



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 5, 2016 – 04:49 PM EST

PDB ID : 5LZB
EMDB ID: : EMD-4122
Title : Structure of SelB-Sec-tRNA^{Sec} bound to the 70S ribosome in the initial binding state (IB)
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 : 5.30 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

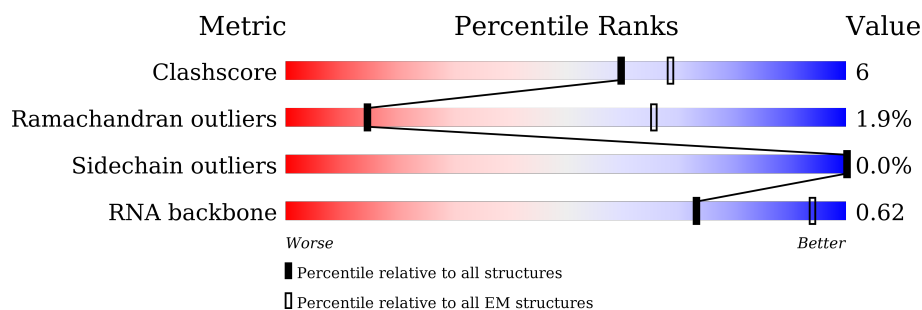
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



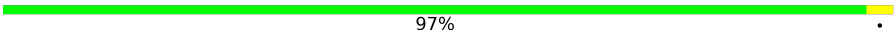

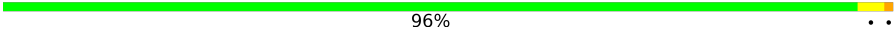

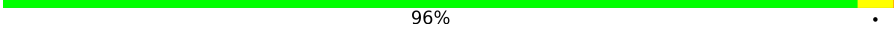
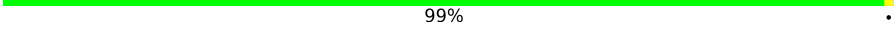

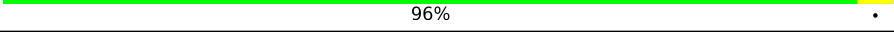
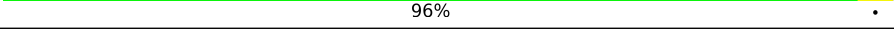

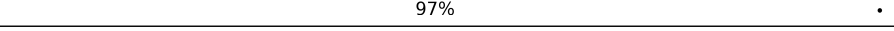
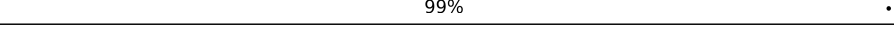
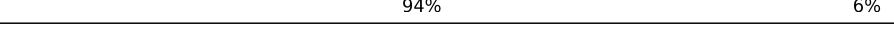

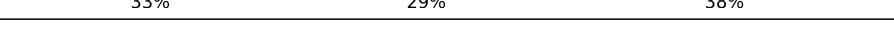

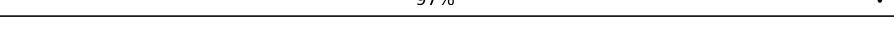


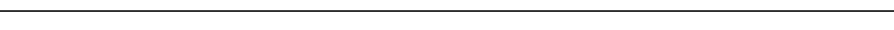

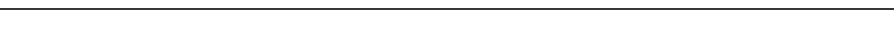
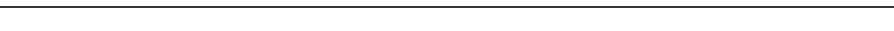


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	a	1539	75% 22% .
2	b	218	96% .
3	c	206	97% .
4	d	205	97% .
5	e	157	95% 5%
6	f	100	95% 5%
7	g	151	97% .
8	h	129	98% .












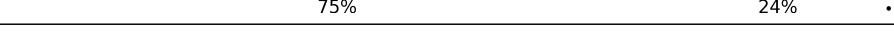







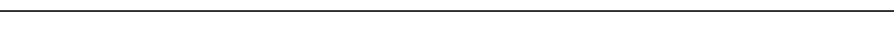

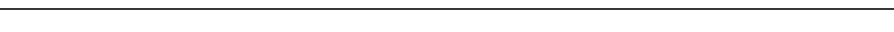
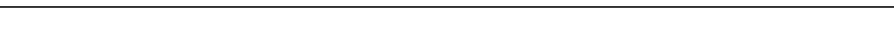


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Mol	Chain	Length	Quality of chain
9	i	127	 97% .
10	j	98	 92% 7% .
11	k	116	 96% ..
12	l	123	 93% 7%
13	m	114	 96% ..
14	n	100	 99% .
15	o	88	 93% 6% .
16	p	82	 96% .
17	q	80	 96% .
18	r	65	 92% 8%
19	s	79	 97% .
20	t	85	 99% .
21	u	65	 94% 6%
22	v	77	 66% 34%
23	x	48	 33% 29% 38%
24	y	95	 44% 39% 17%
25	z	614	 97% .
26	A	2903	 62% 31% 6% .
27	B	120	 64% 29% 5% .
28	C	271	 82% 17%
29	D	209	 78% 22%
30	E	201	 87% 13%
31	F	177	 81% 18% .
32	G	176	 74% 23% .
33	I	141	 78% 21% ..

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Mol	Chain	Length	Quality of chain
34	H	149	 83% 15% .
35	J	142	 82% 17% .
36	K	122	 78% 21% .
37	L	143	 78% 22% .
38	M	136	 81% 18% .
39	N	120	 82% 18%
40	O	116	 83% 17%
41	P	114	 81% 19%
42	Q	117	 85% 15%
43	R	103	 80% 20%
44	S	110	 87% 11% .
45	T	93	 75% 24% .
46	U	102	 67% 31% .
47	V	94	 86% 14%
48	W	75	 83% 17%
49	X	77	 91% 9%
50	Y	63	 83% 16% .
51	Z	58	 76% 24%
52	0	56	 84% 16%
53	1	50	 76% 24%
54	2	46	 87% 13%
55	3	64	 86% 13% .
56	4	38	 82% 16% .
57	6	66	 73% 21% 6%
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

There are 64 unique types of molecules in this entry. The entry contains 152991 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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-tRNA^{Sec}.

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

- Molecule 25 is a protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	614	Total	C	N	O	S	1	0
			4863	3049	904	893	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	C	N	O	0	0
			947	604	192	151		

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

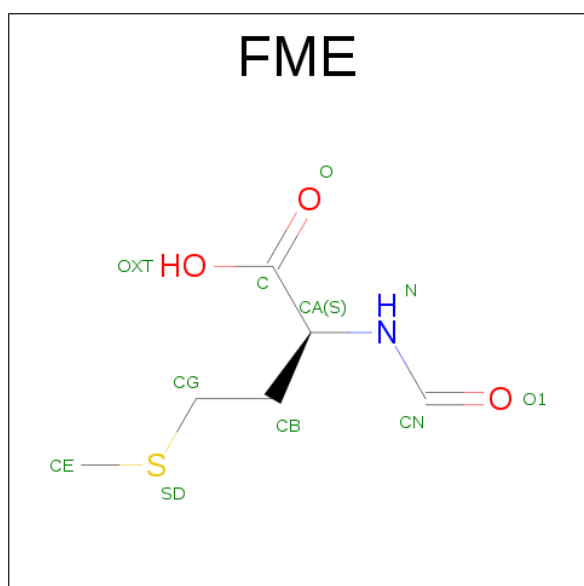
- Molecule 57 is a protein called 50S ribosomal protein L31.

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 tRNA^{Sec} (low occupancy).

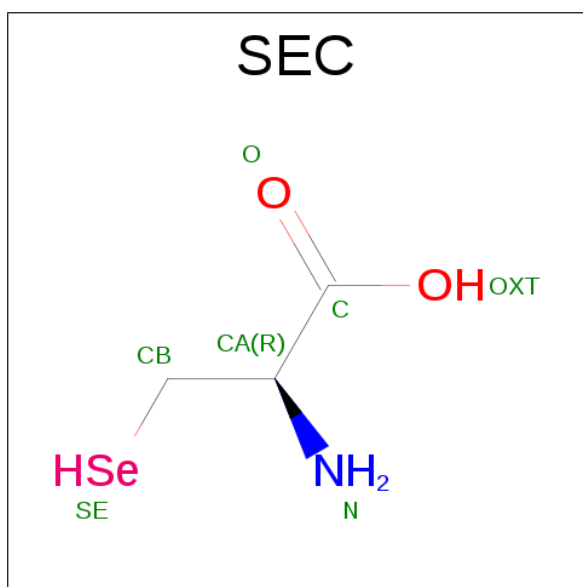
Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



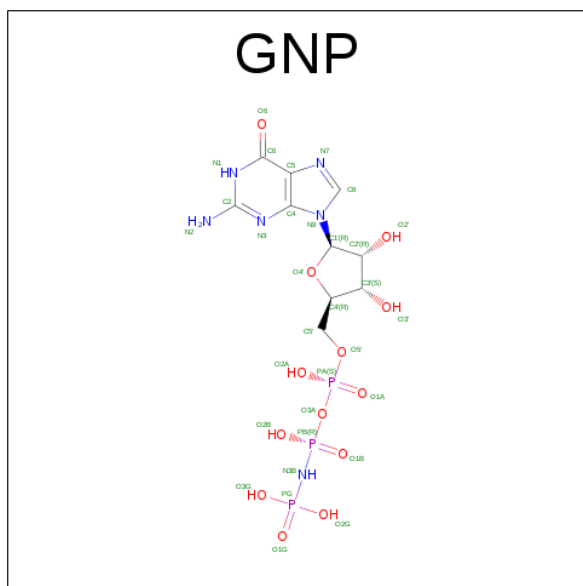
Mol	Chain	Residues	Atoms					AltConf
59	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is SELENOCYSTEINE (three-letter code: SEC) (formula: C₃H₇NO₂Se).



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: C₁₀H₁₇N₆O₁₃P₃).



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

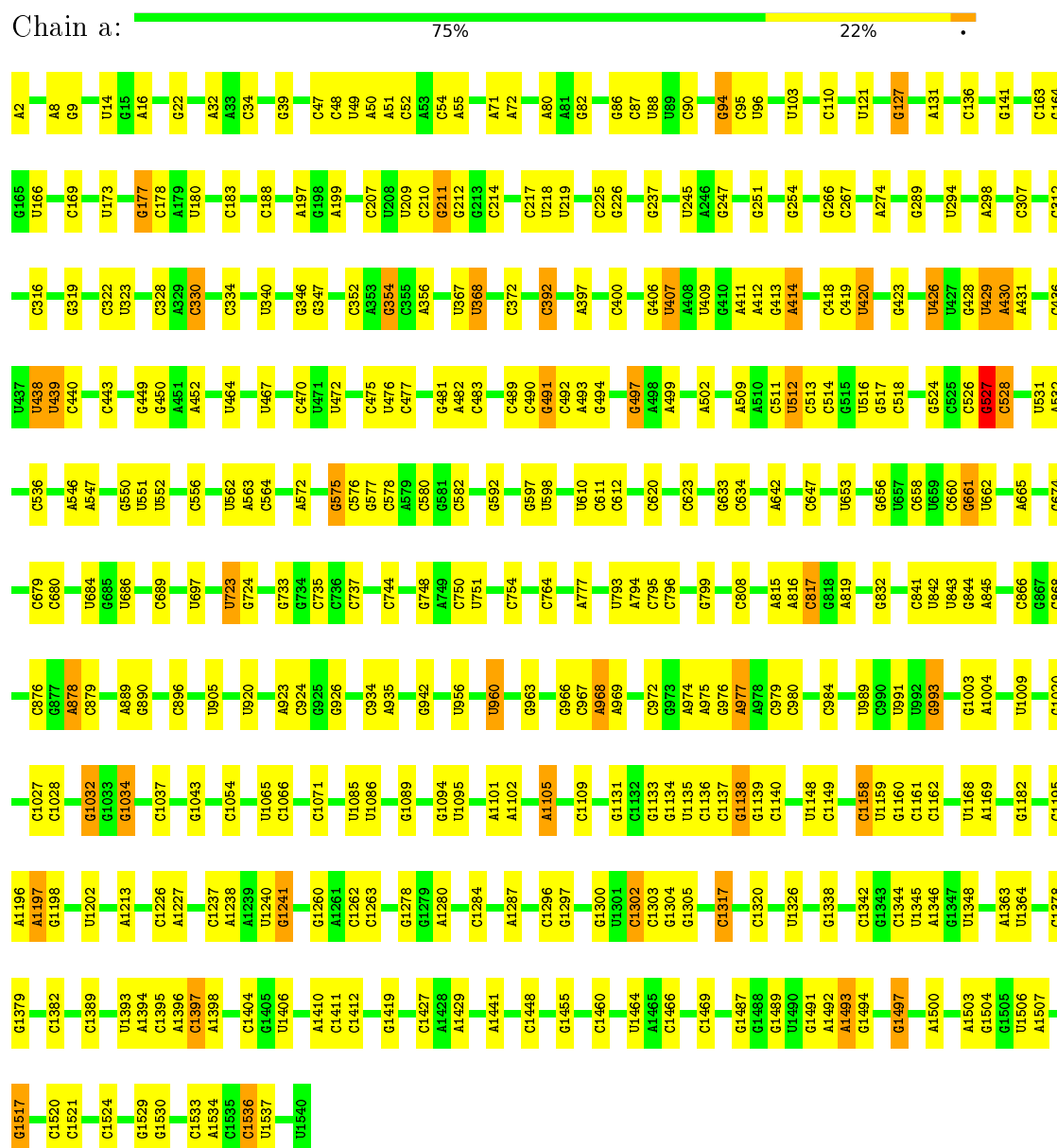
- Molecule 64 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S ribosomal RNA



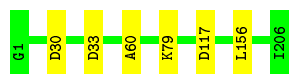
- Molecule 2: 30S ribosomal protein S2

Chain b:  96% .



- Molecule 3: 30S ribosomal protein S3

Chain c:  97% .



- Molecule 4: 30S ribosomal protein S4

Chain d:  97% .



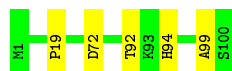
- Molecule 5: 30S ribosomal protein S5

Chain e:  95% 5%



- Molecule 6: 30S ribosomal protein S6

Chain f:  95% 5%



- Molecule 7: 30S ribosomal protein S7

Chain g:  97% .



- Molecule 8: 30S ribosomal protein S8

Chain h:  98% .



- Molecule 9: 30S ribosomal protein S9

Chain i:  97% .



- Molecule 10: 30S ribosomal protein S10

Chain j: 92% 7%



- Molecule 11: 30S ribosomal protein S11

Chain k: 96% ..



- Molecule 12: 30S ribosomal protein S12

Chain l: 93% 7%



- Molecule 13: 30S ribosomal protein S13

Chain m: 96% ..



- Molecule 14: 30S ribosomal protein S14

Chain n: 99% .



- Molecule 15: 30S ribosomal protein S15

Chain o: 93% 6% .



- Molecule 16: 30S ribosomal protein S16

Chain p: 96% .



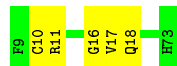
- Molecule 17: 30S ribosomal protein S17

Chain q:  96% .



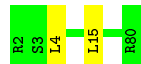
- Molecule 18: 30S ribosomal protein S18

Chain r:  92% 8%



- Molecule 19: 30S ribosomal protein S19

Chain s:  97% .



- Molecule 20: 30S ribosomal protein S20

Chain t:  99% .



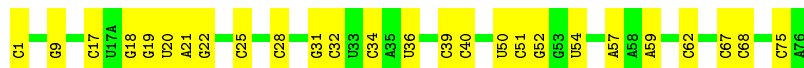
- Molecule 21: 30S ribosomal protein S21

Chain u:  94% 6%

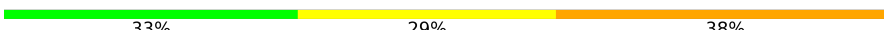


- Molecule 22: fMet-tRNA^{fMet}

Chain v:  66% 34%



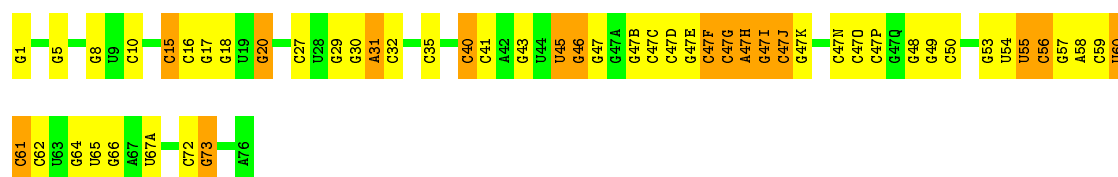
- Molecule 23: SECIS mRNA

Chain x:  33% 29% 38%



- Molecule 24: Sec-tRNA^{Sec}

Chain y:  44% 39% 17%



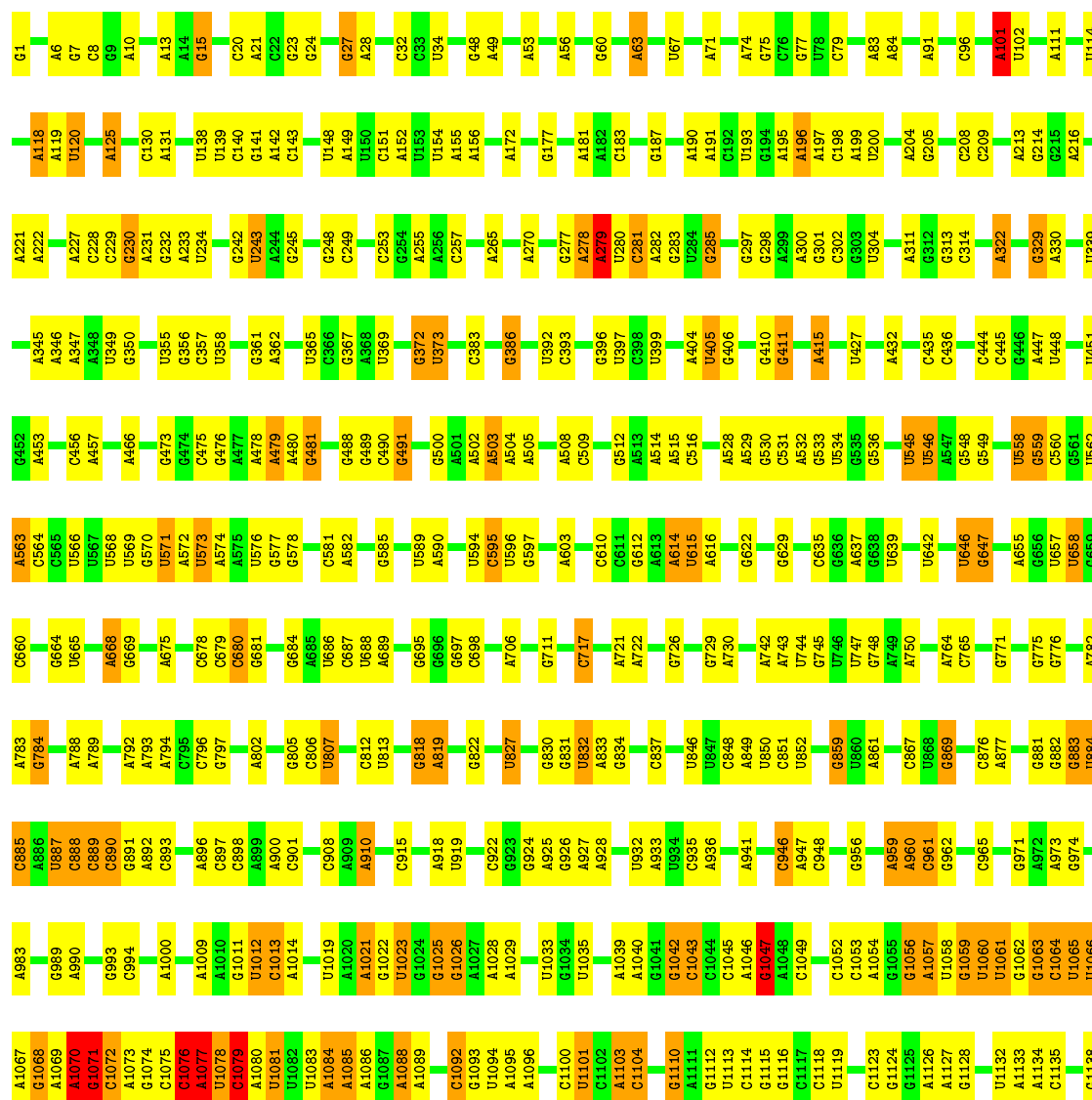
- Molecule 25: Selenocysteine-specific elongation factor

Chain z: 97%



- Molecule 26: 23S ribosomal RNA

Chain A: 62% 31% 6%

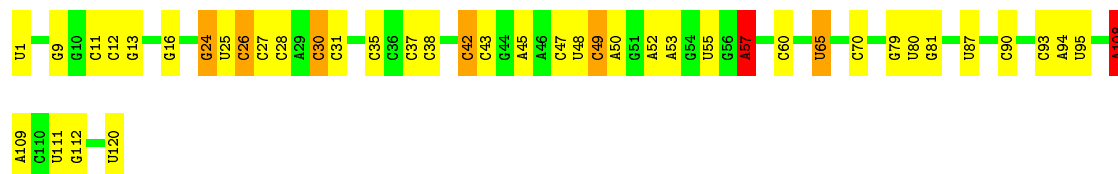






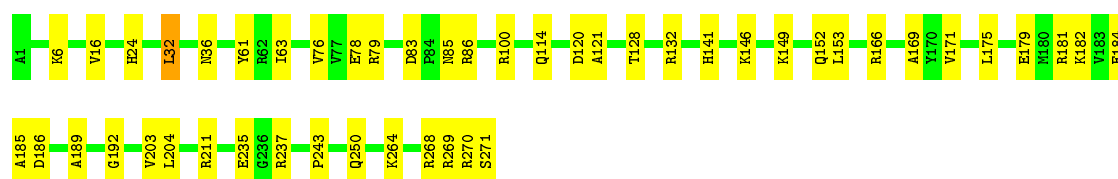

• Molecule 27: 5S ribosomal RNA

Chain B: 64% 29% 5%



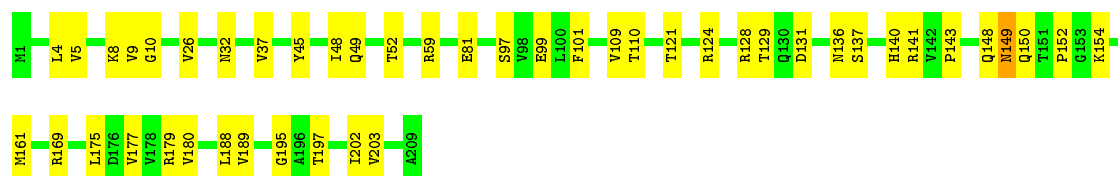
• Molecule 28: 50S ribosomal protein L2

Chain C: 82% 17%



• Molecule 29: 50S ribosomal protein L3

Chain D: 78% 22%



• Molecule 30: 50S ribosomal protein L4

Chain E: 87% 13%



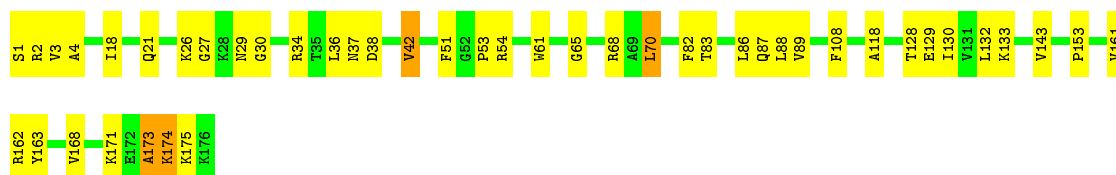
• Molecule 31: 50S ribosomal protein L5

Chain F: 81% 18%



• Molecule 32: 50S ribosomal protein L6

Chain G: 74% 23%



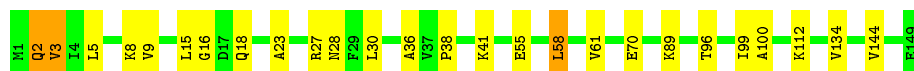
- Molecule 33: 50S ribosomal protein L11

Chain I: 78% 21% ..



- Molecule 34: 50S ribosomal protein L9

Chain H: 83% 15% .



- Molecule 35: 50S ribosomal protein L13

Chain J: 82% 17% .



- Molecule 36: 50S ribosomal protein L14

Chain K: 78% 21% .



- Molecule 37: 50S ribosomal protein L15

Chain L: 78% 22% .



- Molecule 38: 50S ribosomal protein L16

Chain M: 81% 18% .



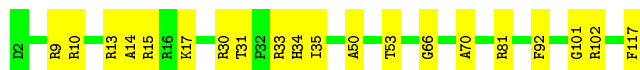
- Molecule 39: 50S ribosomal protein L17

Chain N: 82% 18%



- Molecule 40: 50S ribosomal protein L18

Chain O: 83% 17%



- Molecule 41: 50S ribosomal protein L19

Chain P: 81% 19%



- Molecule 42: 50S ribosomal protein L20

Chain Q: 85% 15%



- Molecule 43: 50S ribosomal protein L21

Chain R: 80% 20%



- Molecule 44: 50S ribosomal protein L22

Chain S: 87% 11%



- Molecule 45: 50S ribosomal protein L23

Chain T: 75% 24%

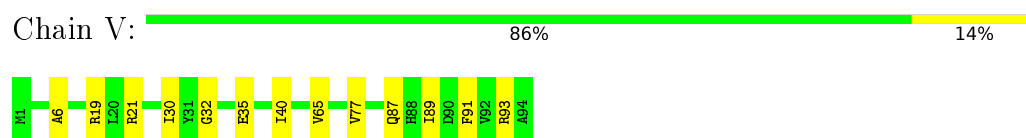


- Molecule 46: 50S ribosomal protein L24

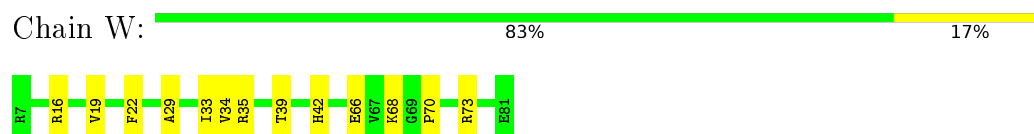
Chain U: 67% 31%



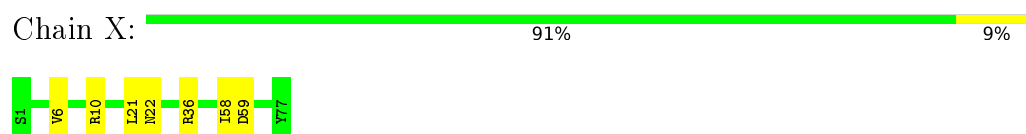
- Molecule 47: 50S ribosomal protein L25



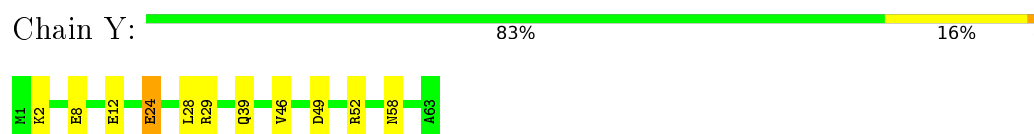
- Molecule 48: 50S ribosomal protein L27



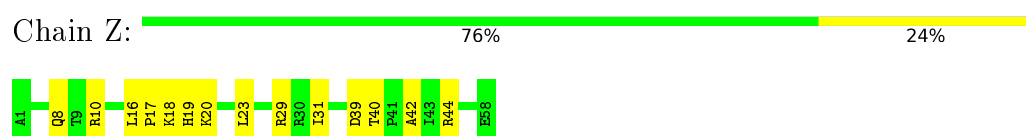
- Molecule 49: 50S ribosomal protein L28



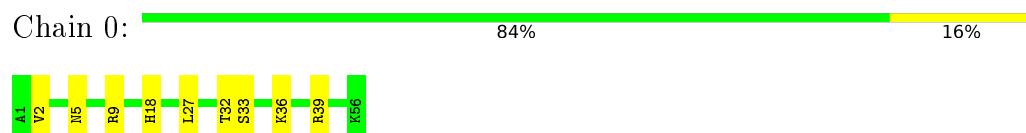
- Molecule 50: 50S ribosomal protein L29



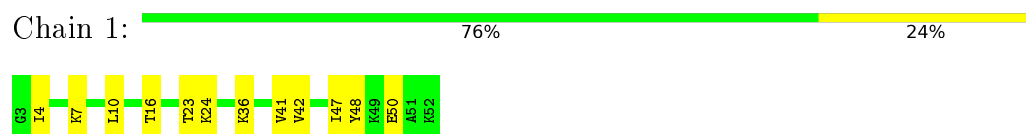
- Molecule 51: 50S ribosomal protein L30



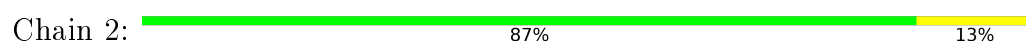
- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



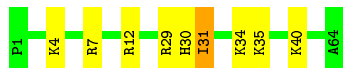
- Molecule 54: 50S ribosomal protein L34





- Molecule 55: 50S ribosomal protein L35

Chain 3: 86% 13% .



