Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Dec 5, 2016 – 02:07 PM EST

PDB ID	:	5LZC
EMDB ID:	:	EMD-4123
Title	:	Structure of SelB-Sec-tRNASec bound to the 70S ribosome in the codon reading state (CR)
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	:	4.80 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 (i) symbol.

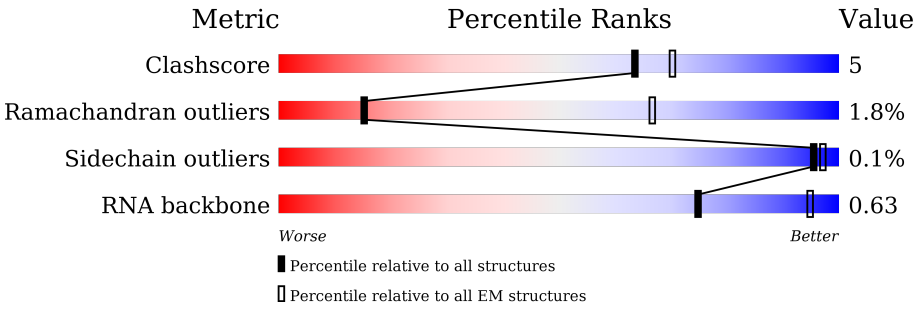
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.80 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 <=5%

Mol	Chain	Length	Quality of chain
1	a	1539	73% 25% .
2	b	218	95% .
3	c	206	97% .
4	d	205	96% .
5	e	157	97% .
6	f	100	89% 10% .
7	g	151	97% .
8	h	129	97% .

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Mol	Chain	Length	Quality of chain
9	i	127	94% 6%
10	j	98	93% 6%
11	k	116	97%
12	l	123	94% 5%
13	m	114	94% 6%
14	n	100	96%
15	o	88	94% 6%
16	p	82	96%
17	q	80	96%
18	r	65	92% 8%
19	s	79	97%
20	t	85	100%
21	u	65	94% 6%
22	v	77	68% 31%
23	x	48	38% 29% 33%
24	y	95	61% 35%
25	z	614	96%
26	A	2903	67% 27% 6%
27	B	120	73% 22%
28	C	271	85% 15%
29	D	209	79% 21%
30	E	201	85% 15%
31	F	177	80% 19%
32	G	176	66% 33%
33	I	141	67% 32%

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Mol	Chain	Length	Quality of chain
34	H	149	82% 17%
35	J	142	87% 13%
36	K	122	84% 16%
37	L	143	86% 13%
38	M	136	84% 16%
39	N	120	90% 10%
40	O	116	85% 15%
41	P	114	90% 10%
42	Q	117	85% 15%
43	R	103	83% 17%
44	S	110	90% 9%
45	T	93	82% 18%
46	U	102	80% 17%
47	V	94	91% 9%
48	W	75	84% 15%
49	X	77	91% 9%
50	Y	63	86% 14%
51	Z	58	81% 17%
52	0	56	93% 7%
53	1	50	88% 12%
54	2	46	83% 17%
55	3	64	89% 11%
56	4	38	76% 21%
57	6	66	79% 20%
58	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 criteria:

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

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 152981 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
			Total	C	N	O	P		
1	a	1539	33029	14738	6052	10700	1539	0	0

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

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

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

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

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

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

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

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

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

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

- 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 fMet-tRNAfMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	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 Sec-tRNASec.

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 protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	614	Total	C	N	O	S	0	0
			4853	3043	901	892	17		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2903	Total	C	N	O	P	0	0
			62335	27815	11467	20150	2903		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

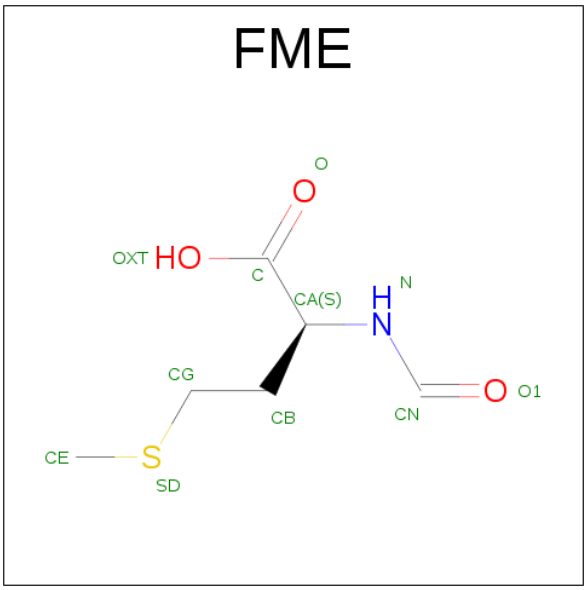
- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 58 is a RNA chain called CCA 3' end of E-site tRNASec (low occupancy).

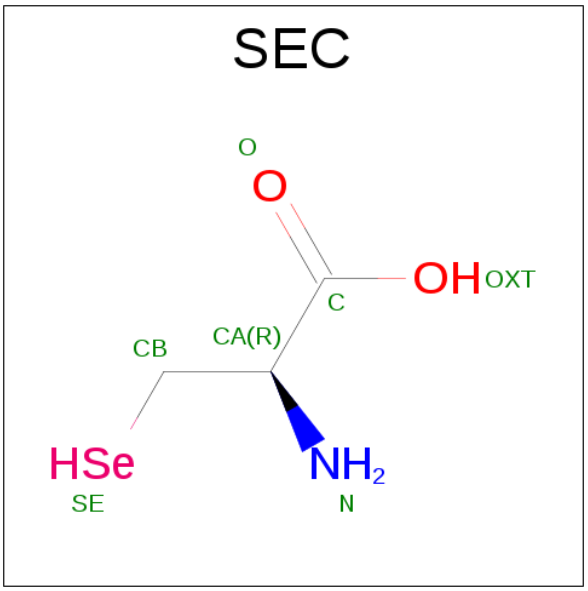
Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



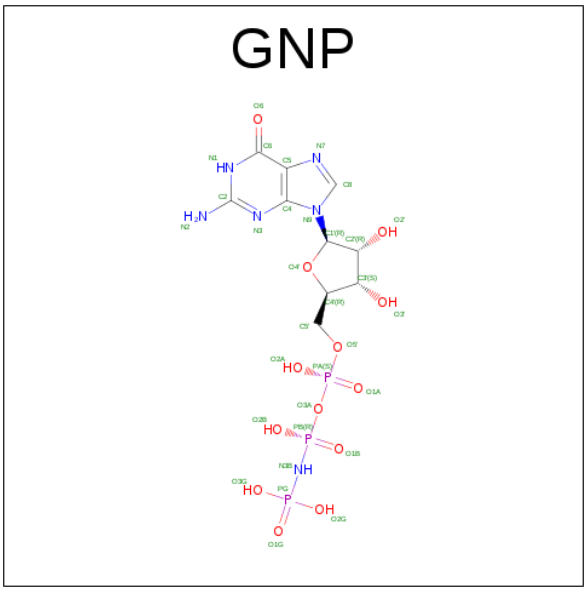
Mol	Chain	Residues	Atoms					AltConf
59	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is SELENOCYSTEINE (three-letter code: SEC) (formula: $C_3H_7NO_2Se$).



Mol	Chain	Residues	Atoms					AltConf
60	y	1	Total	C	N	O	Se	0
			6	3	1	1	1	

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
61	z	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
62	z	1	Total Mg 1 1	0

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
63	4	1	Total Zn 1 1	0
63	6	1	Total Zn 1 1	0

- Molecule 64 is water.

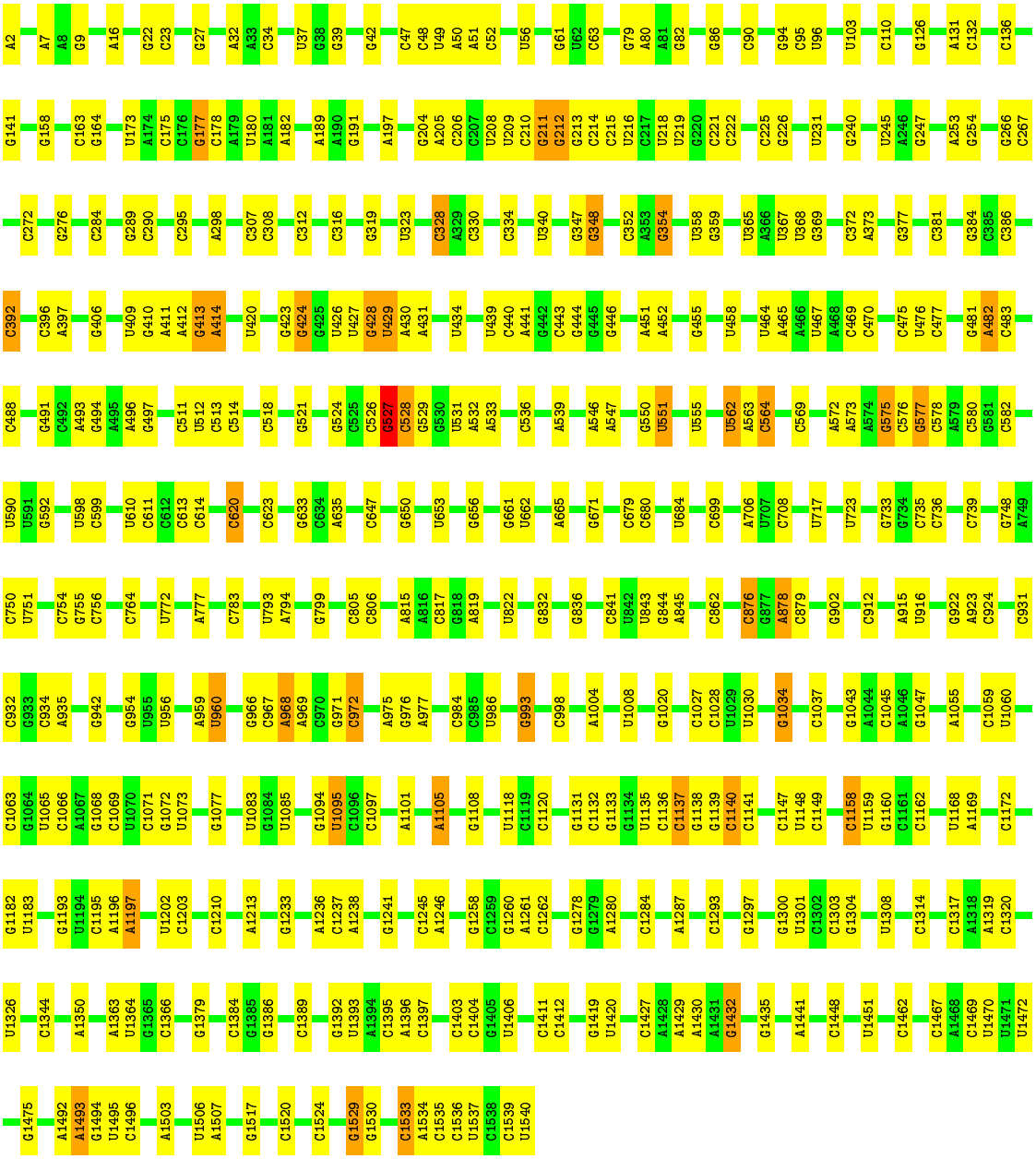
Mol	Chain	Residues	Atoms	AltConf
64	z	2	Total O 2 2	0

3 Residue-property plots (i)

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.

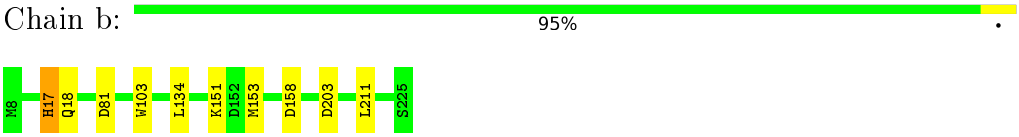
- Molecule 1: 16S ribosomal RNA

Chain a: 73% 25%



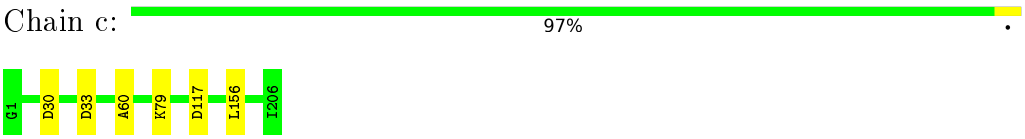
• Molecule 2: 30S ribosomal protein S2

Chain b:



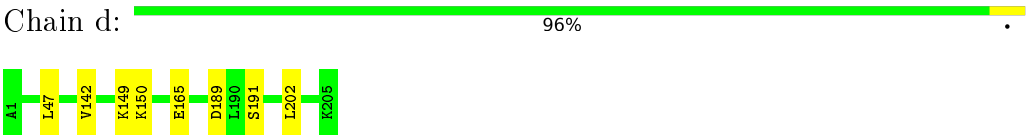
• Molecule 3: 30S ribosomal protein S3

Chain c:



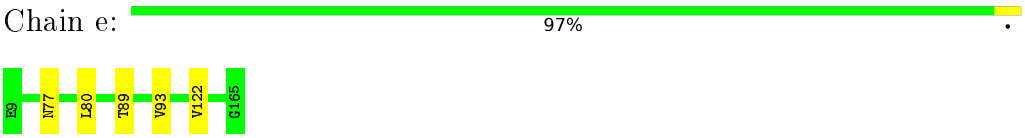
• Molecule 4: 30S ribosomal protein S4

Chain d:



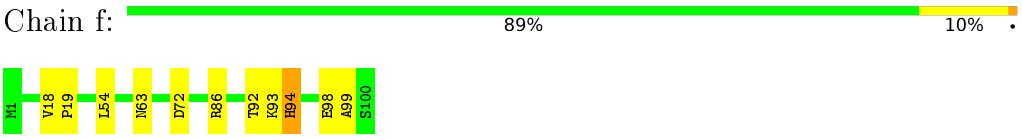
• Molecule 5: 30S ribosomal protein S5

Chain e:



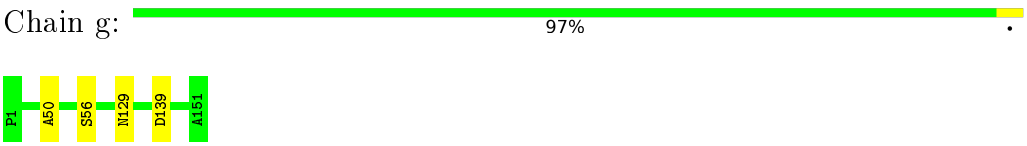
• Molecule 6: 30S ribosomal protein S6

Chain f:



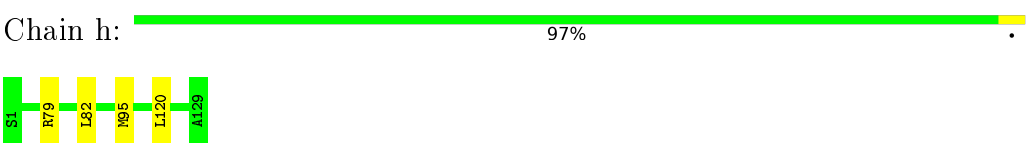
• Molecule 7: 30S ribosomal protein S7

Chain g:



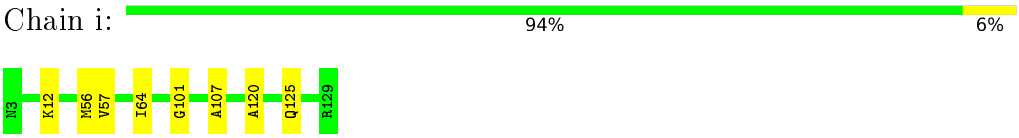
• Molecule 8: 30S ribosomal protein S8

Chain h:



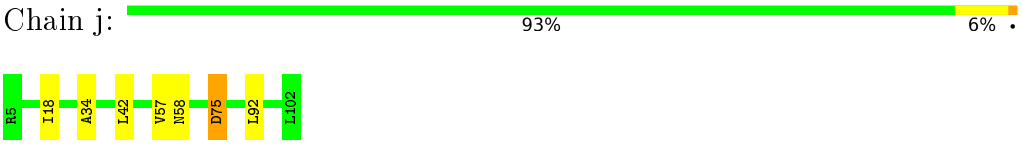
• Molecule 9: 30S ribosomal protein S9

Chain i:



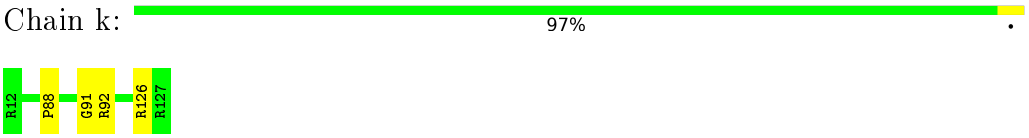
- Molecule 10: 30S ribosomal protein S10

Chain j:



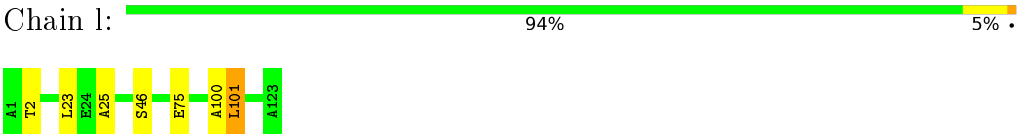
- Molecule 11: 30S ribosomal protein S11

Chain k:



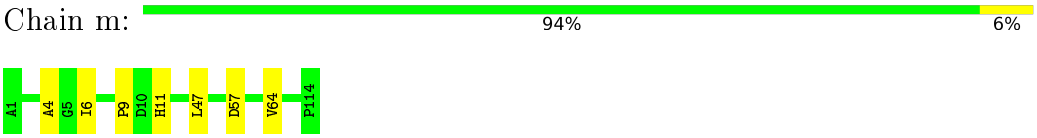
- Molecule 12: 30S ribosomal protein S12

Chain l:



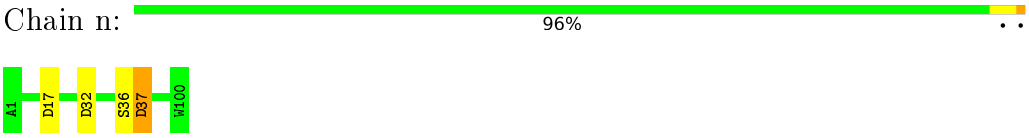
- Molecule 13: 30S ribosomal protein S13

Chain m:



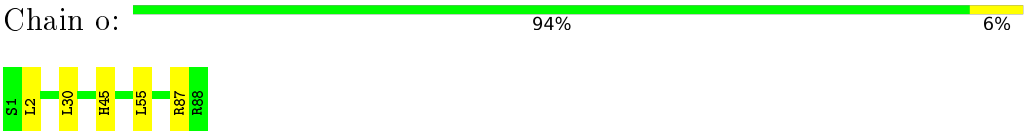
- Molecule 14: 30S ribosomal protein S14

Chain n:



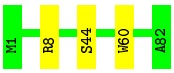
- Molecule 15: 30S ribosomal protein S15

Chain o:



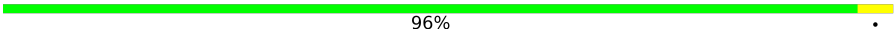
- Molecule 16: 30S ribosomal protein S16

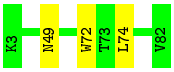
Chain p:



• Molecule 17: 30S ribosomal protein S17

Chain q:



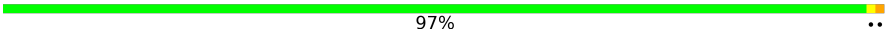


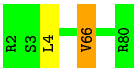
• Molecule 18: 30S ribosomal protein S18

Chain r:

• Molecule 19: 30S ribosomal protein S19

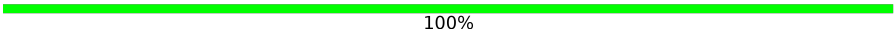
Chain s:





• Molecule 20: 30S ribosomal protein S20

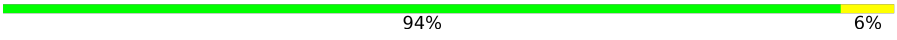
Chain t:

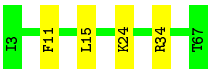


There are no outlier residues recorded for this chain.

• Molecule 21: 30S ribosomal protein S21

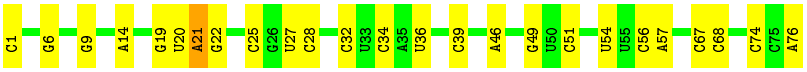
Chain u:





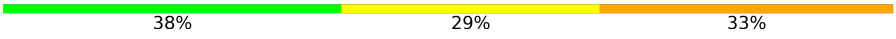
• Molecule 22: fMet-tRNAfMet

Chain v:



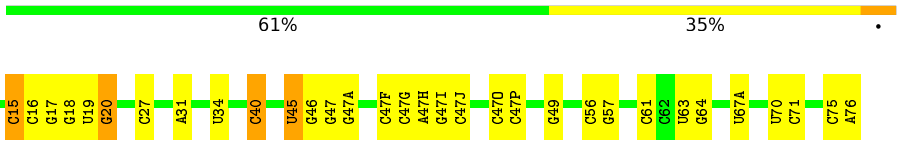
• Molecule 23: SECIS mRNA

Chain x:



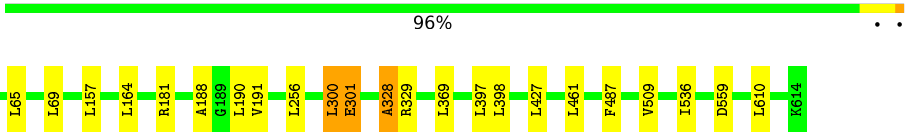
• Molecule 24: Sec-tRNASec

Chain y:



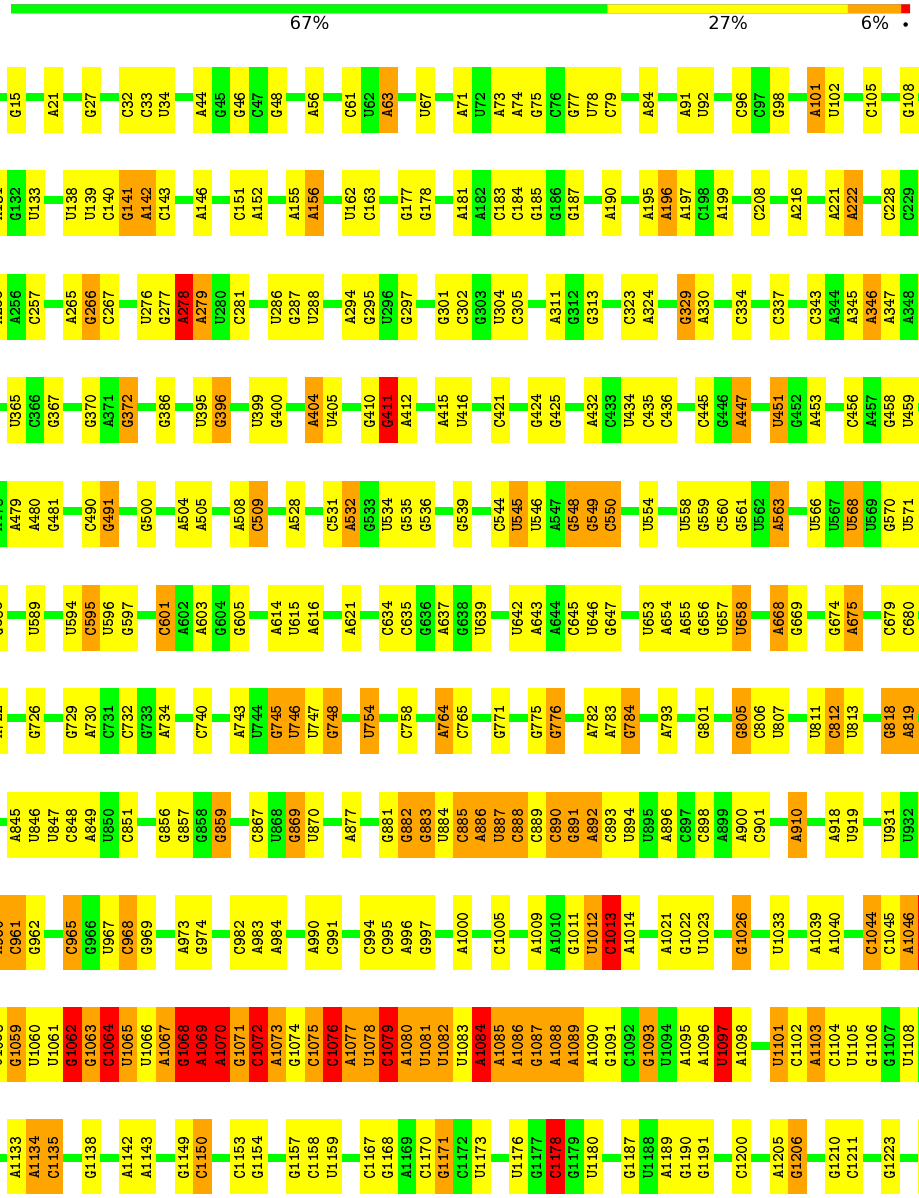
• Molecule 25: Selenocysteine-specific elongation factor

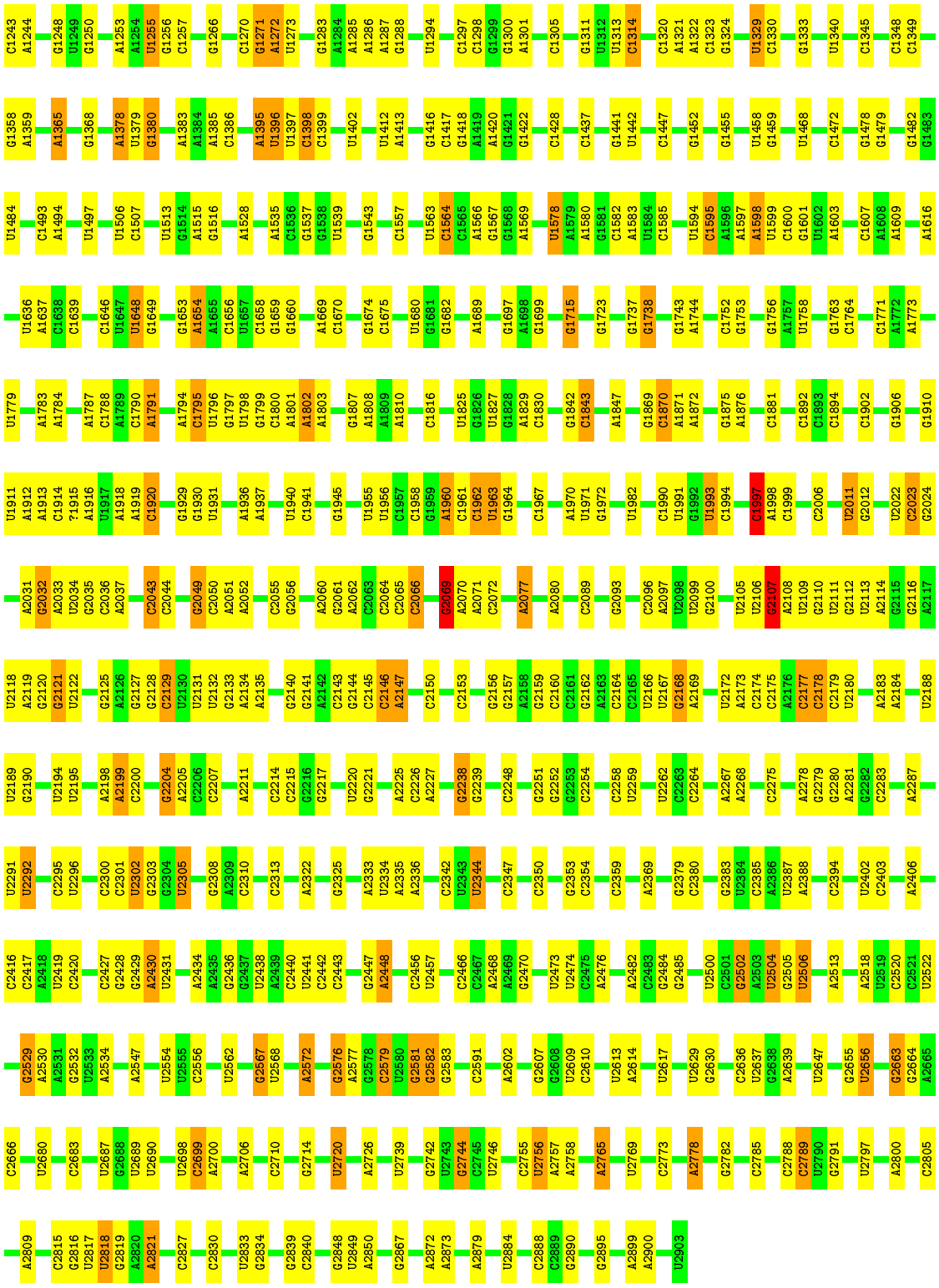
Chain z:



• Molecule 26: 23S ribosomal RNA

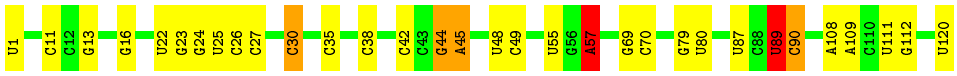
Chain A:





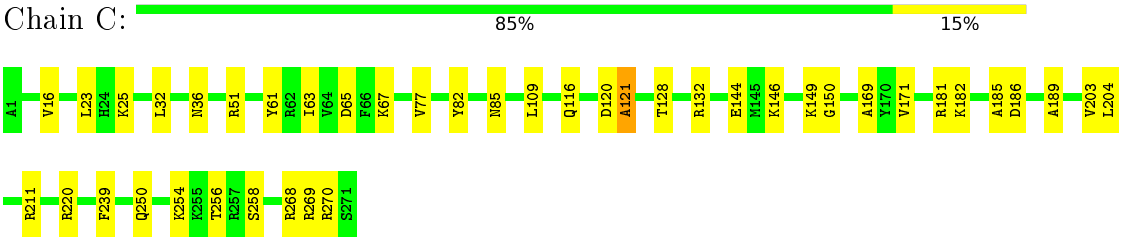
- Molecule 27: 5S ribosomal RNA

Chain B:



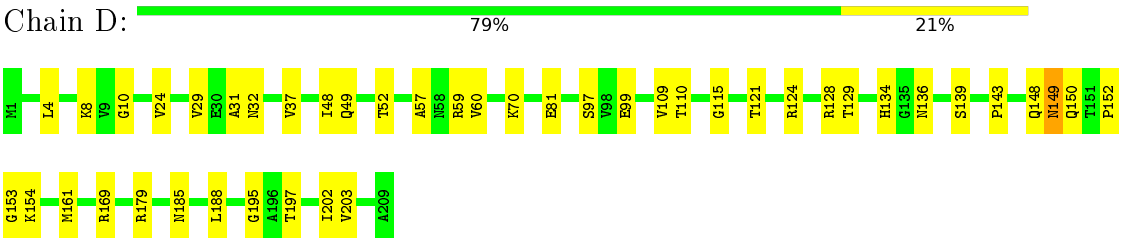
- Molecule 28: 50S ribosomal protein L2

Chain C:



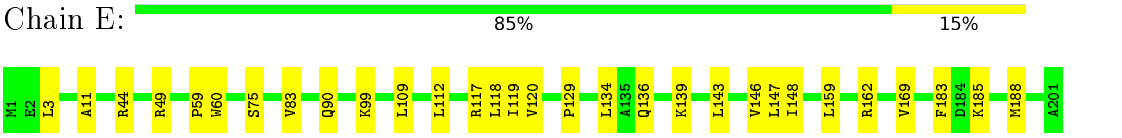
- Molecule 29: 50S ribosomal protein L3

Chain D:



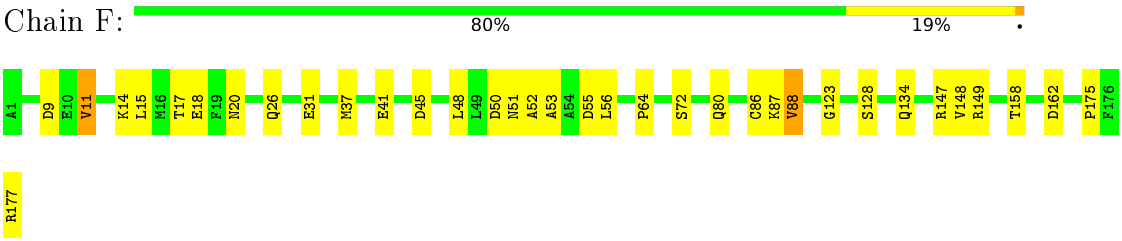
- Molecule 30: 50S ribosomal protein L4

Chain E:



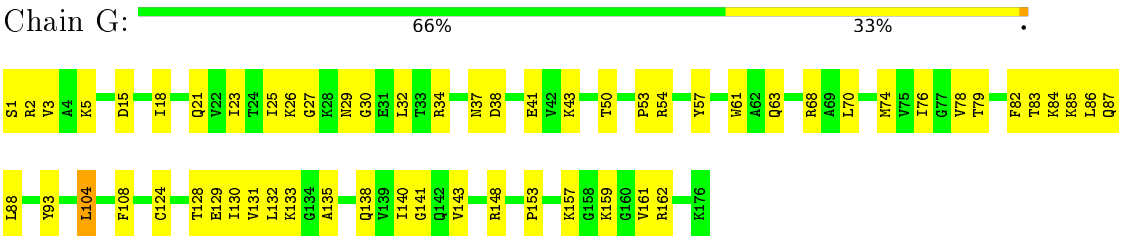
- Molecule 31: 50S ribosomal protein L5

Chain F:



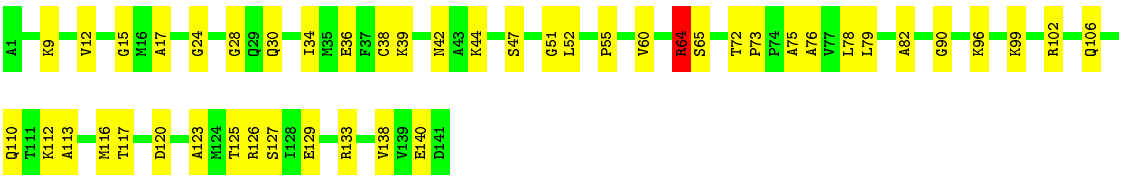
- Molecule 32: 50S ribosomal protein L6

Chain G:

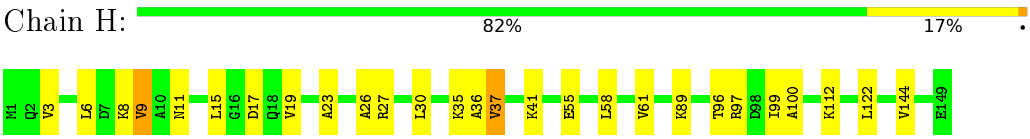


- Molecule 33: 50S ribosomal protein L11

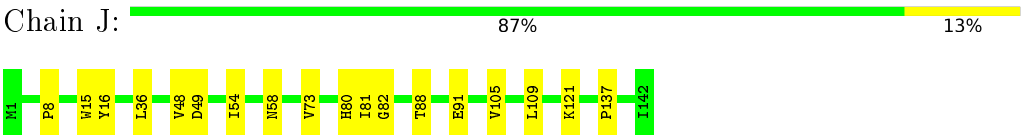
Chain I:



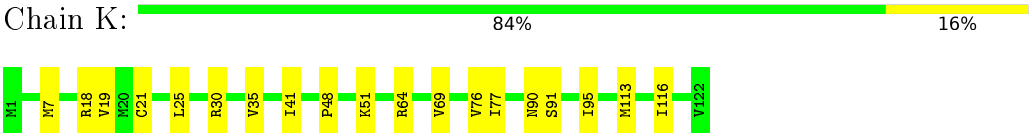
• Molecule 34: 50S ribosomal protein L9



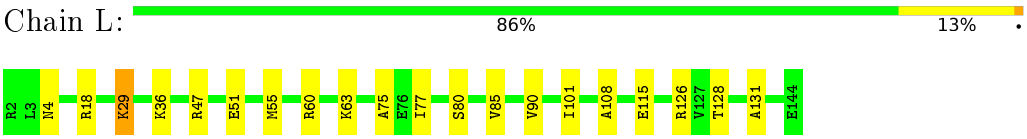
• Molecule 35: 50S ribosomal protein L13



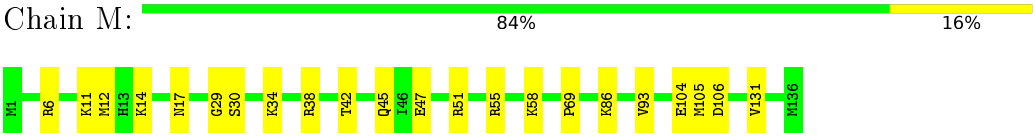
• Molecule 36: 50S ribosomal protein L14



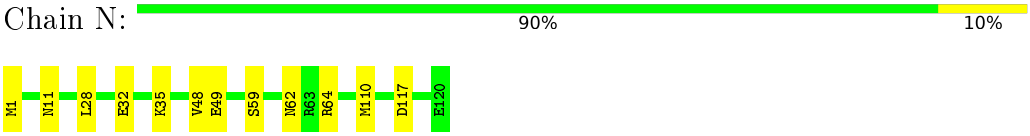
• Molecule 37: 50S ribosomal protein L15



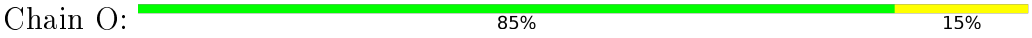
• Molecule 38: 50S ribosomal protein L16



• Molecule 39: 50S ribosomal protein L17



• Molecule 40: 50S ribosomal protein L18

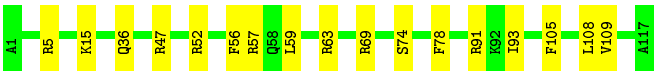


• Molecule 41: 50S ribosomal protein L19

Chain P:

• Molecule 42: 50S ribosomal protein L20

Chain Q:

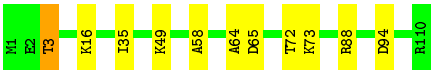


• Molecule 43: 50S ribosomal protein L21

Chain R:

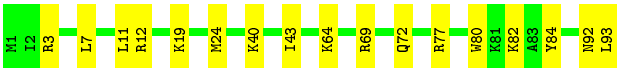
• Molecule 44: 50S ribosomal protein L22

Chain S:



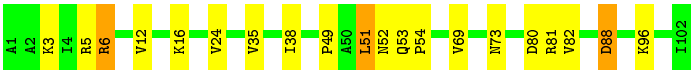
• Molecule 45: 50S ribosomal protein L23

Chain T:



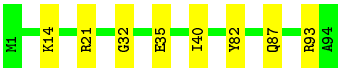
• Molecule 46: 50S ribosomal protein L24

Chain U:



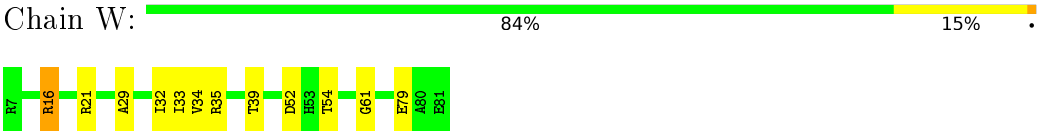
• Molecule 47: 50S ribosomal protein L25

Chain V:



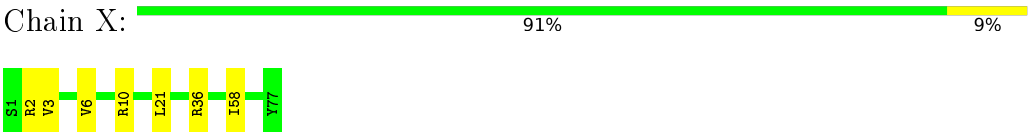
- Molecule 48: 50S ribosomal protein L27

Chain W:



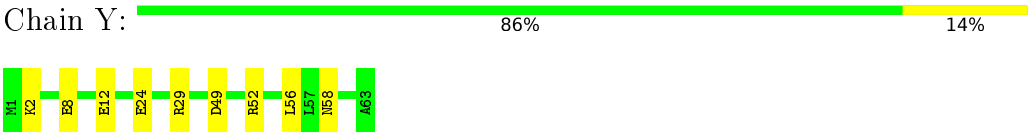
- Molecule 49: 50S ribosomal protein L28

Chain X:



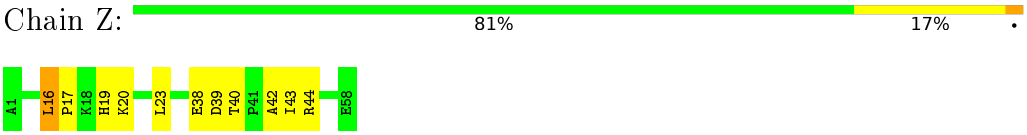
- Molecule 50: 50S ribosomal protein L29

Chain Y:



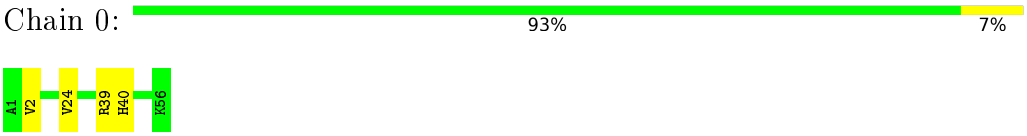
- Molecule 51: 50S ribosomal protein L30

Chain Z:



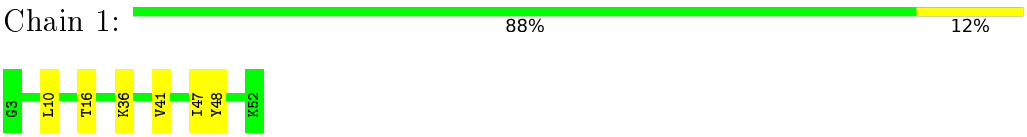
- Molecule 52: 50S ribosomal protein L32

Chain 0:



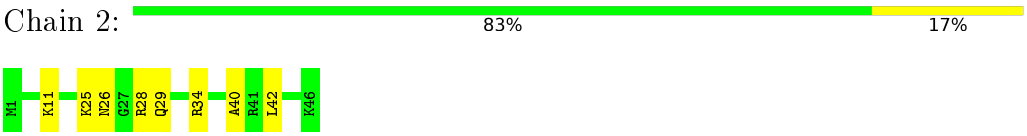
- Molecule 53: 50S ribosomal protein L33

Chain 1:



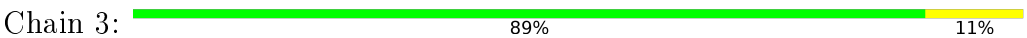
- Molecule 54: 50S ribosomal protein L34

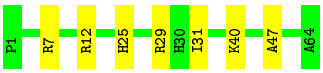
Chain 2:



- Molecule 55: 50S ribosomal protein L35

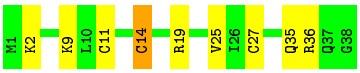
Chain 3:





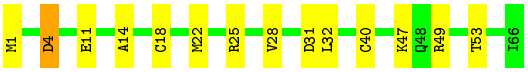
• Molecule 56: 50S ribosomal protein L36

Chain 4:



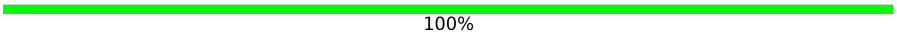
• Molecule 57: 50S ribosomal protein L31

Chain 6:



• Molecule 58: CCA 3' end of E-site tRNASec (low occupancy)

Chain w:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	11658	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 ($e^-/Å^2$)	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: GNP, MA6, 2MA, 2MG, 1MG, 3TD, G7M, SEC, UR3, 5MU, ZN, 6IA, 5MC, 6MZ, FME, OMC, MG, OMG, H2U, OMU, 4OC, 4SU, 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	0.60	4/36701 (0.0%)	1.38	560/57246 (1.0%)
10	j	0.45	0/797	0.91	2/1077 (0.2%)
11	k	0.54	0/886	0.86	0/1195
12	l	0.49	0/969	0.80	1/1300 (0.1%)
13	m	0.42	0/893	0.85	3/1193 (0.3%)
14	n	0.45	0/806	0.80	2/1074 (0.2%)
15	o	0.40	0/722	0.76	2/964 (0.2%)
16	p	0.52	0/659	0.86	1/884 (0.1%)
17	q	0.44	0/658	0.84	1/881 (0.1%)
18	r	0.38	0/512	0.84	1/689 (0.1%)
19	s	0.38	0/653	0.77	1/877 (0.1%)
2	b	0.49	0/1736	0.88	4/2338 (0.2%)
20	t	0.46	0/671	0.75	0/888
21	u	0.42	0/501	0.79	1/668 (0.1%)
22	v	0.65	1/1745 (0.1%)	1.47	33/2716 (1.2%)
23	x	0.92	2/1145 (0.2%)	1.88	45/1781 (2.5%)
24	y	0.70	1/2168 (0.0%)	1.52	35/3375 (1.0%)
25	z	0.50	0/4952	0.97	23/6712 (0.3%)
26	A	0.57	16/69240 (0.0%)	1.25	623/108014 (0.6%)
27	B	0.56	1/2873 (0.0%)	1.21	16/4478 (0.4%)
28	C	0.42	0/2122	0.75	1/2852 (0.0%)
29	D	0.47	0/1586	0.73	0/2134
3	c	0.41	0/1652	0.75	3/2225 (0.1%)
30	E	0.45	0/1571	0.74	1/2113 (0.0%)
31	F	0.54	1/1435 (0.1%)	0.85	3/1926 (0.2%)
32	G	0.55	0/1343	0.89	1/1816 (0.1%)
33	I	0.49	0/1046	0.96	2/1410 (0.1%)
34	H	0.41	0/1122	0.78	2/1515 (0.1%)
35	J	0.43	0/1152	0.66	0/1551
36	K	0.45	0/948	0.74	0/1268
37	L	0.43	0/1054	0.76	0/1403

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
38	M	0.42	0/1093	0.73	0/1460
39	N	0.45	0/974	0.68	0/1301
4	d	0.57	0/1665	0.98	4/2227 (0.2%)
40	O	0.43	0/902	0.73	2/1209 (0.2%)
41	P	0.45	0/929	0.68	0/1242
42	Q	0.42	0/960	0.63	1/1278 (0.1%)
43	R	0.45	0/829	0.76	0/1107
44	S	0.41	0/864	0.73	0/1156
45	T	0.46	0/745	0.78	0/994
46	U	0.46	0/788	0.86	3/1051 (0.3%)
47	V	0.44	0/766	0.73	1/1025 (0.1%)
48	W	0.39	0/582	0.72	0/769
49	X	0.36	0/635	0.74	2/848 (0.2%)
5	e	0.46	0/1170	0.86	1/1573 (0.1%)
50	Y	0.49	0/510	0.90	1/677 (0.1%)
51	Z	0.38	0/453	0.71	2/605 (0.3%)
52	0	0.36	0/450	0.76	0/599
53	1	0.35	0/417	0.75	0/554
54	2	0.43	0/380	0.75	0/498
55	3	0.41	0/513	0.70	1/676 (0.1%)
56	4	0.60	1/303 (0.3%)	0.86	1/397 (0.3%)
57	6	0.44	0/532	0.87	2/709 (0.3%)
58	w	0.41	0/68	1.01	0/103
6	f	0.52	1/836 (0.1%)	0.92	3/1128 (0.3%)
7	g	0.47	0/1196	0.79	1/1602 (0.1%)
8	h	0.46	0/989	0.83	4/1326 (0.3%)
9	i	0.48	0/1034	0.86	2/1375 (0.1%)
All	All	0.55	28/164901 (0.0%)	1.19	1398/246052 (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
12	l	0	2
14	n	0	2
18	r	0	1
2	b	0	1
25	z	0	2
26	A	2	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	C	0	1
34	H	0	1
46	U	0	1
6	f	0	1
9	i	0	2
All	All	4	14

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	1	U	OP3-P	-10.72	1.48	1.61
24	y	1	G	OP3-P	-10.71	1.48	1.61
26	A	1	G	OP3-P	-10.60	1.48	1.61
23	x	87	A	OP3-P	-10.53	1.48	1.61
22	v	1	C	OP3-P	-10.48	1.48	1.61
1	a	2	A	OP3-P	-10.45	1.48	1.61
26	A	571	U	C4-O4	9.54	1.31	1.23
1	a	723	U	C4-O4	-7.43	1.17	1.23
6	f	18	VAL	C-N	6.66	1.46	1.34
26	A	1071	G	C6-O6	-6.58	1.18	1.24
31	F	11	VAL	CB-CG1	-6.43	1.39	1.52
26	A	1963	U	C5-C6	-6.43	1.28	1.34
26	A	278	A	N9-C4	6.24	1.41	1.37
56	4	27	CYS	CB-SG	6.19	1.92	1.82
26	A	1071	G	N3-C4	6.16	1.39	1.35
26	A	1071	G	C5-C4	-6.08	1.34	1.38
1	a	413	G	N9-C4	-5.86	1.33	1.38
26	A	1093	G	C6-O6	-5.85	1.18	1.24
26	A	571	U	C4-C5	5.67	1.48	1.43
26	A	1071	G	N9-C4	5.63	1.42	1.38
23	x	115	A	O3'-P	5.57	1.67	1.61
26	A	1058	U	C4-O4	-5.51	1.19	1.23
26	A	2211	A	N9-C4	5.35	1.41	1.37
26	A	1093	G	N1-C2	-5.28	1.33	1.37
26	A	1093	G	C6-N1	-5.21	1.35	1.39
1	a	212	G	C2-N3	-5.19	1.28	1.32
26	A	1313	U	N1-C2	5.15	1.43	1.38
26	A	1057	A	N9-C4	-5.06	1.34	1.37

