal protein S15

Chain o:  92% 7% .



- Molecule 16: 30S ribosomal protein S16

Chain p: 94% ..



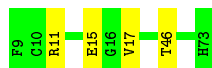
- Molecule 17: 30S ribosomal protein S17

Chain q: 96% ..



- Molecule 18: 30S ribosomal protein S18

Chain r: 94% 6%



- Molecule 19: 30S ribosomal protein S19

Chain s: 96% ..



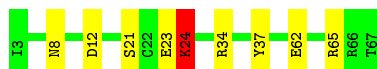
- Molecule 20: 30S ribosomal protein S20

Chain t: 100%

There are no outlier residues recorded for this chain.

- Molecule 21: 30S ribosomal protein S21

Chain u: 86% 12% .



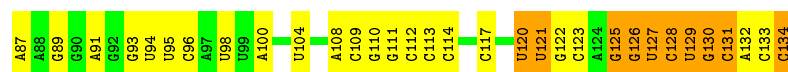
- Molecule 22: tRNA^{fMet}

Chain v: 65% 31% .



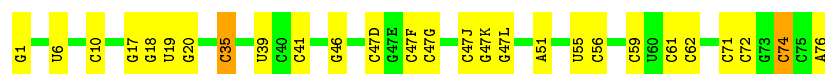
- Molecule 23: SECIS mRNA

Chain x:  33% 46% 21%



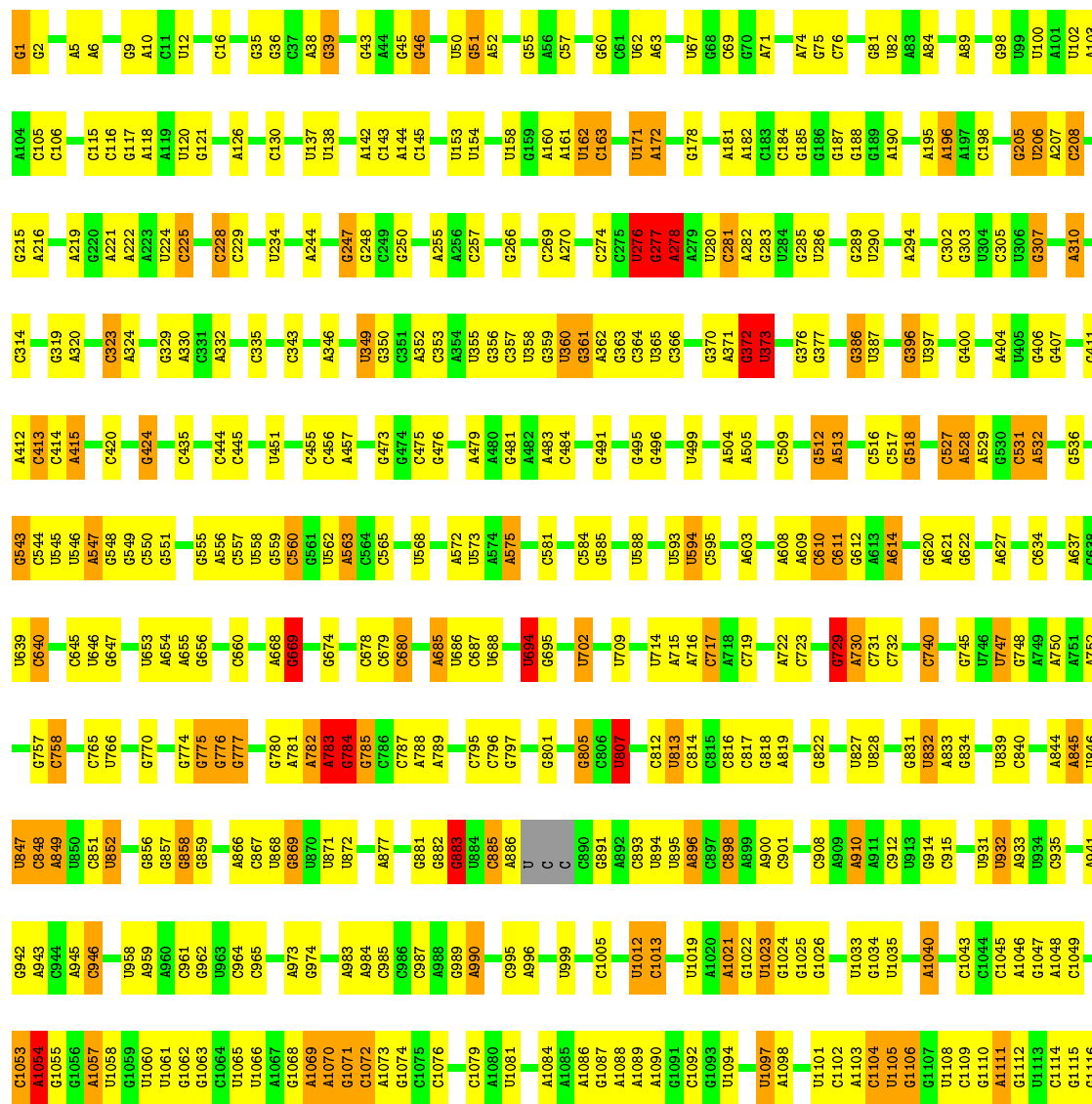
• Molecule 24: fMetSec-tRNA^{Sec}

Chain y:  72% 26%

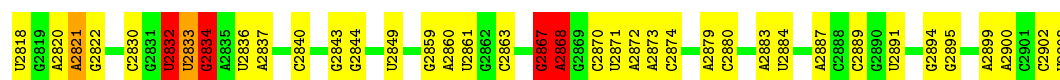


• Molecule 25: 23S ribosomal RNA

Chain A:  62% 29% 8%

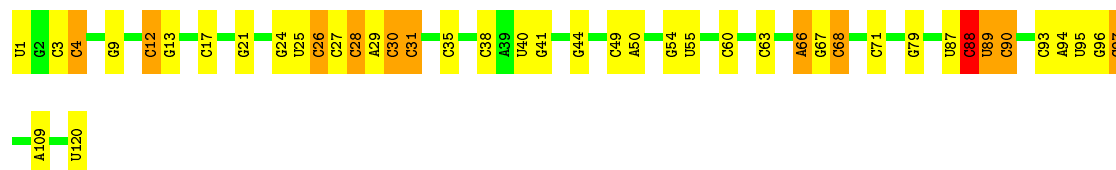




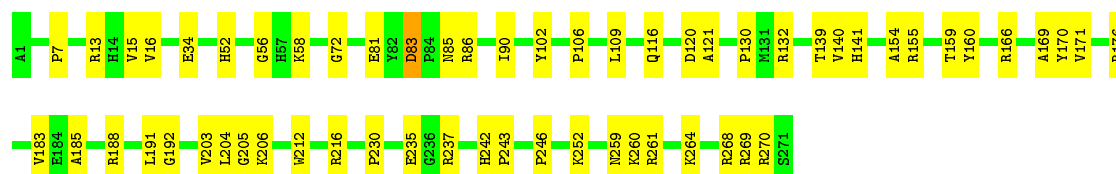
- Molecule 26: 5S ribosomal RNA

Chain B: 64% 26% 9%



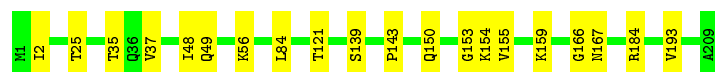
- Molecule 27: 50S ribosomal protein L2

Chain C: 78% 21%



- Molecule 28: 50S ribosomal protein L3

Chain D: 90% 10%



- Molecule 29: 50S ribosomal protein L4

Chain E: 88% 11%



- Molecule 30: 50S ribosomal protein L5

Chain F: 84% 16%

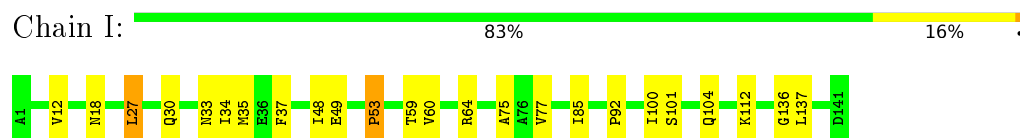


- Molecule 31: 50S ribosomal protein L6

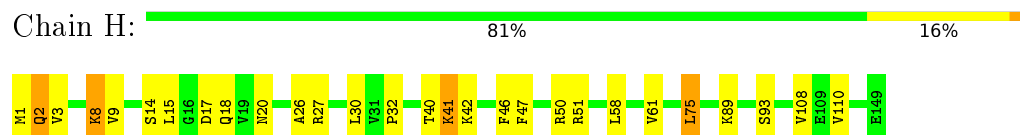
Chain G: 86% 14%



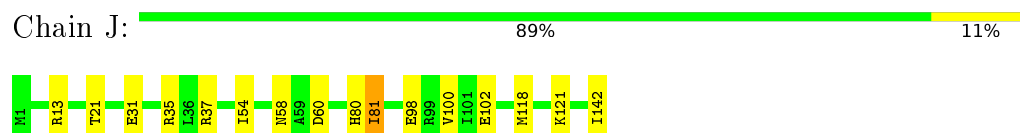
- Molecule 32: 50S ribosomal protein L11



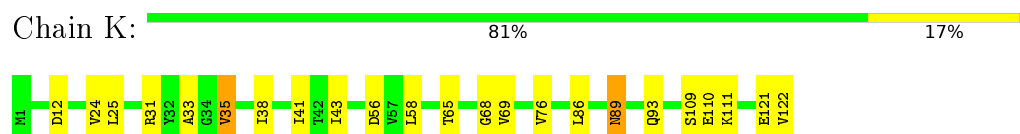
- Molecule 33: 50S ribosomal protein L9



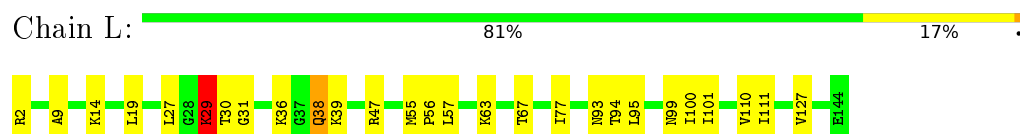
- Molecule 34: 50S ribosomal protein L13



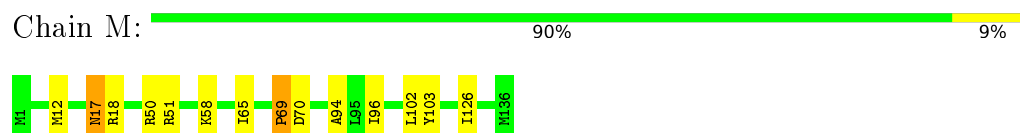
- Molecule 35: 50S ribosomal protein L14



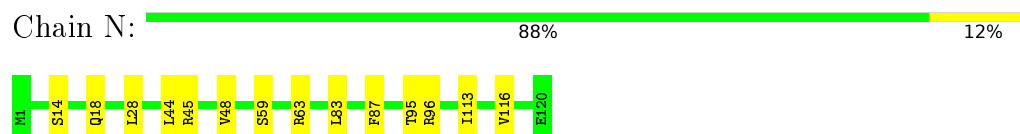
- Molecule 36: 50S ribosomal protein L15




- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17




- Molecule 39: 50S ribosomal protein L18

Chain O:  89% 11%




- Molecule 40: 50S ribosomal protein L19

Chain P:  82% 18%




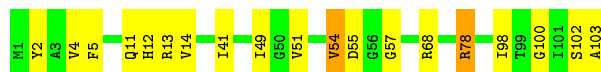
- Molecule 41: 50S ribosomal protein L20

Chain Q:  90% 9%




- Molecule 42: 50S ribosomal protein L21

Chain R:  82% 17%




- Molecule 43: 50S ribosomal protein L22

Chain S:  86% 14%




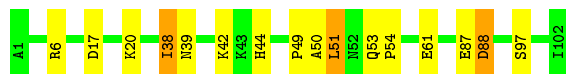
- Molecule 44: 50S ribosomal protein L23

Chain T:  84% 16%




- Molecule 45: 50S ribosomal protein L24

Chain U:  84% 13%



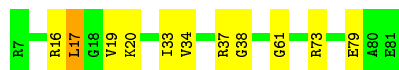
- Molecule 46: 50S ribosomal protein L25

Chain V:  82% 18%



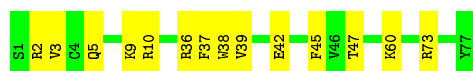
- Molecule 47: 50S ribosomal protein L27

Chain W: 85% 13%



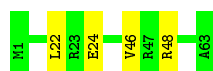
- Molecule 48: 50S ribosomal protein L28

Chain X: 82% 18%



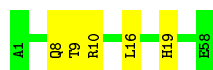
- Molecule 49: 50S ribosomal protein L29

Chain Y: 94% 6%



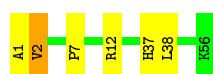
- Molecule 50: 50S ribosomal protein L30

Chain Z: 91% 9%



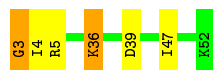
- Molecule 51: 50S ribosomal protein L32

Chain 0: 89% 9%



- Molecule 52: 50S ribosomal protein L33

Chain 1: 88% 8%

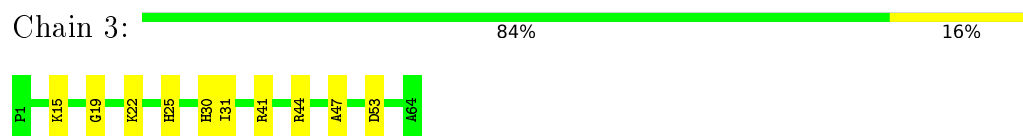


- Molecule 53: 50S ribosomal protein L34

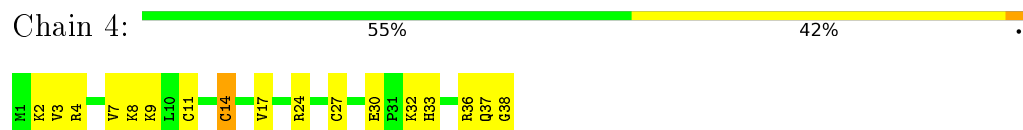
Chain 2: 83% 17%



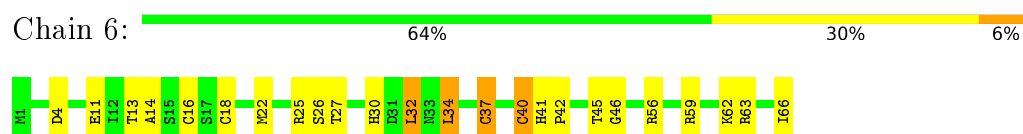
- Molecule 54: 50S ribosomal protein L35



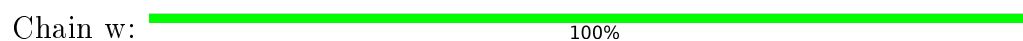
- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L31



- Molecule 57: CCA 3' end of E-site tRNA^{Sec} (low occupancy)



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	130705	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 3TD, ZN, 6IA, OMG, 5MC, MA6, G7M, OMC, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 4SU, 1MG, PSU

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 >2	RMSZ	# Z >2
1	a	0.84	6/36701 (0.0%)	1.37	537/57246 (0.9%)
10	j	0.44	0/797	0.78	0/1077
11	k	0.46	0/886	0.71	1/1195 (0.1%)
12	l	0.43	0/969	0.77	1/1300 (0.1%)
13	m	0.46	0/893	0.82	3/1193 (0.3%)
14	n	0.51	0/806	0.68	0/1074
15	o	0.45	0/722	0.73	2/964 (0.2%)
16	p	0.53	0/659	0.84	1/884 (0.1%)
17	q	0.49	0/658	0.78	1/881 (0.1%)
18	r	0.46	0/512	0.74	1/689 (0.1%)
19	s	0.50	0/653	0.87	3/877 (0.3%)
2	b	0.44	0/1736	0.69	1/2338 (0.0%)
20	t	0.44	0/671	0.64	0/888
21	u	0.53	0/501	0.98	2/668 (0.3%)
22	v	0.79	1/1747 (0.1%)	1.48	44/2721 (1.6%)
23	x	0.91	3/1145 (0.3%)	1.67	32/1781 (1.8%)
24	y	0.67	1/2162 (0.0%)	1.42	33/3351 (1.0%)
25	A	0.93	12/69171 (0.0%)	1.32	778/107904 (0.7%)
26	B	0.76	1/2873 (0.0%)	1.41	53/4478 (1.2%)
27	C	0.54	0/2122	0.74	2/2852 (0.1%)
28	D	0.48	0/1586	0.70	0/2134
29	E	0.49	0/1571	0.67	2/2113 (0.1%)
3	c	0.44	0/1652	0.63	0/2225
30	F	0.48	0/1435	0.74	1/1926 (0.1%)
31	G	0.45	0/1343	0.66	2/1816 (0.1%)
32	I	0.43	0/1046	0.71	1/1410 (0.1%)
33	H	0.40	0/1122	0.70	1/1515 (0.1%)
34	J	0.50	0/1152	0.64	0/1551
35	K	0.53	0/948	0.74	1/1268 (0.1%)
36	L	0.50	0/1054	0.78	1/1403 (0.1%)
37	M	0.47	0/1093	0.68	1/1460 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	N	0.49	0/974	0.68	0/1301
39	O	0.45	0/902	0.61	0/1209
4	d	0.42	0/1665	0.64	0/2227
40	P	0.50	0/929	0.70	1/1242 (0.1%)
41	Q	0.59	0/960	0.68	1/1278 (0.1%)
42	R	0.47	0/829	0.72	2/1107 (0.2%)
43	S	0.47	0/864	0.66	1/1156 (0.1%)
44	T	0.44	0/745	0.60	0/994
45	U	0.49	0/788	0.82	4/1051 (0.4%)
46	V	0.44	0/766	0.62	1/1025 (0.1%)
47	W	0.49	0/582	0.64	0/769
48	X	0.49	0/635	0.59	0/848
49	Y	0.42	0/510	0.61	0/677
5	e	0.49	0/1170	0.74	2/1573 (0.1%)
50	Z	0.39	0/453	0.65	0/605
51	0	0.51	0/450	0.75	0/599
52	1	0.47	0/417	0.78	1/554 (0.2%)
53	2	0.49	0/380	0.65	0/498
54	3	0.49	0/513	0.65	0/676
55	4	0.79	1/303 (0.3%)	1.05	1/397 (0.3%)
56	6	0.60	1/532 (0.2%)	1.09	4/709 (0.6%)
57	w	0.28	0/68	1.00	0/103
6	f	0.51	0/836	0.85	3/1128 (0.3%)
7	g	0.42	0/1196	0.62	0/1602
8	h	0.47	0/989	0.69	0/1326
9	i	0.49	1/1034 (0.1%)	0.78	1/1375 (0.1%)
All	All	0.79	27/159876 (0.0%)	1.22	1527/239211 (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	a	2	0
10	j	0	3
12	l	0	2
13	m	0	2
15	o	0	1
16	p	0	1
17	q	0	1
19	s	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
21	u	0	2
25	A	2	0
27	C	0	1
28	D	0	1
29	E	0	1
30	F	0	1
33	H	0	3
35	K	0	1
36	L	0	1
45	U	0	2
5	e	0	3
51	0	0	1
52	1	0	1
54	3	0	1
6	f	0	2
9	i	0	2
All	All	4	35

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	1	G	OP3-P	-10.82	1.48	1.61
25	A	1	G	OP3-P	-10.72	1.48	1.61
22	v	1	C	OP3-P	-10.66	1.48	1.61
26	B	1	U	OP3-P	-10.62	1.48	1.61
1	a	2	A	OP3-P	-10.55	1.48	1.61
23	x	87	A	OP3-P	-10.53	1.48	1.61
55	4	27	CYS	CB-SG	8.23	1.96	1.82
1	a	1034	G	C6-O6	-7.96	1.17	1.24
25	A	1784	A	N7-C5	-7.30	1.34	1.39
25	A	984	A	N9-C4	-7.18	1.33	1.37
25	A	528	A	N9-C4	-6.99	1.33	1.37
25	A	783	A	N7-C5	-5.80	1.35	1.39
23	x	128	C	O3'-P	5.71	1.68	1.61
1	a	2	A	N7-C5	-5.68	1.35	1.39
25	A	360	U	C4-O4	-5.59	1.19	1.23
25	A	1105	U	C2-N3	-5.57	1.33	1.37
25	A	278	A	N9-C4	5.56	1.41	1.37
1	a	354	G	C6-N1	-5.48	1.35	1.39
25	A	787	C	O3'-P	-5.47	1.54	1.61
23	x	125	G	O3'-P	5.35	1.67	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1312	G	O3'-P	-5.34	1.54	1.61
25	A	1081	U	C4-O4	-5.33	1.19	1.23
1	a	1140	C	N3-C4	-5.32	1.30	1.33
56	6	40	CYS	CB-SG	5.19	1.91	1.82
25	A	1779	U	C5-C6	-5.16	1.29	1.34
9	i	90	ASP	CB-CG	5.07	1.62	1.51
25	A	528	A	N7-C5	-5.04	1.36	1.39

