



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 5, 2016 – 06:47 PM EST

PDB ID : 5LZD
EMDB ID: : EMD-4124
Title : Structure of SelB-Sec-tRNA^{Sec} bound to the 70S ribosome in the GTPase activated state (GA)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2016-09-29
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

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

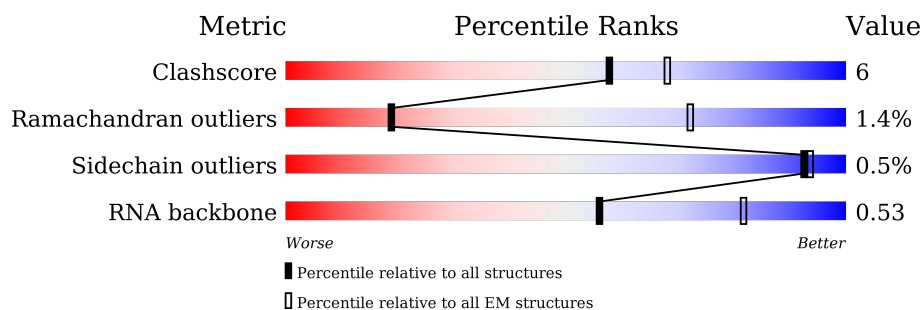
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.





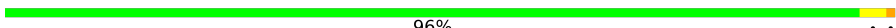










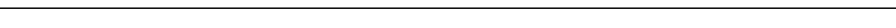



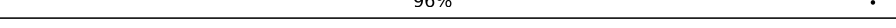







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	80% 18% .
2	b	218	93% 6% .
3	c	206	98% .
4	d	205	95% 5%
5	e	157	96% .
6	f	100	94% 5% .
7	g	151	97% .
8	h	129	96% ..

























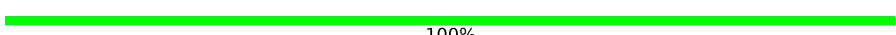
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Mol	Chain	Length	Quality of chain
9	i	127	 94% 5% .
10	j	98	 93% 6% .
11	k	116	 96% . .
12	l	123	 92% 7% .
13	m	114	 92% 8%
14	n	100	 94% 6%
15	o	88	 94% 6%
16	p	82	 99% .
17	q	80	 90% 10%
18	r	65	 94% 6%
19	s	86	 93% 6% .
20	t	85	 98% .
21	u	65	 89% 11%
22	v	77	 79% 19% .
23	x	48	 40% 38% 23%
24	y	95	 68% 32%
25	z	614	 96% .
26	A	2903	 63% 30% 6% .
27	B	120	 61% 32% 6% .
28	C	271	 77% 22% .
29	D	209	 77% 23%
30	E	201	 69% 30% .
31	F	177	 68% 29% . .
32	G	176	 72% 28%
33	I	141	 77% 22% .

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Mol	Chain	Length	Quality of chain
34	H	149	 77% 21% .
35	J	142	 78% 22%
36	K	122	 77% 21% .
37	L	143	 77% 22% .
38	M	136	 76% 22% .
39	N	120	 84% 14% .
40	O	116	 78% 22%
41	P	114	 70% 30%
42	Q	117	 86% 14%
43	R	103	 81% 19%
44	S	110	 75% 25% .
45	T	93	 76% 24%
46	U	102	 61% 36% .
47	V	94	 79% 21%
48	W	75	 92% 8%
49	X	77	 79% 19% .
50	Y	63	 81% 19%
51	Z	58	 74% 24% .
52	0	56	 73% 25% .
53	1	50	 76% 24%
54	2	46	 89% 11%
55	3	64	 84% 14% .
56	4	38	 68% 26% 5%
57	6	66	 74% 24% .
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 65 unique types of molecules in this entry. The entry contains 153177 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	86	Total	C	N	O	S	0	0
			687	438	131	116	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	0	0
			4853	3043	901	892	17		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Q	117	Total	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		

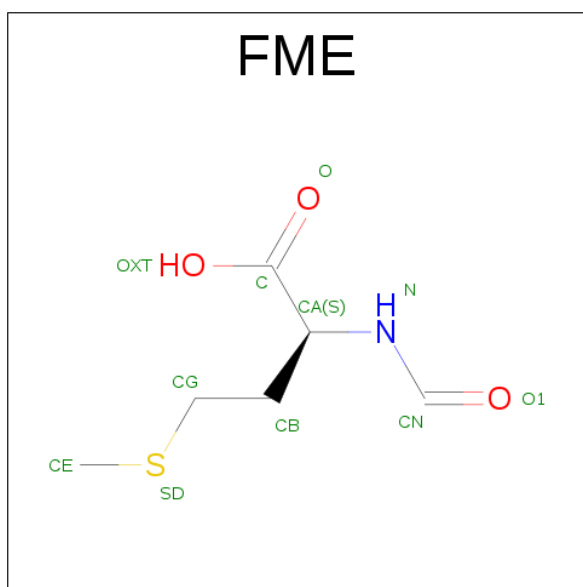
- Molecule 59 is CHLORIDE ION (three-letter code: CL)(formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
59	a	1	Total	Cl	0
			1	1	

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

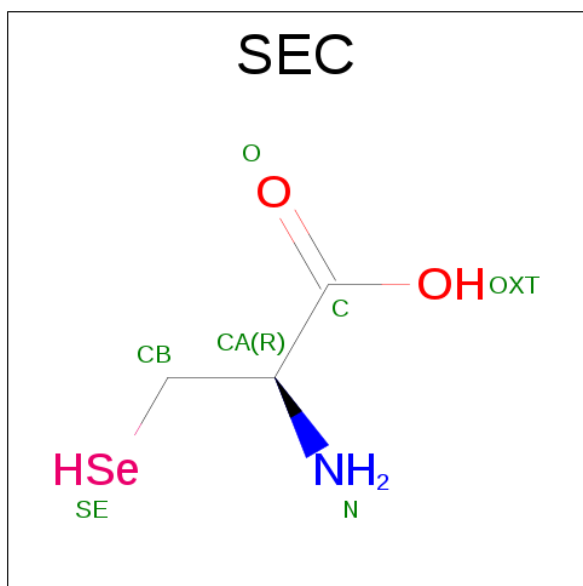
Mol	Chain	Residues	Atoms		AltConf
60	B	2	Total	Mg	0
			2	2	
60	a	30	Total	Mg	0
			30	30	
60	z	1	Total	Mg	0
			1	1	
60	A	111	Total	Mg	0
			111	111	
60	v	1	Total	Mg	0
			1	1	
60	n	1	Total	Mg	0
			1	1	
60	y	1	Total	Mg	0
			1	1	

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



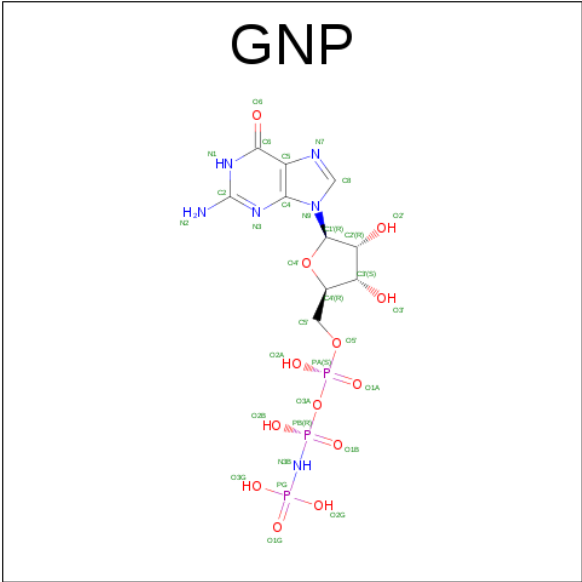
Mol	Chain	Residues	Atoms					AltConf
61	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 62 is SELENOCYSTEINE (three-letter code: SEC) (formula: $C_3H_7NO_2Se$).



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

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	4	1	Total	Zn	0
			1	1	
64	6	1	Total	Zn	0
			1	1	

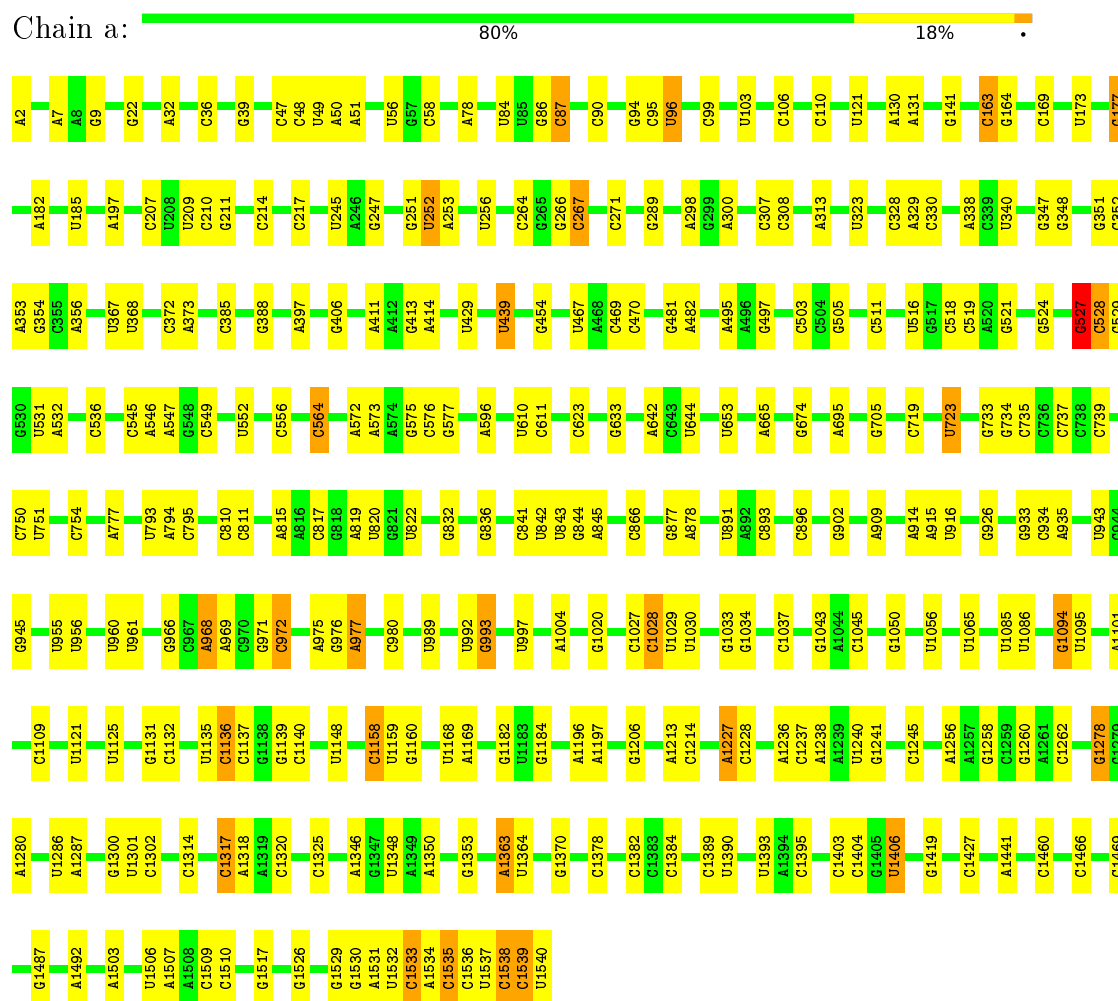
- Molecule 65 is water.

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

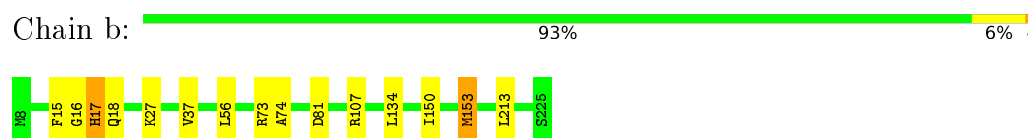
3 Residue-property plots

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



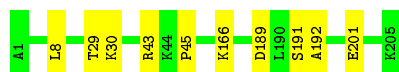
- Molecule 3: 30S ribosomal protein S3

Chain c:  98% .



- Molecule 4: 30S ribosomal protein S4

Chain d:  95% 5% .



- Molecule 5: 30S ribosomal protein S5

Chain e:  96% .



- Molecule 6: 30S ribosomal protein S6

Chain f:  94% 5% .



- Molecule 7: 30S ribosomal protein S7

Chain g:  97% .



- Molecule 8: 30S ribosomal protein S8

Chain h:  96% . .



- Molecule 9: 30S ribosomal protein S9

Chain i:  94% 5% .



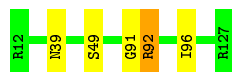
- Molecule 10: 30S ribosomal protein S10

Chain j:  93% 6% .



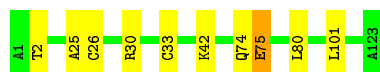
- Molecule 11: 30S ribosomal protein S11

Chain k: 96% ..



- Molecule 12: 30S ribosomal protein S12

Chain l: 92% 7% .



- Molecule 13: 30S ribosomal protein S13

Chain m: 92% 8%



- Molecule 14: 30S ribosomal protein S14

Chain n: 94% 6%



- Molecule 15: 30S ribosomal protein S15

Chain o: 94% 6%



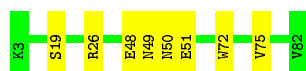
- Molecule 16: 30S ribosomal protein S16

Chain p: 99% .



- Molecule 17: 30S ribosomal protein S17

Chain q: 90% 10%



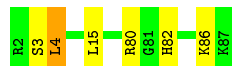
- Molecule 18: 30S ribosomal protein S18

Chain r:  94% 6%



- Molecule 19: 30S ribosomal protein S19

Chain s:  93% 6%




- Molecule 20: 30S ribosomal protein S20

Chain t:  98%




- Molecule 21: 30S ribosomal protein S21

Chain u:  89% 11%



- Molecule 22: fMet-tRNA^{fMet}

Chain v:  79% 19%



- Molecule 23: SECIS mRNA

Chain x:  40% 38% 23%



- Molecule 24: Sec-tRNA^{Sec}

Chain y:  68% 32%



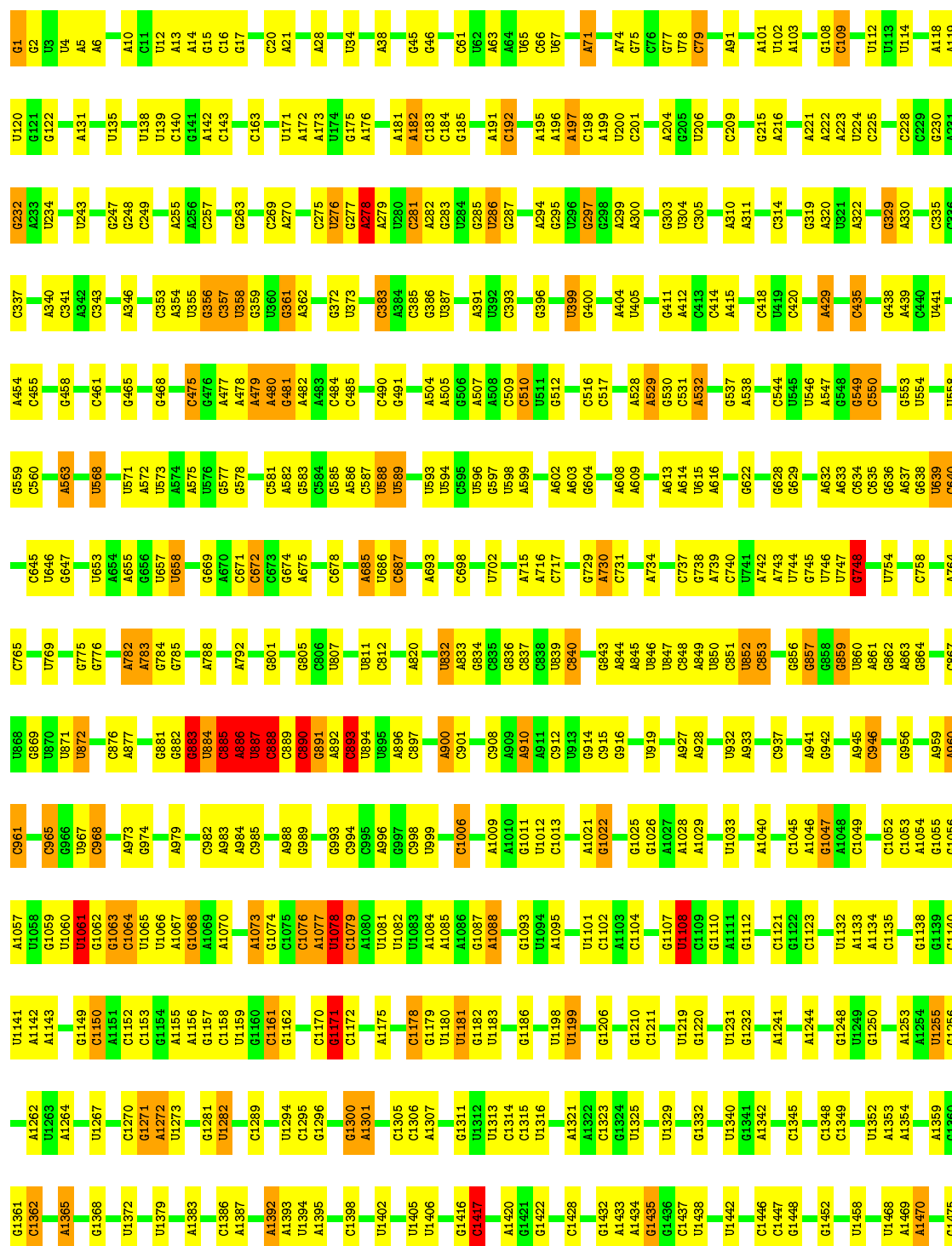
- Molecule 25: Selenocysteine-specific elongation factor

Chain z:  96%



- Molecule 26: 23S ribosomal RNA

Chain A: 63% 30% 6%

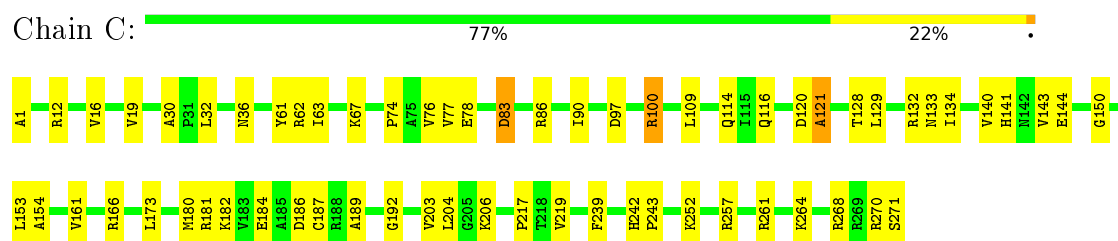




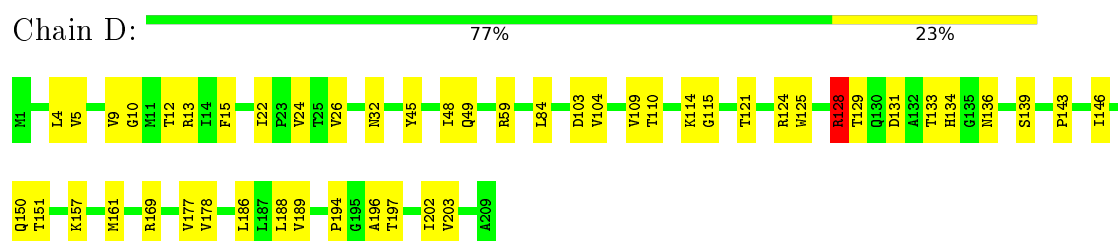
Response	Percentage
Yes	61%
No	32%
Don't know	6%



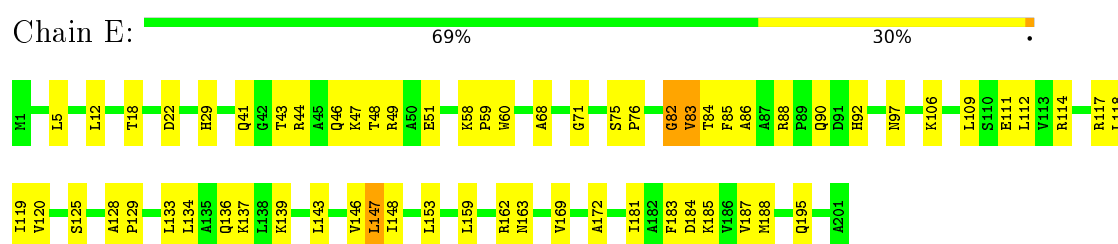
- Molecule 28: 50S ribosomal protein L2



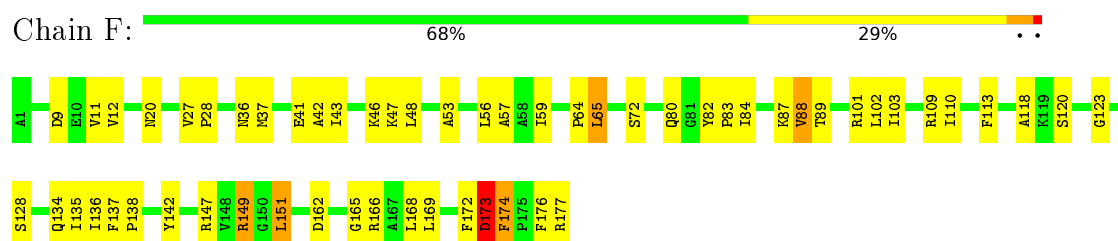
- Molecule 29: 50S ribosomal protein L3



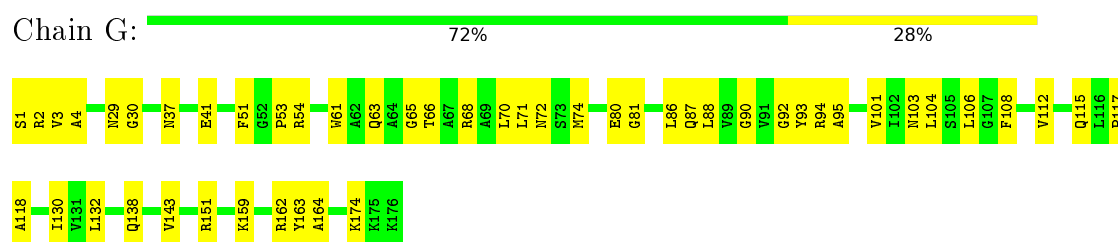
- Molecule 30: 50S ribosomal protein L4




- Molecule 31: 50S ribosomal protein L5

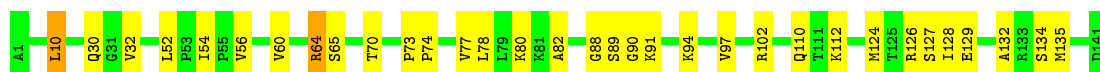


- Molecule 32: 50S ribosomal protein L6




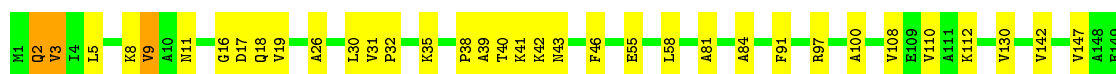
- Molecule 33: 50S ribosomal protein L11