- Molecule 56: 50S ribosomal protein L36

Chain 4: 82% 16% .



- Molecule 57: 50S ribosomal protein L31

Chain 6: 73% 21% 6%



- Molecule 58: CCA 3' end of E-site tRNA^{Sec} (low occupancy)

Chain w: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	8002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.58	3/36701 (0.0%)	1.30	392/57246 (0.7%)
10	j	0.44	0/797	0.87	1/1077 (0.1%)
11	k	0.48	0/886	0.87	3/1195 (0.3%)
12	l	0.43	0/969	0.79	1/1300 (0.1%)
13	m	0.42	0/893	0.90	1/1193 (0.1%)
14	n	0.45	0/806	0.82	1/1074 (0.1%)
15	o	0.42	0/722	0.81	3/964 (0.3%)
16	p	0.55	0/659	0.78	0/884
17	q	0.45	0/658	0.88	0/881
18	r	0.36	0/512	0.67	0/689
19	s	0.37	0/653	0.73	2/877 (0.2%)
2	b	0.45	0/1736	0.85	4/2338 (0.2%)
20	t	0.43	0/671	0.77	0/888
21	u	0.43	0/501	0.85	1/668 (0.1%)
22	v	0.62	2/1745 (0.1%)	1.33	25/2716 (0.9%)
23	x	0.88	1/1145 (0.1%)	1.84	45/1781 (2.5%)
24	y	0.89	2/2168 (0.1%)	1.92	110/3375 (3.3%)
25	z	0.47	0/4963	0.89	12/6727 (0.2%)
26	A	0.57	13/69240 (0.0%)	1.24	539/108014 (0.5%)
27	B	0.58	1/2873 (0.0%)	1.24	27/4478 (0.6%)
28	C	0.42	0/2122	0.77	1/2852 (0.0%)
29	D	0.45	0/1586	0.75	0/2134
3	c	0.41	0/1652	0.76	3/2225 (0.1%)
30	E	0.43	0/1571	0.75	2/2113 (0.1%)
31	F	0.52	1/1435 (0.1%)	0.90	4/1926 (0.2%)
32	G	0.47	0/1343	0.82	3/1816 (0.2%)
33	I	0.49	0/1046	0.97	5/1410 (0.4%)
34	H	0.40	0/1122	0.74	1/1515 (0.1%)
35	J	0.42	0/1152	0.70	2/1551 (0.1%)
36	K	0.47	0/948	0.75	0/1268
37	L	0.42	0/1054	0.75	0/1403

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	M	0.43	0/1093	0.74	1/1460 (0.1%)
39	N	0.43	0/974	0.68	0/1301
4	d	0.49	0/1665	0.93	3/2227 (0.1%)
40	O	0.43	0/902	0.72	0/1209
41	P	0.43	0/929	0.72	1/1242 (0.1%)
42	Q	0.41	0/960	0.58	1/1278 (0.1%)
43	R	0.42	0/829	0.79	0/1107
44	S	0.39	0/864	0.80	2/1156 (0.2%)
45	T	0.44	0/745	0.77	0/994
46	U	0.43	0/788	0.91	1/1051 (0.1%)
47	V	0.47	0/766	0.72	0/1025
48	W	0.39	0/582	0.69	0/769
49	X	0.35	0/635	0.70	1/848 (0.1%)
5	e	0.45	0/1170	0.88	0/1573
50	Y	0.48	0/510	0.92	2/677 (0.3%)
51	Z	0.40	0/453	0.72	1/605 (0.2%)
52	0	0.44	0/450	0.80	0/599
53	1	0.36	0/417	0.77	0/554
54	2	0.40	0/380	0.69	0/498
55	3	0.40	0/513	0.63	0/676
56	4	0.48	0/303	0.80	1/397 (0.3%)
57	6	0.46	0/532	1.01	5/709 (0.7%)
58	w	0.32	0/68	0.98	0/103
6	f	0.51	0/836	0.85	1/1128 (0.1%)
7	g	0.46	0/1196	0.81	2/1602 (0.1%)
8	h	0.43	0/989	0.78	1/1326 (0.1%)
9	i	0.47	0/1034	0.84	0/1375
All	All	0.55	23/164912 (0.0%)	1.17	1211/246067 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
10	j	0	2
11	k	0	1
12	l	0	2
13	m	0	2
15	o	0	1
18	r	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	2
25	z	0	3
26	A	2	0
28	C	0	1
33	I	0	2
34	H	0	3
36	K	0	1
38	M	0	1
44	S	0	1
46	U	0	2
5	e	0	1
55	3	0	1
All	All	4	28

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	1	G	OP3-P	-10.71	1.48	1.61
22	v	1	C	OP3-P	-10.67	1.48	1.61
23	x	87	A	OP3-P	-10.65	1.48	1.61
1	a	2	A	OP3-P	-10.60	1.48	1.61
27	B	1	U	OP3-P	-10.57	1.48	1.61
26	A	1	G	OP3-P	-10.57	1.48	1.61
26	A	2169	A	C8-N7	-9.34	1.25	1.31
26	A	571	U	C4-O4	8.22	1.30	1.23
1	a	723	U	C4-O4	-6.98	1.18	1.23
26	A	2059	A	N9-C4	-6.42	1.34	1.37
26	A	1171	G	C6-N1	6.16	1.43	1.39
26	A	2167	U	N1-C2	-6.15	1.33	1.38
26	A	1085	A	N7-C5	-6.04	1.35	1.39
31	F	11	VAL	CB-CG1	-5.89	1.40	1.52
26	A	2169	A	N7-C5	-5.56	1.35	1.39
26	A	1313	U	N1-C2	5.49	1.43	1.38
24	y	61	C	C5-C6	-5.45	1.29	1.34
26	A	574	A	N9-C4	-5.16	1.34	1.37
26	A	1178	C	N3-C4	-5.09	1.30	1.33
26	A	101	A	N9-C4	-5.08	1.34	1.37
22	v	57	A	N7-C5	-5.07	1.36	1.39
26	A	278	A	N9-C4	5.03	1.40	1.37
1	a	80	A	N9-C4	-5.00	1.34	1.37