All (1398) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1044	C	N1-C2-O2	18.02	129.71	118.90
1	a	452	A	O5'-P-OP1	-17.50	89.70	110.70
26	A	1044	C	C6-N1-C2	-16.95	113.52	120.30
26	A	1071	G	C5-C6-N1	16.75	119.88	111.50
26	A	1071	G	C2-N3-C4	16.40	120.10	111.90
26	A	1044	C	N3-C2-O2	-15.40	111.12	121.90
26	A	1071	G	N3-C4-N9	15.16	135.09	126.00
26	A	1044	C	C5-C6-N1	15.00	128.50	121.00
1	a	1158	C	N1-C2-O2	14.94	127.86	118.90
1	a	1158	C	N3-C2-O2	-14.05	112.07	121.90
1	a	206	C	C6-N1-C2	-14.04	114.68	120.30
1	a	968	A	N1-C6-N6	-13.81	110.31	118.60
22	v	74	C	N1-C2-O2	13.75	127.15	118.90
26	A	1072	C	O5'-P-OP1	-13.59	93.47	105.70
26	A	1313	U	N1-C2-O2	13.55	132.29	122.80
26	A	1087	G	N7-C8-N9	13.54	119.87	113.10
26	A	1071	G	N3-C4-C5	-13.44	121.88	128.60
23	x	121	U	C5-C6-N1	12.55	128.97	122.70
26	A	1313	U	N3-C2-O2	-12.54	113.42	122.20
22	v	74	C	N3-C2-O2	-12.36	113.25	121.90
26	A	1072	C	O5'-P-OP2	-12.11	94.81	105.70
26	A	1076	C	C6-N1-C2	-11.92	115.53	120.30
26	A	2325	G	O5'-P-OP1	11.84	124.91	110.70
1	a	206	C	C5-C6-N1	11.75	126.87	121.00
25	z	40	LEU	CB-CG-CD2	-11.73	91.05	111.00
26	A	1054	A	N9-C4-C5	-11.72	101.11	105.80
26	A	1071	G	P-O3'-C3'	-11.67	105.69	119.70
27	B	45	A	C5-C6-N6	-11.20	114.74	123.70
23	x	127	U	P-O3'-C3'	10.91	132.80	119.70
26	A	67	U	C5-C4-O4	-10.90	119.36	125.90
26	A	1087	G	C8-N9-C4	-10.84	102.06	106.40
26	A	1071	G	C5-C6-O6	-10.84	122.10	128.60
26	A	67	U	N3-C4-O4	10.80	126.96	119.40
26	A	2583	G	O5'-P-OP2	-10.77	96.01	105.70
1	a	34	C	C6-N1-C2	-10.73	116.01	120.30
26	A	1313	U	C2-N1-C1'	10.64	130.47	117.70
26	A	2302	U	N3-C2-O2	-10.64	114.75	122.20
26	A	1178	C	N1-C2-O2	10.45	125.17	118.90
1	a	470	C	C5-C6-N1	10.45	126.22	121.00
26	A	2252	G	N1-C6-O6	-10.42	113.65	119.90
26	A	2617	U	N3-C2-O2	-10.42	114.91	122.20
26	A	1072	C	OP1-P-OP2	10.41	135.21	119.60
1	a	1034	G	C5-C6-O6	-10.40	122.36	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1993	U	N3-C2-O2	-10.37	114.94	122.20
26	A	281	C	C6-N1-C2	-10.31	116.18	120.30
26	A	2179	C	N3-C2-O2	-10.26	114.72	121.90
1	a	614	C	N1-C2-O2	10.26	125.06	118.90
1	a	469	C	C5-C6-N1	10.25	126.12	121.00
1	a	528	C	N1-C2-O2	10.05	124.93	118.90
1	a	494	G	C5-C6-O6	-10.03	122.58	128.60
26	A	1941	C	N1-C2-O2	10.01	124.91	118.90
1	a	397	A	C2-N3-C4	9.98	115.59	110.60
26	A	669	G	N3-C4-C5	-9.74	123.73	128.60
26	A	1068	G	C8-N9-C4	-9.74	102.50	106.40
26	A	1088	A	N1-C6-N6	-9.70	112.78	118.60
1	a	470	C	C6-N1-C2	-9.63	116.45	120.30
1	a	469	C	C6-N1-C2	-9.63	116.45	120.30
24	y	47(P)	C	C6-N1-C2	-9.63	116.45	120.30
22	v	74	C	C6-N1-C2	-9.60	116.46	120.30
1	a	575	G	N3-C2-N2	-9.52	113.23	119.90
23	x	93	G	C5-C6-O6	-9.51	122.89	128.60
26	A	962	G	O5'-P-OP1	-9.48	97.17	105.70
26	A	1072	C	C5-C6-N1	9.42	125.71	121.00
26	A	79	C	C6-N1-C2	-9.41	116.54	120.30
23	x	121	U	C6-N1-C2	-9.39	115.36	121.00
23	x	93	G	N1-C6-O6	9.31	125.48	119.90
23	x	120	U	N3-C4-O4	-9.31	112.88	119.40
1	a	526	C	N1-C2-O2	9.28	124.47	118.90
1	a	968	A	O5'-P-OP2	-9.20	97.42	105.70
1	a	476	U	C5-C6-N1	9.13	127.27	122.70
1	a	34	C	C5-C6-N1	9.10	125.55	121.00
26	A	1084	A	N7-C8-N9	9.09	118.34	113.80
26	A	832	U	N3-C2-O2	-9.04	115.87	122.20
1	a	1412	C	C6-N1-C2	-9.04	116.69	120.30
26	A	281	C	C5-C6-N1	9.03	125.52	121.00
26	A	1941	C	N3-C2-O2	-9.00	115.60	121.90
26	A	571	U	C5-C4-O4	8.96	131.28	125.90
1	a	483	C	C6-N1-C2	-8.96	116.72	120.30
1	a	1197	A	O5'-P-OP1	-8.93	97.66	105.70
24	y	67(A)	U	C5-C6-N1	8.93	127.17	122.70
26	A	1054	A	C4-C5-N7	8.92	115.16	110.70
1	a	526	C	C6-N1-C2	-8.90	116.74	120.30
1	a	723	U	N3-C4-C5	8.89	119.93	114.60
26	A	1086	A	C8-N9-C4	-8.86	102.25	105.80
1	a	563	A	N1-C2-N3	-8.85	124.88	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	464	U	C5-C6-N1	8.81	127.11	122.70
1	a	878	A	N9-C4-C5	-8.80	102.28	105.80
1	a	1379	G	N3-C2-N2	-8.80	113.74	119.90
1	a	428	G	N3-C4-N9	-8.77	120.73	126.00
1	a	1384	C	C6-N1-C2	-8.69	116.82	120.30
26	A	1084	A	C8-N9-C4	-8.66	102.34	105.80
1	a	428	G	N3-C2-N2	-8.65	113.84	119.90
26	A	353	C	C5-C6-N1	8.63	125.32	121.00
1	a	163	C	C6-N1-C2	-8.62	116.85	120.30
1	a	90	C	C6-N1-C2	-8.59	116.86	120.30
26	A	1076	C	N3-C4-C5	-8.56	118.48	121.90
26	A	901	C	N1-C2-O2	8.56	124.03	118.90
26	A	2466	C	O5'-P-OP1	-8.54	98.02	105.70
26	A	669	G	C2-N3-C4	8.54	116.17	111.90
27	B	45	A	N1-C6-N6	8.53	123.72	118.60
26	A	1178	C	N3-C2-O2	-8.53	115.93	121.90
26	A	1564	C	C5-C6-N1	8.51	125.25	121.00
1	a	215	C	C5-C6-N1	8.49	125.25	121.00
1	a	993	G	N3-C4-N9	8.48	131.09	126.00
26	A	278	A	C2-N3-C4	8.48	114.84	110.60
1	a	680	C	C6-N1-C2	-8.43	116.93	120.30
24	y	56	C	N1-C2-O2	8.41	123.95	118.90
1	a	598	U	N3-C2-O2	-8.40	116.32	122.20
26	A	2267	A	N1-C6-N6	-8.40	113.56	118.60
3	c	33	ASP	CB-CG-OD1	8.39	125.85	118.30
26	A	546	U	N3-C2-O2	-8.36	116.34	122.20
26	A	2267	A	C2-N3-C4	8.36	114.78	110.60
6	f	72	ASP	CB-CG-OD1	8.34	125.80	118.30
26	A	2211	A	C2-N3-C4	8.33	114.77	110.60
26	A	2420	C	C5-C6-N1	8.30	125.15	121.00
26	A	1044	C	N1-C1'-C2'	-8.29	102.88	112.00
26	A	991	C	O5'-P-OP2	-8.28	98.25	105.70
18	r	15	GLU	C-N-CA	8.26	139.64	122.30
26	A	891	G	C5-C6-O6	-8.26	123.64	128.60
1	a	968	A	C5-C6-N6	8.24	130.29	123.70
2	b	81	ASP	CB-CG-OD1	8.23	125.71	118.30
26	A	1077	A	C8-N9-C4	8.21	109.09	105.80
26	A	889	C	N1-C2-O2	8.21	123.83	118.90
26	A	885	C	C5-C4-N4	-8.20	114.46	120.20
24	y	47	G	N9-C4-C5	8.19	108.68	105.40
1	a	214	C	C6-N1-C2	-8.18	117.03	120.30
26	A	1386	C	C6-N1-C2	-8.18	117.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	412	A	O4'-C1'-N9	8.18	114.74	108.20
26	A	1200	C	C6-N1-C2	-8.14	117.05	120.30
26	A	1071	G	C4'-C3'-O3'	8.12	129.25	113.00
1	a	656	G	N3-C2-N2	-8.11	114.22	119.90
26	A	2179	C	N1-C2-O2	8.09	123.76	118.90
1	a	1395	C	N3-C2-O2	-8.08	116.25	121.90
26	A	1054	A	N1-C2-N3	-8.07	125.26	129.30
1	a	1344	C	C6-N1-C2	-8.06	117.08	120.30
26	A	2637	U	C5-C6-N1	8.06	126.73	122.70
26	A	1059	G	C6-N1-C2	8.05	129.93	125.10
26	A	1044	C	C4'-C3'-O3'	8.03	129.07	113.00
23	x	131	C	C6-N1-C2	-8.02	117.09	120.30
1	a	563	A	N9-C4-C5	-8.01	102.60	105.80
25	z	69	LEU	CA-CB-CG	-8.01	96.88	115.30
26	A	571	U	N3-C4-C5	-8.00	109.80	114.60
26	A	1046	A	N9-C1'-C2'	-7.98	103.22	112.00
1	a	316	C	C6-N1-C2	-7.98	117.11	120.30
26	A	1076	C	N3-C2-O2	-7.96	116.33	121.90
1	a	225	C	C6-N1-C2	-7.95	117.12	120.30
1	a	993	G	N9-C4-C5	-7.95	102.22	105.40
26	A	1843	C	C5-C6-N1	7.94	124.97	121.00
46	U	51	LEU	CA-CB-CG	7.94	133.56	115.30
6	f	94	HIS	N-CA-CB	-7.92	96.34	110.60
26	A	668	A	N1-C2-N3	-7.90	125.35	129.30
1	a	1448	C	N1-C2-O2	7.89	123.64	118.90
1	a	1537	U	C5-C4-O4	-7.88	121.17	125.90
24	y	7	C	C5-C6-N1	7.87	124.94	121.00
1	a	494	G	C4-C5-N7	7.87	113.95	110.80
1	a	684	U	N3-C2-O2	-7.82	116.73	122.20
1	a	967	5MC	OP2-P-O3'	7.82	122.39	105.20
26	A	669	G	N3-C4-N9	7.80	130.68	126.00
1	a	410	G	C8-N9-C4	-7.79	103.28	106.40
1	a	1034	G	N1-C6-O6	7.78	124.57	119.90
24	y	63	U	C5-C4-O4	-7.75	121.25	125.90
26	A	1087	G	C5-N7-C8	-7.75	100.42	104.30
1	a	413	G	N3-C4-N9	-7.75	121.35	126.00
1	a	614	C	N3-C4-N4	7.75	123.42	118.00
26	A	901	C	N3-C2-O2	-7.75	116.48	121.90
1	a	1008	U	N3-C2-O2	-7.74	116.78	122.20
1	a	413	G	N3-C4-C5	7.71	132.46	128.60
26	A	1086	A	N7-C8-N9	7.71	117.66	113.80
1	a	580	C	N1-C2-O2	7.71	123.53	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	580	C	C6-N1-C2	-7.71	117.22	120.30
24	y	47	G	C8-N9-C4	-7.70	103.32	106.40
26	A	2502	G	O5'-P-OP2	7.69	119.93	110.70
7	g	139	ASP	CB-CG-OD1	7.69	125.22	118.30
26	A	1077	A	N9-C4-C5	-7.69	102.72	105.80
26	A	2121	G	N1-C6-O6	-7.66	115.31	119.90
26	A	1079	C	N1-C2-O2	7.64	123.49	118.90
25	z	181	ARG	NE-CZ-NH1	-7.63	116.49	120.30
27	B	45	A	N9-C4-C5	-7.63	102.75	105.80
24	y	70	U	N3-C2-O2	-7.62	116.86	122.20
26	A	1108	U	C5-C6-N1	7.62	126.51	122.70
30	E	134	LEU	CB-CG-CD2	-7.61	98.06	111.00
26	A	890	C	C2-N1-C1'	7.59	127.15	118.80
26	A	885	C	N3-C4-N4	7.59	123.31	118.00
1	a	1105	A	N9-C4-C5	-7.58	102.77	105.80
25	z	301	GLU	N-CA-CB	-7.58	96.95	110.60
26	A	1097	U	C5-C6-N1	7.56	126.48	122.70
1	a	679	C	C6-N1-C2	-7.56	117.28	120.30
26	A	1752	C	C5-C6-N1	7.55	124.78	121.00
1	a	434	U	C5-C6-N1	7.54	126.47	122.70
1	a	968	A	C6-C5-N7	7.54	137.58	132.30
24	y	20	G	N9-C4-C5	-7.54	102.39	105.40
26	A	1079	C	N3-C2-O2	-7.54	116.63	121.90
26	A	2195	U	N3-C2-O2	-7.53	116.93	122.20
26	A	1071	G	C6-N1-C2	-7.51	120.59	125.10
1	a	1524	C	N1-C2-O2	7.51	123.41	118.90
26	A	1294	U	N3-C2-O2	-7.50	116.95	122.20
23	x	115	A	P-O3'-C3'	7.49	128.69	119.70
25	z	427	LEU	CB-CG-CD2	-7.49	98.27	111.00
1	a	491	G	C4-C5-N7	7.48	113.79	110.80
26	A	812	C	N1-C2-O2	7.48	123.39	118.90
26	A	2617	U	N1-C2-O2	7.48	128.04	122.80
1	a	63	C	C6-N1-C2	-7.47	117.31	120.30
1	a	580	C	C2-N1-C1'	7.46	127.00	118.80
26	A	1081	U	C5-C6-N1	7.45	126.43	122.70
27	B	11	C	C6-N1-C2	-7.45	117.32	120.30
26	A	84	A	C5-N7-C8	7.45	107.62	103.90
1	a	526	C	C5-C6-N1	7.44	124.72	121.00
27	B	45	A	C4-C5-N7	7.44	114.42	110.70
26	A	883	G	C6-C5-N7	-7.43	125.94	130.40
26	A	1021	A	C2-N3-C4	7.43	114.32	110.60
26	A	1058	U	C5-C4-O4	-7.43	121.44	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1384	C	C2-N1-C1'	7.43	126.97	118.80
24	y	15	C	N1-C2-O2	7.42	123.35	118.90
27	B	45	A	C5-C6-N1	7.40	121.40	117.70
26	A	1669	A	N1-C2-N3	-7.39	125.61	129.30
1	a	876	C	C6-N1-C2	-7.39	117.35	120.30
26	A	668	A	N9-C4-C5	-7.38	102.85	105.80
57	6	18	CYS	CA-CB-SG	-7.38	100.72	114.00
1	a	215	C	C6-N1-C2	-7.38	117.35	120.30
14	n	32	ASP	CB-CG-OD1	7.37	124.93	118.30
1	a	984	C	C6-N1-C2	-7.36	117.36	120.30
1	a	1245	C	C5-C6-N1	7.36	124.68	121.00
23	x	93	G	C4-C5-N7	7.33	113.73	110.80
26	A	1047	G	N3-C4-C5	7.32	132.26	128.60
26	A	1994	C	C6-N1-C2	-7.32	117.37	120.30
26	A	784	G	O5'-P-OP1	-7.31	99.12	105.70
1	a	491	G	N9-C4-C5	-7.31	102.48	105.40
13	m	57	ASP	CB-CG-OD1	7.30	124.87	118.30
26	A	2177	C	C6-N1-C2	-7.30	117.38	120.30
1	a	1037	C	C6-N1-C2	-7.29	117.38	120.30
26	A	1068	G	N3-C4-C5	-7.29	124.96	128.60
26	A	1386	C	C5-C6-N1	7.29	124.64	121.00
26	A	1072	C	C4'-C3'-O3'	-7.28	94.11	109.40
26	A	353	C	C6-N1-C2	-7.28	117.39	120.30
24	y	63	U	N3-C4-O4	7.28	124.49	119.40
1	a	316	C	C2-N1-C1'	7.27	126.80	118.80
1	a	63	C	C5-C6-N1	7.26	124.63	121.00
23	x	126	G	O5'-P-OP2	7.25	119.39	110.70
26	A	2359	C	C6-N1-C2	-7.25	117.40	120.30
1	a	1045	C	N1-C2-O2	7.24	123.24	118.90
1	a	1366	C	N1-C2-O2	7.22	123.23	118.90
24	y	45	U	P-O3'-C3'	7.22	128.36	119.70
26	A	783	A	C2-N3-C4	7.19	114.19	110.60
26	A	1082	U	C2-N1-C1'	7.19	126.33	117.70
1	a	1493	A	C6-N1-C2	7.18	122.91	118.60
26	A	1081	U	C6-N1-C2	-7.18	116.69	121.00
1	a	177	G	C2-N3-C4	7.16	115.48	111.90
26	A	1047	G	N3-C4-N9	-7.16	121.70	126.00
1	a	1097	C	C6-N1-C2	-7.16	117.44	120.30
1	a	477	C	C5-C6-N1	7.15	124.58	121.00
26	A	1065	U	C5-C6-N1	-7.15	119.12	122.70
1	a	420	U	C5-C6-N1	7.15	126.28	122.70
26	A	1936	A	N1-C6-N6	-7.15	114.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1420	U	N3-C2-O2	-7.14	117.20	122.20
26	A	1114	C	C5-C6-N1	7.14	124.57	121.00
26	A	1578	U	N3-C2-O2	-7.14	117.20	122.20
26	A	1843	C	C6-N1-C2	-7.14	117.45	120.30
1	a	1034	G	C4-C5-N7	7.13	113.65	110.80
1	a	923	A	N7-C8-N9	7.13	117.36	113.80
1	a	614	C	C5-C6-N1	7.13	124.56	121.00
25	z	397	LEU	CB-CG-CD1	7.13	123.12	111.00
1	a	34	C	C2-N1-C1'	7.13	126.64	118.80
26	A	1097	U	O5'-P-OP1	7.13	119.25	110.70
26	A	1071	G	O3'-P-O5'	7.12	117.53	104.00
26	A	1082	U	N3-C4-O4	7.12	124.38	119.40
1	a	1149	C	C6-N1-C2	-7.12	117.45	120.30
1	a	1412	C	C2-N1-C1'	7.11	126.62	118.80
26	A	2420	C	C6-N1-C2	-7.11	117.46	120.30
1	a	879	C	C5-C6-N1	7.09	124.55	121.00
21	u	15	LEU	CA-CB-CG	7.09	131.60	115.30
26	A	2699	C	C5-C6-N1	7.09	124.54	121.00
25	z	26	ASP	CB-CG-OD1	7.08	124.68	118.30
1	a	1195	C	C6-N1-C2	-7.08	117.47	120.30
1	a	1241	G	C2-N3-C4	7.08	115.44	111.90
22	v	67	C	C6-N1-C2	-7.08	117.47	120.30
26	A	2394	C	N1-C2-O2	7.07	123.14	118.90
1	a	1493	A	N1-C2-N3	-7.07	125.77	129.30
1	a	1172	C	N1-C2-O2	7.06	123.14	118.90
1	a	1539	C	N1-C2-O2	-7.06	114.67	118.90
26	A	806	C	C6-N1-C2	-7.06	117.48	120.30
26	A	946	C	C6-N1-C2	-7.05	117.48	120.30
50	Y	49	ASP	CB-CG-OD1	7.05	124.64	118.30
25	z	301	GLU	CA-CB-CG	7.04	128.88	113.40
26	A	2177	C	N1-C2-O2	7.03	123.12	118.90
24	y	7	C	C6-N1-C2	-7.03	117.49	120.30
26	A	162	U	C2-N3-C4	-7.03	122.78	127.00
26	A	1049	C	N1-C2-O2	7.03	123.11	118.90
1	a	1524	C	C6-N1-C2	-7.02	117.49	120.30
1	a	993	G	C4-C5-N7	7.02	113.61	110.80
1	a	1105	A	N1-C2-N3	-7.01	125.79	129.30
1	a	1293	C	C6-N1-C2	-7.01	117.49	120.30
26	A	2080	A	N9-C4-C5	-7.01	102.99	105.80
22	v	32	C	N1-C2-O2	7.01	123.10	118.90
1	a	984	C	C5-C6-N1	7.00	124.50	121.00
1	a	750	C	C6-N1-C2	-7.00	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1395	C	N1-C2-O2	7.00	123.10	118.90
1	a	429	U	O4'-C1'-N1	-7.00	102.60	108.20
26	A	1093	G	N1-C6-O6	-6.99	115.70	119.90
1	a	580	C	C5-C6-N1	6.99	124.50	121.00
1	a	954	G	N9-C4-C5	-6.99	102.60	105.40
22	v	74	C	N3-C4-C5	-6.99	119.11	121.90
1	a	993	G	C6-C5-N7	-6.98	126.21	130.40
1	a	614	C	C5-C4-N4	-6.97	115.32	120.20
26	A	1059	G	C4-C5-N7	6.97	113.59	110.80
22	v	32	C	N3-C2-O2	-6.97	117.02	121.90
26	A	545	U	C5-C6-N1	6.97	126.19	122.70
1	a	878	A	C4-C5-N7	6.96	114.18	110.70
1	a	1047	G	N1-C6-O6	-6.96	115.72	119.90
1	a	368	U	N3-C2-O2	-6.96	117.33	122.20
1	a	452	A	N1-C2-N3	-6.96	125.82	129.30
56	4	14	CYS	CA-CB-SG	6.96	126.53	114.00
1	a	308	C	N3-C4-N4	6.96	122.87	118.00
1	a	136	C	N1-C2-O2	6.95	123.07	118.90
55	3	31	ILE	CG1-CB-CG2	-6.95	96.11	111.40
1	a	1412	C	C5-C6-N1	6.95	124.47	121.00
25	z	164	LEU	CA-CB-CG	-6.95	99.32	115.30
26	A	1053	C	C6-N1-C2	-6.95	117.52	120.30
26	A	101	A	C2-N3-C4	-6.94	107.13	110.60
26	A	1054	A	C6-C5-N7	-6.94	127.44	132.30
26	A	1787	A	N9-C4-C5	-6.94	103.02	105.80
1	a	90	C	N3-C2-O2	-6.94	117.05	121.90
1	a	103	U	N3-C2-O2	-6.93	117.35	122.20
1	a	368	U	C2-N3-C4	-6.93	122.84	127.00
1	a	1195	C	C5-C6-N1	6.93	124.46	121.00
1	a	878	A	N1-C2-N3	-6.92	125.84	129.30
26	A	302	C	C6-N1-C2	-6.92	117.53	120.30
24	y	47(O)	C	C6-N1-C2	-6.92	117.53	120.30
4	d	202	LEU	CB-CG-CD2	-6.91	99.25	111.00
26	A	1085	A	C8-N9-C4	-6.91	103.04	105.80
26	A	2683	C	N1-C2-O2	6.91	123.04	118.90
1	a	1137	C	C2-N3-C4	6.90	123.35	119.90
1	a	50	A	C2-N3-C4	6.90	114.05	110.60
1	a	1535	C	N1-C2-O2	6.89	123.03	118.90
1	a	799	G	N1-C6-O6	-6.88	115.77	119.90
1	a	1095	U	O5'-P-OP1	-6.88	99.51	105.70
1	a	1411	C	C5-C6-N1	6.87	124.44	121.00
1	a	1071	C	C6-N1-C2	-6.86	117.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	177	G	N3-C4-C5	-6.86	125.17	128.60
26	A	1564	C	C6-N1-C2	-6.85	117.56	120.30
26	A	84	A	N7-C8-N9	-6.85	110.38	113.80
26	A	1313	U	C6-N1-C1'	-6.85	111.61	121.20
24	y	7	C	N1-C2-O2	6.84	123.01	118.90
1	a	680	C	C5-C6-N1	6.84	124.42	121.00
26	A	1158	C	C5-C6-N1	6.84	124.42	121.00
26	A	595	C	C5-C6-N1	6.84	124.42	121.00
26	A	1046	A	C4'-C3'-O3'	6.83	126.67	113.00
26	A	2758	A	N1-C6-N6	-6.83	114.50	118.60
26	A	1111	A	N1-C2-N3	-6.83	125.89	129.30
1	a	598	U	N1-C2-O2	6.82	127.58	122.80
23	x	93	G	C6-C5-N7	-6.82	126.31	130.40
22	v	34	C	N1-C2-O2	6.81	122.99	118.90
26	A	2175	C	N1-C2-O2	6.81	122.98	118.90
26	A	2215	C	C5-C6-N1	6.81	124.40	121.00
26	A	889	C	N3-C2-O2	-6.80	117.14	121.90
1	a	1392	G	C4-C5-N7	6.80	113.52	110.80
1	a	959	A	N7-C8-N9	6.78	117.19	113.80
23	x	121	U	OP1-P-OP2	-6.78	109.43	119.60
26	A	544	C	C6-N1-C2	-6.78	117.59	120.30
26	A	2175	C	N3-C2-O2	-6.78	117.16	121.90
26	A	2215	C	C6-N1-C2	-6.78	117.59	120.30
1	a	1245	C	N1-C2-O2	6.78	122.97	118.90
26	A	2143	C	C6-N1-C2	-6.78	117.59	120.30
1	a	528	C	N3-C2-O2	-6.77	117.16	121.90
1	a	1384	C	N1-C2-O2	6.77	122.96	118.90
26	A	1075	C	O5'-P-OP2	6.77	118.82	110.70
26	A	2267	A	N1-C2-N3	-6.77	125.92	129.30
1	a	359	G	N1-C6-O6	-6.76	115.84	119.90
24	y	47	G	N3-C2-N2	-6.75	115.17	119.90
23	x	120	U	C5-C6-N1	-6.75	119.33	122.70
26	A	2474	U	N3-C2-O2	-6.74	117.48	122.20
1	a	527	G7M	P-O3'-C3'	6.72	127.77	119.70
26	A	806	C	C5-C6-N1	6.72	124.36	121.00
26	A	847	U	N3-C2-O2	-6.72	117.50	122.20
26	A	2576	G	C2-N3-C4	6.72	115.26	111.90
26	A	550	C	C6-N1-C2	-6.72	117.61	120.30
26	A	1539	U	C5-C6-N1	6.72	126.06	122.70
33	I	64	ARG	N-CA-CB	-6.71	98.52	110.60
1	a	354	G	N9-C4-C5	-6.71	102.72	105.40
1	a	491	G	N1-C6-O6	6.71	123.92	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1087	G	C4-N9-C1'	6.71	135.22	126.50
1	a	954	G	N1-C6-O6	6.71	123.92	119.90
1	a	308	C	N1-C2-O2	6.70	122.92	118.90
26	A	1058	U	N3-C4-C5	6.70	118.62	114.60
12	l	101	LEU	N-CA-CB	-6.69	97.01	110.40
1	a	158	G	N1-C6-O6	-6.68	115.89	119.90
26	A	2177	C	N3-C2-O2	-6.68	117.22	121.90
23	x	120	U	C5-C4-O4	6.67	129.90	125.90
1	a	1059	C	C6-N1-C2	-6.67	117.63	120.30
26	A	1752	C	C6-N1-C2	-6.67	117.63	120.30
26	A	2699	C	C6-N1-C2	-6.66	117.64	120.30
24	y	27	C	C6-N1-C2	-6.66	117.64	120.30
22	v	36	U	N3-C2-O2	-6.66	117.54	122.20
1	a	620	C	N1-C2-O2	6.65	122.89	118.90
1	a	328	C	N1-C2-O2	-6.65	114.91	118.90
1	a	493	A	C8-N9-C4	-6.64	103.14	105.80
1	a	736	C	C6-N1-C2	-6.64	117.64	120.30
1	a	428	G	C2-N3-C4	-6.63	108.58	111.90
26	A	1047	G	C4-N9-C1'	-6.63	117.88	126.50
26	A	2637	U	C6-N1-C2	-6.63	117.02	121.00
26	A	1071	G	C4-C5-N7	6.63	113.45	110.80
1	a	441	A	O4'-C1'-N9	6.63	113.50	108.20
31	F	88	VAL	CG1-CB-CG2	-6.62	100.30	110.90
1	a	290	C	N1-C2-O2	6.62	122.87	118.90
1	a	455	G	N9-C4-C5	-6.62	102.75	105.40
26	A	1054	A	N1-C6-N6	6.62	122.57	118.60
26	A	1047	G	C2-N3-C4	-6.62	108.59	111.90
1	a	427	U	N1-C2-N3	6.62	118.87	114.90
26	A	1956	U	N3-C2-O2	-6.61	117.57	122.20
26	A	2072	C	C5-C6-N1	6.61	124.31	121.00
1	a	575	G	N9-C4-C5	6.61	108.04	105.40
26	A	302	C	C5-C6-N1	6.61	124.31	121.00
1	a	822	U	N3-C2-O2	-6.60	117.58	122.20
1	a	240	G	N1-C6-O6	6.59	123.86	119.90
26	A	278	A	N3-C4-C5	-6.59	122.19	126.80
26	A	890	C	C6-N1-C1'	-6.59	112.90	120.80
1	a	1406	U	N3-C2-O2	-6.58	117.59	122.20
26	A	2473	U	N3-C2-O2	-6.58	117.59	122.20
26	A	2069	G7M	P-O3'-C3'	6.58	127.60	119.70
1	a	661	G	N9-C4-C5	-6.57	102.77	105.40
24	y	71	C	C5-C6-N1	6.57	124.28	121.00
1	a	526	C	N3-C2-O2	-6.56	117.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	189	ASP	CB-CG-OD1	6.56	124.21	118.30
1	a	1147	C	N3-C4-C5	6.56	124.52	121.90
1	a	410	G	N7-C8-N9	6.56	116.38	113.10
1	a	1392	G	N9-C4-C5	-6.55	102.78	105.40
26	A	84	A	C8-N9-C4	6.55	108.42	105.80
1	a	1158	C	C6-N1-C2	-6.55	117.68	120.30
25	z	300	LEU	CB-CG-CD1	-6.55	99.86	111.00
1	a	429	U	C5-C6-N1	-6.54	119.43	122.70
23	x	121	U	N3-C4-O4	6.54	123.98	119.40
26	A	2037	A	N1-C2-N3	-6.54	126.03	129.30
1	a	424	G	N3-C4-N9	-6.54	122.08	126.00
26	A	545	U	C6-N1-C2	-6.54	117.08	121.00
26	A	2050	C	C5-C6-N1	6.54	124.27	121.00
26	A	2072	C	C6-N1-C2	-6.54	117.69	120.30
1	a	397	A	N3-C4-N9	6.54	132.63	127.40
1	a	493	A	N7-C8-N9	6.53	117.07	113.80
1	a	475	C	C6-N1-C2	-6.53	117.69	120.30
26	A	658	U	C5-C6-N1	6.53	125.97	122.70
1	a	451	A	O5'-P-OP1	-6.52	99.83	105.70
1	a	526	C	N3-C4-N4	6.52	122.57	118.00
26	A	2394	C	N3-C2-O2	-6.52	117.34	121.90
26	A	2302	U	N1-C2-N3	6.52	118.81	114.90
26	A	1052	C	C5-C6-N1	6.51	124.25	121.00
26	A	1795	C	C5-C6-N1	6.51	124.25	121.00
26	A	2080	A	N1-C2-N3	-6.51	126.05	129.30
26	A	1348	C	N1-C2-O2	6.50	122.80	118.90
26	A	2050	C	C6-N1-C2	-6.50	117.70	120.30
26	A	2388	A	C5-N7-C8	6.50	107.15	103.90
1	a	754	C	C2-N1-C1'	6.49	125.94	118.80
1	a	968	A	C4-C5-N7	-6.49	107.45	110.70
1	a	1034	G	N9-C4-C5	-6.49	102.81	105.40
1	a	723	U	C4-C5-C6	-6.49	115.81	119.70
1	a	923	A	C5-N7-C8	-6.48	100.66	103.90
26	A	1013	C	C6-N1-C2	-6.48	117.71	120.30
1	a	751	U	N3-C2-O2	-6.47	117.67	122.20
27	B	26	C	C6-N1-C2	-6.47	117.71	120.30
1	a	1326	U	N3-C2-O2	-6.47	117.67	122.20
1	a	414	A	C6-N1-C2	6.47	122.48	118.60
23	x	97	A	C5-C6-N1	6.47	120.93	117.70
1	a	1533	C	C6-N1-C2	-6.46	117.72	120.30
26	A	208	C	C5-C6-N1	6.46	124.23	121.00
26	A	1054	A	N3-C4-N9	6.45	132.56	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1176	U	N1-C2-O2	6.45	127.32	122.80
1	a	656	G	C6-N1-C2	-6.45	121.23	125.10
1	a	756	C	N1-C2-O2	6.45	122.77	118.90
1	a	212	G	C5-C6-O6	6.45	132.47	128.60
26	A	1077	A	O4'-C1'-N9	-6.45	103.04	108.20
1	a	126	G	N1-C6-O6	-6.45	116.03	119.90
1	a	424	G	O5'-P-OP2	-6.45	99.90	105.70
24	y	61	C	C6-N1-C2	-6.44	117.72	120.30
24	y	20	G	C8-N9-C4	6.44	108.97	106.40
26	A	1941	C	C6-N1-C2	-6.43	117.73	120.30
1	a	959	A	C8-N9-C4	-6.43	103.23	105.80
1	a	276	G	N3-C2-N2	-6.42	115.40	119.90
1	a	993	G	C5-C6-O6	-6.42	124.75	128.60
2	b	158	ASP	CB-CG-OD1	6.42	124.08	118.30
24	y	56	C	N3-C2-O2	-6.42	117.41	121.90
26	A	1941	C	C2-N1-C1'	6.42	125.86	118.80
1	a	330	C	N1-C2-O2	6.41	122.75	118.90
22	v	57	A	C5-N7-C8	6.41	107.11	103.90
1	a	214	C	C5-C6-N1	6.41	124.20	121.00
1	a	1245	C	C6-N1-C2	-6.40	117.74	120.30
1	a	110	C	N1-C2-O2	6.40	122.74	118.90
1	a	272	C	N1-C2-O2	6.40	122.74	118.90
1	a	219	U	C5-C6-N1	6.39	125.90	122.70
22	v	39	C	C6-N1-C2	-6.39	117.74	120.30
26	A	231	A	N9-C4-C5	-6.39	103.24	105.80
26	A	1059	G	C5-C6-N1	-6.39	108.31	111.50
1	a	136	C	C2-N1-C1'	6.39	125.83	118.80
8	h	120	LEU	CB-CG-CD1	6.38	121.84	111.00
1	a	614	C	C6-N1-C2	-6.37	117.75	120.30
1	a	216	U	C5-C6-N1	6.37	125.89	122.70
26	A	687	C	N1-C2-O2	6.37	122.72	118.90
1	a	52	C	C6-N1-C2	-6.37	117.75	120.30
1	a	409	U	C5-C6-N1	6.36	125.88	122.70
1	a	1496	C	C6-N1-C2	-6.36	117.75	120.30
33	I	64	ARG	CA-CB-CG	6.36	127.39	113.40
1	a	723	U	N1-C2-O2	6.36	127.25	122.80
26	A	208	C	C6-N1-C2	-6.36	117.76	120.30
26	A	1059	G	C5-N7-C8	-6.36	101.12	104.30
1	a	1148	U	N3-C2-O2	-6.36	117.75	122.20
1	a	1262	C	N1-C2-O2	6.36	122.71	118.90
1	a	132	C	C6-N1-C2	-6.35	117.76	120.30
26	A	867	C	N1-C2-O2	6.35	122.71	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1314	C	C6-N1-C2	-6.35	117.76	120.30
26	A	2252	G	C5-C6-N1	6.35	114.67	111.50
1	a	611	C	N1-C2-O2	6.34	122.71	118.90
26	A	2214	C	N1-C2-O2	6.34	122.70	118.90
1	a	536	C	C5-C6-N1	6.34	124.17	121.00
1	a	1344	C	N1-C2-O2	6.33	122.70	118.90
1	a	180	U	C5-C6-N1	6.33	125.87	122.70
1	a	599	C	C5-C6-N1	6.33	124.17	121.00
26	A	2342	C	C5-C6-N1	6.32	124.16	121.00
26	A	445	C	N3-C2-O2	-6.32	117.48	121.90
10	j	75	ASP	CB-CG-OD1	6.32	123.98	118.30
26	A	56	A	N1-C2-N3	-6.32	126.14	129.30
26	A	46	G	O5'-P-OP2	-6.31	100.02	105.70
1	a	1395	C	N3-C4-N4	-6.30	113.59	118.00
26	A	1069	A	N7-C8-N9	6.30	116.95	113.80
26	A	1087	G	C6-C5-N7	-6.30	126.62	130.40
49	X	21	LEU	CA-CB-CG	6.30	129.79	115.30
26	A	231	A	C5-C6-N6	-6.30	118.66	123.70
26	A	509	C	C6-N1-C2	-6.28	117.79	120.30
26	A	2011	U	N3-C2-O2	-6.27	117.81	122.20
1	a	423	G	C2-N3-C4	6.27	115.03	111.90
1	a	1406	U	N1-C2-O2	6.27	127.19	122.80
26	A	634	C	C6-N1-C2	-6.27	117.79	120.30
24	y	47(F)	C	C6-N1-C2	-6.27	117.79	120.30
3	c	117	ASP	CB-CG-OD1	6.26	123.94	118.30
26	A	729	G	N3-C4-C5	-6.26	125.47	128.60
25	z	610	LEU	CA-CB-CG	6.26	129.69	115.30
26	A	571	U	C4-C5-C6	6.24	123.45	119.70
1	a	312	C	C6-N1-C2	-6.24	117.81	120.30
26	A	1484	U	N3-C2-O2	-6.24	117.83	122.20
1	a	377	G	N1-C6-O6	-6.23	116.16	119.90
1	a	368	U	N1-C2-N3	6.23	118.64	114.90
1	a	569	C	C6-N1-C2	-6.23	117.81	120.30
1	a	284	C	C6-N1-C2	-6.23	117.81	120.30
26	A	984	A	N7-C8-N9	6.23	116.92	113.80
1	a	420	U	C6-N1-C2	-6.23	117.27	121.00
1	a	956	U	N3-C2-O2	-6.22	117.84	122.20
26	A	888	C	O4'-C1'-N1	6.22	113.18	108.20
26	A	101	A	N1-C2-N3	6.22	132.41	129.30
1	a	211	G	N3-C4-C5	-6.22	125.49	128.60
26	A	886	A	P-O3'-C3'	6.22	127.16	119.70
1	a	1314	C	C5-C6-N1	6.21	124.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1171	G	N3-C4-N9	-6.21	122.27	126.00
1	a	491	G	C6-C5-N7	-6.21	126.67	130.40
26	A	965	C	C5-C6-N1	6.21	124.11	121.00
26	A	1993	U	N1-C2-O2	6.21	127.14	122.80
26	A	1069	A	C8-N9-C4	-6.20	103.32	105.80
1	a	276	G	N1-C6-O6	-6.20	116.18	119.90
26	A	847	U	N1-C2-O2	6.20	127.14	122.80
26	A	1990	C	C5-C6-N1	6.20	124.10	121.00
26	A	2150	C	C6-N1-C2	-6.20	117.82	120.30
26	A	1795	C	C6-N1-C2	-6.20	117.82	120.30
1	a	308	C	C2-N1-C1'	6.19	125.61	118.80
1	a	50	A	N1-C6-N6	-6.18	114.89	118.60
24	y	61	C	C5-C6-N1	6.18	124.09	121.00
26	A	889	C	C2-N1-C1'	6.18	125.60	118.80
23	x	120	U	P-O3'-C3'	6.18	127.11	119.70
1	a	528	C	C2-N1-C1'	6.18	125.59	118.80
1	a	1427	C	C6-N1-C2	-6.17	117.83	120.30
1	a	469	C	C2-N1-C1'	6.17	125.59	118.80
1	a	1389	C	N1-C2-O2	6.17	122.60	118.90
26	A	1936	A	N1-C2-N3	6.17	132.39	129.30
26	A	1982	U	O5'-P-OP2	-6.17	100.15	105.70
26	A	1539	U	N3-C4-O4	6.17	123.72	119.40
1	a	563	A	C4-C5-N7	6.17	113.78	110.70
1	a	647	C	C6-N1-C2	-6.16	117.83	120.30
26	A	1159	U	N3-C2-O2	-6.16	117.89	122.20
23	x	120	U	C2-N1-C1'	-6.16	110.31	117.70
22	v	39	C	C5-C6-N1	6.16	124.08	121.00
1	a	16	A	C6-N1-C2	6.14	122.29	118.60
1	a	428	G	N3-C4-C5	6.14	131.67	128.60
1	a	783	C	C6-N1-C2	-6.14	117.84	120.30
27	B	49	C	C5-C6-N1	6.14	124.07	121.00
1	a	1386	G	N1-C6-O6	-6.13	116.22	119.90
23	x	113	C	O4'-C1'-N1	6.13	113.11	108.20
26	A	758	C	N3-C2-O2	-6.13	117.61	121.90
26	A	1101	U	N3-C2-O2	-6.13	117.91	122.20
26	A	140	C	C6-N1-C2	-6.13	117.85	120.30
8	h	79	ARG	CG-CD-NE	-6.12	98.94	111.80
26	A	2211	A	N3-C4-N9	6.12	132.30	127.40
1	a	213	G	C4-N9-C1'	6.12	134.46	126.50
26	A	334	C	C6-N1-C2	-6.12	117.85	120.30
1	a	876	C	C5-C6-N1	6.12	124.06	121.00
22	v	25	C	N1-C2-O2	6.12	122.57	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1462	C	N1-C2-O2	6.12	122.57	118.90
1	a	1077	G	N3-C4-N9	-6.11	122.33	126.00
26	A	898	C	C5-C6-N1	6.11	124.06	121.00
1	a	424	G	N9-C4-C5	6.11	107.84	105.40
1	a	577	G	C5-C6-O6	-6.10	124.94	128.60
1	a	1071	C	C2-N1-C1'	6.10	125.51	118.80
1	a	536	C	C6-N1-C2	-6.10	117.86	120.30
26	A	1071	G	O4'-C1'-N9	6.10	113.08	108.20
1	a	954	G	C4-C5-N7	6.09	113.24	110.80
26	A	1173	U	C6-N1-C2	-6.09	117.34	121.00
1	a	440	C	C6-N1-C2	-6.09	117.86	120.30
1	a	494	G	N1-C6-O6	6.09	123.56	119.90
26	A	1075	C	C4-C5-C6	6.09	120.45	117.40
1	a	735	C	C6-N1-C2	-6.08	117.87	120.30
26	A	984	A	C2-N3-C4	6.08	113.64	110.60
26	A	1101	U	N1-C2-O2	6.08	127.06	122.80
46	U	88	ASP	CB-CG-OD1	6.08	123.77	118.30
10	j	18	ILE	CG1-CB-CG2	-6.08	98.03	111.40
26	A	851	C	C5-C6-N1	6.07	124.04	121.00
26	A	2217	G	C2-N3-C4	6.07	114.94	111.90
1	a	528	C	C6-N1-C2	-6.07	117.87	120.30
1	a	954	G	C6-C5-N7	-6.07	126.76	130.40
1	a	386	C	C6-N1-C2	-6.07	117.87	120.30
26	A	2416	C	C5-C6-N1	6.07	124.03	121.00
1	a	528	C	C5-C6-N1	6.06	124.03	121.00
26	A	1830	C	C6-N1-C2	-6.06	117.88	120.30
1	a	1072	G	N1-C6-O6	6.06	123.53	119.90
26	A	883	G	N9-C4-C5	-6.05	102.98	105.40
26	A	1402	U	N3-C2-O2	-6.05	117.97	122.20
26	A	1068	G	N7-C8-N9	6.05	116.12	113.10
1	a	1411	C	C6-N1-C2	-6.05	117.88	120.30
2	b	134	LEU	CA-CB-CG	6.05	129.21	115.30
1	a	1448	C	C2-N1-C1'	6.04	125.45	118.80
26	A	1669	A	C2-N3-C4	6.04	113.62	110.60
15	o	30	LEU	CB-CG-CD2	-6.04	100.73	111.00
26	A	595	C	C6-N1-C2	-6.04	117.89	120.30
1	a	1197	A	N1-C2-N3	-6.04	126.28	129.30
26	A	687	C	N3-C2-O2	-6.04	117.68	121.90
26	A	1244	A	N9-C4-C5	-6.04	103.39	105.80
1	a	513	C	N1-C2-O2	6.03	122.52	118.90
26	A	729	G	N3-C4-N9	6.03	129.62	126.00
42	Q	108	LEU	CA-CB-CG	6.03	129.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	867	C	N3-C2-O2	-6.03	117.68	121.90
26	A	1046	A	N7-C8-N9	6.03	116.81	113.80
26	A	2254	C	C6-N1-C2	-6.02	117.89	120.30
1	a	1469	C	N3-C2-O2	-6.02	117.68	121.90
1	a	1469	C	N1-C2-O2	6.02	122.51	118.90
1	a	960	U	N3-C2-O2	-6.02	117.98	122.20
1	a	614	C	N3-C2-O2	-6.02	117.69	121.90
1	a	661	G	C5-C6-O6	-6.02	124.99	128.60
26	A	2252	G	C2-N3-C4	6.02	114.91	111.90
1	a	514	C	C6-N1-C2	-6.01	117.89	120.30
23	x	125	G	N9-C1'-C2'	-6.01	105.38	112.00
26	A	2765	A	C2-N3-C4	6.01	113.61	110.60
27	B	55	U	N3-C2-O2	-6.01	117.99	122.20
1	a	526	C	C2-N1-C1'	6.01	125.41	118.80
1	a	551	U	C5-C4-O4	-6.01	122.29	125.90
23	x	124	A	N9-C1'-C2'	-6.01	105.39	112.00
26	A	257	C	N1-C2-O2	6.01	122.51	118.90
26	A	571	U	C5-C6-N1	-6.01	119.69	122.70
26	A	2275	C	N1-C2-O2	6.01	122.51	118.90
26	A	1049	C	N3-C2-O2	-6.00	117.70	121.90
26	A	1669	A	N3-C4-N9	6.00	132.20	127.40
1	a	431	A	N1-C6-N6	-6.00	115.00	118.60
1	a	661	G	N1-C6-O6	6.00	123.50	119.90
24	y	16	C	C2-N3-C4	6.00	122.90	119.90
1	a	536	C	N1-C2-O2	5.99	122.50	118.90
1	a	1392	G	C6-C5-N7	-5.99	126.81	130.40
1	a	680	C	C2-N1-C1'	5.99	125.38	118.80
1	a	613	C	O5'-P-OP1	-5.98	100.32	105.70
26	A	2789	C	C5-C6-N1	5.98	123.99	121.00
1	a	464	U	C6-N1-C2	-5.98	117.41	121.00
26	A	1294	U	N1-C2-O2	5.97	126.98	122.80
26	A	1071	G	N9-C4-C5	-5.97	103.01	105.40
1	a	1172	C	C5-C6-N1	5.96	123.98	121.00
26	A	2044	C	C6-N1-C2	-5.96	117.92	120.30
1	a	923	A	C4-C5-N7	5.96	113.68	110.70
26	A	1680	U	N3-C2-O2	-5.95	118.03	122.20
1	a	1524	C	N3-C2-O2	-5.95	117.73	121.90
26	A	1723	G	C5-C6-N1	5.95	114.48	111.50
26	A	2066	C	C6-N1-C2	-5.95	117.92	120.30
1	a	397	A	N1-C2-N3	-5.95	126.33	129.30
26	A	1931	U	N3-C2-O2	-5.95	118.04	122.20
1	a	539	A	N1-C2-N3	-5.94	126.33	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1060	U	N1-C2-O2	5.94	126.96	122.80
26	A	1059	G	C2-N3-C4	-5.94	108.93	111.90
26	A	2591	C	C6-N1-C2	-5.94	117.92	120.30
1	a	1470	U	N3-C2-O2	-5.94	118.04	122.20
1	a	1496	C	N1-C2-O2	5.93	122.46	118.90
26	A	546	U	N1-C2-O2	5.93	126.95	122.80
26	A	887	U	N3-C2-O2	-5.93	118.05	122.20
1	a	661	G	C4-C5-N7	5.93	113.17	110.80
26	A	668	A	C4-C5-N7	5.93	113.66	110.70
26	A	2744	G	C5-N7-C8	5.93	107.26	104.30
1	a	699	C	C6-N1-C2	-5.92	117.93	120.30
1	a	915	A	N1-C6-N6	-5.92	115.05	118.60
1	a	577	G	N1-C6-O6	5.92	123.45	119.90
26	A	2666	C	N1-C2-O2	5.92	122.45	118.90
1	a	1120	C	N1-C2-O2	5.92	122.45	118.90
26	A	1072	C	C2-N1-C1'	5.92	125.31	118.80
1	a	488	C	C6-N1-C2	-5.91	117.94	120.30
1	a	1197	A	N9-C4-C5	-5.91	103.44	105.80
23	x	125	G	P-O3'-C3'	-5.91	112.61	119.70
26	A	668	A	C6-N1-C2	5.91	122.15	118.60
26	A	901	C	C6-N1-C2	-5.89	117.94	120.30
26	A	2529	G	N3-C4-N9	5.89	129.54	126.00
1	a	211	G	C2-N3-C4	5.89	114.84	111.90
26	A	1052	C	C6-N1-C2	-5.89	117.94	120.30
1	a	1203	C	C6-N1-C2	-5.89	117.94	120.30
1	a	1386	G	N9-C4-C5	5.89	107.75	105.40