Chain I:  77% 22%




- Molecule 34: 50S ribosomal protein L9

Chain H:  77% 21%




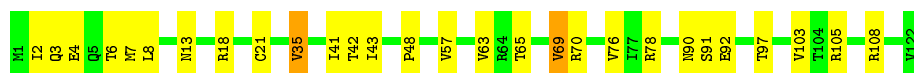
- Molecule 35: 50S ribosomal protein L13

Chain J:  78% 22%




- Molecule 36: 50S ribosomal protein L14

Chain K:  77% 21%




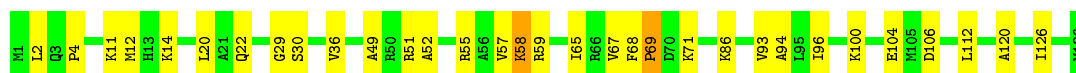
- Molecule 37: 50S ribosomal protein L15

Chain L:  77% 22%




- Molecule 38: 50S ribosomal protein L16

Chain M:  76% 22%




- Molecule 39: 50S ribosomal protein L17

Chain N:  84% 14%



- Molecule 40: 50S ribosomal protein L18

Chain O:  78% 22%



- Molecule 41: 50S ribosomal protein L19

Chain P: 70% 30%



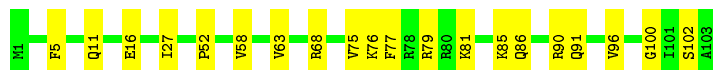
- Molecule 42: 50S ribosomal protein L20

Chain Q: 86% 14%



- Molecule 43: 50S ribosomal protein L21

Chain R: 81% 19%



- Molecule 44: 50S ribosomal protein L22

Chain S: 75% 25%



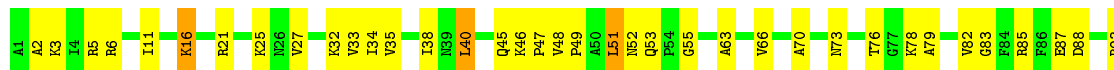
- Molecule 45: 50S ribosomal protein L23

Chain T: 76% 24%



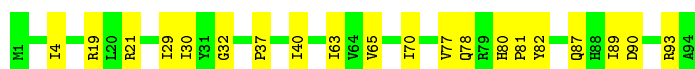
- Molecule 46: 50S ribosomal protein L24

Chain U: 61% 36%



- Molecule 47: 50S ribosomal protein L25

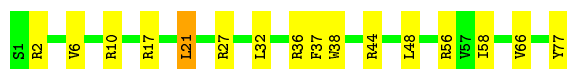
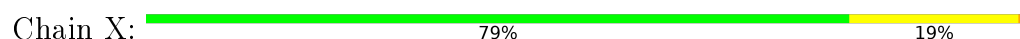
Chain V: 79% 21%



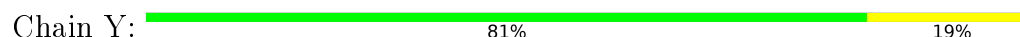
- Molecule 48: 50S ribosomal protein L27



- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29



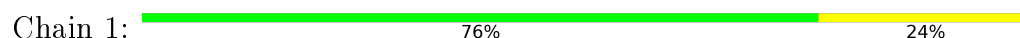
- Molecule 51: 50S ribosomal protein L30



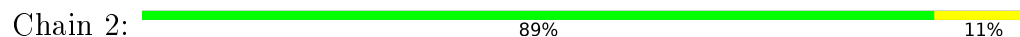
- Molecule 52: 50S ribosomal protein L32




- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35

Chain 3:  84% 14% .



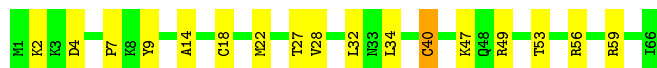
- Molecule 56: 50S ribosomal protein L36

Chain 4:  68% 26% 5%



- Molecule 57: 50S ribosomal protein L31

Chain 6:  74% 24% .



- 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	159729	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, CL, 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	2/36701 (0.0%)	1.18	255/57246 (0.4%)
10	j	0.50	0/797	0.95	1/1077 (0.1%)
11	k	0.53	0/886	0.88	2/1195 (0.2%)
12	l	0.64	2/969 (0.2%)	0.93	3/1300 (0.2%)
13	m	0.52	0/893	0.98	5/1193 (0.4%)
14	n	0.53	0/806	0.90	3/1074 (0.3%)
15	o	0.44	0/722	0.81	3/964 (0.3%)
16	p	0.49	0/659	0.77	0/884
17	q	0.60	0/658	1.07	3/881 (0.3%)
18	r	0.42	0/512	0.82	2/689 (0.3%)
19	s	0.45	0/703	0.89	2/944 (0.2%)
2	b	0.51	2/1736 (0.1%)	0.90	6/2338 (0.3%)
20	t	0.47	0/671	0.81	2/888 (0.2%)
21	u	0.53	0/501	1.06	2/668 (0.3%)
22	v	0.58	1/1745 (0.1%)	1.18	13/2716 (0.5%)
23	x	0.76	2/1145 (0.2%)	1.63	31/1781 (1.7%)
24	y	0.53	1/2168 (0.0%)	1.27	26/3375 (0.8%)
25	z	0.46	1/4952 (0.0%)	0.89	13/6712 (0.2%)
26	A	0.62	10/69240 (0.0%)	1.22	593/108014 (0.5%)
27	B	0.58	1/2873 (0.0%)	1.28	30/4478 (0.7%)
28	C	0.50	1/2122 (0.0%)	0.81	3/2852 (0.1%)
29	D	0.49	0/1586	0.81	2/2134 (0.1%)
3	c	0.44	0/1652	0.82	4/2225 (0.2%)
30	E	0.47	0/1571	0.81	4/2113 (0.2%)
31	F	0.61	1/1435 (0.1%)	1.00	9/1926 (0.5%)
32	G	0.45	0/1343	0.79	2/1816 (0.1%)
33	I	0.40	0/1046	0.73	1/1410 (0.1%)
34	H	0.41	0/1122	0.72	0/1515
35	J	0.46	0/1152	0.72	0/1551
36	K	0.53	1/948 (0.1%)	0.85	1/1268 (0.1%)
37	L	0.42	0/1054	0.78	1/1403 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	M	0.44	0/1093	0.78	0/1460
39	N	0.50	0/974	0.78	1/1301 (0.1%)
4	d	0.49	0/1665	0.87	2/2227 (0.1%)
40	O	0.48	0/902	0.75	1/1209 (0.1%)
41	P	0.45	0/929	0.82	3/1242 (0.2%)
42	Q	0.50	0/960	0.68	1/1278 (0.1%)
43	R	0.47	0/829	0.77	0/1107
44	S	0.46	0/864	0.80	2/1156 (0.2%)
45	T	0.45	0/745	0.73	0/994
46	U	0.52	0/788	0.90	3/1051 (0.3%)
47	V	0.47	0/766	0.71	0/1025
48	W	0.46	0/582	0.75	0/769
49	X	0.42	0/635	0.77	1/848 (0.1%)
5	e	0.51	0/1170	0.88	2/1573 (0.1%)
50	Y	0.52	0/510	0.97	2/677 (0.3%)
51	Z	0.41	0/453	0.78	1/605 (0.2%)
52	0	0.51	1/450 (0.2%)	0.93	2/599 (0.3%)
53	1	0.42	0/417	0.85	1/554 (0.2%)
54	2	0.45	0/380	0.73	0/498
55	3	0.43	0/513	0.73	0/676
56	4	0.75	2/303 (0.7%)	0.93	2/397 (0.5%)
57	6	0.47	0/532	1.00	4/709 (0.6%)
58	w	0.39	0/68	0.94	0/103
6	f	0.56	0/836	0.87	2/1128 (0.2%)
7	g	0.48	0/1196	0.81	2/1602 (0.1%)
8	h	0.46	0/989	0.86	5/1326 (0.4%)
9	i	0.55	0/1034	0.97	4/1375 (0.3%)
All	All	0.57	28/164951 (0.0%)	1.12	1063/246119 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
10	j	0	3
11	k	0	2
12	l	0	2
16	p	0	1
17	q	0	2
2	b	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	u	0	1
25	z	0	1
26	A	2	0
28	C	0	1
30	E	0	1
31	F	0	2
32	G	0	2
34	H	0	3
4	d	0	1
44	S	0	1
46	U	0	2
53	1	0	1
55	3	0	1
6	f	0	1
All	All	4	30

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	1	U	OP3-P	-10.85	1.48	1.61
24	y	1	G	OP3-P	-10.68	1.48	1.61
22	v	1	C	OP3-P	-10.68	1.48	1.61
26	A	1	G	OP3-P	-10.59	1.48	1.61
1	a	2	A	OP3-P	-10.59	1.48	1.61
23	x	87	A	OP3-P	-10.57	1.48	1.61
26	A	571	U	C4-O4	8.50	1.30	1.23
12	l	26	CYS	CB-SG	-8.20	1.68	1.82
1	a	723	U	C4-O4	-7.13	1.18	1.23
31	F	11	VAL	CB-CG1	-7.10	1.38	1.52
26	A	1963	U	C2-O2	-7.07	1.16	1.22
56	4	27	CYS	CB-SG	6.97	1.94	1.82
56	4	11	CYS	CB-SG	6.63	1.93	1.82
52	0	2	VAL	CB-CG2	-6.37	1.39	1.52
36	K	69	VAL	CB-CG1	-5.79	1.40	1.52
2	b	27	LYS	C-N	5.74	1.45	1.34
26	A	2173	A	N9-C4	5.71	1.41	1.37
26	A	278	A	N9-C4	5.58	1.41	1.37
25	z	322	VAL	CB-CG2	-5.54	1.41	1.52
26	A	1936	A	C2-N3	-5.48	1.28	1.33
2	b	37	VAL	CB-CG2	-5.46	1.41	1.52
23	x	128	C	O3'-P	5.46	1.67	1.61
26	A	2211	A	N9-C4	5.26	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	356	G	N7-C5	-5.25	1.36	1.39
12	I	33	CYS	CB-SG	-5.13	1.73	1.81
26	A	571	U	C5-C6	-5.13	1.29	1.34
26	A	1936	A	N3-C4	-5.04	1.31	1.34
28	C	30	ALA	C-N	5.01	1.43	1.34