All (1527) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	529	G	C5-C6-O6	-14.39	119.96	128.60
24	y	35	C	C5-C6-N1	13.59	127.79	121.00
1	a	1027	C	C5-C6-N1	13.56	127.78	121.00
25	A	1313	U	N3-C2-O2	-12.91	113.16	122.20
24	y	35	C	C6-N1-C2	-12.72	115.21	120.30
25	A	1313	U	N1-C2-O2	12.61	131.63	122.80
1	a	215	C	N1-C2-O2	12.52	126.41	118.90
1	a	1003	G	N3-C2-N2	-12.32	111.27	119.90
25	A	278	A	C2-N3-C4	11.81	116.50	110.60
25	A	1081	U	N3-C2-O2	-11.45	114.19	122.20
1	a	1034	G	C5-C6-O6	-11.40	121.76	128.60
1	a	1034	G	C5-C6-N1	11.25	117.13	111.50
23	x	120	U	N1-C2-O2	11.08	130.56	122.80
56	6	32	LEU	CA-CB-CG	11.08	140.78	115.30
25	A	62	U	N1-C2-O2	11.04	130.53	122.80
25	A	1087	G	N3-C2-N2	-11.03	112.18	119.90
23	x	120	U	N3-C2-O2	-10.93	114.55	122.20
1	a	1134	G	N3-C2-N2	-10.81	112.33	119.90
25	A	2103	C	N1-C2-O2	-10.72	112.47	118.90
26	B	12	C	N1-C2-O2	10.70	125.32	118.90
25	A	783	A	N7-C8-N9	10.58	119.09	113.80
25	A	137	U	N3-C2-O2	-10.55	114.81	122.20
23	x	133	C	N1-C2-O2	10.54	125.23	118.90
26	B	4	C	C5-C6-N1	10.50	126.25	121.00
1	a	206	C	N1-C2-O2	-10.46	112.62	118.90
25	A	281	C	C6-N1-C2	-10.41	116.14	120.30
25	A	1101	U	N3-C2-O2	-10.38	114.94	122.20
1	a	1455	G	N1-C6-O6	10.36	126.11	119.90
25	A	1920	C	C6-N1-C2	-10.30	116.18	120.30
25	A	783	A	C8-N9-C4	-10.17	101.73	105.80
1	a	719	C	N1-C2-O2	10.16	125.00	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1507	C	C6-N1-C2	-10.16	116.24	120.30
1	a	355	C	N3-C2-O2	-10.13	114.81	121.90
1	a	355	C	N1-C2-O2	10.12	124.97	118.90
23	x	125	G	N9-C1'-C2'	-10.10	100.87	114.00
1	a	1395	C	N1-C2-O2	10.07	124.94	118.90
1	a	1349	A	O5'-P-OP1	-10.06	96.65	105.70
26	B	4	C	C6-N1-C2	-10.05	116.28	120.30
25	A	2072	C	C5-C6-N1	9.96	125.98	121.00
25	A	2072	C	C6-N1-C2	-9.94	116.32	120.30
1	a	719	C	N3-C2-O2	-9.88	114.99	121.90
25	A	1105	U	N3-C2-O2	-9.81	115.33	122.20
25	A	1180	U	C5-C4-O4	-9.79	120.03	125.90
25	A	2036	C	C6-N1-C2	-9.78	116.39	120.30
1	a	1141	C	N1-C2-O2	9.77	124.76	118.90
1	a	1027	C	C4-C5-C6	-9.76	112.52	117.40
1	a	1404	C	C6-N1-C2	-9.70	116.42	120.30
25	A	2036	C	C5-C6-N1	9.69	125.84	121.00
26	B	97	C	C2-N1-C1'	9.65	129.41	118.80
1	a	168	G	C5-C6-O6	-9.64	122.82	128.60
1	a	1317	C	N1-C2-O2	9.63	124.68	118.90
25	A	1081	U	N3-C4-C5	9.59	120.36	114.60
25	A	1314	C	C6-N1-C2	-9.59	116.46	120.30
25	A	283	G	N3-C2-N2	-9.55	113.21	119.90
25	A	546	U	N3-C2-O2	-9.55	115.51	122.20
25	A	1993	U	N1-C2-O2	9.54	129.47	122.80
1	a	1317	C	N3-C2-O2	-9.52	115.24	121.90
1	a	1140	C	N1-C2-O2	9.51	124.60	118.90
26	B	30	C	C6-N1-C2	-9.49	116.50	120.30
25	A	62	U	N3-C2-O2	-9.49	115.56	122.20
24	y	59	C	N1-C2-O2	9.47	124.58	118.90
1	a	529	G	N1-C6-O6	9.46	125.58	119.90
25	A	783	A	C5-N7-C8	-9.43	99.18	103.90
16	p	44	SER	N-CA-CB	-9.42	96.37	110.50
22	v	67	C	N1-C2-O2	9.42	124.55	118.90
1	a	1325	C	C6-N1-C2	-9.42	116.53	120.30
1	a	215	C	N3-C2-O2	-9.40	115.32	121.90
1	a	1034	G	C4-C5-N7	9.40	114.56	110.80
1	a	1395	C	N3-C2-O2	-9.39	115.33	121.90
1	a	186	C	N1-C2-O2	9.38	124.53	118.90
25	A	1081	U	N1-C2-O2	9.38	129.36	122.80
25	A	1313	U	C2-N1-C1'	9.37	128.95	117.70
1	a	503	C	C6-N1-C2	-9.35	116.56	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	120	U	N3-C2-O2	-9.33	115.67	122.20
25	A	1920	C	C5-C6-N1	9.33	125.66	121.00
25	A	2791	G	N3-C2-N2	-9.28	113.40	119.90
1	a	1455	G	C5-C6-O6	-9.26	123.04	128.60
1	a	221	C	N1-C2-O2	9.25	124.45	118.90
23	x	133	C	N3-C2-O2	-9.19	115.47	121.90
25	A	12	U	N3-C2-O2	-9.19	115.77	122.20
1	a	217	C	C6-N1-C2	-9.18	116.63	120.30
22	v	71	C	C6-N1-C2	-9.09	116.67	120.30
1	a	1149	C	N1-C2-O2	9.08	124.34	118.90
25	A	669	G	C2-N3-C4	9.06	116.43	111.90
25	A	1081	U	C2-N3-C4	-8.95	121.63	127.00
1	a	564	C	N1-C2-O2	8.95	124.27	118.90
1	a	457	G	N1-C6-O6	-8.92	114.55	119.90
25	A	1507	C	C5-C6-N1	8.87	125.44	121.00
25	A	962	G	O5'-P-OP1	-8.85	97.73	105.70
26	B	12	C	N3-C2-O2	-8.85	115.70	121.90
1	a	1027	C	C2-N3-C4	8.81	124.31	119.90
1	a	575	G	N3-C2-N2	-8.79	113.74	119.90
25	A	353	C	N1-C2-O2	8.76	124.16	118.90
25	A	557	C	N1-C2-O2	8.75	124.15	118.90
1	a	660	C	N1-C2-O2	8.73	124.14	118.90
25	A	2762	C	C6-N1-C2	-8.70	116.82	120.30
25	A	2409	G	C5-C6-O6	-8.70	123.38	128.60
25	A	2103	C	C2-N3-C4	-8.67	115.56	119.90
25	A	2473	U	N1-C2-O2	8.67	128.87	122.80
26	B	97	C	N1-C2-O2	8.67	124.10	118.90
25	A	1005	C	N1-C2-O2	8.65	124.09	118.90
25	A	2683	C	N1-C2-O2	8.65	124.09	118.90
22	v	51	C	N1-C2-O2	8.65	124.09	118.90
25	A	121	G	N1-C6-O6	8.63	125.08	119.90
25	A	281	C	C5-C6-N1	8.63	125.32	121.00
1	a	215	C	C6-N1-C2	-8.59	116.86	120.30
25	A	1102	C	N1-C2-O2	8.59	124.06	118.90
25	A	557	C	C6-N1-C2	-8.59	116.86	120.30
25	A	807	U	N3-C2-O2	-8.59	116.19	122.20
1	a	623	C	C6-N1-C2	-8.58	116.87	120.30
26	B	97	C	C6-N1-C2	-8.57	116.87	120.30
25	A	277	G	N7-C8-N9	8.55	117.38	113.10
1	a	500	G	N1-C6-O6	8.55	125.03	119.90
25	A	758	C	N3-C2-O2	-8.54	115.92	121.90
25	A	62	U	C2-N1-C1'	8.54	127.94	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	810	C	C5-C6-N1	8.53	125.26	121.00
22	v	41	C	N1-C2-O2	8.53	124.02	118.90
1	a	385	C	C6-N1-C2	-8.52	116.89	120.30
25	A	883	G	N7-C8-N9	8.51	117.36	113.10
1	a	1028	C	N1-C2-O2	-8.50	113.80	118.90
25	A	2410	G	N3-C2-N2	-8.48	113.96	119.90
25	A	1102	C	N3-C2-O2	-8.47	115.97	121.90
1	a	58	C	N1-C2-O2	-8.43	113.84	118.90
1	a	18	C	C5-C6-N1	8.43	125.21	121.00
26	B	38	C	N1-C2-O2	8.42	123.95	118.90
25	A	1993	U	N3-C2-O2	-8.39	116.33	122.20
25	A	1539	U	C5-C6-N1	8.38	126.89	122.70
22	v	56	C	N1-C2-O2	8.37	123.92	118.90
26	B	30	C	C5-C6-N1	8.37	125.18	121.00
13	m	65	GLU	N-CA-CB	-8.34	95.58	110.60
25	A	2834	G	N7-C8-N9	8.34	117.27	113.10
25	A	669	G	N3-C4-C5	-8.33	124.44	128.60
56	6	18	CYS	CA-CB-SG	-8.31	99.04	114.00
25	A	1498	C	N3-C4-N4	8.30	123.81	118.00
26	B	17	C	N1-C2-O2	8.30	123.88	118.90
23	x	133	C	N1-C1'-C2'	-8.29	102.88	112.00
25	A	2884	U	N3-C2-O2	-8.29	116.40	122.20
26	B	31	C	N1-C2-O2	8.29	123.87	118.90
1	a	102	G	C6-N1-C2	-8.29	120.13	125.10
1	a	544	G	N1-C6-O6	8.27	124.86	119.90
25	A	2226	C	N1-C2-O2	8.26	123.86	118.90
25	A	1087	G	C6-N1-C2	-8.26	120.14	125.10
25	A	1178	C	N1-C2-O2	8.25	123.85	118.90
25	A	2226	C	N3-C2-O2	-8.25	116.12	121.90
25	A	807	U	N1-C2-O2	8.24	128.57	122.80
1	a	1158	C	C2-N1-C1'	8.24	127.86	118.80
25	A	407	G	N1-C6-O6	-8.24	114.96	119.90
25	A	2011	U	N3-C2-O2	-8.22	116.45	122.20
1	a	998	C	N3-C2-O2	-8.21	116.15	121.90
25	A	2742	G	N1-C6-O6	-8.21	114.97	119.90
25	A	413	C	C6-N1-C2	-8.21	117.02	120.30
1	a	1149	C	C6-N1-C2	-8.16	117.03	120.30
22	v	19	G	N1-C6-O6	-8.16	115.00	119.90
1	a	626	G	N1-C6-O6	8.16	124.79	119.90
25	A	581	C	C6-N1-C2	-8.16	117.04	120.30
26	B	4	C	N1-C2-O2	8.15	123.79	118.90
25	A	105	C	C6-N1-C2	-8.14	117.04	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1716	U	C5-C6-N1	8.13	126.77	122.70
1	a	215	C	N3-C4-N4	8.12	123.69	118.00
25	A	1894	C	N1-C2-O2	8.12	123.77	118.90
25	A	2410	G	C6-N1-C2	-8.11	120.23	125.10
1	a	737	C	C6-N1-C2	-8.09	117.06	120.30
1	a	110	C	N1-C2-O2	8.09	123.75	118.90
25	A	2473	U	N3-C2-O2	-8.09	116.54	122.20
1	a	1003	G	C6-N1-C2	-8.08	120.25	125.10
25	A	1314	C	C5-C6-N1	8.08	125.04	121.00
25	A	1104	C	N1-C2-O2	8.08	123.75	118.90
2	b	73	ARG	N-CA-CB	-8.07	96.07	110.60
1	a	751	U	N3-C2-O2	-8.07	116.55	122.20
22	v	67	C	C6-N1-C2	-8.06	117.08	120.30
22	v	71	C	N3-C2-O2	-8.06	116.26	121.90
25	A	1451	C	N1-C2-O2	-8.04	114.07	118.90
1	a	450	G	N1-C6-O6	-8.04	115.08	119.90
25	A	2762	C	N1-C2-O2	8.03	123.72	118.90
1	a	1326	U	N3-C2-O2	-8.02	116.58	122.20
1	a	1149	C	N3-C2-O2	-8.02	116.29	121.90
25	A	2406	A	O5'-P-OP2	-8.01	98.49	105.70
1	a	102	G	N3-C2-N2	-8.01	114.30	119.90
24	y	47(D)	C	C2-N3-C4	-7.97	115.91	119.90
26	B	120	U	N1-C2-O2	7.96	128.38	122.80
19	s	5	LYS	CB-CA-C	-7.96	94.48	110.40
1	a	1056	U	N3-C2-O2	-7.95	116.63	122.20
1	a	355	C	C6-N1-C2	-7.93	117.13	120.30
25	A	1680	U	N3-C2-O2	-7.92	116.66	122.20
1	a	206	C	C2-N3-C4	-7.91	115.95	119.90
1	a	564	C	N3-C2-O2	-7.90	116.37	121.90
1	a	221	C	N3-C2-O2	-7.89	116.38	121.90
1	a	248	C	N1-C2-O2	7.88	123.62	118.90
25	A	866	A	C5-C6-N6	-7.86	117.41	123.70
25	A	1779	U	C4-C5-C6	7.84	124.41	119.70
1	a	529	G	C4-C5-N7	7.84	113.94	110.80
1	a	503	C	C5-C6-N1	7.83	124.92	121.00
25	A	1345	C	C6-N1-C2	-7.83	117.17	120.30
25	A	12	U	N1-C2-O2	7.83	128.28	122.80
26	B	26	C	N1-C2-O2	7.82	123.59	118.90
9	i	90	ASP	N-CA-CB	-7.82	96.53	110.60
25	A	1178	C	N3-C2-O2	-7.82	116.43	121.90
25	A	867	C	N1-C2-O2	7.82	123.59	118.90
25	A	2704	C	C5-C6-N1	7.80	124.90	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1027	C	C6-N1-C2	-7.79	117.19	120.30
22	v	34	C	C5-C6-N1	7.78	124.89	121.00
25	A	1402	U	N3-C2-O2	-7.78	116.76	122.20
1	a	1158	C	C6-N1-C2	-7.78	117.19	120.30
25	A	353	C	C6-N1-C2	-7.77	117.19	120.30
25	A	2125	G	N3-C4-C5	-7.77	124.72	128.60
25	A	547	A	C2-N3-C4	7.76	114.48	110.60
25	A	2794	C	N3-C4-N4	7.76	123.43	118.00
25	A	2262	U	C4-C5-C6	7.76	124.36	119.70
1	a	1383	C	N1-C2-O2	7.71	123.53	118.90
25	A	121	G	C6-C5-N7	-7.71	125.77	130.40
1	a	37	U	N3-C2-O2	-7.70	116.81	122.20
1	a	460	A	N1-C2-N3	-7.70	125.45	129.30
25	A	1816	C	N1-C2-O2	7.70	123.52	118.90
26	B	4	C	N3-C4-N4	7.68	123.38	118.00
23	x	126	G	P-O3'-C3'	7.68	128.91	119.70
1	a	998	C	N1-C2-O2	7.67	123.50	118.90
1	a	1262	C	N1-C2-O2	7.66	123.50	118.90
25	A	2416	C	C5-C6-N1	7.66	124.83	121.00
1	a	626	G	C5-C6-O6	-7.66	124.00	128.60
25	A	314	C	C6-N1-C2	-7.66	117.23	120.30
25	A	543	G	N1-C6-O6	7.65	124.49	119.90
1	a	528	C	C6-N1-C2	-7.65	117.24	120.30
1	a	385	C	C5-C6-N1	7.64	124.82	121.00
22	v	61	C	N1-C2-O2	7.64	123.49	118.90
25	A	2617	U	N3-C2-O2	-7.64	116.85	122.20
1	a	126	G	N1-C6-O6	7.63	124.48	119.90
25	A	2868	A	N7-C8-N9	7.63	117.62	113.80
25	A	1005	C	N3-C2-O2	-7.62	116.57	121.90
1	a	959	A	N7-C8-N9	7.60	117.60	113.80
43	S	62	ASP	C-N-CA	7.59	138.25	122.30
1	a	1262	C	N3-C2-O2	-7.59	116.59	121.90
1	a	1195	C	N1-C2-O2	7.59	123.45	118.90
1	a	168	G	N1-C6-O6	7.58	124.45	119.90
25	A	557	C	N3-C2-O2	-7.58	116.60	121.90
25	A	206	U	C5-C6-N1	7.58	126.49	122.70
1	a	177	G	C2-N3-C4	7.57	115.69	111.90
1	a	1034	G	N9-C4-C5	-7.56	102.38	105.40
1	a	1172	C	C6-N1-C2	-7.54	117.28	120.30
1	a	1140	C	N3-C2-O2	-7.53	116.63	121.90
25	A	2403	C	C6-N1-C2	-7.51	117.29	120.30
25	A	2409	G	N1-C6-O6	7.51	124.41	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2874	C	N1-C2-O2	7.50	123.40	118.90
22	v	67	C	C5-C6-N1	7.49	124.75	121.00
25	A	281	C	N1-C2-O2	7.49	123.39	118.90
25	A	2834	G	C8-N9-C4	-7.49	103.40	106.40
25	A	359	G	N1-C6-O6	-7.48	115.41	119.90
1	a	580	C	N1-C2-O2	7.48	123.39	118.90
25	A	1941	C	N1-C2-O2	7.48	123.39	118.90
22	v	56	C	C6-N1-C2	-7.47	117.31	120.30
25	A	722	A	N1-C2-N3	-7.47	125.57	129.30
25	A	1305	C	N1-C2-O2	7.46	123.38	118.90
25	A	2069	G7M	P-O3'-C3'	7.46	128.65	119.70
1	a	126	G	C6-C5-N7	-7.46	125.93	130.40
25	A	694	U	N3-C2-O2	-7.46	116.98	122.20
25	A	1461	C	C6-N1-C2	-7.45	117.32	120.30
1	a	1141	C	N3-C2-O2	-7.44	116.69	121.90
1	a	989	U	N3-C2-O2	-7.43	117.00	122.20
1	a	110	C	N3-C2-O2	-7.40	116.72	121.90
1	a	840	C	N3-C4-C5	7.40	124.86	121.90
1	a	661	G	N1-C6-O6	7.39	124.33	119.90
25	A	314	C	C5-C6-N1	7.38	124.69	121.00
1	a	1043	G	N1-C6-O6	-7.37	115.48	119.90
25	A	2793	C	N1-C2-O2	7.37	123.32	118.90
25	A	1348	C	N1-C2-O2	7.37	123.32	118.90
25	A	2669	G	N3-C2-N2	-7.37	114.74	119.90
1	a	943	U	N3-C2-O2	-7.37	117.04	122.20
25	A	1774	C	N3-C2-O2	-7.33	116.77	121.90
1	a	58	C	C2-N3-C4	-7.33	116.23	119.90
1	a	1448	C	N3-C2-O2	-7.32	116.77	121.90
23	x	111	G	N1-C6-O6	-7.32	115.51	119.90
29	E	82	GLY	CA-C-O	-7.32	107.43	120.60
25	A	1830	C	C6-N1-C2	-7.32	117.37	120.30
25	A	2192	U	C5-C6-N1	7.32	126.36	122.70
25	A	845	A	N1-C2-N3	-7.29	125.66	129.30
25	A	2769	U	N3-C2-O2	-7.29	117.10	122.20
1	a	116	A	O5'-P-OP2	-7.29	99.14	105.70
1	a	623	C	C5-C6-N1	7.29	124.64	121.00
1	a	89	U	C5-C4-O4	-7.28	121.53	125.90
1	a	215	C	C2-N1-C1'	7.28	126.81	118.80
25	A	2125	G	C2-N3-C4	7.28	115.54	111.90
25	A	2762	C	N3-C2-O2	-7.27	116.81	121.90
1	a	406	G	N1-C6-O6	7.27	124.26	119.90
25	A	2759	G	N1-C6-O6	-7.27	115.54	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	506	G	N1-C6-O6	7.26	124.26	119.90
25	A	784	G	OP1-P-O3'	7.26	121.18	105.20
1	a	840	C	N3-C4-N4	-7.26	112.92	118.00
1	a	93	U	C5-C6-N1	7.25	126.32	122.70
1	a	78	A	N1-C2-N3	-7.24	125.68	129.30
1	a	1448	C	N1-C2-O2	7.24	123.25	118.90
1	a	810	C	C6-N1-C2	-7.24	117.40	120.30
23	x	127	U	P-O3'-C3'	7.24	128.39	119.70
22	v	41	C	N3-C2-O2	-7.24	116.83	121.90
1	a	33	A	N7-C8-N9	7.23	117.42	113.80
25	A	1438	U	C5-C6-N1	7.22	126.31	122.70
25	A	758	C	C6-N1-C2	-7.21	117.42	120.30
1	a	1497	G	N1-C6-O6	-7.21	115.58	119.90
25	A	847	U	N1-C2-O2	7.20	127.84	122.80
1	a	413	G	N3-C4-N9	7.20	130.32	126.00
1	a	527	G7M	P-O3'-C3'	7.18	128.32	119.70
25	A	281	C	N3-C4-N4	7.17	123.02	118.00
25	A	984	A	C2-N3-C4	-7.16	107.02	110.60
24	y	47(L)	G	N3-C2-N2	-7.16	114.89	119.90
25	A	1947	C	C6-N1-C2	-7.16	117.44	120.30
25	A	2666	C	N1-C2-O2	7.16	123.19	118.90
25	A	1462	C	N1-C2-O2	7.15	123.19	118.90
25	A	1104	C	C2-N3-C4	7.15	123.47	119.90
25	A	1151	A	N1-C2-N3	-7.15	125.72	129.30
22	v	34	C	C6-N1-C2	-7.15	117.44	120.30
1	a	52	C	C6-N1-C2	-7.14	117.44	120.30
25	A	883	G	C8-N9-C4	-7.14	103.54	106.40
25	A	867	C	N3-C2-O2	-7.14	116.90	121.90
25	A	2742	G	C5-C6-N1	7.13	115.06	111.50
6	f	53	LYS	N-CA-CB	7.12	123.42	110.60
25	A	2326	C	C5-C6-N1	7.12	124.56	121.00
1	a	1195	C	N3-C2-O2	-7.12	116.92	121.90
25	A	1102	C	C6-N1-C2	-7.12	117.45	120.30
25	A	758	C	N1-C2-O2	7.10	123.16	118.90
25	A	2710	C	C6-N1-C2	-7.09	117.46	120.30
25	A	2805	C	C6-N1-C2	-7.09	117.47	120.30
1	a	126	G	N9-C4-C5	-7.09	102.56	105.40
25	A	847	U	N3-C2-O2	-7.09	117.24	122.20
25	A	1666	G	N1-C6-O6	-7.09	115.65	119.90
56	6	37	CYS	CA-CB-SG	7.08	126.75	114.00
1	a	723	U	C5-C6-N1	7.08	126.24	122.70
25	A	420	C	N1-C2-O2	7.08	123.15	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	34	C	N1-C2-O2	7.08	123.15	118.90
25	A	2456	C	C5-C6-N1	7.07	124.53	121.00
24	y	74	C	C6-N1-C2	-7.07	117.47	120.30
1	a	335	C	C6-N1-C2	-7.05	117.48	120.30
25	A	894	U	N3-C2-O2	-7.05	117.27	122.20
25	A	1578	U	N3-C2-O2	-7.05	117.27	122.20
24	y	74	C	C5-C6-N1	7.04	124.52	121.00
25	A	2791	G	C6-N1-C2	-7.04	120.88	125.10
25	A	2553	G	N1-C6-O6	7.04	124.12	119.90
25	A	281	C	C2-N3-C4	7.04	123.42	119.90
25	A	866	A	N1-C6-N6	7.04	122.82	118.60
26	B	4	C	C2-N3-C4	7.04	123.42	119.90
36	L	77	ILE	CG1-CB-CG2	-7.03	95.93	111.40
1	a	375	U	N3-C2-O2	-7.03	117.28	122.20
21	u	24	LYS	N-CA-CB	-7.02	97.96	110.60
25	A	2745	C	N1-C2-O2	7.02	123.11	118.90
26	B	97	C	C5-C6-N1	7.02	124.51	121.00
1	a	1003	G	N1-C2-N2	7.01	122.51	116.20
25	A	2063	C	C6-N1-C2	-7.01	117.50	120.30
25	A	2868	A	C8-N9-C4	-7.01	103.00	105.80
1	a	868	C	N1-C2-O2	7.01	123.11	118.90
25	A	1564	C	C5-C6-N1	7.00	124.50	121.00
25	A	1589	U	N3-C2-O2	-7.00	117.30	122.20
1	a	1134	G	N1-C2-N2	7.00	122.50	116.20
25	A	2884	U	N1-C2-O2	7.00	127.70	122.80
25	A	353	C	C5-C6-N1	6.99	124.50	121.00
1	a	719	C	C6-N1-C2	-6.99	117.50	120.30
25	A	2683	C	N3-C2-O2	-6.99	117.01	121.90
25	A	528	A	C5-N7-C8	-6.99	100.41	103.90
25	A	353	C	N3-C4-N4	6.98	122.89	118.00
25	A	1567	G	P-O3'-C3'	6.98	128.07	119.70
25	A	67	U	C5-C4-O4	-6.97	121.72	125.90
25	A	2424	C	N3-C4-C5	6.97	124.69	121.90
25	A	2610	C	P-O3'-C3'	6.97	128.07	119.70
25	A	1054	A	N1-C2-N3	-6.97	125.81	129.30
25	A	581	C	C5-C6-N1	6.97	124.48	121.00
25	A	359	G	N3-C2-N2	-6.96	115.03	119.90
25	A	1180	U	N3-C4-O4	6.96	124.27	119.40
1	a	1320	C	N1-C2-O2	6.96	123.08	118.90
26	B	31	C	N3-C2-O2	-6.96	117.03	121.90
25	A	278	A	N1-C6-N6	-6.95	114.43	118.60
25	A	2160	C	N3-C4-N4	-6.94	113.14	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	257	C	N1-C2-O2	6.94	123.06	118.90
25	A	1498	C	C2-N1-C1'	6.94	126.43	118.80
24	y	47(J)	C	N3-C4-C5	6.93	124.67	121.90
25	A	894	U	N1-C2-O2	6.93	127.65	122.80
1	a	455	G	N1-C6-O6	6.93	124.06	119.90
1	a	1011	C	C6-N1-C2	-6.92	117.53	120.30
25	A	528	A	N7-C8-N9	6.92	117.26	113.80
1	a	457	G	N3-C2-N2	-6.92	115.06	119.90
1	a	397	A	C2-N3-C4	6.91	114.06	110.60
1	a	1010	U	N3-C2-O2	-6.91	117.36	122.20
25	A	67	U	N3-C4-O4	6.90	124.23	119.40
1	a	960	U	P-O3'-C3'	6.90	127.97	119.70
25	A	278	A	N3-C4-C5	-6.89	121.97	126.80
1	a	957	U	N3-C2-O2	-6.89	117.38	122.20
1	a	1282	C	C6-N1-C2	-6.89	117.54	120.30
23	x	127	U	O4'-C1'-N1	6.88	113.70	108.20
25	A	2061	G	P-O3'-C3'	6.88	127.95	119.70
25	A	2128	G	C6-C5-N7	-6.88	126.27	130.40
1	a	99	C	C5-C6-N1	6.88	124.44	121.00
1	a	217	C	N3-C2-O2	-6.88	117.09	121.90
25	A	2308	G	N1-C6-O6	-6.88	115.77	119.90
45	U	88	ASP	N-CA-CB	6.87	122.97	110.60
25	A	1105	U	C2-N3-C4	-6.87	122.88	127.00
1	a	1109	C	C6-N1-C2	-6.87	117.55	120.30
1	a	1034	G	N3-C4-N9	6.87	130.12	126.00
25	A	1210	G	C2-N3-C4	6.87	115.33	111.90
25	A	1111	A	P-O3'-C3'	6.86	127.93	119.70
25	A	1331	G	N1-C6-O6	-6.86	115.78	119.90
25	A	694	U	N1-C2-O2	6.86	127.60	122.80
25	A	2769	U	N1-C2-O2	6.85	127.60	122.80
1	a	1143	G	N3-C2-N2	-6.85	115.11	119.90
25	A	1104	C	C6-N1-C2	-6.85	117.56	120.30
25	A	2785	C	C6-N1-C2	-6.85	117.56	120.30
25	A	1795	C	C5-C6-N1	6.85	124.42	121.00
25	A	1098	A	C5-C6-N6	-6.84	118.22	123.70
1	a	611	C	N1-C2-O2	6.84	123.00	118.90
25	A	1451	C	C2-N3-C4	-6.84	116.48	119.90
1	a	156	C	N1-C2-O2	-6.84	114.80	118.90
1	a	1277	C	N1-C2-O2	6.84	123.00	118.90
1	a	472	U	N3-C2-O2	-6.83	117.42	122.20
25	A	1005	C	C6-N1-C2	-6.83	117.57	120.30
1	a	998	C	C6-N1-C2	-6.83	117.57	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	240	G	N1-C6-O6	6.82	123.99	119.90
1	a	61	G	N1-C6-O6	6.82	123.99	119.90
25	A	912	C	N1-C2-O2	6.82	122.99	118.90
25	A	343	C	C6-N1-C2	-6.81	117.58	120.30
25	A	198	C	C5-C6-N1	6.81	124.41	121.00
25	A	1070	A	P-O3'-C3'	6.81	127.87	119.70
1	a	1326	U	N1-C2-O2	6.80	127.56	122.80
25	A	484	C	N1-C2-O2	6.80	122.98	118.90
1	a	545	C	N3-C4-C5	6.79	124.62	121.90
25	A	2553	G	C5-C6-O6	-6.79	124.53	128.60
25	A	2762	C	C2-N1-C1'	6.79	126.27	118.80
41	Q	27	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	a	1037	C	N3-C2-O2	-6.78	117.15	121.90
25	A	234	U	N3-C2-O2	-6.78	117.46	122.20
25	A	1021	A	C2-N3-C4	6.78	113.99	110.60
25	A	1900	A	P-O3'-C3'	6.78	127.83	119.70
22	v	51	C	C6-N1-C2	-6.77	117.59	120.30
25	A	2405	G	OP2-P-O3'	6.76	120.08	105.20
26	B	12	C	C2-N1-C1'	6.76	126.24	118.80
1	a	1389	C	N1-C2-O2	6.76	122.96	118.90
25	A	363	G	N1-C6-O6	6.76	123.95	119.90
25	A	1979	U	N3-C2-O2	-6.76	117.47	122.20
1	a	529	G	N9-C4-C5	-6.75	102.70	105.40
25	A	783	A	C4-C5-N7	6.75	114.07	110.70
1	a	545	C	C4-C5-C6	-6.74	114.03	117.40
25	A	2076	U	N3-C2-O2	-6.74	117.48	122.20
25	A	2666	C	N3-C2-O2	-6.74	117.18	121.90
1	a	89	U	C5-C6-N1	6.74	126.07	122.70
24	y	61	C	C6-N1-C2	-6.74	117.61	120.30
26	B	88	C	N1-C2-O2	6.73	122.94	118.90
22	v	56	C	N3-C2-O2	-6.72	117.19	121.90
25	A	373	U	N3-C2-O2	-6.72	117.49	122.20
1	a	972	C	C6-N1-C2	-6.72	117.61	120.30
1	a	1306	A	C8-N9-C4	-6.72	103.11	105.80
25	A	106	C	C6-N1-C2	-6.72	117.61	120.30
25	A	2870	C	C6-N1-C2	-6.72	117.61	120.30
1	a	89	U	N3-C4-O4	6.72	124.10	119.40
25	A	932	U	N1-C2-N3	6.72	118.93	114.90
1	a	142	G	N1-C6-O6	-6.71	115.87	119.90
25	A	1564	C	C6-N1-C2	-6.71	117.62	120.30
25	A	1737	G	C2-N3-C4	6.71	115.25	111.90
25	A	435	C	N1-C2-O2	6.70	122.92	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	845	A	C2-N3-C4	6.69	113.95	110.60
25	A	276	U	N1-C2-O2	6.69	127.48	122.80
1	a	213	G	C8-N9-C4	-6.69	103.72	106.40
1	a	737	C	C5-C6-N1	6.69	124.34	121.00
1	a	1383	C	N3-C2-O2	-6.69	117.22	121.90
1	a	1453	G	C2-N3-C4	6.69	115.24	111.90
25	A	2416	C	C6-N1-C2	-6.69	117.62	120.30
25	A	1159	U	N3-C2-O2	-6.68	117.52	122.20
17	q	69	THR	N-CA-CB	6.68	122.99	110.30
25	A	1119	U	N1-C2-O2	6.68	127.47	122.80
1	a	1284	C	C6-N1-C2	-6.67	117.63	120.30
25	A	2109	U	C5-C6-N1	6.67	126.03	122.70
22	v	71	C	N1-C2-O2	6.66	122.89	118.90
1	a	126	G	C4-C5-N7	6.65	113.46	110.80
25	A	445	C	N3-C2-O2	-6.65	117.25	121.90
25	A	528	A	C2-N3-C4	-6.65	107.28	110.60
25	A	1087	G	N9-C4-C5	6.63	108.05	105.40
25	A	528	A	C8-N9-C4	-6.62	103.15	105.80
1	a	1382	C	N1-C2-O2	6.61	122.87	118.90
25	A	869	G	N1-C6-O6	-6.61	115.93	119.90
1	a	1306	A	N7-C8-N9	6.61	117.11	113.80
1	a	29	U	N3-C2-O2	-6.60	117.58	122.20
1	a	857	C	N1-C2-O2	6.59	122.86	118.90
24	y	61	C	N1-C2-O2	6.59	122.86	118.90
25	A	2178	C	C6-N1-C2	-6.59	117.66	120.30
1	a	1259	C	N1-C2-O2	6.59	122.85	118.90
1	a	1033	G	N1-C6-O6	6.58	123.85	119.90
1	a	284	C	N1-C2-O2	6.58	122.85	118.90
25	A	2574	G	N1-C6-O6	6.58	123.85	119.90
25	A	2758	A	N1-C6-N6	-6.57	114.66	118.60
25	A	373	U	N1-C2-O2	6.56	127.39	122.80
25	A	2456	C	C6-N1-C2	-6.56	117.68	120.30
1	a	1282	C	N1-C2-O2	6.55	122.83	118.90
1	a	213	G	N7-C8-N9	6.55	116.38	113.10
25	A	1584	U	C5-C6-N1	6.55	125.97	122.70
25	A	2863	C	C5-C6-N1	6.54	124.27	121.00
1	a	99	C	C6-N1-C2	-6.54	117.68	120.30
1	a	1173	U	N3-C4-O4	6.54	123.98	119.40
1	a	318	G	N1-C6-O6	-6.54	115.98	119.90
1	a	475	C	C6-N1-C2	-6.54	117.69	120.30
25	A	1578	U	N1-C2-O2	6.53	127.37	122.80
25	A	2125	G	N3-C4-N9	6.53	129.92	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	310	G	N1-C6-O6	6.53	123.81	119.90
25	A	360	U	N3-C4-C5	6.53	118.52	114.60
25	A	1104	C	N3-C4-N4	6.53	122.57	118.00
26	B	26	C	N3-C2-O2	-6.52	117.33	121.90
26	B	31	C	C6-N1-C2	-6.52	117.69	120.30
1	a	1344	C	C6-N1-C2	-6.52	117.69	120.30
25	A	205	G	OP2-P-O3'	6.52	119.54	105.20
1	a	475	C	N1-C2-O2	6.52	122.81	118.90
1	a	1226	C	C2-N3-C4	-6.52	116.64	119.90
25	A	1114	C	C6-N1-C2	-6.52	117.69	120.30
25	A	1119	U	N3-C2-O2	-6.52	117.64	122.20
25	A	121	G	C4-C5-N7	6.52	113.41	110.80
1	a	284	C	C6-N1-C2	-6.51	117.70	120.30
25	A	783	A	C6-C5-N7	-6.51	127.74	132.30
1	a	623	C	N1-C2-O2	6.51	122.81	118.90
1	a	1320	C	N3-C2-O2	-6.51	117.34	121.90
1	a	1134	G	C6-N1-C2	-6.50	121.20	125.10
25	A	205	G	P-O3'-C3'	6.50	127.51	119.70
25	A	2248	C	N1-C2-O2	6.50	122.80	118.90
25	A	546	U	C6-N1-C2	-6.50	117.10	121.00
1	a	1011	C	C5-C6-N1	6.50	124.25	121.00
25	A	1297	C	C6-N1-C2	-6.50	117.70	120.30
1	a	739	C	C6-N1-C2	-6.50	117.70	120.30
25	A	1644	C	C6-N1-C2	-6.50	117.70	120.30
1	a	165	G	N1-C6-O6	6.49	123.80	119.90
1	a	450	G	N3-C2-N2	-6.49	115.36	119.90
24	y	35	C	N3-C4-N4	6.49	122.54	118.00
1	a	126	G	N3-C2-N2	6.49	124.44	119.90
25	A	274	C	N3-C4-N4	-6.49	113.46	118.00
26	B	38	C	N3-C2-O2	-6.48	117.36	121.90
25	A	81	G	N1-C6-O6	-6.48	116.01	119.90
25	A	282	A	N1-C2-N3	-6.48	126.06	129.30
25	A	1760	C	C6-N1-C2	-6.47	117.71	120.30
19	s	5	LYS	CB-CG-CD	6.47	128.42	111.60
22	v	34	C	C2-N1-C1'	6.47	125.91	118.80
1	a	660	C	N3-C2-O2	-6.46	117.38	121.90
25	A	357	C	C6-N1-C2	-6.46	117.71	120.30
25	A	228	C	P-O3'-C3'	6.46	127.45	119.70
1	a	528	C	C5-C6-N1	6.46	124.23	121.00
25	A	281	C	N3-C4-C5	-6.45	119.32	121.90
25	A	372	G	P-O3'-C3'	6.44	127.43	119.70
25	A	435	C	N3-C2-O2	-6.44	117.39	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1294	U	N3-C2-O2	-6.44	117.69	122.20
25	A	2658	C	N1-C2-O2	6.44	122.77	118.90
1	a	1510	C	N1-C2-O2	6.44	122.77	118.90
25	A	2325	G	N1-C6-O6	6.44	123.76	119.90
25	A	2863	C	C6-N1-C2	-6.44	117.72	120.30
25	A	847	U	C2-N1-C1'	6.44	125.42	117.70
25	A	868	U	N3-C2-O2	-6.44	117.69	122.20
23	x	125	G	C4'-C3'-O3'	6.43	125.87	113.00
1	a	1393	U	N3-C2-O2	-6.43	117.70	122.20
25	A	908	C	C6-N1-C2	-6.43	117.73	120.30
25	A	2056	G	N1-C6-O6	6.43	123.76	119.90
1	a	215	C	C2-N3-C4	6.42	123.11	119.90
13	m	57	ASP	CB-CG-OD1	6.42	124.08	118.30
25	A	1081	U	C5-C4-O4	-6.42	122.05	125.90
1	a	1389	C	C5-C6-N1	6.41	124.21	121.00
25	A	611	C	C6-N1-C2	-6.41	117.73	120.30
1	a	126	G	N3-C4-N9	6.41	129.85	126.00
25	A	121	G	C5-C6-O6	-6.41	124.76	128.60
1	a	193	C	N1-C2-O2	6.40	122.74	118.90
25	A	484	C	C5-C6-N1	6.40	124.20	121.00
25	A	1662	U	N3-C2-O2	-6.40	117.72	122.20
25	A	2407	A	O5'-P-OP2	-6.40	99.94	105.70
25	A	640	C	C6-N1-C2	-6.40	117.74	120.30
25	A	2799	A	N1-C6-N6	6.40	122.44	118.60
25	A	1804	C	C6-N1-C2	-6.39	117.75	120.30
25	A	121	G	N9-C4-C5	-6.38	102.85	105.40
25	A	2243	U	N3-C2-O2	-6.38	117.73	122.20
25	A	813	U	N3-C2-O2	-6.38	117.73	122.20
6	f	98	GLU	N-CA-CB	6.38	122.08	110.60
25	A	2767	C	C6-N1-C2	-6.38	117.75	120.30
25	A	1105	U	N1-C2-O2	6.37	127.26	122.80
25	A	1114	C	N1-C2-O2	6.37	122.72	118.90
1	a	414	A	O5'-P-OP2	-6.36	99.97	105.70
1	a	846	G	C6-C5-N7	-6.36	126.58	130.40
22	v	49	G	N1-C6-O6	6.36	123.72	119.90
25	A	2128	G	N1-C6-O6	6.36	123.72	119.90
1	a	1344	C	N3-C2-O2	-6.36	117.45	121.90
25	A	2164	C	N1-C2-O2	6.36	122.71	118.90
23	x	91	A	N1-C2-N3	-6.35	126.12	129.30
25	A	1267	U	N1-C2-O2	6.35	127.25	122.80
24	y	47(D)	C	N1-C2-N3	6.35	123.64	119.20
26	B	97	C	N3-C2-O2	-6.33	117.47	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	67	C	C2-N3-C4	6.33	123.07	119.90
23	x	134	C	C6-N1-C2	-6.33	117.77	120.30
25	A	281	C	C2-N1-C1'	6.33	125.76	118.80
1	a	660	C	C6-N1-C2	-6.32	117.77	120.30
25	A	2065	C	C6-N1-C2	-6.32	117.77	120.30
1	a	1037	C	C6-N1-C2	-6.32	117.77	120.30
1	a	1129	C	OP1-P-O3'	6.32	119.10	105.20
25	A	1894	C	N3-C2-O2	-6.32	117.48	121.90
24	y	71	C	N1-C2-O2	6.32	122.69	118.90
25	A	51	G	P-O3'-C3'	6.31	127.27	119.70
25	A	2720	U	N3-C2-O2	-6.31	117.78	122.20
25	A	1752	C	C6-N1-C2	-6.31	117.78	120.30
25	A	669	G	C4-N9-C1'	6.30	134.69	126.50
25	A	1114	C	C5-C6-N1	6.30	124.15	121.00
25	A	1498	C	C5-C4-N4	-6.30	115.79	120.20
26	B	28	C	C6-N1-C2	-6.30	117.78	120.30
25	A	932	U	C2-N3-C4	-6.29	123.22	127.00
25	A	1054	A	C6-N1-C2	6.29	122.38	118.60
1	a	896	C	C5-C6-N1	6.29	124.15	121.00
25	A	965	C	C6-N1-C2	-6.29	117.79	120.30
25	A	172	A	N1-C2-N3	-6.28	126.16	129.30
26	B	120	U	C2-N1-C1'	6.28	125.23	117.70
1	a	1173	U	C5-C6-N1	6.28	125.84	122.70
1	a	413	G	OP2-P-O3'	6.27	119.00	105.20
25	A	1574	C	C6-N1-C2	-6.27	117.79	120.30
1	a	52	C	C5-C6-N1	6.27	124.13	121.00
1	a	1303	C	N1-C2-O2	6.27	122.66	118.90
25	A	2669	G	C6-N1-C2	-6.26	121.34	125.10
25	A	2794	C	C5-C4-N4	-6.26	115.81	120.20
1	a	222	C	C6-N1-C2	-6.26	117.80	120.30
25	A	2704	C	C6-N1-C2	-6.26	117.80	120.30
25	A	2171	A	N1-C6-N6	6.25	122.35	118.60
1	a	221	C	C6-N1-C2	-6.25	117.80	120.30
1	a	1140	C	C6-N1-C2	-6.25	117.80	120.30
25	A	565	C	N1-C2-O2	6.25	122.65	118.90
24	y	41	C	C6-N1-C2	-6.25	117.80	120.30
25	A	1348	C	N3-C2-O2	-6.24	117.53	121.90
1	a	459	A	N1-C2-N3	-6.24	126.18	129.30
1	a	846	G	N1-C6-O6	6.24	123.64	119.90
25	A	1135	C	OP1-P-O3'	6.24	118.93	105.20
25	A	2767	C	C5-C6-N1	6.24	124.12	121.00
1	a	240	G	C5-C6-O6	-6.23	124.86	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	56	C	C2-N1-C1'	6.23	125.66	118.80
23	x	128	C	C3'-C2'-C1'	6.23	106.49	101.50
1	a	890	G	C8-N9-C4	6.23	108.89	106.40
25	A	1774	C	N1-C2-O2	6.23	122.64	118.90
1	a	1226	C	N1-C2-O2	-6.23	115.16	118.90
1	a	1463	U	C5-C6-N1	6.23	125.81	122.70
25	A	2214	C	N3-C2-O2	-6.23	117.54	121.90
1	a	1197	A	O5'-P-OP2	-6.22	100.10	105.70
1	a	1427	C	C6-N1-C2	-6.22	117.81	120.30
25	A	783	A	N1-C6-N6	6.22	122.33	118.60
25	A	1212	G	P-O3'-C3'	6.22	127.17	119.70
22	v	67	C	C2-N1-C1'	6.22	125.64	118.80
56	6	34	LEU	CA-CB-CG	6.22	129.61	115.30
24	y	6	U	N3-C2-O2	-6.22	117.85	122.20
1	a	487	A	C2-N3-C4	6.21	113.71	110.60
1	a	717	U	N3-C2-O2	-6.21	117.85	122.20
25	A	407	G	N3-C2-N2	-6.21	115.55	119.90
26	B	4	C	C2-N1-C1'	6.21	125.63	118.80
45	U	88	ASP	N-CA-C	-6.21	94.24	111.00
25	A	1958	C	C6-N1-C2	-6.21	117.82	120.30
1	a	193	C	N3-C2-O2	-6.20	117.56	121.90
25	A	57	C	C5-C6-N1	6.20	124.10	121.00
25	A	2576	G	N3-C4-N9	6.20	129.72	126.00
1	a	988	G	C6-N1-C2	-6.20	121.38	125.10
25	A	2200	C	C6-N1-C2	-6.20	117.82	120.30
26	B	68	C	C6-N1-C2	-6.19	117.82	120.30
1	a	1245	C	C5-C6-N1	6.19	124.09	121.00
25	A	2591	C	C6-N1-C2	-6.19	117.83	120.30
35	K	12	ASP	CB-CG-OD1	6.19	123.87	118.30
25	A	702	U	C5-C6-N1	6.19	125.79	122.70
1	a	231	U	N3-C2-O2	-6.18	117.87	122.20
5	e	77	ASN	N-CA-CB	-6.18	99.47	110.60
23	x	108	A	C2-N3-C4	6.18	113.69	110.60
25	A	1314	C	C2-N1-C1'	6.18	125.60	118.80
25	A	413	C	N1-C2-O2	6.18	122.61	118.90
25	A	669	G	N3-C4-N9	6.18	129.71	126.00
25	A	1567	G	OP2-P-O3'	6.18	118.79	105.20
1	a	1496	C	C6-N1-C2	-6.18	117.83	120.30
25	A	1345	C	C5-C6-N1	6.16	124.08	121.00
1	a	386	C	N3-C4-N4	6.16	122.31	118.00
1	a	988	G	N3-C2-N2	-6.16	115.59	119.90
22	v	51	C	N3-C2-O2	-6.16	117.59	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1182	G	OP2-P-O3'	6.16	118.75	105.20
25	A	1104	C	C5-C6-N1	6.16	124.08	121.00
25	A	2129	C	C6-N1-C2	-6.16	117.84	120.30
1	a	264	C	C6-N1-C2	-6.16	117.84	120.30
25	A	358	U	N3-C2-O2	-6.15	117.89	122.20
1	a	1353	G	N1-C6-O6	-6.14	116.21	119.90
26	B	60	C	C5-C6-N1	6.14	124.07	121.00
25	A	2076	U	N1-C2-O2	6.14	127.10	122.80
1	a	186	C	C5-C6-N1	6.14	124.07	121.00
25	A	1348	C	C6-N1-C2	-6.14	117.84	120.30
25	A	2226	C	C6-N1-C2	-6.14	117.84	120.30
25	A	2745	C	N3-C2-O2	-6.14	117.61	121.90
25	A	2128	G	N3-C4-N9	6.13	129.68	126.00
1	a	126	G	C5-C6-O6	-6.13	124.92	128.60
1	a	1277	C	C6-N1-C2	-6.13	117.85	120.30
26	B	68	C	C5-C6-N1	6.13	124.07	121.00
1	a	977	A	C2-N3-C4	6.13	113.66	110.60
1	a	67	C	C6-N1-C2	-6.13	117.85	120.30
25	A	611	C	C5-C6-N1	6.12	124.06	121.00
25	A	1994	C	N3-C2-O2	-6.12	117.61	121.90
25	A	206	U	C6-N1-C2	-6.12	117.33	121.00
1	a	266	G	O4'-C1'-N9	-6.12	103.30	108.20
1	a	1056	U	N1-C2-O2	6.12	127.09	122.80
1	a	1173	U	C5-C4-O4	-6.12	122.23	125.90
25	A	1267	U	N3-C2-O2	-6.12	117.91	122.20
25	A	2326	C	O4'-C1'-N1	6.12	113.10	108.20
22	v	67	C	N3-C4-N4	6.12	122.28	118.00
25	A	1200	C	C6-N1-C2	-6.12	117.85	120.30
25	A	1648	U	N3-C2-O2	-6.12	117.92	122.20
25	A	1656	C	C6-N1-C2	-6.11	117.86	120.30
1	a	1087	G	N1-C2-N3	6.11	127.56	123.90
25	A	1376	C	N1-C2-O2	6.11	122.56	118.90
1	a	896	C	C6-N1-C2	-6.11	117.86	120.30
22	v	3	C	C6-N1-C2	-6.11	117.86	120.30
23	x	125	G	C3'-C2'-C1'	6.10	106.38	101.50
25	A	2666	C	C6-N1-C2	-6.10	117.86	120.30
25	A	2326	C	C4-C5-C6	-6.10	114.35	117.40
1	a	1158	C	N3-C2-O2	-6.09	117.63	121.90
1	a	1282	C	N3-C2-O2	-6.09	117.64	121.90
1	a	544	G	C5-C6-O6	-6.09	124.95	128.60
25	A	353	C	C2-N1-C1'	6.09	125.50	118.80
25	A	557	C	C2-N1-C1'	6.09	125.50	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	144	G	N1-C6-O6	6.09	123.55	119.90
55	4	14	CYS	CA-CB-SG	6.09	124.96	114.00
25	A	2782	G	C6-C5-N7	-6.09	126.75	130.40
1	a	883	C	N1-C2-O2	6.08	122.55	118.90
1	a	419	C	N1-C2-O2	-6.08	115.25	118.90
25	A	137	U	N1-C2-O2	6.08	127.06	122.80
1	a	500	G	C6-C5-N7	-6.08	126.75	130.40
1	a	868	C	N3-C2-O2	-6.08	117.65	121.90
1	a	890	G	O4'-C1'-N9	6.07	113.06	108.20
25	A	353	C	C2-N3-C4	6.07	122.94	119.90
1	a	1382	C	N3-C2-O2	-6.07	117.65	121.90
1	a	1237	C	OP1-P-O3'	6.07	118.56	105.20
25	A	640	C	C5-C6-N1	6.07	124.03	121.00
18	r	15	GLU	C-N-CA	6.07	135.04	122.30
1	a	957	U	N1-C2-N3	6.06	118.54	114.90
1	a	356	A	N1-C2-N3	6.06	132.33	129.30
25	A	335	C	C6-N1-C2	-6.06	117.88	120.30
25	A	2691	C	C6-N1-C2	-6.06	117.88	120.30
25	A	1945	G	C5-C6-O6	-6.06	124.96	128.60
1	a	310	G	C5-C6-O6	-6.05	124.97	128.60
1	a	215	C	C5-C6-N1	6.05	124.03	121.00
1	a	506	G	C5-C6-O6	-6.05	124.97	128.60
1	a	840	C	C2-N3-C4	-6.05	116.88	119.90
25	A	2646	C	C6-N1-C2	-6.05	117.88	120.30
25	A	901	C	N1-C2-O2	6.04	122.53	118.90
22	v	34	C	C2-N3-C4	6.04	122.92	119.90
25	A	1048	A	N7-C8-N9	6.04	116.82	113.80
1	a	475	C	N3-C2-O2	-6.03	117.68	121.90
26	B	97	C	N3-C4-N4	6.03	122.22	118.00
1	a	1195	C	C6-N1-C2	-6.03	117.89	120.30
1	a	408	A	N1-C2-N3	-6.03	126.29	129.30
42	R	78	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	a	1277	C	N3-C2-O2	-6.01	117.69	121.90
1	a	1297	G	P-O3'-C3'	6.01	126.91	119.70
1	a	1383	C	C6-N1-C2	-6.01	117.90	120.30
1	a	186	C	N3-C2-O2	-6.00	117.70	121.90
25	A	1101	U	N1-C2-O2	6.00	127.00	122.80
1	a	1225	A	C2-N3-C4	6.00	113.60	110.60
5	e	89	THR	N-CA-CB	-6.00	98.90	110.30
25	A	435	C	C6-N1-C2	-6.00	117.90	120.30
25	A	1237	A	N7-C8-N9	6.00	116.80	113.80
1	a	717	U	N1-C2-O2	6.00	127.00	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2716	C	N1-C2-O2	6.00	122.50	118.90
13	m	78	ARG	NE-CZ-NH1	6.00	123.30	120.30
25	A	1313	U	C6-N1-C1'	-5.99	112.81	121.20
1	a	979	C	C6-N1-C2	-5.99	117.91	120.30
1	a	636	U	C5-C6-N1	5.99	125.69	122.70
25	A	866	A	C4-C5-N7	5.99	113.69	110.70
25	A	634	C	C5-C6-N1	5.98	123.99	121.00
25	A	2832	U	P-O3'-C3'	5.98	126.88	119.70
25	A	1413	A	N1-C2-N3	-5.98	126.31	129.30
25	A	2805	C	N1-C2-O2	5.98	122.49	118.90
25	A	2884	U	C2-N1-C1'	5.98	124.87	117.70
1	a	1363	A	C2-N3-C4	5.97	113.59	110.60
1	a	717	U	OP2-P-O3'	5.97	118.34	105.20
1	a	1182	G	P-O3'-C3'	5.97	126.87	119.70
25	A	1303	G	N1-C6-O6	5.97	123.48	119.90
25	A	2177	C	C6-N1-C2	-5.97	117.91	120.30
1	a	1507	A	N1-C2-N3	-5.97	126.31	129.30
24	y	35	C	N1-C2-O2	5.97	122.48	118.90
1	a	225	C	C6-N1-C2	-5.97	117.91	120.30