26	A	2769	U	N3-C2-O2	-5.88	118.08	122.20
1	a	932	C	C6-N1-C2	-5.88	117.95	120.30
26	A	1582	C	C6-N1-C2	-5.88	117.95	120.30
22	v	57	A	N7-C8-N9	-5.88	110.86	113.80
26	A	1082	U	C5-C4-O4	-5.88	122.37	125.90
26	A	1044	C	C2-N1-C1'	5.87	125.26	118.80
26	A	1257	C	C6-N1-C2	-5.87	117.95	120.30
1	a	998	C	N1-C2-O2	5.86	122.42	118.90
1	a	998	C	N3-C2-O2	-5.86	117.80	121.90
1	a	1118	U	C5-C4-O4	-5.86	122.38	125.90
1	a	1202	U	N3-C2-O2	-5.86	118.10	122.20
1	a	1435	G	N1-C6-O6	5.86	123.42	119.90
26	A	813	U	N3-C2-O2	-5.86	118.10	122.20
26	A	2576	G	N3-C4-C5	-5.86	125.67	128.60
1	a	521	G	N1-C6-O6	-5.86	116.39	119.90
26	A	445	C	N1-C2-O2	5.86	122.41	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1384	C	N3-C2-O2	-5.85	117.80	121.90
26	A	343	C	N1-C2-O2	5.85	122.41	118.90
1	a	61	G	N9-C4-C5	-5.85	103.06	105.40
26	A	890	C	N1-C2-O2	5.85	122.41	118.90
1	a	1027	C	N3-C4-C5	5.84	124.24	121.90
23	x	120	U	C4'-C3'-O3'	-5.84	97.14	109.40
26	A	1243	C	C6-N1-C2	-5.84	117.97	120.30
1	a	465	A	O4'-C1'-N9	5.83	112.87	108.20
26	A	1068	G	C6-C5-N7	-5.83	126.90	130.40
22	v	51	C	C6-N1-C2	-5.83	117.97	120.30
1	a	1149	C	N1-C2-O2	5.83	122.40	118.90
26	A	1298	C	C6-N1-C2	-5.83	117.97	120.30
1	a	1066	C	N3-C2-O2	-5.83	117.82	121.90
23	x	131	C	N1-C1'-C2'	-5.83	105.59	112.00
1	a	1384	C	C5-C6-N1	5.82	123.91	121.00
26	A	346	A	N1-C2-N3	5.82	132.21	129.30
26	A	1539	U	C5-C4-O4	-5.82	122.41	125.90
26	A	1936	A	C5-C6-N6	5.82	128.35	123.70
1	a	323	U	C5-C4-O4	-5.81	122.41	125.90
26	A	305	C	C5-C6-N1	5.81	123.91	121.00
1	a	772	U	N3-C2-O2	-5.81	118.13	122.20
26	A	1936	A	N9-C4-C5	5.81	108.12	105.80
26	A	2143	C	N3-C2-O2	-5.81	117.83	121.90
1	a	960	U	N1-C2-O2	5.80	126.86	122.80
26	A	162	U	N1-C2-N3	5.80	118.38	114.90
26	A	1994	C	C5-C6-N1	5.80	123.90	121.00
26	A	1349	C	N1-C2-O2	5.80	122.38	118.90
25	z	398	LEU	CA-CB-CG	5.79	128.63	115.30
26	A	1159	U	N1-C2-O2	5.79	126.86	122.80
26	A	2656	U	N3-C2-O2	-5.79	118.14	122.20
1	a	1147	C	N3-C4-N4	-5.79	113.95	118.00
23	x	131	C	O4'-C1'-N1	5.79	112.83	108.20
26	A	56	A	N9-C4-C5	-5.79	103.48	105.80
1	a	563	A	C6-N1-C2	5.79	122.07	118.60
1	a	27	G	N1-C6-O6	5.79	123.37	119.90
1	a	410	G	N3-C4-C5	-5.78	125.71	128.60
26	A	305	C	C6-N1-C2	-5.78	117.99	120.30
26	A	2044	C	C5-C6-N1	5.78	123.89	121.00
26	A	2200	C	C6-N1-C2	-5.78	117.99	120.30
1	a	539	A	N9-C4-C5	-5.78	103.49	105.80
26	A	2416	C	C6-N1-C2	-5.78	117.99	120.30
26	A	668	A	N1-C6-N6	5.78	122.07	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	222	C	N1-C2-O2	5.78	122.36	118.90
1	a	614	C	C2-N1-C1'	5.78	125.15	118.80
1	a	513	C	C5-C6-N1	5.77	123.89	121.00
1	a	610	U	N3-C2-O2	-5.77	118.16	122.20
1	a	414	A	N1-C2-N3	-5.77	126.42	129.30
1	a	562	U	N3-C2-O2	-5.77	118.16	122.20
26	A	119	A	N1-C6-N6	-5.77	115.14	118.60
26	A	1670	C	C6-N1-C2	-5.77	117.99	120.30
22	v	67	C	N1-C2-O2	5.77	122.36	118.90
26	A	2579	C	C5-C6-N1	5.77	123.88	121.00
1	a	679	C	C5-C6-N1	5.76	123.88	121.00
1	a	1472	U	N3-C2-O2	-5.76	118.17	122.20
26	A	1086	A	N1-C2-N3	5.76	132.18	129.30
26	A	2207	C	C6-N1-C2	-5.76	118.00	120.30
26	A	365	U	C5-C4-O4	-5.76	122.44	125.90
1	a	924	C	C6-N1-C2	-5.76	118.00	120.30
26	A	278	A	C8-N9-C4	-5.76	103.50	105.80
26	A	1053	C	C5-C6-N1	5.76	123.88	121.00
1	a	1132	C	N3-C2-O2	-5.76	117.87	121.90
26	A	1297	C	C6-N1-C2	-5.76	118.00	120.30
26	A	140	C	C5-C6-N1	5.75	123.88	121.00
26	A	729	G	C4-N9-C1'	5.75	133.98	126.50
26	A	1093	G	C5-C6-N1	5.75	114.38	111.50
1	a	1141	C	C6-N1-C2	-5.75	118.00	120.30
1	a	1393	U	N3-C2-O2	-5.75	118.18	122.20
26	A	278	A	N3-C4-N9	5.75	132.00	127.40
1	a	575	G	C6-N1-C2	-5.75	121.65	125.10
26	A	826	U	OP1-P-O3'	5.75	117.84	105.20
26	A	2442	C	N1-C2-O2	5.75	122.35	118.90
26	A	509	C	C5-C6-N1	5.74	123.87	121.00
26	A	1669	A	N9-C4-C5	-5.74	103.50	105.80
26	A	886	A	O4'-C1'-N9	5.74	112.79	108.20
26	A	2179	C	C6-N1-C2	-5.74	118.00	120.30
34	H	37	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	a	204	G	N7-C8-N9	5.74	115.97	113.10
1	a	90	C	C5-C6-N1	5.73	123.87	121.00
26	A	1787	A	C4-C5-N7	5.73	113.56	110.70
26	A	2089	C	C5-C6-N1	5.73	123.86	121.00
1	a	1195	C	N1-C2-O2	5.73	122.34	118.90
1	a	1392	G	N3-C2-N2	5.73	123.91	119.90
26	A	1021	A	C8-N9-C4	-5.73	103.51	105.80
26	A	2529	G	C5-C6-N1	5.72	114.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	458	U	C5-C6-N1	5.72	125.56	122.70
23	x	131	C	C3'-C2'-C1'	5.72	106.07	101.50
26	A	1071	G	N1-C2-N3	-5.72	120.47	123.90
26	A	1945	G	N9-C4-C5	-5.72	103.11	105.40
26	A	2248	C	C6-N1-C2	-5.72	118.01	120.30
1	a	212	G	N3-C2-N2	-5.71	115.90	119.90
1	a	564	C	N1-C2-O2	5.71	122.33	118.90
25	z	181	ARG	CG-CD-NE	-5.71	99.81	111.80
1	a	358	U	N3-C2-O2	-5.71	118.21	122.20
1	a	1395	C	C5-C4-N4	5.71	124.19	120.20
26	A	1114	C	C6-N1-C2	-5.71	118.02	120.30
26	A	2683	C	N3-C2-O2	-5.71	117.91	121.90
1	a	993	G	N3-C2-N2	5.70	123.89	119.90
26	A	2680	U	N3-C2-O2	-5.70	118.21	122.20
1	a	429	U	OP1-P-O3'	5.70	117.74	105.20
26	A	2292	U	C5-C4-O4	-5.70	122.48	125.90
26	A	550	C	C5-C6-N1	5.70	123.85	121.00
26	A	231	A	C4-C5-N7	5.69	113.55	110.70
26	A	2275	C	C2-N1-C1'	5.69	125.06	118.80
1	a	323	U	C5-C6-N1	5.69	125.55	122.70
8	h	82	LEU	CA-CB-CG	5.69	128.39	115.30
1	a	189	A	C5-N7-C8	5.69	106.74	103.90
1	a	993	G	N1-C6-O6	5.68	123.31	119.90
26	A	1059	G	N7-C8-N9	5.68	115.94	113.10
1	a	972	C	N3-C2-O2	-5.68	117.92	121.90
26	A	2873	A	N7-C8-N9	5.68	116.64	113.80
23	x	123	C	N3-C4-C5	5.68	124.17	121.90
26	A	240	C	C6-N1-C2	-5.68	118.03	120.30
26	A	1063	G	C4-C5-N7	5.68	113.07	110.80
26	A	889	C	C6-N1-C2	-5.67	118.03	120.30
1	a	63	C	C2-N1-C1'	5.67	125.03	118.80
1	a	225	C	C5-C6-N1	5.67	123.83	121.00
26	A	2305	U	C6-N1-C2	5.67	124.40	121.00
26	A	1595	C	C5-C6-N1	5.66	123.83	121.00
26	A	1963	U	C2-N3-C4	-5.66	123.60	127.00
1	a	1245	C	N3-C4-N4	5.66	121.96	118.00
26	A	1398	C	C6-N1-C2	-5.66	118.04	120.30
22	v	56	C	N1-C2-O2	5.66	122.29	118.90
26	A	1068	G	C4-C5-C6	5.65	122.19	118.80
1	a	1120	C	C6-N1-C2	-5.65	118.04	120.30
1	a	1412	C	N1-C2-O2	5.65	122.29	118.90
1	a	620	C	N3-C2-O2	-5.65	117.94	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	74	C	C2-N1-C1'	5.65	125.01	118.80
26	A	984	A	C8-N9-C4	-5.65	103.54	105.80
1	a	684	U	C2-N3-C4	-5.64	123.61	127.00
26	A	353	C	C2-N3-C4	5.64	122.72	119.90
26	A	898	C	C6-N1-C2	-5.64	118.04	120.30
27	B	70	C	C6-N1-C2	-5.64	118.04	120.30
17	q	74	LEU	CA-CB-CG	5.64	128.28	115.30
23	x	93	G	N9-C4-C5	-5.64	103.14	105.40
26	A	933	A	N3-C4-N9	5.64	131.91	127.40
1	a	590	U	N3-C2-O2	-5.64	118.25	122.20
26	A	399	U	N3-C2-O2	-5.64	118.25	122.20
1	a	211	G	C8-N9-C4	-5.63	104.15	106.40
1	a	212	G	N1-C6-O6	-5.63	116.52	119.90
1	a	536	C	C2-N1-C1'	5.63	124.99	118.80
1	a	708	C	C6-N1-C2	-5.62	118.05	120.30
1	a	1293	C	C5-C6-N1	5.62	123.81	121.00
1	a	912	C	C6-N1-C2	-5.62	118.05	120.30
1	a	1303	C	N1-C2-O2	5.62	122.27	118.90
8	h	95	MET	CA-CB-CG	5.62	122.85	113.30
25	z	427	LEU	CA-CB-CG	5.62	128.22	115.30
23	x	125	G	C3'-C2'-C1'	5.62	105.99	101.50
26	A	2582	G	OP2-P-O3'	5.62	117.55	105.20
26	A	887	U	N1-C2-O2	5.61	126.73	122.80
26	A	1056	G	C4-C5-N7	5.61	113.05	110.80
1	a	80	A	C6-N1-C2	5.61	121.96	118.60
22	v	68	C	C6-N1-C2	-5.61	118.06	120.30
25	z	65	LEU	CB-CG-CD1	-5.61	101.47	111.00
26	A	1084	A	C5-N7-C8	-5.61	101.10	103.90
26	A	1313	U	C5-C6-N1	5.61	125.50	122.70
1	a	16	A	N1-C2-N3	-5.60	126.50	129.30
1	a	23	C	C6-N1-C2	-5.60	118.06	120.30
26	A	669	G	C4-N9-C1'	5.60	133.78	126.50
1	a	611	C	N3-C2-O2	-5.60	117.98	121.90
24	y	63	U	C5-C6-N1	5.60	125.50	122.70
26	A	1658	C	C5-C6-N1	5.59	123.80	121.00
1	a	764	C	C5-C6-N1	5.59	123.80	121.00
26	A	1070	A	C8-N9-C4	5.59	108.04	105.80
1	a	1162	C	C6-N1-C2	-5.59	118.06	120.30
26	A	5	A	N1-C2-N3	-5.59	126.51	129.30
1	a	1308	U	C5-C6-N1	5.59	125.49	122.70
1	a	1435	G	N9-C4-C5	-5.58	103.17	105.40
26	A	669	G	C8-N9-C4	-5.58	104.17	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1639	C	N1-C2-O2	5.58	122.25	118.90
51	Z	16	LEU	CA-CB-CG	5.58	128.13	115.30
1	a	208	U	O4'-C1'-N1	5.58	112.66	108.20
26	A	1150	C	C6-N1-C2	-5.58	118.07	120.30
26	A	1578	U	N1-C2-O2	5.58	126.70	122.80
26	A	1054	A	C5-C6-N6	-5.57	119.24	123.70
1	a	954	G	C5-C6-O6	-5.57	125.26	128.60
26	A	642	U	N3-C2-O2	-5.57	118.30	122.20
26	A	1894	C	N1-C2-O2	5.57	122.24	118.90
26	A	1595	C	C6-N1-C2	-5.57	118.07	120.30
1	a	577	G	N9-C4-C5	-5.56	103.17	105.40
1	a	878	A	C6-C5-N7	-5.56	128.41	132.30
1	a	1435	G	C6-C5-N7	-5.56	127.06	130.40
26	A	2275	C	C6-N1-C2	-5.56	118.08	120.30
1	a	1535	C	N3-C2-O2	-5.56	118.01	121.90
23	x	117	C	C3'-C2'-C1'	5.56	105.95	101.50
27	B	49	C	C6-N1-C2	-5.56	118.08	120.30
1	a	662	U	C5-C4-O4	-5.56	122.57	125.90
1	a	1344	C	C5-C6-N1	5.56	123.78	121.00
9	i	64	ILE	CG1-CB-CG2	-5.56	99.17	111.40
26	A	2579	C	C6-N1-C2	-5.56	118.08	120.30
23	x	117	C	O5'-P-OP2	-5.55	100.70	105.70
26	A	732	C	C6-N1-C2	-5.55	118.08	120.30
26	A	2873	A	C8-N9-C4	-5.55	103.58	105.80
1	a	514	C	C5-C6-N1	5.55	123.78	121.00
1	a	1072	G	C6-C5-N7	-5.55	127.07	130.40
26	A	1830	C	C5-C6-N1	5.55	123.78	121.00
26	A	1787	A	N1-C2-N3	-5.55	126.53	129.30
26	A	2474	U	N1-C2-O2	5.55	126.69	122.80
26	A	2174	C	N1-C2-O2	5.55	122.23	118.90
24	y	40	C	N1-C2-O2	5.55	122.23	118.90
24	y	57	G	O5'-P-OP1	-5.54	100.71	105.70
26	A	1076	C	N1-C2-O2	5.54	122.23	118.90
1	a	446	G	N3-C2-N2	-5.54	116.02	119.90
26	A	722	A	N1-C2-N3	-5.54	126.53	129.30
1	a	1379	G	C6-N1-C2	-5.54	121.78	125.10
1	a	34	C	N1-C2-O2	5.54	122.22	118.90
26	A	1067	A	O4'-C1'-N9	5.54	112.63	108.20
1	a	56	U	C5-C6-N1	5.53	125.47	122.70
26	A	2562	U	N3-C2-O2	-5.53	118.33	122.20
26	A	1894	C	C6-N1-C2	-5.53	118.09	120.30
1	a	706	A	N9-C4-C5	-5.53	103.59	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	63	C	N1-C2-O2	5.53	122.22	118.90
1	a	968	A	N9-C4-C5	5.53	108.01	105.80
1	a	365	U	C5-C6-N1	5.52	125.46	122.70
1	a	428	G	N1-C2-N3	5.52	127.21	123.90
1	a	580	C	N3-C4-N4	5.52	121.86	118.00
1	a	1261	A	N7-C8-N9	-5.52	111.04	113.80
23	x	128	C	C3'-C2'-C1'	5.52	105.92	101.50
24	y	56	C	C5-C6-N1	5.52	123.76	121.00
26	A	509	C	N1-C2-O2	5.52	122.21	118.90
26	A	1963	U	N1-C2-N3	5.52	118.21	114.90
40	O	108	ASP	CB-CG-OD1	5.52	123.27	118.30
1	a	916	U	N3-C2-O2	-5.52	118.34	122.20
1	a	1133	G	N1-C6-O6	-5.52	116.59	119.90
26	A	105	C	C6-N1-C2	-5.52	118.09	120.30
26	A	890	C	P-O3'-C3'	5.52	126.32	119.70
26	A	1171	G	N3-C2-N2	-5.51	116.04	119.90
26	A	2840	C	C5-C6-N1	5.51	123.76	121.00
26	A	1065	U	C5-C4-O4	-5.51	122.59	125.90
26	A	2036	C	N1-C2-O2	5.51	122.21	118.90
1	a	240	G	C6-C5-N7	-5.51	127.09	130.40
26	A	1062	G	O4'-C1'-N9	5.51	112.61	108.20
1	a	494	G	C5-N7-C8	-5.51	101.55	104.30
1	a	312	C	N1-C2-O2	5.50	122.20	118.90
24	y	20	G	N3-C2-N2	5.50	123.75	119.90
26	A	2720	U	N3-C2-O2	-5.50	118.35	122.20
26	A	1763	G	N7-C8-N9	5.50	115.85	113.10
26	A	1788	C	N1-C2-O2	5.50	122.20	118.90
1	a	577	G	C4-C5-N7	5.50	113.00	110.80
26	A	2562	U	N1-C2-O2	5.49	126.64	122.80
1	a	312	C	C2-N1-C1'	5.49	124.84	118.80
26	A	2122	U	N3-C2-O2	-5.49	118.36	122.20
1	a	455	G	C4-C5-N7	5.49	113.00	110.80
1	a	671	G	N1-C6-O6	-5.49	116.61	119.90
26	A	415	A	N1-C2-N3	-5.49	126.56	129.30
26	A	2211	A	N3-C4-C5	-5.49	122.96	126.80
26	A	416	U	N3-C2-O2	-5.49	118.36	122.20
26	A	1956	U	N1-C2-O2	5.48	126.64	122.80
1	a	1073	U	N3-C2-O2	-5.48	118.36	122.20
26	A	2107	G	C5-N7-C8	5.48	107.04	104.30
1	a	316	C	C5-C6-N1	5.48	123.74	121.00
22	v	28	C	C6-N1-C2	-5.48	118.11	120.30
26	A	2077	A	N1-C2-N3	-5.48	126.56	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	528	A	N7-C8-N9	5.48	116.54	113.80
1	a	110	C	N3-C2-O2	-5.48	118.07	121.90
1	a	1496	C	N3-C2-O2	-5.48	118.07	121.90
26	A	1178	C	C2-N3-C4	5.48	122.64	119.90
23	x	110	G	N3-C4-N9	5.47	129.28	126.00
22	v	74	C	C2-N3-C4	5.47	122.64	119.90
26	A	2342	C	C6-N1-C2	-5.47	118.11	120.30
1	a	1105	A	C4-C5-N7	5.47	113.43	110.70
1	a	1366	C	N3-C2-O2	-5.47	118.07	121.90
26	A	2064	C	C6-N1-C2	-5.47	118.11	120.30
26	A	1960	A	N1-C2-N3	-5.47	126.57	129.30
23	x	126	G	O5'-C5'-C4'	5.46	122.08	111.70
26	A	883	G	N1-C6-O6	5.46	123.18	119.90
26	A	1200	C	C5-C6-N1	5.46	123.73	121.00
26	A	1079	C	C6-N1-C2	-5.46	118.12	120.30
26	A	2448	A	O5'-P-OP2	-5.46	100.79	105.70
26	A	128	C	C6-N1-C2	-5.46	118.12	120.30
26	A	435	C	N1-C2-O2	5.46	122.17	118.90
26	A	1057	A	C4-C5-C6	-5.46	114.27	117.00
26	A	2006	C	N1-C2-O2	5.45	122.17	118.90
26	A	1059	G	C6-C5-N7	-5.45	127.13	130.40
26	A	1398	C	N1-C2-O2	5.45	122.17	118.90
23	x	130	G	C3'-C2'-C1'	5.45	105.86	101.50
24	y	27	C	C5-C6-N1	5.45	123.72	121.00
26	A	281	C	C2-N3-C4	5.45	122.62	119.90
26	A	758	C	C6-N1-C2	-5.45	118.12	120.30
24	y	64	G	N1-C6-O6	-5.45	116.63	119.90
1	a	308	C	C6-N1-C2	-5.44	118.12	120.30
23	x	130	G	N9-C1'-C2'	-5.44	106.01	112.00
26	A	141	G	N3-C4-C5	-5.44	125.88	128.60
26	A	2473	U	N1-C2-O2	5.44	126.61	122.80
26	A	2895	G	N1-C6-O6	5.44	123.17	119.90
1	a	412	A	C8-N9-C4	5.44	107.98	105.80
1	a	1435	G	C4-C5-N7	5.44	112.97	110.80
26	A	1150	C	C5-C6-N1	5.44	123.72	121.00
26	A	1585	C	N1-C2-O2	5.44	122.16	118.90
26	A	1920	C	N1-C2-O2	5.44	122.16	118.90
1	a	82	G	N3-C4-N9	5.44	129.26	126.00
1	a	932	C	C2-N1-C1'	5.43	124.78	118.80
26	A	1138	G	C2-N3-C4	5.43	114.62	111.90
1	a	1237	C	OP1-P-O3'	5.43	117.15	105.20
25	z	369	LEU	CA-CB-CG	5.43	127.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	54	LEU	CB-CG-CD1	5.43	120.23	111.00
1	a	1261	A	C8-N9-C4	5.43	107.97	105.80
1	a	397	A	N3-C4-C5	-5.42	123.00	126.80
26	A	1084	A	O4'-C1'-N9	-5.42	103.86	108.20
1	a	61	G	N1-C6-O6	5.42	123.15	119.90
26	A	1564	C	N1-C2-O2	5.42	122.15	118.90
26	A	2325	G	OP1-P-OP2	-5.42	111.47	119.60
26	A	2656	U	C6-N1-C2	-5.42	117.75	121.00
26	A	1902	C	N1-C2-O2	5.42	122.15	118.90
26	A	1103	A	C2-N3-C4	5.42	113.31	110.60
26	A	2800	A	C4-C5-C6	-5.42	114.29	117.00
26	A	2572	A	O5'-P-OP1	-5.42	100.83	105.70
26	A	44	A	N1-C2-N3	-5.42	126.59	129.30
26	A	991	C	C6-N1-C2	-5.42	118.13	120.30
26	A	346	A	N1-C6-N6	-5.41	115.35	118.60
26	A	546	U	C6-N1-C2	-5.41	117.75	121.00
26	A	1062	G	N1-C2-N2	5.41	121.07	116.20
1	a	968	A	O4'-C1'-N9	5.41	112.53	108.20
1	a	354	G	N3-C4-N9	5.41	129.24	126.00
1	a	610	U	N1-C2-O2	5.41	126.58	122.80
1	a	1071	C	N1-C2-O2	5.41	122.14	118.90
1	a	1245	C	C5-C4-N4	-5.41	116.42	120.20
26	A	832	U	N1-C2-N3	5.41	118.14	114.90
26	A	2636	C	N1-C2-O2	5.41	122.14	118.90
51	Z	23	LEU	CB-CG-CD1	-5.40	101.81	111.00
1	a	126	G	C6-C5-N7	5.40	133.64	130.40
1	a	477	C	C6-N1-C2	-5.40	118.14	120.30
1	a	922	G	N3-C2-N2	5.40	123.68	119.90
1	a	623	C	C2-N1-C1'	5.40	124.74	118.80
1	a	1366	C	C2-N1-C1'	5.39	124.73	118.80
22	v	67	C	C5-C6-N1	5.39	123.70	121.00
26	A	1340	U	N3-C2-O2	-5.39	118.43	122.20
31	F	50	ASP	CB-CG-OD1	5.39	123.15	118.30
1	a	348	G	N1-C6-O6	5.39	123.13	119.90
24	y	47(P)	C	N3-C2-O2	-5.39	118.13	121.90
26	A	1914	C	C6-N1-C2	-5.39	118.14	120.30
26	A	2214	C	N3-C2-O2	-5.39	118.13	121.90
26	A	156	A	N1-C2-N3	-5.39	126.61	129.30
24	y	47(P)	C	C5-C6-N1	5.38	123.69	121.00
25	z	536	ILE	CG1-CB-CG2	-5.38	99.55	111.40
26	A	1314	C	C5-C6-N1	5.38	123.69	121.00
1	a	254	G	N3-C4-N9	5.38	129.23	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	p	60	TRP	CA-CB-CG	-5.38	103.47	113.70
26	A	2252	G	N3-C2-N2	-5.38	116.14	119.90
1	a	377	G	C6-C5-N7	5.38	133.62	130.40
26	A	2815	C	N1-C2-O2	5.38	122.12	118.90
1	a	1262	C	N3-C2-O2	-5.37	118.14	121.90
1	a	1448	C	N3-C2-O2	-5.37	118.14	121.90
26	A	1771	C	C5-C6-N1	5.37	123.68	121.00
26	A	2782	G	C6-C5-N7	-5.37	127.18	130.40
1	a	1293	C	N1-C2-O2	5.37	122.12	118.90
26	A	1958	C	C6-N1-C2	-5.37	118.15	120.30
26	A	2226	C	C6-N1-C2	-5.37	118.15	120.30
26	A	1178	C	C6-N1-C2	-5.37	118.15	120.30
26	A	867	C	C6-N1-C2	-5.36	118.15	120.30
26	A	1963	U	N1-C2-O2	-5.36	119.05	122.80
1	a	132	C	C5-C6-N1	5.36	123.68	121.00
26	A	1135	C	OP1-P-O3'	5.36	116.99	105.20
1	a	27	G	C5-C6-O6	-5.36	125.39	128.60
1	a	931	C	C6-N1-C2	-5.36	118.16	120.30
26	A	568	U	N3-C2-O2	-5.36	118.45	122.20
26	A	1892	C	C5-C6-N1	5.36	123.68	121.00
1	a	592	G	N9-C4-C5	5.35	107.54	105.40
1	a	1303	C	C2-N1-C1'	5.35	124.68	118.80
26	A	1072	C	C5-C4-N4	-5.35	116.45	120.20
1	a	175	C	O5'-P-OP2	-5.34	100.89	105.70
26	A	1064	C	C6-N1-C2	-5.34	118.16	120.30
26	A	1945	G	C4-C5-N7	5.34	112.94	110.80
1	a	348	G	N9-C4-C5	-5.34	103.27	105.40
27	B	26	C	N3-C2-O2	-5.34	118.17	121.90
1	a	1149	C	N3-C2-O2	-5.33	118.17	121.90
26	A	133	U	N3-C2-O2	-5.33	118.47	122.20
1	a	307	C	N1-C2-O2	5.33	122.10	118.90
1	a	359	G	C6-C5-N7	5.33	133.60	130.40
1	a	1344	C	N3-C2-O2	-5.33	118.17	121.90
26	A	1072	C	C5'-C4'-O4'	5.33	115.50	109.10
1	a	1435	G	C5-C6-O6	-5.33	125.40	128.60
26	A	2666	C	N3-C2-O2	-5.33	118.17	121.90
1	a	1261	A	C5-N7-C8	5.33	106.56	103.90
1	a	1403	C	N1-C2-O2	5.32	122.09	118.90
26	A	1557	C	C6-N1-C2	-5.32	118.17	120.30
26	A	2207	C	C5-C6-N1	5.32	123.66	121.00
1	a	551	U	N3-C4-O4	5.32	123.13	119.40
26	A	965	C	C6-N1-C2	-5.32	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1313	U	C6-N1-C2	-5.32	117.81	121.00
26	A	447	A	C6-N1-C2	5.32	121.79	118.60
26	A	982	C	C6-N1-C2	-5.32	118.17	120.30
26	A	2827	C	C6-N1-C2	-5.32	118.17	120.30
23	x	93	G	C5-N7-C8	-5.32	101.64	104.30
26	A	601	C	C6-N1-C2	-5.32	118.17	120.30
26	A	2710	C	C6-N1-C2	-5.32	118.17	120.30
23	x	125	G	C4'-C3'-O3'	5.31	123.63	113.00
26	A	2080	A	C4-C5-N7	5.31	113.36	110.70
22	v	32	C	C6-N1-C2	-5.31	118.18	120.30
26	A	528	A	C2-N3-C4	-5.31	107.94	110.60
26	A	1056	G	C2-N3-C4	-5.31	109.25	111.90
23	x	130	G	O4'-C1'-N9	5.31	112.45	108.20
26	A	44	A	N9-C4-C5	-5.31	103.68	105.80
1	a	1404	C	C6-N1-C2	-5.30	118.18	120.30
1	a	444	G	N9-C1'-C2'	-5.30	106.17	112.00
1	a	426	U	C5-C6-N1	5.30	125.35	122.70
1	a	496	A	C5-C6-N6	-5.30	119.46	123.70
1	a	1524	C	C2-N1-C1'	5.30	124.63	118.80
1	a	240	G	N9-C4-C5	-5.30	103.28	105.40
26	A	1348	C	N3-C2-O2	-5.30	118.19	121.90
26	A	2175	C	C6-N1-C2	-5.30	118.18	120.30
26	A	130	C	C6-N1-C2	-5.29	118.18	120.30
26	A	883	G	N3-C4-N9	5.29	129.18	126.00
26	A	1086	A	C5-N7-C8	-5.29	101.25	103.90
1	a	221	C	N1-C2-O2	5.29	122.07	118.90
26	A	231	A	C8-N9-C4	5.29	107.92	105.80
1	a	1060	U	N3-C2-O2	-5.29	118.50	122.20
26	A	968	C	C5-C6-N1	5.29	123.64	121.00
26	A	2281	A	N9-C4-C5	-5.29	103.69	105.80
1	a	103	U	N1-C2-O2	5.28	126.50	122.80
26	A	1056	G	N3-C4-C5	5.28	131.24	128.60
1	a	1326	U	N1-C2-O2	5.28	126.49	122.80
22	v	19	G	N1-C6-O6	-5.28	116.73	119.90
26	A	2153	C	C6-N1-C2	-5.28	118.19	120.30
26	A	1305	C	N1-C2-O2	5.27	122.06	118.90
1	a	656	G	N9-C4-C5	5.27	107.51	105.40
26	A	1104	C	N1-C2-O2	5.27	122.06	118.90
1	a	428	G	N9-C4-C5	5.27	107.51	105.40
25	z	461	LEU	CA-CB-CG	5.27	127.42	115.30
26	A	2805	C	C6-N1-C2	-5.27	118.19	120.30
1	a	1063	C	C6-N1-C2	-5.27	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2188	U	C5-C4-O4	-5.27	122.74	125.90
26	A	2300	C	N1-C2-O2	5.27	122.06	118.90
1	a	381	C	C6-N1-C2	-5.26	118.19	120.30
22	v	67	C	C2-N1-C1'	5.26	124.59	118.80
23	x	110	G	N3-C4-C5	-5.26	125.97	128.60
26	A	61	C	N1-C2-O2	5.26	122.06	118.90
26	A	845	A	N1-C2-N3	-5.26	126.67	129.30
26	A	959	A	C5-N7-C8	5.26	106.53	103.90
26	A	1472	C	C6-N1-C2	-5.26	118.20	120.30
26	A	2050	C	C2-N3-C4	5.26	122.53	119.90
1	a	529	G	N9-C4-C5	-5.26	103.30	105.40
22	v	25	C	C6-N1-C2	-5.26	118.20	120.30
26	A	1881	C	C6-N1-C2	-5.26	118.20	120.30
1	a	427	U	N1-C2-O2	-5.26	119.12	122.80
22	v	74	C	N3-C4-N4	5.26	121.68	118.00
26	A	2049	G	C6-C5-N7	-5.26	127.25	130.40
1	a	354	G	C4-C5-N7	5.26	112.90	110.80
1	a	986	U	C5-C4-O4	-5.26	122.75	125.90
1	a	912	C	C5-C6-N1	5.25	123.63	121.00
26	A	1123	C	C6-N1-C2	-5.25	118.20	120.30
1	a	426	U	C6-N1-C2	-5.25	117.85	121.00
26	A	411	G	O5'-P-OP2	-5.25	100.97	105.70
1	a	923	A	C6-C5-N7	-5.25	128.63	132.30
26	A	811	U	N3-C4-O4	-5.25	115.73	119.40
1	a	717	U	C5-C4-O4	-5.25	122.75	125.90
26	A	98	G	C2-N3-C4	5.25	114.52	111.90
26	A	1080	A	C8-N9-C4	-5.25	103.70	105.80
25	z	509	VAL	CA-CB-CG1	5.24	118.77	110.90
1	a	308	C	N3-C2-O2	-5.24	118.23	121.90
1	a	482	A	C5-N7-C8	-5.24	101.28	103.90
26	A	281	C	C2-N1-C1'	5.24	124.57	118.80
1	a	1304	G	O5'-P-OP2	-5.24	100.98	105.70
26	A	222	A	O4'-C1'-N9	-5.24	104.01	108.20
26	A	1349	C	C6-N1-C2	-5.24	118.20	120.30
1	a	1197	A	N1-C6-N6	5.24	121.74	118.60
26	A	143	C	C5-C6-N1	5.24	123.62	121.00
26	A	1472	C	C5-C6-N1	5.24	123.62	121.00
1	a	42	G	N1-C6-O6	5.24	123.04	119.90
1	a	218	U	P-O3'-C3'	5.24	125.98	119.70
23	x	119	G	C8-N9-C4	-5.24	104.31	106.40
1	a	205	A	N7-C8-N9	5.23	116.42	113.80
1	a	295	C	N1-C2-O2	5.23	122.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	424	G	C4-C5-N7	-5.23	108.71	110.80
1	a	739	C	C6-N1-C2	-5.23	118.21	120.30
2	b	211	LEU	CA-CB-CG	5.23	127.33	115.30
1	a	1118	U	N3-C4-O4	5.23	123.06	119.40
1	a	878	A	N3-C4-N9	5.23	131.58	127.40
1	a	1148	U	N1-C2-O2	5.23	126.46	122.80
22	v	28	C	N1-C2-O2	5.23	122.04	118.90
1	a	735	C	C5-C6-N1	5.22	123.61	121.00
1	a	1063	C	C5-C6-N1	5.22	123.61	121.00
26	A	544	C	C5-C6-N1	5.22	123.61	121.00
26	A	1997	C	O5'-P-OP2	-5.22	101.00	105.70
26	A	2529	G	C2-N3-C4	5.22	114.51	111.90
1	a	550	G	C2-N3-C4	5.22	114.51	111.90
1	a	551	U	C2-N1-C1'	5.22	123.97	117.70
1	a	1495	U	N3-C2-O2	-5.22	118.54	122.20
1	a	1386	G	C4-C5-N7	-5.22	108.71	110.80
22	v	14	A	C5-C6-N1	5.22	120.31	117.70
26	A	2556	C	N1-C2-O2	5.22	122.03	118.90
1	a	215	C	C2-N1-C1'	5.22	124.54	118.80
26	A	1044	C	C4-C5-C6	-5.22	114.79	117.40
26	A	2888	C	C6-N1-C2	-5.22	118.21	120.30
1	a	61	G	C4-C5-N7	5.21	112.89	110.80
1	a	427	U	C6-N1-C1'	5.21	128.50	121.20
26	A	1044	C	C2-N3-C4	5.21	122.51	119.90
26	A	2556	C	N3-C2-O2	-5.21	118.25	121.90
26	A	266	G	C6-C5-N7	-5.21	127.27	130.40
26	A	1314	C	C2-N1-C1'	5.21	124.53	118.80
32	G	104	LEU	CA-CB-CG	5.21	127.28	115.30
26	A	1380	G	C6-C5-N7	-5.21	127.28	130.40
26	A	2431	U	N3-C2-O2	-5.21	118.56	122.20
1	a	396	C	N1-C2-O2	5.20	122.02	118.90
25	z	559	ASP	CB-CG-OD1	5.20	122.98	118.30
1	a	526	C	C5-C4-N4	-5.20	116.56	120.20
1	a	582	C	N1-C2-O2	5.20	122.02	118.90
1	a	1158	C	C2-N1-C1'	5.20	124.52	118.80
1	a	1448	C	N3-C4-N4	5.20	121.64	118.00
4	d	142	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	a	452	A	C2-N3-C4	5.20	113.20	110.60
26	A	183	C	N1-C2-O2	5.20	122.02	118.90
13	m	64	VAL	CA-CB-CG1	5.20	118.70	110.90
26	A	1089	A	C8-N9-C4	-5.20	103.72	105.80
26	A	21	A	N1-C2-N3	-5.20	126.70	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	528	A	N1-C2-N3	5.20	131.90	129.30
26	A	2064	C	C2-N1-C1'	5.20	124.52	118.80
1	a	1120	C	C2-N1-C1'	5.19	124.51	118.80
25	z	256	LEU	CB-CG-CD2	-5.19	102.18	111.00
26	A	721	A	N9-C4-C5	-5.19	103.72	105.80
26	A	1399	C	C5-C6-N1	5.19	123.60	121.00
1	a	61	G	C5-C6-O6	-5.19	125.49	128.60
26	A	1771	C	C6-N1-C2	-5.19	118.22	120.30
15	o	55	LEU	CA-CB-CG	5.18	127.22	115.30
26	A	2417	C	C6-N1-C2	-5.18	118.23	120.30
1	a	580	C	N3-C2-O2	-5.18	118.27	121.90
27	B	90	C	C6-N1-C2	-5.18	118.23	120.30
1	a	392	C	C6-N1-C2	-5.18	118.23	120.30
1	a	1246	A	N1-C2-N3	-5.18	126.71	129.30
1	a	178	C	N1-C2-O2	5.18	122.01	118.90
26	A	143	C	C6-N1-C2	-5.18	118.23	120.30
26	A	1744	A	C2-N3-C4	5.18	113.19	110.60
1	a	483	C	C5-C6-N1	5.18	123.59	121.00
26	A	548	G	C5-C6-O6	-5.18	125.49	128.60
3	c	30	ASP	CB-CG-OD1	5.17	122.96	118.30
34	H	122	LEU	CB-CG-CD2	-5.17	102.20	111.00
1	a	1412	C	N3-C4-N4	5.17	121.62	118.00
26	A	1447	C	C6-N1-C2	-5.17	118.23	120.30
26	A	2153	C	N1-C2-O2	5.17	122.00	118.90
26	A	2380	C	C6-N1-C2	-5.17	118.23	120.30
1	a	739	C	N1-C2-O2	5.17	122.00	118.90
1	a	1131	G	C5-N7-C8	-5.17	101.72	104.30
1	a	1138	G	C2-N3-C4	5.17	114.48	111.90
26	A	740	C	N1-C2-O2	5.17	122.00	118.90
26	A	1990	C	C6-N1-C2	-5.17	118.23	120.30
26	A	2205	A	N9-C4-C5	-5.17	103.73	105.80
26	A	1080	A	N1-C2-N3	5.16	131.88	129.30
1	a	1392	G	N1-C6-O6	5.16	123.00	119.90
26	A	544	C	C2-N1-C1'	5.16	124.48	118.80
26	A	2080	A	N1-C6-N6	5.16	121.70	118.60
1	a	1069	C	C6-N1-C2	-5.16	118.24	120.30
24	y	6	U	N1-C2-O2	5.16	126.41	122.80
26	A	1044	C	OP2-P-O3'	5.16	116.55	105.20
26	A	1056	G	C5-N7-C8	-5.16	101.72	104.30
26	A	2302	U	N1-C2-O2	5.16	126.41	122.80
26	A	2043	C	N1-C2-O2	5.16	121.99	118.90
26	A	1080	A	C2-N3-C4	-5.15	108.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	27	G	N9-C4-C5	-5.15	103.34	105.40
1	a	79	G	N3-C2-N2	-5.15	116.30	119.90
1	a	739	C	C5-C6-N1	5.15	123.58	121.00
1	a	1448	C	C5-C4-N4	-5.15	116.59	120.20
4	d	149	LYS	C-N-CA	5.15	134.58	121.70
26	A	946	C	C5-C6-N1	5.15	123.58	121.00
26	A	732	C	C5-C6-N1	5.15	123.57	121.00
26	A	1171	G	N1-C6-O6	-5.14	116.81	119.90
40	O	69	ASP	CB-CG-OD1	5.14	122.93	118.30
1	a	878	A	N1-C6-N6	5.14	121.69	118.60
22	v	21	A	C5-C6-N1	5.14	120.27	117.70
28	C	65	ASP	CB-CG-OD1	5.14	122.93	118.30
1	a	496	A	N9-C4-C5	-5.14	103.75	105.80
26	A	754	U	N3-C2-O2	-5.14	118.61	122.20
57	6	4	ASP	CB-CG-OD1	5.13	122.92	118.30
26	A	1105	U	N1-C1'-C2'	-5.13	106.36	112.00
26	A	1455	G	N3-C4-N9	5.13	129.08	126.00
31	F	11	VAL	CG1-CB-CG2	-5.13	102.69	110.90
26	A	1585	C	N3-C2-O2	-5.13	118.31	121.90
1	a	413	G	C2-N3-C4	-5.13	109.34	111.90
49	X	3	VAL	CA-CB-CG2	5.13	118.59	110.90
1	a	1284	C	C6-N1-C2	-5.13	118.25	120.30
1	a	799	G	N9-C4-C5	5.12	107.45	105.40
26	A	2023	C	C6-N1-C2	-5.12	118.25	120.30
1	a	1494	G	N3-C4-N9	5.12	129.07	126.00
1	a	163	C	C5-C6-N1	5.12	123.56	121.00
27	B	89	U	OP1-P-O3'	5.12	116.46	105.20
1	a	555	U	C5-C6-N1	5.12	125.26	122.70
22	v	27	U	N3-C4-O4	5.12	122.98	119.40
1	a	23	C	C5-C6-N1	5.11	123.56	121.00
1	a	213	G	N1-C2-N3	5.11	126.97	123.90
1	a	578	C	C6-N1-C2	-5.11	118.25	120.30
26	A	891	G	N1-C6-O6	5.11	122.97	119.90
26	A	1091	G	N7-C8-N9	-5.11	110.54	113.10
47	V	40	ILE	CG1-CB-CG2	-5.11	100.15	111.40
1	a	219	U	C6-N1-C2	-5.11	117.93	121.00
26	A	101	A	N3-C4-N9	-5.11	123.31	127.40
1	a	191	G	N9-C4-C5	-5.11	103.36	105.40
26	A	1005	C	N1-C2-O2	5.11	121.96	118.90
26	A	2280	G	N9-C4-C5	-5.11	103.36	105.40
1	a	879	C	C6-N1-C2	-5.10	118.26	120.30
1	a	1172	C	C2-N1-C1'	5.10	124.41	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	126	G	C5-C6-O6	5.10	131.66	128.60
24	y	47	G	N3-C4-N9	-5.10	122.94	126.00
26	A	2301	C	C6-N1-C2	-5.10	118.26	120.30
1	a	1529	G	C6-C5-N7	-5.09	127.34	130.40
26	A	1046	A	C8-N9-C4	-5.09	103.76	105.80
26	A	2259	U	N3-C2-O2	-5.09	118.63	122.20
1	a	37	U	N1-C2-N3	5.09	117.96	114.90
26	A	2011	U	N1-C2-O2	5.09	126.36	122.80
1	a	334	C	C5-C6-N1	5.09	123.55	121.00
1	a	491	G	C8-N9-C1'	-5.09	120.38	127.00
26	A	892	A	N1-C2-N3	5.09	131.85	129.30
26	A	1656	C	C6-N1-C2	-5.09	118.26	120.30
1	a	1083	U	N3-C2-O2	-5.09	118.64	122.20
26	A	2895	G	N9-C4-C5	-5.09	103.36	105.40
23	x	108	A	N7-C8-N9	-5.09	111.26	113.80
26	A	807	U	N3-C2-O2	-5.09	118.64	122.20
1	a	340	U	N3-C2-O2	-5.08	118.64	122.20
1	a	377	G	N9-C4-C5	5.08	107.43	105.40
1	a	1392	G	C5-C6-O6	-5.08	125.55	128.60
1	a	82	G	N9-C4-C5	-5.08	103.37	105.40
1	a	1210	C	N1-C2-O2	5.08	121.95	118.90
5	e	80	LEU	CB-CG-CD2	-5.08	102.36	111.00
23	x	121	U	C2-N3-C4	5.08	130.05	127.00
26	A	1105	U	O4'-C1'-N1	5.08	112.26	108.20
1	a	316	C	C6-N1-C1'	-5.07	114.71	120.80
1	a	706	A	N1-C2-N3	-5.07	126.76	129.30
26	A	2252	G	C5-C6-O6	5.07	131.64	128.60
1	a	1432	G	C8-N9-C4	-5.07	104.37	106.40
26	A	1058	U	C4-C5-C6	-5.07	116.66	119.70
1	a	206	C	N3-C4-C5	-5.07	119.87	121.90
1	a	805	C	C5-C6-N1	5.07	123.53	121.00
22	v	49	G	N9-C4-C5	-5.07	103.37	105.40
26	A	2267	A	C5-C6-N1	5.07	120.23	117.70
1	a	993	G	C8-N9-C1'	-5.07	120.41	127.00
1	a	1203	C	N1-C2-O2	5.07	121.94	118.90
26	A	783	A	N3-C4-N9	5.07	131.45	127.40
46	U	6	ARG	N-CA-CB	-5.07	101.48	110.60
23	x	115	A	O3'-P-O5'	5.06	113.62	104.00
1	a	806	C	C6-N1-C2	-5.06	118.28	120.30
1	a	1097	C	N3-C2-O2	-5.06	118.36	121.90
1	a	1467	C	N1-C2-O2	5.06	121.93	118.90
26	A	1005	C	C6-N1-C2	-5.05	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2129	C	N3-C2-O2	-5.05	118.36	121.90
1	a	443	C	C5-C6-N1	5.05	123.53	121.00
1	a	34	C	N3-C4-N4	5.05	121.54	118.00
1	a	439	U	N3-C2-O2	-5.05	118.67	122.20
1	a	1430	A	N9-C4-C5	-5.05	103.78	105.80
22	v	6	G	N1-C6-O6	-5.05	116.87	119.90
26	A	1287	A	C6-N1-C2	5.05	121.63	118.60
26	A	1047	G	O4'-C1'-N9	5.05	112.24	108.20
1	a	862	C	C6-N1-C2	-5.05	118.28	120.30
1	a	1344	C	C2-N1-C1'	5.05	124.35	118.80
26	A	2388	A	N7-C8-N9	-5.05	111.28	113.80
26	A	2121	G	C5-C6-O6	5.04	131.63	128.60
1	a	496	A	N3-C4-N9	5.04	131.44	127.40
26	A	2252	G	C6-C5-N7	5.04	133.43	130.40
1	a	491	G	C5-C6-O6	-5.04	125.58	128.60
13	m	47	LEU	CA-CB-CG	5.04	126.89	115.30
26	A	2194	U	N3-C2-O2	-5.04	118.67	122.20
1	a	1203	C	C5-C6-N1	5.04	123.52	121.00
25	z	157	LEU	CB-CG-CD2	-5.04	102.44	111.00
26	A	146	A	N1-C2-N3	-5.03	126.78	129.30
26	A	1960	A	N9-C4-C5	-5.03	103.79	105.80
1	a	231	U	N3-C2-O2	-5.03	118.68	122.20
1	a	384	G	N9-C4-C5	-5.03	103.39	105.40
1	a	1193	G	N1-C6-O6	-5.03	116.88	119.90
26	A	836	G	C5-C6-O6	-5.03	125.58	128.60
26	A	919	U	N1-C2-O2	5.03	126.32	122.80
27	B	57	A	C2-N3-C4	5.03	113.11	110.60
19	s	66	VAL	CG1-CB-CG2	-5.02	102.86	110.90
25	z	328	ALA	N-CA-CB	5.02	117.13	110.10
9	i	120	ALA	N-CA-CB	5.02	117.13	110.10
26	A	1830	C	C2-N1-C1'	5.02	124.32	118.80
14	n	17	ASP	CB-CG-OD1	5.02	122.81	118.30
26	A	2281	A	N1-C2-N3	-5.02	126.79	129.30
26	A	2468	A	N1-C2-N3	5.02	131.81	129.30
1	a	635	A	N9-C4-C5	-5.01	103.80	105.80
1	a	1140	C	C6-N1-C2	-5.01	118.29	120.30
26	A	1071	G	N9-C1'-C2'	-5.01	106.48	112.00
26	A	2150	C	C5-C6-N1	5.01	123.51	121.00
27	B	120	U	N3-C2-O2	-5.01	118.69	122.20
26	A	968	C	C6-N1-C2	-5.01	118.30	120.30
26	A	1763	G	C8-N9-C4	-5.01	104.39	106.40
26	A	2254	C	N3-C2-O2	-5.01	118.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1470	U	N1-C2-O2	5.01	126.31	122.80
23	x	127	U	C4'-C3'-O3'	-5.01	98.88	109.40
26	A	1599	U	C5-C6-N1	5.01	125.20	122.70
26	A	1993	U	N1-C2-N3	5.01	117.91	114.90
1	a	1068	G	N1-C6-O6	5.00	122.90	119.90
1	a	1540	U	N1-C2-N3	5.00	117.90	114.90
26	A	582	A	N9-C4-C5	-5.00	103.80	105.80
26	A	1600	C	N1-C2-O2	5.00	121.90	118.90
26	A	305	C	N1-C2-O2	5.00	121.90	118.90
26	A	2778	A	N1-C2-N3	-5.00	126.80	129.30
26	A	2769	U	N1-C2-O2	5.00	126.30	122.80