All (1063) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	968	A	N1-C6-N6	-23.76	104.34	118.60
1	a	1158	C	N1-C2-O2	18.14	129.78	118.90
26	A	2059	A	N1-C2-N3	-17.84	120.38	129.30
1	a	1158	C	N3-C2-O2	-17.55	109.61	121.90
1	a	529	G	C5-C6-O6	-15.48	119.31	128.60
1	a	968	A	C5-C6-N6	15.15	135.82	123.70
26	A	890	C	C2-N1-C1'	14.01	134.21	118.80
26	A	887	U	N1-C2-O2	13.17	132.02	122.80
26	A	887	U	N3-C2-O2	-13.10	113.03	122.20
26	A	2059	A	C6-N1-C2	12.82	126.29	118.60
1	a	207	C	N3-C2-O2	-12.33	113.27	121.90
26	A	1963	U	N1-C2-N3	12.26	122.26	114.90
26	A	1941	C	N1-C2-O2	12.21	126.23	118.90
1	a	1158	C	C6-N1-C2	-12.03	115.49	120.30
26	A	890	C	C6-N1-C1'	-12.01	106.39	120.80
26	A	1313	U	N1-C2-O2	12.01	131.21	122.80
1	a	529	G	N1-C6-O6	12.00	127.10	119.90
26	A	890	C	N1-C2-O2	11.90	126.04	118.90
1	a	968	A	N9-C4-C5	11.84	110.54	105.80
26	A	1313	U	N3-C2-O2	-11.44	114.19	122.20
31	F	151	LEU	CB-CG-CD2	-11.43	91.56	111.00
26	A	888	C	C6-N1-C2	-11.15	115.84	120.30
26	A	886	A	P-O3'-C3'	11.10	133.02	119.70
25	z	373	LEU	CB-CG-CD1	-11.04	92.23	111.00
26	A	1963	U	C6-N1-C2	-10.93	114.44	121.00
17	q	26	ARG	NE-CZ-NH2	10.89	125.75	120.30
1	a	207	C	N1-C2-O2	10.89	125.43	118.90
26	A	2179	C	N3-C2-O2	-10.84	114.31	121.90
26	A	894	U	C5-C6-N1	10.75	128.07	122.70
26	A	961	C	O5'-P-OP1	-10.64	96.12	105.70
1	a	968	A	C6-C5-N7	10.64	139.75	132.30
26	A	1498	C	C2-N1-C1'	10.43	130.27	118.80
1	a	1027	C	N1-C2-O2	10.39	125.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2805	C	C5-C6-N1	10.36	126.18	121.00
25	z	398	LEU	CB-CG-CD2	-10.30	93.50	111.00
26	A	1941	C	N3-C2-O2	-10.17	114.78	121.90
26	A	893	C	C6-N1-C2	-10.16	116.24	120.30
23	x	114	C	N1-C2-O2	10.16	124.99	118.90
1	a	307	C	N1-C2-O2	10.07	124.94	118.90
27	B	60	C	C5-C6-N1	9.96	125.98	121.00
26	A	1348	C	N1-C2-O2	9.94	124.86	118.90
26	A	2143	C	C6-N1-C2	-9.93	116.33	120.30
26	A	2473	U	N1-C2-O2	9.91	129.74	122.80
17	q	26	ARG	NE-CZ-NH1	-9.90	115.35	120.30
26	A	2805	C	C6-N1-C2	-9.75	116.40	120.30
26	A	893	C	C5-C6-N1	9.69	125.85	121.00
23	x	131	C	C6-N1-C2	-9.60	116.46	120.30
26	A	2757	A	C6-N1-C2	9.59	124.35	118.60
26	A	640	C	C5-C6-N1	9.45	125.72	121.00
26	A	2683	C	N1-C2-O2	9.44	124.56	118.90
1	a	1314	C	O5'-P-OP2	-9.41	97.23	105.70
26	A	2473	U	N3-C2-O2	-9.41	115.61	122.20
1	a	556	C	C5-C6-N1	9.39	125.69	121.00
26	A	571	U	O4'-C1'-N1	-9.32	100.74	108.20
26	A	341	C	C6-N1-C2	-9.30	116.58	120.30
26	A	1956	U	N1-C2-O2	9.26	129.28	122.80
26	A	901	C	N1-C2-O2	9.23	124.44	118.90
26	A	550	C	C5-C6-N1	9.22	125.61	121.00
1	a	207	C	C6-N1-C2	-9.21	116.62	120.30
1	a	529	G	N9-C4-C5	-9.20	101.72	105.40
1	a	90	C	C6-N1-C2	-9.16	116.63	120.30
26	A	1936	A	N1-C2-N3	9.14	133.87	129.30
27	B	30	C	C6-N1-C2	-9.12	116.65	120.30
49	X	21	LEU	CA-CB-CG	9.11	136.25	115.30
26	A	2179	C	N1-C2-O2	9.10	124.36	118.90
1	a	1158	C	C2-N1-C1'	9.05	128.76	118.80
26	A	528	A	C8-N9-C4	-9.05	102.18	105.80
26	A	1313	U	C2-N1-C1'	9.03	128.53	117.70
1	a	968	A	O4'-C1'-N9	9.02	115.42	108.20
1	a	529	G	C4-C5-N7	8.94	114.37	110.80
32	G	104	LEU	CA-CB-CG	8.90	135.77	115.30
26	A	278	A	C2-N3-C4	8.82	115.01	110.60
26	A	571	U	C5-C4-O4	8.81	131.19	125.90
1	a	87	C	C5-C6-N1	8.80	125.40	121.00
1	a	968	A	C4-C5-N7	-8.78	106.31	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	42	C	N1-C2-O2	8.77	124.16	118.90
26	A	639	U	C5-C6-N1	8.74	127.07	122.70
25	z	79	LEU	CA-CB-CG	8.72	135.36	115.30
27	B	60	C	C6-N1-C2	-8.70	116.82	120.30
1	a	1393	U	N3-C2-O2	-8.68	116.12	122.20
1	a	1538	C	C6-N1-C2	-8.67	116.83	120.30
26	A	2072	C	C6-N1-C2	-8.61	116.86	120.30
23	x	114	C	C2-N1-C1'	8.60	128.26	118.80
26	A	183	C	N3-C2-O2	-8.53	115.93	121.90
26	A	2150	C	C6-N1-C2	-8.51	116.90	120.30
26	A	984	A	C2-N3-C4	8.51	114.85	110.60
1	a	1245	C	C5-C6-N1	8.49	125.25	121.00
24	y	40	C	C6-N1-C2	-8.47	116.91	120.30
26	A	550	C	C6-N1-C2	-8.45	116.92	120.30
26	A	847	U	N3-C2-O2	-8.44	116.30	122.20
26	A	283	G	N3-C2-N2	-8.40	114.02	119.90
1	a	1317	C	N1-C2-O2	8.38	123.93	118.90
1	a	307	C	N3-C2-O2	-8.36	116.05	121.90
21	u	15	LEU	CA-CB-CG	8.35	134.50	115.30
26	A	885	C	N1-C2-O2	-8.34	113.90	118.90
31	F	174	PHE	CB-CG-CD1	8.33	126.63	120.80
1	a	556	C	C6-N1-C2	-8.32	116.97	120.30
26	A	1348	C	N3-C2-O2	-8.31	116.08	121.90
26	A	2043	C	C6-N1-C2	-8.29	116.98	120.30
26	A	1941	C	C2-N1-C1'	8.26	127.89	118.80
26	A	2174	C	N1-C2-O2	8.26	123.86	118.90
26	A	968	C	C6-N1-C2	-8.20	117.02	120.30
26	A	2211	A	C2-N3-C4	8.19	114.70	110.60
26	A	2637	U	C5-C6-N1	8.18	126.79	122.70
26	A	2043	C	C5-C6-N1	8.16	125.08	121.00
25	z	427	LEU	CB-CG-CD2	-8.16	97.12	111.00
26	A	894	U	C6-N1-C2	-8.16	116.11	121.00
26	A	837	C	N3-C2-O2	-8.14	116.20	121.90
26	A	1305	C	C6-N1-C2	-8.14	117.04	120.30
26	A	2646	C	C5-C6-N1	8.12	125.06	121.00
27	B	26	C	N1-C2-O2	8.12	123.77	118.90
1	a	723	U	N3-C4-C5	8.11	119.47	114.60
1	a	1537	U	C2-N1-C1'	8.11	127.43	117.70
1	a	968	A	N9-C1'-C2'	-8.11	103.08	112.00
26	A	183	C	C6-N1-C2	-8.08	117.07	120.30
26	A	2105	U	C5-C6-N1	8.07	126.73	122.70
26	A	2302	U	N3-C2-O2	-8.07	116.55	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	217	C	C6-N1-C2	-8.05	117.08	120.30
1	a	1537	U	N3-C2-O2	-8.04	116.57	122.20
1	a	909	A	O5'-P-OP1	-8.03	98.47	105.70
26	A	343	C	C6-N1-C2	-8.03	117.09	120.30
26	A	2173	A	C2-N3-C4	7.99	114.59	110.60
53	l	5	ARG	NE-CZ-NH1	-7.99	116.30	120.30
26	A	234	U	N3-C2-O2	-7.98	116.62	122.20
26	A	1507	C	C6-N1-C2	-7.98	117.11	120.30
26	A	1314	C	C6-N1-C2	-7.96	117.12	120.30
1	a	217	C	C5-C6-N1	7.96	124.98	121.00
26	A	887	U	C2-N1-C1'	7.96	127.25	117.70
26	A	634	C	C6-N1-C2	-7.96	117.12	120.30
26	A	2188	U	C5-C6-N1	7.95	126.68	122.70
51	Z	23	LEU	CB-CG-CD1	-7.95	97.49	111.00
1	a	1245	C	C6-N1-C2	-7.92	117.13	120.30
1	a	90	C	C5-C6-N1	7.85	124.92	121.00
26	A	198	C	C5-C6-N1	7.85	124.92	121.00
26	A	1267	U	N1-C2-O2	7.84	128.29	122.80
1	a	413	G	C5-C6-O6	-7.84	123.90	128.60
1	a	96	U	C5-C6-N1	7.84	126.62	122.70
26	A	1052	C	C5-C6-N1	7.83	124.91	121.00
26	A	571	U	N3-C4-C5	-7.82	109.91	114.60
26	A	1669	A	C2-N3-C4	7.79	114.49	110.60
26	A	2473	U	C2-N1-C1'	7.79	127.04	117.70
26	A	2646	C	C6-N1-C2	-7.78	117.19	120.30
26	A	1956	U	N3-C2-O2	-7.78	116.75	122.20
23	x	127	U	P-O3'-C3'	7.76	129.01	119.70
26	A	358	U	N3-C2-O2	-7.75	116.77	122.20
13	m	8	ILE	CG1-CB-CG2	-7.74	94.37	111.40
26	A	1022	G	N1-C6-O6	-7.74	115.26	119.90
26	A	1499	C	C2-N1-C1'	7.74	127.31	118.80
12	l	75	GLU	N-CA-CB	-7.72	96.71	110.60
26	A	640	C	C6-N1-C2	-7.72	117.21	120.30
56	4	14	CYS	CA-CB-SG	7.71	127.89	114.00
24	y	16	C	C6-N1-C2	-7.70	117.22	120.30
26	A	2292	U	C5-C6-N1	7.70	126.55	122.70
26	A	1063	G	N7-C8-N9	7.70	116.95	113.10
26	A	2617	U	N3-C2-O2	-7.69	116.82	122.20
26	A	2683	C	N3-C2-O2	-7.68	116.52	121.90
26	A	2129	C	O5'-P-OP1	7.68	119.91	110.70
26	A	1963	U	C6-N1-C1'	7.67	131.94	121.20
26	A	528	A	N7-C8-N9	7.67	117.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	32	C	C5-C6-N1	7.67	124.83	121.00
1	a	1537	U	N1-C2-O2	7.67	128.17	122.80
26	A	341	C	C5-C6-N1	7.66	124.83	121.00
1	a	87	C	C6-N1-C2	-7.66	117.23	120.30
26	A	1683	U	C5-C6-N1	7.64	126.52	122.70
26	A	1052	C	C6-N1-C2	-7.64	117.25	120.30
26	A	1920	C	C5-C6-N1	7.63	124.82	121.00
26	A	109	C	C5-C6-N1	7.63	124.81	121.00
27	B	120	U	N3-C2-O2	-7.63	116.86	122.20
1	a	1037	C	C6-N1-C2	-7.57	117.27	120.30
57	6	18	CYS	CA-CB-SG	-7.57	100.38	114.00
23	x	96	C	C6-N1-C2	-7.57	117.27	120.30
26	A	2026	U	C5-C6-N1	7.57	126.48	122.70
26	A	1171	G	C8-N9-C4	-7.55	103.38	106.40
1	a	330	C	N1-C2-O2	7.54	123.42	118.90
26	A	343	C	N1-C2-O2	7.53	123.42	118.90
24	y	40	C	C5-C6-N1	7.52	124.76	121.00
31	F	151	LEU	CB-CG-CD1	7.52	123.79	111.00
26	A	1362	C	C5-C6-N1	7.52	124.76	121.00
26	A	2666	C	N1-C2-O2	7.51	123.41	118.90
26	A	2174	C	N3-C2-O2	-7.51	116.64	121.90
27	B	47	C	N1-C2-O2	7.50	123.40	118.90
1	a	1389	C	C2-N1-C1'	7.49	127.04	118.80
2	b	150	ILE	CG1-CB-CG2	-7.49	94.93	111.40
4	d	189	ASP	CB-CG-OD1	7.46	125.01	118.30
1	a	177	G	C2-N3-C4	7.43	115.61	111.90
26	A	1362	C	C6-N1-C2	-7.43	117.33	120.30
1	a	735	C	C6-N1-C2	-7.43	117.33	120.30
26	A	2305	U	C6-N1-C2	7.41	125.44	121.00
23	x	117	C	O5'-P-OP2	7.41	119.59	110.70
26	A	783	A	C2-N3-C4	7.40	114.30	110.60
26	A	1941	C	C6-N1-C2	-7.39	117.34	120.30
1	a	78	A	N7-C8-N9	7.38	117.49	113.80
26	A	890	C	OP1-P-O3'	7.38	121.43	105.20
26	A	1708	C	C6-N1-C2	-7.38	117.35	120.30
26	A	901	C	N3-C2-O2	-7.36	116.75	121.90
26	A	357	C	C6-N1-C2	-7.36	117.36	120.30
1	a	989	U	N3-C2-O2	-7.35	117.06	122.20
26	A	1435	G	C8-N9-C4	-7.35	103.46	106.40
26	A	183	C	N1-C2-O2	7.34	123.31	118.90
26	A	1021	A	C2-N3-C4	7.34	114.27	110.60
3	c	35	ASP	CB-CG-OD1	7.33	124.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	837	C	N1-C2-O2	7.33	123.30	118.90
26	A	1063	G	C8-N9-C4	-7.33	103.47	106.40
25	z	359	LEU	CB-CG-CD2	7.30	123.41	111.00
26	A	2896	C	C5-C6-N1	7.30	124.65	121.00
26	A	2656	U	C5-C6-N1	7.30	126.35	122.70
1	a	1027	C	N3-C2-O2	-7.29	116.80	121.90
26	A	888	C	N3-C2-O2	-7.29	116.80	121.90
1	a	1109	C	N1-C2-O2	7.27	123.26	118.90
26	A	2250	G	C8-N9-C4	-7.27	103.49	106.40
26	A	2723	C	C5-C6-N1	7.26	124.63	121.00
26	A	1498	C	C5-C6-N1	7.25	124.62	121.00
12	l	80	LEU	CA-CB-CG	7.25	131.97	115.30
25	z	26	ASP	CB-CG-OD1	7.24	124.81	118.30
50	Y	49	ASP	CB-CG-OD1	7.21	124.79	118.30
26	A	234	U	N1-C2-O2	7.21	127.85	122.80
1	a	1406	U	N3-C2-O2	-7.21	117.16	122.20
6	f	98	GLU	N-CA-CB	-7.19	97.66	110.60
26	A	1186	G	O5'-P-OP1	-7.18	99.23	105.70
1	a	1045	C	C5-C6-N1	7.18	124.59	121.00
26	A	669	G	N3-C4-N9	7.17	130.30	126.00
26	A	847	U	N1-C2-O2	7.17	127.81	122.80
26	A	2151	U	C5-C6-N1	7.16	126.28	122.70
26	A	356	G	N7-C8-N9	7.15	116.68	113.10
26	A	358	U	C5-C6-N1	7.15	126.28	122.70
26	A	1708	C	C5-C6-N1	7.15	124.58	121.00
26	A	1920	C	C6-N1-C2	-7.15	117.44	120.30
1	a	1382	C	N1-C2-O2	7.15	123.19	118.90
26	A	669	G	N3-C4-C5	-7.15	125.03	128.60
1	a	439	U	N3-C2-O2	-7.14	117.20	122.20
23	x	125	G	N9-C1'-C2'	-7.14	104.14	112.00
26	A	2179	C	C6-N1-C2	-7.14	117.44	120.30
26	A	2072	C	C5-C6-N1	7.14	124.57	121.00
26	A	1936	A	C2-N3-C4	-7.14	107.03	110.60
1	a	723	U	N3-C4-O4	-7.13	114.41	119.40
26	A	1498	C	C6-N1-C1'	-7.13	112.25	120.80
26	A	2757	A	N1-C2-N3	-7.11	125.74	129.30
1	a	1027	C	C5-C6-N1	7.11	124.56	121.00
27	B	26	C	N3-C2-O2	-7.11	116.92	121.90
26	A	634	C	C5-C6-N1	7.09	124.55	121.00
1	a	611	C	N1-C2-O2	7.09	123.15	118.90
1	a	1427	C	C6-N1-C2	-7.08	117.47	120.30
26	A	314	C	C5-C6-N1	7.08	124.54	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1150	C	C6-N1-C2	-7.08	117.47	120.30
26	A	305	C	C6-N1-C2	-7.07	117.47	120.30
26	A	2739	U	N3-C2-O2	-7.06	117.25	122.20
26	A	1267	U	N3-C2-O2	-7.06	117.26	122.20
1	a	968	A	C8-N9-C4	-7.06	102.98	105.80
26	A	1498	C	C6-N1-C2	-7.06	117.48	120.30
26	A	2723	C	C6-N1-C2	-7.05	117.48	120.30
26	A	891	G	C5-C6-O6	-7.05	124.37	128.60
1	a	1466	C	N1-C2-O2	7.05	123.13	118.90
3	c	33	ASP	CB-CG-OD1	7.04	124.64	118.30
26	A	890	C	C5-C6-N1	7.03	124.51	121.00
26	A	571	U	C5-C6-N1	-7.02	119.19	122.70
23	x	121	U	C2-N1-C1'	7.01	126.11	117.70
26	A	1321	A	C2-N3-C4	7.01	114.10	110.60
15	o	55	LEU	CA-CB-CG	7.00	131.41	115.30
1	a	90	C	N1-C2-O2	7.00	123.10	118.90
26	A	1435	G	N7-C8-N9	7.00	116.60	113.10
26	A	2006	C	C5-C6-N1	7.00	124.50	121.00
26	A	901	C	C2-N1-C1'	7.00	126.50	118.80
26	A	2840	C	C5-C6-N1	7.00	124.50	121.00
1	a	56	U	C5-C6-N1	6.99	126.20	122.70
26	A	901	C	C6-N1-C2	-6.99	117.50	120.30
27	B	27	C	N1-C2-O2	6.98	123.09	118.90
26	A	1963	U	N1-C2-O2	-6.98	117.92	122.80
1	a	503	C	C6-N1-C2	-6.97	117.51	120.30
27	B	37	C	N3-C2-O2	-6.97	117.02	121.90
1	a	1109	C	N3-C2-O2	-6.97	117.02	121.90
9	i	120	ALA	N-CA-CB	6.97	119.85	110.10
1	a	737	C	C6-N1-C2	-6.96	117.52	120.30
26	A	1499	C	N1-C2-O2	6.95	123.07	118.90
1	a	1389	C	C6-N1-C2	-6.95	117.52	120.30
26	A	358	U	C6-N1-C2	-6.95	116.83	121.00
26	A	361	G	N1-C6-O6	6.94	124.06	119.90
1	a	90	C	N3-C2-O2	-6.94	117.04	121.90
2	b	153	MET	CG-SD-CE	-6.93	89.11	100.20
26	A	2656	U	N1-C2-O2	6.93	127.65	122.80
37	L	112	LEU	CA-CB-CG	6.93	131.24	115.30
26	A	867	C	N1-C2-O2	6.93	123.06	118.90
26	A	243	U	N1-C2-O2	6.92	127.64	122.80
26	A	343	C	C2-N1-C1'	6.91	126.40	118.80
26	A	1963	U	C2-N3-C4	-6.91	122.86	127.00
26	A	1340	U	N3-C2-O2	-6.90	117.37	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	16	C	C5-C6-N1	6.90	124.45	121.00
26	A	2069	G7M	P-O3'-C3'	6.89	127.97	119.70
1	a	1403	C	N1-C2-O2	6.89	123.04	118.90
33	I	10	LEU	CA-CB-CG	6.89	131.15	115.30
26	A	314	C	C6-N1-C2	-6.89	117.55	120.30
1	a	1027	C	C6-N1-C2	-6.88	117.55	120.30
26	A	1314	C	C5-C6-N1	6.87	124.44	121.00
1	a	1404	C	C6-N1-C2	-6.87	117.55	120.30
1	a	58	C	C6-N1-C2	-6.87	117.55	120.30
1	a	1466	C	N3-C2-O2	-6.86	117.09	121.90
26	A	297	G	O5'-P-OP1	6.86	118.93	110.70
31	F	102	LEU	CA-CB-CG	6.86	131.08	115.30
1	a	1045	C	C6-N1-C2	-6.85	117.56	120.30
1	a	1469	C	N1-C2-O2	6.85	123.01	118.90
27	B	55	U	N3-C2-O2	-6.85	117.41	122.20
27	B	120	U	N1-C2-O2	6.83	127.58	122.80
26	A	1656	C	C5-C6-N1	6.81	124.41	121.00
1	a	968	A	N1-C2-N3	6.81	132.71	129.30
26	A	2110	G	C5-C6-O6	6.81	132.68	128.60
24	y	32	C	C6-N1-C2	-6.79	117.58	120.30
27	B	37	C	N1-C2-O2	6.78	122.97	118.90
26	A	1294	U	N3-C2-O2	-6.78	117.46	122.20
1	a	980	C	N1-C2-O2	6.76	122.96	118.90
25	z	49	ASP	CB-CG-OD1	6.76	124.39	118.30
26	A	2066	C	C6-N1-C2	-6.75	117.60	120.30
1	a	1389	C	C5-C6-N1	6.75	124.38	121.00
27	B	47	C	N3-C2-O2	-6.75	117.18	121.90
26	A	669	G	C2-N3-C4	6.75	115.27	111.90
26	A	2466	C	O5'-P-OP1	-6.75	99.63	105.70
1	a	413	G	C8-N9-C4	6.74	109.10	106.40
22	v	1	C	N1-C2-O2	6.74	122.94	118.90
1	a	977	A	C2-N3-C4	6.74	113.97	110.60
26	A	2066	C	C5-C6-N1	6.73	124.37	121.00
26	A	885	C	N3-C4-N4	6.73	122.71	118.00
21	u	5	VAL	CG1-CB-CG2	-6.73	100.14	110.90
26	A	1507	C	C5-C6-N1	6.73	124.36	121.00
1	a	207	C	C2-N1-C1'	6.72	126.19	118.80
26	A	1348	C	C6-N1-C2	-6.72	117.61	120.30
1	a	1406	U	N1-C2-O2	6.71	127.50	122.80
1	a	610	U	N3-C2-O2	-6.71	117.50	122.20
31	F	174	PHE	CB-CG-CD2	-6.70	116.11	120.80
26	A	232	G	C8-N9-C4	-6.69	103.72	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	571	U	C4-C5-C6	6.68	123.71	119.70
26	A	889	C	C2-N3-C4	6.68	123.24	119.90
26	A	2666	C	N3-C2-O2	-6.68	117.22	121.90
1	a	1533	C	C6-N1-C2	-6.68	117.63	120.30
1	a	1086	U	N3-C2-O2	-6.67	117.53	122.20
26	A	1774	C	C6-N1-C2	-6.67	117.63	120.30
26	A	1305	C	C5-C6-N1	6.67	124.33	121.00
3	c	117	ASP	CB-CG-OD1	6.64	124.28	118.30
7	g	139	ASP	CB-CG-OD1	6.64	124.28	118.30
1	a	439	U	N1-C2-O2	6.63	127.44	122.80
26	A	2072	C	O4'-C1'-N1	6.63	113.50	108.20
1	a	1056	U	N3-C2-O2	-6.63	117.56	122.20
26	A	399	U	N3-C2-O2	-6.62	117.57	122.20
26	A	1716	U	N1-C2-O2	6.62	127.43	122.80
23	x	114	C	N3-C2-O2	-6.62	117.27	121.90
26	A	589	U	C5-C6-N1	6.61	126.00	122.70
26	A	140	C	C6-N1-C2	-6.59	117.66	120.30
6	f	72	ASP	CB-CG-OD1	6.59	124.23	118.30
1	a	1037	C	C5-C6-N1	6.58	124.29	121.00
26	A	1314	C	C2-N1-C1'	6.58	126.04	118.80
26	A	1442	U	C5-C6-N1	6.57	125.99	122.70
26	A	1061	U	OP2-P-O3'	6.57	119.65	105.20
1	a	549	C	C5-C6-N1	6.56	124.28	121.00
13	m	57	ASP	CB-CG-OD1	6.55	124.20	118.30
1	a	413	G	N9-C4-C5	-6.55	102.78	105.40
19	s	4	LEU	CB-CG-CD1	-6.54	99.87	111.00
1	a	564	C	N1-C2-O2	6.53	122.82	118.90