25	A	1301	A	C2-N3-C4	5.96	113.58	110.60
25	A	278	A	C8-N9-C4	-5.96	103.42	105.80
31	G	165	ASP	CB-CG-OD1	5.96	123.66	118.30
1	a	1100	C	C5-C6-N1	5.96	123.98	121.00
1	a	1460	C	C6-N1-C2	-5.95	117.92	120.30
1	a	1258	G	N1-C6-O6	-5.95	116.33	119.90
25	A	2691	C	C5-C6-N1	5.95	123.97	121.00
25	A	2867	G	C4-C5-N7	5.95	113.18	110.80
1	a	58	C	C5-C4-N4	-5.95	116.04	120.20
1	a	177	G	N3-C4-C5	-5.95	125.63	128.60
1	a	240	G	N9-C4-C5	-5.95	103.02	105.40
1	a	544	G	N9-C4-C5	-5.94	103.02	105.40
1	a	153	C	N1-C2-O2	5.94	122.46	118.90
25	A	1784	A	C5-N7-C8	5.94	106.87	103.90
25	A	1498	C	C6-N1-C2	-5.93	117.93	120.30
27	C	269	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	a	29	U	N1-C2-N3	5.93	118.46	114.90
25	A	2903	U	N1-C2-O2	5.93	126.95	122.80
1	a	483	C	C6-N1-C2	-5.93	117.93	120.30
25	A	2195	U	N3-C2-O2	-5.93	118.05	122.20
1	a	128	G	N1-C6-O6	5.92	123.45	119.90
1	a	141	G	N3-C2-N2	-5.92	115.76	119.90
25	A	413	C	N3-C2-O2	-5.91	117.76	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2542	A	N1-C6-N6	-5.91	115.05	118.60
26	B	97	C	C6-N1-C1'	-5.91	113.70	120.80
1	a	156	C	N3-C4-N4	-5.91	113.86	118.00
25	A	420	C	N3-C2-O2	-5.91	117.77	121.90
25	A	1450	G	N1-C6-O6	-5.90	116.36	119.90
25	A	2424	C	N1-C2-O2	5.90	122.44	118.90
1	a	248	C	N3-C2-O2	-5.90	117.77	121.90
25	A	314	C	N1-C2-O2	5.89	122.44	118.90
25	A	2147	A	C8-N9-C4	-5.89	103.44	105.80
25	A	2867	G	N9-C4-C5	-5.89	103.04	105.40
25	A	2793	C	N3-C2-O2	-5.89	117.78	121.90
25	A	1058	U	C2-N3-C4	5.88	130.53	127.00
25	A	2391	G	P-O3'-C3'	5.88	126.76	119.70
25	A	359	G	N1-C2-N2	5.88	121.49	116.20
25	A	2162	G	C4-N9-C1'	5.88	134.14	126.50
1	a	1007	U	N3-C2-O2	-5.88	118.09	122.20
25	A	898	C	C5-C6-N1	5.88	123.94	121.00
25	A	1624	U	N3-C2-O2	-5.88	118.09	122.20
1	a	64	G	OP2-P-O3'	5.88	118.12	105.20
1	a	611	C	N3-C2-O2	-5.88	117.79	121.90
25	A	281	C	N3-C2-O2	-5.87	117.79	121.90
25	A	610	C	N3-C2-O2	-5.87	117.79	121.90
25	A	1049	C	N1-C2-O2	5.87	122.42	118.90
25	A	1941	C	N3-C2-O2	-5.87	117.79	121.90
25	A	1804	C	C5-C6-N1	5.87	123.94	121.00
1	a	356	A	C6-N1-C2	-5.86	115.08	118.60
1	a	1210	C	C6-N1-C2	-5.86	117.95	120.30
24	y	59	C	N3-C2-O2	-5.86	117.80	121.90
25	A	2785	C	C5-C6-N1	5.86	123.93	121.00
1	a	591	U	N3-C2-O2	-5.85	118.10	122.20
1	a	601	G	N1-C6-O6	5.85	123.41	119.90
22	v	49	G	C6-C5-N7	-5.85	126.89	130.40
1	a	132	C	C6-N1-C2	-5.85	117.96	120.30
25	A	2840	C	C5-C6-N1	5.85	123.92	121.00
23	x	129	U	C5'-C4'-C3'	5.85	125.35	116.00
25	A	2484	G	N1-C6-O6	5.85	123.41	119.90
25	A	678	C	C6-N1-C2	-5.84	117.96	120.30
37	M	70	ASP	CB-CG-OD1	5.84	123.56	118.30
25	A	1731	G	N1-C6-O6	5.84	123.40	119.90
23	x	112	C	C6-N1-C2	-5.83	117.97	120.30
1	a	570	G	N1-C6-O6	-5.83	116.40	119.90
25	A	2164	C	N3-C4-C5	5.83	124.23	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1	39	ASP	CB-CG-OD1	5.83	123.55	118.30
25	A	2181	U	C5-C6-N1	5.83	125.62	122.70
24	y	18	G	N1-C6-O6	5.83	123.40	119.90
1	a	660	C	C2-N1-C1'	5.83	125.21	118.80
32	I	27	LEU	CA-CB-CG	5.83	128.70	115.30
22	v	67	C	N3-C2-O2	-5.82	117.83	121.90
25	A	277	G	C8-N9-C4	-5.82	104.07	106.40
1	a	264	C	C5-C6-N1	5.81	123.91	121.00
25	A	610	C	N1-C2-O2	5.81	122.39	118.90
1	a	1112	C	C6-N1-C2	-5.81	117.98	120.30
1	a	491	G	N1-C6-O6	-5.80	116.42	119.90
25	A	2716	C	C6-N1-C2	-5.80	117.98	120.30
33	H	75	LEU	CA-CB-CG	-5.80	101.95	115.30
22	v	22	G	N1-C6-O6	5.80	123.38	119.90
24	y	59	C	C2-N3-C4	5.80	122.80	119.90
25	A	353	C	N3-C2-O2	-5.80	117.84	121.90
25	A	2300	C	C2-N1-C1'	5.80	125.17	118.80
1	a	200	G	N1-C6-O6	-5.79	116.42	119.90
1	a	529	G	C5-C6-N1	5.79	114.40	111.50
24	y	61	C	C5-C6-N1	5.79	123.90	121.00
25	A	1994	C	C6-N1-C2	-5.79	117.98	120.30
1	a	37	U	N1-C2-O2	5.79	126.85	122.80
25	A	1455	G	C6-C5-N7	-5.79	126.93	130.40
25	A	1784	A	N7-C8-N9	-5.79	110.90	113.80
25	A	1947	C	C5-C6-N1	5.79	123.89	121.00
1	a	350	G	N1-C6-O6	-5.79	116.43	119.90
25	A	1138	G	N1-C6-O6	-5.78	116.43	119.90
1	a	56	U	N3-C4-O4	5.78	123.45	119.40
1	a	1442	G	N1-C6-O6	-5.78	116.43	119.90
1	a	1147	C	N1-C2-O2	5.78	122.37	118.90
25	A	1180	U	C2-N1-C1'	5.78	124.64	117.70
1	a	1524	C	C5-C6-N1	5.78	123.89	121.00
25	A	2215	C	C5-C6-N1	5.78	123.89	121.00
1	a	525	C	N3-C4-C5	5.78	124.21	121.90
25	A	420	C	C2-N1-C1'	5.78	125.15	118.80
25	A	1057	A	N1-C2-N3	-5.78	126.41	129.30
25	A	1737	G	N3-C4-C5	-5.78	125.71	128.60
25	A	2805	C	N3-C2-O2	-5.78	117.86	121.90
25	A	1386	C	C6-N1-C2	-5.77	117.99	120.30
1	a	18	C	C6-N1-C2	-5.77	117.99	120.30
25	A	1622	G	N1-C6-O6	5.77	123.36	119.90
1	a	406	G	C5-C6-O6	-5.77	125.14	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	434	U	N3-C2-O2	-5.76	118.16	122.20
25	A	935	C	N1-C2-O2	5.76	122.36	118.90
25	A	2063	C	N3-C2-O2	-5.76	117.86	121.90
25	A	2566	A	O4'-C1'-N9	5.76	112.81	108.20
1	a	890	G	P-O3'-C3'	5.76	126.61	119.70
1	a	1510	C	N3-C4-N4	5.76	122.03	118.00
1	a	188	C	C6-N1-C2	-5.76	118.00	120.30
25	A	2385	C	N1-C2-O2	5.76	122.35	118.90
25	A	286	U	N3-C2-O2	-5.75	118.17	122.20
25	A	1455	G	C4-C5-N7	5.75	113.10	110.80
23	x	111	G	C5-C6-N1	5.75	114.37	111.50
1	a	413	G	N3-C4-C5	-5.75	125.73	128.60
1	a	1038	C	C6-N1-C2	-5.75	118.00	120.30
1	a	413	G	C4-N9-C1'	5.74	133.97	126.50
25	A	2214	C	N1-C2-O2	5.74	122.34	118.90
1	a	922	G	N1-C6-O6	-5.74	116.46	119.90
25	A	852	U	C5-C6-N1	5.73	125.57	122.70
1	a	660	C	N3-C4-N4	5.73	122.01	118.00
26	B	4	C	C5-C4-N4	-5.73	116.19	120.20
1	a	393	A	O5'-P-OP2	-5.72	100.55	105.70
1	a	1455	G	C6-C5-N7	-5.72	126.97	130.40
25	A	278	A	C5-C6-N1	5.72	120.56	117.70
25	A	1013	C	N1-C2-O2	5.72	122.33	118.90
24	y	46	G	N3-C2-N2	5.72	123.91	119.90
25	A	1787	A	N1-C2-N3	-5.72	126.44	129.30
1	a	1002	G	N1-C6-O6	-5.71	116.47	119.90
25	A	1669	A	C2-N3-C4	5.71	113.46	110.60
25	A	1169	A	C5-C6-N1	5.71	120.56	117.70
1	a	406	G	C6-C5-N7	-5.71	126.97	130.40
26	B	38	C	C6-N1-C2	-5.71	118.02	120.30
26	B	30	C	N1-C2-O2	5.71	122.33	118.90
25	A	1546	G	N1-C6-O6	-5.71	116.47	119.90
25	A	105	C	N1-C2-O2	5.71	122.32	118.90
25	A	512	G	P-O3'-C3'	5.70	126.54	119.70
1	a	186	C	C6-N1-C2	-5.70	118.02	120.30
1	a	193	C	C6-N1-C2	-5.70	118.02	120.30
25	A	984	A	N3-C4-C5	5.70	130.79	126.80
1	a	544	G	C8-N9-C4	5.70	108.68	106.40
25	A	1289	C	N1-C2-O2	5.70	122.32	118.90
1	a	719	C	C2-N1-C1'	5.69	125.06	118.80
1	a	1510	C	C6-N1-C2	-5.69	118.02	120.30
1	a	1031	C	C6-N1-C2	-5.69	118.02	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2047	C	N1-C2-O2	5.69	122.31	118.90
25	A	818	G	C6-C5-N7	-5.69	126.99	130.40
25	A	2264	C	N1-C2-O2	-5.68	115.49	118.90
25	A	352	A	N1-C2-N3	-5.68	126.46	129.30
25	A	543	G	C6-C5-N7	-5.68	126.99	130.40
1	a	61	G	C5-C6-O6	-5.68	125.19	128.60
25	A	550	C	C5-C6-N1	5.68	123.84	121.00
25	A	901	C	N3-C2-O2	-5.68	117.92	121.90
25	A	366	C	C6-N1-C2	-5.68	118.03	120.30
1	a	1034	G	C6-N1-C2	-5.67	121.69	125.10
25	A	1063	G	C5-C6-O6	-5.67	125.19	128.60
25	A	847	U	C6-N1-C2	-5.67	117.60	121.00
22	v	51	C	N3-C4-N4	5.67	121.97	118.00
26	B	38	C	N3-C4-N4	5.67	121.97	118.00
25	A	1148	U	C5-C6-N1	5.67	125.53	122.70
25	A	1945	G	N1-C6-O6	5.67	123.30	119.90
25	A	2867	G	P-O3'-C3'	5.67	126.50	119.70
1	a	1129	C	C6-N1-C2	-5.67	118.03	120.30
1	a	505	G	N1-C6-O6	5.67	123.30	119.90
25	A	286	U	N1-C2-O2	5.66	126.77	122.80
25	A	2730	C	C6-N1-C2	-5.66	118.04	120.30
1	a	524	G	N1-C6-O6	5.66	123.30	119.90
25	A	62	U	C5-C6-N1	5.66	125.53	122.70
25	A	2023	C	N1-C2-O2	5.66	122.29	118.90
26	B	27	C	N1-C2-O2	5.66	122.29	118.90
25	A	2716	C	C5-C6-N1	5.65	123.83	121.00
25	A	1463	C	C6-N1-C2	-5.65	118.04	120.30
25	A	2874	C	N3-C2-O2	-5.65	117.94	121.90
25	A	818	G	N3-C4-N9	5.65	129.39	126.00
25	A	130	C	N3-C4-C5	5.65	124.16	121.90
25	A	1157	G	N3-C4-N9	5.64	129.39	126.00
1	a	221	C	C2-N1-C1'	5.64	125.00	118.80
1	a	671	G	N1-C6-O6	5.64	123.28	119.90
1	a	1003	G	N9-C4-C5	5.64	107.65	105.40
25	A	484	C	C6-N1-C2	-5.64	118.05	120.30
25	A	1103	A	OP1-P-O3'	5.64	117.60	105.20
25	A	1295	C	N1-C2-O2	5.64	122.28	118.90
25	A	2354	C	C6-N1-C2	-5.63	118.05	120.30
1	a	215	C	N3-C4-C5	-5.63	119.65	121.90
1	a	626	G	C6-C5-N7	-5.63	127.02	130.40
25	A	1086	A	N1-C2-N3	5.63	132.12	129.30
26	B	3	C	N1-C2-O2	5.63	122.28	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	34	C	N3-C4-N4	5.63	121.94	118.00
25	A	277	G	C5-N7-C8	-5.63	101.49	104.30
1	a	737	C	N1-C2-O2	5.63	122.28	118.90
1	a	1134	G	C5-C6-O6	-5.63	125.22	128.60
1	a	1143	G	N1-C6-O6	-5.63	116.52	119.90
25	A	2752	C	N1-C2-O2	5.63	122.28	118.90
30	F	172	PHE	C-N-CA	5.63	135.76	121.70
1	a	1432	G	P-O3'-C3'	5.62	126.45	119.70
25	A	283	G	N1-C2-N2	5.62	121.26	116.20
25	A	171	U	N3-C2-O2	-5.62	118.27	122.20
25	A	2056	G	C6-C5-N7	-5.62	127.03	130.40
25	A	2403	C	C5-C6-N1	5.62	123.81	121.00
22	v	71	C	C5-C6-N1	5.62	123.81	121.00
25	A	1314	C	N1-C2-O2	5.61	122.27	118.90
25	A	1931	U	C5-C6-N1	5.61	125.51	122.70
1	a	413	G	C8-N9-C1'	-5.61	119.70	127.00
1	a	506	G	C6-C5-N7	-5.61	127.03	130.40
24	y	71	C	C6-N1-C2	-5.61	118.06	120.30
25	A	2410	G	C5-C6-O6	-5.61	125.23	128.60
25	A	2574	G	C5-C6-O6	-5.61	125.23	128.60
25	A	1317	G	N1-C6-O6	5.61	123.27	119.90
23	x	91	A	N9-C4-C5	-5.61	103.56	105.80
25	A	495	G	N1-C6-O6	5.61	123.26	119.90
25	A	2297	A	N1-C2-N3	-5.60	126.50	129.30
1	a	144	G	C6-C5-N7	-5.60	127.04	130.40
25	A	121	G	N3-C4-N9	5.60	129.36	126.00
25	A	1683	U	N3-C2-O2	-5.60	118.28	122.20
25	A	740	C	C5-C6-N1	5.60	123.80	121.00
1	a	543	U	N3-C2-O2	-5.59	118.28	122.20
1	a	1303	C	N3-C2-O2	-5.59	117.98	121.90
1	a	168	G	C4-C5-N7	5.59	113.04	110.80
1	a	1255	G	N1-C6-O6	-5.59	116.55	119.90
25	A	413	C	C5-C6-N1	5.59	123.79	121.00
25	A	849	A	N7-C8-N9	5.59	116.59	113.80
22	v	28	C	N1-C2-O2	5.59	122.25	118.90
25	A	896	A	N1-C6-N6	5.59	121.95	118.60
1	a	588	G	N3-C4-C5	-5.58	125.81	128.60
1	a	598	U	N3-C2-O2	-5.58	118.29	122.20
22	v	51	C	C5-C6-N1	5.58	123.79	121.00
1	a	906	A	C5-C6-N6	-5.58	119.24	123.70
25	A	2164	C	N3-C4-N4	-5.58	114.10	118.00
25	A	2103	C	C5-C4-N4	-5.58	116.30	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	234	U	N1-C2-O2	5.57	126.70	122.80
25	A	2566	A	P-O3'-C3'	5.57	126.38	119.70
25	A	513	A	N7-C8-N9	5.57	116.58	113.80
25	A	2108	A	N1-C2-N3	5.57	132.08	129.30
1	a	1404	C	C5-C6-N1	5.57	123.78	121.00
25	A	154	U	N3-C2-O2	-5.56	118.31	122.20
25	A	1352	U	N3-C2-O2	-5.56	118.31	122.20
1	a	194	C	C6-N1-C2	-5.56	118.08	120.30
1	a	626	G	N3-C2-N2	5.56	123.79	119.90
1	a	1041	G	N1-C6-O6	5.56	123.23	119.90
24	y	62	C	C6-N1-C2	-5.56	118.08	120.30
25	A	1533	C	N3-C4-N4	-5.56	114.11	118.00
22	v	56	C	N3-C4-C5	-5.55	119.68	121.90
23	x	133	C	C3'-C2'-C1'	5.55	105.94	101.50
25	A	1531	C	N3-C4-N4	-5.55	114.11	118.00
25	A	2889	C	N1-C2-O2	5.55	122.23	118.90
1	a	1088	G	C5-C6-O6	-5.55	125.27	128.60
25	A	420	C	C6-N1-C2	-5.55	118.08	120.30
1	a	41	G	N3-C4-C5	-5.55	125.83	128.60
1	a	507	C	N3-C4-C5	5.55	124.12	121.90
25	A	1795	C	C6-N1-C2	-5.55	118.08	120.30
1	a	441	A	C2-N3-C4	5.55	113.37	110.60
1	a	1262	C	C6-N1-C2	-5.55	118.08	120.30
25	A	2171	A	C5-C6-N6	-5.55	119.26	123.70
25	A	2870	C	C5-C6-N1	5.55	123.77	121.00
26	B	21	G	N1-C6-O6	-5.55	116.57	119.90
1	a	1459	G	N1-C6-O6	5.54	123.23	119.90
11	k	126	ARG	NE-CZ-NH2	-5.54	117.53	120.30
25	A	1940	U	P-O3'-C3'	5.54	126.35	119.70
25	A	2292	U	C5-C6-N1	5.54	125.47	122.70
25	A	1087	G	N1-C2-N3	5.54	127.22	123.90
25	A	2178	C	C5-C6-N1	5.54	123.77	121.00
1	a	1325	C	N3-C2-O2	-5.54	118.03	121.90
25	A	687	C	N1-C2-O2	5.54	122.22	118.90
25	A	444	C	C6-N1-C2	-5.53	118.09	120.30
25	A	2863	C	N1-C2-O2	5.53	122.22	118.90
25	A	2791	G	N1-C2-N2	5.53	121.18	116.20
1	a	93	U	C6-N1-C2	-5.53	117.68	121.00
25	A	276	U	N3-C2-O2	-5.53	118.33	122.20
25	A	1048	A	C8-N9-C4	-5.53	103.59	105.80
25	A	1499	C	N3-C4-N4	-5.53	114.13	118.00
25	A	1539	U	C5-C4-O4	-5.53	122.58	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1833	C	N3-C2-O2	-5.53	118.03	121.90
25	A	1993	U	C2-N1-C1'	5.53	124.33	117.70
25	A	2056	G	C5-C6-O6	-5.52	125.28	128.60
25	A	362	A	C8-N9-C4	-5.52	103.59	105.80
25	A	2466	C	O5'-P-OP1	-5.52	100.73	105.70
25	A	2636	C	C2-N1-C1'	5.52	124.87	118.80
25	A	2794	C	C2-N1-C1'	5.52	124.87	118.80
1	a	1369	C	N3-C2-O2	-5.52	118.04	121.90
1	a	960	U	N1-C2-O2	5.52	126.66	122.80
22	v	49	G	C4-C5-N7	5.52	113.01	110.80
1	a	980	C	N1-C2-O2	5.51	122.21	118.90
25	A	581	C	O5'-P-OP1	-5.51	100.74	105.70
25	A	2438	U	N3-C2-O2	-5.51	118.34	122.20
1	a	1460	C	N1-C2-O2	5.51	122.21	118.90
25	A	1395	A	O4'-C1'-N9	5.51	112.61	108.20
1	a	1147	C	N3-C2-O2	-5.51	118.05	121.90
25	A	360	U	C4-C5-C6	-5.51	116.40	119.70
25	A	565	C	N3-C2-O2	-5.51	118.05	121.90
1	a	643	C	C6-N1-C2	-5.50	118.10	120.30
1	a	1317	C	C6-N1-C2	-5.50	118.10	120.30
24	y	61	C	C2-N3-C4	5.50	122.65	119.90
25	A	965	C	C5-C6-N1	5.50	123.75	121.00
1	a	891	U	C5-C6-N1	5.50	125.45	122.70
25	A	2592	G	N3-C2-N2	5.50	123.75	119.90
23	x	126	G	N7-C8-N9	5.50	115.85	113.10
1	a	168	G	C6-C5-N7	-5.50	127.10	130.40
1	a	1522	U	C6-N1-C2	-5.50	117.70	121.00
1	a	96	U	N1-C2-O2	5.50	126.65	122.80
25	A	359	G	C2-N3-C4	5.50	114.65	111.90
25	A	445	C	C6-N1-C2	-5.50	118.10	120.30
1	a	623	C	C2-N1-C1'	5.49	124.84	118.80
1	a	910	C	N3-C2-O2	-5.49	118.06	121.90
25	A	208	C	C5-C6-N1	5.49	123.75	121.00
1	a	1348	U	N3-C2-O2	-5.49	118.36	122.20
1	a	206	C	N1-C2-N3	5.49	123.04	119.20
1	a	504	C	C5-C6-N1	5.49	123.74	121.00
25	A	1760	C	C5-C6-N1	5.49	123.74	121.00
23	x	93	G	N1-C6-O6	5.49	123.19	119.90
25	A	62	U	C2-N3-C4	5.49	130.29	127.00
25	A	396	G	N1-C6-O6	5.49	123.19	119.90
1	a	269	C	C6-N1-C2	-5.48	118.11	120.30
25	A	362	A	N7-C8-N9	5.48	116.54	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1462	C	N3-C2-O2	-5.48	118.06	121.90
1	a	67	C	N3-C2-O2	-5.48	118.06	121.90
1	a	575	G	C6-N1-C2	-5.48	121.81	125.10
1	a	671	G	C5-C6-O6	-5.48	125.31	128.60
25	A	717	C	C6-N1-C2	-5.48	118.11	120.30
25	A	2814	A	C8-N9-C4	-5.47	103.61	105.80
1	a	102	G	C4-C5-N7	-5.47	108.61	110.80
1	a	1124	G	N1-C6-O6	-5.47	116.62	119.90
26	B	27	C	N3-C2-O2	-5.47	118.07	121.90
1	a	1149	C	N3-C4-N4	5.47	121.83	118.00
25	A	2518	A	C2-N3-C4	5.46	113.33	110.60
6	f	53	LYS	N-CA-C	-5.46	96.25	111.00
25	A	1098	A	N1-C6-N6	5.46	121.88	118.60
1	a	959	A	C5-N7-C8	-5.46	101.17	103.90
25	A	1830	C	C5-C6-N1	5.46	123.73	121.00
1	a	33	A	C8-N9-C4	-5.46	103.62	105.80
1	a	1448	C	N3-C4-C5	5.45	124.08	121.90
25	A	1081	U	C4-C5-C6	-5.45	116.43	119.70
1	a	358	U	N3-C2-O2	-5.45	118.39	122.20
26	B	17	C	C6-N1-C2	-5.45	118.12	120.30
1	a	1073	U	N3-C2-O2	-5.44	118.39	122.20
1	a	284	C	C5-C6-N1	5.44	123.72	121.00
26	B	31	C	C2-N1-C1'	5.44	124.79	118.80
1	a	155	A	N1-C2-N3	-5.44	126.58	129.30
1	a	1499	A	OP2-P-O3'	5.44	117.17	105.20
22	v	6	G	N1-C6-O6	-5.44	116.64	119.90
25	A	1362	C	C6-N1-C2	-5.44	118.12	120.30
1	a	1071	C	N1-C2-O2	5.44	122.16	118.90
1	a	910	C	N1-C2-O2	5.43	122.16	118.90
25	A	1894	C	C2-N1-C1'	5.43	124.78	118.80
25	A	2416	C	N1-C2-O2	5.43	122.16	118.90
23	x	130	G	N9-C1'-C2'	-5.43	106.02	112.00
1	a	1369	C	C6-N1-C2	-5.43	118.13	120.30
23	x	125	G	C4-N9-C1'	-5.43	119.44	126.50
25	A	1499	C	N1-C2-O2	-5.43	115.64	118.90
25	A	2592	G	N1-C6-O6	5.43	123.16	119.90
1	a	73	C	N3-C4-N4	-5.43	114.20	118.00
1	a	866	C	C6-N1-C2	-5.43	118.13	120.30
25	A	816	C	C6-N1-C2	-5.43	118.13	120.30
1	a	330	C	N1-C2-O2	5.42	122.16	118.90
25	A	81	G	N3-C2-N2	-5.42	116.10	119.90
25	A	1930	G	P-O3'-C3'	5.42	126.21	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1816	C	N3-C2-O2	-5.42	118.11	121.90
25	A	1402	U	N1-C2-O2	5.42	126.59	122.80
25	A	536	G	N1-C6-O6	-5.42	116.65	119.90
25	A	1306	C	N3-C4-C5	5.42	124.07	121.90
25	A	16	C	C6-N1-C2	-5.42	118.13	120.30
25	A	2834	G	C5-N7-C8	-5.42	101.59	104.30
25	A	2628	C	C6-N1-C2	-5.42	118.13	120.30
1	a	412	A	OP2-P-O3'	5.41	117.11	105.20
1	a	667	G	N1-C6-O6	-5.41	116.65	119.90
25	A	283	G	C6-N1-C2	-5.41	121.85	125.10
1	a	2	A	C5-N7-C8	5.41	106.61	103.90
25	A	2056	G	C4-C5-N7	5.41	112.96	110.80
1	a	563	A	N3-C4-N9	5.41	131.73	127.40
25	A	775	G	O4'-C1'-N9	5.41	112.53	108.20
25	A	1994	C	N1-C2-O2	5.41	122.14	118.90
1	a	385	C	N1-C2-O2	5.40	122.14	118.90
25	A	1104	C	C2-N1-C1'	5.40	124.75	118.80
1	a	1043	G	C5-C6-N1	5.40	114.20	111.50
25	A	931	U	C5-C6-N1	5.40	125.40	122.70
25	A	1564	C	N1-C2-O2	5.40	122.14	118.90
25	A	2889	C	C6-N1-C2	-5.40	118.14	120.30
25	A	1461	C	N1-C2-O2	5.40	122.14	118.90
1	a	379	C	N3-C4-C5	5.40	124.06	121.90
1	a	578	C	C6-N1-C2	-5.40	118.14	120.30
25	A	407	G	C5-C6-O6	5.40	131.84	128.60
25	A	584	C	N1-C2-O2	5.40	122.14	118.90
25	A	1682	G	N3-C4-N9	5.40	129.24	126.00
21	u	24	LYS	CA-CB-CG	5.39	125.27	113.40
25	A	2720	U	N1-C2-O2	5.39	126.58	122.80
1	a	1498	UR3	OP1-P-O3'	5.39	117.06	105.20
25	A	2321	U	C4-C5-C6	5.39	122.94	119.70
1	a	528	C	N1-C2-O2	5.39	122.13	118.90
25	A	1761	C	N1-C2-O2	5.39	122.13	118.90
26	B	17	C	C5-C6-N1	5.38	123.69	121.00
26	B	120	U	C6-N1-C2	-5.38	117.77	121.00
1	a	1271	A	N1-C2-N3	-5.38	126.61	129.30
25	A	1507	C	C2-N3-C4	5.38	122.59	119.90
25	A	2117	A	N1-C2-N3	-5.38	126.61	129.30
1	a	1325	C	C5-C6-N1	5.38	123.69	121.00
25	A	2192	U	N3-C4-O4	5.38	123.17	119.40
23	x	132	A	P-O5'-C5'	5.38	129.50	120.90
26	B	4	C	OP1-P-OP2	-5.38	111.53	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2903	U	N3-C2-O2	-5.38	118.44	122.20
1	a	455	G	C6-C5-N7	-5.37	127.18	130.40
25	A	1680	U	N1-C2-O2	5.37	126.56	122.80
25	A	680	C	C5-C6-N1	5.37	123.69	121.00
25	A	1625	C	N3-C4-C5	5.37	124.05	121.90
1	a	186	C	C5-C4-N4	-5.37	116.44	120.20
1	a	1404	C	N3-C4-C5	-5.37	119.75	121.90
1	a	1113	C	C6-N1-C2	-5.37	118.15	120.30
25	A	1945	G	C4-C5-N7	5.37	112.95	110.80
1	a	341	C	N3-C4-N4	-5.37	114.24	118.00
1	a	1172	C	C5-C6-N1	5.37	123.68	121.00
29	E	82	GLY	N-CA-C	5.37	126.52	113.10
1	a	524	G	C5-C6-O6	-5.36	125.38	128.60
1	a	822	U	C6-N1-C2	-5.36	117.78	121.00
1	a	893	C	C6-N1-C2	-5.36	118.16	120.30
25	A	137	U	N1-C2-N3	5.36	118.12	114.90
23	x	131	C	C3'-C2'-C1'	5.36	105.79	101.50
45	U	38	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	a	890	G	OP2-P-O3'	5.36	116.99	105.20
25	A	188	G	N3-C2-N2	-5.36	116.15	119.90
25	A	278	A	N1-C2-N3	-5.36	126.62	129.30
25	A	1455	G	N1-C6-O6	5.36	123.11	119.90
1	a	1112	C	N3-C2-O2	-5.36	118.15	121.90
1	a	1459	G	C5-C6-O6	-5.35	125.39	128.60
25	A	2450	A	N1-C2-N3	-5.35	126.62	129.30
25	A	1843	C	N1-C2-O2	5.35	122.11	118.90
25	A	82	U	N1-C2-O2	5.35	126.54	122.80
1	a	820	U	P-O3'-C3'	5.35	126.12	119.70
25	A	82	U	N3-C2-O2	-5.35	118.46	122.20
25	A	1588	G	N1-C6-O6	5.35	123.11	119.90
15	o	88	ARG	N-CA-CB	5.35	120.22	110.60
1	a	208	U	N1-C2-O2	5.34	126.54	122.80
25	A	546	U	N1-C2-O2	5.34	126.54	122.80
1	a	154	U	N1-C2-O2	5.34	126.54	122.80
25	A	832	U	N1-C2-N3	5.34	118.11	114.90
25	A	2585	U	C5-C6-N1	5.34	125.37	122.70
25	A	2394	C	N1-C2-O2	5.34	122.11	118.90
25	A	1487	U	N3-C2-O2	-5.34	118.46	122.20
25	A	1908	C	C6-N1-C2	-5.34	118.16	120.30
25	A	2347	C	C6-N1-C2	-5.34	118.16	120.30
40	P	113	LEU	CA-CB-CG	5.34	127.58	115.30
1	a	75	G	N1-C6-O6	-5.34	116.70	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	500	G	C5-C6-O6	-5.34	125.40	128.60
25	A	12	U	C2-N1-C1'	5.34	124.10	117.70
25	A	528	A	C5-C6-N1	-5.34	115.03	117.70
25	A	2742	G	C6-N1-C2	-5.33	121.90	125.10
25	A	965	C	N1-C2-O2	5.33	122.10	118.90
25	A	1352	U	N1-C2-O2	5.33	126.53	122.80
25	A	307	G	N3-C2-N2	-5.33	116.17	119.90
1	a	605	U	N3-C2-O2	-5.33	118.47	122.20
1	a	355	C	C2-N1-C1'	5.33	124.66	118.80
25	A	2306	C	C5-C6-N1	5.33	123.66	121.00
25	A	2364	C	N1-C2-O2	-5.33	115.70	118.90
1	a	1148	U	N3-C2-O2	-5.32	118.47	122.20
25	A	943	A	O5'-P-OP1	-5.32	100.91	105.70
25	A	1315	C	N1-C2-O2	5.32	122.09	118.90
25	A	2069	G7M	OP2-P-O3'	5.32	116.90	105.20
25	A	2283	C	N3-C4-C5	5.32	124.03	121.90
25	A	215	G	OP1-P-O3'	5.32	116.90	105.20
19	s	54	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	a	1345	U	N1-C2-O2	-5.31	119.08	122.80
25	A	1104	C	N3-C4-C5	-5.31	119.77	121.90
25	A	740	C	N1-C2-O2	5.31	122.09	118.90
25	A	2745	C	C6-N1-C2	-5.31	118.17	120.30
25	A	2759	G	N3-C2-N2	-5.31	116.18	119.90
25	A	1963	U	C5-C6-N1	5.31	125.36	122.70
1	a	267	C	N1-C2-O2	5.31	122.09	118.90
23	x	121	U	N1-C2-O2	5.31	126.52	122.80
25	A	343	C	C5-C6-N1	5.31	123.66	121.00
1	a	1107	C	O5'-P-OP1	-5.31	100.92	105.70
1	a	1086	U	N3-C2-O2	-5.31	118.49	122.20
25	A	2043	C	C2-N1-C1'	5.31	124.64	118.80
1	a	601	G	C5-C6-O6	-5.30	125.42	128.60
25	A	1730	C	OP2-P-O3'	5.30	116.87	105.20
1	a	1406	U	N3-C2-O2	-5.30	118.49	122.20
25	A	2566	A	OP2-P-O3'	5.30	116.86	105.20
25	A	1317	G	C6-C5-N7	-5.30	127.22	130.40
25	A	278	A	N3-C4-N9	5.30	131.64	127.40
1	a	810	C	N1-C2-O2	5.30	122.08	118.90
25	A	363	G	C6-C5-N7	-5.29	127.22	130.40
1	a	661	G	C6-C5-N7	-5.29	127.22	130.40
1	a	1490	U	N3-C2-O2	-5.29	118.50	122.20
1	a	450	G	C5-C6-O6	5.29	131.78	128.60
25	A	1069	A	OP1-P-O3'	5.29	116.84	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	671	G	C4-C5-N7	5.29	112.92	110.80
25	A	1090	A	N1-C2-N3	-5.29	126.66	129.30
1	a	1497	G	N3-C2-N2	-5.29	116.20	119.90
25	A	1833	C	N1-C2-O2	5.29	122.07	118.90
25	A	2248	C	C5-C6-N1	5.29	123.64	121.00
1	a	735	C	N1-C2-O2	5.28	122.07	118.90
1	a	1253	G	N1-C6-O6	-5.28	116.73	119.90
1	a	514	C	C5-C6-N1	5.28	123.64	121.00
25	A	2043	C	C5-C6-N1	5.28	123.64	121.00
25	A	2059	A	OP2-P-O3'	5.28	116.82	105.20
25	A	2282	G	N1-C6-O6	-5.28	116.73	119.90
25	A	2474	U	N3-C2-O2	-5.28	118.50	122.20
25	A	415	A	N1-C2-N3	-5.28	126.66	129.30
25	A	1644	C	C5-C6-N1	5.28	123.64	121.00
1	a	671	G	N9-C4-C5	-5.28	103.29	105.40
25	A	2297	A	C6-N1-C2	5.28	121.77	118.60
1	a	240	G	C4-C5-N7	5.28	112.91	110.80
1	a	563	A	C2-N3-C4	5.28	113.24	110.60
1	a	737	C	N3-C4-N4	5.27	121.69	118.00
1	a	989	U	N1-C2-O2	5.27	126.49	122.80
23	x	114	C	N1-C2-O2	5.27	122.06	118.90
1	a	457	G	C6-C5-N7	5.27	133.56	130.40
25	A	12	U	C6-N1-C2	-5.27	117.84	121.00
25	A	62	U	C6-N1-C2	-5.26	117.84	121.00
25	A	776	G	N3-C4-C5	-5.26	125.97	128.60
25	A	2200	C	N1-C2-O2	5.26	122.06	118.90
26	B	71	C	N1-C2-O2	5.26	122.06	118.90
1	a	375	U	N1-C2-O2	5.26	126.48	122.80
25	A	2023	C	C6-N1-C2	-5.26	118.19	120.30
25	A	2417	C	C6-N1-C2	-5.26	118.20	120.30
25	A	2394	C	N3-C2-O2	-5.26	118.22	121.90
25	A	1054	A	N9-C4-C5	-5.26	103.70	105.80
1	a	910	C	C6-N1-C2	-5.26	118.20	120.30
1	a	1060	U	N3-C2-O2	-5.26	118.52	122.20
1	a	1172	C	N1-C2-O2	5.26	122.05	118.90
1	a	754	C	OP1-P-O3'	5.25	116.75	105.20
25	A	2678	C	C5-C6-N1	5.25	123.63	121.00
1	a	87	C	C5-C6-N1	5.25	123.62	121.00
25	A	1164	C	N1-C2-O2	5.24	122.05	118.90
25	A	2215	C	C6-N1-C2	-5.24	118.20	120.30
1	a	18	C	C4-C5-C6	-5.24	114.78	117.40
1	a	396	C	C6-N1-C2	-5.24	118.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	271	C	N1-C2-O2	5.24	122.04	118.90
1	a	661	G	C4-C5-N7	5.24	112.90	110.80
25	A	69	C	N1-C2-O2	5.24	122.04	118.90
1	a	225	C	C5-C6-N1	5.24	123.62	121.00
25	A	2329	U	C5-C6-N1	5.24	125.32	122.70
1	a	168	G	N3-C4-N9	5.24	129.14	126.00
1	a	1158	C	N1-C2-O2	5.24	122.04	118.90
25	A	1892	C	C5-C6-N1	5.24	123.62	121.00
25	A	1101	U	N1-C2-N3	5.23	118.04	114.90
1	a	754	C	C2-N1-C1'	5.23	124.56	118.80
25	A	933	A	C2-N3-C4	5.23	113.22	110.60
1	a	1537	U	C5-C6-N1	5.23	125.31	122.70
25	A	1105	U	N3-C4-O4	-5.23	115.74	119.40
1	a	995	C	N1-C2-O2	5.23	122.04	118.90
25	A	163	C	C6-N1-C2	-5.23	118.21	120.30
25	A	2164	C	N3-C2-O2	-5.22	118.24	121.90
25	A	2752	C	N3-C2-O2	-5.22	118.24	121.90
1	a	213	G	C4-N9-C1'	5.22	133.29	126.50
1	a	1100	C	C6-N1-C2	-5.22	118.21	120.30
1	a	496	A	C2-N3-C4	5.22	113.21	110.60
25	A	143	C	C6-N1-C2	-5.22	118.21	120.30
25	A	987	C	N3-C4-C5	5.22	123.99	121.90
25	A	484	C	C2-N1-C1'	5.22	124.54	118.80
25	A	1269	A	N1-C2-N3	-5.22	126.69	129.30
25	A	105	C	N3-C2-O2	-5.21	118.25	121.90
25	A	557	C	C5-C6-N1	5.21	123.61	121.00
25	A	396	G	C6-C5-N7	-5.21	127.27	130.40
1	a	623	C	N3-C2-O2	-5.21	118.25	121.90
1	a	1227	A	C2-N3-C4	5.21	113.21	110.60
25	A	777	G	N1-C6-O6	5.21	123.03	119.90
1	a	33	A	C5-N7-C8	-5.21	101.30	103.90
1	a	34	C	C5-C6-N1	5.21	123.60	121.00
22	v	49	G	N3-C2-N2	5.21	123.55	119.90
25	A	2306	C	C6-N1-C2	-5.21	118.22	120.30
15	o	86	LEU	CA-CB-CG	5.21	127.28	115.30
25	A	1559	U	P-O3'-C3'	5.21	125.94	119.70
24	y	72	C	C6-N1-C2	-5.20	118.22	120.30
25	A	777	G	C6-C5-N7	-5.20	127.28	130.40
25	A	1055	G	N3-C2-N2	-5.20	116.26	119.90
1	a	413	G	C2-N3-C4	5.20	114.50	111.90
25	A	894	U	C2-N1-C1'	5.20	123.94	117.70
25	A	2162	G	N3-C4-N9	5.20	129.12	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	776	G	C2-N3-C4	5.20	114.50	111.90
25	A	2651	C	C6-N1-C2	-5.20	118.22	120.30
1	a	840	C	N1-C2-O2	-5.20	115.78	118.90
25	A	274	C	N3-C4-C5	5.19	123.98	121.90
25	A	1101	U	C2-N3-C4	-5.19	123.89	127.00
1	a	240	G	C8-N9-C4	5.19	108.47	106.40
25	A	2162	G	N3-C4-C5	-5.18	126.01	128.60
46	V	92	VAL	CG1-CB-CG2	-5.18	102.60	110.90
25	A	2325	G	C5-C6-O6	-5.18	125.49	128.60
25	A	363	G	C5-C6-N1	-5.17	108.91	111.50
22	v	74	C	C5-C6-N1	5.17	123.59	121.00
24	y	35	C	C2-N1-C1'	5.17	124.49	118.80
1	a	1225	A	C4-N9-C1'	5.17	135.60	126.30
25	A	1035	U	N3-C2-O2	-5.17	118.58	122.20
25	A	2409	G	C6-C5-N7	-5.17	127.30	130.40
1	a	661	G	N9-C4-C5	-5.17	103.33	105.40
1	a	1136	C	C5-C6-N1	5.17	123.58	121.00
1	a	1225	A	N1-C2-N3	-5.17	126.72	129.30
25	A	560	C	C5-C6-N1	5.17	123.58	121.00
45	U	51	LEU	N-CA-CB	-5.17	100.07	110.40
1	a	1033	G	C6-C5-N7	-5.16	127.30	130.40
25	A	349	U	N1-C2-O2	5.16	126.41	122.80
25	A	848	C	N1-C2-O2	5.16	122.00	118.90
1	a	386	C	C5-C4-N4	-5.16	116.59	120.20
1	a	1536	C	C6-N1-C2	-5.16	118.24	120.30
22	v	49	G	N9-C4-C5	-5.16	103.34	105.40
24	y	39	U	N3-C4-O4	5.16	123.01	119.40
25	A	817	C	N1-C2-O2	5.16	122.00	118.90
25	A	2262	U	N3-C4-O4	5.16	123.01	119.40
26	B	63	C	C6-N1-C2	-5.16	118.24	120.30
25	A	1538	G	C2-N3-C4	-5.16	109.32	111.90
25	A	2799	A	C4-C5-N7	5.15	113.28	110.70
1	a	452	A	N1-C2-N3	-5.15	126.72	129.30
25	A	550	C	C4-C5-C6	-5.15	114.83	117.40
25	A	680	C	C6-N1-C2	-5.15	118.24	120.30
25	A	2105	U	C2-N3-C4	5.15	130.09	127.00
25	A	2797	U	N1-C2-O2	5.15	126.41	122.80
25	A	740	C	C6-N1-C2	-5.15	118.24	120.30
25	A	1945	G	N3-C4-N9	5.15	129.09	126.00
25	A	2222	C	N3-C2-O2	-5.15	118.30	121.90
1	a	457	G	C2-N3-C4	5.15	114.47	111.90
22	v	1	C	C6-N1-C2	-5.15	118.24	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2222	C	N1-C2-O2	5.15	121.99	118.90
1	a	88	U	C5-C6-N1	5.15	125.27	122.70
24	y	35	C	C2-N3-C4	5.14	122.47	119.90
25	A	1394	U	C5-C6-N1	5.14	125.27	122.70
25	A	1583	A	C2-N3-C4	5.14	113.17	110.60
25	A	1630	A	C6-N1-C2	-5.14	115.51	118.60
1	a	1031	C	C5-C6-N1	5.14	123.57	121.00
12	l	23	LEU	CA-CB-CG	5.14	127.12	115.30
25	A	516	C	N1-C2-O2	5.14	121.98	118.90
25	A	2056	G	N9-C4-C5	-5.14	103.34	105.40
25	A	2443	C	N1-C2-O2	5.14	121.98	118.90
42	R	78	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	a	1088	G	N9-C4-C5	-5.14	103.34	105.40
24	y	18	G	C2-N3-C4	-5.14	109.33	111.90
25	A	805	G	N9-C4-C5	-5.14	103.35	105.40
1	a	1412	C	N1-C2-O2	5.13	121.98	118.90
1	a	544	G	C4-C5-N7	5.13	112.85	110.80
1	a	781	A	C2-N3-C4	5.13	113.17	110.60
24	y	56	C	N1-C2-O2	-5.13	115.82	118.90
25	A	1611	C	N1-C2-O2	5.13	121.98	118.90
25	A	2624	G	N1-C6-O6	5.12	122.97	119.90
23	x	100	A	C2-N3-C4	5.12	113.16	110.60
25	A	143	C	N1-C2-O2	5.12	121.97	118.90
25	A	257	C	N3-C2-O2	-5.12	118.31	121.90
25	A	1398	C	C2-N1-C1'	5.12	124.43	118.80
25	A	594	U	C5-C6-N1	5.12	125.26	122.70
25	A	2215	C	N1-C2-O2	5.12	121.97	118.90
1	a	1341	U	N3-C2-O2	-5.12	118.62	122.20
25	A	1584	U	C6-N1-C2	-5.12	117.93	121.00
25	A	2011	U	N1-C2-O2	5.12	126.38	122.80
25	A	2515	C	C5-C6-N1	5.12	123.56	121.00
1	a	83	C	C5-C6-N1	5.12	123.56	121.00
26	B	66	A	OP1-P-O3'	5.12	116.46	105.20
25	A	1880	U	C2-N1-C1'	5.12	123.84	117.70
25	A	69	C	N3-C2-O2	-5.11	118.32	121.90
25	A	2861	U	C5-C6-N1	5.11	125.26	122.70
25	A	709	U	N3-C2-O2	-5.11	118.62	122.20
31	G	136	ASP	CB-CG-OD1	5.11	122.90	118.30
25	A	1967	C	N1-C2-O2	5.11	121.97	118.90
1	a	524	G	C6-C5-N7	-5.11	127.34	130.40
22	v	56	C	C2-N3-C4	5.11	122.45	119.90
25	A	1874	C	N1-C2-O2	5.11	121.96	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2601	C	C5-C6-N1	5.11	123.55	121.00
25	A	1723	G	C5-C6-N1	5.10	114.05	111.50
25	A	2739	U	N1-C2-O2	5.10	126.37	122.80
25	A	1212	G	OP2-P-O3'	5.10	116.42	105.20
25	A	1108	U	N3-C2-O2	-5.10	118.63	122.20
25	A	2561	U	C2-N3-C4	-5.10	123.94	127.00
1	a	154	U	N3-C2-O2	-5.10	118.63	122.20
27	C	83	ASP	CB-CG-OD1	5.09	122.89	118.30
1	a	217	C	N1-C2-O2	5.09	121.95	118.90
1	a	661	G	C5-C6-O6	-5.09	125.55	128.60
25	A	946	C	C6-N1-C2	-5.09	118.26	120.30
1	a	348	G	C6-C5-N7	-5.09	127.35	130.40
1	a	147	G	C5-C6-O6	-5.08	125.55	128.60
1	a	796	C	C6-N1-C2	-5.08	118.27	120.30
25	A	158	U	N3-C2-O2	-5.08	118.64	122.20
25	A	531	C	C6-N1-C2	5.08	122.33	120.30
1	a	213	G	N1-C2-N3	5.08	126.95	123.90
25	A	2592	G	C6-C5-N7	-5.08	127.35	130.40
1	a	454	G	N7-C8-N9	5.08	115.64	113.10
25	A	55	G	N1-C6-O6	-5.08	116.85	119.90
25	A	307	G	N3-C4-N9	-5.08	122.95	126.00
26	B	97	C	C5-C4-N4	-5.08	116.64	120.20
25	A	105	C	N3-C4-C5	-5.08	119.87	121.90
25	A	305	C	C5-C6-N1	5.08	123.54	121.00
1	a	744	C	N3-C4-C5	5.07	123.93	121.90
25	A	2109	U	C6-N1-C2	-5.07	117.96	121.00
25	A	2192	U	C5-C4-O4	-5.07	122.86	125.90
1	a	1225	A	N3-C4-N9	5.07	131.46	127.40
1	a	1509	C	C6-N1-C2	-5.07	118.27	120.30
23	x	121	U	N3-C2-O2	-5.07	118.65	122.20
25	A	1669	A	C4-N9-C1'	5.07	135.43	126.30
25	A	1761	C	N3-C2-O2	-5.07	118.35	121.90
25	A	2515	C	C6-N1-C2	-5.07	118.27	120.30
26	B	79	G	C5-C6-N1	5.07	114.03	111.50
25	A	2091	C	N1-C2-O2	-5.07	115.86	118.90
1	a	370	C	N1-C2-O2	5.07	121.94	118.90
1	a	457	G	N9-C4-C5	5.07	107.43	105.40
1	a	1202	U	N3-C2-O2	-5.07	118.65	122.20
25	A	832	U	N3-C2-O2	-5.07	118.66	122.20
25	A	1198	U	N3-C2-O2	-5.07	118.65	122.20
1	a	1141	C	N3-C4-N4	5.06	121.54	118.00
25	A	115	C	C6-N1-C2	-5.06	118.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	195	A	OP1-P-O3'	5.06	116.33	105.20
1	a	90	C	C6-N1-C2	-5.06	118.28	120.30
1	a	215	C	C5-C4-N4	-5.06	116.66	120.20
25	A	2798	U	N1-C2-O2	5.06	126.34	122.80
1	a	248	C	C2-N1-C1'	5.06	124.36	118.80
22	v	61	C	N3-C2-O2	-5.06	118.36	121.90
25	A	1891	G	C4-N9-C1'	5.06	133.07	126.50
25	A	2300	C	N1-C2-O2	5.06	121.94	118.90
1	a	955	U	C5-C6-N1	5.06	125.23	122.70
25	A	145	C	N1-C2-O2	5.06	121.93	118.90
25	A	795	C	C5-C6-N1	5.06	123.53	121.00
25	A	1581	G	N1-C6-O6	5.05	122.93	119.90
25	A	2152	G	N7-C8-N9	5.05	115.63	113.10
1	a	740	U	N3-C2-O2	-5.05	118.66	122.20
25	A	282	A	C6-N1-C2	5.05	121.63	118.60
25	A	719	C	C6-N1-C2	-5.05	118.28	120.30
25	A	964	C	C6-N1-C2	-5.05	118.28	120.30
25	A	1734	G	N1-C6-O6	5.05	122.93	119.90
25	A	2791	G	C5-C6-O6	-5.05	125.57	128.60
25	A	62	U	C6-N1-C1'	-5.05	114.13	121.20
25	A	495	G	C5-C6-O6	-5.05	125.57	128.60
1	a	1037	C	N1-C2-O2	5.04	121.93	118.90
1	a	452	A	C2-N3-C4	5.04	113.12	110.60
1	a	654	G	C6-C5-N7	-5.04	127.37	130.40
1	a	1279	G	C8-N9-C4	-5.04	104.38	106.40
25	A	732	C	N1-C2-O2	5.04	121.92	118.90
25	A	2302	U	C6-N1-C2	-5.04	117.98	121.00
25	A	363	G	C2-N3-C4	-5.04	109.38	111.90
24	y	59	C	C2-N1-C1'	5.03	124.34	118.80
26	B	3	C	P-O3'-C3'	5.03	125.74	119.70
1	a	102	G	C5-C6-N1	5.03	114.02	111.50
1	a	1113	C	N1-C2-O2	5.03	121.92	118.90
25	A	999	U	N3-C2-O2	-5.03	118.68	122.20
25	A	2840	C	C6-N1-C2	-5.03	118.29	120.30
25	A	2863	C	N3-C4-N4	5.03	121.52	118.00
1	a	943	U	N1-C2-O2	5.03	126.32	122.80
25	A	89	A	N1-C2-N3	-5.03	126.78	129.30
25	A	153	U	N3-C2-O2	-5.03	118.68	122.20
25	A	740	C	N3-C4-N4	5.03	121.52	118.00
25	A	1343	G	N3-C4-N9	5.03	129.02	126.00
1	a	175	C	O5'-P-OP2	-5.03	101.18	105.70
25	A	653	U	O5'-P-OP2	-5.02	101.18	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	x	129	U	O4'-C1'-N1	5.02	112.22	108.20
25	A	2419	U	C6-N1-C2	-5.02	117.99	121.00
1	a	135	C	C6-N1-C2	-5.02	118.29	120.30
25	A	731	C	N1-C2-O2	5.02	121.91	118.90
25	A	2065	C	C5-C6-N1	5.02	123.51	121.00
1	a	56	U	C5-C6-N1	5.02	125.21	122.70
1	a	470	C	C6-N1-C2	-5.02	118.29	120.30
25	A	208	C	C6-N1-C2	-5.02	118.29	120.30
25	A	867	C	C6-N1-C2	-5.02	118.29	120.30
25	A	1200	C	C5-C6-N1	5.02	123.51	121.00
1	a	1149	C	C5-C6-N1	5.02	123.51	121.00
1	a	1372	U	N3-C2-O2	-5.02	118.69	122.20
25	A	766	U	C6-N1-C2	-5.01	117.99	121.00
1	a	58	C	N3-C4-C5	5.01	123.90	121.90
1	a	450	G	C6-C5-N7	5.01	133.41	130.40
24	y	39	U	C5-C4-O4	-5.01	122.90	125.90
25	A	848	C	C6-N1-C2	-5.01	118.30	120.30
25	A	729	G	C6-C5-N7	-5.00	127.40	130.40
1	a	1510	C	C5-C4-N4	-5.00	116.70	120.20
24	y	56	C	N3-C4-C5	5.00	123.90	121.90
25	A	349	U	N3-C2-O2	-5.00	118.70	122.20
25	A	1539	U	N3-C4-O4	5.00	122.90	119.40
25	A	2128	G	C4-C5-C6	5.00	121.80	118.80
1	a	295	C	N1-C2-O2	5.00	121.90	118.90
25	A	1892	C	C6-N1-C2	-5.00	118.30	120.30
25	A	2025	C	N1-C2-O2	5.00	121.90	118.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4',C3'
25	A	2069	G7M	C4',C3'