All (4) chirality outliers are listed below:

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

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	C	120	ASP	Peptide
34	H	8	LYS	Peptide
46	U	5	ARG	Peptide
2	b	17	HIS	Mainchain
6	f	93	LYS	Peptide
9	i	101	GLY	Mainchain
9	i	56	MET	Mainchain
12	l	100	ALA	Mainchain,Peptide
14	n	36	SER	Peptide
14	n	37	ASP	Mainchain
18	r	10	CYS	Mainchain
25	z	190	LEU	Peptide
25	z	300	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33029	0	16643	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
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	1642	0	839	0	0
23	x	1025	0	518	0	0
24	y	2031	0	1039	0	0
25	z	4853	0	4831	0	0
26	A	62335	0	31374	337	0
27	B	2570	0	1301	12	0
28	C	2083	0	2157	24	0
29	D	1565	0	1616	25	0
30	E	1552	0	1619	21	0
31	F	1411	0	1447	21	0
32	G	1323	0	1374	39	0
33	I	1032	0	1088	31	0
34	H	1111	0	1148	12	0
35	J	1129	0	1162	11	0
36	K	939	0	1012	12	0
37	L	1045	0	1117	15	0
38	M	1074	0	1157	15	0
39	N	961	0	1000	8	0
40	O	892	0	923	11	0
41	P	917	0	965	8	0
42	Q	947	0	1022	15	0
43	R	816	0	839	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	S	857	0	922	7	0
45	T	739	0	807	10	0
46	U	780	0	834	11	0
47	V	753	0	780	5	0
48	W	575	0	592	8	0
49	X	625	0	655	4	0
50	Y	509	0	543	6	0
51	Z	449	0	491	7	0
52	0	444	0	461	2	0
53	1	410	0	440	4	0
54	2	377	0	418	5	0
55	3	504	0	574	5	0
56	4	302	0	339	6	0
57	6	523	0	521	6	0
58	w	62	0	34	0	0
59	v	10	0	10	0	0
60	y	6	0	3	0	0
61	z	32	0	13	0	0
62	z	1	0	0	0	0
63	4	1	0	0	0	0
63	6	1	0	0	0	0
64	z	2	0	0	0	0
All	All	152981	0	104086	607	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 5.