26	A	283	G	C6-N1-C2	-6.53	121.18	125.10
57	6	34	LEU	CB-CG-CD1	-6.53	99.90	111.00
1	a	527	G7M	P-O3'-C3'	6.53	127.53	119.70
26	A	2617	U	N1-C2-O2	6.52	127.37	122.80
10	j	75	ASP	CB-CG-OD1	6.52	124.17	118.30
1	a	1240	U	C4-C5-C6	6.51	123.61	119.70
26	A	198	C	C6-N1-C2	-6.51	117.70	120.30
1	a	989	U	N1-C2-O2	6.51	127.36	122.80
26	A	143	C	C6-N1-C2	-6.50	117.70	120.30
1	a	1539	C	N1-C2-O2	-6.50	115.00	118.90
26	A	635	C	C6-N1-C2	-6.50	117.70	120.30
26	A	182	A	N7-C8-N9	6.50	117.05	113.80
26	A	2329	U	C5-C6-N1	6.49	125.95	122.70
26	A	1656	C	C6-N1-C2	-6.49	117.70	120.30
26	A	2250	G	N7-C8-N9	6.49	116.34	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	413	G	C4-C5-N7	6.49	113.39	110.80
26	A	2822	G	C5-C6-O6	-6.48	124.71	128.60
26	A	885	C	C5-C4-N4	-6.48	115.67	120.20
26	A	1498	C	N1-C2-O2	6.46	122.77	118.90
26	A	2558	C	C5-C6-N1	6.46	124.23	121.00
1	a	611	C	N3-C2-O2	-6.45	117.38	121.90
26	A	933	A	C2-N3-C4	6.45	113.83	110.60
26	A	361	G	C5-C6-O6	-6.45	124.73	128.60
26	A	890	C	N3-C2-O2	-6.45	117.38	121.90
1	a	1317	C	N3-C2-O2	-6.45	117.39	121.90
1	a	968	A	N3-C4-N9	-6.44	122.25	127.40
1	a	1028	C	N1-C2-O2	6.44	122.77	118.90
26	A	2305	U	C5-C4-O4	-6.44	122.04	125.90
1	a	110	C	N1-C2-O2	6.43	122.76	118.90
1	a	811	C	N1-C2-O2	6.43	122.76	118.90
23	x	114	C	C6-N1-C1'	-6.42	113.09	120.80
26	A	1886	U	N3-C2-O2	-6.42	117.70	122.20
1	a	795	C	C5-C6-N1	6.42	124.21	121.00
26	A	1947	C	C6-N1-C2	-6.42	117.73	120.30
26	A	2515	C	C5-C6-N1	6.42	124.21	121.00
14	n	32	ASP	CB-CG-OD1	6.41	124.07	118.30
30	E	134	LEU	CA-CB-CG	6.41	130.03	115.30
1	a	529	G	C6-C5-N7	-6.40	126.56	130.40
26	A	358	U	N1-C2-O2	6.39	127.27	122.80
26	A	343	C	N3-C2-O2	-6.38	117.43	121.90
17	q	75	VAL	CA-CB-CG2	6.38	120.47	110.90
1	a	610	U	N1-C2-O2	6.38	127.26	122.80
26	A	628	G	C4-N9-C1'	6.38	134.79	126.50
26	A	1816	C	N1-C2-O2	6.38	122.73	118.90
26	A	888	C	O4'-C1'-N1	6.35	113.28	108.20
1	a	529	G	C8-N9-C4	6.35	108.94	106.40
1	a	735	C	C5-C6-N1	6.35	124.17	121.00
2	b	81	ASP	CB-CG-OD1	6.34	124.01	118.30
26	A	305	C	C5-C6-N1	6.34	124.17	121.00
26	A	758	C	C6-N1-C2	-6.33	117.77	120.30
1	a	1393	U	N1-C2-O2	6.33	127.23	122.80
26	A	1446	C	C5-C6-N1	6.33	124.16	121.00
26	A	2118	U	C5-C4-O4	-6.33	122.10	125.90
26	A	2254	C	N1-C2-O2	6.32	122.69	118.90
26	A	2150	C	C5-C6-N1	6.31	124.16	121.00
26	A	1402	U	N3-C2-O2	-6.31	117.78	122.20
26	A	67	U	N3-C4-O4	6.31	123.82	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1537	U	C5-C6-N1	6.31	125.85	122.70
2	b	134	LEU	CA-CB-CG	6.30	129.79	115.30
26	A	2559	C	C6-N1-C2	-6.30	117.78	120.30
26	A	2248	C	N1-C2-O2	6.29	122.68	118.90
40	O	69	ASP	CB-CG-OD1	6.29	123.96	118.30
26	A	2637	U	N1-C2-O2	6.29	127.20	122.80
26	A	399	U	N1-C2-O2	6.29	127.20	122.80
1	a	106	C	C6-N1-C2	-6.28	117.79	120.30
26	A	999	U	N3-C2-O2	-6.28	117.81	122.20
22	v	67	C	C6-N1-C2	-6.28	117.79	120.30
26	A	1446	C	C6-N1-C2	-6.27	117.79	120.30
24	y	70	U	N3-C2-O2	-6.26	117.82	122.20
26	A	912	C	N1-C2-O2	6.25	122.65	118.90
26	A	2656	U	C2-N1-C1'	6.25	125.19	117.70
46	U	51	LEU	CA-CB-CG	6.24	129.66	115.30
26	A	1880	U	N3-C2-O2	-6.24	117.83	122.20
25	z	107	LEU	CB-CG-CD2	-6.24	100.40	111.00
1	a	177	G	N3-C4-C5	-6.24	125.48	128.60
26	A	853	C	C5-C6-N1	6.24	124.12	121.00
52	0	2	VAL	CG1-CB-CG2	-6.24	100.92	110.90
24	y	73	G	N3-C4-C5	6.23	131.71	128.60
26	A	1104	C	C6-N1-C2	-6.23	117.81	120.30
30	E	109	LEU	CA-CB-CG	6.23	129.62	115.30
41	P	71	ARG	CG-CD-NE	-6.23	98.72	111.80
26	A	960	A	OP1-P-O3'	6.22	118.89	105.20
46	U	40	LEU	CA-CB-CG	6.22	129.60	115.30
1	a	1382	C	N3-C2-O2	-6.22	117.55	121.90
9	i	93	LEU	CA-CB-CG	6.22	129.60	115.30
26	A	2254	C	N3-C2-O2	-6.21	117.55	121.90
26	A	832	U	N3-C2-O2	-6.21	117.85	122.20
26	A	2637	U	N3-C2-O2	-6.20	117.86	122.20
14	n	60	ARG	CG-CD-NE	-6.19	98.79	111.80
1	a	545	C	C6-N1-C2	-6.19	117.82	120.30
1	a	750	C	C6-N1-C2	-6.19	117.82	120.30
1	a	1325	C	C6-N1-C2	-6.19	117.82	120.30
1	a	955	U	N1-C2-O2	6.18	127.13	122.80
25	z	610	LEU	CA-CB-CG	6.18	129.51	115.30
26	A	2043	C	C2-N1-C1'	6.17	125.59	118.80
26	A	206	U	N1-C2-O2	6.17	127.12	122.80
1	a	397	A	C2-N3-C4	6.17	113.68	110.60
1	a	1350	A	O5'-P-OP1	-6.17	100.15	105.70
26	A	2300	C	C6-N1-C2	-6.17	117.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	356	G	C8-N9-C4	-6.16	103.94	106.40
26	A	243	U	N3-C2-O2	-6.16	117.89	122.20
26	A	206	U	N3-C2-O2	-6.15	117.89	122.20
23	x	104	U	N3-C2-O2	-6.15	117.89	122.20
26	A	2739	U	N1-C2-O2	6.15	127.11	122.80
26	A	1352	U	N3-C2-O2	-6.15	117.90	122.20
26	A	965	C	C6-N1-C2	-6.14	117.84	120.30
1	a	968	A	C4-C5-C6	-6.14	113.93	117.00
26	A	1486	U	C5-C6-N1	6.14	125.77	122.70
26	A	2756	U	OP1-P-O3'	6.13	118.69	105.20
1	a	552	U	C6-N1-C2	-6.13	117.32	121.00
26	A	2248	C	C5-C6-N1	6.13	124.06	121.00
1	a	1509	C	C6-N1-C2	-6.12	117.85	120.30
1	a	896	C	C6-N1-C2	-6.12	117.85	120.30
1	a	1237	C	OP1-P-O3'	6.12	118.66	105.20
24	y	27	C	C6-N1-C2	-6.12	117.85	120.30
1	a	1469	C	N3-C2-O2	-6.12	117.62	121.90
1	a	1403	C	N3-C2-O2	-6.11	117.62	121.90
1	a	300	A	C8-N9-C4	-6.11	103.36	105.80
26	A	628	G	C8-N9-C1'	-6.11	119.06	127.00
26	A	2302	U	C6-N1-C2	-6.11	117.33	121.00
26	A	192	C	N1-C2-O2	6.11	122.56	118.90
27	B	49	C	C6-N1-C2	-6.11	117.86	120.30
1	a	340	U	N3-C2-O2	-6.11	117.93	122.20
1	a	368	U	N1-C2-N3	6.11	118.56	114.90
1	a	893	C	C6-N1-C2	-6.10	117.86	120.30
1	a	1029	U	C5-C6-N1	6.10	125.75	122.70
41	P	113	LEU	CA-CB-CG	6.09	129.31	115.30
26	A	2492	U	N1-C2-O2	6.08	127.06	122.80
26	A	2188	U	C6-N1-C2	-6.08	117.35	121.00
26	A	2615	U	N1-C2-O2	6.08	127.06	122.80
1	a	267	C	O5'-P-OP2	-6.08	100.23	105.70
26	A	919	U	N3-C2-O2	-6.07	117.95	122.20
1	a	252	U	N3-C2-O2	-6.07	117.95	122.20
23	x	114	C	C5-C6-N1	6.07	124.04	121.00
26	A	2759	G	N1-C6-O6	-6.07	116.26	119.90
26	A	2797	U	C5-C6-N1	6.07	125.73	122.70
26	A	1487	U	C5-C6-N1	6.06	125.73	122.70
26	A	1886	U	N1-C2-O2	6.06	127.04	122.80
26	A	2649	C	C5-C6-N1	6.06	124.03	121.00
1	a	214	C	C6-N1-C2	-6.05	117.88	120.30
26	A	2656	U	N3-C2-O2	-6.05	117.96	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	888	C	C5-C6-N1	6.04	124.02	121.00
26	A	1499	C	C5-C6-N1	6.04	124.02	121.00
23	x	96	C	C5-C6-N1	6.04	124.02	121.00
26	A	2758	A	N1-C6-N6	-6.04	114.97	118.60
26	A	1289	C	C2-N1-C1'	6.04	125.44	118.80
1	a	993	G	N3-C4-N9	6.04	129.62	126.00
26	A	2248	C	C6-N1-C2	-6.03	117.89	120.30
1	a	1532	U	C5-C6-N1	6.03	125.71	122.70
26	A	356	G	C6-C5-N7	-6.03	126.78	130.40
26	A	2730	C	C6-N1-C2	-6.03	117.89	120.30
26	A	1499	C	C6-N1-C2	-6.02	117.89	120.30
1	a	1535	C	N1-C2-O2	6.02	122.51	118.90
1	a	1466	C	C6-N1-C2	-6.02	117.89	120.30
1	a	842	U	C5-C6-N1	6.02	125.71	122.70
1	a	307	C	C6-N1-C2	-6.02	117.89	120.30
26	A	748	G	OP2-P-O3'	6.02	118.44	105.20
26	A	2769	U	N3-C2-O2	-6.01	117.99	122.20
26	A	1104	C	C5-C6-N1	6.01	124.01	121.00
23	x	128	C	C3'-C2'-C1'	6.01	106.31	101.50
26	A	67	U	C5-C4-O4	-6.00	122.30	125.90
26	A	867	C	N3-C2-O2	-6.00	117.70	121.90
26	A	901	C	C5-C6-N1	6.00	124.00	121.00
1	a	338	A	N7-C8-N9	5.99	116.80	113.80
1	a	564	C	N3-C2-O2	-5.99	117.70	121.90
26	A	546	U	C6-N1-C2	-5.99	117.40	121.00
26	A	1199	U	C5-C6-N1	5.99	125.70	122.70
57	6	4	ASP	CB-CG-OD1	5.99	123.69	118.30
1	a	36	C	C5-C6-N1	5.99	123.99	121.00
26	A	2720	U	N3-C2-O2	-5.98	118.01	122.20
52	0	21	LEU	CA-CB-CG	5.98	129.06	115.30
1	a	754	C	N3-C2-O2	-5.97	117.72	121.90
24	y	68	C	C6-N1-C2	-5.97	117.91	120.30
26	A	1150	C	C5-C6-N1	5.97	123.98	121.00
1	a	340	U	N1-C2-O2	5.96	126.97	122.80
26	A	2300	C	C2-N1-C1'	5.96	125.36	118.80
26	A	2408	U	C5-C6-N1	5.95	125.67	122.70
26	A	1931	U	N3-C2-O2	-5.95	118.04	122.20
26	A	2047	C	C6-N1-C2	-5.94	117.92	120.30
23	x	131	C	C5-C6-N1	5.94	123.97	121.00
26	A	1438	U	N3-C2-O2	-5.94	118.05	122.20
26	A	1078	U	OP1-P-OP2	-5.93	110.70	119.60
1	a	385	C	C6-N1-C2	-5.93	117.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	143	C	C5-C6-N1	5.93	123.96	121.00
26	A	1313	U	C6-N1-C1'	-5.93	112.90	121.20
26	A	2636	C	N1-C2-O2	5.92	122.45	118.90
27	B	74	U	N3-C2-O2	-5.92	118.06	122.20
26	A	1539	U	C5-C6-N1	5.92	125.66	122.70
31	F	48	LEU	CA-CB-CG	5.92	128.91	115.30
26	A	639	U	C6-N1-C2	-5.91	117.45	121.00
26	A	1963	U	O4'-C1'-N1	5.91	112.93	108.20
26	A	278	A	N3-C4-C5	-5.91	122.66	126.80
26	A	1788	C	C6-N1-C2	-5.91	117.94	120.30
26	A	2103	C	N1-C2-O2	5.91	122.44	118.90
1	a	972	C	N3-C2-O2	-5.91	117.77	121.90
23	x	129	U	C5'-C4'-C3'	5.91	125.45	116.00
1	a	529	G	N3-C4-N9	5.90	129.54	126.00
1	a	1227	A	N9-C1'-C2'	-5.90	105.52	112.00
1	a	1395	C	N1-C2-O2	5.89	122.44	118.90
18	r	16	GLY	N-CA-C	-5.89	98.36	113.10
2	b	56	LEU	CA-CB-CG	5.89	128.85	115.30
1	a	516	PSU	O3'-P-O5'	-5.88	92.82	104.00
26	A	1658	C	C6-N1-C2	-5.88	117.95	120.30
26	A	2044	C	C6-N1-C2	-5.88	117.95	120.30
26	A	2142	A	C8-N9-C4	-5.88	103.45	105.80
1	a	1314	C	C6-N1-C2	-5.88	117.95	120.30
26	A	1093	G	C5-C6-O6	-5.88	125.07	128.60
26	A	2474	U	N3-C2-O2	-5.88	118.09	122.20
1	a	891	U	N1-C2-O2	5.87	126.91	122.80
26	A	1585	C	N1-C2-O2	5.87	122.42	118.90
26	A	2765	A	C2-N3-C4	5.87	113.53	110.60
27	B	42	C	N3-C2-O2	-5.87	117.79	121.90
1	a	1262	C	N1-C2-O2	5.86	122.42	118.90
1	a	300	A	N7-C8-N9	5.86	116.73	113.80
1	a	1240	U	C5-C6-N1	-5.85	119.77	122.70
26	A	2615	U	N3-C2-O2	-5.85	118.10	122.20
26	A	1716	U	N3-C2-O2	-5.85	118.11	122.20
1	a	1427	C	C5-C6-N1	5.85	123.92	121.00
26	A	1123	C	C6-N1-C2	-5.84	117.96	120.30
26	A	1848	A	N7-C8-N9	5.84	116.72	113.80
26	A	1064	C	C6-N1-C2	-5.84	117.97	120.30
39	N	79	LEU	CA-CB-CG	5.84	128.73	115.30
26	A	200	U	N1-C2-O2	5.84	126.89	122.80
26	A	2515	C	C6-N1-C2	-5.84	117.97	120.30
26	A	1171	G	N7-C8-N9	5.83	116.02	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	Q	108	LEU	CA-CB-CG	5.83	128.71	115.30
1	a	1148	U	N1-C2-O2	5.83	126.88	122.80
1	a	1348	U	N1-C2-O2	5.83	126.88	122.80
20	t	4	LYS	N-CA-CB	5.82	121.08	110.60
24	y	67(A)	U	C5-C6-N1	5.82	125.61	122.70
23	x	133	C	N1-C2-O2	5.82	122.39	118.90
1	a	896	C	C5-C6-N1	5.82	123.91	121.00
26	A	2142	A	N7-C8-N9	5.82	116.71	113.80
26	A	2821	A	O5'-P-OP2	-5.82	100.46	105.70
26	A	1931	U	N1-C2-O2	5.81	126.87	122.80
26	A	2896	C	C6-N1-C2	-5.81	117.98	120.30
1	a	470	C	C6-N1-C2	-5.80	117.98	120.30
22	v	1	C	N3-C2-O2	-5.80	117.84	121.90
26	A	672	C	C6-N1-C2	-5.80	117.98	120.30
25	z	397	LEU	CB-CG-CD1	5.80	120.86	111.00
1	a	719	C	N3-C2-O2	-5.79	117.84	121.90
26	A	1776	G	C4-N9-C1'	5.79	134.03	126.50
26	A	356	G	C4-N9-C1'	5.79	134.02	126.50
26	A	672	C	C5-C6-N1	5.79	123.89	121.00
1	a	58	C	C5-C6-N1	5.78	123.89	121.00
26	A	2575	C	C6-N1-C2	-5.77	117.99	120.30
26	A	857	G	N7-C8-N9	5.77	115.98	113.10
1	a	1278	G	C2-N3-C4	5.77	114.78	111.90
26	A	702	U	N1-C2-O2	5.77	126.84	122.80
26	A	1372	U	N3-C2-O2	-5.76	118.17	122.20
1	a	754	C	C2-N1-C1'	5.76	125.14	118.80
1	a	997	U	C5-C6-N1	5.76	125.58	122.70
26	A	1055	G	C2-N3-C4	5.76	114.78	111.90
26	A	1087	G	N7-C8-N9	5.76	115.98	113.10
26	A	1629	U	N3-C2-O2	-5.76	118.17	122.20
26	A	2667	C	C6-N1-C2	-5.76	118.00	120.30
26	A	731	C	C6-N1-C2	-5.75	118.00	120.30
26	A	998	C	C6-N1-C2	-5.75	118.00	120.30
1	a	353	A	OP2-P-O3'	5.75	117.85	105.20
26	A	738	G	N3-C2-N2	-5.75	115.88	119.90
26	A	1774	C	N3-C2-O2	-5.75	117.88	121.90
26	A	2146	C	N1-C2-O2	5.74	122.35	118.90
26	A	889	C	N1-C2-O2	5.74	122.34	118.90
26	A	2465	C	C6-N1-C2	-5.74	118.00	120.30
1	a	1317	C	C2-N1-C1'	5.73	125.11	118.80
1	a	1148	U	N3-C2-O2	-5.73	118.19	122.20
1	a	307	C	C2-N1-C1'	5.73	125.10	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	195	A	OP1-P-O3'	5.73	117.81	105.20
26	A	2716	C	C6-N1-C2	-5.73	118.01	120.30
26	A	2110	G	N3-C4-N9	-5.73	122.56	126.00
26	A	669	G	C4-N9-C1'	5.72	133.94	126.50
26	A	1936	A	N3-C4-N9	-5.72	122.82	127.40
1	a	1403	C	C6-N1-C2	-5.72	118.01	120.30
27	B	27	C	N3-C2-O2	-5.72	117.89	121.90
26	A	2637	U	C2-N1-C1'	5.72	124.56	117.70
14	n	17	ASP	CB-CG-OD1	5.72	123.44	118.30
26	A	2147	A	C8-N9-C4	-5.72	103.51	105.80
26	A	942	G	N1-C6-O6	-5.71	116.47	119.90
26	A	393	C	C6-N1-C2	-5.71	118.02	120.30
26	A	182	A	C8-N9-C4	-5.71	103.52	105.80
26	A	114	U	N3-C2-O2	-5.71	118.21	122.20
2	b	213	LEU	CB-CG-CD1	5.71	120.70	111.00
26	A	281	C	C6-N1-C2	-5.70	118.02	120.30
26	A	937	C	C6-N1-C2	-5.70	118.02	120.30
26	A	2637	U	C6-N1-C2	-5.70	117.58	121.00
26	A	965	C	C5-C6-N1	5.70	123.85	121.00
23	x	87	A	OP1-P-O3'	5.69	117.73	105.20
26	A	919	U	N1-C2-O2	5.69	126.79	122.80
26	A	109	C	C6-N1-C2	-5.69	118.02	120.30
1	a	469	C	N1-C2-O2	5.69	122.31	118.90
1	a	1241	G	C2-N3-C4	5.69	114.74	111.90
26	A	853	C	C6-N1-C2	-5.69	118.03	120.30
1	a	256	U	C5-C6-N1	5.68	125.54	122.70
26	A	2537	U	N3-C2-O2	-5.68	118.22	122.20
1	a	611	C	C6-N1-C2	-5.68	118.03	120.30
26	A	884	U	N1-C2-O2	-5.68	118.82	122.80
26	A	885	C	C6-N1-C2	-5.68	118.03	120.30
26	A	343	C	C5-C6-N1	5.68	123.84	121.00
26	A	2158	A	C8-N9-C4	-5.68	103.53	105.80
26	A	278	A	N3-C4-N9	5.67	131.94	127.40
41	P	71	ARG	NE-CZ-NH1	-5.67	117.47	120.30
23	x	121	U	N1-C2-O2	5.67	126.77	122.80
26	A	2558	C	C6-N1-C2	-5.67	118.03	120.30
1	a	795	C	C6-N1-C2	-5.67	118.03	120.30
1	a	78	A	C8-N9-C4	-5.66	103.53	105.80
23	x	113	C	OP1-P-O3'	5.66	117.65	105.20
24	y	40	C	C2-N1-C1'	5.66	125.02	118.80
26	A	310	A	O5'-P-OP1	-5.66	100.61	105.70
26	A	546	U	N3-C2-O2	-5.66	118.24	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1086	U	N1-C2-O2	5.65	126.76	122.80
26	A	2710	C	C6-N1-C2	-5.65	118.04	120.30
26	A	1152	C	C6-N1-C2	-5.65	118.04	120.30
1	a	1538	C	C5-C6-N1	5.65	123.82	121.00
26	A	420	C	C6-N1-C2	-5.65	118.04	120.30
26	A	886	A	O3'-P-O5'	5.65	114.73	104.00
11	k	96	ILE	CG1-CB-CG2	-5.65	98.98	111.40
26	A	2769	U	N1-C2-O2	5.64	126.75	122.80
26	A	658	U	C5-C6-N1	5.64	125.52	122.70
26	A	1470	A	N7-C8-N9	5.64	116.62	113.80
26	A	2746	U	C5-C6-N1	5.64	125.52	122.70
1	a	1537	U	C6-N1-C2	-5.64	117.62	121.00
26	A	2066	C	O4'-C1'-N1	5.64	112.71	108.20
23	x	130	G	N9-C1'-C2'	-5.64	105.80	112.00
26	A	852	U	C5-C6-N1	5.63	125.52	122.70
24	y	35	C	C6-N1-C2	-5.63	118.05	120.30
26	A	1323	C	O5'-P-OP1	-5.63	100.63	105.70
13	m	47	LEU	CA-CB-CG	5.63	128.25	115.30
26	A	353	C	C6-N1-C2	-5.63	118.05	120.30
26	A	2870	C	C6-N1-C2	-5.63	118.05	120.30
27	B	49	C	C5-C6-N1	5.63	123.81	121.00
26	A	418	C	C6-N1-C2	-5.62	118.05	120.30
1	a	943	U	N3-C2-O2	-5.62	118.27	122.20
26	A	840	C	C6-N1-C2	-5.62	118.05	120.30
26	A	883	G	C6-C5-N7	-5.62	127.03	130.40
30	E	153	LEU	CA-CB-CG	5.62	128.23	115.30
1	a	313	A	N7-C8-N9	5.62	116.61	113.80
26	A	79	C	C6-N1-C2	-5.62	118.05	120.30
26	A	915	C	C2-N1-C1'	5.61	124.97	118.80
26	A	1832	C	C5-C6-N1	5.61	123.81	121.00
5	e	35	LEU	CB-CG-CD1	-5.61	101.46	111.00
26	A	335	C	C6-N1-C2	-5.61	118.06	120.30
26	A	2591	C	C6-N1-C2	-5.61	118.06	120.30
26	A	2267	A	N1-C2-N3	-5.61	126.50	129.30
1	a	915	A	N1-C6-N6	-5.60	115.24	118.60
26	A	1880	U	N1-C2-O2	5.60	126.72	122.80
26	A	2109	U	C5-C6-N1	5.60	125.50	122.70
36	K	92	GLU	CA-CB-CG	5.60	125.72	113.40
1	a	1094	G	O4'-C1'-N9	5.60	112.68	108.20
26	A	1759	A	C2-N3-C4	5.60	113.40	110.60
26	A	2430	A	O5'-P-OP2	5.60	117.42	110.70
1	a	163	C	N1-C2-O2	5.59	122.26	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	73	G	N3-C4-N9	-5.59	122.64	126.00
1	a	264	C	C6-N1-C2	-5.59	118.06	120.30
26	A	135	U	C5-C6-N1	5.59	125.49	122.70