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	0	1	ALA	Mainchain
52	1	3	GLY	Mainchain
54	3	30	HIS	Peptide
27	C	120	ASP	Peptide
28	D	166	GLY	Peptide
29	E	82	GLY	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
30	F	173	ASP	Mainchain
33	H	2	GLN	Peptide
33	H	41	LYS	Mainchain
33	H	8	LYS	Peptide
35	K	89	ASN	Mainchain
36	L	29	LYS	Mainchain
45	U	50	ALA	Peptide
45	U	87	GLU	Mainchain
2	b	72	LYS	Peptide
5	e	76	ASN	Mainchain,Peptide
5	e	88	HIS	Peptide
6	f	52	ASN	Mainchain
6	f	97	THR	Mainchain
9	i	56	MET	Mainchain,Peptide
10	j	33	GLY	Mainchain,Peptide
10	j	34	ALA	Mainchain
12	l	101	LEU	Mainchain
12	l	23	LEU	Mainchain
13	m	3	ILE	Peptide
13	m	64	VAL	Peptide
15	o	87	ARG	Mainchain
16	p	43	ALA	Peptide
17	q	68	LYS	Mainchain
19	s	4	LEU	Mainchain
21	u	23	GLU	Mainchain
21	u	24	LYS	Mainchain

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	a	33029	0	16644	0	0
2	b	1705	0	1732	0	0
3	c	1625	0	1699	0	0
4	d	1643	0	1710	0	0
5	e	1157	0	1199	0	0
6	f	818	0	808	0	0
7	g	1182	0	1240	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	787	0	828	0	0
11	k	870	0	878	0	0
12	l	955	0	1019	0	0
13	m	884	0	944	0	0
14	n	794	0	836	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	649	0	691	0	0
18	r	505	0	502	0	0
19	s	638	0	665	0	0
20	t	665	0	714	0	0
21	u	496	0	486	0	0
22	v	1644	0	840	0	0
23	x	1025	0	518	0	0
24	y	2031	0	1046	0	0
25	A	62274	0	31342	282	0
26	B	2570	0	1301	8	0
27	C	2083	0	2157	34	0
28	D	1565	0	1616	11	0
29	E	1552	0	1619	17	0
30	F	1411	0	1447	16	0
31	G	1323	0	1374	13	0
32	I	1032	0	1088	10	0
33	H	1111	0	1148	14	0
34	J	1129	0	1162	12	0
35	K	939	0	1012	11	0
36	L	1045	0	1117	18	0
37	M	1074	0	1157	10	0
38	N	961	0	1000	8	0
39	O	892	0	923	7	0
40	P	917	0	965	12	0
41	Q	947	0	1022	9	0
42	R	816	0	839	11	0
43	S	857	0	922	9	0
44	T	739	0	807	8	0
45	U	780	0	834	5	0
46	V	753	0	780	8	0
47	W	575	0	592	8	0
48	X	625	0	655	11	0
49	Y	509	0	543	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	Z	449	0	491	3	0
51	0	444	0	461	3	0
52	1	410	0	440	3	0
53	2	377	0	418	6	0
54	3	504	0	574	6	0
55	4	302	0	340	11	0
56	6	523	0	521	9	0
57	w	62	0	34	0	0
58	4	1	0	0	0	0
58	6	1	0	0	0	0
All	All	148018	0	99207	517	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (517) 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)
25:A:2164:C:H41	25:A:2171:A:H61	1.23	0.85
25:A:1171:G:H1	25:A:1177:G:H1	1.26	0.82
25:A:1171:G:N2	25:A:1178:C:O2	2.18	0.77
55:4:2:LYS:HD2	55:4:4:ARG:HH12	1.50	0.76
25:A:585:G:N7	41:Q:5:ARG:NH1	2.32	0.76
25:A:1270:C:H5''	25:A:1271:G:H5'	1.68	0.74
53:2:24:THR:HG23	53:2:27:GLY:H	1.53	0.73
25:A:1053:C:H42	25:A:1106:G:H1	1.37	0.73
25:A:1798:U:OP2	27:C:270:ARG:NH2	2.23	0.72
30:F:62:GLN:OE1	30:F:94:ARG:NH2	2.23	0.71
25:A:621:A:OP2	36:L:99:ASN:ND2	2.25	0.69
25:A:2691:C:HO2'	25:A:2871:U:HO2'	1.40	0.69
43:S:4:ILE:HG22	43:S:106:VAL:HG22	1.74	0.69
25:A:187:G:N2	25:A:190:A:N7	13.25	0.68
25:A:910:A:H62	37:M:12:MET:HA	1.57	0.68
25:A:1601:G:OP1	44:T:64:LYS:NZ	2.27	0.67
34:J:21:THR:OG1	34:J:58:ASN:ND2	2.27	0.67
27:C:141:HIS:ND1	27:C:192:GLY:O	2.26	0.67
47:W:33:ILE:HG22	47:W:34:VAL:HG23	1.77	0.67
31:G:83:THR:HA	31:G:132:LEU:O	1.95	0.66
25:A:2483:C:O2'	37:M:51:ARG:NH2	2.29	0.66
56:6:14:ALA:HB3	56:6:22:MET:HB2	1.78	0.66
36:L:100:ILE:HG13	36:L:101:ILE:HG23	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:88:ARG:HE	40:P:112:ARG:HH21	1.44	0.66
25:A:881:G:H21	25:A:896:A:H62	1.42	0.65
55:4:2:LYS:NZ	55:4:32:LYS:O	2.31	0.64
25:A:307:G:N2	25:A:310:A:OP2	2.29	0.64
40:P:59:THR:HG22	40:P:72:VAL:HG12	1.80	0.64
42:R:14:VAL:HG21	42:R:98:ILE:HG13	1.80	0.63
46:V:45:ASP:O	46:V:49:ASN:ND2	2.32	0.63
31:G:132:LEU:HB3	31:G:140:ILE:HD11	1.81	0.63
25:A:885:C:O2'	25:A:891:G:N2	2.28	0.63
29:E:146:VAL:HG12	29:E:185:LYS:HB2	1.80	0.63
25:A:1019:U:H3	25:A:1142:A:H62	1.47	0.62
27:C:169:ALA:O	27:C:185:ALA:N	2.29	0.62
25:A:2514:U:H4'	34:J:81:ILE:HD11	1.81	0.62
52:1:36:LYS:HD2	52:1:47:ILE:HG13	1.82	0.61
35:K:121:GLU:HG2	35:K:122:VAL:HG23	1.82	0.61
53:2:12:ARG:HE	53:2:44:VAL:HG21	1.65	0.61
25:A:1040:A:H61	25:A:1115:G:H1	1.46	0.61
48:X:5:GLN:O	48:X:73:ARG:NH2	2.33	0.61
34:J:98:GLU:O	34:J:102:GLU:HB2	2.01	0.60
30:F:43:ILE:HG21	30:F:78:ILE:HG22	1.84	0.59
25:A:1386:C:H2'	25:A:1387:A:C8	2.37	0.59
25:A:196:A:OP2	36:L:47:ARG:NH1	2.36	0.59
25:A:2199:A:OP1	48:X:36:ARG:NH2	2.35	0.59
25:A:1478:G:H1	25:A:1513:U:H3	1.50	0.59
43:S:3:THR:HG21	43:S:58:ALA:HB2	1.83	0.59
27:C:106:PRO:HD2	27:C:109:LEU:HD22	1.84	0.59
25:A:320:A:N3	29:E:163:ASN:ND2	2.51	0.59
29:E:119:ILE:O	29:E:187:VAL:HA	2.03	0.59
35:K:24:VAL:HG13	35:K:33:ALA:HB2	1.84	0.59
25:A:1264:A:H5'	51:0:7:PRO:HG2	1.85	0.59
25:A:750:A:OP1	25:A:1615:C:N4	2.36	0.59
25:A:680:C:O2'	27:C:268:ARG:NH2	60.50	0.59
27:C:7:PRO:HB3	27:C:13:ARG:HG3	1.85	0.58
42:R:4:VAL:HA	42:R:12:HIS:O	2.03	0.58
25:A:2394:C:H5''	36:L:63:LYS:HE3	1.85	0.58
41:Q:99:VAL:O	41:Q:102:LYS:NZ	2.36	0.58
54:3:41:ARG:HG2	54:3:44:ARG:HH21	1.67	0.58
25:A:848:C:H2'	25:A:849:A:C8	2.38	0.58
34:J:21:THR:HG1	34:J:58:ASN:ND2	2.00	0.58
46:V:64:VAL:HA	46:V:68:LYS:O	2.03	0.58
44:T:5:GLU:HA	44:T:8:LEU:HD12	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2676:C:OP1	35:K:31:ARG:NH2	2.37	0.57
47:W:17:LEU:O	47:W:20:LYS:NZ	2.36	0.57
25:A:1515:A:HO2'	25:A:1556:C:HO2'	1.53	0.57
25:A:1173:U:O2'	25:A:1177:G:N2	2.36	0.57
27:C:16:VAL:HB	27:C:203:VAL:HG22	1.87	0.57
33:H:14:SER:OG	33:H:17:ASP:OD2	2.22	0.57
30:F:28:PRO:HB3	30:F:159:ALA:HB2	1.86	0.57
35:K:109:SER:O	35:K:111:LYS:N	2.38	0.57
52:1:3:GLY:O	52:1:5:ARG:N	2.38	0.57
25:A:126:A:H5'	53:2:19:ARG:HG3	1.86	0.57
25:A:413:C:HO2'	25:A:1880:U:HO2'	1.52	0.57
34:J:60:ASP:N	34:J:60:ASP:OD1	2.39	0.56
27:C:170:TYR:HA	27:C:183:VAL:O	2.06	0.56
55:4:3:VAL:HG12	55:4:36:ARG:HD3	1.87	0.56
56:6:11:GLU:OE1	56:6:25:ARG:NH1	2.36	0.56
25:A:2377:A:O2'	39:O:117:PHE:O	2.23	0.56
36:L:95:LEU:HD22	36:L:100:ILE:HD11	1.88	0.56
49:Y:24:GLU:HB3	49:Y:46:VAL:HG21	1.86	0.56
32:I:75:ALA:HB2	32:I:112:LYS:HE3	1.87	0.55
25:A:2375:G:N2	25:A:2378:A:OP2	2.37	0.55
27:C:72:GLY:HA2	27:C:116:GLN:HE21	1.70	0.55
30:F:28:PRO:HB2	30:F:168:LEU:HD22	1.88	0.55
39:O:66:GLY:O	39:O:102:ARG:NH2	2.38	0.55
42:R:57:GLY:HA2	42:R:102:SER:O	2.06	0.55
39:O:30:ARG:HA	39:O:35:ILE:HD12	1.89	0.55
25:A:1326:U:O2'	25:A:2010:G:O2'	2.23	0.55
25:A:2271:G:H5'	47:W:16:ARG:HG2	1.89	0.55
25:A:1094:U:N3	25:A:1097:U:OP2	2.39	0.55
27:C:15:VAL:HG22	27:C:205:GLY:HA3	1.89	0.55
45:U:49:PRO:O	45:U:53:GLN:NE2	2.40	0.55
25:A:2133:G:H21	25:A:2158:A:H61	1.55	0.54
25:A:2123:G:N2	25:A:2175:C:N3	2.56	0.54
31:G:51:PHE:HZ	31:G:71:LEU:HD22	1.71	0.54
32:I:53:PRO:HD2	32:I:77:VAL:HG21	1.88	0.54
25:A:1012:U:OP2	41:Q:69:ARG:NH1	2.39	0.54
47:W:61:GLY:HA3	47:W:79:GLU:O	2.07	0.54
25:A:376:G:H2'	25:A:377:G:H8	1.73	0.54
27:C:86:ARG:HH12	27:C:155:ARG:HH21	1.54	0.54
35:K:35:VAL:HG22	35:K:69:VAL:HG12	1.90	0.54
25:A:2127:G:N2	25:A:2161:C:O2'	2.40	0.54
25:A:2506:U:H3	25:A:2585:U:H3	1.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:747:5MU:H5''	25:A:748:G:H5''	1.90	0.54
25:A:563:A:N3	41:Q:36:GLN:NE2	2.56	0.53
25:A:1223:G:OP1	42:R:68:ARG:NH2	2.42	0.53
25:A:290:U:O2	25:A:350:G:O6	2.27	0.53
31:G:82:PHE:O	31:G:133:LYS:HA	2.08	0.53
33:H:40:THR:O	33:H:42:LYS:N	2.42	0.53
25:A:848:C:H2'	25:A:849:A:H8	1.74	0.53
46:V:58:SER:OG	46:V:59:GLU:OE1	2.25	0.53
25:A:2327:A:H2'	25:A:2328:A:C8	2.44	0.53
25:A:2690:U:OP1	38:N:14:SER:OG	2.26	0.53
25:A:610:C:H2'	25:A:611:C:H6	1.74	0.53
25:A:1072:C:N3	25:A:1092:C:N4	2.55	0.53
25:A:2469:A:N6	25:A:2481:G:O2'	2.42	0.53
29:E:49:ARG:HE	29:E:75:SER:HA	1.74	0.53
33:H:26:ALA:HA	33:H:30:LEU:HB2	1.91	0.53
25:A:160:A:H2'	25:A:161:A:O4'	3.06	0.53
25:A:414:C:H2'	25:A:415:A:C8	2.43	0.53
25:A:269:C:H2'	25:A:270:A:C8	2.83	0.53
25:A:518:G:OP1	43:S:18:ARG:NH1	2.42	0.53
30:F:9:ASP:N	30:F:9:ASP:OD1	2.38	0.53
25:A:2130:U:H4'	25:A:2159:G:H22	1.73	0.52
25:A:276:U:O2'	25:A:278:A:N6	2.42	0.52
26:B:90:C:OP2	37:M:18:ARG:NH2	2.42	0.52
31:G:23:ILE:HD11	31:G:42:VAL:HG11	1.91	0.52
37:M:50:ARG:HD3	37:M:65:ILE:HD11	1.92	0.52
42:R:49:ILE:HG22	42:R:54:VAL:HA	1.90	0.52
27:C:140:VAL:HG12	27:C:191:LEU:HD23	1.91	0.52
25:A:1386:C:H2'	25:A:1387:A:H8	1.74	0.52
25:A:2359:C:O2'	54:3:53:ASP:OD2	2.27	0.52
30:F:72:SER:OG	30:F:80:GLN:N	2.43	0.52
38:N:45:ARG:HG2	38:N:95:THR:HG21	1.90	0.52
25:A:1340:U:OP1	44:T:19:LYS:NZ	2.33	0.52
25:A:1868:C:H2'	25:A:1869:G:O4'	2.09	0.52
25:A:2330:G:H21	47:W:38:GLY:HA2	1.75	0.52
40:P:91:VAL:HG21	40:P:96:LEU:HD21	1.92	0.52
50:Z:8:GLN:NE2	50:Z:10:ARG:O	2.39	0.52
25:A:1972:G:OP2	27:C:237:ARG:NH1	2.43	0.52
25:A:1794:A:H2'	25:A:1795:C:C6	2.45	0.51
25:A:9:G:O2'	25:A:2800:A:N6	2.43	0.51
40:P:26:GLU:HG2	40:P:43:GLU:HB2	1.91	0.51
25:A:560:C:O2'	41:Q:47:ARG:NH2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:94:GLN:OE1	29:E:94:GLN:N	2.43	0.51
39:O:71:ALA:HB2	39:O:102:ARG:HG3	1.93	0.51
28:D:121:THR:HG21	28:D:143:PRO:HB3	1.93	0.51
44:T:58:VAL:HG22	44:T:85:VAL:HG13	1.93	0.51
25:A:558:U:H2'	25:A:559:G:C8	2.46	0.51
25:A:1124:G:H5''	34:J:37:ARG:HG3	41.59	0.51
32:I:100:ILE:HG22	32:I:101:SER:H	1.76	0.51
33:H:2:GLN:HB3	33:H:18:GLN:HB3	1.93	0.51
25:A:780:G:H21	25:A:783:A:H62	1.58	0.50
25:A:1779:U:H5	25:A:1784:A:N7	2.10	0.50
25:A:2267:A:H5''	25:A:2268:A:H5''	1.92	0.50
25:A:881:G:N2	25:A:896:A:H62	2.10	0.50
36:L:93:ASN:O	36:L:95:LEU:N	2.45	0.50
42:R:2:TYR:HA	42:R:14:VAL:O	2.11	0.50
25:A:796:C:H2'	25:A:797:G:C8	2.47	0.50
25:A:1040:A:N6	25:A:1115:G:H1	2.09	0.50
27:C:203:VAL:O	27:C:205:GLY:N	2.43	0.50
25:A:2512:C:O2'	28:D:159:LYS:NZ	2.36	0.50
41:Q:93:ILE:HD12	42:R:13:ARG:HB2	1.92	0.50
47:W:19:VAL:HG22	47:W:34:VAL:HG22	1.93	0.50
25:A:1194:A:OP2	36:L:14:LYS:NZ	2.45	0.50
37:M:69:PRO:HA	37:M:94:ALA:HB2	1.94	0.50
25:A:1918:A:O2'	25:A:1919:A:N7	2.43	0.50
25:A:2618:G:O2'	28:D:155:VAL:O	2.29	0.50
38:N:44:LEU:HD23	38:N:113:ILE:HD13	1.93	0.50
25:A:247:G:O2'	25:A:386:G:N1	2.44	0.49
25:A:277:G:H1'	25:A:361:G:H1	1.78	0.49
42:R:49:ILE:HB	42:R:51:VAL:O	2.13	0.49
43:S:82:MET:HB2	43:S:98:LYS:HB2	1.93	0.49
25:A:1469:A:H2'	25:A:1470:A:C8	2.46	0.49
25:A:2291:U:H2'	25:A:2292:U:C6	2.47	0.49
25:A:355:U:H2'	25:A:356:G:H8	1.78	0.49
55:4:11:CYS:SG	55:4:14:CYS:N	2.86	0.49
40:P:29:VAL:HG12	40:P:80:VAL:HG12	1.94	0.49
45:U:17:ASP:HB3	45:U:20:LYS:HD2	1.94	0.49
25:A:1816:C:N4	27:C:34:GLU:OE2	2.44	0.49
25:A:84:A:N1	25:A:98:G:O2'	2.36	0.49
34:J:35:ARG:HB2	34:J:54:ILE:HD11	1.94	0.49
27:C:130:PRO:HD3	27:C:188:ARG:NH1	2.28	0.49
46:V:20:LEU:HD21	46:V:41:GLU:HG3	1.95	0.49
36:L:19:LEU:HA	36:L:27:LEU:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1858:A:N6	25:A:1884:G:O2'	2.45	0.48
25:A:269:C:H2'	25:A:270:A:H8	2.14	0.48
42:R:5:PHE:O	42:R:11:GLN:HA	2.13	0.48
25:A:770:G:H5''	53:2:10:LEU:HD23	1.94	0.48
25:A:639:U:H2'	25:A:640:C:C6	2.49	0.48
28:D:37:VAL:HG22	28:D:48:ILE:HG22	1.94	0.48
33:H:108:VAL:HG12	33:H:110:VAL:H	1.78	0.48
40:P:20:ARG:HH12	40:P:112:ARG:HD3	1.78	0.48
36:L:57:LEU:HD22	54:3:53:ASP:HB3	1.96	0.48
29:E:106:LYS:HG3	29:E:200:LEU:HD23	1.94	0.48
25:A:1278:C:H2'	25:A:1279:G:H8	1.78	0.48
25:A:2391:G:H2'	25:A:2424:C:N4	2.29	0.48
25:A:2832:U:H4'	25:A:2833:U:H5'	1.95	0.48
25:A:856:G:H2'	25:A:857:G:C8	2.48	0.48
54:3:22:LYS:HA	54:3:47:ALA:O	2.14	0.48
25:A:1073:A:H2'	25:A:1074:G:O4'	2.14	0.48
25:A:2514:U:H2'	25:A:2515:C:C6	2.49	0.48
25:A:2813:A:H2'	25:A:2814:A:C8	2.49	0.48
25:A:414:C:H2'	25:A:415:A:H8	1.78	0.48
25:A:558:U:H2'	25:A:559:G:H8	1.79	0.48
25:A:181:A:H2'	25:A:182:A:C8	2.48	0.48
25:A:2065:C:H4'	25:A:2251:OMG:HM23	1.94	0.48
31:G:94:ARG:HB2	31:G:105:SER:HB3	1.96	0.48
34:J:80:HIS:CE1	34:J:81:ILE:HG22	2.49	0.48
38:N:96:ARG:HH22	38:N:116:VAL:HG13	1.78	0.48
35:K:76:VAL:H	40:P:72:VAL:HG22	1.79	0.48
25:A:1326:U:HO2'	25:A:2010:G:HO2'	1.59	0.48
34:J:31:GLU:HG2	34:J:142:ILE:HG12	1.95	0.48
25:A:5:A:H2'	25:A:6:A:C8	2.49	0.47
28:D:25:THR:HG21	28:D:193:VAL:HG22	1.96	0.47
25:A:694:U:OP1	27:C:58:LYS:NZ	2.43	0.47
25:A:184:C:H2'	25:A:185:G:H8	1.79	0.47
25:A:2040:G:H2'	25:A:2041:U:O4'	2.14	0.47
25:A:2333:A:OP2	47:W:73:ARG:NH2	2.43	0.47
25:A:1723:G:H2'	25:A:1724:G:O4'	2.15	0.47
29:E:15:SER:HB2	29:E:18:THR:HB	1.97	0.47
25:A:2087:G:H2'	25:A:2088:A:C8	2.50	0.47
35:K:43:ILE:HD13	35:K:56:ASP:HB2	1.95	0.47
25:A:2013:A:H4'	43:S:96:ILE:HG22	1.97	0.47
55:4:9:LYS:HG3	55:4:14:CYS:HB2	1.96	0.47
25:A:1054:A:H61	25:A:1105:U:H3	1.60	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2813:A:H2'	25:A:2814:A:H8	1.80	0.47
33:H:47:PHE:HA	33:H:51:ARG:HB2	1.95	0.47
45:U:61:GLU:N	45:U:61:GLU:OE1	2.47	0.47
25:A:1109:C:N3	25:A:1110:G:N2	2.62	0.47
25:A:277:G:H8	25:A:360:U:O4	1.97	0.47
47:W:37:ARG:HA	47:W:37:ARG:HD3	1.58	0.47
25:A:373:U:OP2	25:A:400:G:N1	2.47	0.47
25:A:2626:C:H2'	25:A:2627:G:C8	2.50	0.47
25:A:612:G:N2	25:A:614:A:O2'	2.48	0.47
25:A:839:U:H2'	25:A:840:C:C6	2.50	0.47
25:A:877:A:O2'	25:A:900:A:N6	2.48	0.47
55:4:17:VAL:HG23	55:4:24:ARG:HB2	1.97	0.46
25:A:1071:G:N2	25:A:1089:A:O2'	2.44	0.46
25:A:370:G:O2'	25:A:424:G:OP1	2.32	0.46
25:A:2092:U:OP2	33:H:27:ARG:NH2	2.31	0.46
32:I:85:ILE:HD11	32:I:137:LEU:HD21	1.96	0.46
34:J:13:ARG:HE	34:J:121:LYS:HZ1	1.63	0.46
48:X:37:PHE:O	48:X:45:PHE:HA	2.16	0.46
25:A:688:U:P	53:2:2:LYS:HZ1	2.37	0.46
54:3:25:HIS:CE1	54:3:47:ALA:HB2	2.50	0.46
25:A:1251:C:O2'	25:A:1253:A:OP2	2.34	0.46
25:A:1387:A:H2'	25:A:1388:G:H8	1.80	0.46
25:A:1548:A:H2'	25:A:1549:A:C8	2.51	0.46
25:A:2183:A:H2'	25:A:2184:A:C8	2.50	0.46
25:A:910:A:N3	25:A:2264:C:O2'	2.41	0.46
25:A:1715:G:HO2'	25:A:1716:U:H6	1.63	0.46
25:A:2626:C:H2'	25:A:2627:G:H8	1.81	0.46
25:A:2713:U:H3'	25:A:2714:G:H5''	1.97	0.46
25:A:280:U:H2'	25:A:281:C:C6	2.51	0.46
27:C:56:GLY:HA2	27:C:212:TRP:HA	1.98	0.46
25:A:2709:G:OP1	38:N:18:GLN:NE2	2.48	0.46
31:G:174:LYS:HG2	31:G:175:LYS:H	1.81	0.46
25:A:76:C:OP1	49:Y:48:ARG:NH1	2.49	0.46
27:C:230:PRO:HD2	27:C:246:PRO:HA	1.97	0.46
30:F:62:GLN:HE21	30:F:88:VAL:HG13	1.80	0.46
25:A:532:A:H5'	41:Q:27:ARG:HH12	1.81	0.46
33:H:46:PHE:HB3	33:H:50:ARG:HD2	1.97	0.46
33:H:75:LEU:HA	33:H:75:LEU:HD23	1.57	0.46
32:I:18:ASN:HD21	32:I:34:ILE:HG22	1.81	0.46
39:O:40:ILE:HG12	39:O:47:VAL:HG12	1.98	0.46
25:A:1746:A:H2'	25:A:1747:U:C6	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2415:G:H2'	25:A:2416:C:C6	2.52	0.45
46:V:58:SER:O	46:V:73:LYS:NZ	2.49	0.45
53:2:3:ARG:HD3	53:2:3:ARG:HA	1.63	0.45
25:A:1434:A:H2'	25:A:1435:G:C8	2.51	0.45
25:A:1736:U:H2'	25:A:1737:G:O4'	2.16	0.45
25:A:729:G:H5''	25:A:730:A:O5'	2.16	0.45
25:A:882:G:O2'	25:A:883:G:H8	1.99	0.45
27:C:132:ARG:NH1	33:H:93:SER:OG	2.49	0.45
33:H:58:LEU:HA	33:H:61:VAL:HG22	1.98	0.45
35:K:58:LEU:HD11	35:K:86:LEU:HD13	1.98	0.45
25:A:1432:G:H2'	25:A:1433:A:C8	2.50	0.45
25:A:2584:U:H2'	25:A:2585:U:H5''	1.99	0.45
55:4:11:CYS:HB3	55:4:33:HIS:CE1	2.52	0.45
25:A:1597:A:H5''	25:A:1598:A:H5'	1.98	0.45
25:A:2467:C:OP1	55:4:8:LYS:NZ	2.39	0.45
25:A:729:G:C5	27:C:206:LYS:HB2	2.51	0.45
30:F:5:ASP:OD1	30:F:6:TYR:N	2.49	0.45
25:A:1023:U:H2'	25:A:1024:G:C8	3.90	0.45
25:A:171:U:H2'	25:A:172:A:H8	1.81	0.45
25:A:851:C:H2'	25:A:852:U:C6	2.52	0.45
27:C:166:ARG:HG3	27:C:171:VAL:HG22	1.99	0.45
25:A:2285:C:OP2	52:1:5:ARG:NH1	2.50	0.45
25:A:1817:G:OP1	27:C:86:ARG:NH2	2.49	0.45
32:I:30:GLN:HB3	32:I:60:VAL:HG11	1.99	0.45
55:4:7:VAL:HG13	55:4:38:GLY:HA3	1.99	0.45
25:A:1365:A:OP1	48:X:2:ARG:NH1	2.47	0.45
25:A:1744:A:H3'	25:A:1745:A:H8	1.82	0.45
25:A:1796:U:H2'	25:A:1797:G:H8	1.81	0.45
25:A:1:G:H2'	25:A:2:G:C8	2.52	0.45
27:C:259:ASN:O	27:C:261:ARG:N	2.44	0.45
25:A:2830:C:H5''	28:D:56:LYS:NZ	2.32	0.45
37:M:96:ILE:HG21	37:M:126:ILE:HD13	1.98	0.45
25:A:224:U:H2'	25:A:225:C:C6	4.03	0.45
29:E:7:ASP:OD1	29:E:7:ASP:N	2.48	0.45
44:T:63:VAL:HB	44:T:80:TRP:O	2.17	0.45
25:A:1023:U:OP2	25:A:1025:G:O2'	2.35	0.44
25:A:1:G:H2'	25:A:2:G:H8	1.81	0.44
25:A:499:U:H5''	45:U:42:LYS:HE2	1.99	0.44
25:A:871:U:H2'	25:A:872:U:C6	2.53	0.44
30:F:113:PHE:HD2	56:6:41:HIS:HE1	1.64	0.44
25:A:289:G:H2'	25:A:290:U:O4'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:674:G:H1'	29:E:69:ARG:HH12	1.81	0.44
25:A:781:A:OP1	27:C:216:ARG:NH2	2.47	0.44
25:A:942:G:OP2	36:L:39:LYS:NZ	2.45	0.44
25:A:832:U:H5'	36:L:38:GLN:HB3	1.99	0.44
25:A:1915:3TD:H10B	25:A:1916:A:C6	2.52	0.44
25:A:278:A:N1	25:A:361:G:C6	2.85	0.44
51:O:37:HIS:ND1	51:O:38:LEU:O	2.35	0.44
25:A:483:A:O4'	45:U:44:HIS:HB3	2.17	0.44
27:C:83:ASP:HB2	27:C:90:ILE:HG12	2.00	0.44
31:G:53:PRO:HG3	31:G:61:TRP:CE2	2.52	0.44
30:F:108:PRO:HB3	56:6:41:HIS:CD2	2.53	0.44
25:A:1278:C:H2'	25:A:1279:G:C8	2.52	0.44
25:A:1838:C:H4'	25:A:1839:G:H5''	2.00	0.44
31:G:53:PRO:HG3	31:G:61:TRP:CD2	2.53	0.44
39:O:25:ARG:HA	39:O:91:SER:O	2.18	0.44
25:A:1434:A:H2'	25:A:1435:G:O4'	2.63	0.44
27:C:252:LYS:HE2	27:C:252:LYS:HB2	1.84	0.44
29:E:154:ASP:OD1	29:E:154:ASP:N	2.49	0.44
25:A:568:U:H1'	25:A:2030:6MZ:H9C1	1.98	0.44
25:A:2098:U:H2'	25:A:2099:U:O4'	2.18	0.44
25:A:2788:C:H2'	25:A:2789:C:C6	2.52	0.44
25:A:610:C:H2'	25:A:611:C:C6	2.52	0.44
30:F:92:GLY:O	30:F:95:MET:HG2	2.17	0.44
35:K:65:THR:HG23	35:K:68:GLY:H	1.82	0.44
38:N:83:LEU:HD22	38:N:87:PHE:HE2	1.83	0.44
25:A:2328:A:H2'	25:A:2329:U:C6	2.53	0.44
30:F:30:VAL:HG23	30:F:155:ILE:HG23	2.00	0.44
37:M:102:LEU:HD11	37:M:126:ILE:HD11	2.00	0.44
40:P:21:PRO:HD3	40:P:49:ILE:HD12	1.99	0.44
25:A:1646:C:H5''	25:A:1647:U:H5''	2.00	0.43
35:K:41:ILE:HG13	35:K:58:LEU:O	2.18	0.43
54:3:15:LYS:HE2	54:3:19:GLY:HA2	2.00	0.43
25:A:1607:C:N4	25:A:1622:G:OP2	2.41	0.43
25:A:528:A:N1	25:A:2042:A:H2'	2.33	0.43
25:A:2834:G:H2'	25:A:2879:A:H61	1.83	0.43
25:A:1804:C:H2'	25:A:1805:A:H8	1.82	0.43
25:A:1869:G:N2	25:A:1872:A:OP2	2.49	0.43
25:A:2243:U:H2'	25:A:2244:U:C6	2.54	0.43
25:A:679:C:H2'	25:A:680:C:C6	2.53	0.43
27:C:86:ARG:NH1	27:C:155:ARG:HH21	2.16	0.43
32:I:104:GLN:OE1	32:I:104:GLN:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:V:77:VAL:HG23	46:V:89:ILE:HG12	2.00	0.43
25:A:161:A:H3'	25:A:162:U:H5''	1.99	0.43
25:A:2812:G:H2'	25:A:2813:A:C8	2.54	0.43
25:A:2867:G:O2'	25:A:2868:A:H8	2.01	0.43
33:H:1:MET:O	33:H:20:ASN:ND2	2.51	0.43
55:4:30:GLU:O	55:4:33:HIS:HB2	2.19	0.43
25:A:1023:U:H2'	25:A:1024:G:H8	3.36	0.43
25:A:1509:A:H2'	25:A:1510:G:C8	2.52	0.43
25:A:2036:C:H6	25:A:2036:C:H5'	1.83	0.43
25:A:2899:A:H2'	25:A:2900:A:C8	2.53	0.43
25:A:319:G:H1	25:A:323:C:H5	1.67	0.43
40:P:24:THR:O	40:P:86:LYS:HB2	2.18	0.43
25:A:1932:A:H2'	25:A:1933:G:O4'	2.18	0.43
25:A:302:C:H2'	25:A:303:G:H8	1.83	0.43
25:A:2024:G:O3'	28:D:154:LYS:NZ	2.48	0.43
55:4:36:ARG:HG2	55:4:37:GLN:HB3	2.00	0.43
56:6:42:PRO:O	56:6:46:GLY:N	2.48	0.43
25:A:1437:C:H2'	25:A:1438:U:C6	2.54	0.43
25:A:2258:C:O2'	25:A:2427:C:OP2	2.37	0.43
25:A:2104:C:H2'	25:A:2105:U:H6	1.84	0.43
25:A:476:G:N1	25:A:479:A:OP2	2.48	0.43
25:A:883:G:H1	25:A:893:C:H42	1.67	0.43
31:G:37:ASN:OD1	31:G:38:ASP:N	2.52	0.43
48:X:39:VAL:HG12	48:X:42:GLU:H	1.84	0.43
25:A:1487:U:H2'	25:A:1488:C:C6	2.54	0.43
25:A:882:G:H22	25:A:895:U:H1'	1.84	0.43
33:H:32:PRO:HA	48:X:38:TRP:CD1	2.54	0.43
32:I:30:GLN:HG2	32:I:60:VAL:HB	2.00	0.43
41:Q:59:LEU:HD21	41:Q:63:ARG:HH12	1.84	0.43
42:R:41:ILE:HD13	42:R:103:ALA:HA	2.01	0.43
25:A:1614:A:H61	43:S:88:ARG:H	1.66	0.43
25:A:2140:G:H2'	25:A:2141:G:C8	2.53	0.42
25:A:2141:G:H2'	25:A:2142:A:H8	1.83	0.42
30:F:30:VAL:HG22	30:F:95:MET:HE1	2.00	0.42
39:O:2:ASP:O	39:O:5:SER:OG	2.34	0.42
25:A:38:A:H2'	25:A:39:G:O4'	2.18	0.42
25:A:715:A:H2'	25:A:716:A:C8	3.10	0.42
25:A:2599:G:C8	27:C:235:GLU:HG2	2.54	0.42
25:A:1126:A:H4'	25:A:1127:A:H5''	2.01	0.42
25:A:1469:A:H2'	25:A:1470:A:H8	1.84	0.42
26:B:30:C:H2'	26:B:31:C:H5'	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:93:C:H2'	26:B:94:A:C8	2.55	0.42
40:P:12:MET:O	40:P:14:GLN:NE2	2.52	0.42
56:6:62:LYS:HG2	56:6:63:ARG:NH1	2.34	0.42
25:A:1197:G:H2'	25:A:1198:U:H6	1.84	0.42
25:A:608:A:H2'	25:A:609:A:C8	2.54	0.42
28:D:184:ARG:HH12	40:P:6:GLN:HG2	1.84	0.42
25:A:2843:G:H2'	25:A:2844:G:O4'	2.20	0.42
56:6:56:ARG:O	56:6:59:ARG:HG2	2.20	0.42
25:A:116:C:H2'	25:A:117:G:O4'	2.18	0.42
26:B:28:C:H2'	26:B:29:A:C8	2.55	0.42
25:A:990:A:N1	42:R:78:ARG:NH1	2.67	0.42
43:S:17:VAL:HB	43:S:76:VAL:HG11	2.01	0.42
25:A:1387:A:H2'	25:A:1388:G:C8	2.54	0.42
25:A:685:A:H5''	25:A:788:A:H62	1.84	0.42
34:J:118:MET:HA	34:J:121:LYS:HG2	2.02	0.42
41:Q:97:ILE:HG22	41:Q:105:PHE:HB2	2.02	0.42
25:A:1353:A:H2'	25:A:1354:A:C8	2.54	0.42
25:A:745:1MG:HM11	25:A:745:1MG:HN21	1.69	0.42
31:G:94:ARG:HD2	31:G:127:GLN:HE21	1.85	0.42
25:A:144:A:H4'	44:T:2:ILE:HD11	2.02	0.42
25:A:2086:U:H2'	25:A:2087:G:C8	2.55	0.42
25:A:2301:C:H2'	25:A:2302:U:C6	2.55	0.42
35:K:25:LEU:HD12	35:K:38:ILE:HG22	2.02	0.42
25:A:2821:A:H2'	25:A:2822:G:O4'	2.20	0.42
26:B:95:U:H2'	26:B:96:G:H8	1.85	0.42
38:N:28:LEU:HD23	38:N:48:VAL:HG21	2.02	0.42
48:X:36:ARG:HA	48:X:47:THR:HA	2.01	0.42
56:6:37:CYS:O	56:6:41:HIS:HB2	2.20	0.41
25:A:2087:G:H2'	25:A:2088:A:H8	1.83	0.41
25:A:207:A:H2'	25:A:208:C:O4'	2.20	0.41
26:B:88:C:O2'	26:B:89:U:O5'	2.28	0.41
36:L:29:LYS:O	36:L:30:THR:OG1	2.38	0.41
50:Z:9:THR:OG1	50:Z:10:ARG:N	2.53	0.41
25:A:2376:A:H2'	25:A:2377:A:O4'	2.19	0.41
25:A:562:U:H5''	25:A:563:A:C5	11.89	0.41
25:A:660:C:H5''	29:E:94:GLN:HG3	2.01	0.41
25:A:782:A:H4'	25:A:783:A:H5'	2.01	0.41
26:B:49:C:H2'	26:B:50:A:C8	2.56	0.41
29:E:117:ARG:NH1	36:L:2:ARG:HG2	2.35	0.41
29:E:52:VAL:HG21	29:E:82:GLY:H	1.85	0.41
30:F:5:ASP:O	30:F:8:LYS:HB2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:153:PRO:HA	31:G:159:LYS:O	2.20	0.41
25:A:1213:A:H1'	25:A:1237:A:C2	2.55	0.41
25:A:527:C:C4	25:A:2779:U:H2'	2.55	0.41
25:A:45:G:H2'	25:A:46:G:C8	6.06	0.41
25:A:5:A:H2'	25:A:6:A:H8	1.84	0.41
25:A:2572:A:N7	28:D:150:GLN:HG2	2.35	0.41
34:J:37:ARG:HD3	34:J:37:ARG:HA	4.44	0.41
25:A:2757:A:N1	31:G:66:THR:OG1	2.47	0.41
25:A:397:U:OP2	48:X:9:LYS:NZ	2.36	0.41
25:A:801:G:O4'	29:E:49:ARG:NH2	2.54	0.41
25:A:833:A:H2'	25:A:834:G:C8	2.55	0.41
27:C:242:HIS:HA	27:C:243:PRO:HD3	1.90	0.41
25:A:364:C:H2'	25:A:365:U:C6	2.55	0.41
28:D:35:THR:OG1	28:D:49:GLN:HG3	2.20	0.41
40:P:46:VAL:HG22	40:P:60:VAL:HG22	2.01	0.41
43:S:17:VAL:HA	43:S:43:ALA:HB1	2.03	0.41
25:A:2800:A:C2	25:A:2895:G:H1'	2.56	0.41
25:A:517:C:OP1	51:O:12:ARG:NH2	2.54	0.41
25:A:669:G:H2'	25:A:669:G:N3	2.35	0.41
36:L:110:VAL:HG21	36:L:127:VAL:HG22	2.01	0.41
37:M:65:ILE:HG12	37:M:103:TYR:CE1	2.56	0.41
25:A:171:U:H2'	25:A:172:A:C8	2.56	0.41
25:A:2141:G:H2'	25:A:2142:A:C8	2.56	0.41
25:A:2784:U:H2'	25:A:2785:C:C6	2.55	0.41
25:A:620:G:H4'	25:A:621:A:O5'	2.21	0.41
32:I:92:PRO:HG3	32:I:136:GLY:HA2	2.03	0.41
25:A:475:C:O2	25:A:479:A:N6	2.53	0.41
25:A:593:U:H2'	25:A:594:U:C6	2.56	0.41
33:H:8:LYS:HE3	33:H:8:LYS:HB3	1.90	0.41
25:A:2247:A:H2'	25:A:2248:C:H6	1.86	0.41
25:A:2698:U:H2'	25:A:2699:C:C6	2.56	0.41
28:D:2:ILE:HG21	28:D:84:LEU:HD23	2.03	0.41
29:E:49:ARG:HH21	29:E:49:ARG:HD3	1.74	0.41
37:M:96:ILE:HA	37:M:96:ILE:HD12	1.93	0.41
25:A:1538:G:H2'	25:A:1539:U:C6	2.56	0.41
32:I:48:ILE:HG13	32:I:49:GLU:H	1.86	0.41
43:S:59:GLU:HA	43:S:64:ALA:HB2	2.03	0.41
44:T:57:VAL:O	44:T:86:THR:OG1	2.29	0.41
25:A:244:A:H5''	36:L:67:THR:HG21	2.03	0.41
25:A:594:U:H2'	25:A:595:C:C6	2.55	0.41
27:C:159:THR:HG23	27:C:176:ARG:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:60:SER:OG	30:F:61:GLY:N	2.54	0.41
56:6:26:SER:OG	56:6:27:THR:N	2.53	0.40
25:A:2297:A:N1	25:A:2321:U:H5	2.18	0.40
25:A:807:U:H1'	25:A:2445:2MG:H5'	2.02	0.40
25:A:2610:C:H4'	25:A:2611:C:H5'	2.02	0.40
25:A:575:A:OP2	25:A:2055:C:N4	2.51	0.40
25:A:857:G:H2'	25:A:858:G:O4'	2.21	0.40
36:L:29:LYS:O	36:L:31:GLY:N	2.54	0.40
36:L:55:MET:HA	36:L:56:PRO:HD3	1.97	0.40
25:A:1170:C:H2'	25:A:1171:G:C8	2.56	0.40
37:M:17:ASN:ND2	37:M:17:ASN:O	2.55	0.40
38:N:59:SER:O	38:N:63:ARG:HG2	2.21	0.40
44:T:29:THR:O	44:T:33:LYS:HB2	13.65	0.40
48:X:3:VAL:HG22	48:X:10:ARG:HB3	2.03	0.40
25:A:1141:U:H4'	25:A:1142:A:O4'	2.20	0.40
25:A:1158:C:H2'	25:A:1159:U:H6	1.86	0.40
25:A:1178:C:H2'	25:A:1179:G:C8	2.56	0.40
25:A:1534:U:O2	25:A:1537:G:N2	2.50	0.40
25:A:1565:C:O2'	25:A:1566:A:H2'	2.20	0.40
25:A:2353:G:H2'	25:A:2354:C:O4'	2.21	0.40
25:A:2620:C:H2'	25:A:2621:G:O4'	2.22	0.40
25:A:372:G:H5''	48:X:60:LYS:HZ1	1.86	0.40
27:C:81:GLU:HG3	27:C:102:TYR:HE1	1.87	0.40
27:C:264:LYS:HE3	27:C:264:LYS:HB2	1.87	0.40
30:F:123:GLY:HA2	30:F:162:ASP:HB3	2.03	0.40
29:E:26:ALA:HB2	36:L:9:ALA:HB2	2.03	0.40
46:V:56:PHE:CE1	46:V:61:LEU:HD21	2.57	0.40
25:A:1410:G:H2'	25:A:1411:U:H6	1.87	0.40
25:A:1779:U:H5''	25:A:1780:A:H5''	2.03	0.40
25:A:2685:G:H2'	25:A:2686:G:H8	1.87	0.40
25:A:2836:U:H2'	25:A:2837:A:C8	2.56	0.40
25:A:2859:G:H2'	25:A:2860:A:C8	2.57	0.40
25:A:679:C:H2'	25:A:680:C:H6	1.86	0.40
26:B:54:G:H2'	26:B:55:U:H6	1.86	0.40
46:V:72:VAL:HG12	46:V:93:ARG:HA	2.02	0.40
50:Z:16:LEU:HB2	50:Z:19:HIS:ND1	2.37	0.40
25:A:2185:U:H2'	25:A:2186:G:C8	2.57	0.40
25:A:2834:G:H2'	25:A:2879:A:N6	2.36	0.40
25:A:372:G:H5''	48:X:60:LYS:NZ	2.36	0.40
25:A:784:G:H5'	25:A:785:G:OP1	2.21	0.40
25:A:813:U:H2'	25:A:814:C:C6	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:139:THR:HG23	27:C:160:TYR:HB2	2.03	0.40
29:E:149:ILE:HD11	29:E:172:ALA:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/218 (99%)	190 (88%)	23 (11%)	3 (1%)	14	58
3	c	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	13	56
4	d	203/205 (99%)	181 (89%)	19 (9%)	3 (2%)	13	56
5	e	155/157 (99%)	139 (90%)	9 (6%)	7 (4%)	3	30
6	f	98/100 (98%)	83 (85%)	10 (10%)	5 (5%)	2	26
7	g	149/151 (99%)	136 (91%)	10 (7%)	3 (2%)	9	51
8	h	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	12	55
9	i	125/127 (98%)	105 (84%)	14 (11%)	6 (5%)	3	28
10	j	96/98 (98%)	83 (86%)	8 (8%)	5 (5%)	2	25
11	k	114/116 (98%)	102 (90%)	10 (9%)	2 (2%)	11	53
12	l	121/123 (98%)	101 (84%)	14 (12%)	6 (5%)	3	27
13	m	112/114 (98%)	100 (89%)	8 (7%)	4 (4%)	4	37
14	n	98/100 (98%)	86 (88%)	8 (8%)	4 (4%)	3	33
15	o	86/88 (98%)	73 (85%)	9 (10%)	4 (5%)	3	29
16	p	80/82 (98%)	69 (86%)	7 (9%)	4 (5%)	3	27
17	q	78/80 (98%)	65 (83%)	11 (14%)	2 (3%)	7	45
18	r	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	3	28
19	s	77/79 (98%)	71 (92%)	5 (6%)	1 (1%)	15	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	t	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
21	u	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	14
27	C	269/271 (99%)	245 (91%)	19 (7%)	5 (2%)	10	51
28	D	207/209 (99%)	191 (92%)	13 (6%)	3 (1%)	14	58
29	E	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	13	56
30	F	175/177 (99%)	160 (91%)	13 (7%)	2 (1%)	17	63
31	G	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	11	54
32	I	139/141 (99%)	120 (86%)	15 (11%)	4 (3%)	6	42
33	H	147/149 (99%)	125 (85%)	17 (12%)	5 (3%)	5	39
34	J	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	14	58
35	K	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	5	39
36	L	141/143 (99%)	127 (90%)	10 (7%)	4 (3%)	6	43
37	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	13	56
38	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
39	O	114/116 (98%)	104 (91%)	9 (8%)	1 (1%)	21	68
40	P	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
41	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
42	R	101/103 (98%)	89 (88%)	9 (9%)	3 (3%)	5	42
43	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
44	T	91/93 (98%)	78 (86%)	11 (12%)	2 (2%)	8	49
45	U	100/102 (98%)	87 (87%)	7 (7%)	6 (6%)	2	21
46	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
47	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	14	58
48	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
49	Y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	12	55
50	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
51	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	10	51
52	1	48/50 (96%)	47 (98%)	0	1 (2%)	9	50
53	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
54	3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	12	55
55	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	6	64/66 (97%)	58 (91%)	5 (8%)	1 (2%)	12	55
All	All	5717/5817 (98%)	5151 (90%)	439 (8%)	127 (2%)	13	49