All (1211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	452	A	O5'-P-OP1	-19.89	86.83	110.70
1	a	450	G	O5'-P-OP1	16.99	131.09	110.70
26	A	1026	G	O5'-P-OP1	-15.92	91.37	105.70
26	A	2169	A	C5-N7-C8	15.84	111.82	103.90
26	A	1178	C	N1-C2-O2	15.82	128.39	118.90
26	A	1178	C	N3-C2-O2	-15.14	111.30	121.90
26	A	120	U	C5-C4-O4	-14.70	117.08	125.90
26	A	2059	A	N1-C2-N3	-14.28	122.16	129.30
26	A	890	C	N1-C2-O2	14.17	127.40	118.90
1	a	1158	C	N1-C2-O2	13.98	127.29	118.90
26	A	1171	G	N3-C2-N2	-13.97	110.12	119.90
26	A	120	U	N3-C4-O4	13.94	129.16	119.40
26	A	1313	U	N1-C2-O2	13.34	132.14	122.80
26	A	1071	G	C5-C6-O6	-13.14	120.72	128.60
1	a	1158	C	N3-C2-O2	-12.84	112.92	121.90
1	a	1304	G	O5'-P-OP2	-12.64	94.32	105.70
26	A	1313	U	N3-C2-O2	-12.56	113.41	122.20
24	y	47(I)	G	O5'-P-OP2	-12.20	94.72	105.70
26	A	2146	C	O5'-P-OP1	12.19	125.33	110.70
26	A	1186	G	O5'-P-OP2	12.09	125.20	110.70
1	a	1198	G	O5'-P-OP2	-11.90	94.99	105.70
24	y	61	C	C6-N1-C2	-11.44	115.72	120.30
26	A	1313	U	C2-N1-C1'	11.27	131.22	117.70
1	a	1197	A	O5'-P-OP1	-11.26	95.57	105.70
26	A	2109	U	C5-C6-N1	11.05	128.23	122.70
46	U	51	LEU	CA-CB-CG	10.88	140.32	115.30
23	x	117	C	N1-C2-O2	10.85	125.41	118.90
26	A	1093	G	C5-C6-O6	-10.75	122.15	128.60
26	A	2169	A	C4-C5-N7	-10.70	105.35	110.70
22	v	51	C	C6-N1-C2	-10.52	116.09	120.30
24	y	61	C	C4-C5-C6	10.45	122.62	117.40
24	y	61	C	N3-C4-C5	-10.39	117.74	121.90
24	y	41	C	C5-C6-N1	10.34	126.17	121.00
26	A	2305	U	C5-C4-O4	-10.29	119.72	125.90
24	y	47(D)	C	C6-N1-C2	-10.19	116.22	120.30
24	y	47(D)	C	C5-C6-N1	10.13	126.06	121.00
26	A	1071	G	N1-C6-O6	10.10	125.96	119.90
1	a	1054	C	O5'-P-OP2	-10.06	96.65	105.70
23	x	117	C	N3-C2-O2	-10.02	114.89	121.90
1	a	968	A	N1-C6-N6	-9.97	112.61	118.60
26	A	647	G	O5'-P-OP1	-9.92	96.77	105.70
1	a	1296	C	C6-N1-C2	-9.89	116.34	120.30
26	A	436	C	O5'-P-OP2	-9.84	96.84	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	51	C	C5-C6-N1	9.80	125.90	121.00
26	A	1993	U	N3-C2-O2	-9.78	115.35	122.20
26	A	2059	A	C6-N1-C2	9.73	124.44	118.60
26	A	1186	G	O5'-P-OP1	-9.71	96.96	105.70
26	A	887	U	N3-C2-O2	-9.71	115.41	122.20
26	A	2637	U	C5-C6-N1	9.70	127.55	122.70
26	A	2583	G	O5'-P-OP2	-9.70	96.97	105.70
24	y	48	G	N1-C6-O6	9.62	125.67	119.90
33	I	32	VAL	CG1-CB-CG2	-9.59	95.56	110.90
1	a	656	G	N3-C2-N2	-9.58	113.19	119.90
24	y	48	G	C5-C6-O6	-9.58	122.85	128.60
24	y	43	G	O4'-C1'-N9	9.54	115.83	108.20
26	A	67	U	C5-C4-O4	-9.48	120.21	125.90
26	A	1539	U	C5-C6-N1	9.46	127.43	122.70
26	A	1093	G	N9-C4-C5	-9.42	101.63	105.40
26	A	1079	C	N1-C2-O2	9.38	124.53	118.90
1	a	414	A	N1-C6-N6	-9.35	112.99	118.60
26	A	2147	A	C8-N9-C4	-9.34	102.06	105.80
1	a	597	G	O5'-P-OP2	-9.30	97.33	105.70
1	a	214	C	C5-C6-N1	9.29	125.65	121.00
1	a	1158	C	C6-N1-C2	-9.27	116.59	120.30
24	y	41	C	C6-N1-C2	-9.22	116.61	120.30
57	6	18	CYS	CA-CB-SG	-9.22	97.40	114.00
26	A	890	C	C2-N3-C4	9.16	124.48	119.90
26	A	2302	U	N3-C2-O2	-9.16	115.79	122.20
26	A	281	C	C5-C6-N1	9.15	125.58	121.00
1	a	214	C	C6-N1-C2	-9.14	116.64	120.30
24	y	47(N)	C	C6-N1-C2	-9.14	116.64	120.30
23	x	117	C	C6-N1-C2	-9.10	116.66	120.30
26	A	1783	A	O5'-P-OP2	-9.09	97.52	105.70
1	a	72	A	O5'-P-OP2	-9.08	97.53	105.70
1	a	1158	C	C2-N1-C1'	9.05	128.75	118.80
26	A	67	U	N3-C4-O4	9.03	125.72	119.40
26	A	545	U	C6-N1-C2	-9.03	115.58	121.00
23	x	125	G	N9-C1'-C2'	-9.02	102.07	112.00
26	A	2150	C	C6-N1-C2	-8.94	116.72	120.30
24	y	61	C	N1-C2-O2	8.94	124.27	118.90
26	A	2428	G	O5'-P-OP1	8.94	121.43	110.70
26	A	1171	G	N9-C4-C5	8.92	108.97	105.40
24	y	47(C)	C	C6-N1-C2	-8.87	116.75	120.30
26	A	2359	C	C6-N1-C2	-8.84	116.76	120.30
26	A	2617	U	N3-C2-O2	-8.79	116.04	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	62	C	N3-C2-O2	-8.79	115.75	121.90
26	A	2325	G	O5'-P-OP1	8.68	121.11	110.70
1	a	1241	G	C2-N3-C4	8.66	116.23	111.90
26	A	281	C	C6-N1-C2	-8.65	116.84	120.30
26	A	647	G	O5'-P-OP2	8.63	121.06	110.70
24	y	61	C	N3-C2-O2	-8.63	115.86	121.90
1	a	528	C	N1-C2-O2	8.60	124.06	118.90
26	A	887	U	N1-C2-O2	8.60	128.82	122.80
1	a	563	A	N9-C4-C5	-8.54	102.38	105.80
24	y	48	G	O4'-C1'-N9	-8.54	101.36	108.20
3	c	33	ASP	CB-CG-OD1	8.52	125.97	118.30
26	A	545	U	C5-C6-N1	8.49	126.95	122.70
24	y	73	G	C4-C5-N7	8.42	114.17	110.80
26	A	1042	G	P-O3'-C3'	8.40	129.78	119.70
1	a	1412	C	C6-N1-C2	-8.37	116.95	120.30
26	A	1104	C	C6-N1-C2	-8.35	116.96	120.30
26	A	546	U	C5-C6-N1	8.35	126.87	122.70
24	y	60	U	N1-C2-O2	-8.32	116.98	122.80
26	A	610	C	C6-N1-C2	-8.32	116.97	120.30
1	a	392	C	C6-N1-C2	-8.32	116.97	120.30
23	x	127	U	P-O3'-C3'	8.31	129.67	119.70
26	A	571	U	N3-C4-C5	-8.31	109.61	114.60
24	y	57	G	O5'-P-OP2	8.24	120.59	110.70
26	A	1093	G	C4-C5-N7	8.24	114.10	110.80
21	u	15	LEU	CA-CB-CG	8.23	134.23	115.30
1	a	1296	C	N1-C2-O2	8.22	123.83	118.90
1	a	972	C	C6-N1-C2	-8.22	117.01	120.30
24	y	30	G	N9-C4-C5	-8.21	102.12	105.40
27	B	24	G	C5-C6-O6	-8.19	123.69	128.60
26	A	2150	C	C5-C6-N1	8.18	125.09	121.00
25	z	328	ALA	N-CA-C	-8.18	88.92	111.00
26	A	1080	A	C8-N9-C4	-8.18	102.53	105.80
26	A	1076	C	C6-N1-C2	-8.14	117.05	120.30
26	A	2714	G	O5'-P-OP2	8.13	120.46	110.70
1	a	1296	C	C5-C6-N1	8.12	125.06	121.00
1	a	723	U	N3-C4-C5	8.12	119.47	114.60
26	A	2109	U	C6-N1-C2	-8.11	116.13	121.00
26	A	2502	G	O5'-P-OP2	8.11	120.43	110.70
26	A	1076	C	C5-C6-N1	8.07	125.04	121.00
15	o	30	LEU	CB-CG-CD2	-8.06	97.30	111.00
1	a	1397	C	C6-N1-C2	8.05	123.52	120.30
24	y	61	C	C2-N1-C1'	8.05	127.66	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2267	A	C2-N3-C4	8.05	114.63	110.60
26	A	2169	A	N7-C8-N9	-8.05	109.78	113.80
26	A	2147	A	N7-C8-N9	8.02	117.81	113.80
26	A	2109	U	C2-N3-C4	7.99	131.79	127.00
1	a	477	C	C6-N1-C2	-7.97	117.11	120.30
1	a	419	C	C6-N1-C2	-7.96	117.12	120.30
26	A	84	A	C8-N9-C4	7.96	108.98	105.80
26	A	2269	G	O5'-P-OP1	-7.93	98.56	105.70
1	a	799	G	N1-C6-O6	-7.92	115.15	119.90
24	y	61	C	N3-C4-N4	7.90	123.53	118.00
1	a	34	C	C6-N1-C2	-7.89	117.14	120.30
27	B	24	G	N1-C6-O6	7.89	124.63	119.90
1	a	1395	C	N1-C2-O2	7.88	123.63	118.90
26	A	2637	U	C6-N1-C2	-7.88	116.28	121.00
26	A	891	G	C5-C6-O6	-7.87	123.88	128.60
26	A	890	C	C4-C5-C6	-7.85	113.47	117.40
26	A	1047	G	O4'-C1'-N9	7.85	114.48	108.20
23	x	117	C	C2-N1-C1'	7.84	127.43	118.80
26	A	2466	C	O5'-P-OP1	-7.84	98.65	105.70
1	a	750	C	C6-N1-C2	-7.83	117.17	120.30
1	a	392	C	N1-C2-O2	7.82	123.59	118.90
26	A	1386	C	C5-C6-N1	7.79	124.90	121.00
26	A	962	G	O5'-P-OP1	-7.78	98.70	105.70
1	a	513	C	C6-N1-C2	-7.76	117.19	120.30
6	f	72	ASP	CB-CG-OD1	7.76	125.28	118.30
26	A	2758	A	N1-C6-N6	-7.75	113.95	118.60
26	A	669	G	N3-C4-C5	-7.74	124.73	128.60
26	A	885	C	C6-N1-C2	-7.73	117.21	120.30
26	A	1270	C	C5-C6-N1	7.73	124.86	121.00
26	A	883	G	C6-C5-N7	-7.72	125.77	130.40
26	A	1564	C	C5-C6-N1	7.72	124.86	121.00
26	A	2359	C	C5-C6-N1	7.72	124.86	121.00
26	A	1656	C	C5-C6-N1	7.71	124.86	121.00
26	A	2474	U	N3-C2-O2	-7.71	116.80	122.20
33	I	64	ARG	CA-CB-CG	7.71	130.35	113.40
26	A	546	U	C6-N1-C2	-7.70	116.38	121.00
13	m	57	ASP	CB-CG-OD1	7.68	125.21	118.30
1	a	1397	C	N3-C4-N4	-7.65	112.65	118.00
26	A	2166	U	C6-N1-C2	-7.64	116.42	121.00
1	a	924	C	C6-N1-C2	-7.64	117.25	120.30
26	A	2416	C	C5-C6-N1	7.64	124.82	121.00
26	A	571	U	C5-C4-O4	7.63	130.48	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1074	G	N3-C2-N2	-7.62	114.56	119.90
26	A	1656	C	C6-N1-C2	-7.62	117.25	120.30
1	a	754	C	C2-N1-C1'	7.61	127.17	118.80
7	g	139	ASP	CB-CG-OD1	7.61	125.14	118.30
1	a	492	C	C5-C6-N1	7.60	124.80	121.00
1	a	993	G	N9-C4-C5	-7.59	102.36	105.40
4	d	190	LEU	CB-CG-CD1	7.59	123.90	111.00
27	B	11	C	C6-N1-C2	-7.59	117.27	120.30
1	a	430	A	O5'-P-OP1	-7.58	98.88	105.70
1	a	993	G	N3-C4-N9	7.56	130.54	126.00
1	a	34	C	C5-C6-N1	7.56	124.78	121.00
26	A	1271	G	O4'-C1'-N9	7.55	114.24	108.20
26	A	2143	C	C6-N1-C2	-7.53	117.29	120.30
26	A	2896	C	C5-C6-N1	7.53	124.76	121.00
1	a	1034	G	C4-C5-N7	7.51	113.81	110.80
24	y	27	C	C6-N1-C2	-7.49	117.30	120.30
26	A	1171	G	N1-C2-N2	7.49	122.94	116.20
1	a	476	U	C5-C6-N1	7.47	126.44	122.70
24	y	30	G	N3-C4-N9	7.46	130.48	126.00
1	a	737	C	C6-N1-C2	-7.42	117.33	120.30
1	a	1102	A	N9-C4-C5	-7.42	102.83	105.80
26	A	231	A	N9-C4-C5	-7.42	102.83	105.80
26	A	53	A	C5-C6-N6	-7.41	117.77	123.70
26	A	647	G	OP1-P-OP2	-7.41	108.49	119.60
1	a	968	A	O5'-P-OP2	-7.41	99.03	105.70
26	A	890	C	N3-C4-N4	-7.40	112.82	118.00
26	A	1171	G	C6-N1-C2	-7.40	120.66	125.10
26	A	2165	C	O5'-P-OP2	-7.38	99.06	105.70
1	a	563	A	N1-C2-N3	-7.38	125.61	129.30
24	y	47	G	C8-N9-C4	-7.38	103.45	106.40
1	a	490	C	C6-N1-C2	-7.38	117.35	120.30
1	a	878	A	N9-C4-C5	-7.38	102.85	105.80
1	a	1034	G	N9-C4-C5	-7.38	102.45	105.40
26	A	2562	U	N3-C2-O2	-7.37	117.04	122.20
1	a	180	U	C5-C6-N1	7.36	126.38	122.70
26	A	1665	A	O5'-P-OP2	-7.35	99.09	105.70
26	A	669	G	N3-C4-N9	7.34	130.40	126.00
26	A	1982	U	O5'-P-OP2	-7.34	99.09	105.70
1	a	1263	C	C5-C6-N1	7.33	124.67	121.00
1	a	1397	C	N3-C4-C5	7.33	124.83	121.90
14	n	32	ASP	CB-CG-OD1	7.33	124.90	118.30
26	A	1079	C	N3-C2-O2	-7.33	116.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	575	G	N3-C2-N2	-7.32	114.77	119.90
1	a	1027	C	N1-C2-O2	7.30	123.28	118.90
1	a	1262	C	N1-C2-O2	7.29	123.28	118.90
26	A	813	U	N3-C2-O2	-7.29	117.10	122.20
26	A	2473	U	N3-C2-O2	-7.28	117.10	122.20
24	y	59	C	C5-C6-N1	7.27	124.64	121.00
25	z	398	LEU	CA-CB-CG	7.26	132.01	115.30
26	A	2746	U	C5-C6-N1	7.26	126.33	122.70
27	B	60	C	C6-N1-C2	-7.26	117.40	120.30
26	A	1171	G	N3-C4-N9	-7.26	121.65	126.00
26	A	2582	G	OP2-P-O3'	7.25	121.16	105.20
1	a	1071	C	C6-N1-C2	-7.25	117.40	120.30
2	b	81	ASP	CB-CG-OD1	7.24	124.82	118.30
26	A	1386	C	C6-N1-C2	-7.24	117.41	120.30
1	a	1148	U	N3-C2-O2	-7.24	117.14	122.20
24	y	59	C	C6-N1-C2	-7.22	117.41	120.30
24	y	47(B)	G	N7-C8-N9	7.21	116.71	113.10
26	A	1060	U	O5'-P-OP1	-7.20	99.22	105.70
1	a	1493	A	N1-C2-N3	-7.20	125.70	129.30
1	a	620	C	N1-C2-O2	7.19	123.21	118.90
1	a	472	U	C5-C6-N1	7.16	126.28	122.70
26	A	2161	C	N1-C2-O2	-7.15	114.61	118.90
26	A	1476	U	N3-C2-O2	-7.13	117.20	122.20
1	a	217	C	C5-C6-N1	7.13	124.57	121.00
1	a	414	A	C2-N3-C4	7.12	114.16	110.60
26	A	2110	G	N3-C4-N9	-7.12	121.73	126.00
1	a	419	C	N3-C2-O2	-7.11	116.92	121.90
26	A	1080	A	N7-C8-N9	7.11	117.36	113.80
24	y	47(P)	C	C6-N1-C2	-7.11	117.46	120.30
31	F	88	VAL	CG1-CB-CG2	-7.11	99.52	110.90
1	a	80	A	C6-N1-C2	7.11	122.86	118.60
1	a	477	C	C5-C6-N1	7.10	124.55	121.00
24	y	47(N)	C	C5-C6-N1	7.10	124.55	121.00
27	B	60	C	C5-C6-N1	7.10	124.55	121.00
50	Y	49	ASP	CB-CG-OD1	7.08	124.67	118.30
24	y	55	PSU	P-O3'-C3'	7.07	128.19	119.70
1	a	163	C	C6-N1-C2	-7.07	117.47	120.30
1	a	392	C	C5-C6-N1	7.07	124.53	121.00
26	A	183	C	N1-C2-O2	7.07	123.14	118.90
30	E	82	GLY	N-CA-C	7.07	130.76	113.10
1	a	397	A	C2-N3-C4	7.06	114.13	110.60
22	v	39	C	C5-C6-N1	7.05	124.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1202	U	N3-C2-O2	-7.05	117.27	122.20
1	a	397	A	N3-C4-N9	7.04	133.03	127.40
1	a	409	U	C5-C6-N1	7.04	126.22	122.70
26	A	1074	G	N1-C2-N2	7.03	122.53	116.20
1	a	512	U	C5-C6-N1	7.03	126.21	122.70
24	y	30	G	C6-C5-N7	-7.01	126.19	130.40
1	a	492	C	C6-N1-C2	-7.00	117.50	120.30
24	y	47(C)	C	C5-C6-N1	6.97	124.49	121.00
23	x	126	G	P-O3'-C3'	6.97	128.06	119.70
26	A	114	U	N1-C2-O2	6.97	127.68	122.80
26	A	79	C	C6-N1-C2	-6.96	117.52	120.30
25	z	328	ALA	N-CA-CB	6.94	119.82	110.10
1	a	392	C	C2-N1-C1'	6.93	126.43	118.80
24	y	73	G	N9-C4-C5	-6.93	102.63	105.40
26	A	1936	A	N1-C6-N6	-6.92	114.45	118.60
26	A	1313	U	C6-N1-C1'	-6.91	111.52	121.20
26	A	2442	C	N1-C2-O2	6.91	123.05	118.90
26	A	1071	G	N9-C4-C5	-6.91	102.64	105.40
31	F	11	VAL	CG1-CB-CG2	-6.90	99.86	110.90
26	A	2474	U	N1-C2-O2	6.89	127.62	122.80
25	z	445	LEU	CB-CG-CD2	-6.88	99.30	111.00
26	A	1104	C	C5-C6-N1	6.87	124.43	121.00
26	A	2195	U	N3-C2-O2	-6.87	117.39	122.20
26	A	53	A	N1-C6-N6	6.86	122.71	118.60
1	a	1448	C	N1-C2-O2	6.85	123.01	118.90
26	A	2636	C	N1-C2-O2	6.85	123.01	118.90
26	A	445	C	N3-C2-O2	-6.85	117.11	121.90
26	A	2755	C	N1-C2-O2	6.85	123.01	118.90
26	A	1294	U	N3-C2-O2	-6.83	117.42	122.20
26	A	883	G	N7-C8-N9	6.83	116.52	113.10
24	y	48	G	C4-C5-N7	6.83	113.53	110.80
1	a	1296	C	N3-C2-O2	-6.82	117.12	121.90
26	A	884	U	N1-C2-N3	6.82	118.99	114.90
22	v	32	C	N1-C2-O2	6.82	122.99	118.90
33	I	79	LEU	CB-CG-CD2	-6.82	99.41	111.00
1	a	868	C	C6-N1-C2	-6.82	117.57	120.30
22	v	50	U	C5-C6-N1	6.82	126.11	122.70
26	A	2167	U	N1-C2-O2	-6.82	118.03	122.80
1	a	1034	G	N1-C6-O6	6.81	123.99	119.90
24	y	40	C	C5-C6-N1	6.81	124.41	121.00
24	y	47(G)	C	N1-C2-O2	-6.81	114.81	118.90
1	a	88	U	C6-N1-C2	-6.81	116.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	x	118	G	N7-C8-N9	6.81	116.50	113.10
44	S	64	ALA	N-CA-CB	6.80	119.62	110.10
1	a	1263	C	C6-N1-C2	-6.80	117.58	120.30
26	A	2326	C	C6-N1-C2	-6.79	117.58	120.30
26	A	2512	C	C6-N1-C2	-6.79	117.58	120.30
27	B	120	U	N3-C2-O2	-6.79	117.45	122.20
1	a	407	U	O5'-P-OP2	6.78	118.84	110.70
26	A	2069	G7M	P-O3'-C3'	6.77	127.82	119.70
26	A	84	A	N7-C8-N9	-6.75	110.42	113.80
26	A	140	C	C6-N1-C2	-6.75	117.60	120.30
1	a	428	G	N3-C4-N9	-6.72	121.97	126.00
26	A	1071	G	C4-C5-N7	6.72	113.49	110.80
1	a	429	U	OP1-P-O3'	6.71	119.97	105.20
26	A	546	U	N3-C2-O2	-6.71	117.50	122.20
27	B	55	U	N3-C2-O2	-6.71	117.51	122.20
1	a	923	A	N7-C8-N9	6.71	117.15	113.80
26	A	283	G	N3-C2-N2	-6.69	115.22	119.90
24	y	20	G	C2-N3-C4	-6.69	108.56	111.90
1	a	526	C	C6-N1-C2	-6.68	117.63	120.30
26	A	2080	A	N9-C4-C5	-6.68	103.13	105.80
1	a	407	U	C6-N1-C2	-6.67	117.00	121.00
23	x	133	C	C6-N1-C2	-6.67	117.63	120.30
24	y	48	G	N9-C4-C5	-6.67	102.73	105.40
26	A	2574	G	O5'-P-OP1	6.67	118.71	110.70
26	A	2163	A	O5'-P-OP1	6.66	118.70	110.70
27	B	57	A	N7-C8-N9	6.66	117.13	113.80
26	A	8	C	C5-C6-N1	6.66	124.33	121.00
26	A	2267	A	N1-C6-N6	-6.66	114.60	118.60
1	a	1344	C	C6-N1-C2	-6.64	117.64	120.30
1	a	1466	C	N3-C2-O2	-6.63	117.25	121.90
26	A	1178	C	C6-N1-C2	-6.63	117.65	120.30
22	v	19	G	O4'-C1'-N9	-6.62	102.90	108.20
26	A	890	C	N3-C2-O2	-6.62	117.27	121.90
1	a	397	A	N9-C4-C5	-6.62	103.15	105.80
1	a	1105	A	N9-C4-C5	-6.62	103.15	105.80
22	v	32	C	N3-C2-O2	-6.62	117.27	121.90
26	A	208	C	C5-C6-N1	6.62	124.31	121.00
1	a	88	U	C5-C6-N1	6.61	126.01	122.70
26	A	528	A	N7-C8-N9	6.61	117.11	113.80
26	A	1664	A	O5'-P-OP1	6.61	118.63	110.70
26	A	1083	U	N1-C2-O2	-6.60	118.18	122.80
1	a	1037	C	C6-N1-C2	-6.60	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	42	C	N1-C2-O2	6.60	122.86	118.90
26	A	528	A	C8-N9-C4	-6.60	103.16	105.80
1	a	1393	U	N3-C2-O2	-6.60	117.58	122.20
26	A	642	U	C6-N1-C2	-6.60	117.04	121.00
26	A	399	U	N3-C2-O2	-6.60	117.58	122.20
1	a	443	C	C5-C6-N1	6.59	124.30	121.00
1	a	1109	C	N1-C2-O2	6.59	122.85	118.90
1	a	993	G	C6-C5-N7	-6.59	126.45	130.40
26	A	889	C	N1-C2-O2	6.59	122.85	118.90
23	x	109	C	C6-N1-C2	-6.58	117.67	120.30
26	A	1313	U	C5-C6-N1	6.58	125.99	122.70
1	a	1497	G	N3-C4-N9	6.58	129.95	126.00
24	y	72	C	C2-N1-C1'	6.58	126.03	118.80
1	a	136	C	C2-N1-C1'	6.57	126.02	118.80
1	a	527	G7M	P-O3'-C3'	6.57	127.58	119.70
1	a	611	C	N1-C2-O2	6.57	122.84	118.90
26	A	2626	C	C5-C6-N1	6.56	124.28	121.00
1	a	592	G	C8-N9-C4	-6.56	103.78	106.40
26	A	534	U	C5-C6-N1	6.56	125.98	122.70
1	a	536	C	C6-N1-C2	-6.56	117.68	120.30
26	A	1093	G	C8-N9-C4	6.55	109.02	106.40
1	a	1109	C	C6-N1-C2	-6.55	117.68	120.30
26	A	837	C	N3-C2-O2	-6.55	117.31	121.90
1	a	1195	C	C6-N1-C2	-6.55	117.68	120.30
26	A	231	A	C8-N9-C4	6.55	108.42	105.80
26	A	806	C	C6-N1-C2	-6.54	117.69	120.30
26	A	1072	C	O5'-P-OP2	-6.54	99.81	105.70
1	a	620	C	N3-C2-O2	-6.53	117.33	121.90
26	A	1075	C	N1-C2-O2	6.53	122.82	118.90
26	A	1093	G	N1-C6-O6	6.53	123.82	119.90
26	A	1669	A	N3-C4-N9	6.51	132.61	127.40
1	a	563	A	C4-C5-N7	6.51	113.95	110.70
26	A	2502	G	O5'-P-OP1	-6.50	99.85	105.70
26	A	1064	C	N1-C2-O2	-6.50	115.00	118.90
1	a	136	C	N1-C2-O2	6.50	122.80	118.90
1	a	418	C	C6-N1-C2	-6.49	117.70	120.30
1	a	1427	C	C6-N1-C2	-6.49	117.70	120.30
26	A	2162	G	N1-C6-O6	-6.49	116.01	119.90
1	a	513	C	C5-C6-N1	6.49	124.24	121.00
1	a	1517	G	N3-C2-N2	-6.47	115.37	119.90
26	A	1075	C	C2-N1-C1'	6.47	125.92	118.80
27	B	37	C	N1-C2-O2	6.47	122.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	90	C	C6-N1-C2	-6.47	117.71	120.30
26	A	445	C	N1-C2-O2	6.47	122.78	118.90
26	A	571	U	C4-C5-C6	6.47	123.58	119.70
1	a	661	G	N9-C4-C5	-6.46	102.81	105.40
26	A	2060	A	OP2-P-O3'	6.45	119.39	105.20
1	a	1469	C	N1-C2-O2	6.45	122.77	118.90
56	4	14	CYS	CA-CB-SG	6.45	125.60	114.00
26	A	1956	U	N3-C2-O2	-6.44	117.69	122.20
23	x	109	C	C5-C6-N1	6.44	124.22	121.00
1	a	475	C	C6-N1-C2	-6.43	117.73	120.30
26	A	1056	G	N1-C6-O6	6.43	123.76	119.90
26	A	2702	G	N1-C6-O6	-6.43	116.05	119.90
1	a	656	G	C6-N1-C2	-6.42	121.25	125.10
26	A	183	C	N3-C2-O2	-6.42	117.40	121.90
24	y	30	G	C8-N9-C1'	-6.42	118.65	127.00
26	A	2188	U	C5-C6-N1	6.42	125.91	122.70
1	a	493	A	C8-N9-C4	-6.42	103.23	105.80
1	a	449	G	C4-C5-N7	6.41	113.37	110.80
1	a	744	C	C5-C6-N1	6.41	124.21	121.00
26	A	669	G	C2-N3-C4	6.41	115.11	111.90
26	A	1294	U	N1-C2-O2	6.41	127.29	122.80
1	a	217	C	C6-N1-C2	-6.41	117.74	120.30
1	a	1027	C	C5-C6-N1	6.41	124.20	121.00
26	A	560	C	C5-C6-N1	6.41	124.20	121.00
26	A	891	G	C6-C5-N7	-6.41	126.56	130.40
1	a	963	G	N3-C2-N2	-6.40	115.42	119.90
26	A	1064	C	C6-N1-C2	-6.40	117.74	120.30
33	I	64	ARG	N-CA-CB	-6.39	99.10	110.60
26	A	646	U	OP2-P-O3'	6.39	119.25	105.20
26	A	615	U	C5-C4-O4	-6.39	122.07	125.90
23	x	124	A	N9-C4-C5	-6.38	103.25	105.80
1	a	110	C	N1-C2-O2	6.38	122.73	118.90
1	a	723	U	N1-C2-O2	6.38	127.27	122.80
23	x	104	U	N3-C2-O2	-6.38	117.74	122.20
26	A	399	U	N1-C2-O2	6.37	127.26	122.80
26	A	783	A	C2-N3-C4	6.37	113.79	110.60
26	A	1059	G	C5-C6-O6	-6.37	124.78	128.60
26	A	891	G	N3-C4-N9	6.37	129.82	126.00
1	a	896	C	C5-C6-N1	6.37	124.18	121.00