26	A	1047	G	O4'-C1'-N9	5.59	112.67	108.20
26	A	897	C	C6-N1-C2	-5.58	118.07	120.30
26	A	353	C	C5-C6-N1	5.58	123.79	121.00
24	y	56	C	C6-N1-C2	-5.58	118.07	120.30
24	y	36	A	C2-N3-C4	5.57	113.39	110.60
24	y	47(P)	C	C6-N1-C2	-5.57	118.07	120.30
26	A	2006	C	C6-N1-C2	-5.57	118.07	120.30
26	A	2295	C	C6-N1-C2	-5.57	118.07	120.30
1	a	866	C	C6-N1-C2	-5.57	118.07	120.30
26	A	628	G	C6-C5-N7	-5.57	127.06	130.40
26	A	1685	C	C6-N1-C2	-5.56	118.07	120.30
22	v	39	C	C5-C6-N1	5.56	123.78	121.00
26	A	454	A	OP2-P-O3'	5.56	117.44	105.20
24	y	69	U	C5-C6-N1	5.56	125.48	122.70
26	A	2248	C	C2-N1-C1'	5.56	124.91	118.80
26	A	275	C	N1-C2-O2	5.55	122.23	118.90
26	A	479	A	OP1-P-O3'	5.55	117.42	105.20
26	A	1804	C	C6-N1-C2	-5.55	118.08	120.30
26	A	1578	U	N3-C2-O2	-5.55	118.31	122.20
26	A	2153	C	C6-N1-C2	-5.55	118.08	120.30
1	a	552	U	C5-C6-N1	5.55	125.47	122.70
26	A	2179	C	C5-C4-N4	5.55	124.08	120.20
26	A	2164	C	N1-C2-O2	5.54	122.22	118.90
26	A	888	C	C2-N1-C1'	5.53	124.89	118.80
1	a	1028	C	N3-C2-O2	-5.53	118.03	121.90
26	A	2683	C	C2-N1-C1'	5.53	124.88	118.80
1	a	99	C	C6-N1-C2	-5.53	118.09	120.30
1	a	470	C	C5-C6-N1	5.53	123.76	121.00
26	A	281	C	C5-C6-N1	5.53	123.76	121.00
1	a	891	U	N3-C2-O2	-5.53	118.33	122.20
26	A	2173	A	N3-C4-C5	-5.53	122.93	126.80
1	a	368	U	C2-N3-C4	-5.52	123.69	127.00
26	A	544	C	C6-N1-C2	-5.52	118.09	120.30
28	C	83	ASP	CB-CG-OD1	5.52	123.27	118.30
1	a	1158	C	C5-C6-N1	5.51	123.76	121.00
26	A	1282	U	C5-C6-N1	5.51	125.46	122.70
12	l	25	ALA	N-CA-CB	5.51	117.82	110.10
26	A	1658	C	C5-C6-N1	5.51	123.76	121.00
1	a	820	U	OP2-P-O3'	5.51	117.32	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	810	C	N1-C2-O2	5.51	122.20	118.90
26	A	353	C	C2-N1-C1'	5.51	124.86	118.80
24	y	40	C	N1-C2-O2	5.51	122.20	118.90
26	A	2130	U	N1-C2-O2	5.51	126.66	122.80
26	A	2492	U	N3-C2-O2	-5.51	118.34	122.20
26	A	2430	A	C2-N3-C4	5.51	113.35	110.60
26	A	200	U	N3-C2-O2	-5.50	118.35	122.20
26	A	1843	C	C6-N1-C2	-5.50	118.10	120.30
9	i	89	TYR	CA-CB-CG	5.49	123.84	113.40
1	a	811	C	N3-C2-O2	-5.49	118.06	121.90
26	A	2200	C	C5-C6-N1	5.49	123.75	121.00
26	A	1398	C	C5-C6-N1	5.49	123.74	121.00
26	A	1157	G	C4-N9-C1'	5.49	133.63	126.50
44	S	84	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	a	644	U	N3-C2-O2	-5.48	118.36	122.20
26	A	985	C	C6-N1-C2	-5.48	118.11	120.30
32	G	70	LEU	CA-CB-CG	5.48	127.91	115.30
26	A	2840	C	C6-N1-C2	-5.48	118.11	120.30
27	B	37	C	C6-N1-C2	-5.48	118.11	120.30
26	A	737	C	C6-N1-C2	-5.47	118.11	120.30
28	C	153	LEU	CB-CG-CD1	5.47	120.31	111.00
1	a	163	C	N3-C2-O2	-5.47	118.07	121.90
26	A	887	U	C6-N1-C2	-5.47	117.72	121.00
1	a	1384	C	C2-N1-C1'	5.46	124.81	118.80
26	A	12	U	N3-C2-O2	-5.46	118.37	122.20
26	A	2822	G	C4-C5-N7	5.46	112.99	110.80
27	B	26	C	C6-N1-C2	-5.46	118.11	120.30
8	h	58	LEU	CA-CB-CG	5.46	127.86	115.30
26	A	872	U	C5-C6-N1	5.46	125.43	122.70
1	a	737	C	C5-C6-N1	5.46	123.73	121.00
26	A	2194	U	C5-C6-N1	5.46	125.43	122.70
1	a	214	C	C5-C6-N1	5.46	123.73	121.00
1	a	1184	G	N3-C4-C5	-5.46	125.87	128.60
26	A	912	C	C2-N1-C1'	5.46	124.80	118.80
1	a	454	G	N7-C8-N9	5.46	115.83	113.10
26	A	2757	A	C5-C6-N1	-5.45	114.97	117.70
27	B	55	U	N1-C2-O2	5.45	126.62	122.80
1	a	1027	C	C2-N1-C1'	5.45	124.79	118.80
1	a	1404	C	C5-C6-N1	5.45	123.72	121.00
26	A	1349	C	C6-N1-C2	-5.45	118.12	120.30
26	A	2716	C	C5-C6-N1	5.45	123.72	121.00
26	A	512	G	O4'-C1'-N9	5.45	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	t	78	LEU	CB-CG-CD2	-5.44	101.75	111.00
25	z	107	LEU	CA-CB-CG	5.44	127.81	115.30
26	A	475	C	C6-N1-C2	-5.44	118.12	120.30
31	F	65	LEU	CA-CB-CG	5.44	127.81	115.30
8	h	79	ARG	NE-CZ-NH2	5.44	123.02	120.30
26	A	1087	G	C8-N9-C4	-5.44	104.23	106.40
23	x	118	G	C5'-C4'-O4'	5.43	115.62	109.10
1	a	308	C	C5-C6-N1	5.42	123.71	121.00
1	a	1348	U	N3-C2-O2	-5.42	118.41	122.20
1	a	1384	C	C6-N1-C2	-5.42	118.13	120.30
26	A	968	C	C5-C6-N1	5.42	123.71	121.00
26	A	1348	C	C2-N1-C1'	5.41	124.75	118.80
56	4	27	CYS	CA-CB-SG	5.41	123.74	114.00
26	A	143	C	C2-N1-C1'	5.41	124.75	118.80
23	x	131	C	N1-C1'-C2'	-5.41	106.05	112.00
26	A	122	G	C6-C5-N7	-5.41	127.16	130.40
26	A	1629	U	C6-N1-C2	-5.40	117.76	121.00
1	a	313	A	C8-N9-C4	-5.40	103.64	105.80
1	a	469	C	N3-C2-O2	-5.40	118.12	121.90
26	A	257	C	N1-C2-O2	5.40	122.14	118.90
1	a	956	U	N3-C2-O2	-5.39	118.42	122.20
26	A	2822	G	N1-C6-O6	5.39	123.14	119.90
26	A	1121	C	C6-N1-C2	-5.39	118.14	120.30
26	A	2636	C	C2-N1-C1'	5.39	124.73	118.80
1	a	723	U	N1-C2-O2	5.39	126.57	122.80
26	A	999	U	N1-C2-O2	5.39	126.57	122.80
1	a	623	C	C6-N1-C2	-5.39	118.14	120.30
26	A	2068	U	C5-C6-N1	5.38	125.39	122.70
26	A	702	U	C2-N1-C1'	5.38	124.16	117.70
26	A	1438	U	C5-C6-N1	5.38	125.39	122.70
1	a	1531	A	N7-C8-N9	5.37	116.49	113.80
26	A	529	A	O5'-P-OP2	-5.37	100.86	105.70
26	A	1352	U	N1-C2-O2	5.37	126.56	122.80
26	A	1747	U	C5-C6-N1	5.37	125.38	122.70
1	a	271	C	C6-N1-C2	-5.37	118.15	120.30
26	A	201	C	N3-C2-O2	-5.37	118.14	121.90
26	A	2901	C	C2-N1-C1'	5.37	124.70	118.80
23	x	131	C	C3'-C2'-C1'	5.36	105.79	101.50
26	A	532	A	C2-N3-C4	5.36	113.28	110.60
26	A	2103	C	N3-C2-O2	-5.36	118.15	121.90
28	C	100	ARG	NE-CZ-NH1	-5.36	117.62	120.30
26	A	1438	U	N1-C2-O2	5.36	126.55	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1662	U	N3-C2-O2	-5.36	118.45	122.20
50	Y	37	LEU	CA-CB-CG	5.35	127.61	115.30
24	y	73	G	C4-N9-C1'	-5.35	119.55	126.50
1	a	330	C	N3-C2-O2	-5.35	118.16	121.90
1	a	972	C	C6-N1-C2	-5.35	118.16	120.30
26	A	257	C	N3-C2-O2	-5.35	118.16	121.90
26	A	1085	A	C8-N9-C4	-5.34	103.66	105.80
26	A	2267	A	C2-N3-C4	5.34	113.27	110.60
27	B	30	C	C2-N1-C1'	5.34	124.68	118.80
30	E	147	LEU	CA-CB-CG	5.34	127.59	115.30
26	A	481	G	N9-C4-C5	-5.34	103.26	105.40
23	x	120	U	OP1-P-O3'	5.34	116.94	105.20
1	a	323	U	C5-C6-N1	5.34	125.37	122.70
26	A	2816	G	N3-C2-N2	-5.34	116.16	119.90
26	A	1022	G	C5-C6-O6	5.33	131.80	128.60
26	A	1843	C	C5-C6-N1	5.33	123.67	121.00
26	A	2785	C	C6-N1-C2	-5.33	118.17	120.30
1	a	1131	G	N7-C8-N9	5.33	115.76	113.10
23	x	129	U	P-O5'-C5'	5.32	129.42	120.90
26	A	886	A	O4'-C1'-N9	5.32	112.46	108.20
8	h	79	ARG	CA-CB-CG	5.32	125.10	113.40
1	a	1510	C	C6-N1-C2	-5.32	118.17	120.30
8	h	95	MET	CA-CB-CG	5.32	122.33	113.30
9	i	93	LEU	CB-CG-CD2	-5.32	101.96	111.00
26	A	2110	G	N1-C6-O6	-5.32	116.71	119.90
26	A	2720	U	N1-C2-O2	5.31	126.52	122.80
26	A	1941	C	C5-C6-N1	5.31	123.66	121.00
26	A	1956	U	C5-C6-N1	5.31	125.36	122.70
25	z	397	LEU	CB-CG-CD2	-5.31	101.97	111.00
26	A	635	C	C5-C6-N1	5.31	123.66	121.00
26	A	283	G	N9-C4-C5	5.31	107.52	105.40
26	A	1936	A	N9-C4-C5	5.31	107.92	105.80
26	A	286	U	C5-C6-N1	5.30	125.35	122.70
1	a	955	U	N3-C2-O2	-5.30	118.49	122.20
26	A	2745	C	C6-N1-C2	-5.30	118.18	120.30
26	A	2767	C	C6-N1-C2	-5.30	118.18	120.30
1	a	185	U	C5-C6-N1	5.29	125.35	122.70
1	a	103	U	N3-C2-O2	-5.29	118.50	122.20
1	a	1125	U	C5-C4-O4	-5.29	122.73	125.90
26	A	2173	A	N3-C4-N9	5.29	131.63	127.40
29	D	49	GLN	CA-CB-CG	5.29	125.03	113.40
26	A	687	C	N1-C2-O2	5.29	122.07	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2147	A	N7-C8-N9	5.29	116.44	113.80
23	x	133	C	C2-N1-C1'	5.28	124.61	118.80
26	A	885	C	OP1-P-O3'	5.28	116.82	105.20
26	A	886	A	OP1-P-OP2	-5.28	111.68	119.60
4	d	8	LEU	CA-CB-CG	5.28	127.45	115.30
22	v	1	C	C6-N1-C2	-5.28	118.19	120.30
22	v	75	C	C6-N1-C2	-5.28	118.19	120.30
26	A	1348	C	C5-C6-N1	5.28	123.64	121.00
26	A	1417	C	N1-C2-O2	5.27	122.06	118.90
26	A	2165	C	N3-C2-O2	-5.27	118.21	121.90
22	v	56	C	C6-N1-C2	-5.27	118.19	120.30
26	A	915	C	N1-C2-O2	5.27	122.06	118.90
26	A	2089	C	C6-N1-C2	-5.27	118.19	120.30
26	A	2141	G	C8-N9-C4	-5.27	104.29	106.40
1	a	1533	C	C5-C6-N1	5.27	123.64	121.00
1	a	945	G	N3-C4-N9	5.27	129.16	126.00
22	v	67	C	C2-N1-C1'	5.27	124.60	118.80
26	A	1108	U	C5-C6-N1	5.27	125.33	122.70
31	F	173	ASP	N-CA-C	-5.27	96.78	111.00
26	A	998	C	C5-C6-N1	5.26	123.63	121.00
26	A	1053	C	C6-N1-C2	-5.26	118.19	120.30
26	A	1398	C	C6-N1-C2	-5.26	118.19	120.30
26	A	1669	A	N3-C4-C5	-5.26	123.12	126.80
1	a	674	G	N7-C8-N9	5.26	115.73	113.10
26	A	1316	U	N3-C2-O2	-5.26	118.52	122.20
26	A	1941	C	C6-N1-C1'	-5.26	114.49	120.80
27	B	31	C	C2-N1-C1'	5.26	124.58	118.80
26	A	885	C	C5'-C4'-O4'	5.25	115.41	109.10
1	a	1109	C	C6-N1-C2	-5.25	118.20	120.30
22	v	34	C	N1-C2-O2	5.25	122.05	118.90
26	A	209	C	C6-N1-C2	-5.25	118.20	120.30
27	B	64	G	N9-C4-C5	-5.25	103.30	105.40
23	x	133	C	N3-C2-O2	-5.25	118.23	121.90
26	A	1536	C	P-O3'-C3'	5.25	125.99	119.70
26	A	2782	G	C6-C5-N7	-5.25	127.25	130.40
1	a	754	C	N1-C2-O2	5.24	122.05	118.90
26	A	1881	C	C6-N1-C2	-5.24	118.20	120.30
26	A	1893	C	N1-C2-O2	5.24	122.05	118.90
1	a	169	C	N1-C2-O2	5.24	122.05	118.90
23	x	104	U	N1-C2-O2	5.24	126.47	122.80
26	A	897	C	N1-C2-O2	5.24	122.05	118.90
26	A	2123	G	C8-N9-C4	-5.24	104.31	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	51	C	C5-C6-N1	5.24	123.62	121.00
5	e	80	LEU	CA-CB-CG	5.23	127.33	115.30
26	A	1816	C	N3-C2-O2	-5.23	118.24	121.90
1	a	877	G	O4'-C1'-N9	5.23	112.38	108.20
24	y	19	H2U	P-O3'-C3'	5.23	125.97	119.70
24	y	56	C	C5-C6-N1	5.23	123.61	121.00
26	A	1675	C	C6-N1-C2	-5.23	118.21	120.30
26	A	1894	C	C6-N1-C2	-5.22	118.21	120.30
26	A	888	C	N3-C4-C5	-5.22	119.81	121.90
13	m	91	ARG	CB-CG-CD	-5.22	98.03	111.60
24	y	48	G	C5-C6-O6	-5.21	125.47	128.60
26	A	1499	C	C6-N1-C1'	-5.21	114.55	120.80
1	a	56	U	C6-N1-C2	-5.21	117.87	121.00
26	A	2089	C	C5-C6-N1	5.21	123.60	121.00
7	g	65	LEU	CA-CB-CG	5.21	127.28	115.30
26	A	2211	A	N3-C4-C5	-5.21	123.16	126.80
26	A	946	C	C6-N1-C2	-5.20	118.22	120.30
26	A	2403	C	C6-N1-C2	-5.20	118.22	120.30
1	a	169	C	N3-C2-O2	-5.20	118.26	121.90
3	c	30	ASP	CB-CG-OD1	5.20	122.98	118.30
1	a	1132	C	N1-C2-O2	5.19	122.02	118.90
27	B	19	C	C5-C6-N1	5.19	123.60	121.00
15	o	86	LEU	C-N-CA	5.18	134.66	121.70
26	A	890	C	C4-C5-C6	-5.18	114.81	117.40
26	A	2130	U	N3-C2-O2	-5.18	118.57	122.20
26	A	2305	U	C5-C6-N1	-5.18	120.11	122.70
26	A	2165	C	N1-C2-O2	5.18	122.01	118.90
27	B	30	C	C5-C6-N1	5.18	123.59	121.00
46	U	83	GLY	N-CA-C	-5.18	100.15	113.10
26	A	458	G	O4'-C1'-N9	5.18	112.34	108.20
26	A	1685	C	C5-C6-N1	5.18	123.59	121.00
26	A	2151	U	C6-N1-C2	-5.17	117.90	121.00
1	a	1121	U	C5-C6-N1	5.17	125.29	122.70
1	a	110	C	N3-C2-O2	-5.17	118.28	121.90
26	A	2628	C	C6-N1-C2	-5.17	118.23	120.30
1	a	536	C	C2-N1-C1'	5.17	124.48	118.80
1	a	1395	C	N3-C2-O2	-5.17	118.28	121.90
26	A	1589	U	C5-C6-N1	5.16	125.28	122.70
26	A	2200	C	C6-N1-C2	-5.16	118.23	120.30
27	B	3	C	C5-C6-N1	5.16	123.58	121.00
26	A	2556	C	N1-C2-O2	5.16	122.00	118.90
26	A	1006	C	C6-N1-C2	-5.16	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	x	130	G	C3'-C2'-C1'	5.16	105.63	101.50
26	A	897	C	N3-C2-O2	-5.16	118.29	121.90
1	a	751	U	N3-C2-O2	-5.16	118.59	122.20
26	A	1161	C	O4'-C1'-N1	5.15	112.32	108.20
26	A	2036	C	C5-C6-N1	5.15	123.58	121.00
26	A	1157	G	N3-C4-N9	5.15	129.09	126.00
26	A	1055	G	N3-C4-C5	-5.14	126.03	128.60
26	A	2302	U	N1-C2-N3	5.14	117.99	114.90
1	a	163	C	C6-N1-C2	-5.14	118.24	120.30
26	A	209	C	C5-C6-N1	5.14	123.57	121.00
26	A	2306	C	C6-N1-C2	-5.14	118.24	120.30
26	A	1402	U	N1-C2-O2	5.14	126.40	122.80
26	A	1803	A	N7-C8-N9	5.14	116.37	113.80
26	A	1822	C	C6-N1-C2	-5.14	118.24	120.30
26	A	356	G	C4-C5-C6	5.14	121.88	118.80
26	A	2232	C	C5-C6-N1	5.14	123.57	121.00
18	r	28	LEU	CA-CB-CG	5.13	127.11	115.30
1	a	916	U	N3-C2-O2	-5.13	118.61	122.20
31	F	88	VAL	CG1-CB-CG2	-5.13	102.69	110.90
26	A	1725	U	N3-C2-O2	-5.13	118.61	122.20
26	A	890	C	C5-C4-N4	-5.13	116.61	120.20
26	A	2755	C	C6-N1-C2	-5.13	118.25	120.30
27	B	3	C	C6-N1-C2	-5.12	118.25	120.30
1	a	1318	A	C8-N9-C4	5.12	107.85	105.80
26	A	391	A	C2-N3-C4	5.12	113.16	110.60
26	A	2141	G	N7-C8-N9	5.12	115.66	113.10
26	A	114	U	C2-N1-C1'	5.12	123.84	117.70
26	A	1486	U	C6-N1-C2	-5.12	117.93	121.00
11	k	92	ARG	N-CA-CB	-5.12	101.39	110.60
26	A	1289	C	N1-C2-O2	5.12	121.97	118.90
26	A	1993	U	N3-C2-O2	-5.12	118.62	122.20
26	A	2044	C	C5-C6-N1	5.12	123.56	121.00
1	a	822	U	N3-C2-O2	-5.11	118.62	122.20
26	A	1512	C	C6-N1-C2	-5.11	118.26	120.30
26	A	1788	C	C5-C6-N1	5.11	123.56	121.00
26	A	807	U	N3-C2-O2	-5.11	118.63	122.20
26	A	276	U	OP2-P-O3'	5.10	116.42	105.20
8	h	82	LEU	CA-CB-CG	5.10	127.02	115.30
22	v	25	C	N1-C2-O2	5.10	121.96	118.90
26	A	485	C	C6-N1-C2	-5.10	118.26	120.30
15	o	55	LEU	CB-CG-CD2	-5.09	102.34	111.00
26	A	361	G	N7-C8-N9	5.09	115.65	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	891	G	OP1-P-OP2	-5.09	111.96	119.60
26	A	960	A	P-O3'-C3'	5.09	125.81	119.70
26	A	2099	U	C5-C6-N1	5.09	125.24	122.70
26	A	1052	C	N1-C2-O2	5.09	121.95	118.90
26	A	2576	G	C2-N3-C4	5.08	114.44	111.90
1	a	980	C	N3-C2-O2	-5.08	118.34	121.90
25	z	167	ARG	CA-CB-CG	-5.08	102.22	113.40
1	a	252	U	N1-C2-O2	5.08	126.35	122.80
13	m	33	LEU	CA-CB-CG	-5.08	103.62	115.30
26	A	225	C	C6-N1-C2	-5.07	118.27	120.30
29	D	128	ARG	CG-CD-NE	5.07	122.46	111.80
22	v	16	C	C5-C6-N1	5.07	123.54	121.00
1	a	623	C	C5-C6-N1	5.07	123.53	121.00
1	a	1390	U	N3-C2-O2	-5.07	118.65	122.20
26	A	16	C	C6-N1-C2	-5.07	118.27	120.30
26	A	769	U	C6-N1-C2	-5.06	117.96	121.00
44	S	64	ALA	N-CA-CB	5.06	117.19	110.10
1	a	1136	C	N1-C2-O2	5.06	121.94	118.90
23	x	109	C	P-O3'-C3'	5.06	125.78	119.70
1	a	1460	C	C6-N1-C2	-5.06	118.28	120.30
24	y	71	C	C6-N1-C2	-5.06	118.28	120.30
1	a	1526	G	OP2-P-O3'	5.06	116.33	105.20
19	s	15	LEU	CA-CB-CG	5.06	126.93	115.30
26	A	461	C	C6-N1-C2	-5.05	118.28	120.30
26	A	1157	G	C8-N9-C1'	-5.05	120.43	127.00
26	A	1848	A	C8-N9-C4	-5.05	103.78	105.80
26	A	2188	U	N3-C4-O4	5.05	122.94	119.40
1	a	739	C	C6-N1-C2	-5.05	118.28	120.30
26	A	1657	U	N3-C2-O2	-5.05	118.66	122.20
22	v	34	C	C2-N1-C1'	5.05	124.36	118.80
26	A	373	U	N1-C2-O2	5.05	126.33	122.80
26	A	2473	U	C5-C6-N1	5.05	125.22	122.70
26	A	860	U	N1-C2-O2	5.05	126.33	122.80
26	A	243	U	C2-N1-C1'	5.04	123.75	117.70
26	A	702	U	N3-C2-O2	-5.04	118.67	122.20
26	A	1812	U	N3-C2-O2	-5.04	118.67	122.20
26	A	2794	C	N1-C2-O2	5.04	121.93	118.90
26	A	900	A	N1-C6-N6	-5.04	115.58	118.60
26	A	1049	C	N1-C2-O2	5.04	121.92	118.90
26	A	1914	C	N1-C2-O2	5.04	121.92	118.90
26	A	889	C	C2-N1-C1'	5.04	124.34	118.80
26	A	2232	C	C6-N1-C2	-5.03	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	47(N)	C	C6-N1-C2	-5.02	118.29	120.30
26	A	383	C	N1-C2-O2	5.02	121.91	118.90
57	6	40	CYS	CB-CA-C	-5.02	100.36	110.40
26	A	1585	C	N3-C2-O2	-5.01	118.39	121.90
26	A	2039	U	N3-C2-O2	-5.01	118.69	122.20
26	A	2441	U	N3-C2-O2	-5.01	118.69	122.20
26	A	2751	G	N3-C4-C5	-5.01	126.09	128.60
24	y	71	C	C5-C6-N1	5.01	123.51	121.00
26	A	484	C	C5-C6-N1	5.01	123.51	121.00
26	A	1049	C	C2-N1-C1'	5.01	124.31	118.80
27	B	6	G	N3-C2-N2	-5.01	116.39	119.90
1	a	385	C	C5-C6-N1	5.01	123.50	121.00
26	A	1611	C	C2-N1-C1'	5.01	124.31	118.80
26	A	1803	A	N1-C2-N3	5.01	131.80	129.30
26	A	2248	C	N3-C2-O2	-5.01	118.39	121.90
1	a	528	C	C6-N1-C2	-5.01	118.30	120.30
1	a	1363	A	C2-N3-C4	5.01	113.10	110.60
26	A	2556	C	N3-C2-O2	-5.01	118.39	121.90
1	a	705	G	N3-C4-C5	-5.00	126.10	128.60
26	A	2143	C	N3-C2-O2	-5.00	118.40	121.90
26	A	435	C	N3-C2-O2	-5.00	118.40	121.90
26	A	2109	U	C6-N1-C2	-5.00	118.00	121.00