All (607) 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)
26:A:2167:U:C2	26:A:2169:A:N7	2.27	1.01
26:A:1047:G:N2	26:A:1111:A:N7	2.12	0.96
26:A:410:G:N3	26:A:432:A:N6	41.76	0.92
26:A:279:A:N6	26:A:361:G:N3	2.18	0.90
26:A:410:G:N2	26:A:432:A:N7	41.35	0.84
33:I:17:ALA:HB2	33:I:42:ASN:HD21	1.46	0.79
26:A:1059:G:H1	33:I:127:SER:HG	1.31	0.77
26:A:1039:A:H61	26:A:1116:G:H1	1.34	0.75
39:N:35:LYS:NZ	39:N:110:MET:SD	2.62	0.73
26:A:1044:C:O2'	26:A:1111:A:N1	2.24	0.71
26:A:1082:U:O4	26:A:1086:A:N7	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1082:U:N3	26:A:1086:A:N6	2.39	0.70
32:G:15:ASP:HB3	32:G:26:LYS:HB3	1.73	0.70
33:I:30:GLN:HB3	33:I:60:VAL:HG11	1.73	0.69
26:A:545:U:O2	26:A:548:G:O6	2.11	0.69
30:E:49:ARG:HE	30:E:75:SER:HA	1.58	0.69
26:A:1056:G:O2'	26:A:1103:A:N6	2.26	0.68
28:C:181:ARG:NH1	28:C:182:LYS:O	2.27	0.68
26:A:1068:G:N3	26:A:1095:A:O2'	2.27	0.68
26:A:2830:C:OP2	29:D:59:ARG:NH2	2.27	0.67
47:V:32:GLY:O	47:V:93:ARG:NH2	2.28	0.67
26:A:1250:G:N7	37:L:18:ARG:NH2	2.43	0.66
26:A:2167:U:N3	26:A:2169:A:N7	2.42	0.66
26:A:2344:U:OP1	53:1:36:LYS:NZ	2.27	0.66
26:A:491:G:O6	44:S:49:LYS:NZ	2.28	0.66
29:D:128:ARG:NH1	29:D:129:THR:O	2.28	0.66
33:I:64:ARG:NH1	33:I:65:SER:OG	2.29	0.66
32:G:54:ARG:HB2	32:G:57:TYR:HD2	1.61	0.66
45:T:19:LYS:NZ	45:T:84:TYR:OH	2.29	0.66
53:1:16:THR:HG21	53:1:41:VAL:HG11	1.78	0.65
37:L:63:LYS:O	55:3:29:ARG:NH1	2.29	0.65
33:I:78:LEU:O	33:I:82:ALA:HB3	1.96	0.64
31:F:41:GLU:OE2	31:F:147:ARG:NH2	2.29	0.64
48:W:16:ARG:O	48:W:35:ARG:NH1	2.31	0.64
26:A:2199:A:OP1	49:X:36:ARG:NH2	2.31	0.64
44:S:3:THR:HG21	44:S:58:ALA:HB2	1.79	0.63
26:A:764:A:N3	28:C:211:ARG:NH1	2.46	0.63
26:A:2167:U:O2	26:A:2169:A:N7	2.32	0.63
32:G:132:LEU:HD13	32:G:143:VAL:HG23	1.80	0.63
26:A:1798:U:OP2	28:C:270:ARG:NH2	2.31	0.63
27:B:48:U:OP1	40:O:30:ARG:NH2	2.32	0.62
29:D:109:VAL:HG12	29:D:203:VAL:HG12	1.82	0.62
26:A:2334:U:O2'	40:O:13:ARG:NH2	2.31	0.62
26:A:2530:A:O2'	26:A:2534:A:N6	2.33	0.62
26:A:1783:A:HO2'	26:A:2607:G:HO2'	1.47	0.62
32:G:32:LEU:HD11	32:G:135:ALA:HB1	1.80	0.62
57:6:28:VAL:HG11	57:6:32:LEU:HD23	1.82	0.61
30:E:159:LEU:HA	30:E:162:ARG:HE	1.64	0.61
26:A:1039:A:N6	26:A:1116:G:H1	1.98	0.61
26:A:2848:G:O2'	26:A:2867:G:N2	2.33	0.61
38:M:47:GLU:OE1	38:M:51:ARG:NH1	2.34	0.61
26:A:771:G:OP2	54:2:11:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2221:G:H21	28:C:146:LYS:HE2	1.64	0.61
26:A:77:G:OP1	50:Y:52:ARG:NH2	2.34	0.61
32:G:21:GLN:OE1	32:G:54:ARG:NH2	2.30	0.60
29:D:97:SER:OG	29:D:99:GLU:OE1	2.14	0.60
26:A:1827:U:OP2	28:C:220:ARG:NH1	2.35	0.60
26:A:197:A:N6	26:A:2430:A:O2'	2.35	0.60
26:A:532:A:N1	26:A:2035:G:N2	2.50	0.60
31:F:134:GLN:NE2	31:F:149:ARG:O	2.34	0.60
28:C:16:VAL:HG12	28:C:203:VAL:HG22	1.83	0.60
26:A:573:U:OP2	43:R:80:ARG:NH2	2.34	0.60
26:A:187:G:N2	26:A:190:A:OP2	11.54	0.60
33:I:36:GLU:OE2	33:I:64:ARG:NH2	2.35	0.60
26:A:1056:G:N1	26:A:1102:C:OP2	2.23	0.60
26:A:956:G:N2	26:A:960:A:OP2	2.34	0.60
34:H:9:VAL:HG22	34:H:35:LYS:HD3	1.83	0.60
26:A:1059:G:N1	33:I:127:SER:OG	2.34	0.60
30:E:148:ILE:HB	30:E:169:VAL:HG22	1.84	0.59
26:A:475:C:O2	26:A:479:A:N6	2.36	0.59
45:T:11:LEU:O	50:Y:29:ARG:NH1	2.31	0.59
26:A:245:G:N7	55:3:7:ARG:NH2	2.50	0.59
26:A:1248:G:OP1	30:E:44:ARG:NH2	2.36	0.59
26:A:276:U:O2'	26:A:278:A:N6	2.36	0.59
30:E:117:ARG:NH2	30:E:183:PHE:O	2.36	0.59
26:A:1063:G:C4	33:I:90:GLY:HA2	2.38	0.58
26:A:1601:G:OP1	45:T:64:LYS:NZ	2.35	0.58
26:A:698:C:O2'	26:A:734:A:N6	2.36	0.58
37:L:77:ILE:HD13	37:L:101:ILE:HD11	1.85	0.58
43:R:69:GLY:O	43:R:90:ARG:NE	2.29	0.58
26:A:329:G:H1	46:U:16:LYS:HZ3	1.51	0.58
32:G:29:ASN:OD1	32:G:30:GLY:N	2.37	0.58
31:F:51:ASN:O	31:F:55:ASP:HB2	2.03	0.58
26:A:2742:G:OP1	56:4:36:ARG:NH1	2.37	0.58
26:A:1083:U:H1'	26:A:1084:A:H8	1.69	0.58
26:A:1056:G:H5"	26:A:1086:A:H2	1.69	0.58
36:K:25:LEU:O	36:K:30:ARG:NH1	2.37	0.58
26:A:337:C:OP1	46:U:3:LYS:NZ	2.36	0.57
26:A:1093:G:H1	26:A:1097:U:H5"	1.69	0.57
26:A:1378:A:O2'	26:A:1380:G:OP2	2.22	0.57
26:A:910:A:N3	26:A:2264:C:O2'	2.38	0.57
29:D:32:ASN:OD1	29:D:52:THR:OG1	2.22	0.57
26:A:1288:G:OP2	26:A:1288:G:N2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1082:U:H3	26:A:1086:A:N6	2.03	0.57
26:A:1869:G:N2	26:A:1872:A:OP2	2.37	0.57
26:A:2099:U:H3	26:A:2190:G:H1	1.51	0.57
32:G:34:ARG:HG2	32:G:70:LEU:HD13	1.87	0.57
33:I:110:GLN:HA	33:I:113:ALA:HB2	1.85	0.57
33:I:96:LYS:HG3	33:I:138:VAL:HG21	1.85	0.56
26:A:877:A:O2'	26:A:900:A:N6	2.29	0.56
26:A:2121:G:OP1	26:A:2168:G:N2	2.38	0.56
26:A:2220:U:H5"	34:H:97:ARG:HH21	1.70	0.56
26:A:2809:A:OP2	26:A:2890:G:N1	2.38	0.56
26:A:1365:A:OP1	49:X:2:ARG:NH1	2.39	0.56
26:A:404:A:N6	26:A:421:C:O2'	2.38	0.56
33:I:52:LEU:HD23	33:I:73:PRO:HB3	1.87	0.56
26:A:1528:A:N6	26:A:1543:G:O2'	2.39	0.56
26:A:2167:U:N3	26:A:2169:A:C8	2.74	0.56
26:A:959:A:N3	26:A:2457:PSU:O2'	2.36	0.56
26:A:818:G:H21	26:A:1189:A:H62	1.54	0.55
29:D:148:GLN:HB2	29:D:152:PRO:HG2	1.87	0.55
33:I:129:GLU:HB3	33:I:133:ARG:HH12	1.71	0.55
38:M:17:ASN:O	38:M:38:ARG:NH1	2.38	0.55
44:S:88:ARG:NH2	44:S:94:ASP:OD2	2.39	0.55
26:A:279:A:H61	26:A:361:G:H1'	1.70	0.55
56:4:25:VAL:HB	56:4:35:GLN:HB2	1.89	0.55
26:A:545:U:O2	26:A:548:G:C6	2.59	0.55
41:P:90:ALA:HA	41:P:112:ARG:HE	1.71	0.55
50:Y:2:LYS:HD2	50:Y:56:LEU:HD11	1.88	0.55
26:A:1011:G:OP1	42:Q:74:SER:OG	2.24	0.55
26:A:776:G:N7	26:A:793:A:O2'	2.35	0.55
32:G:87:GLN:HA	32:G:129:GLU:HA	1.88	0.55
35:J:105:VAL:HG12	35:J:109:LEU:HD23	1.89	0.55
26:A:754:U:O2'	26:A:1272:A:N1	2.39	0.55
26:A:1682:G:OP2	26:A:1699:G:N2	2.40	0.55
26:A:805:G:H22	26:A:828:U:H5"	1.71	0.55
26:A:563:A:N6	26:A:884:U:O2	105.48	0.55
26:A:1060:U:O2'	35:J:58:ASN:ND2	83.47	0.55
38:M:30:SER:N	38:M:106:ASP:OD1	2.37	0.55
26:A:1086:A:O2'	26:A:1087:G:N7	2.39	0.54
26:A:2788:C:O2'	26:A:2809:A:N3	2.36	0.54
26:A:1807:G:N2	26:A:1810:A:OP2	2.38	0.54
26:A:2485:G:OP1	38:M:45:GLN:NE2	2.41	0.54
26:A:1153:C:OP1	42:Q:91:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1077:A:H3'	26:A:1078:U:O4'	2.07	0.54
26:A:961:C:OP1	26:A:2456:C:O2'	2.21	0.54
43:R:60:LYS:HB2	43:R:99:THR:O	2.07	0.54
51:Z:39:ASP:OD2	51:Z:44:ARG:NH1	2.40	0.54
26:A:1365:A:O3'	49:X:10:ARG:NH2	2.40	0.54
26:A:1385:A:O2'	26:A:1396:U:O2	2.25	0.54
41:P:24:THR:HG22	41:P:87:ARG:HB3	1.89	0.54
26:A:1170:C:N3	26:A:1178:C:N4	2.56	0.54
32:G:3:VAL:HG22	32:G:68:ARG:HH21	1.72	0.54
26:A:870:U:OP1	38:M:6:ARG:NE	2.41	0.54
46:U:49:PRO:O	46:U:53:GLN:NE2	2.36	0.54
26:A:743:A:O2'	26:A:1659:G:OP1	2.26	0.54
26:A:2258:C:O2'	26:A:2427:C:OP2	2.25	0.54
40:O:30:ARG:HB2	40:O:102:ARG:HH11	1.73	0.54
26:A:793:A:OP2	26:A:2071:A:O2'	2.25	0.53
32:G:43:LYS:O	32:G:50:THR:OG1	2.26	0.53
26:A:2051:A:N6	26:A:2614:A:O2'	2.41	0.53
26:A:578:G:OP1	26:A:1255:U:O2'	2.25	0.53
29:D:136:ASN:OD1	29:D:139:SER:OG	2.23	0.53
26:A:1026:G:OP2	26:A:1134:A:O2'	2.26	0.53
26:A:2419:U:OP1	55:3:40:LYS:NZ	2.40	0.53
36:K:69:VAL:O	36:K:76:VAL:HA	2.09	0.53
26:A:2024:G:O3'	29:D:154:LYS:NZ	2.40	0.53
26:A:2296:U:OP2	40:O:9:ARG:NH2	2.41	0.53
26:A:2114:A:N3	26:A:2166:U:O2'	2.38	0.53
26:A:1071:G:H1'	26:A:1089:A:H2'	1.90	0.53
32:G:29:ASN:ND2	32:G:79:THR:O	2.42	0.53
45:T:12:ARG:HA	50:Y:29:ARG:HH22	1.72	0.53
26:A:2052:A:O2'	29:D:149:ASN:O	2.26	0.53
26:A:196:A:OP2	37:L:47:ARG:NH1	2.42	0.53
29:D:10:GLY:H	29:D:197:THR:HG23	1.74	0.52
26:A:2522:U:O2'	26:A:2647:U:OP1	2.23	0.52
26:A:1012:U:OP2	42:Q:69:ARG:NH1	2.40	0.52
26:A:1072:C:O5'	26:A:1077:A:N6	2.42	0.52
28:C:132:ARG:NH1	28:C:186:ASP:OD1	2.37	0.52
26:A:32:C:N4	26:A:447:A:OP2	2.42	0.52
26:A:994:C:OP1	42:Q:52:ARG:NH2	2.43	0.52
28:C:61:TYR:HA	28:C:85:ASN:HD21	1.74	0.52
51:Z:38:GLU:OE1	51:Z:40:THR:OG1	2.28	0.52
38:M:51:ARG:O	38:M:55:ARG:HB2	2.10	0.52
26:A:2532:G:N2	26:A:2663:G:O2'	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:304:U:H3	26:A:313:G:H1	1.57	0.52
27:B:27:C:OP1	40:O:34:HIS:NE2	2.38	0.52
28:C:128:THR:HA	28:C:189:ALA:O	2.10	0.52
26:A:1047:G:N2	26:A:1111:A:C8	2.71	0.52
26:A:221:A:N1	26:A:265:A:O2'	2.38	0.52
26:A:601:C:O2'	30:E:99:LYS:NZ	2.43	0.52
26:A:1797:G:HO2'	28:C:256:THR:HG1	1.58	0.52
41:P:1:SER:OG	41:P:2:ASN:N	2.43	0.52
40:O:50:ALA:O	40:O:81:ARG:NH2	2.43	0.52
26:A:1080:A:H2'	26:A:1081:U:O4'	2.10	0.52
26:A:1437:C:HO2'	26:A:1516:G:HO2'	1.58	0.52
26:A:532:A:OP1	26:A:561:G:N2	2.41	0.52
33:I:102:ARG:HH22	33:I:133:ARG:HH22	1.57	0.52
26:A:2011:U:OP2	44:S:16:LYS:NZ	2.29	0.51
26:A:2109:U:H3	26:A:2180:U:H3	1.58	0.51
26:A:2839:G:H4'	39:N:49:GLU:HG2	1.93	0.51
26:A:491:G:N2	26:A:1321:A:OP1	2.40	0.51
33:I:99:LYS:HE3	33:I:140:GLU:HB2	1.92	0.51
26:A:372:G:O2'	26:A:400:G:O6	2.25	0.51
32:G:53:PRO:HG3	32:G:61:TRP:CE2	2.45	0.51
32:G:1:SER:OG	32:G:2:ARG:N	2.43	0.51
32:G:38:ASP:O	32:G:54:ARG:NH1	2.44	0.51
35:J:16:TYR:HB2	35:J:54:ILE:HG22	1.91	0.51
26:A:1047:G:N1	26:A:1110:G:O2'	2.43	0.51
26:A:1227:G:OP2	42:Q:15:LYS:NZ	2.40	0.51
26:A:1715:G:O2'	26:A:1743:G:O6	2.26	0.51
26:A:1270:C:H5"	26:A:1271:G:H5'	1.92	0.51
30:E:120:VAL:HG12	30:E:188:MET:HB2	1.91	0.51
32:G:86:LEU:HB2	32:G:130:ILE:HG13	1.92	0.51
37:L:55:MET:HB3	37:L:60:ARG:HH11	1.74	0.51
36:K:64:ARG:NE	41:P:67:GLU:OE1	2.42	0.51
48:W:21:ARG:HH21	48:W:33:ILE:HD13	1.75	0.51
32:G:2:ARG:HA	32:G:5:LYS:HG3	1.93	0.51
26:A:424:G:H2'	26:A:425:G:H8	2.79	0.51
26:A:856:G:H2'	26:A:857:G:C8	2.46	0.51
46:U:73:ASN:ND2	46:U:80:ASP:OD2	2.43	0.51
26:A:1395:A:O2'	26:A:1397:U:OP2	2.29	0.51
26:A:956:G:N7	38:M:14:LYS:NZ	2.55	0.51
28:C:32:LEU:HD13	28:C:63:ILE:HB	1.92	0.51
29:D:124:ARG:NH2	29:D:161:MET:O	2.44	0.51
39:N:28:LEU:HD22	39:N:48:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:463:G:N2	26:A:466:A:OP2	2.38	0.50
35:J:36:LEU:HD11	35:J:54:ILE:HG12	1.93	0.50
38:M:29:GLY:H	38:M:104:GLU:HG3	1.76	0.50
26:A:1047:G:HO2'	26:A:1110:G:H1	1.55	0.50
26:A:2100:G:H1	26:A:2189:U:H3	1.58	0.50
26:A:2818:U:H2'	26:A:2819:G:C8	2.46	0.50
26:A:859:G:OP2	26:A:869:G:N1	21.96	0.50
31:F:37:MET:HG3	31:F:56:LEU:HD12	1.93	0.50
33:I:120:ASP:H	33:I:123:ALA:HB3	1.75	0.50
26:A:1060:U:OP2	33:I:76:ALA:N	2.43	0.50
31:F:14:LYS:O	31:F:17:THR:OG1	2.30	0.50
32:G:124:CYS:HB3	32:G:130:ILE:HG22	1.94	0.50
26:A:745:1MG:HO2'	26:A:748:G:HO2'	1.59	0.50
27:B:30:C:H1'	27:B:57:A:H61	1.75	0.50
32:G:26:LYS:NZ	32:G:27:GLY:O	2.37	0.50
32:G:76:ILE:HD12	32:G:82:PHE:HE1	1.76	0.50
26:A:910:A:H62	38:M:12:MET:HA	1.75	0.50
26:A:1323:C:N4	26:A:1324:G:O6	2.45	0.50
31:F:31:GLU:OE2	31:F:158:THR:OG1	2.21	0.50
30:E:112:LEU:HB3	30:E:118:LEU:HB2	1.94	0.50
36:K:76:VAL:H	41:P:72:VAL:HG22	1.77	0.50
43:R:6:GLN:HE22	43:R:39:LEU:HD11	1.76	0.50
26:A:1802:A:H2'	26:A:1803:A:C8	2.47	0.50
30:E:112:LEU:O	30:E:118:LEU:N	2.41	0.50
39:N:59:SER:OG	39:N:62:ASN:OD1	2.28	0.50
26:A:2720:U:H5"	41:P:52:ARG:HH22	1.76	0.50
26:A:1961:C:H2'	26:A:1962:5MC:C2	2.46	0.50
26:A:881:G:N2	26:A:896:A:N7	2.59	0.50
26:A:1825:U:OP2	28:C:51:ARG:NH2	2.45	0.50
56:4:9:LYS:NZ	56:4:14:CYS:O	2.43	0.49
26:A:411:G:OP2	26:A:2406:A:O2'	2.30	0.49
29:D:37:VAL:HA	29:D:48:ILE:HG22	1.94	0.49
36:K:21:CYS:HA	36:K:41:ILE:HG22	1.93	0.49
26:A:1653:G:N1	39:N:11:ASN:OD1	2.45	0.49
35:J:49:ASP:OD1	35:J:121:LYS:NZ	2.45	0.49
48:W:21:ARG:NH2	48:W:32:ILE:O	2.45	0.49
26:A:1796:U:H2'	26:A:1797:G:H8	1.76	0.49
26:A:589:U:O2'	30:E:90:GLN:NE2	2.46	0.49
46:U:35:VAL:HB	46:U:38:ILE:HG13	1.94	0.49
26:A:1737:G:N2	26:A:1737:G:OP2	2.32	0.49
26:A:1753:G:N2	26:A:1756:G:OP2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:79:G:O6	47:V:14:LYS:NZ	2.33	0.49
26:A:635:C:OP2	37:L:126:ARG:NH2	2.45	0.49
26:A:601:C:O2'	26:A:605:G:OP1	2.29	0.49
35:J:80:HIS:O	35:J:82:GLY:N	2.46	0.49
37:L:80:SER:OG	37:L:115:GLU:OE2	2.30	0.49
38:M:42:THR:HA	38:M:93:VAL:HA	1.93	0.49
26:A:2303:G:O2'	31:F:128:SER:OG	2.29	0.49
26:A:355:U:H2'	26:A:356:G:H8	1.77	0.49
33:I:9:LYS:HG3	33:I:55:PRO:HB3	1.94	0.49
46:U:82:VAL:O	46:U:96:LYS:NZ	2.46	0.49
47:V:21:ARG:NH1	47:V:87:GLN:O	2.38	0.49
55:3:25:HIS:HE2	55:3:47:ALA:HB2	1.78	0.49
26:A:1111:A:N3	26:A:1112:G:H1'	2.28	0.49
26:A:1528:A:OP2	26:A:1543:G:N2	2.43	0.49
26:A:301:G:OP2	46:U:81:ARG:NH1	2.46	0.49
26:A:195:A:O3'	37:L:47:ARG:NH2	2.46	0.49
26:A:801:G:O4'	30:E:49:ARG:NH2	2.45	0.49
51:Z:16:LEU:HD12	51:Z:17:PRO:HD2	1.94	0.49
56:4:11:CYS:SG	56:4:14:CYS:N	2.85	0.49
32:G:41:GLU:HG3	32:G:54:ARG:HG2	1.95	0.49
34:H:99:ILE:HD11	34:H:144:VAL:HG21	1.94	0.49
26:A:1654:A:OP2	39:N:1:MET:N	2.46	0.49
31:F:56:LEU:HD22	31:F:64:PRO:HG3	1.93	0.49
33:I:112:LYS:O	33:I:116:MET:N	2.44	0.49
34:H:100:ALA:HB2	34:H:112:LYS:HD3	1.94	0.48
45:T:40:LYS:HA	45:T:43:ILE:HG12	1.94	0.48
26:A:2655:G:H1'	26:A:2656:U:H5	1.78	0.48
26:A:424:G:H2'	26:A:425:G:C8	3.50	0.48
26:A:477:A:N6	26:A:500:G:O2'	2.46	0.48
30:E:129:PRO:HB3	30:E:159:LEU:HD11	1.94	0.48
26:A:1918:A:O2'	26:A:1920:C:N4	2.46	0.48
57:6:14:ALA:HB3	57:6:22:MET:HB2	1.95	0.48
26:A:1223:G:N1	26:A:1226:A:OP2	2.45	0.48
27:B:57:A:N3	31:F:26:GLN:NE2	2.61	0.48
45:T:80:TRP:HZ3	45:T:82:LYS:HB3	1.78	0.48
26:A:1311:G:H21	26:A:1603:A:H62	1.61	0.48
26:A:2756:U:OP2	56:4:19:ARG:NE	2.44	0.48
29:D:121:THR:HG21	29:D:143:PRO:HB3	1.95	0.48
53:1:36:LYS:HB3	53:1:47:ILE:HD13	1.96	0.48
26:A:1057:A:H2	33:I:117:THR:HG21	1.79	0.48
26:A:675:A:N3	26:A:2443:C:O2'	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:R:68:ARG:NH1	43:R:90:ARG:O	2.47	0.48
56:4:2:LYS:HE2	56:4:35:GLN:HE21	1.79	0.48
26:A:1082:U:C2	26:A:1086:A:N6	2.81	0.48
31:F:64:PRO:HA	31:F:88:VAL:HG23	1.95	0.47
26:A:535:G:H1	26:A:558:U:H3	1.62	0.47
26:A:892:A:H2'	26:A:893:C:C6	2.49	0.47
31:F:45:ASP:HB3	31:F:48:LEU:HD23	1.95	0.47
51:Z:40:THR:HG22	51:Z:42:ALA:H	1.78	0.47
49:X:6:VAL:HG21	49:X:58:ILE:HD11	1.95	0.47
26:A:1283:G:N2	26:A:1329:U:O4	2.42	0.47
30:E:136:GLN:HA	30:E:139:LYS:HG2	1.95	0.47
26:A:2698:U:H2'	26:A:2699:C:C6	2.50	0.47
26:A:570:G:O3'	26:A:819:A:O2'	20.99	0.47
31:F:72:SER:OG	31:F:80:GLN:N	2.47	0.47
33:I:75:ALA:HB1	33:I:79:LEU:HD13	1.96	0.47
26:A:558:U:H2'	26:A:559:G:C8	2.48	0.47
32:G:84:LYS:HB2	32:G:132:LEU:HD12	1.96	0.47
26:A:2353:G:O2'	48:W:29:ALA:O	2.29	0.47
26:A:1083:U:H1'	26:A:1084:A:C8	2.47	0.47
26:A:1167:C:H2'	26:A:1168:G:H8	1.78	0.47
26:A:2821:A:OP1	29:D:115:GLY:N	2.47	0.47
26:A:459:U:OP1	54:2:40:ALA:N	2.48	0.47
26:A:1071:G:H1'	26:A:1089:A:C8	2.49	0.47
44:S:35:ILE:HG13	52:0:24:VAL:HG12	1.96	0.47
26:A:2032:G:O2'	29:D:150:GLN:NE2	2.48	0.47
28:C:169:ALA:O	28:C:185:ALA:N	2.46	0.47
26:A:2706:A:O2'	39:N:64:ARG:NH1	2.48	0.47
26:A:349:U:H2'	26:A:350:G:H8	1.80	0.47
27:B:22:U:H2'	27:B:23:G:C8	2.49	0.47
29:D:49:GLN:HB3	29:D:81:GLU:HB3	1.97	0.47
26:A:1064:C:O2'	26:A:1074:G:N2	2.41	0.46
32:G:86:LEU:HD22	32:G:130:ILE:HD11	1.97	0.46
38:M:34:LYS:HE3	38:M:131:VAL:HG11	1.97	0.46
43:R:63:VAL:HG12	43:R:96:VAL:HG12	1.96	0.46
26:A:2438:U:O2'	26:A:2440:C:OP1	2.28	0.46
26:A:532:A:N6	26:A:1206:G:O2'	62.09	0.46
32:G:18:ILE:HG13	32:G:23:ILE:HG22	1.97	0.46
26:A:1078:U:H5'	26:A:1079:C:H5"	1.96	0.46
26:A:1870:C:O2'	26:A:1871:A:O4'	2.33	0.46
26:A:2655:G:O2'	26:A:2664:G:O6	2.32	0.46
32:G:85:LYS:HG3	32:G:131:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:T:92:ASN:OD1	45:T:93:LEU:N	2.49	0.46
26:A:746:PSU:H5"	26:A:748:G:H1'	1.95	0.46
31:F:17:THR:OG1	31:F:18:GLU:OE1	2.33	0.46
40:O:14:ALA:HA	40:O:17:LYS:HE3	1.98	0.46
35:J:8:PRO:HG3	35:J:48:VAL:HG23	1.97	0.46
26:A:1689:A:H61	26:A:1697:G:H2'	1.81	0.46
47:V:35:GLU:HB2	47:V:93:ARG:NH2	2.31	0.46
57:6:49:ARG:O	57:6:53:THR:OG1	2.25	0.46
26:A:1062:G:C8	26:A:1070:A:H5"	2.51	0.46
26:A:574:A:N6	26:A:2034:U:OP1	2.49	0.46
32:G:83:THR:HA	32:G:132:LEU:O	2.16	0.46
26:A:451:U:O2	26:A:453:A:N6	2.49	0.45
29:D:8:LYS:NZ	29:D:195:GLY:O	2.36	0.45
32:G:27:GLY:HA3	32:G:78:VAL:HB	1.96	0.45
26:A:1915:3TD:H2'	26:A:1916:A:O4'	2.16	0.45
26:A:2295:C:OP1	40:O:10:ARG:NH1	2.50	0.45
26:A:594:U:H2'	26:A:595:C:C6	2.51	0.45
26:A:1059:G:H1'	33:I:116:MET:SD	2.57	0.45
54:2:26:ASN:HD22	54:2:29:GLN:HE22	1.64	0.45
26:A:539:G:H1	26:A:554:U:H3	1.64	0.45
26:A:882:G:N3	26:A:896:A:N6	2.65	0.45
30:E:119:ILE:HD11	30:E:143:LEU:HD21	1.99	0.45
26:A:1242:U:O2	37:L:4:ASN:ND2	2.49	0.45
46:U:51:LEU:HD23	46:U:52:ASN:H	1.80	0.45
26:A:1190:G:H2'	26:A:1191:G:H8	1.81	0.45
26:A:2577:A:H2'	26:A:2614:A:H62	1.82	0.45
26:A:2313:C:H4'	31:F:87:LYS:HD3	1.97	0.45
45:T:69:ARG:NH2	45:T:72:GLN:O	2.49	0.45
46:U:12:VAL:HA	46:U:69:VAL:HG12	1.99	0.45
34:H:6:LEU:HD11	34:H:37:VAL:HG23	1.97	0.45
36:K:7:MET:HA	36:K:19:VAL:O	2.17	0.45
26:A:1114:C:H2'	26:A:1115:G:C8	2.52	0.45
26:A:1563:U:H2'	26:A:1564:C:C6	2.52	0.45
26:A:177:G:N2	26:A:177:G:OP2	2.32	0.45
26:A:2106:U:O4	26:A:2178:C:N4	2.50	0.45
26:A:434:U:O2	26:A:436:C:N4	2.50	0.45
26:A:566:U:H5"	37:L:29:LYS:HE3	1.99	0.45
29:D:179:ARG:HD2	29:D:188:LEU:HD12	1.99	0.45
32:G:37:ASN:HD22	32:G:63:GLN:CD	2.20	0.45
32:G:82:PHE:O	32:G:133:LYS:HA	2.17	0.45
26:A:2336:A:H61	48:W:39:THR:HG21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:268:ARG:NH1	28:C:269:ARG:O	2.49	0.45
33:I:55:PRO:HD2	33:I:72:THR:O	2.17	0.45
40:O:94:ARG:HB2	40:O:97:PHE:O	2.16	0.45
26:A:536:G:H4'	42:Q:56:PHE:HZ	1.81	0.45
26:A:1056:G:H5"	26:A:1086:A:C2	2.49	0.45
26:A:1422:G:H4'	36:K:48:PRO:HB3	99.58	0.45
51:Z:17:PRO:HA	51:Z:20:LYS:HG2	1.98	0.44
26:A:2699:C:H2'	26:A:2700:A:H8	1.82	0.44
26:A:679:C:H2'	26:A:680:C:H6	1.95	0.44
28:C:23:LEU:HD21	28:C:82:TYR:HB2	1.99	0.44
35:J:88:THR:OG1	35:J:91:GLU:OE1	2.33	0.44
36:K:7:MET:HB3	36:K:18:ARG:HE	1.83	0.44
26:A:141:G:N2	26:A:142:A:N3	2.65	0.44
26:A:2144:G:O2'	26:A:2147:A:N6	2.50	0.44
26:A:2788:C:H2'	26:A:2789:C:C6	2.53	0.44
26:A:458:G:O2'	26:A:469:G:O6	2.36	0.44
33:I:102:ARG:HH22	33:I:133:ARG:NH2	2.14	0.44
31:F:52:ALA:HB2	31:F:149:ARG:HH21	1.81	0.44
35:J:15:TRP:HB3	35:J:137:PRO:HB3	2.00	0.44
26:A:1073:A:H2'	26:A:1074:G:O4'	2.18	0.44
26:A:1266:G:O2'	26:A:2012:G:O6	2.26	0.44
26:A:2096:C:H2'	26:A:2097:A:H8	1.82	0.44
26:A:286:U:H2'	26:A:287:G:C8	2.53	0.44
42:Q:78:PHE:CE1	42:Q:109:VAL:HG22	2.53	0.44
42:Q:59:LEU:HD11	42:Q:63:ARG:HH21	1.82	0.44
26:A:1320:C:N3	26:A:1330:C:N4	2.66	0.44
26:A:345:A:O2'	26:A:347:A:N6	2.43	0.44
36:K:77:ILE:HG13	41:P:71:ARG:HG3	1.99	0.44
33:I:44:LYS:HA	33:I:47:SER:HB3	1.99	0.44
33:I:15:GLY:H	33:I:51:GLY:HA2	1.83	0.44
37:L:63:LYS:HA	55:3:12:ARG:HG2	1.99	0.44
26:A:1083:U:N3	26:A:1085:A:H5"	2.33	0.44
26:A:2146:C:H4'	26:A:2147:A:C5	2.52	0.44
48:W:33:ILE:HG22	48:W:34:VAL:HG23	1.99	0.44
26:A:1412:U:H2'	26:A:1413:A:C8	2.53	0.44
26:A:297:G:N2	26:A:301:G:N7	23.75	0.44
30:E:143:LEU:HD23	30:E:146:VAL:HG11	2.00	0.44
31:F:123:GLY:HA2	31:F:162:ASP:HB2	2.00	0.44
26:A:918:A:N3	27:B:80:U:O2'	2.49	0.43
27:B:13:G:N2	27:B:16:G:N3	2.63	0.43
42:Q:93:ILE:HG21	43:R:4:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1081:U:H2'	26:A:1082:U:H6	1.83	0.43
26:A:2183:A:H2'	26:A:2184:A:C8	2.53	0.43
26:A:572:A:OP2	43:R:80:ARG:NH1	2.47	0.43
26:A:958:U:O2	27:B:89:U:O2'	2.30	0.43
38:M:11:LYS:HD3	38:M:86:LYS:HG2	2.00	0.43
26:A:549:G:H2'	26:A:550:C:C6	2.53	0.43
26:A:1779:U:O2	26:A:1783:A:N6	2.51	0.43
26:A:1794:A:H2'	26:A:1795:C:C6	2.54	0.43
26:A:1999:C:O2	26:A:2687:U:O2'	2.34	0.43
26:A:2096:C:H2'	26:A:2097:A:C8	2.53	0.43
26:A:560:C:O2'	42:Q:47:ARG:NH2	2.52	0.43
32:G:88:LEU:HD23	32:G:93:TYR:HB3	2.00	0.43
50:Y:8:GLU:OE1	50:Y:12:GLU:HB2	2.18	0.43
54:2:34:ARG:NE	54:2:42:LEU:O	2.41	0.43
26:A:395:U:O2'	26:A:396:G:N7	2.43	0.43
26:A:657:U:H2'	26:A:658:U:C6	2.54	0.43
26:A:819:A:OP2	26:A:1187:G:N2	2.45	0.43
34:H:58:LEU:HA	34:H:61:VAL:HG22	1.99	0.43
35:J:73:VAL:HG12	35:J:88:THR:HG22	2.00	0.43
26:A:1997:C:H2'	26:A:1998:A:H8	1.84	0.43
26:A:1418:G:H1'	26:A:1580:A:H61	1.84	0.43
26:A:1636:U:H2'	26:A:1637:A:C8	2.54	0.43
26:A:2506:U:OP2	26:A:2576:G:N2	2.47	0.43
26:A:2699:C:H2'	26:A:2700:A:C8	2.54	0.43
26:A:2773:C:OP1	29:D:169:ARG:NH2	2.51	0.43
26:A:2899:A:H2'	26:A:2900:A:C8	2.54	0.43
32:G:148:ARG:HA	32:G:161:VAL:HB	2.01	0.43
36:K:113:MET:HA	36:K:116:ILE:HG22	2.00	0.43
26:A:2482:A:H61	38:M:55:ARG:HH12	1.66	0.43
44:S:72:THR:OG1	44:S:73:LYS:N	2.51	0.43
26:A:1441:G:H2'	26:A:1442:U:C6	2.54	0.43
26:A:1842:G:H2'	26:A:1843:C:C6	2.53	0.43
26:A:833:A:H2'	26:A:834:G:H8	1.83	0.43
31:F:53:ALA:HA	31:F:64:PRO:HG2	2.00	0.43
32:G:153:PRO:HG2	32:G:162:ARG:HG2	2.00	0.43
45:T:3:ARG:HH12	45:T:7:LEU:HD21	1.84	0.43
26:A:1790:C:H2'	26:A:1791:A:C5	2.54	0.42
26:A:558:U:H2'	26:A:559:G:H8	1.83	0.42
28:C:144:GLU:OE1	28:C:150:GLY:N	2.52	0.42
32:G:1:SER:HB3	32:G:61:TRP:HB3	2.00	0.42
26:A:2077:A:OP1	26:A:2238:G:N2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:968:C:H2'	26:A:969:G:H8	1.84	0.42
32:G:84:LYS:HE2	32:G:140:ILE:HG22	2.01	0.42
34:H:17:ASP:HB3	34:H:19:VAL:HG13	2.01	0.42
33:I:106:GLN:NE2	33:I:125:THR:OG1	2.52	0.42
33:I:113:ALA:HA	33:I:116:MET:HB2	2.00	0.42
33:I:28:GLY:HA3	33:I:34:ILE:HD11	2.01	0.42
33:I:38:CYS:SG	33:I:39:LYS:N	2.92	0.42
26:A:995:C:OP2	42:Q:52:ARG:NH2	2.52	0.42
46:U:52:ASN:OD1	46:U:53:GLN:N	2.52	0.42
38:M:34:LYS:HD3	47:V:82:TYR:HA	2.00	0.42
54:2:25:LYS:O	54:2:28:ARG:N	2.50	0.42
26:A:1081:U:H2'	26:A:1082:U:C6	2.53	0.42
26:A:1093:G:H21	26:A:1098:A:H62	1.66	0.42
26:A:1506:U:H2'	26:A:1507:C:C6	2.54	0.42
26:A:2135:A:H61	26:A:2156:G:H2'	1.85	0.42
26:A:78:U:H3	26:A:108:G:H1	1.67	0.42
26:A:1047:G:O2'	26:A:1110:G:N1	2.43	0.42
26:A:1397:U:P	26:A:1398:C:H41	2.43	0.42
26:A:997:G:OP2	42:Q:57:ARG:NH1	2.52	0.42
34:H:26:ALA:HA	34:H:30:LEU:HB2	2.00	0.42
36:K:51:LYS:HE2	36:K:95:ILE:HD12	2.01	0.42
26:A:1478:G:H1	26:A:1513:U:H3	1.68	0.42
26:A:151:C:H2'	26:A:152:A:H8	1.85	0.42
26:A:177:G:H3'	26:A:178:G:H8	1.85	0.42
26:A:563:A:N3	42:Q:36:GLN:NE2	2.65	0.42
32:G:84:LYS:HE3	32:G:141:GLY:HA2	2.01	0.42
32:G:70:LEU:O	32:G:74:MET:HG3	2.19	0.42
40:O:39:VAL:HG22	40:O:49:VAL:HB	2.02	0.42
26:A:1270:C:O2'	26:A:1648:U:OP2	2.31	0.42
26:A:2204:G:H4'	28:C:149:LYS:HD3	2.02	0.42
26:A:2302:U:H2'	26:A:2303:G:C8	2.54	0.42
26:A:2576:G:O2'	26:A:2579:C:OP2	2.30	0.42
28:C:171:VAL:O	28:C:182:LYS:HA	2.19	0.42
48:W:61:GLY:HA3	48:W:79:GLU:O	2.19	0.42
57:6:11:GLU:OE1	57:6:25:ARG:NH1	2.43	0.42
26:A:2816:G:H2'	26:A:2817:U:C6	2.55	0.42
28:C:77:VAL:HG11	28:C:109:LEU:HD11	2.01	0.42
29:D:29:VAL:O	29:D:185:ASN:HB3	2.20	0.42
29:D:24:VAL:HG21	29:D:188:LEU:HB3	2.01	0.42
26:A:1075:C:H3'	26:A:1076:C:O4'	2.20	0.42
26:A:545:U:C2	26:A:548:G:O6	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:679:C:H2'	26:A:680:C:C6	2.65	0.42
27:B:111:U:H2'	27:B:112:G:C8	2.54	0.42
31:F:177:ARG:OXT	57:6:47:LYS:NZ	2.49	0.42
37:L:128:THR:HG23	37:L:131:ALA:H	1.84	0.42
40:O:66:GLY:O	40:O:102:ARG:NH2	2.44	0.42
26:A:2581:G:H22	26:A:2610:C:H2'	1.85	0.42
26:A:33:C:O2	26:A:447:A:N6	2.53	0.42
26:A:581:C:H2'	26:A:582:A:C8	2.54	0.42
26:A:643:A:H2	26:A:2369:A:HO2'	1.66	0.42
26:A:697:G:H2'	26:A:698:C:C6	2.54	0.42
26:A:833:A:H1'	37:L:51:GLU:HB2	2.02	0.42
26:A:1322:A:H2	26:A:1333:G:HO2'	1.67	0.41
26:A:370:G:O2'	26:A:424:G:OP1	2.38	0.41
26:A:848:C:H2'	26:A:849:A:H8	1.85	0.41
51:Z:16:LEU:HB3	51:Z:19:HIS:ND1	2.35	0.41
26:A:1054:A:C6	26:A:1106:G:C6	3.08	0.41
26:A:818:G:N2	26:A:1189:A:H62	2.18	0.41
26:A:323:C:O2'	26:A:1205:A:N6	2.53	0.41
26:A:155:A:H2'	26:A:156:A:H8	1.85	0.41
26:A:967:U:H2'	26:A:968:C:C6	2.55	0.41
30:E:109:LEU:HA	30:E:112:LEU:HG	2.03	0.41
30:E:146:VAL:HG12	30:E:185:LYS:HB2	2.02	0.41
41:P:24:THR:HA	41:P:45:VAL:HA	2.02	0.41
26:A:1285:A:H61	26:A:1329:U:H5'	1.86	0.41
28:C:250:GLN:HB3	28:C:254:LYS:HD2	2.02	0.41
30:E:59:PRO:HB2	30:E:60:TRP:CE3	2.55	0.41
34:H:23:ALA:HB1	34:H:27:ARG:HH21	1.85	0.41
34:H:55:GLU:HA	34:H:58:LEU:HG	2.02	0.41
43:R:38:VAL:HG13	43:R:54:VAL:HG12	2.02	0.41
26:A:1069:A:N3	26:A:1096:A:H5'	2.36	0.41
26:A:1149:G:H2'	26:A:1150:C:C6	2.55	0.41
26:A:1597:A:H5"	26:A:1598:A:H5'	2.02	0.41
42:Q:105:PHE:O	42:Q:109:VAL:HG23	2.19	0.41
52:0:39:ARG:HG3	52:0:40:HIS:ND1	2.36	0.41
26:A:2291:U:H2'	26:A:2292:U:C6	2.55	0.41
26:A:882:G:H1	26:A:894:U:H3	1.67	0.41
28:C:116:GLN:HB3	28:C:121:ALA:HB1	2.02	0.41
26:A:1567:G:H22	28:C:25:LYS:HA	1.85	0.41
29:D:110:THR:HB	29:D:202:ILE:HG13	2.02	0.41
31:F:9:ASP:OD1	31:F:9:ASP:N	2.52	0.41
32:G:88:LEU:N	32:G:128:THR:O	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1081:U:H4'	33:I:126:ARG:HE	1.85	0.41
28:C:36:ASN:HB2	28:C:61:TYR:HB2	2.03	0.41
35:J:80:HIS:C	35:J:82:GLY:H	2.24	0.41
38:M:30:SER:N	38:M:105:MET:O	2.54	0.41
26:A:111:A:O2'	50:Y:58:ASN:ND2	2.51	0.41
26:A:1737:G:O2'	26:A:1738:G:O4'	2.37	0.41
26:A:585:G:N7	42:Q:5:ARG:NH1	2.69	0.41
26:A:1594:U:H2'	26:A:1595:C:C6	2.56	0.41
26:A:2140:G:H2'	26:A:2141:G:C8	2.56	0.41
26:A:354:A:H2'	26:A:355:U:O4'	2.20	0.41
26:A:572:A:OP2	43:R:79:ARG:NH2	2.53	0.41
29:D:57:ALA:HA	29:D:60:VAL:HG22	2.02	0.41
26:A:1013:C:H2'	26:A:1014:A:H8	1.86	0.41
26:A:1069:A:O2'	26:A:1096:A:O2'	2.21	0.41
26:A:2065:C:H2'	26:A:2066:C:H6	1.86	0.41
26:A:2500:U:O2'	26:A:2504:PSU:OP1	2.39	0.41
26:A:534:U:H2'	26:A:535:G:H8	1.86	0.41
26:A:63:A:O2'	45:T:77:ARG:NE	2.52	0.41
26:A:674:G:H2'	26:A:675:A:H8	4.09	0.41
26:A:745:1MG:HM11	26:A:745:1MG:HN21	1.71	0.41
27:B:16:G:N2	27:B:69:G:H1'	2.36	0.41
26:A:1910:G:H2'	26:A:1911:PSU:O4'	2.20	0.41
26:A:2567:G:H2'	26:A:2568:U:C6	2.56	0.41
26:A:4:U:H2'	26:A:5:A:H8	1.86	0.41
26:A:848:C:H2'	26:A:849:A:C8	2.56	0.41
29:D:4:LEU:HB2	29:D:32:ASN:ND2	2.36	0.41
30:E:147:LEU:HD23	30:E:183:PHE:CD2	2.56	0.41
31:F:11:VAL:HG23	31:F:15:LEU:HD13	2.03	0.41
36:K:90:ASN:OD1	36:K:91:SER:N	2.54	0.41
26:A:1000:A:OP2	26:A:1154:G:N1	2.42	0.41
26:A:2107:G:H2'	26:A:2108:A:C8	2.56	0.41
26:A:2834:G:H2'	26:A:2879:A:H61	1.86	0.41
26:A:287:G:H2'	26:A:288:U:H6	1.86	0.41
26:A:635:C:O2'	26:A:639:U:OP1	2.39	0.41
28:C:67:LYS:HA	28:C:150:GLY:HA2	2.03	0.41
31:F:37:MET:HB2	31:F:86:CYS:SG	2.61	0.41
32:G:25:ILE:HG12	32:G:78:VAL:HG21	2.03	0.41
37:L:75:ALA:O	37:L:108:ALA:HA	2.21	0.41
26:A:1059:G:H1	33:I:127:SER:CB	2.34	0.40
26:A:2746:U:H1'	32:G:138:GLN:HE22	1.86	0.40
26:A:2809:A:P	26:A:2890:G:H1	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:44:G:OP2	57:6:1:MET:N	2.51	0.40
34:H:96:THR:O	34:H:99:ILE:HG22	2.21	0.40
26:A:1478:G:H2'	26:A:1479:G:H8	1.86	0.40
26:A:2785:C:O3'	29:D:70:LYS:NZ	2.53	0.40
26:A:656:G:H2'	26:A:657:U:C6	2.85	0.40
30:E:136:GLN:HA	30:E:139:LYS:HE3	2.03	0.40
46:U:24:VAL:HA	46:U:35:VAL:HG22	2.01	0.40
26:A:1283:G:N1	26:A:1286:A:OP2	2.54	0.40
26:A:48:G:N2	26:A:177:G:OP2	2.54	0.40
30:E:3:LEU:O	30:E:11:ALA:HA	2.21	0.40
53:1:10:LEU:HG	53:1:48:TYR:HB3	2.03	0.40
37:L:85:VAL:HG11	37:L:90:VAL:HG12	2.04	0.40
26:A:1266:G:C8	44:S:16:LYS:HE3	2.57	0.40
26:A:184:C:H2'	26:A:185:G:H8	1.87	0.40
26:A:2262:U:OP1	26:A:2387:U:O2'	2.36	0.40
26:A:596:U:H2'	26:A:597:G:H8	1.86	0.40
32:G:37:ASN:OD1	32:G:38:ASP:N	2.55	0.40
34:H:30:LEU:HD23	34:H:36:ALA:HB3	2.02	0.40
39:N:28:LEU:O	39:N:32:GLU:HA	2.21	0.40
43:R:16:GLU:OE1	43:R:100:GLY:N	2.55	0.40
48:W:52:ASP:HB3	48:W:54:THR:HG22	2.04	0.40
51:Z:40:THR:HB	51:Z:43:ILE:HG12	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%)	186 (86%)	24 (11%)	6 (3%)	6 45
3	c	204/206 (99%)	192 (94%)	9 (4%)	3 (2%)	13 58
4	d	203/205 (99%)	187 (92%)	12 (6%)	4 (2%)	9 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	e	155/157 (99%)	142 (92%)	9 (6%)	4 (3%)	7 46
6	f	98/100 (98%)	86 (88%)	5 (5%)	7 (7%)	1 22
7	g	149/151 (99%)	139 (93%)	7 (5%)	3 (2%)	9 52
8	h	127/129 (98%)	116 (91%)	11 (9%)	0	100 100
9	i	125/127 (98%)	111 (89%)	10 (8%)	4 (3%)	5 42
10	j	96/98 (98%)	83 (86%)	7 (7%)	6 (6%)	2 26
11	k	114/116 (98%)	103 (90%)	7 (6%)	4 (4%)	4 40
12	l	121/123 (98%)	110 (91%)	6 (5%)	5 (4%)	3 35
13	m	112/114 (98%)	102 (91%)	6 (5%)	4 (4%)	4 40
14	n	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	19 65
15	o	86/88 (98%)	76 (88%)	7 (8%)	3 (4%)	4 40
16	p	80/82 (98%)	72 (90%)	6 (8%)	2 (2%)	7 47
17	q	78/80 (98%)	69 (88%)	7 (9%)	2 (3%)	7 46
18	r	63/65 (97%)	58 (92%)	2 (3%)	3 (5%)	3 32
19	s	77/79 (98%)	70 (91%)	5 (6%)	2 (3%)	7 46
20	t	83/85 (98%)	78 (94%)	5 (6%)	0	100 100
21	u	63/65 (97%)	55 (87%)	5 (8%)	3 (5%)	3 32
25	z	612/614 (100%)	588 (96%)	18 (3%)	6 (1%)	19 65
28	C	269/271 (99%)	252 (94%)	13 (5%)	4 (2%)	13 58
29	D	207/209 (99%)	191 (92%)	12 (6%)	4 (2%)	10 53
30	E	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	34 77
31	F	175/177 (99%)	157 (90%)	15 (9%)	3 (2%)	11 56
32	G	174/176 (99%)	167 (96%)	5 (3%)	2 (1%)	17 64
33	I	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	8 50
34	H	147/149 (99%)	134 (91%)	7 (5%)	6 (4%)	3 35
35	J	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	26 71
36	K	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	24 69
37	L	141/143 (99%)	128 (91%)	11 (8%)	2 (1%)	14 58
38	M	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	13 58
39	N	118/120 (98%)	111 (94%)	6 (5%)	1 (1%)	24 69
40	O	114/116 (98%)	105 (92%)	9 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
42	Q	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
43	R	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	9	52
44	S	108/110 (98%)	103 (95%)	2 (2%)	3 (3%)	6	45
45	T	91/93 (98%)	81 (89%)	9 (10%)	1 (1%)	17	64
46	U	100/102 (98%)	89 (89%)	8 (8%)	3 (3%)	5	44
47	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
48	W	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	14	58
49	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
50	Y	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	12	57
51	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
52	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	10	53
53	1	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
54	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
55	3	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
56	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
57	6	64/66 (97%)	57 (89%)	4 (6%)	3 (5%)	3	32
All	All	6329/6431 (98%)	5850 (92%)	362 (6%)	117 (2%)	15	54