24	y	56	C	C6-N1-C2	-6.37	117.75	120.30
26	A	1075	C	N3-C2-O2	-6.36	117.45	121.90
26	A	1348	C	N1-C2-O2	6.36	122.72	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	20	G	N1-C2-N3	6.36	127.72	123.90
26	A	114	U	N3-C2-O2	-6.36	117.75	122.20
1	a	419	C	C6-N1-C1'	6.36	128.43	120.80
26	A	2110	G	C5-C6-O6	6.36	132.41	128.60
24	y	47(K)	G	N3-C4-C5	6.36	131.78	128.60
1	a	307	C	N1-C2-O2	6.35	122.71	118.90
1	a	1326	U	N3-C2-O2	-6.35	117.76	122.20
24	y	65	U	O5'-P-OP1	-6.34	99.99	105.70
26	A	2011	U	N3-C2-O2	-6.34	117.76	122.20
1	a	1202	U	N1-C2-O2	6.34	127.24	122.80
26	A	2305	U	C6-N1-C2	6.34	124.80	121.00
26	A	1025	G	OP1-P-O3'	6.33	119.13	105.20
1	a	754	C	C6-N1-C1'	-6.33	113.20	120.80
1	a	868	C	C5-C6-N1	6.33	124.17	121.00
1	a	1404	C	N1-C2-O2	6.33	122.69	118.90
1	a	968	A	C5-C6-N6	6.32	128.75	123.70
26	A	2840	C	C5-C6-N1	6.32	124.16	121.00
27	B	26	C	N3-C2-O2	-6.32	117.48	121.90
26	A	2160	C	C6-N1-C2	-6.31	117.78	120.30
1	a	177	G	N3-C4-C5	-6.31	125.45	128.60
26	A	2267	A	N1-C2-N3	-6.30	126.15	129.30
26	A	1669	A	N9-C4-C5	-6.30	103.28	105.80
24	y	48	G	C6-C5-N7	-6.29	126.62	130.40
8	h	95	MET	CA-CB-CG	6.29	124.00	113.30
26	A	1539	U	C5-C4-O4	-6.29	122.12	125.90
1	a	177	G	C2-N3-C4	6.29	115.05	111.90
26	A	1101	U	N3-C2-O2	-6.29	117.80	122.20
1	a	1066	C	N3-C2-O2	-6.29	117.50	121.90
2	b	134	LEU	CA-CB-CG	6.29	129.76	115.30
26	A	1200	C	C6-N1-C2	-6.29	117.79	120.30
26	A	1178	C	C5-C4-N4	6.28	124.60	120.20
26	A	2691	C	C5-C6-N1	6.28	124.14	121.00
27	B	49	C	C6-N1-C2	-6.28	117.79	120.30
26	A	2394	C	C6-N1-C2	-6.28	117.79	120.30
25	z	559	ASP	CB-CG-OD1	6.28	123.95	118.30
1	a	1412	C	C5-C6-N1	6.27	124.14	121.00
26	A	1096	A	C8-N9-C4	-6.27	103.29	105.80
26	A	2442	C	N3-C2-O2	-6.27	117.51	121.90
1	a	1302	C	C6-N1-C2	6.26	122.80	120.30
1	a	979	C	N1-C2-O2	6.26	122.65	118.90
26	A	898	C	C6-N1-C2	-6.25	117.80	120.30
1	a	1302	C	OP1-P-O3'	-6.25	91.45	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	26	C	N1-C2-O2	6.25	122.65	118.90
26	A	357	C	C6-N1-C2	-6.25	117.80	120.30
26	A	1313	U	C6-N1-C2	-6.24	117.26	121.00
11	k	96	ILE	CG1-CB-CG2	-6.24	97.68	111.40
27	B	26	C	C6-N1-C2	-6.24	117.81	120.30
26	A	1787	A	N9-C4-C5	-6.24	103.31	105.80
26	A	140	C	C5-C6-N1	6.23	124.11	121.00
26	A	2572	A	O5'-P-OP1	-6.22	100.10	105.70
26	A	234	U	N3-C2-O2	-6.22	117.85	122.20
26	A	1101	U	N1-C2-O2	6.21	127.15	122.80
26	A	1012	U	N1-C2-O2	-6.20	118.46	122.80
1	a	977	A	C2-N3-C4	6.20	113.70	110.60
26	A	2394	C	N1-C2-O2	6.20	122.62	118.90
23	x	129	U	O4'-C1'-N1	6.20	113.16	108.20
26	A	1096	A	N7-C8-N9	6.18	116.89	113.80
26	A	2044	C	C6-N1-C2	-6.18	117.83	120.30
1	a	516	PSU	O3'-P-O5'	-6.17	92.28	104.00
1	a	795	C	C6-N1-C2	-6.17	117.83	120.30
4	d	189	ASP	CB-CG-OD1	6.16	123.84	118.30
1	a	989	U	N3-C2-O2	-6.16	117.89	122.20
1	a	1296	C	C2-N1-C1'	6.15	125.57	118.80
1	a	660	C	C5-C6-N1	6.14	124.07	121.00
1	a	180	U	C6-N1-C2	-6.14	117.32	121.00
26	A	231	A	C5-C6-N6	-6.14	118.79	123.70
26	A	444	C	C6-N1-C2	-6.14	117.84	120.30
26	A	1611	C	C6-N1-C2	-6.14	117.85	120.30
23	x	121	U	N3-C2-O2	-6.13	117.91	122.20
26	A	1075	C	C6-N1-C2	-6.13	117.85	120.30
24	y	30	G	N1-C6-O6	6.12	123.58	119.90
26	A	2617	U	N1-C2-O2	6.12	127.09	122.80
1	a	1497	G	N3-C4-C5	-6.12	125.54	128.60
26	A	2043	C	C2-N1-C1'	6.12	125.53	118.80
1	a	397	A	N1-C2-N3	-6.12	126.24	129.30
26	A	891	G	N1-C6-O6	6.11	123.57	119.90
23	x	118	G	C6-C5-N7	-6.11	126.73	130.40
26	A	1021	A	C2-N3-C4	6.11	113.66	110.60
1	a	1493	A	C6-N1-C2	6.10	122.26	118.60
24	y	47(D)	C	C2-N3-C4	6.10	122.95	119.90
23	x	104	U	O4'-C1'-N1	6.10	113.08	108.20
26	A	1171	G	C4-C5-N7	-6.09	108.36	110.80
1	a	1284	C	C6-N1-C2	-6.08	117.87	120.30
24	y	45	U	P-O3'-C3'	6.08	127.00	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2103	C	N3-C2-O2	-6.08	117.64	121.90
26	A	2766	A	N9-C4-C5	-6.08	103.37	105.80
24	y	50	C	C5-C6-N1	6.08	124.04	121.00
1	a	1109	C	N3-C2-O2	-6.08	117.65	121.90
24	y	40	C	C6-N1-C2	-6.08	117.87	120.30
1	a	679	C	C6-N1-C2	-6.07	117.87	120.30
24	y	56	C	C5-C6-N1	6.07	124.03	121.00
1	a	993	G	C4-C5-N7	6.06	113.23	110.80
26	A	2755	C	N3-C2-O2	-6.06	117.66	121.90
26	A	889	C	N3-C2-O2	-6.06	117.66	121.90
3	c	117	ASP	CB-CG-OD1	6.05	123.75	118.30
1	a	1466	C	N1-C2-O2	6.05	122.53	118.90
23	x	129	U	N3-C2-O2	-6.05	117.97	122.20
26	A	283	G	C6-C5-N7	6.05	134.03	130.40
1	a	1195	C	C5-C6-N1	6.04	124.02	121.00
1	a	536	C	C5-C6-N1	6.03	124.02	121.00
23	x	108	A	O4'-C1'-N9	6.03	113.02	108.20
26	A	1181	U	N3-C2-O2	-6.03	117.98	122.20
24	y	16	C	C6-N1-C1'	6.02	128.03	120.80
22	v	36	U	N3-C2-O2	-6.02	117.99	122.20
26	A	1056	G	C5-C6-O6	-6.01	124.99	128.60
22	v	51	C	C2-N1-C1'	6.01	125.41	118.80
26	A	198	C	C5-C6-N1	6.00	124.00	121.00
24	y	30	G	C4-C5-N7	6.00	113.20	110.80
1	a	207	C	C6-N1-C2	-6.00	117.90	120.30
26	A	1723	G	N1-C6-O6	-5.99	116.31	119.90
1	a	438	U	O4'-C1'-N1	5.99	112.99	108.20
1	a	968	A	O4'-C1'-N9	5.99	112.99	108.20
26	A	1279	G	C4-C5-N7	5.99	113.19	110.80
23	x	131	C	O4'-C1'-N1	5.98	112.99	108.20
1	a	799	G	C2-N3-C4	5.98	114.89	111.90
1	a	1393	U	N1-C2-O2	5.98	126.98	122.80
26	A	435	C	OP1-P-OP2	-5.98	110.63	119.60
1	a	464	U	C5-C6-N1	5.97	125.69	122.70
24	y	46	G	N3-C2-N2	-5.97	115.72	119.90
26	A	2837	A	O5'-P-OP2	-5.97	100.33	105.70
1	a	1326	U	N1-C2-O2	5.97	126.98	122.80
1	a	52	C	C6-N1-C2	-5.96	117.91	120.30
1	a	1262	C	N3-C2-O2	-5.96	117.73	121.90
1	a	968	A	N9-C4-C5	5.96	108.19	105.80
1	a	612	C	N1-C2-O2	5.96	122.47	118.90
26	A	1348	C	C6-N1-C2	-5.96	117.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	980	C	C6-N1-C2	-5.95	117.92	120.30
12	l	80	LEU	CA-CB-CG	5.95	128.99	115.30
24	y	56	C	OP2-P-O3'	-5.95	92.11	105.20
26	A	1092	C	N1-C2-O2	5.95	122.47	118.90
1	a	354	G	N9-C4-C5	-5.95	103.02	105.40
26	A	2160	C	N3-C2-O2	-5.95	117.74	121.90
49	X	21	LEU	CA-CB-CG	5.94	128.97	115.30
26	A	2394	C	N3-C2-O2	-5.94	117.74	121.90
26	A	1585	C	N1-C2-O2	5.93	122.46	118.90
26	A	2162	G	C5-C6-O6	5.93	132.16	128.60
26	A	2473	U	N1-C2-O2	5.93	126.95	122.80
23	x	128	C	C3'-C2'-C1'	5.92	106.24	101.50
27	B	120	U	N1-C2-O2	5.92	126.95	122.80
23	x	101	A	N1-C2-N3	-5.92	126.34	129.30
26	A	2179	C	C6-N1-C2	-5.92	117.93	120.30
26	A	1775	U	N3-C2-O2	-5.92	118.06	122.20
1	a	578	C	C6-N1-C2	-5.91	117.93	120.30
22	v	34	C	N1-C2-O2	5.91	122.45	118.90
1	a	423	G	C5-C6-O6	-5.91	125.05	128.60
1	a	16	A	C6-N1-C2	5.91	122.14	118.60
24	y	43	G	C4-N9-C1'	-5.90	118.83	126.50
1	a	1027	C	C6-N1-C2	-5.90	117.94	120.30
1	a	1448	C	C2-N1-C1'	5.90	125.29	118.80
26	A	231	A	C4-C5-N7	5.90	113.65	110.70
1	a	528	C	C2-N1-C1'	5.90	125.28	118.80
26	A	130	C	C6-N1-C2	-5.89	117.94	120.30
26	A	687	C	N1-C2-O2	5.89	122.44	118.90
1	a	494	G	C5-C6-O6	-5.89	125.06	128.60
1	a	483	C	C6-N1-C2	-5.89	117.94	120.30
26	A	890	C	C5-C4-N4	5.88	124.32	120.20
26	A	2550	G	O5'-P-OP1	-5.88	100.40	105.70
26	A	885	C	C5-C6-N1	5.88	123.94	121.00
1	a	368	U	N3-C2-O2	-5.88	118.09	122.20
1	a	346	G	C2-N3-C4	5.87	114.84	111.90
11	k	112	VAL	CA-CB-CG1	5.87	119.71	110.90
27	B	49	C	C5-C6-N1	5.87	123.94	121.00
26	A	560	C	C6-N1-C2	-5.86	117.96	120.30
1	a	166	U	N3-C2-O2	-5.86	118.10	122.20
26	A	1093	G	N3-C4-N9	5.85	129.51	126.00
27	B	37	C	N3-C2-O2	-5.85	117.80	121.90
1	a	1162	C	C6-N1-C2	-5.85	117.96	120.30
24	y	48	G	C8-N9-C1'	-5.85	119.40	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	234	U	N1-C2-O2	5.85	126.89	122.80
26	A	257	C	C6-N1-C2	-5.85	117.96	120.30
1	a	188	C	C6-N1-C2	-5.85	117.96	120.30
1	a	400	C	C5-C6-N1	5.85	123.92	121.00
26	A	1171	G	C8-N9-C4	-5.85	104.06	106.40
1	a	923	A	C6-C5-N7	-5.84	128.21	132.30
25	z	257	LEU	CA-CB-CG	5.84	128.74	115.30
1	a	808	C	C6-N1-C2	-5.84	117.96	120.30
26	A	302	C	C6-N1-C2	-5.84	117.96	120.30
26	A	397	U	C5-C6-N1	5.84	125.62	122.70
26	A	2254	C	N1-C2-O2	5.84	122.40	118.90
1	a	346	G	N3-C4-N9	5.84	129.50	126.00
26	A	1063	G	N3-C4-C5	-5.84	125.68	128.60
1	a	1455	G	N3-C4-N9	5.83	129.50	126.00
26	A	1494	A	N7-C8-N9	5.83	116.72	113.80
44	S	64	ALA	N-CA-C	-5.83	95.25	111.00
24	y	47(G)	C	C6-N1-C2	-5.83	117.97	120.30
24	y	47(B)	G	C8-N9-C4	-5.83	104.07	106.40
26	A	2649	C	C5-C6-N1	5.82	123.91	121.00
1	a	82	G	N3-C4-N9	5.82	129.49	126.00
1	a	879	C	N1-C2-O2	5.82	122.39	118.90
26	A	2606	C	C6-N1-C2	-5.82	117.97	120.30
24	y	27	C	C5-C6-N1	5.82	123.91	121.00
26	A	1049	C	N3-C4-N4	-5.81	113.93	118.00
23	x	130	G	N7-C8-N9	5.81	116.01	113.10
1	a	497	G	N3-C2-N2	-5.81	115.83	119.90
1	a	582	C	C6-N1-C2	-5.81	117.98	120.30
1	a	658	C	N1-C2-O2	5.81	122.39	118.90
1	a	1382	C	N1-C2-O2	5.81	122.39	118.90
26	A	2292	U	C5-C6-N1	5.81	125.60	122.70
1	a	735	C	C6-N1-C2	-5.80	117.98	120.30
22	v	57	A	C5-N7-C8	5.80	106.80	103.90
26	A	1993	U	N1-C2-O2	5.80	126.86	122.80
26	A	2896	C	C6-N1-C2	-5.80	117.98	120.30
1	a	679	C	C5-C6-N1	5.80	123.90	121.00
26	A	383	C	N1-C2-O2	5.80	122.38	118.90
26	A	1081	U	C6-N1-C2	-5.80	117.52	121.00
1	a	980	C	N3-C2-O2	-5.80	117.84	121.90
1	a	684	U	N3-C2-O2	-5.79	118.14	122.20
26	A	229	C	C6-N1-C2	-5.79	117.98	120.30
26	A	1113	U	N3-C2-O2	-5.79	118.14	122.20
26	A	1113	U	N1-C2-O2	5.79	126.85	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	876	C	C6-N1-C2	-5.79	117.98	120.30
26	A	889	C	C6-N1-C2	-5.79	117.98	120.30
26	A	668	A	N9-C4-C5	-5.79	103.48	105.80
26	A	1314	C	C6-N1-C2	-5.79	117.98	120.30
23	x	118	G	N3-C4-N9	5.79	129.47	126.00
1	a	556	C	C5-C6-N1	5.78	123.89	121.00
24	y	57	G	N1-C2-N2	5.78	121.41	116.20
26	A	1103	A	C2-N3-C4	5.78	113.49	110.60
26	A	2120	G	O5'-P-OP1	-5.78	100.49	105.70
1	a	1494	G	O5'-P-OP1	-5.78	100.50	105.70
24	y	15	C	N1-C2-O2	5.78	122.37	118.90
1	a	90	C	C5-C6-N1	5.78	123.89	121.00
25	z	26	ASP	CB-CG-OD1	5.77	123.50	118.30
26	A	1539	U	N3-C4-O4	5.77	123.44	119.40
26	A	2310	C	N1-C2-O2	5.77	122.36	118.90
24	y	73	G	N1-C6-O6	5.77	123.36	119.90
26	A	2147	A	O5'-P-OP1	-5.77	100.51	105.70
32	G	70	LEU	CA-CB-CG	5.77	128.57	115.30
24	y	56	C	C2-N1-C1'	5.76	125.14	118.80
26	A	2305	U	N3-C4-C5	5.76	118.06	114.60
26	A	2146	C	OP1-P-O3'	-5.76	92.52	105.20
26	A	2215	C	C6-N1-C2	-5.76	118.00	120.30
23	x	115	A	O4'-C1'-N9	-5.76	103.59	108.20
24	y	31	A	OP2-P-O3'	5.76	117.87	105.20
1	a	1034	G	C5-C6-O6	-5.76	125.15	128.60
24	y	47(D)	C	N1-C2-O2	5.75	122.35	118.90
26	A	1905	C	N1-C2-O2	5.75	122.35	118.90
26	A	1494	A	C8-N9-C4	-5.75	103.50	105.80
26	A	1760	C	N1-C2-O2	5.75	122.35	118.90
23	x	126	G	N1-C2-N2	-5.74	111.03	116.20
1	a	1226	C	N3-C2-O2	-5.74	117.88	121.90
24	y	30	G	C5-C6-O6	-5.74	125.16	128.60
26	A	1267	U	N3-C2-O2	-5.74	118.18	122.20
26	A	1380	G	N3-C4-N9	5.74	129.44	126.00
27	B	30	C	C6-N1-C2	-5.74	118.00	120.30
26	A	1054	A	O4'-C1'-N9	5.74	112.79	108.20
1	a	656	G	N9-C4-C5	5.74	107.69	105.40
1	a	1378	C	N1-C2-O2	5.74	122.34	118.90
57	6	40	CYS	N-CA-CB	5.74	120.92	110.60
22	v	32	C	C6-N1-C2	-5.73	118.01	120.30
26	A	1279	G	N9-C4-C5	-5.73	103.11	105.40
1	a	491	G	C8-N9-C1'	-5.73	119.55	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	689	C	C6-N1-C2	-5.73	118.01	120.30
26	A	1270	C	C6-N1-C2	-5.73	118.01	120.30
1	a	866	C	C5-C6-N1	5.72	123.86	121.00
1	a	575	G	N9-C4-C5	5.72	107.69	105.40
24	y	1	G	N9-C4-C5	-5.71	103.11	105.40
26	A	2804	U	N3-C2-O2	-5.71	118.20	122.20
1	a	330	C	N1-C2-O2	5.71	122.33	118.90
1	a	1197	A	N9-C4-C5	-5.71	103.52	105.80
26	A	1565	C	C6-N1-C2	-5.71	118.02	120.30
26	A	2043	C	N1-C2-O2	5.71	122.33	118.90
1	a	1536	C	C6-N1-C2	-5.71	118.02	120.30
26	A	1582	C	C6-N1-C2	-5.71	118.02	120.30
26	A	2103	C	N1-C2-O2	5.71	122.33	118.90
24	y	43	G	C8-N9-C1'	5.71	134.42	127.00
24	y	65	U	OP2-P-O3'	5.71	117.75	105.20
26	A	1083	U	C2-N1-C1'	-5.71	110.85	117.70
28	C	32	LEU	CA-CB-CG	5.71	128.43	115.30
1	a	392	C	N3-C2-O2	-5.70	117.91	121.90
1	a	723	U	N3-C4-O4	-5.70	115.41	119.40
23	x	104	U	OP2-P-O3'	5.70	117.74	105.20
1	a	993	G	C8-N9-C1'	-5.70	119.59	127.00
1	a	1028	C	N1-C2-O2	5.70	122.32	118.90
24	y	10	C	C6-N1-C2	-5.70	118.02	120.30
1	a	14	U	C6-N1-C2	-5.69	117.58	121.00
26	A	2512	C	C5-C6-N1	5.68	123.84	121.00
1	a	87	C	N1-C2-O2	5.68	122.31	118.90
26	A	729	G	C4-N9-C1'	5.68	133.88	126.50
26	A	1257	C	C5-C6-N1	5.68	123.84	121.00
1	a	968	A	N9-C1'-C2'	-5.68	105.75	112.00
35	J	81	ILE	CG1-CB-CG2	-5.68	98.91	111.40
23	x	118	G	C4-C5-N7	5.67	113.07	110.80
26	A	680	C	C5-C6-N1	5.67	123.84	121.00
26	A	1760	C	C5-C6-N1	5.67	123.84	121.00
1	a	426	U	N3-C2-O2	-5.67	118.23	122.20
26	A	2080	A	N1-C2-N3	-5.67	126.46	129.30
1	a	923	A	C5-N7-C8	-5.67	101.07	103.90
1	a	1149	C	C6-N1-C2	-5.66	118.03	120.30
26	A	1380	G	C6-C5-N7	-5.66	127.00	130.40
26	A	2065	C	C6-N1-C2	-5.66	118.04	120.30
26	A	1053	C	C6-N1-C2	-5.65	118.04	120.30
26	A	2558	C	C5-C6-N1	5.65	123.83	121.00
26	A	2765	A	C2-N3-C4	5.65	113.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	60	U	N3-C2-O2	5.65	126.15	122.20
25	z	461	LEU	CB-CG-CD1	-5.65	101.40	111.00
26	A	883	G	C4-C5-N7	5.65	113.06	110.80
26	A	2720	U	N3-C2-O2	-5.65	118.25	122.20
1	a	514	C	C6-N1-C2	-5.64	118.04	120.30
1	a	1317	C	C6-N1-C2	-5.64	118.04	120.30
26	A	209	C	C5-C6-N1	5.64	123.82	121.00
1	a	449	G	C5-C6-O6	-5.64	125.21	128.60
1	a	799	G	N3-C2-N2	-5.64	115.95	119.90
26	A	503	A	C8-N9-C4	5.64	108.06	105.80
26	A	1267	U	N1-C2-O2	5.64	126.75	122.80
24	y	15	C	C2-N1-C1'	5.64	125.00	118.80
26	A	558	U	O5'-P-OP1	-5.64	100.63	105.70
1	a	513	C	N1-C2-O2	5.63	122.28	118.90
23	x	125	G	C3'-C2'-C1'	5.63	106.00	101.50
1	a	407	U	C5-C6-N1	5.62	125.51	122.70
26	A	243	U	N1-C2-O2	5.62	126.73	122.80
26	A	729	G	O4'-C1'-N9	5.62	112.69	108.20
24	y	17	G	N3-C4-N9	-5.61	122.63	126.00
26	A	2180	U	C2-N3-C4	5.61	130.37	127.00
1	a	322	C	C6-N1-C2	-5.61	118.06	120.30
1	a	611	C	N3-C2-O2	-5.61	117.97	121.90
26	A	243	U	N3-C2-O2	-5.61	118.28	122.20
26	A	2710	C	C6-N1-C2	-5.61	118.06	120.30
26	A	2637	U	N3-C2-O2	-5.60	118.28	122.20
1	a	54	C	N1-C2-O2	5.60	122.26	118.90
1	a	1303	C	OP2-P-O3'	5.60	117.53	105.20
24	y	5	G	N3-C2-N2	-5.60	115.98	119.90
27	B	70	C	C6-N1-C2	-5.60	118.06	120.30
1	a	920	U	N3-C2-O2	-5.60	118.28	122.20
26	A	2416	C	C6-N1-C2	-5.60	118.06	120.30
32	G	42	VAL	CG1-CB-CG2	-5.60	101.94	110.90
1	a	1469	C	N3-C2-O2	-5.59	117.98	121.90
26	A	2066	C	C6-N1-C2	-5.59	118.06	120.30
26	A	806	C	C5-C6-N1	5.58	123.79	121.00
1	a	1009	U	N3-C4-O4	-5.58	115.50	119.40
26	A	837	C	N1-C2-O2	5.58	122.25	118.90
32	G	173	ALA	C-N-CA	5.58	135.65	121.70
24	y	47(G)	C	C6-N1-C1'	5.58	127.49	120.80
1	a	1133	G	N3-C2-N2	-5.58	116.00	119.90
26	A	279	A	C5-C6-N6	-5.58	119.24	123.70
26	A	1180	U	C2-N1-C1'	5.57	124.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	354	G	N3-C4-N9	5.57	129.34	126.00
1	a	723	U	C4-C5-C6	-5.57	116.36	119.70
1	a	799	G	N9-C4-C5	5.57	107.63	105.40
26	A	2626	C	C6-N1-C2	-5.57	118.07	120.30
1	a	502	A	N9-C4-C5	-5.57	103.57	105.80
24	y	16	C	C2-N1-C1'	-5.57	112.68	118.80
1	a	110	C	N3-C2-O2	-5.56	118.00	121.90
26	A	2044	C	C5-C6-N1	5.56	123.78	121.00
26	A	198	C	C6-N1-C2	-5.55	118.08	120.30
26	A	2214	C	N1-C2-O2	5.55	122.23	118.90
24	y	47(H)	A	O5'-P-OP2	-5.55	100.71	105.70
26	A	1594	U	C5-C6-N1	5.55	125.47	122.70
1	a	647	C	C6-N1-C2	-5.54	118.08	120.30
26	A	1103	A	C5-C6-N1	5.54	120.47	117.70
26	A	84	A	C5-N7-C8	5.54	106.67	103.90
26	A	1076	C	C2-N3-C4	5.54	122.67	119.90
26	A	2179	C	N3-C2-O2	-5.54	118.02	121.90
1	a	443	C	C6-N1-C2	-5.54	118.08	120.30
1	a	956	U	N3-C2-O2	-5.54	118.32	122.20
22	v	1	C	C2-N3-C4	5.54	122.67	119.90
26	A	2276	G	N3-C2-N2	-5.54	116.02	119.90
1	a	312	C	C2-N1-C1'	5.53	124.89	118.80
1	a	1161	C	N1-C2-O2	5.53	122.22	118.90
26	A	610	C	C5-C6-N1	5.53	123.77	121.00
1	a	737	C	C5-C6-N1	5.53	123.77	121.00
1	a	1460	C	C5-C6-N1	5.53	123.77	121.00
26	A	2562	U	N1-C2-O2	5.53	126.67	122.80
51	Z	23	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	a	536	C	C2-N1-C1'	5.53	124.88	118.80
26	A	890	C	N1-C2-N3	-5.53	115.33	119.20
26	A	1971	U	N1-C2-O2	-5.53	118.93	122.80
1	a	90	C	N3-C2-O2	-5.53	118.03	121.90
1	a	960	U	N1-C2-O2	5.53	126.67	122.80
23	x	101	A	N9-C4-C5	-5.52	103.59	105.80
26	A	948	C	C5-C6-N1	5.52	123.76	121.00
26	A	1071	G	OP1-P-O3'	5.52	117.35	105.20
26	A	1564	C	C6-N1-C2	-5.52	118.09	120.30
26	A	1775	U	N1-C2-O2	5.52	126.67	122.80
1	a	307	C	C6-N1-C2	-5.52	118.09	120.30
23	x	125	G	C8-N9-C4	-5.52	104.19	106.40
26	A	2075	U	N3-C4-O4	5.52	123.26	119.40
26	A	2573	C	O5'-P-OP1	5.51	117.32	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2707	U	N1-C2-O2	5.51	126.66	122.80
26	A	231	A	N1-C6-N6	5.51	121.91	118.60
26	A	642	U	N3-C2-O2	-5.51	118.34	122.20
1	a	1395	C	N3-C2-O2	-5.51	118.04	121.90
26	A	393	C	C6-N1-C2	-5.51	118.10	120.30
1	a	662	U	C5-C4-O4	-5.50	122.60	125.90
24	y	47(K)	G	N3-C4-N9	-5.50	122.70	126.00
26	A	559	G	N7-C8-N9	5.50	115.85	113.10
26	A	2462	C	C5-C6-N1	5.50	123.75	121.00
24	y	47(B)	G	C4-N9-C1'	5.49	133.64	126.50
26	A	901	C	N1-C2-O2	5.49	122.20	118.90
1	a	491	G	C4-N9-C1'	5.49	133.64	126.50
1	a	868	C	C2-N1-C1'	5.49	124.84	118.80
1	a	514	C	C5-C6-N1	5.49	123.74	121.00
1	a	1071	C	C2-N1-C1'	5.49	124.84	118.80
26	A	852	U	C5-C4-O4	-5.49	122.61	125.90
1	a	896	C	C6-N1-C2	-5.49	118.11	120.30
23	x	126	G	C2'-C3'-O3'	-5.48	97.44	109.50
26	A	1158	C	O5'-P-OP2	-5.48	100.76	105.70
1	a	513	C	C2-N1-C1'	5.48	124.83	118.80
26	A	2805	C	C6-N1-C2	-5.48	118.11	120.30
1	a	598	U	N3-C2-O2	-5.48	118.36	122.20
26	A	125	A	C8-N9-C4	5.48	107.99	105.80
26	A	1244	A	N9-C4-C5	-5.48	103.61	105.80
26	A	822	G	N7-C8-N9	5.48	115.84	113.10
26	A	2134	A	N1-C6-N6	-5.47	115.32	118.60
1	a	334	C	C6-N1-C2	-5.47	118.11	120.30
26	A	415	A	N9-C4-C5	-5.47	103.61	105.80
26	A	717	C	C6-N1-C2	-5.47	118.11	120.30
1	a	418	C	N1-C2-O2	5.47	122.18	118.90
24	y	47(O)	C	C6-N1-C2	-5.47	118.11	120.30
26	A	1314	C	C5-C6-N1	5.47	123.73	121.00
41	P	113	LEU	CA-CB-CG	5.46	127.87	115.30
1	a	90	C	N1-C2-O2	5.46	122.18	118.90
26	A	1548	A	N9-C4-C5	-5.46	103.61	105.80
1	a	1521	C	C5-C6-N1	5.46	123.73	121.00
22	v	67	C	C6-N1-C2	-5.46	118.12	120.30
26	A	1061	U	OP2-P-O3'	5.46	117.21	105.20