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	73	ARG
5	e	77	ASN
5	e	89	THR
5	e	93	VAL
6	f	53	LYS
6	f	54	LEU
6	f	98	GLU
9	i	57	VAL
9	i	90	ASP
10	j	34	ALA
11	k	88	PRO
12	l	23	LEU
12	l	75	GLU
13	m	4	ALA
13	m	65	GLU
16	p	44	SER
16	p	79	ASN
16	p	80	LYS
17	q	69	THR
18	r	11	ARG
19	s	4	LEU
21	u	24	LYS
27	C	121	ALA
28	D	167	ASN
29	E	83	VAL
30	F	174	PHE
31	G	108	PHE
33	H	3	VAL
33	H	9	VAL
33	H	41	LYS
35	K	35	VAL
35	K	110	GLU
36	L	36	LYS
45	U	6	ARG
45	U	38	ILE
45	U	51	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	U	88	ASP
51	0	2	VAL
52	1	4	ILE
54	3	31	ILE
2	b	18	GLN
3	c	156	LEU
6	f	92	THR
7	g	145	GLU
10	j	57	VAL
13	m	6	ILE
14	n	34	ASN
15	o	46	LYS
18	r	17	VAL
18	r	46	THR
21	u	62	GLU
27	C	204	LEU
28	D	153	GLY
30	F	20	ASN
31	G	174	LYS
36	L	29	LYS
36	L	111	ILE
39	O	63	LYS
42	R	100	GLY
49	Y	22	LEU
56	6	4	ASP
4	d	191	SER
5	e	23	THR
5	e	50	GLY
5	e	102	THR
5	e	122	VAL
6	f	86	ARG
7	g	29	LEU
7	g	83	THR
8	h	47	ASP
9	i	12	LYS
9	i	107	ALA
9	i	125	GLN
10	j	42	LEU
10	j	93	ALA
11	k	92	ARG
13	m	104	ASN
14	n	2	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	n	53	ASP
15	o	2	LEU
16	p	43	ALA
21	u	8	ASN
29	E	80	SER
29	E	122	GLU
32	I	53	PRO
32	I	59	THR
42	R	55	ASP
45	U	54	PRO
45	U	97	SER
3	c	96	VAL
3	c	205	GLU
4	d	29	THR
9	i	31	GLN
10	j	89	ARG
17	q	17	GLU
27	C	52	HIS
28	D	139	SER
31	G	47	ASN
32	I	64	ARG
33	H	15	LEU
35	K	89	ASN
44	T	38	ALA
8	h	2	MET
12	l	2	THR
12	l	21	PRO
12	l	88	ASP
12	l	101	LEU
15	o	27	GLN
15	o	45	HIS
27	C	154	ALA
33	H	89	LYS
36	L	94	THR
37	M	58	LYS
44	T	52	GLU
47	W	17	LEU
4	d	166	LYS
14	n	54	SER
21	u	34	ARG
21	u	65	ARG
27	C	260	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	K	93	GLN
37	M	69	PRO
2	b	27	LYS
42	R	54	VAL
32	I	12	VAL
34	J	81	ILE
34	J	100	VAL