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	17	HIS
2	b	18	GLN
2	b	103	TRP
5	e	89	THR
6	f	92	THR
6	f	94	HIS
6	f	98	GLU
9	i	57	VAL
10	j	34	ALA
10	j	92	LEU
11	k	92	ARG
12	l	101	LEU
13	m	6	ILE
14	n	37	ASP

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Mol	Chain	Res	Type
17	q	49	ASN
18	r	11	ARG
18	r	18	GLN
21	u	34	ARG
25	z	191	VAL
25	z	301	GLU
25	z	487	PHE
28	C	121	ALA
33	I	64	ARG
34	H	9	VAL
35	J	81	ILE
36	K	35	VAL
37	L	36	LYS
43	R	52	PRO
46	U	88	ASP
52	0	2	VAL
57	6	40	CYS
2	b	151	LYS
2	b	153	MET
3	c	79	LYS
3	c	156	LEU
4	d	47	LEU
4	d	150	LYS
4	d	165	GLU
5	e	77	ASN
5	e	93	VAL
5	e	122	VAL
7	g	129	ASN
9	i	107	ALA
10	j	42	LEU
10	j	57	VAL
11	k	91	GLY
12	l	25	ALA
12	l	75	GLU
16	p	44	SER
17	q	72	TRP
18	r	17	VAL
19	s	4	LEU
21	u	24	LYS
25	z	188	ALA
25	z	328	ALA
29	D	31	ALA

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Mol	Chain	Res	Type
29	D	134	HIS
29	D	149	ASN
31	F	20	ASN
31	F	148	VAL
32	G	108	PHE
33	I	24	GLY
34	H	3	VAL
39	N	117	ASP
44	S	64	ALA
44	S	65	ASP
46	U	6	ARG
3	c	60	ALA
4	d	191	SER
6	f	63	ASN
7	g	50	ALA
9	i	12	LYS
9	i	125	GLN
10	j	58	ASN
10	j	75	ASP
13	m	4	ALA
13	m	11	HIS
15	o	2	LEU
15	o	45	HIS
21	u	11	PHE
28	C	204	LEU
31	F	175	PRO
34	H	11	ASN
34	H	15	LEU
34	H	41	LYS
34	H	89	LYS
37	L	29	LYS
38	M	58	LYS
43	R	55	ASP
44	S	3	THR
48	W	16	ARG
2	b	203	ASP
12	l	2	THR
12	l	46	SER
15	o	87	ARG
16	p	8	ARG
28	C	239	PHE
28	C	258	SER

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Mol	Chain	Res	Type
32	G	159	LYS
38	M	69	PRO
45	T	24	MET
50	Y	24	GLU
57	6	31	ASP
6	f	86	ARG
7	g	56	SER
11	k	88	PRO
11	k	126	ARG
25	z	329	ARG
30	E	83	VAL
46	U	54	PRO
57	6	4	ASP
6	f	99	ALA
19	s	66	VAL
6	f	19	PRO
33	I	12	VAL
13	m	9	PRO
29	D	153	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	180 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	102 (99%)	1 (1%)	82	92
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%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
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
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
25	z	501/501 (100%)	499 (100%)	2 (0%)	93	96
28	C	216/216 (100%)	216 (100%)	0	100	100
29	D	164/164 (100%)	164 (100%)	0	100	100
30	E	165/165 (100%)	165 (100%)	0	100	100
31	F	148/148 (100%)	148 (100%)	0	100	100
32	G	137/137 (100%)	135 (98%)	2 (2%)	72	89
33	I	109/109 (100%)	109 (100%)	0	100	100
34	H	114/114 (100%)	114 (100%)	0	100	100
35	J	116/116 (100%)	116 (100%)	0	100	100
36	K	103/103 (100%)	103 (100%)	0	100	100
37	L	102/102 (100%)	102 (100%)	0	100	100
38	M	109/109 (100%)	109 (100%)	0	100	100
39	N	100/100 (100%)	100 (100%)	0	100	100
40	O	86/86 (100%)	86 (100%)	0	100	100
41	P	99/99 (100%)	99 (100%)	0	100	100
42	Q	89/89 (100%)	89 (100%)	0	100	100
43	R	84/84 (100%)	84 (100%)	0	100	100
44	S	93/93 (100%)	93 (100%)	0	100	100
45	T	80/80 (100%)	80 (100%)	0	100	100
46	U	83/83 (100%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	V	78/78 (100%)	78 (100%)	0	100 100
48	W	57/57 (100%)	57 (100%)	0	100 100
49	X	67/67 (100%)	67 (100%)	0	100 100
50	Y	55/55 (100%)	55 (100%)	0	100 100
51	Z	48/48 (100%)	48 (100%)	0	100 100
52	0	47/47 (100%)	47 (100%)	0	100 100
53	1	45/45 (100%)	45 (100%)	0	100 100
54	2	38/38 (100%)	38 (100%)	0	100 100
55	3	51/51 (100%)	51 (100%)	0	100 100
56	4	34/34 (100%)	34 (100%)	0	100 100
57	6	59/59 (100%)	59 (100%)	0	100 100
All	All	5229/5252 (100%)	5224 (100%)	5 (0%)	95 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	23	LEU
25	z	26	ASP
25	z	27	ARG
32	G	104	LEU
32	G	157	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	167	HIS
4	d	135	GLN
9	i	31	GLN
13	m	90	HIS
14	n	59	GLN
15	o	41	HIS
20	t	60	GLN
25	z	47	GLN
25	z	287	HIS
25	z	292	HIS
25	z	474	HIS
28	C	85	ASN

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Mol	Chain	Res	Type
29	D	130	GLN
29	D	150	GLN
30	E	90	GLN
31	F	36	ASN
32	G	72	ASN
32	G	142	GLN
33	I	42	ASN
33	I	106	GLN
34	H	2	GLN
44	S	102	HIS
50	Y	58	ASN
54	2	26	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	176 (11%)	0
22	v	76/77 (98%)	7 (9%)	0
23	x	47/48 (97%)	27 (57%)	0
24	y	93/95 (97%)	20 (21%)	0
26	A	2898/2903 (99%)	381 (13%)	10 (0%)
27	B	119/120 (99%)	14 (11%)	0
58	w	2/3 (66%)	0	0
All	All	4770/4785 (99%)	625 (13%)	10 (0%)

All (625) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	49	U
1	a	51	A
1	a	86	G
1	a	94	G
1	a	95	C
1	a	96	U

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Mol	Chain	Res	Type
1	a	131	A
1	a	141	G
1	a	164	G
1	a	173	U
1	a	177	G
1	a	182	A
1	a	197	A
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	245	U
1	a	247	G
1	a	253	A
1	a	266	G
1	a	267	C
1	a	289	G
1	a	298	A
1	a	319	G
1	a	328	C
1	a	347	G
1	a	348	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	392	C
1	a	406	G
1	a	411	A
1	a	413	G
1	a	414	A
1	a	424	G
1	a	428	G
1	a	429	U
1	a	430	A
1	a	467	U
1	a	481	G
1	a	482	A
1	a	497	G

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Mol	Chain	Res	Type
1	a	511	C
1	a	512	U
1	a	518	C
1	a	524	G
1	a	527	G7M
1	a	528	C
1	a	531	U
1	a	532	A
1	a	533	A
1	a	546	A
1	a	547	A
1	a	551	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	620	C
1	a	633	G
1	a	650	G
1	a	653	U
1	a	665	A
1	a	733	G
1	a	748	G
1	a	755	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	817	C
1	a	819	A
1	a	832	G
1	a	836	G
1	a	841	C
1	a	843	U
1	a	844	G
1	a	845	A
1	a	876	C
1	a	878	A
1	a	902	G

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Mol	Chain	Res	Type
1	a	934	C
1	a	935	A
1	a	942	G
1	a	960	U
1	a	966	2MG
1	a	968	A
1	a	969	A
1	a	971	G
1	a	972	C
1	a	975	A
1	a	976	G
1	a	977	A
1	a	993	G
1	a	1004	A
1	a	1020	G
1	a	1028	C
1	a	1030	U
1	a	1034	G
1	a	1043	G
1	a	1055	A
1	a	1065	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1105	A
1	a	1108	G
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1139	G
1	a	1140	C
1	a	1158	C
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1169	A
1	a	1182	G
1	a	1183	U
1	a	1196	A
1	a	1197	A
1	a	1213	A

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Mol	Chain	Res	Type
1	a	1233	G
1	a	1236	A
1	a	1238	A
1	a	1258	G
1	a	1260	G
1	a	1278	G
1	a	1280	A
1	a	1287	A
1	a	1297	G
1	a	1300	G
1	a	1301	U
1	a	1317	C
1	a	1319	A
1	a	1320	C
1	a	1350	A
1	a	1363	A
1	a	1364	U
1	a	1396	A
1	a	1397	C
1	a	1419	G
1	a	1429	A
1	a	1432	G
1	a	1441	A
1	a	1451	U
1	a	1475	G
1	a	1492	A
1	a	1493	A
1	a	1503	A
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1520	C
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1536	C
22	v	9	G
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	46	A

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Mol	Chain	Res	Type
22	v	54	5MU
22	v	76	A
23	x	88	A
23	x	90	G
23	x	95	U
23	x	96	C
23	x	97	A
23	x	98	U
23	x	108	A
23	x	109	C
23	x	110	G
23	x	113	C
23	x	114	C
23	x	115	A
23	x	116	U
23	x	117	C
23	x	119	G
23	x	120	U
23	x	121	U
23	x	123	C
23	x	124	A
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	133	C
23	x	134	C
24	y	5(A)	A
24	y	8	G
24	y	15	C
24	y	17	G
24	y	18	G
24	y	19	H2U
24	y	20	G
24	y	31	A
24	y	34	U
24	y	40	C
24	y	45	U
24	y	46	G
24	y	47(A)	G

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Mol	Chain	Res	Type
24	y	47(G)	C
24	y	47(H)	A
24	y	47(I)	G
24	y	47(J)	C
24	y	49	G
24	y	75	C
24	y	76	A
26	A	10	A
26	A	15	G
26	A	27	G
26	A	34	U
26	A	63	A
26	A	71	A
26	A	73	A
26	A	74	A
26	A	75	G
26	A	91	A
26	A	92	U
26	A	96	C
26	A	101	A
26	A	102	U
26	A	118	A
26	A	120	U
26	A	131	A
26	A	138	U
26	A	139	U
26	A	142	A
26	A	163	C
26	A	181	A
26	A	196	A
26	A	199	A
26	A	216	A
26	A	222	A
26	A	228	C
26	A	230	G
26	A	232	G
26	A	248	G
26	A	255	A
26	A	266	G
26	A	267	C
26	A	277	G
26	A	278	A

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Mol	Chain	Res	Type
26	A	279	A
26	A	294	A
26	A	295	G
26	A	311	A
26	A	324	A
26	A	329	G
26	A	330	A
26	A	346	A
26	A	353	C
26	A	362	A
26	A	367	G
26	A	372	G
26	A	386	G
26	A	396	G
26	A	404	A
26	A	405	U
26	A	411	G
26	A	412	A
26	A	451	U
26	A	456	C
26	A	480	A
26	A	481	G
26	A	490	C
26	A	491	G
26	A	504	A
26	A	505	A
26	A	508	A
26	A	509	C
26	A	531	C
26	A	532	A
26	A	549	G
26	A	563	A
26	A	568	U
26	A	573	U
26	A	575	A
26	A	603	A
26	A	614	A
26	A	615	U
26	A	616	A
26	A	621	A
26	A	637	A
26	A	645	C