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 (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	1	3	GLY	Peptide
55	3	30	HIS	Peptide
28	C	120	ASP	Peptide
30	E	82	GLY	Peptide
31	F	172	PHE	Peptide
31	F	173	ASP	Mainchain
32	G	117	PRO	Peptide
32	G	174	LYS	Mainchain
34	H	2	GLN	Peptide
34	H	40	THR	Peptide

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Mol	Chain	Res	Type	Group
34	H	8	LYS	Mainchain
44	S	63	GLY	Peptide
46	U	16	LYS	Peptide
46	U	87	GLU	Peptide
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain
4	d	30	LYS	Mainchain
6	f	97	THR	Peptide
10	j	41	PRO	Peptide
10	j	56	HIS	Peptide
10	j	57	VAL	Mainchain
11	k	49	SER	Peptide
11	k	91	GLY	Peptide
12	l	42	LYS	Peptide
12	l	74	GLN	Peptide
16	p	44	SER	Mainchain
17	q	48	GLU	Peptide
17	q	50	ASN	Peptide
21	u	40	PRO	Mainchain
25	z	190	LEU	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	687	0	715	0	0
20	t	665	0	714	0	0
21	u	496	0	486	0	0
22	v	1642	0	839	0	0
23	x	1025	0	518	0	0
24	y	2031	0	1039	0	0
25	z	4853	0	4831	0	0
26	A	62335	0	31374	392	0
27	B	2570	0	1301	24	0
28	C	2083	0	2157	40	0
29	D	1565	0	1616	37	0
30	E	1552	0	1619	42	0
31	F	1411	0	1447	38	0
32	G	1323	0	1374	25	0
33	I	1032	0	1088	28	0
34	H	1111	0	1148	21	0
35	J	1129	0	1162	22	0
36	K	939	0	1012	17	0
37	L	1045	0	1117	22	0
38	M	1074	0	1157	20	0
39	N	961	0	1000	11	0
40	O	892	0	923	17	0
41	P	917	0	965	25	0
42	Q	947	0	1022	15	0
43	R	816	0	839	14	0
44	S	857	0	922	17	0
45	T	739	0	807	16	0
46	U	780	0	834	19	0
47	V	753	0	780	14	0
48	W	575	0	592	5	0
49	X	625	0	655	12	0
50	Y	509	0	543	6	0
51	Z	449	0	491	10	0
52	0	444	0	461	13	0
53	1	410	0	440	6	0
54	2	377	0	418	4	0
55	3	504	0	574	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	4	302	0	340	9	0
57	6	523	0	521	10	0
58	w	62	0	34	0	0
59	a	1	0	0	0	0
60	A	111	0	0	0	0
60	B	2	0	0	0	0
60	a	30	0	0	0	0
60	n	1	0	0	0	0
60	v	1	0	0	0	0
60	y	1	0	0	0	0
60	z	1	0	0	0	0
61	v	10	0	10	0	0
62	y	6	0	3	0	0
63	z	32	0	13	0	0
64	4	1	0	0	0	0
64	6	1	0	0	0	0
65	z	2	0	0	0	0
All	All	153177	0	104137	811	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 (811) 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)
36:K:35:VAL:HG21	36:K:69:VAL:HG12	1.61	0.82
26:A:745:1MG:HO2'	26:A:748:G:HO2'	1.28	0.76
30:E:172:ALA:HB3	30:E:195:GLN:HE21	1.50	0.75
26:A:1597:A:H5''	26:A:1598:A:H5'	1.70	0.74
26:A:329:G:H1	46:U:16:LYS:HZ2	1.35	0.73
31:F:37:MET:HG3	31:F:56:LEU:HD12	1.69	0.73
43:R:63:VAL:HG12	43:R:96:VAL:HG12	1.71	0.73
26:A:563:A:N3	42:Q:36:GLN:NE2	2.38	0.71
32:G:1:SER:HB3	32:G:61:TRP:HB3	1.73	0.70
26:A:320:A:N3	30:E:163:ASN:ND2	2.38	0.70
26:A:888:C:O2'	26:A:890:C:N4	2.25	0.69
26:A:1248:G:OP1	30:E:44:ARG:NH2	2.24	0.69
53:1:36:LYS:HB3	53:1:47:ILE:HD13	1.75	0.69
35:J:36:LEU:HD21	35:J:122:LEU:HB2	1.73	0.69
43:R:58:VAL:H	43:R:102:SER:HB2	1.57	0.68
31:F:110:ILE:HA	31:F:136:ILE:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1270:C:H5'	26:A:1271:G:H5'	1.75	0.68
26:A:2020:A:H62	52:O:5:ASN:HD21	1.39	0.67
39:N:35:LYS:NZ	39:N:110:MET:SD	2.65	0.67
45:T:12:ARG:HA	50:Y:29:ARG:HH22	1.58	0.67
26:A:877:A:O2'	26:A:900:A:N6	2.26	0.67
28:C:78:GLU:OE2	28:C:100:ARG:NH1	2.27	0.67
26:A:910:A:H62	38:M:12:MET:HA	1.60	0.67
28:C:83:ASP:OD2	28:C:86:ARG:NH1	2.27	0.67
30:E:129:PRO:HB3	30:E:159:LEU:HD11	1.77	0.67
29:D:5:VAL:HG22	29:D:202:ILE:HG22	1.78	0.66
26:A:572:A:OP2	43:R:79:ARG:NH2	2.27	0.66
26:A:276:U:O2'	26:A:278:A:N6	2.28	0.66
26:A:2032:G:H21	29:D:151:THR:HB	1.61	0.66
26:A:2032:G:O2'	29:D:150:GLN:NE2	2.29	0.66
26:A:441:U:O2'	30:E:41:GLN:NE2	2.28	0.66
47:V:32:GLY:O	47:V:93:ARG:NH2	2.30	0.65
26:A:468:G:OP2	54:2:37:LYS:NZ	2.29	0.65
26:A:1653:G:H3'	39:N:2:ARG:HG2	1.78	0.65
27:B:30:C:H1'	27:B:57:A:H61	1.61	0.65
40:O:55:GLU:HG3	40:O:57:ALA:H	1.62	0.64
26:A:1250:G:N7	37:L:18:ARG:NH2	2.46	0.64
26:A:2294:G:OP1	40:O:94:ARG:NH1	2.31	0.64
26:A:77:G:OP1	50:Y:52:ARG:NH2	2.29	0.64
27:B:48:U:OP1	40:O:30:ARG:NH2	2.30	0.64
30:E:51:GLU:OE2	30:E:88:ARG:NH1	2.30	0.64
53:1:16:THR:HG21	53:1:41:VAL:HG11	1.79	0.64
26:A:1171:G:N2	26:A:1178:C:N3	2.42	0.64
44:S:11:ARG:NH1	44:S:11:ARG:O	2.31	0.64
26:A:517:C:OP1	52:O:12:ARG:NH2	2.28	0.63
31:F:123:GLY:HA2	31:F:162:ASP:HB2	1.80	0.63
32:G:3:VAL:HG22	32:G:68:ARG:HH21	1.63	0.63
26:A:563:A:OP2	43:R:79:ARG:NH1	2.30	0.63
57:6:28:VAL:HG11	57:6:32:LEU:HD23	1.80	0.63
26:A:1244:A:HO2'	30:E:29:HIS:HE2	1.46	0.63
37:L:57:LEU:HD13	37:L:60:ARG:HH21	1.65	0.62
26:A:269:C:H2'	26:A:270:A:H8	2.10	0.62
31:F:135:ILE:HG21	31:F:142:TYR:HD1	1.64	0.62
35:J:73:VAL:HG12	35:J:88:THR:HG22	1.81	0.62
28:C:16:VAL:HG12	28:C:203:VAL:HG22	1.81	0.62
26:A:908:C:OP2	38:M:22:GLN:NE2	2.33	0.62
28:C:132:ARG:NH1	28:C:186:ASP:OD1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1011:G:OP1	42:Q:74:SER:OG	2.17	0.62
26:A:2199:A:OP1	49:X:36:ARG:NH2	2.32	0.62
26:A:2720:U:H5''	41:P:52:ARG:HH22	1.65	0.62
26:A:2261:C:OP1	48:W:15:LYS:NZ	2.32	0.62
30:E:111:GLU:OE2	30:E:114:ARG:NH2	2.33	0.62
26:A:2839:G:H4'	39:N:49:GLU:HG2	1.81	0.62
33:I:102:ARG:NH1	33:I:129:GLU:OE1	2.32	0.61
26:A:279:A:H61	26:A:361:G:H1'	1.64	0.61
26:A:2636:C:O2'	29:D:45:TYR:OH	2.17	0.61
30:E:125:SER:O	30:E:137:LYS:NZ	2.34	0.61
26:A:587:C:OP2	37:L:21:ARG:NH2	2.32	0.61
30:E:112:LEU:HB3	30:E:118:LEU:HB2	1.83	0.61
31:F:64:PRO:HA	31:F:88:VAL:HG23	1.82	0.61
38:M:69:PRO:HA	38:M:94:ALA:HB2	1.83	0.61
26:A:77:G:H5''	50:Y:2:LYS:HE2	1.82	0.61
26:A:1434:A:H2'	26:A:1435:G:C8	2.36	0.60
26:A:1469:A:H2'	26:A:1470:A:H8	1.66	0.60
46:U:51:LEU:HD23	46:U:52:ASN:H	1.66	0.60
30:E:119:ILE:HD11	30:E:143:LEU:HD11	1.81	0.60
44:S:3:THR:HG21	44:S:58:ALA:HB2	1.84	0.60
49:X:44:ARG:NH2	49:X:77:TYR:OH	2.35	0.60
48:W:33:ILE:HG22	48:W:34:VAL:HG23	1.82	0.60
36:K:76:VAL:H	41:P:72:VAL:HG22	1.66	0.60
33:I:32:VAL:HG23	33:I:60:VAL:HG13	1.82	0.60
26:A:1262:A:H2	52:O:6:LYS:HZ1	1.49	0.60
34:H:5:LEU:HB2	34:H:16:GLY:H	1.66	0.59
26:A:856:G:H2'	26:A:857:G:C8	2.38	0.59
33:I:64:ARG:NH1	33:I:65:SER:OG	2.36	0.59
26:A:1081:U:H4'	33:I:126:ARG:HH21	1.68	0.59
26:A:2333:A:H5'	26:A:2335:A:H1'	1.84	0.59
30:E:49:ARG:HE	30:E:75:SER:HA	1.68	0.59
35:J:36:LEU:HD11	35:J:54:ILE:HG12	1.84	0.59
32:G:51:PHE:HZ	32:G:71:LEU:HD23	1.68	0.59
40:O:14:ALA:HA	40:O:17:LYS:HE3	1.83	0.59
28:C:76:VAL:HG12	28:C:114:GLN:HG3	1.85	0.59
26:A:2313:C:H5''	31:F:87:LYS:HD3	1.83	0.59
35:J:62:VAL:HG11	35:J:101:ILE:HD11	1.84	0.59
33:I:56:VAL:HB	33:I:70:THR:HG23	1.85	0.59
26:A:1365:A:O2'	49:X:10:ARG:NH2	2.36	0.58
26:A:181:A:H2'	26:A:182:A:C8	2.38	0.58
46:U:49:PRO:O	46:U:53:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:54:ILE:HA	33:I:74:PRO:HD3	1.85	0.58
29:D:131:ASP:O	29:D:136:ASN:ND2	2.35	0.58
26:A:2500:U:O2'	26:A:2504:PSU:OP1	2.19	0.58
26:A:1386:C:H2'	26:A:1387:A:H8	1.69	0.58
26:A:568:U:H1'	26:A:2030:6MZ:H9C1	1.86	0.58
45:T:80:TRP:HZ3	45:T:82:LYS:HB3	1.69	0.58
26:A:2511:U:H5''	29:D:128:ARG:HD2	1.85	0.58
28:C:261:ARG:O	28:C:264:LYS:NZ	2.33	0.58
26:A:801:G:O4'	30:E:49:ARG:NH2	2.37	0.58
26:A:979:A:H2'	26:A:982:C:H42	1.68	0.58
46:U:45:GLN:NE2	46:U:55:GLY:O	2.36	0.58
37:L:95:LEU:HD22	37:L:100:ILE:HD11	1.86	0.58
30:E:143:LEU:HD23	30:E:146:VAL:HG21	1.86	0.57
26:A:538:A:H5''	35:J:7:LYS:HE3	1.86	0.57
37:L:74:THR:HG22	37:L:107:PHE:HB2	1.85	0.57
27:B:76:G:H21	47:V:78:GLN:HE22	1.52	0.57
56:4:3:VAL:HB	56:4:37:GLN:HE21	1.70	0.57
26:A:1365:A:OP1	49:X:2:ARG:NH1	2.38	0.57
35:J:80:HIS:O	35:J:82:GLY:N	2.31	0.57
46:U:93:ARG:HB3	46:U:102:ILE:HD13	1.85	0.57
26:A:1306:C:H2'	26:A:1307:A:H8	1.70	0.57
26:A:2305:U:O4	31:F:151:LEU:N	2.38	0.57
28:C:74:PRO:HA	28:C:116:GLN:HB3	1.85	0.57
33:I:129:GLU:HA	33:I:132:ALA:HB3	1.87	0.57
26:A:20:C:H2'	26:A:21:A:H8	1.70	0.57
34:H:81:ALA:HA	34:H:147:VAL:HB	1.85	0.57
28:C:1:ALA:N	28:C:19:VAL:O	2.34	0.57
30:E:18:THR:HA	30:E:106:LYS:HD3	1.86	0.57
31:F:12:VAL:HG12	31:F:27:VAL:HG21	1.86	0.56
32:G:132:LEU:HD13	32:G:143:VAL:HG23	1.87	0.56
26:A:1342:A:OP1	45:T:40:LYS:NZ	2.35	0.56
46:U:11:ILE:HG22	46:U:21:ARG:HB3	1.88	0.56
26:A:1264:A:H5'	52:0:7:PRO:HG2	1.87	0.56
51:Z:38:GLU:OE1	51:Z:40:THR:OG1	2.23	0.56
29:D:10:GLY:H	29:D:197:THR:HG23	1.70	0.56
46:U:32:LYS:HE3	46:U:63:ALA:HB3	1.87	0.56
28:C:154:ALA:HB2	28:C:161:VAL:HG13	1.86	0.56
29:D:109:VAL:HG12	29:D:203:VAL:HG12	1.88	0.56
26:A:322:A:H5'	26:A:340:A:H1'	1.86	0.56
45:T:40:LYS:HA	45:T:43:ILE:HG12	1.86	0.56
38:M:29:GLY:H	38:M:104:GLU:HG3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Q:77:LYS:HG2	42:Q:116:LEU:HD22	1.86	0.56
36:K:70:ARG:HG2	36:K:76:VAL:HG12	1.88	0.56
26:A:2141:G:H2'	26:A:2142:A:C8	2.41	0.56
26:A:399:U:H5''	49:X:56:ARG:HH12	1.71	0.56
26:A:1437:C:HO2'	26:A:1516:G:HO2'	1.46	0.55
26:A:729:G:H5''	26:A:730:A:H5''	1.87	0.55
47:V:29:ILE:HD11	47:V:37:PRO:HB2	1.88	0.55
26:A:516:C:OP1	52:O:9:ARG:NH1	2.39	0.55
26:A:1527:G:N1	26:A:1544:A:OP2	2.37	0.55
26:A:355:U:H2'	26:A:356:G:C8	2.41	0.55
41:P:90:ALA:HB2	41:P:112:ARG:HA	1.88	0.55
26:A:1469:A:H2'	26:A:1470:A:C8	2.41	0.55
37:L:80:SER:OG	37:L:115:GLU:OE2	2.24	0.55
26:A:1078:U:H5'	26:A:1079:C:H5''	1.88	0.55
26:A:1434:A:H2'	26:A:1435:G:H8	1.70	0.55
26:A:956:G:O6	38:M:14:LYS:NZ	2.40	0.55
26:A:886:A:H4'	26:A:887:U:O5'	2.07	0.55
32:G:29:ASN:OD1	32:G:30:GLY:N	2.40	0.55
35:J:78:THR:HG23	35:J:80:HIS:H	1.71	0.55
26:A:1068:G:N2	26:A:1095:A:O2'	2.39	0.55
26:A:1056:G:N1	26:A:1102:C:OP2	2.38	0.55
26:A:1088:A:N6	33:I:134:SER:OG	2.40	0.55
26:A:2140:G:H2'	26:A:2141:G:C8	2.42	0.54
26:A:636:G:C5	37:L:111:ILE:HG21	2.42	0.54
51:Z:8:GLN:NE2	51:Z:10:ARG:O	2.37	0.54
39:N:56:LYS:NZ	39:N:87:PHE:O	2.40	0.54
48:W:21:ARG:HH21	48:W:33:ILE:HD13	1.73	0.54
32:G:37:ASN:ND2	32:G:63:GLN:OE1	2.39	0.54
26:A:1076:C:O2'	33:I:90:GLY:O	2.23	0.54
29:D:177:VAL:HG22	29:D:189:VAL:HG12	1.90	0.54
32:G:101:VAL:HG12	32:G:115:GLN:HA	1.90	0.54
26:A:820:A:H4'	26:A:836:G:H22	1.73	0.54
41:P:24:THR:HG22	41:P:87:ARG:HB3	1.90	0.54
44:S:7:HIS:HD2	44:S:10:ALA:HB2	1.72	0.53
28:C:184:GLU:HG3	28:C:186:ASP:H	1.73	0.53
32:G:1:SER:OG	32:G:2:ARG:N	2.41	0.53
34:H:100:ALA:HB2	34:H:112:LYS:HD3	1.89	0.53
26:A:2123:G:N2	26:A:2175:C:N3	2.57	0.53
30:E:117:ARG:HH21	30:E:184:ASP:HA	1.73	0.53
45:T:65:GLY:O	45:T:76:ARG:NH1	2.42	0.53
26:A:337:C:OP1	46:U:3:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1386:C:H2'	26:A:1387:A:C8	2.43	0.53
46:U:46:LYS:HD2	46:U:47:PRO:HD2	1.89	0.53
46:U:82:VAL:O	46:U:96:LYS:NZ	2.41	0.53
26:A:2128:G:H21	26:A:2173:A:H1'	1.72	0.53
27:B:49:C:H2'	27:B:50:A:H8	1.73	0.53
30:E:47:LYS:HB2	30:E:51:GLU:HG2	1.89	0.53
31:F:53:ALA:HA	31:F:64:PRO:HG2	1.91	0.53
32:G:95:ALA:HB1	32:G:130:ILE:HG23	1.90	0.53
44:S:15:GLN:NE2	52:O:16:ARG:HE	2.07	0.53
34:H:17:ASP:HB3	34:H:19:VAL:HG13	1.91	0.53
51:Z:40:THR:HG22	51:Z:42:ALA:H	1.74	0.53
26:A:2720:U:OP1	41:P:52:ARG:NH2	2.41	0.53
26:A:355:U:H2'	26:A:356:G:H8	1.73	0.53
38:M:30:SER:N	38:M:106:ASP:OD1	2.42	0.53
46:U:35:VAL:HB	46:U:38:ILE:HG13	1.91	0.53
26:A:184:C:H2'	26:A:185:G:H8	1.74	0.52
26:A:1300:G:H4'	26:A:1301:A:H5''	1.91	0.52
31:F:65:LEU:HD13	31:F:87:LYS:HB3	1.91	0.52
46:U:2:ALA:O	46:U:5:ARG:NH2	2.42	0.52
26:A:1802:A:H2'	26:A:1803:A:C8	2.44	0.52
26:A:2377:A:H2'	26:A:2378:A:C8	2.44	0.52
44:S:77:ASP:N	44:S:77:ASP:OD1	2.39	0.52
26:A:1063:G:C8	33:I:135:MET:HA	2.45	0.52
26:A:2313:C:O4'	31:F:36:ASN:ND2	2.42	0.52
26:A:582:A:H2'	26:A:583:G:H8	1.74	0.52
35:J:31:GLU:HG3	35:J:142:ILE:HD13	1.90	0.52
56:4:3:VAL:HG12	56:4:36:ARG:HD3	1.91	0.52
26:A:1059:G:H1	33:I:127:SER:HB3	1.75	0.52
26:A:639:U:H2'	26:A:640:C:C6	2.45	0.52
26:A:745:IMG:O2'	26:A:748:G:O2'	2.17	0.52
31:F:134:GLN:NE2	31:F:149:ARG:O	2.43	0.52
34:H:31:VAL:HG11	34:H:38:PRO:HD3	1.92	0.52
26:A:2188:U:H2'	26:A:2189:U:O4'	2.10	0.52
26:A:2788:C:O2'	26:A:2809:A:N3	2.40	0.52
26:A:286:U:H2'	26:A:287:G:H8	1.75	0.52
26:A:2899:A:H2'	26:A:2900:A:C8	2.45	0.52
45:T:40:LYS:HB2	45:T:58:VAL:HG23	1.90	0.52
26:A:1478:G:H1	26:A:1513:U:H3	1.58	0.52
26:A:2141:G:H2'	26:A:2142:A:H8	1.75	0.52
38:M:58:LYS:HG3	38:M:59:ARG:H	1.75	0.52
41:P:88:ARG:HH21	41:P:112:ARG:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:674:G:H2'	26:A:675:A:H8	4.46	0.51
26:A:715:A:H2'	26:A:716:A:C8	2.80	0.51
27:B:51:G:H2'	27:B:52:A:H8	1.75	0.51
26:A:1503:A:H2'	26:A:1504:A:C8	2.45	0.51
26:A:746:PSU:HO2'	26:A:2611:C:HO2'	1.58	0.51
28:C:36:ASN:HB2	28:C:61:TYR:HB2	1.92	0.51
26:A:2303:G:O2'	31:F:120:SER:O	2.28	0.51
43:R:68:ARG:HH11	43:R:90:ARG:HB2	1.74	0.51
26:A:2032:G:N2	26:A:2572:A:OP2	2.40	0.51
34:H:9:VAL:HG22	34:H:35:LYS:HG2	1.93	0.51
26:A:2258:C:O2'	26:A:2427:C:OP2	2.29	0.51
40:O:62:LEU:HD13	40:O:70:ALA:HA	1.93	0.51
26:A:2848:G:O2'	26:A:2867:G:N2	2.44	0.51
40:O:28:VAL:HG11	40:O:103:VAL:HG23	1.92	0.51
26:A:2172:U:O5'	26:A:2175:C:N4	2.44	0.51
26:A:549:G:H2'	26:A:550:C:C6	2.46	0.51
31:F:46:LYS:HB2	31:F:47:LYS:HD2	1.93	0.51
37:L:62:PRO:HG2	55:3:24:LYS:HB3	1.92	0.51
26:A:1059:G:N2	33:I:128:ILE:HG13	2.26	0.51
27:B:30:C:O2'	27:B:57:A:N1	2.42	0.51
37:L:63:LYS:O	55:3:29:ARG:NH1	2.44	0.51
26:A:1494:A:H2'	26:A:1495:A:C8	2.46	0.51
26:A:729:G:N7	28:C:206:LYS:HB3	2.26	0.51
28:C:77:VAL:HG11	28:C:109:LEU:HD21	1.93	0.51
35:J:32:LEU:HD22	35:J:54:ILE:HD13	1.93	0.51
36:K:21:CYS:HA	36:K:41:ILE:HG22	1.93	0.51
45:T:11:LEU:HG	45:T:32:LEU:HD13	1.92	0.51
26:A:5:A:H2'	26:A:6:A:H8	1.76	0.50
34:H:55:GLU:HA	34:H:58:LEU:HG	1.93	0.50
26:A:1028:A:H2'	26:A:1029:A:C8	2.46	0.50
26:A:1365:A:O5'	49:X:27:ARG:NH2	2.45	0.50
30:E:120:VAL:HG12	30:E:188:MET:HB2	1.93	0.50
33:I:30:GLN:HB3	33:I:60:VAL:HG11	1.92	0.50
26:A:754:U:O2'	26:A:1272:A:N1	2.44	0.50
26:A:2830:C:OP2	29:D:59:ARG:NH2	2.44	0.50
31:F:72:SER:OG	31:F:80:GLN:N	2.43	0.50
26:A:475:C:O2	26:A:479:A:N6	2.44	0.50
26:A:848:C:H2'	26:A:849:A:H8	1.77	0.50
32:G:41:GLU:HG3	32:G:54:ARG:HG2	1.93	0.50
26:A:2065:C:H2'	26:A:2066:C:H6	1.77	0.50
26:A:881:G:N2	26:A:896:A:N7	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:G:53:PRO:HG3	32:G:61:TRP:CE2	2.47	0.50
35:J:118:MET:HA	35:J:121:LYS:HZ3	1.77	0.50
42:Q:43:GLN:HE21	43:R:77:PHE:HB3	1.77	0.50
54:2:25:LYS:O	54:2:28:ARG:N	2.44	0.50
56:4:2:LYS:NZ	56:4:32:LYS:O	2.44	0.50
26:A:1961:C:H2'	26:A:1962:5MC:C2	2.47	0.50
26:A:354:A:H2'	26:A:355:U:O4'	2.12	0.50
26:A:629:G:N3	26:A:639:U:O2'	2.45	0.50
32:G:106:LEU:HD23	32:G:151:ARG:HD2	1.92	0.50
41:P:30:TRP:HE3	41:P:37:LYS:HG2	1.77	0.50
45:T:56:GLU:HB2	45:T:86:THR:HG23	1.94	0.50
55:3:27:ASN:HB3	55:3:35:LYS:HE2	1.93	0.50
26:A:1315:C:O2'	26:A:1392:A:N3	2.41	0.50
26:A:181:A:H2'	26:A:182:A:H8	1.74	0.50
26:A:885:C:H4'	26:A:886:A:H5'	1.94	0.50
26:A:973:A:OP2	43:R:81:LYS:NZ	2.40	0.50
26:A:372:G:O2'	26:A:400:G:O6	2.24	0.49
26:A:28:A:O2'	42:Q:10:ARG:NH2	2.44	0.49
28:C:181:ARG:NH1	28:C:182:LYS:O	2.45	0.49
38:M:52:ALA:HA	38:M:55:ARG:HD3	1.93	0.49
29:D:124:ARG:NH2	29:D:161:MET:O	2.45	0.49
29:D:128:ARG:NH1	29:D:129:THR:O	2.46	0.49
26:A:1432:G:H2'	26:A:1433:A:C8	2.48	0.49
32:G:86:LEU:HD22	32:G:130:ILE:HD11	1.95	0.49
33:I:54:ILE:HG12	33:I:73:PRO:HA	1.94	0.49
30:E:181:ILE:HG23	37:L:2:ARG:HH11	1.77	0.49
26:A:465:G:O3'	54:2:21:ARG:NH1	2.44	0.49
26:A:743:A:O2'	26:A:1659:G:OP1	2.28	0.49
26:A:17:G:H4'	42:Q:24:TYR:HE1	1.78	0.49
26:A:2756:U:OP2	56:4:19:ARG:NE	2.45	0.49
26:A:582:A:H2'	26:A:583:G:C8	2.48	0.49
35:J:45:THR:HB	35:J:48:VAL:HG12	1.93	0.49
43:R:27:ILE:HD11	43:R:63:VAL:HG11	1.94	0.49
50:Y:8:GLU:OE1	50:Y:12:GLU:HB2	2.11	0.49
53:1:10:LEU:HG	53:1:48:TYR:HB3	1.94	0.49
26:A:5:A:H2'	26:A:6:A:C8	2.48	0.49
31:F:118:ALA:O	31:F:166:ARG:NH2	2.46	0.49
43:R:16:GLU:OE1	43:R:100:GLY:N	2.45	0.49
26:A:2804:U:H2'	26:A:2805:C:C6	2.48	0.49
26:A:988:A:C5	51:Z:13:ILE:HD11	2.46	0.49
37:L:85:VAL:HG11	37:L:90:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:N:79:LEU:HA	39:N:83:LEU:HB2	1.94	0.49
26:A:884:U:H3'	26:A:885:C:H5''	1.94	0.49
26:A:729:G:C5	28:C:206:LYS:HB3	2.48	0.49
29:D:13:ARG:O	41:P:11:GLN:NE2	2.45	0.49
30:E:146:VAL:HG12	30:E:185:LYS:HB2	1.95	0.49
30:E:148:ILE:HB	30:E:169:VAL:HG22	1.95	0.49
32:G:92:GLY:HA2	32:G:94:ARG:HH12	1.77	0.49
40:O:30:ARG:HD2	40:O:102:ARG:HH11	1.77	0.49
26:A:2334:U:O2'	40:O:13:ARG:NH2	2.46	0.49
27:B:51:G:H2'	27:B:52:A:C8	2.48	0.49
28:C:16:VAL:HG12	28:C:203:VAL:H	1.78	0.49
32:G:71:LEU:HD12	32:G:74:MET:HB2	1.93	0.49
26:A:833:A:H1'	37:L:51:GLU:HB2	1.94	0.49
49:X:58:ILE:HG12	49:X:66:VAL:HG21	1.95	0.49
26:A:1796:U:H2'	26:A:1797:G:H8	1.78	0.48
26:A:1746:A:H2'	26:A:1747:U:C6	2.48	0.48
26:A:1864:U:OP1	26:A:2410:G:O2'	2.30	0.48
26:A:2065:C:H2'	26:A:2066:C:C6	2.48	0.48
38:M:49:ALA:HB1	38:M:120:ALA:HB1	1.96	0.48
41:P:24:THR:HA	41:P:45:VAL:HA	1.93	0.48
27:B:49:C:H2'	27:B:50:A:C8	2.47	0.48
27:B:5:U:H2'	27:B:6:G:C8	2.49	0.48
31:F:9:ASP:N	31:F:9:ASP:OD1	2.45	0.48
33:I:77:VAL:HA	33:I:80:LYS:HE2	1.94	0.48
35:J:64:VAL:HB	35:J:68:LYS:HD2	1.94	0.48
40:O:92:PHE:HB2	40:O:117:PHE:CD2	2.49	0.48
51:Z:8:GLN:HG2	51:Z:31:ILE:HA	1.94	0.48
30:E:22:ASP:HA	30:E:114:ARG:HH12	1.78	0.48
38:M:71:LYS:HB3	38:M:93:VAL:O	2.14	0.48
47:V:40:ILE:HD12	47:V:65:VAL:HG21	1.95	0.48
26:A:1171:G:H2'	26:A:1172:C:O4'	2.14	0.48
28:C:32:LEU:HD13	28:C:63:ILE:HB	1.95	0.48
34:H:2:GLN:NE2	34:H:18:GLN:OE1	2.43	0.48
41:P:59:THR:HG23	41:P:72:VAL:HG12	1.94	0.48
26:A:172:A:H2'	26:A:173:A:H8	1.78	0.48
26:A:2291:U:H2'	26:A:2292:U:C6	2.48	0.48
26:A:588:U:H2'	26:A:589:U:C6	2.49	0.48
26:A:744:U:H2'	26:A:745:1MG:O4'	2.13	0.48
26:A:833:A:H2'	26:A:834:G:C8	2.49	0.48
44:S:28:LYS:HD3	44:S:70:LYS:HZ3	1.78	0.48
26:A:2126:A:N1	26:A:2162:G:O2'	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2150:C:H2'	26:A:2151:U:O4'	2.14	0.48
26:A:2483:C:O2'	38:M:51:ARG:NH2	2.47	0.48
33:I:78:LEU:O	33:I:82:ALA:HB3	2.14	0.48
48:W:21:ARG:NH2	48:W:32:ILE:O	2.47	0.48
26:A:2087:G:H2'	26:A:2088:A:C8	2.49	0.48
26:A:2303:G:O2'	31:F:128:SER:OG	2.32	0.48
27:B:29:A:O2'	27:B:58:A:N1	2.43	0.48
34:H:130:VAL:HG23	34:H:142:VAL:HG13	1.94	0.48
38:M:57:VAL:HG12	38:M:112:LEU:HG	1.95	0.48
41:P:102:ARG:HD3	41:P:106:ALA:HB1	1.95	0.48
26:A:2525:G:H2'	26:A:2526:G:H8	1.79	0.48
26:A:848:C:H2'	26:A:849:A:C8	2.48	0.48
32:G:88:LEU:HD23	32:G:93:TYR:HB3	1.96	0.48
33:I:88:GLY:HA2	33:I:97:VAL:HG11	1.95	0.48
52:0:9:ARG:HA	52:0:12:ARG:HG2	1.96	0.47
26:A:1361:G:H2'	26:A:1362:C:C6	2.49	0.47
26:A:2428:G:H21	37:L:60:ARG:CZ	2.27	0.47
30:E:159:LEU:HA	30:E:162:ARG:HE	1.79	0.47
41:P:1:SER:OG	41:P:2:ASN:N	2.45	0.47
26:A:1161:C:H2'	26:A:1162:G:H8	1.79	0.47
26:A:843:G:H2'	26:A:844:A:C8	2.49	0.47
33:I:74:PRO:HG2	33:I:77:VAL:HG22	1.96	0.47
26:A:299:A:N3	26:A:319:G:O2'	2.39	0.47
29:D:124:ARG:HH21	29:D:125:TRP:HE1	1.62	0.47
44:S:23:LEU:O	44:S:27:LYS:NZ	2.35	0.47
45:T:80:TRP:CZ3	45:T:82:LYS:HB3	2.49	0.47
43:R:5:PHE:O	43:R:11:GLN:HA	2.14	0.47
26:A:859:G:O2'	26:A:916:G:O6	2.30	0.47
26:A:1798:U:OP2	28:C:270:ARG:NH2	2.46	0.47
52:0:54:ILE:HD12	52:0:56:LYS:H	1.79	0.47
26:A:13:A:O2'	26:A:15:G:N7	2.47	0.47
26:A:560:C:O2'	42:Q:47:ARG:NH2	2.44	0.47
28:C:129:LEU:HD13	28:C:133:ASN:HB2	1.96	0.47
36:K:35:VAL:HG13	36:K:65:THR:HG23	1.95	0.47
26:A:1682:G:H2'	26:A:1683:U:C6	2.50	0.47
26:A:358:U:H2'	26:A:359:G:H8	2.14	0.47
26:A:477:A:H2'	26:A:478:A:C8	2.50	0.47
26:A:959:A:N3	26:A:2457:PSU:O2'	2.39	0.47
26:A:20:C:H2'	26:A:21:A:C8	2.50	0.47
26:A:2646:C:OP2	26:A:2732:G:O2'	2.27	0.47
26:A:269:C:H2'	26:A:270:A:C8	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:658:U:O2	30:E:97:ASN:ND2	2.44	0.47
26:A:994:C:OP1	42:Q:52:ARG:NH2	2.46	0.47
26:A:2344:U:OP1	53:1:36:LYS:NZ	2.32	0.47
31:F:28:PRO:HB2	31:F:168:LEU:HD22	1.96	0.47
36:K:69:VAL:O	36:K:76:VAL:HA	2.15	0.47
47:V:4:ILE:HG13	47:V:63:ILE:HG22	1.97	0.47
28:C:134:ILE:HD13	28:C:140:VAL:HG11	1.96	0.47
36:K:2:ILE:HG23	36:K:6:THR:HB	1.96	0.47
46:U:70:ALA:HB3	46:U:79:ALA:HB1	1.96	0.47
26:A:1:G:H2'	26:A:2:G:C8	2.49	0.47
26:A:2682:A:H61	26:A:2728:U:H1'	1.80	0.47
31:F:41:GLU:OE2	31:F:147:ARG:NH2	2.47	0.47
41:P:30:TRP:HE1	41:P:81:ASP:HB3	1.80	0.47
26:A:1077:A:H3'	26:A:1078:U:O4'	2.14	0.46
26:A:1789:A:H4'	28:C:217:PRO:HB3	1.97	0.46
36:K:42:THR:HB	36:K:57:VAL:HG12	1.97	0.46
49:X:17:ARG:HD2	49:X:21:LEU:HB2	1.96	0.46
26:A:1219:U:H2'	26:A:1220:G:H8	1.80	0.46
28:C:128:THR:HA	28:C:189:ALA:O	2.14	0.46
28:C:67:LYS:HA	28:C:150:GLY:HA2	1.97	0.46
26:A:1676:A:H1'	29:D:133:THR:HG21	1.97	0.46
55:3:31:ILE:O	55:3:35:LYS:NZ	2.45	0.46
56:4:14:CYS:SG	56:4:27:CYS:HB2	2.56	0.46
30:E:59:PRO:HB2	30:E:60:TRP:CE3	2.51	0.46
30:E:84:THR:OG1	30:E:85:PHE:N	2.48	0.46
26:A:537:G:H5''	35:J:5:THR:HG21	1.98	0.46
26:A:2482:A:H61	38:M:55:ARG:HH12	1.62	0.46
39:N:49:GLU:HA	39:N:52:ILE:HG22	1.96	0.46
40:O:12:THR:HA	40:O:15:ARG:HB3	1.97	0.46