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	
2	b	180/180 (100%)	178 (99%)	2 (1%)	80	92
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	172 (100%)	0	100	100
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	103 (100%)	0	100	100
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	75 (99%)	1 (1%)	76	91
16	p	65/65 (100%)	64 (98%)	1 (2%)	72	90
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	41 (93%)	3 (7%)	20	60
27	C	216/216 (100%)	215 (100%)	1 (0%)	92	97
28	D	164/164 (100%)	164 (100%)	0	100	100
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/148 (100%)	148 (100%)	0	100	100
31	G	137/137 (100%)	137 (100%)	0	100	100
32	I	109/109 (100%)	105 (96%)	4 (4%)	41	76
33	H	114/114 (100%)	114 (100%)	0	100	100
34	J	116/116 (100%)	116 (100%)	0	100	100
35	K	103/103 (100%)	103 (100%)	0	100	100
36	L	102/102 (100%)	101 (99%)	1 (1%)	82	93
37	M	109/109 (100%)	108 (99%)	1 (1%)	84	94
38	N	100/100 (100%)	100 (100%)	0	100	100
39	O	86/86 (100%)	86 (100%)	0	100	100
40	P	99/99 (100%)	99 (100%)	0	100	100
41	Q	89/89 (100%)	89 (100%)	0	100	100
42	R	84/84 (100%)	84 (100%)	0	100	100
43	S	93/93 (100%)	93 (100%)	0	100	100
44	T	80/80 (100%)	80 (100%)	0	100	100
45	U	83/83 (100%)	82 (99%)	1 (1%)	78	92
46	V	78/78 (100%)	77 (99%)	1 (1%)	76	91
47	W	57/57 (100%)	57 (100%)	0	100	100
48	X	67/67 (100%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	55 (100%)	0	100	100
50	Z	48/48 (100%)	48 (100%)	0	100	100
51	0	47/47 (100%)	46 (98%)	1 (2%)	61	86
52	1	45/45 (100%)	44 (98%)	1 (2%)	60	85
53	2	38/38 (100%)	38 (100%)	0	100	100
54	3	51/51 (100%)	51 (100%)	0	100	100
55	4	34/34 (100%)	34 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	6	59/59 (100%)	51 (86%)	8 (14%)	5 26
All	All	4728/4751 (100%)	4702 (100%)	26 (0%)	92 97