1	a	103	U	N3-C2-O2	-5.45	118.38	122.20
24	y	48	G	C5-N7-C8	-5.45	101.57	104.30
1	a	984	C	C6-N1-C2	-5.45	118.12	120.30
26	A	1578	U	N3-C2-O2	-5.45	118.38	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	6	32	LEU	CB-CG-CD1	5.45	120.26	111.00
1	a	211	G	N3-C4-C5	-5.44	125.88	128.60
1	a	34	C	C2-N1-C1'	5.44	124.78	118.80
1	a	1066	C	C6-N1-C2	-5.44	118.12	120.30
24	y	57	G	N9-C4-C5	5.43	107.57	105.40
26	A	1340	U	N3-C2-O2	-5.43	118.40	122.20
26	A	2766	A	C5-C6-N6	-5.43	119.35	123.70
1	a	610	U	N3-C2-O2	-5.43	118.40	122.20
2	b	56	LEU	CA-CB-CG	5.43	127.78	115.30
26	A	1624	U	N3-C2-O2	-5.42	118.40	122.20
1	a	16	A	N1-C2-N3	-5.42	126.59	129.30
1	a	322	C	C5-C6-N1	5.42	123.71	121.00
22	v	68	C	C6-N1-C2	-5.42	118.13	120.30
26	A	120	U	C4-C5-C6	5.42	122.95	119.70
26	A	669	G	C4-N9-C1'	5.42	133.55	126.50
1	a	1487	G	N3-C2-N2	-5.42	116.11	119.90
1	a	1131	G	C4-C5-N7	5.42	112.97	110.80
24	y	45	U	C6-N1-C2	-5.42	117.75	121.00
24	y	48	G	C4-N9-C1'	5.42	133.54	126.50
1	a	723	U	N3-C2-O2	-5.41	118.41	122.20
24	y	47(E)	G	N1-C6-O6	-5.41	116.65	119.90
57	6	4	ASP	CB-CG-OD1	5.41	123.17	118.30
26	A	1348	C	N3-C2-O2	-5.41	118.11	121.90
26	A	2118	U	C5-C4-O4	-5.41	122.66	125.90
26	A	1070	A	O5'-P-OP2	5.40	117.19	110.70
1	a	87	C	C6-N1-C2	-5.40	118.14	120.30
23	x	124	A	N3-C4-N9	5.40	131.72	127.40
26	A	2254	C	N3-C2-O2	-5.40	118.12	121.90
26	A	2305	U	C6-N1-C1'	-5.40	113.64	121.20
26	A	278	A	C2-N3-C4	5.39	113.30	110.60
26	A	1708	C	C5-C6-N1	5.39	123.70	121.00
1	a	307	C	N3-C2-O2	-5.39	118.13	121.90
26	A	2902	C	C6-N1-C2	-5.39	118.14	120.30
23	x	129	U	C5'-C4'-C3'	5.39	124.62	116.00
27	B	108	A	N1-C6-N6	5.38	121.83	118.60
26	A	2699	C	C5-C6-N1	5.38	123.69	121.00
1	a	680	C	C6-N1-C2	-5.38	118.15	120.30
26	A	1914	C	C6-N1-C2	-5.38	118.15	120.30
26	A	867	C	N1-C2-O2	5.38	122.13	118.90
24	y	47(G)	C	N1-C2-N3	5.38	122.97	119.20
26	A	141	G	N3-C4-N9	5.38	129.23	126.00
1	a	71	A	OP2-P-O3'	5.38	117.03	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	65	U	N3-C2-O2	-5.38	118.44	122.20
23	x	126	G	N3-C2-N2	5.38	123.66	119.90
22	v	62	C	C5-C6-N1	5.37	123.69	121.00
26	A	827	U	O5'-P-OP1	-5.37	100.86	105.70
26	A	365	U	C5-C4-O4	-5.37	122.68	125.90
27	B	25	U	N3-C2-O2	-5.37	118.44	122.20
26	A	1476	U	C2-N1-C1'	5.37	124.14	117.70
1	a	661	G	C4-C5-N7	5.37	112.95	110.80
19	s	15	LEU	CA-CB-CG	5.37	127.64	115.30
26	A	1723	G	C5-C6-N1	5.37	114.18	111.50
1	a	582	C	N1-C2-O2	5.36	122.12	118.90
26	A	1670	C	C6-N1-C2	-5.36	118.16	120.30
26	A	658	U	C5-C6-N1	5.36	125.38	122.70
26	A	1927	A	OP2-P-O3'	5.36	116.99	105.20
1	a	923	A	C4-C5-N7	5.36	113.38	110.70
23	x	110	G	P-O3'-C3'	-5.36	113.27	119.70
1	a	470	C	C6-N1-C2	-5.36	118.16	120.30
1	a	1158	C	C6-N1-C1'	-5.36	114.37	120.80
1	a	979	C	C6-N1-C2	-5.35	118.16	120.30
26	A	1585	C	N3-C2-O2	-5.35	118.15	121.90
1	a	1302	C	N3-C4-C5	5.35	124.04	121.90
26	A	230	G	N9-C4-C5	-5.35	103.26	105.40
26	A	2165	C	N1-C2-O2	5.35	122.11	118.90
22	v	40	C	C6-N1-C2	-5.35	118.16	120.30
1	a	967	5MC	OP2-P-O3'	5.35	116.96	105.20
1	a	1389	C	C6-N1-C2	-5.35	118.16	120.30
26	A	717	C	C5-C6-N1	5.35	123.67	121.00
24	y	41	C	C2-N1-C1'	5.35	124.68	118.80
26	A	1886	U	N3-C2-O2	-5.35	118.46	122.20
1	a	413	G	N3-C4-C5	5.34	131.27	128.60
26	A	1043	C	O4'-C1'-N1	5.34	112.47	108.20
1	a	420	U	C2-N1-C1'	5.34	124.11	117.70
26	A	444	C	C5-C6-N1	5.33	123.67	121.00
1	a	1102	A	C8-N9-C4	5.33	107.93	105.80
1	a	1241	G	C8-N9-C4	-5.33	104.27	106.40
26	A	2428	G	OP1-P-OP2	-5.33	111.60	119.60
1	a	440	C	C6-N1-C2	-5.33	118.17	120.30
26	A	2180	U	C5-C6-N1	5.33	125.36	122.70
1	a	178	C	C6-N1-C2	-5.33	118.17	120.30
1	a	225	C	C6-N1-C2	-5.33	118.17	120.30
1	a	431	A	N1-C6-N6	-5.33	115.40	118.60
1	a	1460	C	C6-N1-C2	-5.33	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	148	U	C5-C4-O4	-5.33	122.70	125.90
24	y	62	C	N3-C4-N4	-5.33	114.27	118.00
25	z	338	VAL	CG1-CB-CG2	-5.33	102.38	110.90
1	a	751	U	N3-C2-O2	-5.33	118.47	122.20
26	A	947	A	N9-C4-C5	-5.32	103.67	105.80
23	x	131	C	C3'-C2'-C1'	5.32	105.76	101.50
26	A	2302	U	N1-C2-O2	5.32	126.53	122.80
26	A	1498	C	C5-C6-N1	5.32	123.66	121.00
1	a	610	U	N1-C2-O2	5.32	126.52	122.80
1	a	1382	C	N3-C2-O2	-5.32	118.18	121.90
24	y	53	G	C2-N3-C4	-5.31	109.24	111.90
26	A	1990	C	C6-N1-C2	-5.31	118.17	120.30
33	I	10	LEU	CA-CB-CG	5.31	127.52	115.30
1	a	80	A	C5-C6-N1	-5.31	115.05	117.70
1	a	1138	G	C2-N3-C4	5.31	114.55	111.90
22	v	40	C	N1-C2-O2	5.31	122.08	118.90
26	A	2081	U	C5-C6-N1	5.31	125.35	122.70
1	a	323	U	C5-C4-O4	-5.30	122.72	125.90
1	a	764	C	C5-C6-N1	5.30	123.65	121.00
1	a	878	A	C4-C5-N7	5.30	113.35	110.70
1	a	879	C	C5-C6-N1	5.30	123.65	121.00
1	a	1504	G	N3-C4-N9	-5.30	122.82	126.00
24	y	57	G	N3-C4-N9	-5.30	122.82	126.00
26	A	1629	U	N3-C2-O2	-5.30	118.49	122.20
26	A	2007	U	C5-C6-N1	5.30	125.35	122.70
1	a	924	C	C5-C6-N1	5.29	123.65	121.00
42	Q	108	LEU	CA-CB-CG	5.29	127.47	115.30
24	y	72	C	C6-N1-C2	-5.29	118.19	120.30
26	A	2080	A	N1-C6-N6	5.29	121.77	118.60
26	A	1548	A	N1-C2-N3	-5.29	126.66	129.30
1	a	528	C	C5-C6-N1	5.28	123.64	121.00
26	A	1229	C	C6-N1-C2	-5.28	118.19	120.30
24	y	58	A	O5'-P-OP2	-5.28	100.95	105.70
31	F	162	ASP	CB-CG-OD1	5.28	123.05	118.30
1	a	439	U	N3-C2-O2	-5.27	118.51	122.20
26	A	2231	U	C5-C6-N1	5.27	125.33	122.70
24	y	40	C	C2-N1-C1'	5.27	124.60	118.80
27	B	47	C	C6-N1-C2	-5.27	118.19	120.30
23	x	117	C	C5-C6-N1	5.27	123.63	121.00
26	A	233	A	N9-C4-C5	-5.27	103.69	105.80
1	a	620	C	C6-N1-C2	-5.26	118.19	120.30
26	A	283	G	N3-C4-N9	-5.26	122.84	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	67	C	C5-C6-N1	5.26	123.63	121.00
26	A	302	C	C5-C6-N1	5.26	123.63	121.00
24	y	30	G	C4-N9-C1'	5.25	133.33	126.50
26	A	1512	C	C6-N1-C2	-5.25	118.20	120.30
1	a	968	A	C6-C5-N7	5.25	135.97	132.30
1	a	169	C	N3-C2-O2	-5.25	118.23	121.90
26	A	1399	C	C5-C6-N1	5.25	123.62	121.00
1	a	528	C	N3-C2-O2	-5.24	118.23	121.90
1	a	1263	C	N1-C2-O2	5.24	122.05	118.90
1	a	1410	A	N9-C4-C5	-5.24	103.70	105.80
26	A	2259	U	N3-C2-O2	-5.24	118.53	122.20
1	a	1086	U	C5-C6-N1	5.24	125.32	122.70
26	A	2254	C	C6-N1-C2	-5.24	118.20	120.30
26	A	1059	G	OP1-P-O3'	5.24	116.73	105.20
1	a	552	U	C5-C6-N1	5.24	125.32	122.70
26	A	283	G	N1-C6-O6	-5.24	116.76	119.90
26	A	1644	C	N1-C2-O2	5.24	122.04	118.90
26	A	1118	C	C6-N1-C2	-5.23	118.21	120.30
26	A	209	C	C6-N1-C2	-5.23	118.21	120.30
26	A	1257	C	C6-N1-C2	-5.23	118.21	120.30
25	z	610	LEU	CA-CB-CG	5.23	127.33	115.30
1	a	449	G	N9-C4-C5	-5.23	103.31	105.40
1	a	1317	C	N1-C2-O2	5.23	122.04	118.90
1	a	956	U	N1-C2-O2	5.23	126.46	122.80
26	A	101	A	C2-N3-C4	-5.23	107.99	110.60
10	j	75	ASP	CB-CG-OD1	5.23	123.00	118.30
26	A	2565	A	C8-N9-C4	-5.23	103.71	105.80
26	A	143	C	C6-N1-C2	-5.22	118.21	120.30
1	a	1412	C	C2-N1-C1'	5.22	124.54	118.80
27	B	42	C	C6-N1-C2	-5.22	118.21	120.30
1	a	1464	U	N3-C2-O2	-5.22	118.55	122.20
26	A	1958	C	C6-N1-C2	-5.22	118.21	120.30
1	a	580	C	C6-N1-C2	-5.22	118.21	120.30
1	a	582	C	C5-C6-N1	5.22	123.61	121.00
26	A	56	A	N9-C4-C5	-5.22	103.71	105.80
26	A	898	C	C5-C6-N1	5.21	123.61	121.00
1	a	493	A	N7-C8-N9	5.21	116.41	113.80
26	A	813	U	N1-C2-O2	5.21	126.45	122.80
1	a	920	U	N1-C2-O2	5.21	126.44	122.80
26	A	890	C	C2-N1-C1'	5.21	124.53	118.80
26	A	2086	U	N3-C2-O2	-5.21	118.56	122.20
24	y	73	G	C5-C6-O6	-5.20	125.48	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	39	C	C6-N1-C2	-5.20	118.22	120.30
26	A	2028	U	C5-C6-N1	5.20	125.30	122.70
57	6	40	CYS	CB-CA-C	-5.20	100.00	110.40
1	a	397	A	C4-C5-N7	5.20	113.30	110.70
25	z	457	LEU	CA-CB-CG	5.20	127.26	115.30
26	A	2556	C	N3-C2-O2	-5.20	118.26	121.90
1	a	866	C	C6-N1-C2	-5.20	118.22	120.30
24	y	40	C	O5'-P-OP2	-5.20	101.02	105.70
1	a	274	A	N1-C2-N3	-5.19	126.70	129.30
1	a	127	G	N9-C4-C5	-5.19	103.32	105.40
24	y	1	G	C4-C5-N7	5.19	112.88	110.80
26	A	435	C	OP2-P-O3'	5.19	116.62	105.20
26	A	891	G	N3-C4-C5	-5.19	126.00	128.60
26	A	933	A	N3-C4-N9	5.19	131.55	127.40
26	A	346	A	OP2-P-O3'	5.19	116.62	105.20
26	A	314	C	C5-C6-N1	5.19	123.59	121.00
26	A	1077	A	C5-C6-N1	5.19	120.29	117.70
26	A	2226	C	N1-C2-O2	5.19	122.01	118.90
50	Y	28	LEU	CA-CB-CG	5.18	127.22	115.30
26	A	1093	G	C6-C5-N7	-5.18	127.29	130.40
26	A	119	A	C4-C5-C6	-5.18	114.41	117.00
26	A	883	G	N1-C6-O6	5.18	123.01	119.90
23	x	119	G	N9-C4-C5	5.18	107.47	105.40
30	E	82	GLY	CA-C-O	-5.18	111.28	120.60
22	v	50	U	C6-N1-C2	-5.18	117.89	121.00
24	y	32	C	O4'-C1'-N1	5.17	112.34	108.20
26	A	2136	G	C5-C6-O6	-5.17	125.50	128.60
26	A	2766	A	N1-C6-N6	5.17	121.70	118.60
1	a	219	U	C5-C6-N1	5.17	125.29	122.70
24	y	47(P)	C	N3-C2-O2	-5.17	118.28	121.90
15	o	55	LEU	CA-CB-CG	5.17	127.19	115.30
26	A	2310	C	N3-C2-O2	-5.17	118.28	121.90
1	a	431	A	O4'-C1'-N9	5.17	112.33	108.20
26	A	1243	C	C6-N1-C2	-5.17	118.23	120.30
23	x	110	G	C4-N9-C1'	5.16	133.21	126.50
31	F	50	ASP	CB-CG-OD1	5.16	122.95	118.30
1	a	1148	U	C6-N1-C2	-5.16	117.90	121.00
1	a	1109	C	C5-C6-N1	5.16	123.58	121.00
24	y	47(F)	C	C6-N1-C2	-5.16	118.24	120.30
26	A	2430	A	C2-N3-C4	5.16	113.18	110.60
1	a	1003	G	C8-N9-C4	-5.16	104.34	106.40
15	o	86	LEU	CA-CB-CG	5.16	127.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	413	G	O4'-C1'-N9	-5.15	104.08	108.20
26	A	888	C	O4'-C1'-N1	5.15	112.32	108.20
1	a	1034	G	C6-C5-N7	-5.15	127.31	130.40
26	A	687	C	N3-C2-O2	-5.15	118.29	121.90
26	A	1075	C	C6-N1-C1'	-5.15	114.62	120.80
1	a	634	C	C6-N1-C2	-5.14	118.24	120.30
26	A	946	C	C6-N1-C2	-5.14	118.24	120.30
26	A	1771	C	C6-N1-C2	-5.14	118.24	120.30
1	a	199	A	N9-C4-C5	-5.14	103.74	105.80
1	a	1241	G	N3-C4-C5	-5.14	126.03	128.60
26	A	314	C	C6-N1-C2	-5.14	118.24	120.30
26	A	1043	C	C6-N1-C2	-5.14	118.24	120.30
26	A	1081	U	C5-C6-N1	5.14	125.27	122.70
26	A	2469	A	C5-C6-N6	-5.14	119.59	123.70
1	a	340	U	N3-C2-O2	-5.14	118.60	122.20
1	a	1411	C	C6-N1-C2	-5.14	118.24	120.30
26	A	897	C	N3-C2-O2	-5.14	118.30	121.90
26	A	2065	C	N1-C2-O2	5.14	121.98	118.90
1	a	414	A	C5-C6-N1	5.14	120.27	117.70
1	a	1237	C	C5-C6-N1	5.13	123.57	121.00
1	a	1263	C	C2-N1-C1'	5.13	124.45	118.80
11	k	84	MET	CA-CB-CG	5.13	122.03	113.30
1	a	1032	G	N3-C4-N9	5.13	129.08	126.00
1	a	418	C	C5-C6-N1	5.13	123.57	121.00
1	a	923	A	N9-C4-C5	-5.13	103.75	105.80
23	x	119	G	N3-C2-N2	-5.13	116.31	119.90
26	A	2146	C	OP1-P-OP2	-5.13	111.90	119.60
27	B	28	C	C6-N1-C2	-5.13	118.25	120.30
23	x	118	G	C5-N7-C8	-5.13	101.73	104.30
1	a	697	U	N3-C2-O2	-5.13	118.61	122.20
26	A	1181	U	C6-N1-C2	-5.13	117.92	121.00
26	A	283	G	N9-C4-C5	5.13	107.45	105.40
26	A	889	C	C2-N1-C1'	5.13	124.44	118.80
25	z	177	LEU	CB-CG-CD2	-5.12	102.29	111.00
4	d	4	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	a	207	C	N3-C2-O2	-5.12	118.32	121.90
1	a	428	G	N3-C4-C5	5.12	131.16	128.60
7	g	39	GLU	CA-CB-CG	5.12	124.66	113.40
26	A	1350	C	N1-C2-O2	5.12	121.97	118.90
26	A	1499	C	C6-N1-C2	-5.12	118.25	120.30
26	A	1990	C	C5-C6-N1	5.12	123.56	121.00
27	B	120	U	C2-N1-C1'	5.12	123.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1524	C	N1-C2-O2	5.11	121.97	118.90
26	A	851	C	C5-C6-N1	5.11	123.56	121.00
24	y	16	C	N3-C4-N4	-5.11	114.42	118.00
1	a	55	A	C2-N3-C4	5.11	113.16	110.60
1	a	1342	C	C6-N1-C2	-5.11	118.26	120.30
26	A	2548	U	C5-C6-N1	5.11	125.26	122.70
34	H	58	LEU	CA-CB-CG	5.11	127.05	115.30
26	A	278	A	N3-C4-C5	-5.11	123.22	126.80
26	A	668	A	N1-C2-N3	-5.11	126.75	129.30
3	c	30	ASP	CB-CG-OD1	5.11	122.89	118.30
26	A	283	G	N1-C2-N2	5.11	120.79	116.20
1	a	409	U	N3-C2-O2	-5.10	118.63	122.20
26	A	665	U	C5-C6-N1	5.10	125.25	122.70
26	A	807	U	N3-C2-O2	-5.10	118.63	122.20
26	A	2656	U	N1-C2-O2	5.10	126.37	122.80
26	A	867	C	N3-C2-O2	-5.10	118.33	121.90
26	A	1680	U	N3-C2-O2	-5.10	118.63	122.20
1	a	1500	A	C6-N1-C2	5.10	121.66	118.60
2	b	17	HIS	N-CA-C	5.10	124.77	111.00
22	v	28	C	C6-N1-C2	-5.10	118.26	120.30
1	a	419	C	N1-C2-N3	5.09	122.76	119.20
26	A	1476	U	C6-N1-C2	-5.09	117.94	121.00
26	A	53	A	C4-C5-N7	5.09	113.25	110.70
26	A	392	U	N3-C2-O2	-5.09	118.64	122.20
26	A	1158	C	C5-C6-N1	5.09	123.55	121.00
1	a	54	C	N3-C2-O2	-5.09	118.34	121.90
26	A	208	C	C6-N1-C2	-5.09	118.27	120.30
26	A	373	U	C6-N1-C2	-5.09	117.95	121.00
26	A	610	C	C2-N1-C1'	5.09	124.40	118.80
26	A	2558	C	C6-N1-C2	-5.09	118.27	120.30
26	A	2756	U	OP1-P-O3'	5.09	116.39	105.20
1	a	294	U	C5-C6-N1	5.08	125.24	122.70
1	a	1489	G	N3-C2-N2	-5.08	116.34	119.90
26	A	1578	U	N1-C2-O2	5.08	126.36	122.80
38	M	65	ILE	CG1-CB-CG2	-5.08	100.21	111.40
26	A	2716	C	N1-C2-O2	5.08	121.95	118.90
26	A	1812	U	N3-C2-O2	-5.08	118.64	122.20
26	A	2086	U	N1-C2-O2	5.08	126.36	122.80
26	A	1830	C	C6-N1-C2	-5.08	118.27	120.30
27	B	57	A	C8-N9-C4	-5.08	103.77	105.80
26	A	2234	G	N7-C8-N9	5.07	115.64	113.10
24	y	35	C	N1-C2-O2	5.07	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	750	C	N1-C2-N3	5.07	122.75	119.20
26	A	1113	U	O4'-C1'-N1	5.07	112.25	108.20
1	a	489	C	C6-N1-C2	-5.07	118.27	120.30
1	a	879	C	C6-N1-C2	-5.07	118.27	120.30
26	A	1093	G	C5-C6-N1	5.07	114.03	111.50
26	A	2103	C	C6-N1-C2	-5.07	118.27	120.30
1	a	418	C	N3-C2-O2	-5.07	118.35	121.90
23	x	118	G	C4-N9-C1'	5.07	133.09	126.50
24	y	32	C	C6-N1-C1'	5.07	126.88	120.80
26	A	2480	C	C6-N1-C2	-5.07	118.27	120.30
1	a	392	C	N3-C4-N4	5.06	121.54	118.00
22	v	57	A	N7-C8-N9	-5.06	111.27	113.80
24	y	47(J)	C	C6-N1-C2	-5.06	118.28	120.30
1	a	796	C	C6-N1-C2	-5.06	118.28	120.30
26	A	1052	C	C5-C6-N1	5.06	123.53	121.00
26	A	2739	U	N3-C2-O2	-5.06	118.66	122.20
35	J	17	VAL	CG1-CB-CG2	-5.06	102.81	110.90
26	A	883	G	C5-N7-C8	-5.05	101.77	104.30
26	A	2119	A	C5-C6-N6	-5.05	119.66	123.70
1	a	1455	G	C5-C6-O6	-5.05	125.57	128.60
26	A	1437	C	C5-C6-N1	5.05	123.53	121.00
26	A	1646	C	OP1-P-O3'	5.05	116.31	105.20
1	a	1226	C	N1-C2-O2	5.05	121.93	118.90
26	A	358	U	N3-C2-O2	-5.05	118.67	122.20
1	a	1448	C	C5-C6-N1	5.05	123.52	121.00
26	A	2636	C	N3-C2-O2	-5.05	118.37	121.90
23	x	101	A	C6-N1-C2	5.04	121.63	118.60
1	a	80	A	N3-C4-C5	5.04	130.33	126.80
1	a	623	C	C6-N1-C2	-5.04	118.28	120.30
1	a	979	C	N3-C2-O2	-5.04	118.37	121.90
23	x	114	C	O5'-P-OP2	-5.04	101.16	105.70
26	A	2895	G	N9-C4-C5	-5.04	103.38	105.40
1	a	1379	G	N3-C2-N2	-5.04	116.37	119.90
22	v	25	C	C6-N1-C2	-5.04	118.28	120.30
26	A	2405	G	OP2-P-O3'	5.04	116.29	105.20
26	A	832	U	N3-C2-O2	-5.04	118.67	122.20
26	A	1716	U	C6-N1-C2	-5.04	117.98	121.00
26	A	2782	G	N3-C4-N9	5.04	129.02	126.00
26	A	2880	C	C6-N1-C2	-5.04	118.28	120.30
1	a	550	G	N3-C4-C5	-5.03	126.08	128.60
26	A	852	U	C5-C6-N1	5.03	125.22	122.70
26	A	1956	U	N1-C2-O2	5.03	126.32	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	88	U	N3-C2-O2	-5.03	118.68	122.20
1	a	817	C	C2-N1-C1'	5.03	124.33	118.80
26	A	141	G	N3-C4-C5	-5.03	126.09	128.60
26	A	1539	U	C2-N1-C1'	5.03	123.73	117.70
26	A	2065	C	N3-C2-O2	-5.03	118.38	121.90
19	s	4	LEU	CA-CB-CG	5.02	126.86	115.30
26	A	193	U	N3-C2-O2	-5.02	118.68	122.20
26	A	915	C	C2-N1-C1'	5.02	124.33	118.80
1	a	71	A	OP1-P-OP2	-5.02	112.07	119.60
26	A	1774	C	N1-C2-O2	5.02	121.91	118.90
26	A	1279	G	N1-C6-O6	5.02	122.91	119.90
26	A	595	C	C5-C6-N1	5.02	123.51	121.00
24	y	72	C	C5-C6-N1	5.02	123.51	121.00
1	a	218	U	C5-C6-N1	5.02	125.21	122.70
26	A	49	A	O4'-C1'-N9	-5.02	104.19	108.20
26	A	2752	C	N1-C2-O2	5.02	121.91	118.90
1	a	905	U	C6-N1-C2	-5.01	117.99	121.00
26	A	2305	U	C2-N3-C4	-5.01	123.99	127.00
26	A	2656	U	N3-C2-O2	-5.01	118.69	122.20
1	a	674	G	N7-C8-N9	5.01	115.61	113.10
1	a	346	G	C5-C6-N1	5.01	114.00	111.50
24	y	47(B)	G	C6-C5-N7	-5.01	127.39	130.40
26	A	2238	G	N3-C4-N9	5.01	129.00	126.00
1	a	1348	U	N1-C2-O2	5.01	126.31	122.80
1	a	94	G	C5-C6-O6	-5.01	125.60	128.60
22	v	17	C	C6-N1-C2	-5.01	118.30	120.30
26	A	2556	C	N1-C2-O2	5.01	121.90	118.90
24	y	67(A)	U	C5-C6-N1	5.00	125.20	122.70
1	a	689	C	C2-N1-C1'	5.00	124.30	118.80
26	A	2110	G	N3-C4-C5	5.00	131.10	128.60
26	A	2279	G	N9-C4-C5	-5.00	103.40	105.40
1	a	136	C	C5-C6-N1	5.00	123.50	121.00
1	a	656	G	N1-C2-N3	5.00	126.90	123.90
26	A	919	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 (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
55	3	30	HIS	Peptide
28	C	120	ASP	Peptide
34	H	2	GLN	Peptide
34	H	8	LYS	Mainchain,Peptide
33	I	23	VAL	Peptide
33	I	63	ASP	Peptide
36	K	34	GLY	Peptide
38	M	57	VAL	Mainchain
44	S	63	GLY	Peptide
46	U	5	ARG	Peptide
46	U	50	ALA	Peptide
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain
5	e	92	ARG	Peptide
10	j	33	GLY	Peptide
10	j	56	HIS	Peptide
11	k	91	GLY	Peptide
12	l	100	ALA	Peptide
12	l	74	GLN	Peptide
13	m	3	ILE	Peptide
13	m	4	ALA	Mainchain
15	o	87	ARG	Mainchain
18	r	10	CYS	Peptide
18	r	16	GLY	Peptide
25	z	190	LEU	Peptide
25	z	300	LEU	Peptide
25	z	327	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33029	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	787	0	828	0	0
11	k	870	0	878	0	0
12	l	955	0	1019	0	0
13	m	884	0	944	0	0
14	n	794	0	836	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	649	0	691	0	0
18	r	505	0	502	0	0
19	s	638	0	665	0	0
20	t	665	0	714	0	0
21	u	496	0	486	0	0
22	v	1642	0	839	0	0
23	x	1025	0	518	0	0
24	y	2031	0	1039	0	0
25	z	4863	0	4837	0	0
26	A	62335	0	31375	421	0
27	B	2570	0	1301	20	0
28	C	2083	0	2157	30	0
29	D	1565	0	1616	32	0
30	E	1552	0	1619	16	0
31	F	1411	0	1447	20	0
32	G	1323	0	1374	29	0
33	I	1032	0	1088	15	0
34	H	1111	0	1148	13	0
35	J	1129	0	1162	14	0
36	K	939	0	1012	16	0
37	L	1045	0	1117	21	0
38	M	1074	0	1157	17	0
39	N	961	0	1000	14	0
40	O	892	0	923	14	0
41	P	917	0	965	13	0
42	Q	947	0	1022	14	0
43	R	816	0	839	12	0
44	S	857	0	922	9	0
45	T	739	0	807	16	0
46	U	780	0	834	16	0
47	V	753	0	780	10	0
48	W	575	0	592	9	0
49	X	625	0	655	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	Y	509	0	543	8	0
51	Z	449	0	491	10	0
52	0	444	0	461	6	0
53	1	410	0	440	7	0
54	2	377	0	418	4	0
55	3	504	0	574	7	0
56	4	302	0	340	6	0
57	6	523	0	521	10	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	152991	0	104094	728	0