57:6:14:ALA:HB3	57:6:22:MET:HB2	1.97	0.46
27:B:29:A:OP2	40:O:31:THR:OG1	2.32	0.46
31:F:57:ALA:HB2	31:F:64:PRO:HD3	1.98	0.46
32:G:4:ALA:HB2	32:G:65:GLY:HA2	1.97	0.46
26:A:742:A:H2'	26:A:743:A:C8	2.51	0.46
26:A:927:A:H2'	26:A:928:A:C8	2.49	0.46
36:K:13:ASN:HD21	36:K:97:THR:HG1	1.63	0.46
40:O:33:ARG:HG2	40:O:34:HIS:CD2	2.50	0.46
26:A:1601:G:OP1	45:T:64:LYS:NZ	2.35	0.46
26:A:2144:G:N2	26:A:2146:C:O2	2.48	0.46
26:A:2803:G:H2'	26:A:2804:U:C6	2.51	0.46
26:A:674:G:H2'	26:A:675:A:C8	4.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:128:ALA:HB3	30:E:133:LEU:HD21	1.97	0.46
30:E:46:GLN:HE21	30:E:83:VAL:HG21	1.80	0.46
34:H:84:ALA:HA	34:H:91:PHE:H	1.81	0.46
27:B:40:U:H2'	57:6:2:LYS:HE2	1.97	0.46
26:A:2025:C:H2'	26:A:2026:U:C6	2.51	0.46
41:P:28:LYS:HD3	41:P:39:LEU:HD23	1.96	0.46
26:A:1198:U:H2'	26:A:1199:U:C6	2.50	0.46
26:A:2530:A:OP1	26:A:2535:G:N2	2.49	0.46
27:B:30:C:H2'	27:B:31:C:H5'	1.97	0.46
36:K:3:GLN:HG2	36:K:4:GLU:H	1.80	0.46
26:A:1667:G:O2'	26:A:1991:U:O4	2.31	0.46
29:D:24:VAL:HG21	29:D:188:LEU:HB3	1.96	0.46
26:A:2685:G:P	36:K:78:ARG:HH22	2.39	0.46
26:A:2895:G:H2'	26:A:2896:C:C6	2.51	0.46
33:I:128:ILE:O	33:I:132:ALA:N	2.46	0.46
26:A:1405:U:H2'	26:A:1406:U:C6	2.51	0.45
26:A:2821:A:OP1	29:D:115:GLY:N	2.46	0.45
34:H:26:ALA:HA	34:H:30:LEU:HB2	1.97	0.45
26:A:2845:U:H5''	41:P:51:ASN:O	2.16	0.45
47:V:77:VAL:HG23	47:V:89:ILE:HG22	1.97	0.45
26:A:1394:U:H4'	26:A:1603:A:H4'	1.98	0.45
26:A:286:U:H2'	26:A:287:G:C8	2.50	0.45
26:A:1490:A:O2'	28:C:97:ASP:OD1	2.29	0.45
26:A:1061:U:C5	33:I:10:LEU:HB2	2.51	0.45
35:J:88:THR:OG1	35:J:91:GLU:OE1	2.28	0.45
39:N:22:ARG:HG3	39:N:70:THR:HA	1.98	0.45
46:U:76:THR:HG23	46:U:78:LYS:HG2	1.97	0.45
26:A:1231:U:H2'	26:A:1232:G:H8	1.81	0.45
26:A:2798:U:O2	26:A:2799:A:N6	2.49	0.45
27:B:114:C:H2'	27:B:115:A:H8	1.81	0.45
26:A:1735:A:H2'	26:A:1736:U:C6	2.52	0.45
26:A:2619:C:H5''	29:D:157:LYS:HG2	1.99	0.45
31:F:56:LEU:HD22	31:F:64:PRO:HG3	1.98	0.45
26:A:108:G:H2'	26:A:109:C:C6	2.52	0.45
26:A:2267:A:H5''	26:A:2268:A:H5''	1.99	0.45
38:M:20:LEU:HD22	47:V:81:PRO:HG3	1.97	0.45
49:X:2:ARG:HB2	49:X:32:LEU:HD12	1.99	0.45
57:6:56:ARG:O	57:6:59:ARG:HG2	2.17	0.45
26:A:1219:U:H2'	26:A:1220:G:C8	2.50	0.45
26:A:1281:G:H2'	26:A:1282:U:C6	2.51	0.45
26:A:2038:G:H2'	26:A:2039:U:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2803:G:H2'	26:A:2804:U:H6	1.81	0.45
26:A:993:G:H1'	43:R:91:GLN:HE21	1.81	0.45
28:C:12:ARG:HD2	28:C:12:ARG:HA	1.84	0.45
28:C:180:MET:HB2	28:C:268:ARG:H	1.82	0.45
29:D:136:ASN:OD1	29:D:139:SER:OG	2.25	0.45
50:Y:17:GLU:HB3	50:Y:53:VAL:HG11	1.97	0.45
26:A:1158:C:O2'	26:A:1159:U:O5'	3.43	0.45
26:A:2622:U:O2'	26:A:2825:G:N7	2.50	0.45
26:A:739:A:H1'	26:A:740:C:H5	1.82	0.45
26:A:886:A:O2'	26:A:888:C:N3	2.49	0.45
30:E:112:LEU:O	30:E:118:LEU:N	2.47	0.45
31:F:162:ASP:O	31:F:165:GLY:N	2.50	0.45
32:G:87:GLN:HE22	32:G:164:ALA:HA	1.81	0.45
37:L:96:LYS:HE3	37:L:105:ILE:HG22	1.98	0.45
26:A:1353:A:H2'	26:A:1354:A:C8	2.52	0.45
26:A:175:G:H2'	26:A:176:A:C8	2.52	0.45
26:A:2392:A:OP2	26:A:2422:C:N4	2.45	0.45
26:A:1078:U:OP1	33:I:134:SER:HB2	2.17	0.45
41:P:90:ALA:HB3	41:P:110:LYS:HG3	1.98	0.45
26:A:2759:G:H21	32:G:138:GLN:HE22	1.64	0.45
39:N:28:LEU:HD11	39:N:113:ILE:HG12	1.98	0.45
26:A:2723:C:H5'	39:N:3:HIS:HD2	1.82	0.45
39:N:60:VAL:O	39:N:64:ARG:HG2	2.17	0.45
40:O:39:VAL:HG23	40:O:48:LEU:HB2	1.99	0.45
26:A:17:G:H4'	42:Q:24:TYR:CE1	2.51	0.45
49:X:6:VAL:HG21	49:X:58:ILE:HD11	1.99	0.45
26:A:1589:U:H2'	26:A:1590:A:H8	1.82	0.45
26:A:698:C:O2'	26:A:734:A:N6	2.50	0.45
26:A:832:U:H2'	26:A:833:A:C8	2.52	0.45
26:A:882:G:N3	26:A:896:A:N6	2.65	0.45
32:G:90:GLY:HA3	32:G:159:LYS:HD3	1.99	0.45
37:L:135:ILE:HG12	37:L:140:GLY:HA3	1.99	0.45
26:A:1645:G:H5''	26:A:1646:C:H5'	1.98	0.44
30:E:76:PRO:HA	30:E:82:GLY:HA2	1.99	0.44
31:F:42:ALA:O	31:F:82:TYR:OH	2.35	0.44
34:H:108:VAL:HG12	34:H:110:VAL:H	1.82	0.44
39:N:73:ASN:HA	39:N:76:VAL:HG12	1.98	0.44
47:V:21:ARG:HH12	47:V:87:GLN:HA	1.81	0.44
47:V:63:ILE:HD11	47:V:70:ILE:HB	1.99	0.44
26:A:1417:C:O2'	26:A:1587:G:O2'	2.33	0.44
26:A:2127:G:H2'	26:A:2128:G:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:657:U:H2'	26:A:658:U:C6	2.53	0.44
26:A:834:G:H5'	55:3:56:LEU:HD11	1.99	0.44
27:B:40:U:OP2	57:6:2:LYS:NZ	2.50	0.44
30:E:58:LYS:HG2	30:E:71:GLY:HA2	2.00	0.44
44:S:82:MET:HG2	44:S:98:LYS:O	2.17	0.44
46:U:33:VAL:HG13	46:U:66:VAL:HG12	1.98	0.44
26:A:1847:A:O2'	26:A:1848:A:H8	2.00	0.44
26:A:632:A:H2'	26:A:633:A:C8	2.52	0.44
30:E:5:LEU:HD11	30:E:12:LEU:HD13	1.99	0.44
36:K:2:ILE:HG12	36:K:8:LEU:HD21	1.99	0.44
37:L:55:MET:HE3	37:L:59:ARG:NE	2.32	0.44
38:M:11:LYS:HD3	38:M:86:LYS:HG2	1.98	0.44
26:A:2124:G:H21	26:A:2174:C:H41	1.66	0.44
26:A:2514:U:H2'	26:A:2515:C:C6	2.52	0.44
26:A:820:A:H4'	26:A:836:G:N2	2.33	0.44
28:C:100:ARG:HH11	28:C:100:ARG:HD3	1.60	0.44
33:I:89:SER:HB2	33:I:91:LYS:H	1.83	0.44
26:A:1140:C:H5'	35:J:26:GLY:HA3	1.99	0.44
38:M:96:ILE:HD11	38:M:126:ILE:HG12	1.99	0.44
57:6:7:PRO:HB2	57:6:27:THR:HG23	1.99	0.44
57:6:49:ARG:O	57:6:53:THR:OG1	2.25	0.44
26:A:281:C:H2'	26:A:282:A:H8	1.82	0.44
26:A:303:G:H2'	26:A:304:U:C6	2.52	0.44
33:I:73:PRO:HG2	33:I:112:LYS:HD3	1.99	0.44
27:B:50:A:OP1	40:O:68:LYS:HG2	2.18	0.44
26:A:2446:G:N7	26:A:2501:C:O2'	2.50	0.44
26:A:2809:A:H2'	26:A:2810:A:C8	2.53	0.44
26:A:745:1MG:HM11	26:A:745:1MG:HN21	1.69	0.44
35:J:17:VAL:HG23	35:J:137:PRO:HB2	2.00	0.44
53:1:7:LYS:HA	53:1:23:THR:HA	1.98	0.44
26:A:2144:G:O2'	26:A:2147:A:N6	2.51	0.44
26:A:247:G:OP2	26:A:249:C:N4	2.51	0.44
26:A:596:U:H2'	26:A:597:G:H8	1.82	0.44
26:A:4:U:H2'	26:A:5:A:H8	1.82	0.44
33:I:52:LEU:HD23	33:I:54:ILE:HD11	2.00	0.44
40:O:75:GLY:HA3	40:O:109:ALA:HB3	2.00	0.44
41:P:52:ARG:H	41:P:56:SER:HB3	1.83	0.44
26:A:2220:U:H5''	34:H:97:ARG:NH2	2.33	0.44
26:A:1901:A:H4'	28:C:252:LYS:HD3	2.00	0.44
29:D:121:THR:HG21	29:D:143:PRO:HB3	1.99	0.44
34:H:32:PRO:HA	49:X:38:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:P:54:LEU:HA	41:P:76:HIS:CD2	2.52	0.44
29:D:15:PHE:HB3	41:P:78:PRO:HD3	2.00	0.44
26:A:2233:U:H2'	26:A:2234:G:C8	2.53	0.44
26:A:2328:A:H2'	26:A:2329:U:C6	2.53	0.44
31:F:110:ILE:HG12	31:F:113:PHE:HD1	1.83	0.44
37:L:91:ASP:OD1	37:L:91:ASP:N	2.31	0.44
41:P:29:VAL:HG12	41:P:80:VAL:HG22	1.99	0.44
26:A:585:G:N7	42:Q:5:ARG:NH1	2.65	0.44
26:A:833:A:H2'	26:A:834:G:H8	1.83	0.43
27:B:95:U:OP2	47:V:19:ARG:NH2	2.50	0.43
26:A:1156:A:C8	42:Q:50:ARG:HD3	2.53	0.43
26:A:45:G:H2'	26:A:46:G:C8	6.01	0.43
26:A:577:G:H2'	26:A:578:G:C8	2.53	0.43
27:B:114:C:H2'	27:B:115:A:C8	2.53	0.43
33:I:91:LYS:HG3	33:I:94:LYS:HE2	2.00	0.43
37:L:101:ILE:HG21	37:L:105:ILE:HG21	2.01	0.43
52:O:32:THR:HG23	52:O:50:GLY:HA2	2.00	0.43
26:A:1295:C:H2'	26:A:1296:G:H8	1.83	0.43
26:A:2743:U:H2'	26:A:2744:G:O4'	2.18	0.43
26:A:475:C:H4'	26:A:510:C:H5'	1.99	0.43
35:J:118:MET:HA	35:J:121:LYS:NZ	2.33	0.43
44:S:76:VAL:HG22	44:S:103:ILE:HG12	2.00	0.43
26:A:1853:A:H2'	26:A:1854:A:C8	2.54	0.43
26:A:2161:C:O2'	26:A:2162:G:N7	2.48	0.43
26:A:2215:C:H2'	26:A:2216:G:H8	1.83	0.43
26:A:322:A:OP2	30:E:163:ASN:HB2	2.19	0.43
26:A:882:G:H2'	26:A:883:G:C8	2.52	0.43
30:E:5:LEU:HG	30:E:120:VAL:HG23	1.99	0.43
31:F:59:ILE:HD11	31:F:137:PHE:CG	2.53	0.43
32:G:103:ASN:HA	32:G:112:VAL:O	2.18	0.43
45:T:37:ASP:N	45:T:37:ASP:OD1	2.51	0.43
26:A:1716:U:H2'	26:A:1717:A:H8	1.83	0.43
26:A:78:U:H2'	26:A:79:C:C6	2.54	0.43
31:F:101:ARG:NH1	57:6:9:TYR:OH	2.51	0.43
37:L:55:MET:O	37:L:60:ARG:NH1	2.51	0.43
45:T:36:LYS:HD2	45:T:36:LYS:HA	1.86	0.43
26:A:849:A:H2'	26:A:850:U:C6	2.54	0.43
34:H:2:GLN:HG2	34:H:39:ALA:O	2.19	0.43
35:J:88:THR:N	35:J:91:GLU:OE2	2.52	0.43
47:V:30:ILE:HG13	47:V:40:ILE:HG13	2.00	0.43
26:A:1506:U:H2'	26:A:1507:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1689:A:H2'	26:A:1690:A:C8	2.54	0.43
26:A:171:U:H2'	26:A:172:A:C8	2.54	0.43
26:A:2100:G:H2'	26:A:2101:A:H8	1.83	0.43
26:A:357:C:H2'	26:A:358:U:C6	2.54	0.43
26:A:593:U:H2'	26:A:594:U:C6	2.56	0.43
26:A:748:G:OP1	44:S:88:ARG:NH1	2.44	0.43
28:C:242:HIS:HA	28:C:243:PRO:HD3	1.87	0.43
30:E:48:THR:HB	30:E:86:ALA:HB2	1.99	0.43
34:H:42:LYS:HG3	34:H:46:PHE:HE1	1.84	0.43
44:S:17:VAL:HG23	44:S:43:ALA:HB1	2.00	0.43
45:T:3:ARG:HH12	45:T:7:LEU:HD21	1.83	0.43
26:A:2016:U:H1'	52:0:2:VAL:HG23	1.99	0.43
31:F:82:TYR:CD1	31:F:83:PRO:HD2	2.53	0.43
44:S:17:VAL:HG13	44:S:76:VAL:HG11	1.99	0.43
26:A:2742:G:OP1	56:4:36:ARG:NH1	2.52	0.43
26:A:1149:G:H2'	26:A:1150:C:C6	2.54	0.43
26:A:1255:U:H3'	30:E:68:ALA:HB2	2.01	0.43
26:A:2522:U:O2'	26:A:2647:U:OP1	2.31	0.43
26:A:263:G:O2'	26:A:429:A:N3	2.52	0.43
26:A:2680:U:H5'	29:D:194:PRO:HA	2.01	0.43
38:M:67:VAL:HG12	38:M:100:LYS:HE3	2.01	0.43
51:Z:37:ARG:HD3	51:Z:37:ARG:HA	1.78	0.43
26:A:1494:A:H2'	26:A:1495:A:H8	1.82	0.43
26:A:172:A:H2'	26:A:173:A:C8	2.53	0.43
26:A:2327:A:H2'	26:A:2328:A:C8	2.54	0.43
36:K:90:ASN:OD1	36:K:91:SER:N	2.51	0.43
26:A:1387:A:H5'	26:A:1469:A:H1'	2.00	0.42
26:A:71:A:OP1	26:A:112:U:O2'	2.24	0.42
26:A:863:A:H2'	26:A:864:G:C8	2.54	0.42
29:D:12:THR:HG22	29:D:13:ARG:H	1.84	0.42
52:0:1:ALA:HB3	52:0:2:VAL:HG12	2.02	0.42
26:A:608:A:H2'	26:A:609:A:C8	2.54	0.42
26:A:638:G:H2'	26:A:639:U:C6	2.54	0.42
26:A:639:U:H2'	26:A:640:C:H6	1.83	0.42
26:A:839:U:H2'	26:A:840:C:C6	2.54	0.42
26:A:2304:G:H5'	31:F:120:SER:HB2	2.01	0.42
31:F:138:PRO:HB2	57:6:32:LEU:HD22	2.01	0.42
34:H:97:ARG:HD3	34:H:112:LYS:HG2	2.01	0.42
46:U:27:VAL:HG13	46:U:33:VAL:HG12	2.00	0.42
26:A:2014:A:H2'	26:A:2015:A:C8	2.55	0.42
26:A:2623:G:H2'	26:A:2624:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:581:C:H2'	26:A:582:A:H8	1.83	0.42
26:A:967:U:H2'	26:A:968:C:C6	2.54	0.42
29:D:22:ILE:HG21	29:D:178:VAL:HG11	2.00	0.42
46:U:85:ARG:HD3	46:U:94:PHE:CD1	2.55	0.42
26:A:2247:A:H2'	26:A:2248:C:H6	1.83	0.42
26:A:558:U:H2'	26:A:559:G:C8	2.54	0.42
27:B:9:G:H2'	27:B:10:G:H8	1.84	0.42
27:B:42:C:N3	31:F:89:THR:HG22	2.34	0.42
29:D:4:LEU:HB2	29:D:32:ASN:ND2	2.35	0.42
46:U:25:LYS:HB3	46:U:34:ILE:HG23	2.02	0.42
26:A:2074:U:H2'	26:A:2075:U:C6	2.54	0.42
26:A:2108:A:H2'	26:A:2109:U:C6	2.55	0.42
26:A:1798:U:H5''	28:C:257:ARG:HB2	2.01	0.42
29:D:186:LEU:HD13	41:P:7:LEU:HD22	2.01	0.42
47:V:80:HIS:CG	47:V:81:PRO:HD2	2.55	0.42
26:A:1073:A:H2'	26:A:1074:G:O4'	2.20	0.42
26:A:1570:A:H2'	26:A:1571:A:C8	2.54	0.42
26:A:2052:A:H5'	29:D:146:ILE:O	2.19	0.42
26:A:2215:C:H2'	26:A:2216:G:C8	2.54	0.42
26:A:1:G:H2'	26:A:2:G:H8	1.85	0.42
26:A:892:A:H2'	26:A:893:C:H6	1.85	0.42
27:B:5:U:H2'	27:B:6:G:H8	1.84	0.42
31:F:169:LEU:HD23	31:F:176:PHE:HZ	1.85	0.42
31:F:177:ARG:OXT	57:6:47:LYS:NZ	2.52	0.42
37:L:128:THR:HG23	37:L:131:ALA:H	1.85	0.42
29:D:9:VAL:HG12	41:P:4:ILE:HG23	2.02	0.42
43:R:68:ARG:NH1	43:R:90:ARG:HB2	2.33	0.42
44:S:83:LYS:HD3	44:S:95:ARG:HH11	1.85	0.42
52:0:30:ASP:OD1	52:0:31:LYS:N	2.52	0.42
26:A:2698:U:H2'	26:A:2699:C:C6	2.54	0.42
26:A:414:C:H2'	26:A:415:A:C8	2.54	0.42
26:A:892:A:H2'	26:A:893:C:C6	2.55	0.42
29:D:9:VAL:O	29:D:26:VAL:HB	2.18	0.42
51:Z:4:ILE:HG13	51:Z:58:GLU:HG3	2.02	0.42
26:A:1483:G:H1'	26:A:1509:A:H2	1.85	0.42
26:A:1869:G:N2	26:A:1872:A:OP2	2.53	0.42
26:A:223:A:H2'	26:A:224:U:C6	7.48	0.42
27:B:111:U:H2'	27:B:112:G:C8	2.55	0.42
27:B:2:G:H2'	27:B:3:C:C6	2.54	0.42
26:A:2312:U:H5'	31:F:84:ILE:HD11	2.02	0.42
35:J:21:THR:HG22	35:J:61:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1831:G:H2'	26:A:1832:C:C6	2.54	0.42
26:A:2134:A:C6	26:A:2158:A:H5'	2.55	0.42
32:G:162:ARG:HG2	32:G:163:TYR:O	2.20	0.42
33:I:52:LEU:HB3	33:I:54:ILE:HG13	2.02	0.42
41:P:52:ARG:HB2	41:P:55:HIS:HB2	2.02	0.42
53:1:41:VAL:HG13	53:1:42:VAL:HG23	2.02	0.42
26:A:1392:A:H2'	26:A:1393:A:C8	2.54	0.42
26:A:1422:G:H4'	36:K:48:PRO:HB3	99.85	0.42
26:A:1447:C:H2'	26:A:1448:G:H8	1.84	0.42
26:A:2193:G:H2'	26:A:2194:U:C6	2.55	0.42
26:A:2196:C:H2'	26:A:2197:U:C6	2.55	0.42
26:A:2233:U:H2'	26:A:2234:G:H8	1.84	0.42
26:A:479:A:H4'	26:A:480:A:H5'	2.02	0.42
26:A:851:C:H2'	26:A:852:U:C6	2.55	0.42
28:C:132:ARG:O	28:C:166:ARG:NH1	2.46	0.42
29:D:48:ILE:HG23	29:D:84:LEU:HD11	2.02	0.42
31:F:169:LEU:HG	31:F:174:PHE:CE2	2.54	0.42
36:K:63:VAL:HB	36:K:103:VAL:HG12	2.02	0.42
52:0:12:ARG:HH11	52:0:16:ARG:NH1	2.17	0.41
26:A:1794:A:H2'	26:A:1795:C:C6	2.55	0.41
26:A:2557:G:H2'	26:A:2558:C:C6	2.54	0.41
35:J:57:LEU:HD21	35:J:130:HIS:HB3	2.02	0.41
45:T:54:GLU:HG3	45:T:88:LYS:HE2	2.02	0.41
49:X:37:PHE:CD2	49:X:48:LEU:HD12	2.54	0.41
26:A:2759:G:N2	32:G:138:GLN:HE22	2.17	0.41
26:A:2824:C:H2'	26:A:2825:G:O4'	2.20	0.41
28:C:141:HIS:ND1	28:C:192:GLY:O	2.36	0.41
26:A:1817:G:OP1	28:C:86:ARG:NH2	2.53	0.41
30:E:119:ILE:O	30:E:187:VAL:HA	2.19	0.41
45:T:54:GLU:N	45:T:54:GLU:OE1	2.53	0.41
26:A:2333:A:P	48:W:73:ARG:HH22	2.41	0.41
26:A:1475:G:O2'	26:A:1514:G:O6	2.39	0.41
26:A:2102:G:H2'	26:A:2103:C:H6	1.85	0.41
26:A:2124:G:C2	26:A:2125:G:H1'	2.55	0.41
26:A:2183:A:H2'	26:A:2184:A:C8	2.56	0.41
26:A:558:U:H2'	26:A:559:G:H8	1.85	0.41
29:D:84:LEU:HD23	29:D:84:LEU:HA	1.84	0.41
31:F:174:PHE:HD2	31:F:176:PHE:HE2	1.67	0.41
37:L:75:ALA:O	37:L:108:ALA:HA	2.20	0.41
43:R:76:LYS:HB2	43:R:85:LYS:HG2	2.01	0.41
26:A:2095:A:H5''	34:H:11:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:197:A:N6	26:A:2430:A:O2'	2.53	0.41
26:A:320:A:H4'	26:A:322:A:C8	2.56	0.41
26:A:482:A:OP2	26:A:507:A:N6	2.47	0.41
26:A:553:G:H2'	26:A:554:U:H6	1.85	0.41
35:J:73:VAL:HA	35:J:88:THR:HA	2.01	0.41
36:K:7:MET:HB3	36:K:18:ARG:HE	1.85	0.41
26:A:1182:G:H2'	26:A:1183:U:O4'	2.21	0.41
26:A:2124:G:N2	26:A:2171:A:H5''	2.35	0.41
26:A:2334:U:O2	40:O:13:ARG:NH1	2.54	0.41
26:A:598:U:H2'	26:A:599:A:C8	2.55	0.41
28:C:144:GLU:OE1	28:C:150:GLY:N	2.53	0.41
38:M:36:VAL:HG23	47:V:82:TYR:CD2	2.56	0.41
42:Q:78:PHE:HE2	42:Q:94:LEU:HD21	1.85	0.41
44:S:29:VAL:HG11	44:S:69:LEU:HB3	2.02	0.41
56:4:22:VAL:HG13	56:4:24:ARG:HE	1.86	0.41
26:A:1107:G:H2'	26:A:1108:U:C6	2.56	0.41
26:A:38:A:N3	30:E:43:THR:OG1	2.49	0.41
26:A:671:C:H2'	26:A:672:C:H6	1.84	0.41
26:A:876:C:H2'	26:A:877:A:O4'	2.19	0.41
26:A:782:A:N7	28:C:219:VAL:HG21	2.35	0.41
28:C:268:ARG:NH2	28:C:271:SER:OG	2.53	0.41
26:A:2757:A:N1	32:G:66:THR:HG21	2.35	0.41
26:A:1153:C:OP1	42:Q:91:ARG:NH2	2.54	0.41
46:U:48:VAL:O	46:U:53:GLN:HG3	2.20	0.41
26:A:1181:U:H2'	26:A:1182:G:C8	2.56	0.41
26:A:2151:U:H2'	26:A:2152:G:C8	2.56	0.41
26:A:2745:C:H2'	26:A:2746:U:C6	2.55	0.41
26:A:2773:C:OP1	29:D:169:ARG:NH2	2.53	0.41
29:D:103:ASP:OD1	29:D:104:VAL:N	2.54	0.41
30:E:136:GLN:HA	30:E:139:LYS:HG2	2.01	0.41
30:E:90:GLN:OE1	30:E:92:HIS:NE2	2.54	0.41
29:D:13:ARG:NH1	41:P:74:GLN:OE1	2.43	0.41
26:A:993:G:OP2	42:Q:50:ARG:NH2	2.54	0.41
42:Q:97:ILE:HD13	42:Q:97:ILE:HG21	1.89	0.41
26:A:1545:A:H2'	26:A:1546:G:O4'	2.21	0.41
26:A:1744:A:H3'	26:A:1745:A:H8	1.85	0.41
26:A:1902:C:H5''	28:C:239:PHE:HE2	1.84	0.41
26:A:2636:C:H2'	26:A:2637:U:C6	2.55	0.41
26:A:598:U:H2'	26:A:599:A:H8	1.85	0.41
28:C:143:VAL:HG11	28:C:173:LEU:HD11	2.02	0.41
29:D:110:THR:HB	29:D:202:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:43:ILE:HD12	31:F:43:ILE:H	1.86	0.41
55:3:25:HIS:CE1	55:3:47:ALA:HB2	2.56	0.41
26:A:2467:C:OP1	56:4:8:LYS:NZ	2.47	0.41
26:A:2469:A:N6	26:A:2481:G:O2'	2.54	0.41
26:A:685:A:H5''	26:A:788:A:H62	1.86	0.41
29:D:114:LYS:HG2	29:D:196:ALA:HB2	2.02	0.41
36:K:105:ARG:O	36:K:108:ARG:HB2	2.20	0.41
44:S:20:VAL:HG21	44:S:43:ALA:HB3	2.03	0.41
47:V:90:ASP:OD1	47:V:90:ASP:N	2.52	0.41
51:Z:11:SER:O	51:Z:15:ARG:NH1	2.54	0.41
51:Z:23:LEU:HD23	51:Z:23:LEU:HA	1.87	0.41
56:4:14:CYS:HA	56:4:27:CYS:HA	2.03	0.41
26:A:1790:C:H2'	26:A:1791:A:C5	2.55	0.41
26:A:2577:A:H5''	26:A:2578:G:H5'	2.02	0.41
30:E:147:LEU:HD23	30:E:183:PHE:CD2	2.55	0.41
33:I:89:SER:OG	33:I:90:GLY:N	2.53	0.41
51:Z:43:ILE:O	51:Z:46:MET:N	2.50	0.41
55:3:22:LYS:HA	55:3:47:ALA:O	2.21	0.41
26:A:2243:U:H2'	26:A:2244:U:C6	2.56	0.41
26:A:2532:G:N2	26:A:2663:G:O2'	2.54	0.41
26:A:553:G:H2'	26:A:554:U:C6	2.56	0.41
26:A:65:U:H2'	26:A:66:C:H6	1.85	0.41
29:D:133:THR:HG22	29:D:134:HIS:H	1.86	0.41
32:G:80:GLU:HG2	32:G:81:GLY:H	1.86	0.41
34:H:84:ALA:HA	34:H:91:PHE:N	2.36	0.41
38:M:2:LEU:HD21	38:M:65:ILE:HD13	2.02	0.41
43:R:75:VAL:HG22	43:R:86:GLN:HG3	2.02	0.41
44:S:47:VAL:HA	44:S:50:VAL:HG12	2.01	0.41
26:A:1170:C:H2'	26:A:1171:G:C4	2.56	0.40
26:A:852:U:H2'	26:A:853:C:C6	2.55	0.40
34:H:3:VAL:HA	34:H:38:PRO:HA	2.03	0.40
26:A:1138:G:O2'	35:J:104:ALA:O	2.39	0.40
26:A:191:A:H2'	26:A:192:C:C6	2.57	0.40
26:A:61:C:OP2	50:Y:47:ARG:NH1	2.52	0.40
28:C:62:ARG:HG2	28:C:90:ILE:HD11	2.02	0.40
37:L:77:ILE:HD12	37:L:77:ILE:HA	1.79	0.40
26:A:687:C:O4'	54:2:4:THR:HA	2.22	0.40
26:A:1753:G:H5''	41:P:92:ARG:HD3	2.02	0.40
26:A:2788:C:H2'	26:A:2789:C:C6	2.55	0.40
26:A:675:A:N3	26:A:2443:C:O2'	2.44	0.40
26:A:861:A:H2'	26:A:862:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:109:ARG:HD2	31:F:136:ILE:O	2.21	0.40
38:M:4:PRO:HG3	38:M:68:PHE:HE2	1.85	0.40
44:S:7:HIS:CD2	44:S:10:ALA:HB2	2.54	0.40
45:T:67:VAL:HG13	45:T:74:ILE:HD11	2.03	0.40
26:A:693:A:O2'	26:A:1353:A:N3	2.51	0.40
26:A:602:A:O2'	26:A:604:G:O2'	2.29	0.40
26:A:2404:U:H2'	26:A:2405:G:O4'	2.22	0.40
26:A:2715:C:H2'	26:A:2716:C:O4'	2.22	0.40
26:A:438:G:H2'	26:A:439:A:C8	2.56	0.40
26:A:871:U:H2'	26:A:872:U:C6	2.55	0.40
27:B:48:U:H2'	27:B:49:C:C6	2.57	0.40
28:C:116:GLN:HE21	28:C:121:ALA:HA	1.87	0.40
30:E:88:ARG:HA	30:E:88:ARG:HD3	1.85	0.40
34:H:39:ALA:HA	34:H:43:ASN:HB2	2.03	0.40
33:I:110:GLN:HA	33:I:124:MET:HE1	2.02	0.40
40:O:67:ASN:H	40:O:70:ALA:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/218 (99%)	184 (85%)	26 (12%)	6 (3%)	6	41
3	c	204/206 (99%)	191 (94%)	12 (6%)	1 (0%)	34	75
4	d	203/205 (99%)	185 (91%)	13 (6%)	5 (2%)	7	43
5	e	155/157 (99%)	138 (89%)	12 (8%)	5 (3%)	5	38
6	f	98/100 (98%)	81 (83%)	14 (14%)	3 (3%)	5	39
7	g	149/151 (99%)	136 (91%)	11 (7%)	2 (1%)	15	57
8	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	i	125/127 (98%)	105 (84%)	16 (13%)	4 (3%)	5	38
10	j	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3	29
11	k	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	21	65
12	l	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	7	43
13	m	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	6	41
14	n	98/100 (98%)	86 (88%)	9 (9%)	3 (3%)	5	39
15	o	86/88 (98%)	71 (83%)	12 (14%)	3 (4%)	4	35
16	p	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	15	57
17	q	78/80 (98%)	68 (87%)	7 (9%)	3 (4%)	4	32
18	r	63/65 (97%)	55 (87%)	6 (10%)	2 (3%)	5	38
19	s	84/86 (98%)	74 (88%)	5 (6%)	5 (6%)	2	19
20	t	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
21	u	63/65 (97%)	51 (81%)	9 (14%)	3 (5%)	3	25
25	z	612/614 (100%)	581 (95%)	24 (4%)	7 (1%)	17	61
28	C	269/271 (99%)	247 (92%)	20 (7%)	2 (1%)	26	70
29	D	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
30	E	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	34	75
31	F	175/177 (99%)	162 (93%)	10 (6%)	3 (2%)	11	51
32	G	174/176 (99%)	159 (91%)	13 (8%)	2 (1%)	17	61
33	I	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	26	70
34	H	147/149 (99%)	129 (88%)	15 (10%)	3 (2%)	9	48
35	J	140/142 (99%)	134 (96%)	5 (4%)	1 (1%)	26	70
36	K	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	24	67
37	L	141/143 (99%)	128 (91%)	11 (8%)	2 (1%)	14	55
38	M	134/136 (98%)	119 (89%)	13 (10%)	2 (2%)	13	54
39	N	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
40	O	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
41	P	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
42	Q	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
43	R	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	19	63
44	S	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	21	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	T	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
46	U	100/102 (98%)	88 (88%)	10 (10%)	2 (2%)	9	48
47	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
48	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
49	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
50	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	12	53
51	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
52	0	54/56 (96%)	48 (89%)	5 (9%)	1 (2%)	10	49
53	1	48/50 (96%)	46 (96%)	1 (2%)	1 (2%)	9	47
54	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
55	3	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	12	53
56	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
57	6	64/66 (97%)	55 (86%)	8 (12%)	1 (2%)	12	53
All	All	6336/6438 (98%)	5763 (91%)	482 (8%)	91 (1%)	19	55