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	86	CYS
2	b	122	ASP
15	o	87	ARG
16	p	19	VAL
21	u	12	ASP
21	u	21	SER
21	u	37	TYR
27	C	85	ASN
32	I	27	LEU
32	I	33	ASN
32	I	35	MET
32	I	37	PHE
36	L	38	GLN
37	M	17	ASN
45	U	39	ASN
46	V	42	LEU
51	0	2	VAL
52	1	36	LYS
56	6	13	THR
56	6	16	CYS
56	6	30	HIS
56	6	32	LEU
56	6	34	LEU
56	6	40	CYS
56	6	45	THR
56	6	66	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	40	GLN
7	g	147	ASN
11	k	80	ASN
15	o	34	GLN
16	p	79	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	C	44	ASN
27	C	52	HIS
27	C	116	GLN
29	E	41	GLN
31	G	127	GLN
32	I	42	ASN
33	H	20	ASN
34	J	58	ASN
45	U	39	ASN
46	V	78	GLN
48	X	15	ASN
52	1	44	GLN
56	6	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	247 (16%)	0
22	v	76/77 (98%)	15 (19%)	0
23	x	47/48 (97%)	22 (46%)	0
24	y	87/95 (91%)	12 (13%)	0
25	A	2894/2903 (99%)	513 (17%)	34 (1%)
26	B	119/120 (99%)	19 (15%)	3 (2%)
57	w	2/3 (66%)	0	0
All	All	4760/4785 (99%)	828 (17%)	37 (0%)

All (828) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	7	A
1	a	8	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	41	G
1	a	42	G
1	a	47	C
1	a	48	C
1	a	49	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	50	A
1	a	51	A
1	a	61	G
1	a	65	A
1	a	71	A
1	a	79	G
1	a	81	A
1	a	82	G
1	a	83	C
1	a	86	G
1	a	88	U
1	a	94	G
1	a	95	C
1	a	96	U
1	a	116	A
1	a	118	U
1	a	121	U
1	a	126	G
1	a	127	G
1	a	131	A
1	a	168	G
1	a	174	A
1	a	178	C
1	a	181	A
1	a	183	C
1	a	197	A
1	a	208	U
1	a	210	C
1	a	211	G
1	a	226	G
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	264	C
1	a	266	G
1	a	267	C
1	a	281	G
1	a	289	G
1	a	319	G
1	a	328	C
1	a	330	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	340	U
1	a	345	C
1	a	346	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	369	G
1	a	372	C
1	a	373	A
1	a	384	G
1	a	397	A
1	a	398	U
1	a	406	G
1	a	410	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	423	G
1	a	429	U
1	a	441	A
1	a	446	G
1	a	466	A
1	a	467	U
1	a	481	G
1	a	482	A
1	a	486	U
1	a	496	A
1	a	497	G
1	a	499	A
1	a	506	G
1	a	509	A
1	a	511	C
1	a	512	U
1	a	518	C
1	a	527	G7M
1	a	528	C
1	a	532	A
1	a	546	A
1	a	547	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	550	G
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	596	A
1	a	615	G
1	a	617	G
1	a	633	G
1	a	642	A
1	a	654	G
1	a	661	G
1	a	665	A
1	a	671	G
1	a	687	A
1	a	701	U
1	a	702	A
1	a	713	G
1	a	718	A
1	a	723	U
1	a	724	G
1	a	731	G
1	a	733	G
1	a	734	G
1	a	759	A
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	829	G
1	a	832	G
1	a	836	G
1	a	843	U
1	a	844	G
1	a	845	A
1	a	846	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	849	G
1	a	872	A
1	a	873	A
1	a	885	G
1	a	890	G
1	a	891	U
1	a	902	G
1	a	914	A
1	a	926	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	967	5MC
1	a	968	A
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	991	U
1	a	992	U
1	a	993	G
1	a	996	A
1	a	1004	A
1	a	1020	G
1	a	1026	G
1	a	1028	C
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1053	G
1	a	1066	C
1	a	1070	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1126	U
1	a	1130	A
1	a	1132	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1139	G
1	a	1140	C
1	a	1151	A
1	a	1159	U
1	a	1160	G
1	a	1161	C
1	a	1182	G
1	a	1183	U
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1207	2MG
1	a	1212	U
1	a	1213	A
1	a	1214	C
1	a	1223	C
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1236	A
1	a	1238	A
1	a	1241	G
1	a	1257	A
1	a	1260	G
1	a	1280	A
1	a	1286	U
1	a	1287	A
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1332	A
1	a	1346	A
1	a	1353	G
1	a	1363	A
1	a	1364	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1381	U
1	a	1398	A
1	a	1401	G
1	a	1419	G
1	a	1422	G
1	a	1429	A
1	a	1433	A
1	a	1446	A
1	a	1452	C
1	a	1453	G
1	a	1492	A
1	a	1494	G
1	a	1498	UR3
1	a	1499	A
1	a	1503	A
1	a	1504	G
1	a	1505	G
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1534	A
1	a	1535	C
1	a	1540	U
22	v	8	4SU
22	v	9	G
22	v	14	A
22	v	17	C
22	v	17(A)	U
22	v	18	G
22	v	19	G
22	v	20	H2U
22	v	22	G
22	v	47	U
22	v	49	G
22	v	59	A
22	v	60	U
22	v	75	C
22	v	76	A
23	x	89	G
23	x	94	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	x	95	U
23	x	96	C
23	x	98	U
23	x	104	U
23	x	109	C
23	x	110	G
23	x	113	C
23	x	117	C
23	x	120	U
23	x	121	U
23	x	122	G
23	x	123	C
23	x	125	G
23	x	126	G
23	x	127	U
23	x	128	C
23	x	129	U
23	x	130	G
23	x	131	C
23	x	134	C
24	y	10	C
24	y	17	G
24	y	19	H2U
24	y	20	G
24	y	35	C
24	y	47(F)	C
24	y	47(G)	C
24	y	47(K)	G
24	y	51	A
24	y	55	PSU
24	y	74	C
24	y	76	A
25	A	10	A
25	A	35	G
25	A	36	G
25	A	39	G
25	A	43	G
25	A	46	G
25	A	50	U
25	A	51	G
25	A	52	A
25	A	60	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	63	A
25	A	71	A
25	A	74	A
25	A	75	G
25	A	100	U
25	A	102	U
25	A	103	A
25	A	118	A
25	A	120	U
25	A	138	U
25	A	142	A
25	A	162	U
25	A	163	C
25	A	178	G
25	A	196	A
25	A	205	G
25	A	206	U
25	A	216	A
25	A	219	A
25	A	221	A
25	A	222	A
25	A	225	C
25	A	228	C
25	A	229	C
25	A	247	G
25	A	248	G
25	A	250	G
25	A	255	A
25	A	266	G
25	A	276	U
25	A	277	G
25	A	278	A
25	A	285	G
25	A	294	A
25	A	310	A
25	A	323	C
25	A	324	A
25	A	329	G
25	A	330	A
25	A	332	A
25	A	346	A
25	A	349	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	361	G
25	A	371	A
25	A	372	G
25	A	373	U
25	A	386	G
25	A	387	U
25	A	396	G
25	A	404	A
25	A	406	G
25	A	411	G
25	A	412	A
25	A	424	G
25	A	451	U
25	A	455	C
25	A	456	C
25	A	457	A
25	A	473	G
25	A	481	G
25	A	491	G
25	A	496	G
25	A	504	A
25	A	505	A
25	A	509	C
25	A	513	A
25	A	518	G
25	A	527	C
25	A	529	A
25	A	531	C
25	A	532	A
25	A	543	G
25	A	544	C
25	A	545	U
25	A	547	A
25	A	548	G
25	A	549	G
25	A	551	G
25	A	556	A
25	A	563	A
25	A	572	A
25	A	573	U
25	A	575	A
25	A	588	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	603	A
25	A	614	A
25	A	622	G
25	A	627	A
25	A	637	A
25	A	645	C
25	A	646	U
25	A	647	G
25	A	654	A
25	A	655	A
25	A	656	G
25	A	668	A
25	A	669	G
25	A	685	A
25	A	686	U
25	A	694	U
25	A	695	G
25	A	702	U
25	A	714	U
25	A	717	C
25	A	723	C
25	A	729	G
25	A	730	A
25	A	740	C
25	A	747	5MU
25	A	752	A
25	A	757	G
25	A	765	C
25	A	775	G
25	A	776	G
25	A	777	G
25	A	782	A
25	A	783	A
25	A	784	G
25	A	785	G
25	A	789	A
25	A	805	G
25	A	807	U
25	A	812	C
25	A	819	A
25	A	822	G
25	A	827	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	828	U
25	A	831	G
25	A	844	A
25	A	845	A
25	A	846	U
25	A	847	U
25	A	858	G
25	A	859	G
25	A	869	G
25	A	883	G
25	A	885	C
25	A	886	A
25	A	898	C
25	A	910	A
25	A	914	G
25	A	915	C
25	A	932	U
25	A	941	A
25	A	945	A
25	A	946	C
25	A	958	U
25	A	959	A
25	A	961	C
25	A	973	A
25	A	974	G
25	A	983	A
25	A	985	C
25	A	990	A
25	A	995	C
25	A	996	A
25	A	1012	U
25	A	1013	C
25	A	1021	A
25	A	1022	G
25	A	1023	U
25	A	1026	G
25	A	1033	U
25	A	1034	G
25	A	1040	A
25	A	1043	C
25	A	1045	C
25	A	1046	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	1047	G
25	A	1053	C
25	A	1054	A
25	A	1057	A
25	A	1060	U
25	A	1061	U
25	A	1062	G
25	A	1065	U
25	A	1066	U
25	A	1068	G
25	A	1069	A
25	A	1070	A
25	A	1071	G
25	A	1072	C
25	A	1076	C
25	A	1079	C
25	A	1084	A
25	A	1088	A
25	A	1097	U
25	A	1104	C
25	A	1106	G
25	A	1112	G
25	A	1116	G
25	A	1132	U
25	A	1135	C
25	A	1136	G
25	A	1137	G
25	A	1142	A
25	A	1148	U
25	A	1155	A
25	A	1165	A
25	A	1172	C
25	A	1174	U
25	A	1175	A
25	A	1178	C
25	A	1179	G
25	A	1180	U
25	A	1183	U
25	A	1186	G
25	A	1204	A
25	A	1205	A
25	A	1210	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	1211	C
25	A	1212	G
25	A	1213	A
25	A	1227	G
25	A	1237	A
25	A	1238	G
25	A	1247	A
25	A	1248	G
25	A	1250	G
25	A	1251	C
25	A	1253	A
25	A	1256	G
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1287	A
25	A	1300	G
25	A	1301	A
25	A	1306	C
25	A	1314	C
25	A	1325	U
25	A	1326	U
25	A	1332	G
25	A	1345	C
25	A	1352	U
25	A	1365	A
25	A	1368	G
25	A	1379	U
25	A	1383	A
25	A	1386	C
25	A	1395	A
25	A	1416	G
25	A	1417	C
25	A	1421	G
25	A	1428	C
25	A	1429	G
25	A	1453	A
25	A	1454	C
25	A	1458	U
25	A	1459	G
25	A	1475	G
25	A	1482	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	1498	C
25	A	1504	A
25	A	1515	A
25	A	1524	G
25	A	1533	C
25	A	1536	C
25	A	1558	C
25	A	1559	U
25	A	1560	G
25	A	1567	G
25	A	1568	G
25	A	1569	A
25	A	1578	U
25	A	1581	G
25	A	1583	A
25	A	1584	U
25	A	1608	A
25	A	1617	C
25	A	1627	G
25	A	1646	C
25	A	1647	U
25	A	1648	U
25	A	1649	G
25	A	1665	A
25	A	1669	A
25	A	1674	G
25	A	1682	G
25	A	1695	G
25	A	1698	A
25	A	1715	G
25	A	1716	U
25	A	1729	U
25	A	1730	C
25	A	1732	C
25	A	1733	G
25	A	1738	G
25	A	1758	U
25	A	1764	C
25	A	1773	A
25	A	1781	U
25	A	1782	U
25	A	1784	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	1791	A
25	A	1800	C
25	A	1801	A
25	A	1808	A
25	A	1809	A
25	A	1812	U
25	A	1816	C
25	A	1829	A
25	A	1833	C
25	A	1847	A
25	A	1857	G
25	A	1870	C
25	A	1873	G
25	A	1884	G
25	A	1899	A
25	A	1901	A
25	A	1906	G
25	A	1913	A
25	A	1919	A
25	A	1929	G
25	A	1930	G
25	A	1931	U
25	A	1936	A
25	A	1937	A
25	A	1938	A
25	A	1941	C
25	A	1942	C
25	A	1955	U
25	A	1966	A
25	A	1967	C
25	A	1970	A
25	A	1971	U
25	A	1972	G
25	A	1991	U
25	A	1993	U
25	A	1997	C
25	A	2022	U
25	A	2023	C
25	A	2031	A
25	A	2032	G
25	A	2034	U
25	A	2036	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	2043	C
25	A	2044	C
25	A	2049	G
25	A	2050	C
25	A	2055	C
25	A	2056	G
25	A	2060	A
25	A	2061	G
25	A	2062	A
25	A	2069	G7M
25	A	2070	A
25	A	2072	C
25	A	2093	G
25	A	2096	C
25	A	2100	G
25	A	2108	A
25	A	2111	U
25	A	2112	G
25	A	2113	U
25	A	2116	G
25	A	2118	U
25	A	2119	A
25	A	2120	G
25	A	2121	G
25	A	2122	U
25	A	2125	G
25	A	2127	G
25	A	2129	C
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2137	U
25	A	2145	C
25	A	2147	A
25	A	2152	G
25	A	2153	C
25	A	2159	G
25	A	2160	C
25	A	2166	U
25	A	2169	A
25	A	2170	A
25	A	2172	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	2173	A
25	A	2178	C
25	A	2182	U
25	A	2183	A
25	A	2189	U
25	A	2192	U
25	A	2198	A
25	A	2199	A
25	A	2204	G
25	A	2211	A
25	A	2213	U
25	A	2223	G
25	A	2225	A
25	A	2238	G
25	A	2239	G
25	A	2250	G
25	A	2268	A
25	A	2279	G
25	A	2283	C
25	A	2287	A
25	A	2294	G
25	A	2305	U
25	A	2309	A
25	A	2312	U
25	A	2321	U
25	A	2322	A
25	A	2325	G
25	A	2327	A
25	A	2331	G
25	A	2333	A
25	A	2347	C
25	A	2350	C
25	A	2354	C
25	A	2383	G
25	A	2385	C
25	A	2392	A
25	A	2402	U
25	A	2403	C
25	A	2406	A
25	A	2429	G
25	A	2430	A
25	A	2435	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	2441	U
25	A	2445	2MG
25	A	2448	A
25	A	2464	G
25	A	2470	G
25	A	2476	A
25	A	2484	G
25	A	2494	G
25	A	2502	G
25	A	2505	G
25	A	2506	U
25	A	2513	A
25	A	2518	A
25	A	2519	U
25	A	2520	C
25	A	2535	G
25	A	2542	A
25	A	2547	A
25	A	2554	U
25	A	2567	G
25	A	2569	G
25	A	2572	A
25	A	2573	C
25	A	2585	U
25	A	2586	U
25	A	2602	A
25	A	2603	G
25	A	2609	U
25	A	2610	C
25	A	2611	C
25	A	2613	U
25	A	2615	U
25	A	2621	G
25	A	2629	U
25	A	2630	G
25	A	2634	A
25	A	2646	C
25	A	2663	G
25	A	2682	A
25	A	2689	U
25	A	2690	U
25	A	2707	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	2713	U
25	A	2714	G
25	A	2716	C
25	A	2718	G
25	A	2720	U
25	A	2722	G
25	A	2729	G
25	A	2732	G
25	A	2733	A
25	A	2744	G
25	A	2748	A
25	A	2755	C
25	A	2764	A
25	A	2765	A
25	A	2766	A
25	A	2769	U
25	A	2778	A
25	A	2791	G
25	A	2793	C
25	A	2794	C
25	A	2798	U
25	A	2800	A
25	A	2801	G
25	A	2809	A
25	A	2818	U
25	A	2820	A
25	A	2821	A
25	A	2832	U
25	A	2833	U
25	A	2834	G
25	A	2849	U
25	A	2867	G
25	A	2868	A
25	A	2872	A
25	A	2873	A
25	A	2880	C
25	A	2883	A
25	A	2887	A
25	A	2891	U
25	A	2894	G
25	A	2902	C
26	B	4	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	B	9	G
26	B	12	C
26	B	13	G
26	B	24	G
26	B	25	U
26	B	26	C
26	B	35	C
26	B	40	U
26	B	41	G
26	B	44	G
26	B	67	G
26	B	68	C
26	B	87	U
26	B	88	C
26	B	89	U
26	B	90	C
26	B	97	C
26	B	109	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	51	G
25	A	205	G
25	A	228	C
25	A	372	G
25	A	512	G
25	A	555	G
25	A	758	C
25	A	774	G
25	A	989	G
25	A	1070	A
25	A	1111	A
25	A	1182	G
25	A	1190	G
25	A	1212	G
25	A	1236	G
25	A	1240	U
25	A	1432	G
25	A	1458	U
25	A	1567	G
25	A	1715	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	1900	A
25	A	1930	G
25	A	1940	U
25	A	2061	G
25	A	2128	G
25	A	2326	C
25	A	2391	G
25	A	2447	G
25	A	2566	A
25	A	2610	C
25	A	2800	A
25	A	2820	A
25	A	2832	U
25	A	2867	G
26	B	24	G
26	B	66	A
26	B	88	C