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

All (728) 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:279:A:N6	26:A:361:G:N3	2.04	1.05
26:A:2166:U:O2	26:A:2170:A:N6	2.08	0.85
36:K:35:VAL:HG21	36:K:69:VAL:HG12	1.69	0.74
26:A:1072:C:OP1	26:A:1077:A:N6	2.23	0.72
26:A:410:G:N3	26:A:432:A:N6	41.67	0.72
47:V:32:GLY:O	47:V:93:ARG:NH2	2.24	0.70
39:N:35:LYS:NZ	39:N:110:MET:SD	2.64	0.70
32:G:88:LEU:HG	32:G:161:VAL:HG22	1.74	0.68
26:A:1250:G:N7	37:L:18:ARG:NH2	2.40	0.68
26:A:585:G:N7	42:Q:5:ARG:NH1	2.43	0.66
26:A:2296:U:OP2	40:O:9:ARG:NH2	2.28	0.66
26:A:956:G:N7	38:M:14:LYS:NZ	2.43	0.65
26:A:1311:G:H21	26:A:1603:A:H62	1.43	0.65
57:6:28:VAL:HG11	57:6:32:LEU:HD23	1.79	0.64
43:R:48:LYS:NZ	43:R:49:ILE:O	2.30	0.64
26:A:1060:U:O2'	35:J:58:ASN:ND2	81.07	0.64
29:D:128:ARG:NH1	29:D:129:THR:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:32:VAL:HG23	33:I:60:VAL:HG13	1.79	0.64
28:C:181:ARG:NH1	28:C:182:LYS:O	2.31	0.64
26:A:994:C:OP1	42:Q:52:ARG:NH2	2.31	0.64
26:A:2848:G:O2'	26:A:2867:G:N2	2.31	0.64
26:A:850:U:OP1	51:Z:18:LYS:NZ	2.31	0.63
26:A:1454:C:OP1	39:N:63:ARG:NH2	2.31	0.63
26:A:910:A:N3	26:A:2264:C:O2'	2.29	0.63
26:A:2743:U:OP2	26:A:2755:C:N4	2.32	0.63
26:A:2250:G:O2'	26:A:2496:C:OP1	2.16	0.63
26:A:475:C:O2	26:A:479:A:N6	2.31	0.63
27:B:30:C:H1'	27:B:57:A:H61	1.64	0.63
40:O:50:ALA:O	40:O:81:ARG:NH2	2.32	0.63
26:A:764:A:N3	28:C:211:ARG:NH1	2.47	0.62
27:B:48:U:OP1	40:O:30:ARG:NH2	2.31	0.62
31:F:31:GLU:OE2	31:F:158:THR:OG1	2.18	0.62
31:F:101:ARG:NH1	57:6:9:TYR:OH	2.33	0.62
26:A:516:C:OP1	52:0:9:ARG:NH1	2.33	0.61
29:D:37:VAL:HA	29:D:48:ILE:HG22	1.83	0.61
26:A:24:G:N2	44:S:78:GLU:OE2	2.34	0.61
26:A:961:C:OP1	26:A:2456:C:O2'	2.19	0.61
29:D:97:SER:OG	29:D:99:GLU:OE1	2.18	0.61
26:A:2830:C:OP2	29:D:59:ARG:NH2	2.34	0.61
26:A:545:U:O2	26:A:548:G:O6	2.19	0.61
33:I:17:ALA:HB1	33:I:38:CYS:HA	1.81	0.61
26:A:200:U:O2	26:A:386:G:N2	2.32	0.61
26:A:245:G:N7	55:3:7:ARG:NH2	2.48	0.61
35:J:105:VAL:HG12	35:J:109:LEU:HD23	1.83	0.61
31:F:177:ARG:O	57:6:47:LYS:NZ	2.33	0.61
43:R:69:GLY:O	43:R:90:ARG:NE	2.29	0.61
26:A:1056:G:O2'	26:A:1103:A:N6	2.34	0.60
26:A:2334:U:O2'	40:O:13:ARG:NH2	2.34	0.60
26:A:453:A:N3	26:A:457:A:O2'	2.34	0.60
26:A:908:C:OP2	38:M:22:GLN:NE2	2.34	0.60
26:A:1737:G:N2	26:A:1737:G:OP2	2.34	0.60
41:P:8:GLU:HG2	41:P:54:LEU:HD23	1.84	0.60
26:A:750:A:OP1	26:A:1615:C:N4	2.35	0.60
32:G:21:GLN:NE2	32:G:37:ASN:O	2.35	0.60
28:C:182:LYS:NZ	28:C:264:LYS:O	2.34	0.60
26:A:491:G:O6	44:S:49:LYS:NZ	2.34	0.60
26:A:877:A:O2'	26:A:900:A:N6	2.31	0.60
26:A:1753:G:N2	26:A:1756:G:OP2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1000:A:OP2	26:A:1154:G:N1	2.32	0.59
26:A:771:G:OP2	54:2:11:LYS:NZ	2.35	0.59
26:A:959:A:N3	26:A:2457:PSU:O2'	2.32	0.59
26:A:1528:A:OP2	26:A:1543:G:N2	2.34	0.59
32:G:53:PRO:HG3	32:G:61:TRP:CE2	2.37	0.59
57:6:14:ALA:HB3	57:6:22:MET:HB2	1.84	0.59
26:A:1170:C:N3	26:A:1178:C:N4	2.50	0.59
53:1:16:THR:HG21	53:1:41:VAL:HG11	1.83	0.59
26:A:2344:U:OP1	53:1:36:LYS:NZ	2.35	0.59
26:A:2576:G:O2'	26:A:2579:C:OP2	2.21	0.59
26:A:1997:C:OP2	29:D:128:ARG:NH1	2.35	0.59
36:K:69:VAL:O	36:K:76:VAL:HA	2.03	0.59
26:A:1084:A:H2'	26:A:1085:A:C8	2.37	0.58
26:A:1392:A:N6	45:T:18:GLU:OE1	2.35	0.58
26:A:297:G:N2	26:A:300:A:OP2	12.69	0.58
26:A:612:G:OP2	26:A:614:A:N6	2.36	0.58
26:A:2394:C:OP1	55:3:29:ARG:NH1	2.36	0.58
35:J:118:MET:HA	35:J:121:LYS:HZ3	1.67	0.58
26:A:807:U:O2'	26:A:2060:A:N1	2.37	0.58
43:R:63:VAL:HG12	43:R:96:VAL:HG12	1.85	0.58
27:B:57:A:N3	31:F:26:GLN:NE2	2.52	0.58
32:G:4:ALA:HA	32:G:68:ARG:HE	1.67	0.58
26:A:1666:G:HO2'	36:K:6:THR:HG1	1.52	0.58
26:A:684:G:O2'	26:A:788:A:N7	2.35	0.58
28:C:83:ASP:OD2	28:C:86:ARG:NH1	2.36	0.58
28:C:61:TYR:HA	28:C:85:ASN:HD21	1.67	0.58
26:A:2742:G:OP1	56:4:36:ARG:NH1	2.37	0.57
26:A:1127:A:N7	26:A:2488:G:O2'	2.35	0.57
26:A:2520:C:O2'	26:A:2565:A:O2'	2.21	0.57
26:A:956:G:N2	26:A:960:A:OP2	2.35	0.57
26:A:1288:G:OP2	26:A:1288:G:N2	2.32	0.57
51:Z:8:GLN:NE2	51:Z:10:ARG:O	2.36	0.57
26:A:63:A:O2'	45:T:77:ARG:NE	2.36	0.57
40:O:14:ALA:HA	40:O:17:LYS:HE3	1.87	0.57
26:A:1992:G:O2'	26:A:1997:C:N4	2.37	0.57
28:C:78:GLU:OE2	28:C:100:ARG:NH1	2.38	0.57
43:R:58:VAL:H	43:R:102:SER:HB2	1.70	0.57
26:A:1068:G:N3	26:A:1095:A:O2'	2.37	0.57
26:A:660:C:O2'	37:L:13:LYS:NZ	2.38	0.57
26:A:2406:A:OP2	26:A:2411:A:N6	2.38	0.57
32:G:38:ASP:O	32:G:54:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:J:49:ASP:OD1	35:J:121:LYS:NZ	2.38	0.57
26:A:1365:A:O2'	49:X:10:ARG:NH2	2.37	0.57
26:A:2051:A:N6	26:A:2614:A:O2'	2.38	0.57
26:A:1156:A:OP1	42:Q:54:ARG:NH1	2.38	0.56
26:A:2835:A:N6	26:A:2879:A:O4'	2.38	0.56
26:A:563:A:N6	26:A:884:U:O2	105.61	0.56
28:C:243:PRO:O	28:C:250:GLN:NE2	2.38	0.56
34:H:2:GLN:NE2	34:H:18:GLN:OE1	2.38	0.56
26:A:2788:C:O2'	26:A:2809:A:N3	2.32	0.56
41:P:47:ILE:HA	41:P:96:LEU:HD12	1.87	0.56
26:A:536:G:H4'	42:Q:56:PHE:HZ	1.70	0.56
26:A:279:A:H61	26:A:361:G:H1'	1.69	0.56
45:T:80:TRP:HZ3	45:T:82:LYS:HB3	1.70	0.56
26:A:545:U:O2	26:A:548:G:C6	2.59	0.56
26:A:301:G:OP2	46:U:81:ARG:NH1	2.38	0.56
26:A:196:A:OP2	37:L:47:ARG:NH1	2.39	0.56
46:U:49:PRO:O	46:U:53:GLN:NE2	2.38	0.56
26:A:2320:U:O2'	26:A:2333:A:N6	2.39	0.56
36:K:76:VAL:H	41:P:72:VAL:HG22	1.70	0.56
26:A:1315:C:O2'	26:A:1392:A:N3	2.36	0.56
26:A:2522:U:O2'	26:A:2647:U:OP1	2.23	0.56
53:1:36:LYS:HB3	53:1:47:ILE:HD13	1.88	0.56
26:A:859:G:OP2	26:A:869:G:N1	23.51	0.56
29:D:8:LYS:NZ	29:D:195:GLY:O	2.35	0.56
29:D:32:ASN:OD1	29:D:52:THR:OG1	2.21	0.56
38:M:17:ASN:O	38:M:38:ARG:NH1	2.38	0.56
26:A:221:A:N1	26:A:265:A:O2'	2.35	0.56
35:J:73:VAL:HG12	35:J:88:THR:HG22	1.88	0.56
36:K:21:CYS:HA	36:K:41:ILE:HG22	1.88	0.56
26:A:1088:A:N6	33:I:134:SER:OG	2.39	0.55
26:A:1378:A:O2'	26:A:1380:G:OP2	2.23	0.55
43:R:6:GLN:HE22	43:R:39:LEU:HD11	1.70	0.55
26:A:1807:G:N2	26:A:1810:A:OP2	2.38	0.55
51:Z:40:THR:HG22	51:Z:42:ALA:H	1.71	0.55
28:C:132:ARG:NH1	28:C:186:ASP:OD1	2.35	0.55
32:G:88:LEU:N	32:G:128:THR:O	2.33	0.55
40:O:53:THR:HG21	40:O:70:ALA:HB1	1.87	0.55
26:A:1071:G:H1'	26:A:1089:A:H2'	1.88	0.55
31:F:56:LEU:HD22	31:F:64:PRO:HG3	1.88	0.55
26:A:1437:C:HO2'	26:A:1516:G:HO2'	1.54	0.55
26:A:2419:U:OP1	55:3:40:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:32:LEU:HD13	28:C:63:ILE:HB	1.89	0.55
39:N:58:ASP:OD1	39:N:63:ARG:NE	2.38	0.55
26:A:1950:G:N2	26:A:1956:U:O4	2.39	0.55
49:X:6:VAL:HG21	49:X:58:ILE:HD11	1.89	0.55
26:A:298:G:N1	26:A:339:U:OP2	2.39	0.55
36:K:25:LEU:O	36:K:30:ARG:NH1	2.39	0.55
26:A:1153:C:OP1	42:Q:91:ARG:NH2	2.39	0.55
30:E:117:ARG:NH2	30:E:183:PHE:O	2.40	0.54
32:G:1:SER:OG	32:G:2:ARG:N	2.40	0.54
26:A:1869:G:N2	26:A:1872:A:OP2	2.40	0.54
26:A:1889:A:N3	26:A:2086:U:O2'	2.37	0.54
26:A:743:A:O2'	26:A:1659:G:OP1	2.24	0.54
26:A:2172:U:OP1	26:A:2174:C:N4	2.39	0.54
32:G:26:LYS:NZ	32:G:27:GLY:O	2.38	0.54
33:I:64:ARG:NH1	33:I:65:SER:OG	2.40	0.54
45:T:40:LYS:HA	45:T:43:ILE:HG12	1.88	0.54
26:A:197:A:N6	26:A:2430:A:O2'	2.41	0.54
26:A:2469:A:O4'	38:M:55:ARG:NH1	2.40	0.54
28:C:16:VAL:HG12	28:C:203:VAL:HG22	1.90	0.54
26:A:270:A:N1	26:A:369:U:O2'	2.40	0.54
26:A:635:C:O2'	26:A:639:U:OP1	2.26	0.54
26:A:1798:U:OP2	28:C:270:ARG:NH2	2.41	0.54
26:A:27:G:O2'	26:A:512:G:N2	2.41	0.54
26:A:2636:C:O2'	29:D:45:TYR:OH	2.25	0.54
35:J:36:LEU:HD11	35:J:54:ILE:HG12	1.88	0.54
40:O:66:GLY:O	40:O:102:ARG:NH2	2.41	0.54
29:D:131:ASP:O	29:D:136:ASN:ND2	2.41	0.54
26:A:2532:G:O2'	26:A:2657:A:N1	2.41	0.53
32:G:82:PHE:O	32:G:133:LYS:HA	2.08	0.53
26:A:111:A:O2'	50:Y:58:ASN:ND2	2.35	0.53
35:J:16:TYR:HB2	35:J:54:ILE:HG22	1.89	0.53
26:A:2336:A:H61	48:W:39:THR:HG21	1.74	0.53
26:A:2136:G:N2	26:A:2156:G:O2'	2.42	0.53
30:E:105:LEU:HD11	30:E:200:LEU:HD21	1.90	0.53
26:A:910:A:H62	38:M:12:MET:HA	1.72	0.53
26:A:792:A:O2'	26:A:794:A:N7	15.01	0.53
27:B:27:C:OP1	40:O:34:HIS:NE2	2.41	0.53
40:O:92:PHE:HB2	40:O:117:PHE:HD2	1.72	0.53
26:A:2107:G:N2	26:A:2182:U:O2'	2.41	0.53
26:A:2773:C:OP1	29:D:169:ARG:NH2	2.41	0.53
30:E:120:VAL:HG12	30:E:188:MET:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:J:80:HIS:O	35:J:82:GLY:N	2.41	0.53
26:A:415:A:O2'	26:A:1866:A:OP1	2.25	0.53
26:A:1682:G:OP2	26:A:1699:G:N2	2.42	0.53
26:A:1796:U:H2'	26:A:1797:G:H8	1.72	0.53
26:A:304:U:H3	26:A:313:G:H1	1.54	0.53
26:A:1223:G:N2	26:A:1226:A:OP2	2.33	0.53
26:A:1942:C:OP2	26:A:1943:U:O2'	2.26	0.53
26:A:2481:G:HO2'	26:A:2482:A:H8	1.55	0.53
26:A:571:U:O2'	26:A:573:U:OP2	2.27	0.53
34:H:27:ARG:NH2	49:X:59:ASP:OD2	2.42	0.53
26:A:1802:A:H2'	26:A:1803:A:C8	2.44	0.52
26:A:1138:G:O2'	35:J:104:ALA:O	2.28	0.52
32:G:29:ASN:OD1	32:G:30:GLY:N	2.40	0.52
26:A:1065:U:O2	26:A:1066:U:O2'	2.22	0.52
26:A:2144:G:O2'	26:A:2147:A:N6	2.42	0.52
31:F:37:MET:HG3	31:F:56:LEU:HD12	1.91	0.52
26:A:2140:G:N2	26:A:2152:G:N7	2.58	0.52
29:D:109:VAL:HG12	29:D:203:VAL:HG12	1.90	0.52
26:A:2353:G:O2'	48:W:29:ALA:O	2.20	0.52
26:A:489:G:N2	26:A:1321:A:OP1	2.42	0.52
26:A:349:U:H2'	26:A:350:G:H8	1.75	0.52
30:E:159:LEU:HA	30:E:162:ARG:HE	1.74	0.52
26:A:1614:A:N6	44:S:88:ARG:H	2.08	0.52
26:A:1998:A:OP2	29:D:141:ARG:NH1	2.40	0.52
26:A:2755:C:OP1	56:4:19:ARG:NH2	2.42	0.52
27:B:31:C:O2'	27:B:53:A:N1	2.36	0.52
51:Z:16:LEU:HD12	51:Z:17:PRO:HD2	1.91	0.52
26:A:253:C:OP2	55:3:4:LYS:NZ	2.36	0.52
27:B:95:U:OP2	47:V:19:ARG:NH2	2.43	0.52
32:G:87:GLN:HA	32:G:129:GLU:HA	1.90	0.52
26:A:1437:C:O2'	26:A:1516:G:O2'	2.25	0.52
31:F:46:LYS:HB2	31:F:47:LYS:HD2	1.91	0.52
38:M:47:GLU:OE1	38:M:51:ARG:NH1	2.43	0.52
44:S:25:ARG:NH2	44:S:74:ILE:O	2.41	0.52
26:A:1601:G:OP1	45:T:64:LYS:NZ	2.43	0.52
38:M:40:ARG:HG2	38:M:95:LEU:HA	1.91	0.52
26:A:1496:A:N3	26:A:1577:C:O2'	2.39	0.52
29:D:148:GLN:HB2	29:D:152:PRO:HG2	1.92	0.52
44:S:3:THR:HG21	44:S:58:ALA:HB2	1.90	0.51
48:W:66:GLU:HB3	48:W:68:LYS:HG2	1.91	0.51
26:A:1063:G:O6	26:A:1076:C:O2'	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:566:U:H5''	37:L:29:LYS:HE3	1.92	0.51
26:A:187:G:N2	26:A:190:A:OP2	11.77	0.51
26:A:2817:U:OP1	39:N:42:LYS:NZ	2.39	0.51
28:C:153:LEU:HD23	28:C:175:LEU:HD21	1.92	0.51
28:C:128:THR:HA	28:C:189:ALA:O	2.11	0.51
26:A:1071:G:N3	26:A:1089:A:O2'	2.36	0.51
46:U:8:ASP:H	46:U:24:VAL:HG22	1.74	0.51
48:W:16:ARG:O	48:W:35:ARG:NH1	2.44	0.51
26:A:2202:U:O2'	26:A:2204:G:OP1	2.24	0.51
26:A:77:G:OP1	50:Y:52:ARG:NH2	2.41	0.51
26:A:1019:U:OP1	26:A:1035:U:O2'	2.21	0.51
45:T:19:LYS:NZ	45:T:84:TYR:OH	2.40	0.51
26:A:2233:U:H2'	26:A:2234:G:C8	2.46	0.51
26:A:2857:G:N2	26:A:2860:A:OP2	2.36	0.51
33:I:74:PRO:HG2	33:I:77:VAL:HG22	1.93	0.51
44:S:30:SER:OG	44:S:31:GLN:OE1	2.29	0.51
37:L:77:ILE:HD13	37:L:101:ILE:HD11	1.93	0.51
46:U:13:LEU:N	46:U:68:ASN:O	2.32	0.51
56:4:11:CYS:SG	56:4:14:CYS:N	2.85	0.50
26:A:28:A:O2'	42:Q:10:ARG:NH2	2.44	0.50
38:M:71:LYS:HB3	38:M:93:VAL:O	2.11	0.50
26:A:77:G:H5''	50:Y:2:LYS:HE2	1.94	0.50
53:1:41:VAL:HG13	53:1:42:VAL:HG23	1.93	0.50
26:A:2258:C:O2'	26:A:2427:C:OP2	2.22	0.50
26:A:2645:G:N2	26:A:2645:G:OP2	2.43	0.50
31:F:72:SER:OG	31:F:80:GLN:N	2.44	0.50
34:H:3:VAL:HA	34:H:38:PRO:HA	1.93	0.50
37:L:74:THR:HG22	37:L:107:PHE:HB2	1.93	0.50
45:T:65:GLY:O	45:T:76:ARG:NH1	2.43	0.50
53:1:24:LYS:NZ	53:1:50:GLU:OE1	2.42	0.50
26:A:1961:C:H2'	26:A:1962:5MC:C2	2.46	0.50
26:A:200:U:OP1	49:X:22:ASN:ND2	2.44	0.50
26:A:2024:G:O3'	29:D:154:LYS:NZ	2.40	0.50
26:A:2282:G:N2	26:A:2390:U:O2	2.43	0.50
31:F:43:ILE:HG12	31:F:78:ILE:HG22	1.93	0.50
26:A:329:G:H1	46:U:16:LYS:HZ3	1.59	0.50
26:A:564:C:O4'	42:Q:36:GLN:NE2	2.44	0.50
26:A:2045:C:O2	52:0:18:HIS:NE2	2.45	0.50
26:A:1183:U:O3'	51:Z:29:ARG:NH2	2.44	0.50
56:4:9:LYS:HG3	56:4:14:CYS:HB2	1.94	0.50
26:A:2199:A:O4'	34:H:28:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:124:ARG:NH2	29:D:161:MET:O	2.41	0.50
29:D:10:GLY:H	29:D:197:THR:HG23	1.76	0.50
26:A:1011:G:OP1	42:Q:74:SER:OG	2.29	0.50
46:U:15:GLY:O	46:U:18:LYS:NZ	2.39	0.50
26:A:1664:A:H61	26:A:1996:C:H42	1.58	0.50
26:A:411:G:OP2	26:A:2406:A:O2'	2.26	0.50
36:K:7:MET:HA	36:K:19:VAL:O	2.12	0.50
41:P:24:THR:HG22	41:P:87:ARG:HB3	1.94	0.50
26:A:1478:G:H1	26:A:1513:U:H3	1.59	0.50
26:A:2108:A:H2'	26:A:2109:U:C6	2.46	0.50
29:D:4:LEU:HB2	29:D:32:ASN:HD22	1.76	0.50
39:N:56:LYS:NZ	39:N:87:PHE:O	2.44	0.50
40:O:35:ILE:HG22	40:O:66:GLY:HA2	1.93	0.50
55:3:31:ILE:O	55:3:35:LYS:NZ	2.34	0.49
26:A:581:C:H2'	26:A:582:A:H8	1.77	0.49
38:M:69:PRO:HA	38:M:94:ALA:HB2	1.94	0.49
50:Y:24:GLU:HB3	50:Y:46:VAL:HG21	1.94	0.49
26:A:1128:G:N3	26:A:2516:A:O2'	2.37	0.49
26:A:882:G:N3	26:A:896:A:N6	2.59	0.49
54:2:34:ARG:NE	54:2:42:LEU:O	2.45	0.49
37:L:128:THR:HG23	37:L:131:ALA:H	1.75	0.49
26:A:1493:C:OP1	26:A:1495:A:N6	2.45	0.49
26:A:578:G:OP1	26:A:1255:U:O2'	2.30	0.49
26:A:2600:A:H62	28:C:235:GLU:HG3	1.77	0.49
43:R:68:ARG:NH1	43:R:90:ARG:O	2.45	0.49
26:A:2178:C:O2'	26:A:2180:U:OP2	2.29	0.49
28:C:141:HIS:ND1	28:C:192:GLY:O	2.40	0.49
29:D:5:VAL:HG22	29:D:202:ILE:HG22	1.94	0.49
47:V:30:ILE:HG12	47:V:91:PHE:HB2	1.95	0.49
26:A:1021:A:O2'	26:A:1123:C:OP1	2.28	0.49
26:A:2119:A:H61	26:A:2169:A:N6	2.10	0.49
53:1:7:LYS:HA	53:1:23:THR:HA	1.94	0.49
31:F:25:MET:HG3	31:F:26:GLN:HE21	1.78	0.49
32:G:18:ILE:HD11	32:G:42:VAL:HG13	1.95	0.49
26:A:2031:A:N3	26:A:2455:G:O2'	2.41	0.49
26:A:1636:U:H2'	26:A:1637:A:C8	2.48	0.49
26:A:249:C:OP2	26:A:2394:C:O2'	2.27	0.49
26:A:355:U:H2'	26:A:356:G:H8	1.78	0.49
26:A:478:A:N6	26:A:500:G:O2'	2.46	0.49
29:D:101:PHE:HB2	29:D:180:VAL:HG23	1.94	0.49
26:A:688:U:H2'	26:A:689:A:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:148:ILE:HB	30:E:169:VAL:HG22	1.95	0.49
30:E:95:LYS:NZ	30:E:97:ASN:OD1	2.46	0.49
32:G:132:LEU:HD13	32:G:143:VAL:HG23	1.94	0.49
26:A:1527:G:N1	26:A:1544:A:OP2	2.38	0.48
26:A:2482:A:H61	38:M:55:ARG:HH12	1.59	0.48
26:A:1085:A:H2'	26:A:1086:A:O4'	2.13	0.48
45:T:12:ARG:HA	50:Y:29:ARG:HH22	1.78	0.48
26:A:1011:G:OP2	42:Q:65:ASN:ND2	2.47	0.48
34:H:100:ALA:HB2	34:H:112:LYS:HD3	1.95	0.48
37:L:95:LEU:HD22	37:L:100:ILE:HD11	1.95	0.48
38:M:17:ASN:OD1	38:M:97:GLN:NE2	2.46	0.48
26:A:1681:G:H21	26:A:1762:A:H3'	1.78	0.48
26:A:195:A:H2'	26:A:196:A:C4	9.89	0.48
28:C:132:ARG:O	28:C:166:ARG:NH1	2.41	0.48
26:A:1244:A:HO2'	30:E:29:HIS:HE2	1.58	0.48
31:F:28:PRO:HB2	31:F:168:LEU:HD22	1.96	0.48
32:G:86:LEU:HD22	32:G:130:ILE:HD11	1.95	0.48
38:M:30:SER:N	38:M:106:ASP:OD1	2.45	0.48
26:A:2579:C:O3'	29:D:137:SER:OG	2.30	0.48
34:H:30:LEU:HD23	34:H:36:ALA:HB3	1.96	0.48
37:L:75:ALA:O	37:L:108:ALA:HA	2.14	0.48
26:A:1386:C:H2'	26:A:1387:A:H8	1.79	0.48
26:A:488:G:O2'	26:A:491:G:O6	2.32	0.48
30:E:112:LEU:HB3	30:E:118:LEU:HB2	1.96	0.48
26:A:2199:A:OP1	49:X:36:ARG:NH2	2.47	0.48
26:A:1673:G:N2	26:A:1675:C:O4'	2.47	0.48
26:A:1259:G:H2'	26:A:1260:A:H8	1.79	0.47
26:A:2759:G:H1'	32:G:34:ARG:HH22	1.79	0.47
26:A:2849:U:OP1	41:P:92:ARG:NH2	2.47	0.47
26:A:1070:A:OP2	26:A:1077:A:N6	2.40	0.47
26:A:1079:C:N3	33:I:131:THR:OG1	2.48	0.47
26:A:196:A:H61	26:A:831:G:H21	1.62	0.47
46:U:46:LYS:HD2	46:U:47:PRO:HD2	1.96	0.47
26:A:1323:C:N4	26:A:1324:G:O6	2.48	0.47
45:T:51:PHE:O	45:T:92:ASN:ND2	2.47	0.47
26:A:1312:U:O2'	26:A:1314:C:N4	2.46	0.47
26:A:1818:U:O2'	28:C:152:GLN:O	2.28	0.47
45:T:54:GLU:HG3	45:T:88:LYS:HE2	1.96	0.47
26:A:1915:3TD:H3'	26:A:1916:A:H8	1.80	0.47
26:A:32:C:N4	26:A:447:A:OP2	2.47	0.47
41:P:1:SER:OG	41:P:2:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:W:33:ILE:HG22	48:W:34:VAL:HG23	1.96	0.47
26:A:1796:U:H2'	26:A:1797:G:C8	2.50	0.47
26:A:1799:G:OP2	26:A:1819:A:N6	2.44	0.47
26:A:2052:A:O2'	29:D:149:ASN:O	2.31	0.47
26:A:2796:U:O2'	26:A:2798:U:OP2	2.33	0.47
26:A:577:G:H2'	26:A:578:G:C8	2.50	0.47
26:A:1715:G:O2'	26:A:1743:G:O6	2.28	0.47
26:A:1995:U:O2	36:K:32:TYR:OH	2.31	0.47
26:A:1057:A:H2	33:I:117:THR:HG21	1.79	0.47
35:J:8:PRO:HG3	35:J:48:VAL:HG23	1.96	0.47
26:A:1853:A:N3	26:A:2233:U:O2'	2.40	0.47
26:A:2032:G:O2'	29:D:150:GLN:NE2	2.48	0.47
28:C:184:GLU:HG3	28:C:186:ASP:H	1.80	0.47
29:D:4:LEU:HB2	29:D:32:ASN:ND2	2.30	0.47
30:E:112:LEU:O	30:E:118:LEU:N	2.44	0.47
45:T:11:LEU:O	50:Y:29:ARG:NH1	2.38	0.47
46:U:35:VAL:HB	46:U:38:ILE:HG13	1.97	0.47
26:A:818:G:H21	26:A:1189:A:H62	1.62	0.47
26:A:355:U:H2'	26:A:356:G:C8	2.50	0.47
26:A:776:G:N2	26:A:802:A:OP2	23.62	0.47
32:G:88:LEU:HA	32:G:161:VAL:HA	1.96	0.47
26:A:405:U:H3'	29:D:4:LEU:HD21	167.58	0.47
26:A:927:A:H2'	26:A:928:A:C8	2.49	0.47
28:C:179:GLU:HG3	28:C:269:ARG:HA	1.97	0.47
53:1:10:LEU:HG	53:1:48:TYR:HB3	1.97	0.46
26:A:2899:A:H2'	26:A:2900:A:C8	2.50	0.46
26:A:1715:G:H1'	26:A:1716:U:H5	1.81	0.46
26:A:1266:G:O2'	26:A:2012:G:O6	2.32	0.46
26:A:572:A:OP2	43:R:80:ARG:NH1	2.46	0.46
30:E:118:LEU:HD11	30:E:188:MET:HG2	1.97	0.46
43:R:38:VAL:HG13	43:R:54:VAL:HG12	1.97	0.46
26:A:558:U:H2'	26:A:559:G:C8	2.51	0.46
26:A:861:A:N3	27:B:79:G:O2'	2.43	0.46
31:F:16:MET:HE2	31:F:27:VAL:HG13	1.97	0.46
36:K:68:GLY:HA2	36:K:77:ILE:O	2.15	0.46
51:Z:17:PRO:HA	51:Z:20:LYS:HG2	1.96	0.46
26:A:488:G:N1	26:A:491:G:OP2	2.48	0.46
26:A:570:G:O3'	26:A:819:A:O2'	21.16	0.46
26:A:2246:G:H2'	26:A:2247:A:H8	1.81	0.46
26:A:2500:U:O2'	26:A:2504:PSU:OP1	2.33	0.46
26:A:1227:G:OP2	42:Q:15:LYS:NZ	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:265:A:N1	26:A:427:U:O2'	2.40	0.46
26:A:1469:A:H2'	26:A:1470:A:H8	1.80	0.46
26:A:629:G:N3	26:A:639:U:O2'	2.47	0.46
26:A:6:A:H2'	26:A:7:G:H8	1.81	0.46
28:C:169:ALA:O	28:C:185:ALA:N	2.46	0.46
34:H:99:ILE:HD11	34:H:144:VAL:HG21	1.97	0.46
26:A:2022:U:O2	26:A:2616:C:O2'	2.33	0.46
26:A:881:G:N2	26:A:896:A:N7	2.64	0.46
26:A:1615:C:OP2	26:A:1617:C:N4	2.37	0.46
26:A:581:C:H2'	26:A:582:A:C8	2.50	0.46
46:U:24:VAL:HA	46:U:35:VAL:HG22	1.97	0.46
46:U:95:PHE:HB2	46:U:99:SER:HA	1.98	0.46
26:A:1907:G:O6	26:A:1924:C:N4	2.49	0.45
36:K:1:MET:HA	36:K:32:TYR:HB3	1.98	0.45
26:A:1469:A:H2'	26:A:1470:A:C8	2.51	0.45
26:A:155:A:H2'	26:A:156:A:H8	1.81	0.45
26:A:177:G:OP2	26:A:177:G:N2	2.34	0.45
26:A:2229:U:H2'	26:A:2230:G:H8	1.81	0.45
26:A:2446:G:N7	26:A:2501:C:O2'	2.48	0.45
26:A:279:A:H62	26:A:361:G:N2	2.13	0.45
26:A:594:U:H2'	26:A:595:C:C6	2.51	0.45
26:A:200:U:H5'	49:X:22:ASN:HD22	1.81	0.45
26:A:993:G:H1'	43:R:91:GLN:HE21	1.81	0.45
29:D:49:GLN:HB3	29:D:81:GLU:HB3	1.99	0.45
43:R:60:LYS:HB2	43:R:99:THR:O	2.16	0.45
26:A:850:U:H5''	51:Z:18:LYS:HG3	1.99	0.45
26:A:819:A:OP2	26:A:1187:G:N2	2.42	0.45
26:A:832:U:H2'	26:A:833:A:C8	2.52	0.45
33:I:38:CYS:SG	33:I:39:LYS:N	2.89	0.45
38:M:17:ASN:ND2	38:M:96:ILE:O	2.44	0.45
51:Z:39:ASP:OD2	51:Z:44:ARG:NH1	2.49	0.45
36:K:24:VAL:HA	36:K:39:ILE:HG22	1.99	0.45
37:L:63:LYS:HA	55:3:12:ARG:HG2	1.97	0.45
26:A:1068:G:HO2'	26:A:1070:A:H62	1.59	0.45
26:A:1047:G:N2	26:A:1110:G:O2'	2.48	0.45
26:A:1316:U:H2'	26:A:1317:G:C8	2.52	0.45
26:A:1506:U:H2'	26:A:1507:C:C6	2.52	0.45
26:A:1264:A:N6	26:A:2014:A:OP2	2.46	0.45
26:A:2519:U:O4'	26:A:2542:A:N6	2.50	0.45
26:A:546:U:H1'	26:A:548:G:C6	2.51	0.45
31:F:57:ALA:HB2	31:F:64:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:971:G:OP1	26:A:989:G:N1	2.43	0.45
27:B:43:C:OP1	57:6:2:LYS:N	2.44	0.45
36:K:64:ARG:HB2	36:K:83:ALA:HB3	1.99	0.45
38:M:42:THR:HA	38:M:93:VAL:HA	1.99	0.45
26:A:1769:U:H2'	26:A:1770:G:H8	1.82	0.45
26:A:2250:G:H21	26:A:2497:A:P	2.40	0.45
31:F:64:PRO:HA	31:F:88:VAL:HG23	1.98	0.45
41:P:24:THR:HA	41:P:45:VAL:HA	1.99	0.45
26:A:2140:G:H2'	26:A:2141:G:C8	2.52	0.45
26:A:2375:G:N2	26:A:2378:A:OP2	2.45	0.45
45:T:92:ASN:OD1	45:T:93:LEU:N	2.49	0.45
26:A:1278:C:H2'	26:A:1279:G:H8	1.82	0.45
26:A:13:A:O2'	26:A:15:G:N7	2.46	0.45
26:A:1934:C:H2'	26:A:1935:G:C8	2.51	0.45
26:A:1935:G:N2	26:A:1964:G:O4'	2.49	0.45
39:N:49:GLU:HA	39:N:52:ILE:HG22	1.98	0.45
46:U:11:ILE:HG22	46:U:21:ARG:HB3	1.99	0.45
55:3:31:ILE:HG21	55:3:34:LYS:HD3	1.99	0.44
32:G:153:PRO:HB2	32:G:168:VAL:HG11	1.99	0.44
32:G:3:VAL:HG22	32:G:68:ARG:HH21	1.81	0.44
33:I:102:ARG:NH2	33:I:141:ASP:OD1	2.40	0.44
27:B:9:G:OP2	40:O:15:ARG:NH2	2.49	0.44
26:A:2595:G:N2	26:A:2598:A:OP2	2.45	0.44
29:D:121:THR:HG21	29:D:143:PRO:HB3	1.99	0.44
30:E:146:VAL:HG12	30:E:185:LYS:HB2	1.99	0.44
45:T:6:ARG:NH2	45:T:37:ASP:OD2	2.50	0.44
47:V:35:GLU:HB2	47:V:93:ARG:NH2	2.32	0.44
26:A:2291:U:H2'	26:A:2292:U:C6	2.53	0.44
26:A:2581:G:H22	26:A:2610:C:H2'	1.82	0.44
26:A:281:C:H2'	26:A:282:A:C8	2.53	0.44
26:A:833:A:H2'	26:A:834:G:C8	2.53	0.44
46:U:82:VAL:O	46:U:96:LYS:NZ	2.50	0.44
26:A:1395:A:O2'	26:A:1397:U:OP2	2.35	0.44
26:A:1432:G:H2'	26:A:1433:A:C8	2.51	0.44
26:A:1704:C:H2'	26:A:1705:A:H8	1.82	0.44
26:A:345:A:O2'	26:A:347:A:N6	2.42	0.44
26:A:833:A:H2'	26:A:834:G:H8	1.82	0.44
26:A:848:C:H2'	26:A:849:A:H8	1.82	0.44
38:M:29:GLY:H	38:M:104:GLU:HG3	1.82	0.44
26:A:1023:U:OP2	26:A:1025:G:O2'	2.36	0.44
26:A:1167:C:H2'	26:A:1168:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1434:A:H2'	26:A:1435:G:C8	2.52	0.44
26:A:1563:U:H2'	26:A:1564:C:C6	2.52	0.44
29:D:179:ARG:HB3	29:D:188:LEU:HB2	2.00	0.44
36:K:43:ILE:HD11	36:K:54:LYS:HA	1.99	0.44
26:A:516:C:O2'	26:A:1261:C:O2'	2.31	0.44
26:A:2057:G:H2'	26:A:2058:A:H8	1.81	0.44
26:A:2443:C:H2'	26:A:2444:G:H8	1.83	0.44
26:A:834:G:O2'	26:A:2358:A:O2'	2.23	0.44
26:A:918:A:N3	27:B:80:U:O2'	2.46	0.44
26:A:2303:G:O2'	31:F:128:SER:OG	2.23	0.44
35:J:37:ARG:HD3	35:J:39:LYS:HD2	1.98	0.44
50:Y:8:GLU:OE1	50:Y:12:GLU:HB2	2.18	0.44
28:C:268:ARG:NH2	28:C:271:SER:OG	2.50	0.44
28:C:76:VAL:HG12	28:C:114:GLN:HG3	1.99	0.44
32:G:89:VAL:HG21	32:G:162:ARG:NH1	2.33	0.44
39:N:79:LEU:HA	39:N:83:LEU:HB2	1.99	0.44
27:B:12:C:O2'	48:W:70:PRO:O	2.34	0.44
26:A:1571:A:H2'	26:A:1572:A:C8	2.53	0.44
26:A:514:A:N3	26:A:581:C:O2'	2.49	0.44
26:A:151:C:H2'	26:A:152:A:H8	1.82	0.44
26:A:745:1MG:HM11	26:A:745:1MG:HN21	1.70	0.44
33:I:100:ILE:HG22	33:I:101:SER:H	1.82	0.44
36:K:113:MET:HA	36:K:116:ILE:HG22	2.00	0.44
54:2:25:LYS:O	54:2:28:ARG:N	2.50	0.43
26:A:1311:G:H21	26:A:1603:A:N6	2.13	0.43
26:A:926:G:H2'	26:A:927:A:C8	2.53	0.43
34:H:58:LEU:HA	34:H:61:VAL:HG22	1.99	0.43
26:A:1167:C:H2'	26:A:1168:G:H8	1.83	0.43
26:A:1802:A:H2'	26:A:1803:A:H8	1.83	0.43
28:C:24:HIS:CG	28:C:79:ARG:HD2	2.52	0.43
31:F:115:GLY:HA3	31:F:177:ARG:HA	2.00	0.43
26:A:1654:A:OP2	39:N:1:MET:N	2.40	0.43
26:A:1667:G:O2'	26:A:1991:U:O4	2.34	0.43
26:A:2176:A:O2'	26:A:2177:C:O5'	2.30	0.43
26:A:1638:C:O2	26:A:2698:U:O2'	2.35	0.43
26:A:280:U:H2'	26:A:281:C:C6	2.54	0.43
26:A:2850:A:N7	26:A:2868:A:O2'	2.39	0.43
26:A:2885:G:N7	52:O:39:ARG:NH1	2.65	0.43
26:A:1013:C:H2'	26:A:1014:A:H8	1.82	0.43
26:A:1114:C:H2'	26:A:1115:G:C8	2.52	0.43
26:A:1229:C:H2'	26:A:1230:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:119:ILE:O	30:E:187:VAL:HA	2.18	0.43
26:A:2249:U:O2'	26:A:2252:G:OP2	2.37	0.43
26:A:372:G:H1'	26:A:373:U:H5	1.84	0.43
41:P:30:TRP:HE3	41:P:37:LYS:HG2	1.83	0.43
26:A:1538:G:H2'	26:A:1539:U:C6	2.53	0.43
26:A:1652:A:H62	39:N:11:ASN:HD21	1.66	0.43
26:A:1716:U:H2'	26:A:1717:A:H8	1.83	0.43
26:A:2485:G:OP1	38:M:45:GLN:NE2	2.51	0.43
26:A:476:G:O2'	26:A:502:A:N6	2.38	0.43
27:B:80:U:H2'	27:B:81:G:H8	1.83	0.43
35:J:64:VAL:HB	35:J:68:LYS:HD2	2.00	0.43
42:Q:59:LEU:HD11	42:Q:63:ARG:HH21	1.84	0.43
56:4:14:CYS:SG	56:4:27:CYS:HB2	2.59	0.43
26:A:1028:A:H2'	26:A:1029:A:C8	2.54	0.43
26:A:1149:G:H2'	26:A:1150:C:C6	2.54	0.43
26:A:149:A:N1	26:A:172:A:N6	15.47	0.43
26:A:2183:A:H2'	26:A:2184:A:H8	1.82	0.43
26:A:2818:U:H2'	26:A:2819:G:C8	2.54	0.43
26:A:721:A:H2'	26:A:722:A:C8	2.54	0.43
26:A:1322:A:H2	26:A:1333:G:HO2'	1.65	0.43
26:A:742:A:H2'	26:A:743:A:C8	2.54	0.43
26:A:796:C:H2'	26:A:797:G:H8	1.84	0.43
26:A:96:C:OP1	50:Y:39:GLN:NE2	2.52	0.43
29:D:109:VAL:HG22	29:D:175:LEU:HD21	2.00	0.43
26:A:2529:G:H4'	32:G:174:LYS:HD3	2.01	0.43
34:H:55:GLU:HA	34:H:58:LEU:HG	2.00	0.43
37:L:70:LYS:HG3	37:L:73:ILE:HD11	2.00	0.43
27:B:52:A:H2'	40:O:33:ARG:HH22	1.82	0.43
56:4:3:VAL:HG12	56:4:36:ARG:HD3	2.01	0.43
26:A:1103:A:OP2	26:A:1104:C:N4	2.44	0.43
26:A:1727:C:H2'	26:A:1728:C:C6	2.54	0.43
26:A:2070:A:H2'	26:A:2071:A:H8	1.84	0.43
26:A:227:A:O2'	26:A:2407:A:O2'	2.30	0.43
26:A:892:A:H2'	26:A:893:C:H6	1.84	0.43
26:A:1081:U:H5'	33:I:126:ARG:HE	1.84	0.43
26:A:1278:C:H2'	26:A:1279:G:C8	2.53	0.43
26:A:558:U:H2'	26:A:559:G:H8	1.83	0.43
34:H:23:ALA:HB1	34:H:27:ARG:HH21	1.83	0.43
44:S:72:THR:OG1	44:S:73:LYS:N	2.51	0.43
26:A:1934:C:H2'	26:A:1935:G:H8	1.84	0.42
30:E:153:LEU:HD12	30:E:158:PHE:HE2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:T:40:LYS:HB2	45:T:58:VAL:HG23	2.01	0.42
47:V:30:ILE:HG13	47:V:40:ILE:HG13	2.00	0.42
47:V:6:ALA:HB3	47:V:65:VAL:HG22	2.01	0.42
26:A:1486:U:H2'	26:A:1487:U:C6	2.54	0.42
26:A:2246:G:H2'	26:A:2247:A:C8	2.54	0.42
26:A:680:C:H2'	26:A:681:G:C8	2.54	0.42
27:B:65:U:O4	27:B:108:A:O2'	2.31	0.42
26:A:2393:U:O2'	37:L:59:ARG:O	2.33	0.42
51:Z:31:ILE:HG21	51:Z:31:ILE:HD13	1.91	0.42
52:O:27:LEU:HD12	52:O:36:LYS:HE3	2.01	0.42
26:A:1681:G:OP2	26:A:1757:A:N6	2.52	0.42
26:A:568:U:H1'	26:A:2030:6MZ:H9C1	2.01	0.42
26:A:706:A:OP1	28:C:6:LYS:NZ	2.52	0.42
41:P:88:ARG:NH1	41:P:114:ASN:OD1	2.52	0.42
26:A:1798:U:OP2	28:C:269:ARG:NH2	2.53	0.42
26:A:6:A:H2'	26:A:7:G:C8	2.54	0.42
29:D:177:VAL:HG22	29:D:189:VAL:HG12	2.01	0.42
37:L:85:VAL:HG11	37:L:90:VAL:HG12	2.01	0.42
39:N:103:ARG:HG2	39:N:105:GLY:H	1.85	0.42
41:P:29:VAL:HG12	41:P:80:VAL:HG22	2.00	0.42
26:A:1409:U:H2'	26:A:1410:G:H8	1.84	0.42
26:A:2141:G:H2'	26:A:2142:A:C8	2.55	0.42
28:C:146:LYS:HB3	28:C:149:LYS:HE2	2.02	0.42
32:G:83:THR:HA	32:G:132:LEU:O	2.20	0.42
26:A:2684:U:O2'	36:K:78:ARG:NH2	2.52	0.42
36:K:90:ASN:OD1	36:K:91:SER:N	2.50	0.42
41:P:47:ILE:HG22	41:P:99:LEU:HD21	2.01	0.42
26:A:1273:U:O2'	26:A:1275:A:OP1	2.37	0.42
26:A:2109:U:H3	26:A:2180:U:H3	1.68	0.42
26:A:680:C:H2'	26:A:681:G:H8	1.84	0.42
27:B:93:C:H2'	27:B:94:A:H8	1.85	0.42
33:I:102:ARG:O	33:I:106:GLN:HB3	2.20	0.42
37:L:77:ILE:HG13	37:L:78:ARG:H	1.85	0.42
26:A:1664:A:H61	26:A:1996:C:N4	2.17	0.42
26:A:2135:A:H61	26:A:2156:G:H2'	1.85	0.42
26:A:784:G:N2	26:A:792:A:O4'	2.53	0.42
27:B:111:U:H2'	27:B:112:G:H8	1.85	0.42
32:G:37:ASN:OD1	32:G:38:ASP:N	2.53	0.42
45:T:56:GLU:HB2	45:T:86:THR:HG23	2.01	0.42
26:A:2037:A:H2'	26:A:2038:G:C8	2.55	0.42
26:A:2698:U:H2'	26:A:2699:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:9:VAL:O	29:D:26:VAL:HB	2.20	0.42
26:A:1614:A:H61	44:S:88:ARG:H	1.67	0.42
26:A:1252:G:OP2	42:Q:13:HIS:NE2	2.50	0.42
26:A:2107:G:H2'	26:A:2108:A:C4	2.55	0.42
26:A:2567:G:H2'	26:A:2568:U:C6	2.55	0.42
26:A:2899:A:H2'	26:A:2900:A:H8	1.84	0.42
26:A:479:A:N3	26:A:481:G:H5''	2.35	0.42
26:A:657:U:H2'	26:A:658:U:C6	2.54	0.42
26:A:793:A:OP2	26:A:2071:A:O2'	2.29	0.42
27:B:49:C:H2'	27:B:50:A:C8	2.54	0.42
31:F:125:GLY:O	31:F:157:THR:OG1	2.37	0.42
37:L:19:LEU:HD23	37:L:27:LEU:HD13	2.02	0.42
46:U:32:LYS:HE3	46:U:63:ALA:HB3	2.02	0.42
57:6:11:GLU:OE1	57:6:25:ARG:NH1	2.46	0.42
26:A:1485:U:H5'	26:A:1961:C:H5''	99.22	0.42
26:A:1754:A:O3'	41:P:102:ARG:NH2	2.51	0.42
26:A:406:G:H5'	29:D:4:LEU:HG	164.06	0.42
30:E:128:ALA:HB3	30:E:133:LEU:HD21	2.02	0.42
32:G:36:LEU:HD21	32:G:70:LEU:HD11	2.02	0.42
34:H:70:GLU:HB2	34:H:134:VAL:HG11	2.01	0.42
43:R:4:VAL:HG23	43:R:39:LEU:HB2	2.01	0.42
26:A:1353:A:H2'	26:A:1354:A:H8	1.84	0.41
26:A:1386:C:H2'	26:A:1387:A:C8	2.55	0.41
26:A:1737:G:O2'	26:A:1738:G:N3	2.53	0.41
26:A:2183:A:H2'	26:A:2184:A:C8	2.55	0.41
26:A:2514:U:H2'	26:A:2515:C:C6	2.55	0.41
26:A:596:U:H2'	26:A:597:G:H8	1.84	0.41
28:C:36:ASN:HB2	28:C:61:TYR:HB2	2.02	0.41
32:G:4:ALA:HB2	32:G:65:GLY:HA2	2.02	0.41
39:N:79:LEU:O	39:N:84:GLY:N	2.49	0.41
26:A:1503:A:H2'	26:A:1504:A:H8	1.85	0.41
26:A:20:C:H2'	26:A:21:A:H8	1.85	0.41
26:A:576:U:H2'	26:A:577:G:C8	2.54	0.41
34:H:5:LEU:HB2	34:H:16:GLY:H	1.85	0.41
37:L:80:SER:OG	37:L:115:GLU:OE2	2.38	0.41
39:N:56:LYS:NZ	39:N:90:ARG:O	2.51	0.41
46:U:52:ASN:OD1	46:U:53:GLN:N	2.52	0.41
26:A:466:A:OP1	54:2:34:ARG:NH1	2.54	0.41
26:A:1039:A:H61	26:A:1116:G:H1	1.68	0.41
26:A:1190:G:OP1	37:L:30:THR:OG1	2.28	0.41
26:A:1693:U:O4	26:A:1976:U:O2'	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:298:G:O2'	26:A:322:A:N1	2.38	0.41
32:G:51:PHE:HE2	32:G:68:ARG:HA	1.85	0.41
33:I:9:LYS:HB3	33:I:55:PRO:HB2	2.03	0.41
51:Z:16:LEU:HB3	51:Z:19:HIS:ND1	2.35	0.41
26:A:1028:A:OP2	26:A:1126:A:N6	2.36	0.41
26:A:1197:G:N2	26:A:1249:U:O2'	2.54	0.41
33:I:82:ALA:HB1	33:I:108:ILE:HD13	2.02	0.41
33:I:2:LYS:HE2	33:I:61:TYR:CD1	2.55	0.41
35:J:45:THR:HB	35:J:48:VAL:HG12	2.01	0.41
26:A:1250:G:P	37:L:21:ARG:HE	2.42	0.41
57:6:16:CYS:SG	57:6:18:CYS:HB2	2.60	0.41
26:A:1751:U:H2'	26:A:1752:C:C6	2.55	0.41
26:A:2047:C:H2'	26:A:2048:G:H8	1.85	0.41
26:A:2428:G:H21	37:L:60:ARG:HH22	1.69	0.41
39:N:59:SER:OG	39:N:62:ASN:OD1	2.27	0.41
57:6:41:HIS:HD2	57:6:43:PHE:HB2	1.85	0.41
26:A:1078:U:H5'	26:A:1079:C:H5''	2.02	0.41
26:A:2295:C:OP1	40:O:10:ARG:NH1	2.51	0.41
26:A:796:C:H2'	26:A:797:G:C8	2.55	0.41
47:V:35:GLU:HB2	47:V:93:ARG:HH22	1.86	0.41
26:A:1171:G:H2'	26:A:1172:C:O4'	2.20	0.41
26:A:154:U:H2'	26:A:155:A:C8	2.69	0.41
26:A:569:U:O2'	26:A:971:G:N2	2.48	0.41
26:A:882:G:H2'	26:A:883:G:C8	2.55	0.41
31:F:37:MET:HB2	31:F:86:CYS:SG	2.60	0.41
34:H:96:THR:O	34:H:99:ILE:HG22	2.21	0.41
42:Q:78:PHE:CE1	42:Q:109:VAL:HG22	2.55	0.41
26:A:1601:G:H5''	45:T:64:LYS:HZ3	1.85	0.41
26:A:1927:A:H2'	26:A:1928:A:C8	2.56	0.41
26:A:242:G:H1'	26:A:243:U:H5	1.85	0.41
26:A:2530:A:N7	32:G:171:LYS:NZ	2.51	0.41
26:A:935:C:H2'	26:A:936:A:H8	1.85	0.41
32:G:42:VAL:HG23	32:G:51:PHE:CE1	2.55	0.41
47:V:40:ILE:HG23	47:V:40:ILE:HD12	1.87	0.41
26:A:922:C:H1'	48:W:22:PHE:CD2	2.55	0.41
26:A:1244:A:O2'	30:E:29:HIS:NE2	2.42	0.41
26:A:679:C:H2'	26:A:680:C:C6	2.56	0.41
32:G:86:LEU:HG	32:G:163:TYR:HD1	1.85	0.41
46:U:7:ASP:HB2	46:U:23:LYS:HB2	2.02	0.41
26:A:213:A:H2'	26:A:214:G:C8	2.56	0.41
26:A:514:A:H2'	26:A:515:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:171:VAL:O	28:C:182:LYS:HA	2.20	0.41
57:6:14:ALA:HB1	57:6:34:LEU:HD11	2.03	0.41
26:A:1475:G:O2'	26:A:1514:G:O6	2.39	0.41
26:A:1808:A:O2'	26:A:1809:A:O4'	2.35	0.41
26:A:2012:G:N7	44:S:16:LYS:NZ	2.69	0.41
26:A:2591:C:H2'	26:A:2592:G:C8	2.55	0.41
26:A:1939:5MU:OP1	26:A:2604:PSU:O2'	2.39	0.41
26:A:285:G:C6	26:A:356:G:C6	3.08	0.41
26:A:589:U:H2'	26:A:590:A:H8	1.86	0.41
26:A:191:A:O2'	26:A:678:C:O2	2.36	0.41
27:B:57:A:H1'	31:F:26:GLN:HG3	2.03	0.41
48:W:42:HIS:CD2	48:W:73:ARG:HD3	2.56	0.41
26:A:48:G:O2'	26:A:118:A:N1	2.40	0.40
26:A:1274:A:OP1	26:A:1646:C:N4	2.45	0.40
26:A:2086:U:H2'	26:A:2087:G:C8	2.56	0.40
30:E:133:LEU:HA	30:E:136:GLN:HG2	2.02	0.40
31:F:12:VAL:HG12	31:F:27:VAL:HG21	2.02	0.40
41:P:19:PHE:HE2	41:P:46:VAL:HG11	1.87	0.40
57:6:7:PRO:HB2	57:6:27:THR:HG23	2.03	0.40
26:A:1265:A:H61	26:A:2013:A:H5''	1.87	0.40
26:A:1687:G:N1	26:A:1700:A:OP1	2.44	0.40
26:A:2229:U:H2'	26:A:2230:G:C8	2.57	0.40
26:A:924:G:H2'	26:A:925:A:C8	2.56	0.40
26:A:1972:G:OP2	28:C:237:ARG:NH1	2.54	0.40
29:D:110:THR:HB	29:D:202:ILE:HG13	2.04	0.40
35:J:91:GLU:HG3	35:J:95:ARG:HH22	1.86	0.40
38:M:57:VAL:HG12	38:M:112:LEU:HG	2.03	0.40
52:0:32:THR:OG1	52:0:33:SER:N	2.55	0.40
26:A:83:A:N6	26:A:101:A:O2'	2.49	0.40
26:A:1857:G:H22	26:A:1884:G:H2'	1.86	0.40
26:A:1899:A:H4'	26:A:1901:A:H5''	2.03	0.40
26:A:1997:C:H2'	26:A:1998:A:H8	1.86	0.40
26:A:2185:U:H2'	26:A:2186:G:C8	2.56	0.40
26:A:744:U:H2'	26:A:745:1MG:O4'	2.21	0.40
27:B:13:G:N2	27:B:16:G:N3	2.69	0.40
32:G:3:VAL:HG22	32:G:68:ARG:NH2	2.37	0.40
47:V:21:ARG:NH1	47:V:87:GLN:O	2.46	0.40
26:A:2041:U:H2'	26:A:2042:A:C8	2.56	0.40
26:A:2699:C:H2'	26:A:2700:A:C8	2.57	0.40
26:A:500:G:N1	26:A:503:A:OP2	2.50	0.40
26:A:697:G:H2'	26:A:698:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:49:C:H2'	27:B:50:A:H8	1.87	0.40
37:L:89:VAL:HG13	37:L:123:ARG:NH1	2.37	0.40
39:N:33:ILE:HB	39:N:114:GLU:HG3	2.03	0.40
26:A:1151:A:H4'	42:Q:80:ASN:ND2	2.37	0.40
46:U:70:ALA:HB3	46:U:79:ALA:HB1	2.03	0.40
48:W:19:VAL:HA	48:W:34:VAL:HG22	2.03	0.40
26:A:1123:C:H2'	26:A:1124:G:C8	2.56	0.40
26:A:2022:U:H3	52:O:5:ASN:ND2	2.20	0.40
26:A:2087:G:H2'	26:A:2088:A:H8	1.86	0.40
28:C:175:LEU:HD23	28:C:175:LEU:HA	1.84	0.40
37:L:123:ARG:NH2	37:L:143:GLU:OE2	2.55	0.40
40:O:31:THR:HG23	40:O:33:ARG:O	2.22	0.40
43:R:98:ILE:HD12	43:R:98:ILE:HA	1.92	0.40
47:V:77:VAL:HG23	47:V:89:ILE:HG22	2.02	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%)	188 (87%)	24 (11%)	4 (2%)	10	51
3	c	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	13	57
4	d	203/205 (99%)	190 (94%)	8 (4%)	5 (2%)	7	45
5	e	155/157 (99%)	142 (92%)	6 (4%)	7 (4%)	3	33
6	f	98/100 (98%)	81 (83%)	13 (13%)	4 (4%)	3	34
7	g	149/151 (99%)	139 (93%)	7 (5%)	3 (2%)	9	51
8	h	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	24	69
9	i	125/127 (98%)	108 (86%)	13 (10%)	4 (3%)	5	41
10	j	96/98 (98%)	83 (86%)	7 (7%)	6 (6%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	k	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	11	53
12	l	121/123 (98%)	110 (91%)	7 (6%)	4 (3%)	5	40
13	m	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	6	44
14	n	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
15	o	86/88 (98%)	76 (88%)	7 (8%)	3 (4%)	4	39
16	p	80/82 (98%)	72 (90%)	5 (6%)	3 (4%)	4	37
17	q	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	4	37
18	r	63/65 (97%)	57 (90%)	3 (5%)	3 (5%)	3	31
19	s	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
20	t	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	61
21	u	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	3	31
25	z	613/614 (100%)	587 (96%)	20 (3%)	6 (1%)	19	64
28	C	269/271 (99%)	254 (94%)	13 (5%)	2 (1%)	26	71
29	D	207/209 (99%)	197 (95%)	8 (4%)	2 (1%)	19	64
30	E	199/201 (99%)	189 (95%)	8 (4%)	2 (1%)	19	64
31	F	175/177 (99%)	163 (93%)	9 (5%)	3 (2%)	11	54
32	G	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	6	43
33	I	139/141 (99%)	121 (87%)	14 (10%)	4 (3%)	6	43
34	H	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	5	40
35	J	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	26	71
36	K	120/122 (98%)	116 (97%)	2 (2%)	2 (2%)	11	54
37	L	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	14	57
38	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	13	57
39	N	118/120 (98%)	108 (92%)	9 (8%)	1 (1%)	24	69
40	O	114/116 (98%)	103 (90%)	10 (9%)	1 (1%)	21	66
41	P	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
42	Q	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
43	R	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	9	51
44	S	108/110 (98%)	102 (94%)	4 (4%)	2 (2%)	10	51
45	T	91/93 (98%)	79 (87%)	11 (12%)	1 (1%)	17	63
46	U	100/102 (98%)	89 (89%)	5 (5%)	6 (6%)	2	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
48	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
49	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
50	Y	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	12	55
51	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
52	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	10	51
53	1	48/50 (96%)	46 (96%)	1 (2%)	1 (2%)	9	50
54	2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	8	48
55	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	12	55
56	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
57	6	64/66 (97%)	57 (89%)	5 (8%)	2 (3%)	5	41
All	All	6330/6431 (98%)	5844 (92%)	368 (6%)	118 (2%)	14	51