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Mol	Chain	Res	Type
26	A	646	U
26	A	647	G
26	A	653	U
26	A	654	A
26	A	655	A
26	A	668	A
26	A	675	A
26	A	686	U
26	A	717	C
26	A	726	G
26	A	730	A
26	A	745	1MG
26	A	746	PSU
26	A	747	5MU
26	A	748	G
26	A	764	A
26	A	765	C
26	A	775	G
26	A	776	G
26	A	782	A
26	A	784	G
26	A	805	G
26	A	812	C
26	A	819	A
26	A	846	U
26	A	859	G
26	A	869	G
26	A	882	G
26	A	883	G
26	A	885	C
26	A	886	A
26	A	887	U
26	A	888	C
26	A	890	C
26	A	891	G
26	A	910	A
26	A	931	U
26	A	941	A
26	A	946	C
26	A	961	C
26	A	965	C
26	A	973	A

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Mol	Chain	Res	Type
26	A	974	G
26	A	983	A
26	A	990	A
26	A	996	A
26	A	1009	A
26	A	1012	U
26	A	1013	C
26	A	1022	G
26	A	1023	U
26	A	1026	G
26	A	1033	U
26	A	1040	A
26	A	1045	C
26	A	1046	A
26	A	1047	G
26	A	1054	A
26	A	1055	G
26	A	1057	A
26	A	1061	U
26	A	1062	G
26	A	1064	C
26	A	1065	U
26	A	1066	U
26	A	1067	A
26	A	1068	G
26	A	1069	A
26	A	1070	A
26	A	1072	C
26	A	1073	A
26	A	1076	C
26	A	1078	U
26	A	1079	C
26	A	1084	A
26	A	1088	A
26	A	1090	A
26	A	1097	U
26	A	1101	U
26	A	1110	G
26	A	1112	G
26	A	1133	A
26	A	1134	A
26	A	1135	C

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Mol	Chain	Res	Type
26	A	1142	A
26	A	1143	A
26	A	1157	G
26	A	1171	G
26	A	1178	C
26	A	1180	U
26	A	1206	G
26	A	1210	G
26	A	1211	C
26	A	1253	A
26	A	1255	U
26	A	1256	G
26	A	1271	G
26	A	1272	A
26	A	1273	U
26	A	1300	G
26	A	1301	A
26	A	1314	C
26	A	1329	U
26	A	1345	C
26	A	1359	A
26	A	1365	A
26	A	1368	G
26	A	1378	A
26	A	1379	U
26	A	1383	A
26	A	1395	A
26	A	1396	U
26	A	1416	G
26	A	1417	C
26	A	1420	A
26	A	1428	C
26	A	1452	G
26	A	1458	U
26	A	1459	G
26	A	1468	U
26	A	1482	G
26	A	1493	C
26	A	1494	A
26	A	1497	U
26	A	1515	A
26	A	1535	A

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Mol	Chain	Res	Type
26	A	1537	G
26	A	1566	A
26	A	1569	A
26	A	1578	U
26	A	1583	A
26	A	1598	A
26	A	1607	C
26	A	1609	A
26	A	1616	A
26	A	1646	C
26	A	1648	U
26	A	1649	G
26	A	1654	A
26	A	1660	G
26	A	1674	G
26	A	1675	C
26	A	1715	G
26	A	1738	G
26	A	1758	U
26	A	1764	C
26	A	1773	A
26	A	1784	A
26	A	1791	A
26	A	1799	G
26	A	1800	C
26	A	1801	A
26	A	1802	A
26	A	1808	A
26	A	1816	C
26	A	1829	A
26	A	1847	A
26	A	1870	C
26	A	1876	A
26	A	1906	G
26	A	1912	A
26	A	1913	A
26	A	1919	A
26	A	1929	G
26	A	1930	G
26	A	1937	A
26	A	1940	U
26	A	1955	U

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Mol	Chain	Res	Type
26	A	1960	A
26	A	1962	5MC
26	A	1963	U
26	A	1964	G
26	A	1967	C
26	A	1970	A
26	A	1971	U
26	A	1972	G
26	A	1991	U
26	A	1993	U
26	A	1997	C
26	A	2022	U
26	A	2023	C
26	A	2031	A
26	A	2032	G
26	A	2033	A
26	A	2043	C
26	A	2049	G
26	A	2055	C
26	A	2056	G
26	A	2060	A
26	A	2061	G
26	A	2062	A
26	A	2069	G7M
26	A	2070	A
26	A	2093	G
26	A	2105	U
26	A	2107	G
26	A	2110	G
26	A	2111	U
26	A	2112	G
26	A	2113	U
26	A	2116	G
26	A	2118	U
26	A	2119	A
26	A	2120	G
26	A	2125	G
26	A	2127	G
26	A	2128	G
26	A	2129	C
26	A	2131	U
26	A	2132	U

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Mol	Chain	Res	Type
26	A	2133	G
26	A	2134	A
26	A	2145	C
26	A	2146	C
26	A	2147	A
26	A	2157	G
26	A	2159	G
26	A	2160	C
26	A	2162	G
26	A	2164	C
26	A	2168	G
26	A	2172	U
26	A	2173	A
26	A	2177	C
26	A	2178	C
26	A	2198	A
26	A	2199	A
26	A	2204	G
26	A	2225	A
26	A	2227	A
26	A	2238	G
26	A	2239	G
26	A	2251	OMG
26	A	2268	A
26	A	2278	A
26	A	2279	G
26	A	2283	C
26	A	2287	A
26	A	2305	U
26	A	2308	G
26	A	2310	C
26	A	2322	A
26	A	2333	A
26	A	2335	A
26	A	2344	U
26	A	2347	C
26	A	2350	C
26	A	2354	C
26	A	2379	G
26	A	2383	G
26	A	2385	C
26	A	2402	U

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Mol	Chain	Res	Type
26	A	2403	C
26	A	2428	G
26	A	2429	G
26	A	2430	A
26	A	2434	A
26	A	2436	G
26	A	2441	U
26	A	2447	G
26	A	2448	A
26	A	2470	G
26	A	2476	A
26	A	2484	G
26	A	2502	G
26	A	2504	PSU
26	A	2505	G
26	A	2506	U
26	A	2513	A
26	A	2518	A
26	A	2520	C
26	A	2529	G
26	A	2547	A
26	A	2554	U
26	A	2567	G
26	A	2572	A
26	A	2581	G
26	A	2582	G
26	A	2602	A
26	A	2609	U
26	A	2613	U
26	A	2629	U
26	A	2630	G
26	A	2639	A
26	A	2663	G
26	A	2689	U
26	A	2690	U
26	A	2714	G
26	A	2726	A
26	A	2739	U
26	A	2744	G
26	A	2755	C
26	A	2757	A
26	A	2765	A

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Mol	Chain	Res	Type
26	A	2778	A
26	A	2791	G
26	A	2797	U
26	A	2818	U
26	A	2821	A
26	A	2833	U
26	A	2849	U
26	A	2850	A
26	A	2872	A
26	A	2884	U
27	B	24	G
27	B	25	U
27	B	30	C
27	B	35	C
27	B	38	C
27	B	42	C
27	B	44	G
27	B	45	A
27	B	57	A
27	B	87	U
27	B	89	U
27	B	90	C
27	B	108	A
27	B	109	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	818	G
26	A	886	A
26	A	890	C
26	A	960	A
26	A	1045	C
26	A	1066	U
26	A	1072	C
26	A	1358	G
26	A	1875	G
26	A	2756	U

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

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	$\#\|Z\| > 2$
26	6MZ	A	1618	26	17,25,26	1.07	1 (5%)	15,36,39	2.47	2 (13%)
26	2MG	A	1835	26	18,26,27	1.15	2 (11%)	21,38,41	2.24	6 (28%)
26	PSU	A	1911	26	15,21,22	1.40	2 (13%)	16,30,33	2.03	3 (18%)
26	3TD	A	1915	26	15,22,23	3.28	6 (40%)	17,32,35	2.15	5 (29%)
26	PSU	A	1917	26	15,21,22	1.07	0	16,30,33	2.45	4 (25%)
26	5MU	A	1939	26	13,22,23	0.64	0	16,32,35	2.56	2 (12%)
26	5MC	A	1962	26	14,22,23	1.23	1 (7%)	17,32,35	1.69	4 (23%)
26	6MZ	A	2030	26	17,25,26	1.08	1 (5%)	15,36,39	1.83	2 (13%)
26	G7M	A	2069	26	18,26,27	1.24	2 (11%)	21,39,42	2.49	8 (38%)
26	OMG	A	2251	26,22	18,26,27	1.18	2 (11%)	21,38,41	1.89	4 (19%)
26	2MG	A	2445	26	18,26,27	1.20	2 (11%)	21,38,41	2.21	5 (23%)
26	H2U	A	2449	26	17,21,22	1.23	4 (23%)	23,30,33	1.51	5 (21%)
26	PSU	A	2457	26	15,21,22	1.51	1 (6%)	16,30,33	2.21	4 (25%)
26	OMC	A	2498	26	15,22,23	0.69	0	20,31,34	1.18	2 (10%)
26	2MA	A	2503	26	17,25,26	1.50	3 (17%)	18,37,40	3.99	2 (11%)
26	PSU	A	2504	26	15,21,22	1.11	1 (6%)	16,30,33	2.33	4 (25%)
26	OMU	A	2552	26	14,22,23	0.68	0	19,31,34	1.74	1 (5%)
26	PSU	A	2580	26	15,21,22	1.29	1 (6%)	16,30,33	2.19	3 (18%)
26	PSU	A	2604	26	15,21,22	1.07	2 (13%)	16,30,33	2.17	4 (25%)
26	PSU	A	2605	26	15,21,22	1.26	2 (13%)	16,30,33	2.17	4 (25%)
26	1MG	A	745	26	17,26,27	1.52	3 (17%)	19,39,42	0.98	1 (5%)
26	PSU	A	746	26	15,21,22	1.64	1 (6%)	16,30,33	2.07	2 (12%)
26	5MU	A	747	26	13,22,23	0.64	1 (7%)	16,32,35	2.75	2 (12%)
26	PSU	A	955	26	15,21,22	1.26	1 (6%)	16,30,33	2.18	4 (25%)
1	2MG	a	1207	1	18,26,27	1.21	2 (11%)	21,38,41	2.26	6 (28%)
1	4OC	a	1402	1	15,23,24	0.54	0	21,32,35	1.82	3 (14%)
1	5MC	a	1407	1	14,22,23	1.42	2 (14%)	17,32,35	0.90	0
1	UR3	a	1498	1	13,22,23	0.76	0	18,32,35	0.89	0
1	2MG	a	1516	1	18,26,27	1.23	2 (11%)	21,38,41	2.20	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MA6	a	1518	1	18,26,27	0.94	1 (5%)	15,38,41	2.46	2 (13%)
1	MA6	a	1519	1	18,26,27	0.96	1 (5%)	15,38,41	2.40	4 (26%)
1	PSU	a	516	1	15,21,22	1.40	1 (6%)	16,30,33	2.12	3 (18%)
1	G7M	a	527	1	18,26,27	1.26	2 (11%)	21,39,42	2.84	10 (47%)
1	2MG	a	966	1	18,26,27	1.23	2 (11%)	21,38,41	2.47	6 (28%)
1	5MC	a	967	1	14,22,23	1.65	1 (7%)	17,32,35	0.96	0
22	H2U	v	20	22	17,21,22	1.10	2 (11%)	23,30,33	1.86	4 (17%)
22	5MU	v	54	22	13,22,23	0.63	1 (7%)	16,32,35	2.61	2 (12%)
22	PSU	v	55	22	15,21,22	1.38	2 (13%)	16,30,33	2.34	4 (25%)
22	4SU	v	8	22	12,21,22	0.63	0	15,30,33	1.01	1 (6%)
24	H2U	y	19	24	17,21,22	1.04	2 (11%)	23,30,33	2.07	4 (17%)
24	6IA	y	37	24	20,29,30	0.89	1 (5%)	22,41,44	3.36	6 (27%)
24	5MU	y	54	24	13,22,23	0.60	0	16,32,35	2.96	2 (12%)
24	PSU	y	55	24	15,21,22	1.42	2 (13%)	16,30,33	2.25	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
26	6MZ	A	1618	26	-	0/5/27/28	0/3/3/3
26	2MG	A	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
26	3TD	A	1915	26	-	0/7/25/26	0/2/2/2
26	PSU	A	1917	26	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/3/25/26	0/2/2/2
26	5MC	A	1962	26	-	0/3/25/26	0/2/2/2
26	6MZ	A	2030	26	-	0/5/27/28	0/3/3/3
26	G7M	A	2069	26	2/2/5/5	0/3/25/26	0/3/3/3
26	OMG	A	2251	26,22	-	0/5/27/28	0/3/3/3
26	2MG	A	2445	26	-	0/5/27/28	0/3/3/3
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
26	OMC	A	2498	26	-	0/5/27/28	0/2/2/2
26	2MA	A	2503	26	-	0/3/25/26	0/3/3/3
26	PSU	A	2504	26	-	0/7/25/26	0/2/2/2
26	OMU	A	2552	26	-	0/5/27/28	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
26	1MG	A	745	26	-	0/3/25/26	0/3/3/3
26	PSU	A	746	26	-	0/7/25/26	0/2/2/2
26	5MU	A	747	26	-	0/3/25/26	0/2/2/2
26	PSU	A	955	26	-	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
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 (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	746	PSU	C5-C1'	-5.40	1.47	1.52
26	A	2457	PSU	C5-C1'	-4.60	1.48	1.52
1	a	516	PSU	C5-C1'	-4.20	1.48	1.52
22	v	55	PSU	C5-C1'	-4.06	1.48	1.52
26	A	1911	PSU	C5-C1'	-3.90	1.48	1.52
24	y	55	PSU	C5-C1'	-3.86	1.48	1.52
26	A	2580	PSU	C5-C1'	-3.75	1.49	1.52
26	A	1915	3TD	O4-C4	-3.54	1.15	1.24
26	A	955	PSU	C5-C1'	-3.51	1.49	1.52
26	A	2605	PSU	C5-C1'	-3.36	1.49	1.52
26	A	2504	PSU	C5-C1'	-2.93	1.49	1.52
26	A	2449	H2U	C2-N3	-2.69	1.33	1.38
24	y	19	H2U	C2-N3	-2.66	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2069	G7M	O2'-C2'	-2.56	1.36	1.43
26	A	2604	PSU	C5-C1'	-2.54	1.50	1.52
22	v	20	H2U	C2-N3	-2.53	1.33	1.38
26	A	2449	H2U	C4-N3	-2.51	1.33	1.37
22	v	20	H2U	C4-N3	-2.39	1.33	1.37
1	a	527	G7M	O2'-C2'	-2.36	1.37	1.43
26	A	1911	PSU	O4'-C1'	-2.33	1.40	1.44
26	A	2449	H2U	C6-N1	-2.32	1.44	1.47
24	y	19	H2U	C4-N3	-2.31	1.33	1.37
1	a	1407	5MC	C2-N3	-2.23	1.33	1.38
26	A	2605	PSU	C2-N3	-2.20	1.33	1.38
26	A	2449	H2U	C2-N1	-2.17	1.32	1.35
24	y	55	PSU	C2-N1	-2.10	1.33	1.38
26	A	2604	PSU	C2-N3	-2.08	1.33	1.38
22	v	54	5MU	C2-N3	-2.03	1.34	1.38
22	v	55	PSU	C2-N3	-2.02	1.34	1.38
26	A	747	5MU	C2-N3	-2.01	1.34	1.38
26	A	1915	3TD	C5-C1'	2.03	1.54	1.52
26	A	745	1MG	C6-N1	2.03	1.41	1.38
26	A	2503	2MA	C5-C4	2.55	1.46	1.40
26	A	2503	2MA	C6-N6	2.67	1.33	1.29
26	A	2251	OMG	C5-C4	3.00	1.47	1.40
26	A	1835	2MG	C5-C4	3.06	1.47	1.40
1	a	1519	MA6	C5-C4	3.07	1.47	1.40
24	y	37	6IA	C5-C4	3.10	1.47	1.40
1	a	1516	2MG	C5-C4	3.13	1.47	1.40
26	A	2445	2MG	C5-C4	3.17	1.47	1.40
1	a	1207	2MG	C5-C4	3.22	1.47	1.40
1	a	1518	MA6	C5-C4	3.40	1.48	1.40
1	a	966	2MG	C5-C4	3.46	1.48	1.40
26	A	1835	2MG	C6-C5	3.52	1.48	1.41
26	A	2251	OMG	C6-C5	3.58	1.48	1.41
26	A	2069	G7M	C6-C5	3.59	1.48	1.41
1	a	966	2MG	C6-C5	3.59	1.48	1.41
26	A	2030	6MZ	C5-C4	3.60	1.48	1.40
1	a	1207	2MG	C6-C5	3.61	1.48	1.41
1	a	1516	2MG	C6-C5	3.62	1.48	1.41
26	A	1618	6MZ	C5-C4	3.71	1.48	1.40
26	A	2445	2MG	C6-C5	3.72	1.48	1.41
26	A	745	1MG	C5-C4	3.74	1.48	1.40
26	A	1962	5MC	C5-C4	3.77	1.47	1.41
1	a	527	G7M	C6-C5	3.90	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	745	1MG	C6-C5	4.30	1.49	1.40
1	a	1407	5MC	C5-C4	4.45	1.48	1.41
26	A	2503	2MA	C6-C5	4.48	1.49	1.40
26	A	1915	3TD	C2-N1	5.23	1.49	1.38
26	A	1915	3TD	C4-N3	5.39	1.46	1.38
26	A	1915	3TD	C6-N1	5.62	1.46	1.34
1	a	967	5MC	C5-C4	5.65	1.50	1.41
26	A	1915	3TD	C6-C5	7.25	1.48	1.38

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	747	5MU	C5-C4-N3	-8.43	118.27	125.35
24	y	37	6IA	C12-N6-C6	-8.33	113.83	123.46
24	y	54	5MU	C5-C4-N3	-8.14	118.52	125.35
24	y	37	6IA	N3-C2-N1	-8.09	122.52	128.87
1	a	1518	MA6	N3-C2-N1	-7.67	122.84	128.87
26	A	1939	5MU	C5-C4-N3	-7.31	119.21	125.35
22	v	54	5MU	C5-C4-N3	-7.21	119.30	125.35
24	y	19	H2U	C5-C6-N1	-7.14	102.94	110.76
1	a	1519	MA6	N3-C2-N1	-6.97	123.40	128.87
26	A	1915	3TD	C5-C1'-C2'	-6.39	104.59	115.44
1	a	966	2MG	CM2-N2-C2	-6.15	116.12	123.03
22	v	20	H2U	C5-C6-N1	-6.12	104.06	110.76
1	a	527	G7M	C5-C6-N1	-5.88	115.83	123.52
26	A	2069	G7M	C5-C6-N1	-5.77	115.98	123.52
26	A	1618	6MZ	N3-C2-N1	-5.66	124.43	128.87
26	A	2030	6MZ	N3-C2-N1	-5.53	124.53	128.87
1	a	1516	2MG	C5-C6-N1	-4.40	117.77	123.52
26	A	746	PSU	C5-C6-N1	-4.35	118.31	124.38
26	A	2445	2MG	C5-C6-N1	-4.29	117.92	123.52
26	A	2445	2MG	CM2-N2-C2	-4.23	118.28	123.03
26	A	2251	OMG	C5-C6-N1	-4.13	118.12	123.52
1	a	1207	2MG	C5-C6-N1	-4.10	118.17	123.52
26	A	2457	PSU	C5-C6-N1	-4.06	118.72	124.38
26	A	1911	PSU	C5-C6-N1	-3.99	118.81	124.38
1	a	966	2MG	C5-C6-N1	-3.92	118.39	123.52
24	y	55	PSU	C5-C6-N1	-3.89	118.96	124.38
1	a	516	PSU	C5-C6-N1	-3.85	119.01	124.38
26	A	1835	2MG	C5-C6-N1	-3.84	118.50	123.52
24	y	37	6IA	C1'-N9-C4	-3.70	122.67	126.81
22	v	20	H2U	C4-N3-C2	-3.68	122.43	125.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	19	H2U	C4-N3-C2	-3.68	122.44	125.77
26	A	2605	PSU	C5-C6-N1	-3.66	119.28	124.38
26	A	2604	PSU	C5-C6-N1	-3.64	119.31	124.38
26	A	2251	OMG	N3-C2-N1	-3.63	122.62	127.56
26	A	2580	PSU	C5-C6-N1	-3.62	119.33	124.38
22	v	55	PSU	C5-C6-N1	-3.55	119.43	124.38
1	a	1207	2MG	C6-C5-C4	-3.48	116.88	120.86
1	a	1402	4OC	CM4-N4-C4	-3.48	119.94	122.87
26	A	2504	PSU	C5-C6-N1	-3.41	119.62	124.38
26	A	955	PSU	C5-C6-N1	-3.40	119.64	124.38
26	A	955	PSU	C5-C1'-C2'	-3.39	109.68	115.44
24	y	55	PSU	C5-C1'-C2'	-3.33	109.78	115.44
26	A	2251	OMG	C6-C5-C4	-3.17	117.24	120.86
26	A	2605	PSU	C5-C1'-C2'	-3.17	110.06	115.44
26	A	1835	2MG	CM2-N2-C2	-3.13	119.51	123.03
22	v	55	PSU	C5-C1'-C2'	-3.13	110.13	115.44
1	a	1516	2MG	C6-C5-C4	-3.06	117.36	120.86
26	A	2504	PSU	C5-C1'-C2'	-3.01	110.32	115.44
26	A	1915	3TD	C5-C6-N1	-2.99	120.22	124.38
22	v	8	4SU	C5-C4-N3	-2.97	120.42	123.56
1	a	1519	MA6	C10-N6-C9	-2.81	106.78	115.96
26	A	745	1MG	C6-C5-C4	-2.81	117.92	119.93
26	A	1835	2MG	C6-C5-C4	-2.77	117.69	120.86
26	A	2449	H2U	C4-N3-C2	-2.68	123.33	125.77
1	a	527	G7M	N3-C2-N1	-2.65	123.95	127.56
26	A	2498	OMC	CM2-O2'-C2'	-2.59	107.33	114.58
1	a	1207	2MG	CM2-N2-C2	-2.56	120.16	123.03
26	A	2069	G7M	N3-C2-N1	-2.52	124.13	127.56
26	A	2604	PSU	C5-C1'-C2'	-2.52	111.16	115.44
26	A	2445	2MG	C6-C5-C4	-2.47	118.04	120.86
26	A	2503	2MA	C6-C5-C4	-2.40	115.36	119.67
1	a	527	G7M	C4'-O4'-C1'	-2.33	107.17	109.64
1	a	1207	2MG	N3-C2-N1	-2.33	122.70	126.19
26	A	1917	PSU	C5-C6-N1	-2.33	121.14	124.38
26	A	2449	H2U	O2-C2-N1	-2.26	120.21	123.17
26	A	2069	G7M	C4'-O4'-C1'	-2.21	107.30	109.64
26	A	1835	2MG	N3-C2-N1	-2.19	122.91	126.19
26	A	1962	5MC	C5-C4-N3	-2.19	117.53	121.26
1	a	1516	2MG	N3-C2-N1	-2.18	122.92	126.19
1	a	1516	2MG	CM2-N2-C2	-2.15	120.62	123.03
1	a	966	2MG	C6-C5-C4	-2.12	118.44	120.86
26	A	1962	5MC	CM5-C5-C4	-2.11	119.24	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2457	PSU	O2'-C2'-C1'	-2.09	107.38	111.93
1	a	1519	MA6	C1'-N9-C4	-2.06	124.50	126.81
26	A	1915	3TD	C4-C5-C1'	2.04	124.70	121.24
1	a	527	G7M	O2'-C2'-C1'	2.05	118.04	111.61
26	A	1962	5MC	CM5-C5-C6	2.08	122.83	118.63
26	A	1917	PSU	O4'-C1'-C2'	2.10	106.96	104.69
24	y	37	6IA	C13-C12-N6	2.10	116.19	112.25
1	a	527	G7M	C5'-C4'-C3'	2.13	123.45	115.20
26	A	2449	H2U	N3-C2-N1	2.15	118.63	116.64
24	y	37	6IA	C5-C6-N6	2.21	124.08	120.61
26	A	2604	PSU	O4'-C1'-C2'	2.24	107.11	104.69
26	A	955	PSU	O4'-C1'-C2'	2.32	107.20	104.69
24	y	55	PSU	O4'-C1'-C2'	2.33	107.20	104.69
26	A	2504	PSU	O4'-C1'-C2'	2.42	107.31	104.69
26	A	1915	3TD	O4'-C1'-C2'	2.42	107.31	104.69
22	v	20	H2U	C5-C4-N3	2.44	119.20	116.62
24	y	19	H2U	C5-C4-N3	2.46	119.22	116.62
26	A	2605	PSU	O4'-C1'-C2'	2.60	107.50	104.69
26	A	1911	PSU	O4'-C1'-C2'	2.64	107.55	104.69
22	v	20	H2U	C6-N1-C2	2.66	126.27	122.16
26	A	2580	PSU	O4'-C1'-C2'	2.83	107.75	104.69
22	v	55	PSU	O4'-C1'-C2'	2.91	107.83	104.69
26	A	2069	G7M	O3'-C3'-C2'	2.94	121.35	111.86
26	A	2069	G7M	C1'-N9-C4	2.98	130.14	126.81
26	A	2457	PSU	O4'-C1'-C2'	3.01	107.95	104.69
1	a	966	2MG	C1'-N9-C4	3.04	130.20	126.81
26	A	2449	H2U	C5-C4-N3	3.11	119.90	116.62
26	A	1917	PSU	C4-C5-C1'	3.18	126.57	121.22
1	a	527	G7M	O3'-C3'-C2'	3.19	122.17	111.86
26	A	2069	G7M	O3'-C3'-C4'	3.39	121.13	111.01
1	a	527	G7M	O3'-C3'-C4'	3.40	121.17	111.01
26	A	2069	G7M	N7-C8-N9	3.55	113.92	108.67
26	A	2449	H2U	C6-N1-C2	3.59	127.71	122.16
26	A	1915	3TD	C5-C4-N3	3.61	121.60	118.65
1	a	527	G7M	N7-C8-N9	3.70	114.14	108.67
1	a	516	PSU	O4'-C1'-C2'	3.72	108.71	104.69
26	A	2498	OMC	C6-C5-C4	3.82	118.93	117.44
24	y	19	H2U	C1'-N1-C2	4.03	123.83	118.19
26	A	2030	6MZ	C2-N1-C6	4.07	119.40	116.47
1	a	1402	4OC	C2-N3-C4	4.11	120.66	115.43
1	a	966	2MG	C6-N1-C2	4.19	121.24	115.24
26	A	1835	2MG	C6-N1-C2	4.48	121.66	115.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2445	2MG	C6-N1-C2	4.48	121.66	115.24
1	a	1519	MA6	C2-N1-C6	4.49	122.23	111.64
1	a	1518	MA6	C2-N1-C6	4.63	122.57	111.64
1	a	1207	2MG	C6-N1-C2	4.98	122.37	115.24
1	a	1516	2MG	C6-N1-C2	4.98	122.37	115.24
26	A	1962	5MC	N4-C4-N3	5.09	124.38	116.92
1	a	1516	2MG	C2-N3-C4	5.39	120.90	114.99
26	A	2251	OMG	C6-N1-C2	5.39	122.20	115.88
1	a	1402	4OC	C6-C5-C4	5.40	119.54	117.42
26	A	2445	2MG	C2-N3-C4	5.55	121.07	114.99
1	a	527	G7M	C1'-N9-C4	5.67	133.13	126.81
1	a	1207	2MG	C2-N3-C4	5.74	121.28	114.99
26	A	2069	G7M	C6-N1-C2	5.78	122.65	115.88
26	A	1911	PSU	C4-N3-C2	5.79	119.99	115.16
1	a	527	G7M	C6-N1-C2	5.83	122.71	115.88
1	a	966	2MG	C2-N3-C4	5.98	121.55	114.99
1	a	516	PSU	C4-N3-C2	6.03	120.19	115.16
26	A	746	PSU	C4-N3-C2	6.10	120.25	115.16
26	A	2605	PSU	C4-N3-C2	6.30	120.41	115.16
26	A	1835	2MG	C2-N3-C4	6.33	121.93	114.99
26	A	955	PSU	C4-N3-C2	6.35	120.46	115.16
26	A	2457	PSU	C4-N3-C2	6.44	120.53	115.16
24	y	55	PSU	C4-N3-C2	6.49	120.57	115.16
26	A	2604	PSU	C4-N3-C2	6.58	120.65	115.16
26	A	1939	5MU	C4-N3-C2	6.79	120.82	115.16
26	A	2552	OMU	C4-N3-C2	6.83	121.41	114.21
26	A	747	5MU	C4-N3-C2	6.84	120.86	115.16
26	A	2580	PSU	C4-N3-C2	6.92	120.93	115.16
22	v	55	PSU	C4-N3-C2	7.09	121.07	115.16
22	v	54	5MU	C4-N3-C2	7.16	121.13	115.16
26	A	2504	PSU	C4-N3-C2	7.35	121.29	115.16
26	A	1618	6MZ	C2-N1-C6	7.46	121.83	116.47
24	y	54	5MU	C4-N3-C2	8.25	122.04	115.16
26	A	1917	PSU	C4-N3-C2	8.34	122.11	115.16
24	y	37	6IA	C2-N1-C6	9.20	123.09	116.47
26	A	2503	2MA	C2-N3-C4	16.39	123.19	115.29

All (4) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
26	A	2069	G7M	C4'
26	A	2069	G7M	C3'

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	1911	PSU	1	0
26	A	1915	3TD	1	0
26	A	1962	5MC	1	0
26	A	2457	PSU	1	0
26	A	2504	PSU	1	0
26	A	745	1MG	2	0
26	A	746	PSU	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
59	FME	v	101	22	8,9,10	0.85	0	5,9,11	0.83	0
60	SEC	y	701	24	1,5,6	0.78	0	1,5,7	2.98	1 (100%)
61	GNP	z	701	62	29,34,34	2.63	8 (27%)	28,54,54	1.54	6 (21%)

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
59	FME	v	101	22	-	1/6/9/11	0/0/0/0
60	SEC	y	701	24	-	0/0/4/6	0/0/0/0
61	GNP	z	701	62	-	0/16/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	z	701	GNP	C4-N9	-10.19	1.34	1.47
61	z	701	GNP	C8-N9	-3.80	1.35	1.47
61	z	701	GNP	C5-C6	-2.75	1.48	1.53
61	z	701	GNP	C2-N1	-2.25	1.34	1.44
61	z	701	GNP	PB-O1B	2.59	1.48	1.46
61	z	701	GNP	PB-N3B	3.78	1.73	1.63
61	z	701	GNP	C1'-N9	3.86	1.49	1.42
61	z	701	GNP	PG-N3B	3.94	1.74	1.63

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	z	701	GNP	PA-O3A-PB	-3.01	121.77	132.71
60	y	701	SEC	O-C-CA	-2.98	117.73	125.72
61	z	701	GNP	O3G-PG-O1G	-2.61	106.70	113.58
61	z	701	GNP	O5'-C5'-C4'	2.63	118.58	109.09
61	z	701	GNP	C2'-C3'-C4'	2.68	108.11	102.64
61	z	701	GNP	C4-C5-N7	2.75	106.97	102.67
61	z	701	GNP	C8-N9-C4	3.09	108.31	104.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	v	101	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.