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

43 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
25	6MZ	A	1618	25	17,25,26	1.04	1 (5%)	15,36,39	2.79	2 (13%)
25	2MG	A	1835	25	18,26,27	0.87	2 (11%)	21,38,41	2.23	7 (33%)
25	PSU	A	1911	25	15,21,22	1.53	4 (26%)	16,30,33	2.08	3 (18%)
25	3TD	A	1915	25	15,22,23	3.06	5 (33%)	17,32,35	1.83	3 (17%)
25	PSU	A	1917	25	15,21,22	1.50	4 (26%)	16,30,33	2.03	3 (18%)
25	5MU	A	1939	25	13,22,23	0.92	1 (7%)	16,32,35	2.04	2 (12%)
25	5MC	A	1962	25	14,22,23	1.12	1 (7%)	17,32,35	1.36	2 (11%)
25	6MZ	A	2030	25	17,25,26	1.05	1 (5%)	15,36,39	2.62	2 (13%)
25	G7M	A	2069	25	18,26,27	1.17	2 (11%)	21,39,42	2.50	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	OMG	A	2251	25,22	18,26,27	1.00	2 (11%)	21,38,41	1.85	4 (19%)
25	2MG	A	2445	25	18,26,27	0.99	2 (11%)	21,38,41	2.20	5 (23%)
25	H2U	A	2449	25	17,21,22	1.36	4 (23%)	23,30,33	2.10	5 (21%)
25	PSU	A	2457	25	15,21,22	2.10	4 (26%)	16,30,33	2.39	4 (25%)
25	OMC	A	2498	25	15,22,23	0.99	2 (13%)	20,31,34	1.25	1 (5%)
25	2MA	A	2503	25	17,25,26	1.45	3 (17%)	18,37,40	3.57	1 (5%)
25	PSU	A	2504	25	15,21,22	1.65	2 (13%)	16,30,33	2.30	4 (25%)
25	OMU	A	2552	25	14,22,23	0.72	1 (7%)	19,31,34	1.58	1 (5%)
25	PSU	A	2580	25	15,21,22	1.65	4 (26%)	16,30,33	2.14	3 (18%)
25	PSU	A	2604	25	15,21,22	1.58	3 (20%)	16,30,33	2.68	4 (25%)
25	PSU	A	2605	25	15,21,22	1.41	4 (26%)	16,30,33	1.90	3 (18%)
25	1MG	A	745	25	17,26,27	1.48	2 (11%)	19,39,42	1.04	2 (10%)
25	PSU	A	746	25	15,21,22	1.72	3 (20%)	16,30,33	2.22	3 (18%)
25	5MU	A	747	25	13,22,23	0.71	1 (7%)	16,32,35	2.68	2 (12%)
25	PSU	A	955	25	15,21,22	1.56	5 (33%)	16,30,33	2.10	4 (25%)
1	2MG	a	1207	1	18,26,27	1.10	2 (11%)	21,38,41	2.21	8 (38%)
1	4OC	a	1402	1	15,23,24	0.75	0	21,32,35	1.64	3 (14%)
1	5MC	a	1407	1	14,22,23	1.16	1 (7%)	17,32,35	1.09	1 (5%)
1	UR3	a	1498	1	13,22,23	0.71	0	18,32,35	0.92	1 (5%)
1	2MG	a	1516	1	18,26,27	1.10	2 (11%)	21,38,41	2.22	5 (23%)
1	MA6	a	1518	1	18,26,27	1.01	1 (5%)	15,38,41	2.43	3 (20%)
1	MA6	a	1519	1	18,26,27	0.82	1 (5%)	15,38,41	2.44	4 (26%)
1	PSU	a	516	1	15,21,22	1.42	3 (20%)	16,30,33	2.25	3 (18%)
1	G7M	a	527	1	18,26,27	1.14	2 (11%)	21,39,42	2.52	8 (38%)
1	2MG	a	966	1	18,26,27	1.08	2 (11%)	21,38,41	2.40	6 (28%)
1	5MC	a	967	1	14,22,23	1.23	1 (7%)	17,32,35	0.94	1 (5%)
22	H2U	v	20	22	17,21,22	1.01	2 (11%)	23,30,33	1.71	4 (17%)
22	5MU	v	54	22	13,22,23	0.62	1 (7%)	16,32,35	2.89	2 (12%)
22	PSU	v	55	22	15,21,22	1.23	2 (13%)	16,30,33	2.26	4 (25%)
22	4SU	v	8	22	12,21,22	0.78	0	15,30,33	1.00	1 (6%)
24	H2U	y	19	24	17,21,22	1.04	2 (11%)	23,30,33	1.29	4 (17%)
24	6IA	y	37	24	20,29,30	1.01	2 (10%)	22,41,44	2.24	4 (18%)
24	5MU	y	54	24	13,22,23	0.57	0	16,32,35	2.94	2 (12%)
24	PSU	y	55	24	15,21,22	1.56	3 (20%)	16,30,33	2.46	4 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	6MZ	A	1618	25	-	0/5/27/28	0/3/3/3
25	2MG	A	1835	25	-	0/5/27/28	0/3/3/3
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	3TD	A	1915	25	-	0/7/25/26	0/2/2/2
25	PSU	A	1917	25	-	0/7/25/26	0/2/2/2
25	5MU	A	1939	25	-	0/3/25/26	0/2/2/2
25	5MC	A	1962	25	-	0/3/25/26	0/2/2/2
25	6MZ	A	2030	25	-	0/5/27/28	0/3/3/3
25	G7M	A	2069	25	2/2/5/5	0/3/25/26	0/3/3/3
25	OMG	A	2251	25,22	-	0/5/27/28	0/3/3/3
25	2MG	A	2445	25	-	0/5/27/28	0/3/3/3
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	OMC	A	2498	25	-	0/5/27/28	0/2/2/2
25	2MA	A	2503	25	-	0/3/25/26	0/3/3/3
25	PSU	A	2504	25	-	0/7/25/26	0/2/2/2
25	OMU	A	2552	25	-	0/5/27/28	0/2/2/2
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	1MG	A	745	25	-	0/3/25/26	0/3/3/3
25	PSU	A	746	25	-	0/7/25/26	0/2/2/2
25	5MU	A	747	25	-	0/3/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	0/3/25/26	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/3/25/26	0/2/2/2
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
22	5MU	v	54	22	-	0/3/25/26	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	4SU	v	8	22	-	0/3/25/26	0/2/2/2
24	H2U	y	19	24	-	0/7/38/39	0/2/2/2
24	6IA	y	37	24	-	0/9/31/32	0/3/3/3
24	5MU	y	54	24	-	0/3/25/26	0/2/2/2
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2457	PSU	C5-C1'	-6.68	1.46	1.52
25	A	746	PSU	C5-C1'	-5.19	1.47	1.52
25	A	2504	PSU	C5-C1'	-5.13	1.47	1.52
24	y	55	PSU	C5-C1'	-4.90	1.48	1.52
25	A	2604	PSU	C5-C1'	-4.59	1.48	1.52
25	A	2580	PSU	C5-C1'	-4.57	1.48	1.52
25	A	1911	PSU	C5-C1'	-4.46	1.48	1.52
25	A	1917	PSU	C5-C1'	-4.20	1.48	1.52
1	a	516	PSU	C5-C1'	-4.06	1.48	1.52
25	A	955	PSU	C5-C1'	-3.67	1.49	1.52
25	A	2605	PSU	C5-C1'	-3.62	1.49	1.52
25	A	2449	H2U	C4-N3	-3.25	1.32	1.37
22	v	55	PSU	C5-C1'	-3.15	1.49	1.52
25	A	1915	3TD	O4-C4	-3.04	1.16	1.24
25	A	2449	H2U	C2-N3	-2.81	1.32	1.38
25	A	1939	5MU	C2-N3	-2.77	1.32	1.38
25	A	2457	PSU	C2-N3	-2.71	1.32	1.38
24	y	19	H2U	C4-N3	-2.67	1.33	1.37
25	A	2069	G7M	O2'-C2'	-2.59	1.36	1.43
25	A	2580	PSU	O4'-C1'	-2.54	1.40	1.44
25	A	955	PSU	C2-N1	-2.54	1.32	1.38
22	v	55	PSU	C2-N3	-2.53	1.32	1.38
22	v	20	H2U	C2-N3	-2.52	1.33	1.38
24	y	19	H2U	C2-N3	-2.50	1.33	1.38
25	A	2580	PSU	C2-N1	-2.46	1.33	1.38
25	A	955	PSU	C2-N3	-2.45	1.33	1.38
25	A	2605	PSU	C2-N3	-2.43	1.33	1.38
1	a	527	G7M	O2'-C2'	-2.41	1.37	1.43
25	A	746	PSU	O4'-C1'	-2.39	1.40	1.44
25	A	1917	PSU	O4'-C1'	-2.28	1.40	1.44
25	A	2604	PSU	C2-N3	-2.28	1.33	1.38
25	A	2580	PSU	C2-N3	-2.27	1.33	1.38
25	A	2504	PSU	C2-N3	-2.27	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	747	5MU	C2-N3	-2.27	1.33	1.38
25	A	2457	PSU	O4'-C1'	-2.26	1.40	1.44
25	A	1917	PSU	C2-N1	-2.26	1.33	1.38
25	A	2449	H2U	C2-N1	-2.23	1.32	1.35
25	A	2605	PSU	O4'-C1'	-2.23	1.41	1.44
25	A	2498	OMC	C6-N1	-2.23	1.32	1.35
25	A	1911	PSU	O4'-C1'	-2.22	1.41	1.44
25	A	2457	PSU	C2-N1	-2.21	1.33	1.38
25	A	2449	H2U	C6-N1	-2.20	1.44	1.47
1	a	516	PSU	C2-N3	-2.18	1.33	1.38
25	A	955	PSU	O4'-C1'	-2.15	1.41	1.44
25	A	2604	PSU	C2-N1	-2.14	1.33	1.38
25	A	1917	PSU	C2-N3	-2.14	1.33	1.38
22	v	20	H2U	C4-N3	-2.14	1.34	1.37
25	A	955	PSU	C2'-C1'	-2.12	1.51	1.53
25	A	1911	PSU	C2-N3	-2.11	1.33	1.38
25	A	746	PSU	C2-N1	-2.10	1.33	1.38
25	A	1911	PSU	C2-N1	-2.10	1.33	1.38
24	y	37	6IA	C2'-C1'	-2.10	1.50	1.53
24	y	55	PSU	C2-N3	-2.06	1.33	1.38
25	A	2605	PSU	C2-N1	-2.05	1.33	1.38
25	A	2498	OMC	C2-N3	-2.05	1.33	1.38
1	a	516	PSU	C2-N1	-2.04	1.33	1.38
24	y	55	PSU	O4'-C1'	-2.03	1.41	1.44
22	v	54	5MU	C2-N3	-2.01	1.34	1.38
25	A	2552	OMU	C2-N3	-2.00	1.34	1.38
25	A	1835	2MG	C5-C4	2.31	1.45	1.40
25	A	2445	2MG	C5-C4	2.40	1.45	1.40
1	a	1519	MA6	C5-C4	2.47	1.46	1.40
25	A	2251	OMG	C5-C4	2.48	1.46	1.40
1	a	966	2MG	C5-C4	2.59	1.46	1.40
25	A	1835	2MG	C6-C5	2.60	1.46	1.41
25	A	2503	2MA	C5-C4	2.66	1.46	1.40
1	a	1516	2MG	C5-C4	2.72	1.46	1.40
24	y	37	6IA	C5-C4	2.81	1.46	1.40
1	a	1518	MA6	C5-C4	2.90	1.47	1.40
25	A	2069	G7M	C6-C5	2.94	1.47	1.41
1	a	1207	2MG	C5-C4	2.99	1.47	1.40
25	A	2445	2MG	C6-C5	3.05	1.47	1.41
25	A	2251	OMG	C6-C5	3.08	1.47	1.41
1	a	1207	2MG	C6-C5	3.18	1.47	1.41
1	a	966	2MG	C6-C5	3.24	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	527	G7M	C6-C5	3.34	1.48	1.41
25	A	2503	2MA	C6-N6	3.34	1.35	1.29
1	a	1516	2MG	C6-C5	3.47	1.48	1.41
25	A	2030	6MZ	C5-C4	3.57	1.48	1.40
25	A	1618	6MZ	C5-C4	3.63	1.48	1.40
25	A	1962	5MC	C5-C4	3.65	1.47	1.41
25	A	745	1MG	C5-C4	3.65	1.48	1.40
1	a	1407	5MC	C5-C4	3.68	1.47	1.41
25	A	2503	2MA	C6-C5	3.84	1.47	1.40
1	a	967	5MC	C5-C4	4.14	1.47	1.41
25	A	745	1MG	C6-C5	4.21	1.49	1.40
25	A	1915	3TD	C4-N3	4.74	1.45	1.38
25	A	1915	3TD	C2-N1	4.93	1.48	1.38
25	A	1915	3TD	C6-N1	5.14	1.45	1.34
25	A	1915	3TD	C6-C5	7.17	1.48	1.38

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	54	5MU	C5-C4-N3	-8.65	118.08	125.35
22	v	54	5MU	C5-C4-N3	-8.37	118.32	125.35
25	A	747	5MU	C5-C4-N3	-7.60	118.97	125.35
25	A	1618	6MZ	N3-C2-N1	-7.37	123.08	128.87
25	A	2449	H2U	C5-C6-N1	-7.24	102.83	110.76
1	a	1519	MA6	N3-C2-N1	-7.13	123.27	128.87
1	a	1518	MA6	N3-C2-N1	-6.88	123.47	128.87
24	y	37	6IA	N3-C2-N1	-6.27	123.95	128.87
25	A	2030	6MZ	N3-C2-N1	-6.27	123.95	128.87
25	A	1939	5MU	C5-C4-N3	-6.11	120.22	125.35
25	A	2069	G7M	C5-C6-N1	-5.88	115.84	123.52
22	v	20	H2U	C5-C6-N1	-5.72	104.50	110.76
25	A	2457	PSU	C5-C1'-C2'	-5.38	106.30	115.44
25	A	2604	PSU	C5-C1'-C2'	-5.38	106.30	115.44
25	A	1915	3TD	C5-C1'-C2'	-5.37	106.32	115.44
1	a	527	G7M	C5-C6-N1	-5.13	116.81	123.52
25	A	2251	OMG	C5-C6-N1	-4.39	117.79	123.52
1	a	1402	4OC	CM4-N4-C4	-4.36	119.19	122.87
24	y	55	PSU	C5-C1'-C2'	-4.34	108.07	115.44
25	A	2504	PSU	C5-C1'-C2'	-4.33	108.08	115.44
25	A	2457	PSU	C5-C6-N1	-4.33	118.35	124.38
25	A	2449	H2U	C4-N3-C2	-4.25	121.92	125.77
1	a	1207	2MG	C5-C6-N1	-4.10	118.17	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1516	2MG	C5-C6-N1	-4.06	118.22	123.52
25	A	746	PSU	C5-C6-N1	-3.95	118.87	124.38
25	A	2445	2MG	C5-C6-N1	-3.93	118.38	123.52
24	y	55	PSU	C5-C6-N1	-3.93	118.90	124.38
25	A	1835	2MG	C6-C5-C4	-3.89	116.42	120.86
25	A	746	PSU	C5-C1'-C2'	-3.85	108.91	115.44
25	A	2504	PSU	C5-C6-N1	-3.83	119.04	124.38
1	a	966	2MG	C5-C6-N1	-3.60	118.82	123.52
25	A	2605	PSU	C5-C6-N1	-3.58	119.39	124.38
25	A	2445	2MG	CM2-N2-C2	-3.53	119.06	123.03
24	y	37	6IA	C12-N6-C6	-3.52	119.39	123.46
1	a	966	2MG	C6-C5-C4	-3.51	116.84	120.86
25	A	1911	PSU	C5-C6-N1	-3.51	119.49	124.38
1	a	1518	MA6	C10-N6-C9	-3.44	104.74	115.96
22	v	55	PSU	C5-C6-N1	-3.36	119.70	124.38
22	v	20	H2U	C4-N3-C2	-3.35	122.73	125.77
1	a	1516	2MG	C6-C5-C4	-3.33	117.05	120.86
25	A	1917	PSU	C5-C6-N1	-3.29	119.79	124.38
1	a	1516	2MG	CM2-N2-C2	-3.16	119.48	123.03
1	a	516	PSU	C5-C6-N1	-3.14	120.00	124.38
22	v	8	4SU	C5-C4-N3	-3.14	120.23	123.56
25	A	2251	OMG	N3-C2-N1	-3.11	123.32	127.56
1	a	527	G7M	N3-C2-N1	-3.10	123.35	127.56
25	A	2580	PSU	C5-C6-N1	-3.08	120.08	124.38
25	A	1835	2MG	C5-C6-N1	-3.07	119.51	123.52
1	a	966	2MG	N3-C2-N1	-3.06	121.61	126.19
1	a	1207	2MG	C6-C5-C4	-3.02	117.41	120.86
25	A	2604	PSU	C5-C6-N1	-3.00	120.19	124.38
25	A	2445	2MG	C6-C5-C4	-3.00	117.43	120.86
25	A	1915	3TD	C5-C6-N1	-2.98	120.23	124.38
1	a	1519	MA6	C10-N6-C9	-2.92	106.43	115.96
25	A	2251	OMG	C6-C5-C4	-2.80	117.65	120.86
25	A	745	1MG	C6-C5-C4	-2.79	117.93	119.93
25	A	1962	5MC	CM5-C5-C4	-2.79	118.52	121.47
25	A	2069	G7M	N3-C2-N1	-2.73	123.85	127.56
25	A	1835	2MG	CM2-N2-C2	-2.68	120.02	123.03
25	A	955	PSU	C5-C6-N1	-2.66	120.67	124.38
24	y	19	H2U	C4-N3-C2	-2.63	123.38	125.77
25	A	1835	2MG	N3-C2-N1	-2.49	122.46	126.19
22	v	55	PSU	C5-C1'-C2'	-2.36	111.43	115.44
1	a	527	G7M	C4'-O4'-C1'	-2.35	107.16	109.64
1	a	1207	2MG	CM2-N2-C2	-2.33	120.41	123.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1519	MA6	C1'-N9-C4	-2.29	124.25	126.81
25	A	955	PSU	O2'-C2'-C1'	-2.27	107.00	111.93
24	y	37	6IA	C2'-C1'-N9	-2.24	107.48	113.47
24	y	19	H2U	C5-C6-N1	-2.22	108.33	110.76
1	a	1207	2MG	N3-C2-N1	-2.08	123.07	126.19
25	A	745	1MG	C1'-N9-C4	-2.07	124.50	126.81
25	A	2449	H2U	O2-C2-N1	-2.01	120.54	123.17
25	A	2449	H2U	C6-N1-C2	2.07	125.36	122.16
1	a	1207	2MG	C1'-N9-C4	2.12	129.17	126.81
25	A	2449	H2U	C1'-N1-C2	2.16	121.21	118.19
1	a	966	2MG	N2-C2-N3	2.18	119.47	116.94
25	A	955	PSU	O4'-C1'-C2'	2.21	107.08	104.69
25	A	2605	PSU	O4'-C1'-C2'	2.24	107.11	104.69
25	A	1835	2MG	N2-C2-N3	2.32	119.64	116.94
22	v	20	H2U	C6-N1-C2	2.33	125.76	122.16
1	a	1498	UR3	C3U-N3-C4	2.34	121.48	118.21
1	a	1207	2MG	N2-C2-N3	2.40	119.73	116.94
24	y	19	H2U	C6-N1-C2	2.41	125.88	122.16
1	a	967	5MC	N4-C4-N3	2.43	120.48	116.92
25	A	2604	PSU	O4'-C1'-C2'	2.44	107.33	104.69
22	v	20	H2U	C5-C4-N3	2.50	119.26	116.62
25	A	1911	PSU	O4'-C1'-C2'	2.62	107.52	104.69
25	A	2504	PSU	O4'-C1'-C2'	2.63	107.53	104.69
25	A	2069	G7M	O3'-C3'-C2'	2.65	120.41	111.86
25	A	2580	PSU	O4'-C1'-C2'	2.78	107.69	104.69
25	A	2457	PSU	O4'-C1'-C2'	2.78	107.70	104.69
24	y	55	PSU	O4'-C1'-C2'	2.79	107.71	104.69
25	A	1915	3TD	O4'-C1'-C2'	2.80	107.72	104.69
1	a	527	G7M	N7-C8-N9	2.82	112.84	108.67
1	a	1407	5MC	N4-C4-N3	2.86	121.11	116.92
25	A	1917	PSU	O4'-C1'-C2'	2.86	107.78	104.69
1	a	1402	4OC	C6-C5-C4	2.89	118.56	117.42
24	y	19	H2U	N3-C2-N1	2.92	119.35	116.64
22	v	55	PSU	O4'-C1'-C2'	3.07	108.01	104.69
1	a	516	PSU	O4'-C1'-C2'	3.07	108.01	104.69
25	A	2069	G7M	C1'-N9-C4	3.11	130.28	126.81
25	A	1962	5MC	N4-C4-N3	3.18	121.58	116.92
1	a	527	G7M	O3'-C3'-C2'	3.25	122.36	111.86
25	A	2069	G7M	N7-C8-N9	3.26	113.50	108.67
25	A	2069	G7M	O3'-C3'-C4'	3.38	121.11	111.01
1	a	527	G7M	O3'-C3'-C4'	3.45	121.30	111.01
1	a	527	G7M	C1'-N9-C4	3.88	131.14	126.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2498	OMC	C6-C5-C4	4.19	119.08	117.44
1	a	1402	4OC	C2-N3-C4	4.36	120.97	115.43
25	A	2445	2MG	C6-N1-C2	4.48	121.66	115.24
1	a	1519	MA6	C2-N1-C6	4.49	122.24	111.64
25	A	1835	2MG	C6-N1-C2	4.53	121.73	115.24
1	a	1518	MA6	C2-N1-C6	4.55	122.38	111.64
1	a	1516	2MG	C6-N1-C2	4.60	121.83	115.24
25	A	1939	5MU	C4-N3-C2	4.83	119.19	115.16
1	a	1207	2MG	C6-N1-C2	4.88	122.22	115.24
1	a	966	2MG	C6-N1-C2	4.90	122.26	115.24
25	A	2251	OMG	C6-N1-C2	5.31	122.11	115.88
1	a	527	G7M	C6-N1-C2	5.40	122.21	115.88
1	a	1207	2MG	C2-N3-C4	5.41	120.92	114.99
25	A	2457	PSU	C4-N3-C2	5.44	119.70	115.16
25	A	2605	PSU	C4-N3-C2	5.57	119.81	115.16
1	a	1516	2MG	C2-N3-C4	5.72	121.26	114.99
25	A	2445	2MG	C2-N3-C4	5.76	121.31	114.99
25	A	1835	2MG	C2-N3-C4	5.97	121.53	114.99
25	A	2069	G7M	C6-N1-C2	6.02	122.93	115.88
25	A	2552	OMU	C4-N3-C2	6.18	120.72	114.21
25	A	2504	PSU	C4-N3-C2	6.26	120.38	115.16
25	A	1917	PSU	C4-N3-C2	6.35	120.45	115.16
25	A	746	PSU	C4-N3-C2	6.43	120.52	115.16
25	A	1911	PSU	C4-N3-C2	6.44	120.53	115.16
24	y	37	6IA	C2-N1-C6	6.79	121.35	116.47
22	v	55	PSU	C4-N3-C2	6.85	120.88	115.16
24	y	55	PSU	C4-N3-C2	6.86	120.88	115.16
1	a	966	2MG	C2-N3-C4	7.01	122.67	114.99
25	A	2580	PSU	C4-N3-C2	7.04	121.03	115.16
25	A	955	PSU	C4-N3-C2	7.13	121.10	115.16
25	A	747	5MU	C4-N3-C2	7.25	121.20	115.16
25	A	2030	6MZ	C2-N1-C6	7.41	121.80	116.47
1	a	516	PSU	C4-N3-C2	7.45	121.37	115.16
22	v	54	5MU	C4-N3-C2	7.53	121.44	115.16
24	y	54	5MU	C4-N3-C2	7.62	121.52	115.16
25	A	1618	6MZ	C2-N1-C6	7.65	121.97	116.47
25	A	2604	PSU	C4-N3-C2	7.89	121.74	115.16
25	A	2503	2MA	C2-N3-C4	14.80	122.42	115.29

All (4) chirality outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
-----	-------	-----	------	------

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4'
1	a	527	G7M	C3'
25	A	2069	G7M	C4'
25	A	2069	G7M	C3'

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1915	3TD	1	0
25	A	2030	6MZ	1	0
25	A	2251	OMG	1	0
25	A	2445	2MG	1	0
25	A	745	1MG	1	0
25	A	747	5MU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	y	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	5(A):A	O3'	6:U	P	3.00
1	y	47(Q):G	O3'	48:G	P	3.00
1	y	67(A):U	O3'	68:C	P	3.00
1	y	5:G	O3'	5(A):A	P	2.99
1	y	67:A	O3'	67(A):U	P	2.99
1	y	47:G	O3'	47(A):G	P	2.97