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
2	b	151	LYS
5	e	89	THR
6	f	94	HIS
9	i	57	VAL
9	i	125	GLN
10	j	34	ALA
10	j	57	VAL
10	j	92	LEU
11	k	92	ARG
12	l	101	LEU
13	m	4	ALA
13	m	6	ILE
15	o	46	LYS
15	o	87	ARG
16	p	44	SER
17	q	16	MET
17	q	49	ASN
25	z	191	VAL
25	z	301	GLU
25	z	328	ALA
28	C	121	ALA

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Mol	Chain	Res	Type
30	E	83	VAL
32	G	174	LYS
32	G	175	LYS
33	I	64	ARG
34	H	9	VAL
35	J	81	ILE
37	L	36	LYS
38	M	58	LYS
44	S	64	ALA
46	U	51	LEU
46	U	88	ASP
52	0	2	VAL
53	1	4	ILE
55	3	31	ILE
3	c	60	ALA
3	c	79	LYS
4	d	165	GLU
4	d	191	SER
5	e	77	ASN
5	e	93	VAL
8	h	44	PHE
9	i	107	ALA
10	j	42	LEU
11	k	91	GLY
12	l	25	ALA
18	r	11	ARG
18	r	18	GLN
21	u	25	ALA
25	z	487	PHE
32	G	108	PHE
33	I	24	GLY
34	H	3	VAL
34	H	41	LYS
36	K	35	VAL
39	N	117	ASP
43	R	52	PRO
43	R	53	PHE
46	U	6	ARG
46	U	18	LYS
57	6	40	CYS
57	6	43	PHE
4	d	47	LEU

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Mol	Chain	Res	Type
5	e	23	THR
6	f	99	ALA
7	g	129	ASN
9	i	12	LYS
15	o	2	LEU
16	p	43	ALA
21	u	24	LYS
21	u	34	ARG
28	C	204	LEU
29	D	140	HIS
29	D	149	ASN
32	G	118	ALA
33	I	69	VAL
34	H	15	LEU
37	L	29	LYS
2	b	17	HIS
3	c	156	LEU
5	e	122	VAL
7	g	57	GLU
10	j	58	ASN
12	l	2	THR
12	l	46	SER
17	q	72	TRP
20	t	26	MET
31	F	20	ASN
32	G	173	ALA
34	H	89	LYS
44	S	3	THR
45	T	88	LYS
54	2	40	ALA
2	b	120	SER
4	d	150	LYS
5	e	158	LYS
6	f	92	THR
7	g	56	SER
10	j	75	ASP
25	z	345	ARG
30	E	122	GLU
31	F	149	ARG
36	K	92	GLU
40	O	101	GLY
46	U	97	SER

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Mol	Chain	Res	Type
46	U	98	ASN
50	Y	24	GLU
4	d	4	LEU
13	m	11	HIS
38	M	69	PRO
5	e	24	VAL
16	p	49	GLY
18	r	17	VAL
25	z	600	GLY
31	F	135	ILE
6	f	19	PRO
33	I	12	VAL

5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	502/501 (100%)	502 (100%)	0	100	100
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%)	137 (100%)	0	100	100
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	5230/5252 (100%)	5229 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	23	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	138	GLN
5	e	121	ASN
9	i	4	GLN
9	i	109	GLN
9	i	125	GLN
14	n	42	ASN
15	o	36	ASN
15	o	45	HIS
17	q	44	HIS
18	r	51	GLN
19	s	51	HIS
19	s	56	HIS
25	z	47	GLN
25	z	292	HIS
25	z	388	GLN
25	z	483	HIS
25	z	529	GLN
28	C	85	ASN
28	C	89	ASN
28	C	250	GLN
29	D	150	GLN
30	E	90	GLN
31	F	26	GLN

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Mol	Chain	Res	Type
32	G	114	HIS
32	G	138	GLN
34	H	2	GLN
34	H	18	GLN
36	K	29	HIS
37	L	35	HIS
41	P	55	HIS
43	R	91	GLN
44	S	102	HIS
46	U	73	ASN
50	Y	58	ASN
52	0	5	ASN
56	4	33	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	197 (12%)	0
22	v	76/77 (98%)	10 (13%)	0
23	x	47/48 (97%)	29 (61%)	0
24	y	93/95 (97%)	23 (24%)	0
26	A	2898/2903 (99%)	414 (14%)	5 (0%)
27	B	119/120 (99%)	11 (9%)	0
58	w	2/3 (66%)	0	0
All	All	4770/4785 (99%)	684 (14%)	5 (0%)

All (684) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	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	50	A
1	a	51	A
1	a	86	G
1	a	94	G

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Mol	Chain	Res	Type
1	a	95	C
1	a	96	U
1	a	121	U
1	a	127	G
1	a	131	A
1	a	141	G
1	a	164	G
1	a	173	U
1	a	177	G
1	a	183	C
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	237	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	254	G
1	a	266	G
1	a	267	C
1	a	289	G
1	a	298	A
1	a	316	C
1	a	319	G
1	a	328	C
1	a	330	C
1	a	347	G
1	a	352	C
1	a	354	G
1	a	356	A
1	a	367	U
1	a	368	U
1	a	372	C
1	a	392	C
1	a	406	G
1	a	407	U
1	a	411	A
1	a	412	A
1	a	414	A

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Mol	Chain	Res	Type
1	a	420	U
1	a	426	U
1	a	429	U
1	a	430	A
1	a	436	C
1	a	438	U
1	a	439	U
1	a	467	U
1	a	481	G
1	a	482	A
1	a	491	G
1	a	497	G
1	a	499	A
1	a	509	A
1	a	511	C
1	a	512	U
1	a	517	G
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	546	A
1	a	547	A
1	a	551	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	633	G
1	a	642	A
1	a	653	U
1	a	661	G
1	a	665	A
1	a	686	U
1	a	723	U
1	a	724	G
1	a	733	G
1	a	748	G

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Mol	Chain	Res	Type
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	816	A
1	a	817	C
1	a	819	A
1	a	832	G
1	a	841	C
1	a	842	U
1	a	843	U
1	a	844	G
1	a	845	A
1	a	876	C
1	a	878	A
1	a	889	A
1	a	890	G
1	a	926	G
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	974	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	991	U
1	a	993	G
1	a	1004	A
1	a	1020	G
1	a	1032	G
1	a	1034	G
1	a	1043	G
1	a	1065	U
1	a	1085	U
1	a	1089	G
1	a	1094	G
1	a	1095	U
1	a	1101	A

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Mol	Chain	Res	Type
1	a	1105	A
1	a	1134	G
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1138	G
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	1196	A
1	a	1197	A
1	a	1213	A
1	a	1227	A
1	a	1238	A
1	a	1240	U
1	a	1241	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	1302	C
1	a	1305	G
1	a	1317	C
1	a	1320	C
1	a	1338	G
1	a	1345	U
1	a	1346	A
1	a	1363	A
1	a	1364	U
1	a	1394	A
1	a	1396	A
1	a	1397	C
1	a	1398	A
1	a	1406	U
1	a	1419	G

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Mol	Chain	Res	Type
1	a	1429	A
1	a	1441	A
1	a	1491	G
1	a	1492	A
1	a	1493	A
1	a	1497	G
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
1	a	1537	U
22	v	9	G
22	v	18	G
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	31	G
22	v	52	G
22	v	54	5MU
22	v	59	A
22	v	75	C
23	x	88	A
23	x	90	G
23	x	96	C
23	x	98	U
23	x	104	U
23	x	108	A
23	x	109	C
23	x	110	G
23	x	111	G
23	x	112	C
23	x	113	C
23	x	114	C
23	x	115	A
23	x	116	U
23	x	117	C

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Mol	Chain	Res	Type
23	x	118	G
23	x	119	G
23	x	120	U
23	x	121	U
23	x	123	C
23	x	125	G
23	x	126	G
23	x	127	U
23	x	128	C
23	x	129	U
23	x	130	G
23	x	131	C
23	x	133	C
23	x	134	C
24	y	8	G
24	y	15	C
24	y	18	G
24	y	20	G
24	y	29	G
24	y	31	A
24	y	40	C
24	y	45	U
24	y	46	G
24	y	47(F)	C
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	54	5MU
24	y	55	PSU
24	y	56	C
24	y	60	U
24	y	61	C
24	y	64	G
24	y	66	G
24	y	73	G
26	A	10	A
26	A	15	G
26	A	23	G
26	A	27	G
26	A	34	U

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Mol	Chain	Res	Type
26	A	60	G
26	A	63	A
26	A	71	A
26	A	74	A
26	A	75	G
26	A	91	A
26	A	101	A
26	A	102	U
26	A	118	A
26	A	120	U
26	A	125	A
26	A	131	A
26	A	138	U
26	A	139	U
26	A	142	A
26	A	181	A
26	A	196	A
26	A	199	A
26	A	204	A
26	A	205	G
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	277	G
26	A	278	A
26	A	279	A
26	A	285	G
26	A	311	A
26	A	322	A
26	A	329	G
26	A	330	A
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

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Mol	Chain	Res	Type
26	A	411	G
26	A	448	U
26	A	451	U
26	A	456	C
26	A	473	G
26	A	479	A
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	529	A
26	A	530	G
26	A	531	C
26	A	532	A
26	A	533	G
26	A	549	G
26	A	562	U
26	A	563	A
26	A	573	U
26	A	603	A
26	A	614	A
26	A	615	U
26	A	616	A
26	A	622	G
26	A	637	A
26	A	646	U
26	A	647	G
26	A	655	A
26	A	664	G
26	A	668	A
26	A	675	A
26	A	686	U
26	A	695	G
26	A	711	G
26	A	717	C
26	A	726	G
26	A	730	A
26	A	747	5MU

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Mol	Chain	Res	Type
26	A	748	G
26	A	765	C
26	A	775	G
26	A	782	A
26	A	784	G
26	A	789	A
26	A	805	G
26	A	812	C
26	A	819	A
26	A	827	U
26	A	830	G
26	A	846	U
26	A	859	G
26	A	869	G
26	A	885	C
26	A	887	U
26	A	888	C
26	A	889	C
26	A	890	C
26	A	910	A
26	A	932	U
26	A	941	A
26	A	946	C
26	A	959	A
26	A	961	C
26	A	965	C
26	A	973	A
26	A	974	G
26	A	983	A
26	A	990	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	1042	G
26	A	1043	C
26	A	1045	C
26	A	1046	A

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Mol	Chain	Res	Type
26	A	1047	G
26	A	1057	A
26	A	1058	U
26	A	1059	G
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	1071	G
26	A	1073	A
26	A	1076	C
26	A	1077	A
26	A	1078	U
26	A	1079	C
26	A	1084	A
26	A	1088	A
26	A	1092	C
26	A	1094	U
26	A	1100	C
26	A	1101	U
26	A	1110	G
26	A	1112	G
26	A	1119	U
26	A	1132	U
26	A	1133	A
26	A	1134	A
26	A	1135	C
26	A	1142	A
26	A	1143	A
26	A	1157	G
26	A	1171	G
26	A	1175	A
26	A	1178	C
26	A	1180	U
26	A	1206	G
26	A	1210	G
26	A	1211	C

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Mol	Chain	Res	Type
26	A	1236	G
26	A	1248	G
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	1311	G
26	A	1314	C
26	A	1325	U
26	A	1329	U
26	A	1345	C
26	A	1359	A
26	A	1365	A
26	A	1378	A
26	A	1379	U
26	A	1383	A
26	A	1392	A
26	A	1394	U
26	A	1395	A
26	A	1401	G
26	A	1403	A
26	A	1407	G
26	A	1416	G
26	A	1417	C
26	A	1420	A
26	A	1428	C
26	A	1437	C
26	A	1452	G
26	A	1455	G
26	A	1458	U
26	A	1460	U
26	A	1468	U
26	A	1482	G
26	A	1490	A
26	A	1493	C
26	A	1497	U
26	A	1509	A
26	A	1515	A

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Mol	Chain	Res	Type
26	A	1532	A
26	A	1534	U
26	A	1535	A
26	A	1536	C
26	A	1537	G
26	A	1566	A
26	A	1569	A
26	A	1578	U
26	A	1583	A
26	A	1608	A
26	A	1609	A
26	A	1619	G
26	A	1639	C
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	1808	A
26	A	1816	C
26	A	1829	A
26	A	1833	C
26	A	1847	A
26	A	1870	C
26	A	1871	A
26	A	1876	A
26	A	1906	G
26	A	1913	A
26	A	1927	A
26	A	1929	G

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Mol	Chain	Res	Type
26	A	1930	G
26	A	1937	A
26	A	1941	C
26	A	1955	U
26	A	1960	A
26	A	1962	5MC
26	A	1963	U
26	A	1964	G
26	A	1967	C
26	A	1971	U
26	A	1972	G
26	A	1991	U
26	A	1992	G
26	A	1993	U
26	A	1997	C
26	A	2002	G
26	A	2021	C
26	A	2022	U
26	A	2023	C
26	A	2031	A
26	A	2032	G
26	A	2043	C
26	A	2051	A
26	A	2052	A
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	2080	A
26	A	2100	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

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Mol	Chain	Res	Type
26	A	2120	G
26	A	2125	G
26	A	2127	G
26	A	2129	C
26	A	2131	U
26	A	2132	U
26	A	2133	G
26	A	2134	A
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	2168	G
26	A	2171	A
26	A	2172	U
26	A	2173	A
26	A	2177	C
26	A	2178	C
26	A	2179	C
26	A	2182	U
26	A	2198	A
26	A	2204	G
26	A	2210	U
26	A	2211	A
26	A	2212	A
26	A	2225	A
26	A	2238	G
26	A	2239	G
26	A	2250	G
26	A	2251	OMG
26	A	2268	A
26	A	2278	A
26	A	2283	C
26	A	2287	A
26	A	2305	U
26	A	2308	G
26	A	2310	C
26	A	2312	U
26	A	2319	G
26	A	2322	A

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Mol	Chain	Res	Type
26	A	2333	A
26	A	2334	U
26	A	2335	A
26	A	2336	A
26	A	2342	C
26	A	2347	C
26	A	2350	C
26	A	2354	C
26	A	2357	G
26	A	2383	G
26	A	2385	C
26	A	2402	U
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	2445	2MG
26	A	2447	G
26	A	2448	A
26	A	2470	G
26	A	2476	A
26	A	2478	A
26	A	2480	C
26	A	2484	G
26	A	2494	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	2525	G
26	A	2529	G
26	A	2547	A
26	A	2554	U
26	A	2567	G
26	A	2581	G
26	A	2582	G

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Mol	Chain	Res	Type
26	A	2585	U
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	2718	G
26	A	2726	A
26	A	2733	A
26	A	2744	G
26	A	2755	C
26	A	2758	A
26	A	2764	A
26	A	2765	A
26	A	2778	A
26	A	2791	G
26	A	2793	C
26	A	2797	U
26	A	2809	A
26	A	2818	U
26	A	2821	A
26	A	2833	U
26	A	2849	U
26	A	2872	A
26	A	2879	A
26	A	2884	U
27	B	24	G
27	B	26	C
27	B	35	C
27	B	38	C
27	B	42	C
27	B	45	A
27	B	57	A
27	B	87	U
27	B	90	C
27	B	108	A
27	B	109	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	818	G
26	A	960	A
26	A	1042	G
26	A	1358	G
26	A	1875	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	6MZ	A	1618	26	17,25,26	1.05	1 (5%)	15,36,39	2.63	2 (13%)
26	2MG	A	1835	26	18,26,27	1.20	2 (11%)	21,38,41	2.53	7 (33%)
26	PSU	A	1911	26	15,21,22	1.22	2 (13%)	16,30,33	2.03	3 (18%)
26	3TD	A	1915	26	15,22,23	3.21	6 (40%)	17,32,35	2.05	5 (29%)
26	PSU	A	1917	26	15,21,22	1.11	2 (13%)	16,30,33	2.39	4 (25%)
26	5MU	A	1939	26	13,22,23	0.61	0	16,32,35	2.47	2 (12%)
26	5MC	A	1962	26	14,22,23	1.20	1 (7%)	17,32,35	1.50	1 (5%)
26	6MZ	A	2030	26	17,25,26	1.09	1 (5%)	15,36,39	1.76	3 (20%)
26	G7M	A	2069	26	18,26,27	1.25	3 (16%)	21,39,42	2.63	9 (42%)
26	OMG	A	2251	26,22	18,26,27	1.22	2 (11%)	21,38,41	1.95	4 (19%)
26	2MG	A	2445	26	18,26,27	1.21	2 (11%)	21,38,41	2.25	5 (23%)
26	H2U	A	2449	26	17,21,22	1.17	3 (17%)	23,30,33	1.99	4 (17%)
26	PSU	A	2457	26	15,21,22	1.40	1 (6%)	16,30,33	2.19	4 (25%)
26	OMC	A	2498	26	15,22,23	0.59	0	20,31,34	1.36	2 (10%)
26	2MA	A	2503	26	17,25,26	1.75	3 (17%)	18,37,40	2.93	1 (5%)
26	PSU	A	2504	26	15,21,22	1.11	2 (13%)	16,30,33	2.27	4 (25%)
26	OMU	A	2552	26	14,22,23	0.67	0	19,31,34	1.78	1 (5%)
26	PSU	A	2580	26	15,21,22	1.40	1 (6%)	16,30,33	2.21	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PSU	A	2604	26	15,21,22	1.14	1 (6%)	16,30,33	2.12	3 (18%)
26	PSU	A	2605	26	15,21,22	1.40	2 (13%)	16,30,33	2.18	4 (25%)
26	1MG	A	745	26	17,26,27	1.58	3 (17%)	19,39,42	2.01	3 (15%)
26	PSU	A	746	26	15,21,22	1.62	1 (6%)	16,30,33	2.23	3 (18%)
26	5MU	A	747	26	13,22,23	0.57	0	16,32,35	2.75	2 (12%)
26	PSU	A	955	26	15,21,22	1.24	2 (13%)	16,30,33	2.29	4 (25%)
1	2MG	a	1207	1	18,26,27	1.17	2 (11%)	21,38,41	2.24	6 (28%)
1	4OC	a	1402	1	15,23,24	0.56	0	21,32,35	1.93	3 (14%)
1	5MC	a	1407	1	14,22,23	1.35	1 (7%)	17,32,35	0.85	1 (5%)
1	UR3	a	1498	1	13,22,23	0.70	0	18,32,35	0.91	1 (5%)
1	2MG	a	1516	1	18,26,27	1.24	2 (11%)	21,38,41	2.20	6 (28%)
1	MA6	a	1518	1	18,26,27	0.93	1 (5%)	15,38,41	2.58	3 (20%)
1	MA6	a	1519	1	18,26,27	0.99	1 (5%)	15,38,41	2.65	3 (20%)
1	PSU	a	516	1	15,21,22	1.11	1 (6%)	16,30,33	2.16	3 (18%)
1	G7M	a	527	1	18,26,27	1.25	2 (11%)	21,39,42	2.99	10 (47%)
1	2MG	a	966	1	18,26,27	1.15	2 (11%)	21,38,41	2.26	7 (33%)
1	5MC	a	967	1	14,22,23	1.36	1 (7%)	17,32,35	0.95	1 (5%)
22	H2U	v	20	22	17,21,22	1.05	2 (11%)	23,30,33	1.73	5 (21%)
22	5MU	v	54	22	13,22,23	0.61	0	16,32,35	2.72	2 (12%)
22	PSU	v	55	22	15,21,22	1.21	2 (13%)	16,30,33	2.26	4 (25%)
22	4SU	v	8	22	12,21,22	0.63	0	15,30,33	1.07	1 (6%)
24	H2U	y	19	24	17,21,22	1.29	3 (17%)	23,30,33	3.00	6 (26%)
24	6IA	y	37	24	20,29,30	0.92	1 (5%)	22,41,44	2.83	4 (18%)
24	5MU	y	54	24	13,22,23	0.60	0	16,32,35	2.66	3 (18%)
24	PSU	y	55	24	15,21,22	1.62	3 (20%)	16,30,33	2.16	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	-	1/7/25/26	0/2/2/2
26	PSU	A	1917	26	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	746	PSU	C5-C1'	-5.28	1.47	1.52
26	A	2457	PSU	C5-C1'	-4.34	1.48	1.52
26	A	2580	PSU	C5-C1'	-4.25	1.48	1.52
26	A	2605	PSU	C5-C1'	-4.25	1.48	1.52
24	y	55	PSU	C5-C1'	-3.64	1.49	1.52
26	A	1915	3TD	O4-C4	-3.53	1.15	1.24
26	A	955	PSU	C5-C1'	-3.36	1.49	1.52
24	y	19	H2U	C2-N3	-3.21	1.32	1.38
24	y	55	PSU	C2-N1	-3.20	1.31	1.38
26	A	1911	PSU	C5-C1'	-3.12	1.49	1.52
26	A	2604	PSU	C5-C1'	-3.02	1.49	1.52
22	v	55	PSU	C5-C1'	-2.96	1.49	1.52
26	A	2449	H2U	C2-N3	-2.81	1.32	1.38
26	A	2449	H2U	C4-N3	-2.74	1.33	1.37
26	A	2504	PSU	C5-C1'	-2.74	1.49	1.52
24	y	55	PSU	C6-C5	-2.61	1.34	1.38
1	a	516	PSU	C5-C1'	-2.61	1.50	1.52
1	a	527	G7M	O2'-C2'	-2.56	1.36	1.43
26	A	2069	G7M	O2'-C2'	-2.56	1.36	1.43
22	v	20	H2U	C2-N3	-2.53	1.33	1.38
22	v	20	H2U	C4-N3	-2.50	1.33	1.37
24	y	19	H2U	O4-C4	-2.46	1.18	1.23
24	y	19	H2U	C4-N3	-2.43	1.33	1.37
22	v	55	PSU	C2-N3	-2.39	1.33	1.38
26	A	1917	PSU	C5-C1'	-2.32	1.50	1.52
26	A	2449	H2U	C2-N1	-2.07	1.32	1.35
26	A	2605	PSU	C2-N3	-2.07	1.33	1.38
26	A	1911	PSU	O4'-C1'	-2.06	1.41	1.44
26	A	2504	PSU	C2-N3	-2.04	1.33	1.38
26	A	1917	PSU	C2-N1	-2.02	1.34	1.38
26	A	955	PSU	C2-N1	-2.01	1.34	1.38
26	A	1915	3TD	C5-C1'	2.07	1.54	1.52
26	A	2069	G7M	C8-N9	2.10	1.37	1.33
26	A	745	1MG	C6-N1	2.19	1.41	1.38
26	A	1835	2MG	C5-C4	3.00	1.47	1.40
26	A	2251	OMG	C5-C4	3.01	1.47	1.40
26	A	2445	2MG	C5-C4	3.09	1.47	1.40
1	a	1207	2MG	C5-C4	3.09	1.47	1.40
24	y	37	6IA	C5-C4	3.19	1.47	1.40
1	a	1516	2MG	C5-C4	3.20	1.47	1.40
1	a	1519	MA6	C5-C4	3.23	1.47	1.40
1	a	966	2MG	C5-C4	3.28	1.47	1.40
1	a	1518	MA6	C5-C4	3.28	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	966	2MG	C6-C5	3.29	1.48	1.41
26	A	2503	2MA	C6-N6	3.44	1.35	1.29
1	a	1207	2MG	C6-C5	3.56	1.48	1.41
26	A	2503	2MA	C5-C4	3.57	1.48	1.40
26	A	2069	G7M	C6-C5	3.60	1.48	1.41
26	A	2030	6MZ	C5-C4	3.64	1.48	1.40
26	A	745	1MG	C5-C4	3.64	1.48	1.40
26	A	2251	OMG	C6-C5	3.66	1.48	1.41
26	A	1618	6MZ	C5-C4	3.67	1.48	1.40
26	A	1962	5MC	C5-C4	3.72	1.47	1.41
1	a	1516	2MG	C6-C5	3.74	1.48	1.41
26	A	1835	2MG	C6-C5	3.74	1.48	1.41
26	A	2445	2MG	C6-C5	3.79	1.49	1.41
1	a	527	G7M	C6-C5	3.85	1.49	1.41
26	A	745	1MG	C6-C5	4.35	1.49	1.40
1	a	1407	5MC	C5-C4	4.64	1.48	1.41
26	A	1915	3TD	C4-N3	4.65	1.45	1.38
1	a	967	5MC	C5-C4	4.78	1.48	1.41
26	A	2503	2MA	C6-C5	4.92	1.49	1.40
26	A	1915	3TD	C2-N1	5.30	1.49	1.38
26	A	1915	3TD	C6-N1	5.57	1.46	1.34
26	A	1915	3TD	C6-C5	7.29	1.48	1.38

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	37	6IA	N3-C2-N1	-8.03	122.56	128.87
26	A	747	5MU	C5-C4-N3	-7.87	118.74	125.35
24	y	19	H2U	C4-N3-C2	-7.87	118.63	125.77
1	a	1519	MA6	N3-C2-N1	-7.76	122.78	128.87
1	a	1518	MA6	N3-C2-N1	-7.49	122.99	128.87
22	v	54	5MU	C5-C4-N3	-7.45	119.09	125.35
26	A	1939	5MU	C5-C4-N3	-7.11	119.38	125.35
24	y	54	5MU	C5-C4-N3	-6.64	119.78	125.35
24	y	19	H2U	C5-C6-N1	-6.52	103.61	110.76
26	A	1618	6MZ	N3-C2-N1	-6.49	123.78	128.87
26	A	745	1MG	C1'-N9-C4	-6.08	120.02	126.81
1	a	527	G7M	C5-C6-N1	-6.05	115.62	123.52
26	A	2449	H2U	C5-C6-N1	-5.98	104.21	110.76
26	A	2069	G7M	C5-C6-N1	-5.82	115.92	123.52
26	A	1915	3TD	C5-C1'-C2'	-5.39	106.29	115.44
22	v	20	H2U	C5-C6-N1	-5.19	105.07	110.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	55	PSU	C5-C1'-C2'	-4.92	107.09	115.44
26	A	2449	H2U	C4-N3-C2	-4.89	121.33	125.77
26	A	745	1MG	C6-C5-C4	-4.88	116.44	119.93
26	A	1835	2MG	CM2-N2-C2	-4.72	117.73	123.03
24	y	19	H2U	O4-C4-C5	-4.64	112.36	122.29
26	A	2030	6MZ	N3-C2-N1	-4.46	125.37	128.87
26	A	2251	OMG	C5-C6-N1	-4.42	117.74	123.52
26	A	2445	2MG	CM2-N2-C2	-4.29	118.21	123.03
1	a	966	2MG	C5-C6-N1	-4.28	117.93	123.52
1	a	1516	2MG	C5-C6-N1	-4.23	117.99	123.52
26	A	746	PSU	C5-C6-N1	-4.15	118.59	124.38
1	a	1207	2MG	C5-C6-N1	-4.12	118.14	123.52
26	A	2445	2MG	C5-C6-N1	-4.12	118.14	123.52
26	A	955	PSU	C5-C1'-C2'	-4.11	108.45	115.44
26	A	2457	PSU	C5-C6-N1	-4.04	118.75	124.38
26	A	2605	PSU	C5-C6-N1	-4.02	118.77	124.38
1	a	1402	4OC	CM4-N4-C4	-3.82	119.65	122.87
26	A	2504	PSU	C5-C1'-C2'	-3.78	109.01	115.44
26	A	746	PSU	C5-C1'-C2'	-3.77	109.03	115.44
26	A	1911	PSU	C5-C6-N1	-3.63	119.31	124.38
26	A	2580	PSU	C5-C6-N1	-3.60	119.36	124.38
26	A	2604	PSU	C5-C6-N1	-3.57	119.41	124.38
26	A	1835	2MG	C5-C6-N1	-3.56	118.87	123.52
22	v	20	H2U	C4-N3-C2	-3.56	122.54	125.77
26	A	2504	PSU	C5-C6-N1	-3.48	119.53	124.38
22	v	55	PSU	C5-C6-N1	-3.41	119.62	124.38
1	a	1519	MA6	C10-N6-C9	-3.35	105.01	115.96
26	A	2605	PSU	C5-C1'-C2'	-3.35	109.75	115.44
26	A	1915	3TD	C5-C6-N1	-3.33	119.74	124.38
26	A	2251	OMG	N3-C2-N1	-3.32	123.04	127.56
1	a	516	PSU	C5-C6-N1	-3.29	119.79	124.38
26	A	2251	OMG	C6-C5-C4	-3.27	117.12	120.86
22	v	8	4SU	C5-C4-N3	-3.27	120.10	123.56
1	a	1516	2MG	C6-C5-C4	-3.18	117.22	120.86
26	A	1835	2MG	C6-C5-C4	-3.15	117.26	120.86
22	v	55	PSU	C5-C1'-C2'	-3.09	110.19	115.44
26	A	955	PSU	C5-C6-N1	-3.04	120.14	124.38
1	a	1207	2MG	C6-C5-C4	-3.00	117.43	120.86
1	a	1207	2MG	CM2-N2-C2	-2.85	119.83	123.03
1	a	527	G7M	C4'-O4'-C1'	-2.81	106.67	109.64
1	a	1516	2MG	CM2-N2-C2	-2.69	120.01	123.03
26	A	2069	G7M	C4'-O4'-C1'	-2.65	106.84	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2445	2MG	C6-C5-C4	-2.62	117.86	120.86
1	a	527	G7M	N3-C2-N1	-2.54	124.10	127.56
1	a	966	2MG	C6-C5-C4	-2.50	118.00	120.86
26	A	1917	PSU	C5-C6-N1	-2.50	120.89	124.38
26	A	1835	2MG	N3-C2-N1	-2.46	122.51	126.19
24	y	37	6IA	C12-N6-C6	-2.35	120.74	123.46
26	A	2069	G7M	N3-C2-N1	-2.33	124.38	127.56
26	A	2498	OMC	CM2-O2'-C2'	-2.28	108.18	114.58
1	a	1518	MA6	C10-N6-C9	-2.25	108.61	115.96
24	y	55	PSU	O2'-C2'-C1'	-2.24	107.05	111.93
1	a	1207	2MG	N3-C2-N1	-2.23	122.85	126.19
1	a	1516	2MG	N3-C2-N1	-2.11	123.03	126.19
26	A	2449	H2U	O2-C2-N1	-2.10	120.43	123.17
1	a	966	2MG	N3-C2-N1	-2.09	123.06	126.19
26	A	2457	PSU	C5-C1'-C2'	-2.05	111.95	115.44
26	A	745	1MG	O2'-C2'-C1'	-2.02	105.30	111.61
1	a	1407	5MC	N4-C4-N3	2.05	119.92	116.92
24	y	19	H2U	O4-C4-N3	2.07	123.70	120.46
1	a	967	5MC	N4-C4-N3	2.08	119.97	116.92
22	v	20	H2U	N3-C2-N1	2.13	118.61	116.64
26	A	1915	3TD	C4-C5-C1'	2.14	124.86	121.24
1	a	527	G7M	O4'-C4'-C5'	2.16	117.01	109.29
1	a	1498	UR3	C3U-N3-C4	2.16	121.24	118.21
22	v	20	H2U	C6-N1-C2	2.18	125.53	122.16
26	A	1917	PSU	O4'-C1'-C2'	2.20	107.07	104.69
22	v	20	H2U	C5-C4-N3	2.25	119.00	116.62
26	A	2069	G7M	C5'-C4'-C3'	2.29	124.07	115.20
26	A	955	PSU	O4'-C1'-C2'	2.31	107.19	104.69
24	y	54	5MU	C5M-C5-C6	2.34	123.36	118.63
26	A	2504	PSU	O4'-C1'-C2'	2.34	107.22	104.69
26	A	2604	PSU	O4'-C1'-C2'	2.39	107.27	104.69
26	A	1911	PSU	O4'-C1'-C2'	2.49	107.39	104.69
1	a	527	G7M	C5'-C4'-C3'	2.54	125.03	115.20
24	y	37	6IA	C13-C12-N6	2.57	117.06	112.25
26	A	1915	3TD	O4'-C1'-C2'	2.69	107.60	104.69
26	A	2605	PSU	O4'-C1'-C2'	2.73	107.65	104.69
26	A	2069	G7M	O3'-C3'-C2'	2.74	120.71	111.86
22	v	55	PSU	O4'-C1'-C2'	2.84	107.76	104.69
26	A	1835	2MG	N2-C2-N1	3.00	120.42	116.94
1	a	516	PSU	O4'-C1'-C2'	3.02	107.95	104.69
26	A	2457	PSU	O4'-C1'-C2'	3.03	107.97	104.69
26	A	1917	PSU	C4-C5-C1'	3.03	126.32	121.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	C1'-N9-C4	3.07	130.23	126.81
1	a	966	2MG	N2-C2-N3	3.07	120.51	116.94
1	a	527	G7M	O3'-C3'-C4'	3.18	120.50	111.01
24	y	55	PSU	O4'-C1'-C2'	3.18	108.13	104.69
26	A	2580	PSU	O4'-C1'-C2'	3.21	108.16	104.69
26	A	2030	6MZ	C2-N1-C6	3.22	118.79	116.47
1	a	527	G7M	O3'-C3'-C2'	3.25	122.37	111.86
26	A	2069	G7M	C1'-N9-C4	3.47	130.68	126.81
24	y	19	H2U	C6-N1-C2	3.56	127.66	122.16
26	A	2030	6MZ	C1'-N9-C4	3.61	130.84	126.81
26	A	1915	3TD	C5-C4-N3	3.77	121.72	118.65
26	A	2069	G7M	O3'-C3'-C4'	3.80	122.36	111.01
26	A	2069	G7M	N7-C8-N9	3.85	114.36	108.67
1	a	1402	4OC	C2-N3-C4	3.86	120.34	115.43
26	A	2449	H2U	C6-N1-C2	3.88	128.15	122.16
26	A	1835	2MG	C6-N1-C2	4.28	121.37	115.24
26	A	2445	2MG	C6-N1-C2	4.38	121.52	115.24
1	a	527	G7M	N7-C8-N9	4.51	115.33	108.67
26	A	2498	OMC	C6-C5-C4	4.71	119.28	117.44
1	a	1207	2MG	C6-N1-C2	4.80	122.11	115.24
26	A	1962	5MC	N4-C4-N3	4.80	123.95	116.92
1	a	1516	2MG	C6-N1-C2	4.91	122.27	115.24
1	a	1518	MA6	C2-N1-C6	4.92	123.25	111.64
1	a	966	2MG	C6-N1-C2	5.03	122.44	115.24
1	a	1519	MA6	C2-N1-C6	5.08	123.62	111.64
24	y	55	PSU	C4-N3-C2	5.34	119.61	115.16
1	a	1516	2MG	C2-N3-C4	5.43	120.95	114.99
26	A	2251	OMG	C6-N1-C2	5.44	122.25	115.88
1	a	966	2MG	C2-N3-C4	5.45	120.97	114.99
26	A	2069	G7M	C6-N1-C2	5.72	122.58	115.88
1	a	527	G7M	C6-N1-C2	5.82	122.70	115.88
26	A	2445	2MG	C2-N3-C4	5.90	121.46	114.99
1	a	1207	2MG	C2-N3-C4	5.92	121.49	114.99
26	A	2605	PSU	C4-N3-C2	6.02	120.18	115.16
1	a	1402	4OC	C6-C5-C4	6.14	119.83	117.42
26	A	1911	PSU	C4-N3-C2	6.20	120.33	115.16
1	a	527	G7M	C1'-N9-C4	6.26	133.79	126.81
26	A	1939	5MU	C4-N3-C2	6.42	120.52	115.16
26	A	2457	PSU	C4-N3-C2	6.42	120.52	115.16
26	A	746	PSU	C4-N3-C2	6.44	120.53	115.16
26	A	2604	PSU	C4-N3-C2	6.57	120.64	115.16
26	A	2504	PSU	C4-N3-C2	6.68	120.73	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	55	PSU	C4-N3-C2	6.70	120.74	115.16
26	A	955	PSU	C4-N3-C2	6.74	120.78	115.16
26	A	2552	OMU	C4-N3-C2	6.84	121.41	114.21
1	a	516	PSU	C4-N3-C2	6.89	120.91	115.16
24	y	19	H2U	C5-C4-N3	6.93	123.94	116.62
26	A	2580	PSU	C4-N3-C2	6.95	120.95	115.16
26	A	1835	2MG	C2-N3-C4	7.22	122.91	114.99
24	y	54	5MU	C4-N3-C2	7.32	121.26	115.16
26	A	747	5MU	C4-N3-C2	7.39	121.32	115.16
22	v	54	5MU	C4-N3-C2	7.50	121.42	115.16
26	A	1618	6MZ	C2-N1-C6	7.67	121.99	116.47
26	A	1917	PSU	C4-N3-C2	8.04	121.86	115.16
24	y	37	6IA	C2-N1-C6	9.61	123.38	116.47
26	A	2503	2MA	C2-N3-C4	11.82	120.98	115.29

All (4) chirality outliers are listed below:

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

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	1915	3TD	O4'-C1'-C5-C4

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	1915	3TD	1	0
26	A	1939	5MU	1	0
26	A	1962	5MC	1	0
26	A	2030	6MZ	1	0
26	A	2457	PSU	1	0
26	A	2504	PSU	1	0
26	A	2604	PSU	1	0
26	A	745	1MG	2	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	0.94	0	5,9,11	1.16	0
60	SEC	y	701	24	1,5,6	0.71	0	1,5,7	1.58	0
61	GNP	z	701	62	29,34,34	2.64	7 (24%)	28,54,54	1.42	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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	z	701	GNP	C4-N9	-10.50	1.33	1.47
61	z	701	GNP	C8-N9	-3.95	1.34	1.47
61	z	701	GNP	C5-C6	-3.34	1.47	1.53
61	z	701	GNP	C2-N1	-2.29	1.34	1.44
61	z	701	GNP	C1'-N9	3.10	1.48	1.42
61	z	701	GNP	PG-N3B	3.89	1.74	1.63
61	z	701	GNP	PB-N3B	4.12	1.74	1.63

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
61	z	701	GNP	O3G-PG-O1G	-2.75	106.34	113.58
61	z	701	GNP	C2'-C1'-N9	-2.13	107.72	113.44
61	z	701	GNP	PA-O3A-PB	-2.11	125.07	132.71
61	z	701	GNP	C3'-C2'-C1'	2.05	105.56	101.44
61	z	701	GNP	C4-C5-N7	3.44	108.04	102.67
61	z	701	GNP	C8-N9-C4	3.51	108.79	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.