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
2	b	73	ARG
5	e	93	VAL
6	f	94	HIS
6	f	98	GLU
9	i	57	VAL
10	j	34	ALA
10	j	42	LEU
10	j	57	VAL
10	j	92	LEU
11	k	92	ARG
12	l	75	GLU
14	n	34	ASN
14	n	57	SER
17	q	49	ASN
17	q	51	GLU
18	r	11	ARG
18	r	17	VAL
19	s	82	HIS

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Mol	Chain	Res	Type
19	s	86	LYS
25	z	191	VAL
25	z	487	PHE
28	C	121	ALA
30	E	83	VAL
31	F	173	ASP
32	G	118	ALA
33	I	64	ARG
34	H	9	VAL
35	J	81	ILE
36	K	35	VAL
37	L	36	LYS
38	M	58	LYS
44	S	64	ALA
46	U	6	ARG
46	U	88	ASP
52	0	2	VAL
55	3	31	ILE
2	b	17	HIS
2	b	153	MET
5	e	89	THR
6	f	92	THR
9	i	120	ALA
9	i	125	GLN
12	l	101	LEU
19	s	80	ARG
25	z	328	ALA
25	z	490	GLU
32	G	108	PHE
34	H	41	LYS
57	6	40	CYS
2	b	74	ALA
3	c	61	LYS
4	d	45	PRO
4	d	191	SER
4	d	192	ALA
9	i	107	ALA
13	m	4	ALA
13	m	65	GLU
16	p	44	SER
21	u	24	LYS
25	z	301	GLU

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Mol	Chain	Res	Type
28	C	204	LEU
31	F	149	ARG
2	b	15	PHE
4	d	29	THR
5	e	122	VAL
7	g	50	ALA
7	g	149	ALA
14	n	2	LYS
15	o	87	ARG
17	q	72	TRP
19	s	4	LEU
25	z	85	ASP
50	Y	22	LEU
13	m	6	ILE
15	o	45	HIS
15	o	75	ALA
21	u	19	LYS
21	u	34	ARG
31	F	20	ASN
37	L	29	LYS
5	e	23	THR
12	l	2	THR
19	s	3	SER
34	H	3	VAL
25	z	600	GLY
38	M	69	PRO
4	d	166	LYS
5	e	24	VAL
43	R	52	PRO
53	1	4	ILE

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%)	179 (99%)	1 (1%)	90 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	170 (99%)	2 (1%)	78	91
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	86 (99%)	1 (1%)	80	92
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	102 (98%)	2 (2%)	65	87
9	i	105/105 (100%)	104 (99%)	1 (1%)	82	93
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	88 (99%)	1 (1%)	80	92
12	l	103/103 (100%)	102 (99%)	1 (1%)	82	93
13	m	92/92 (100%)	91 (99%)	1 (1%)	80	92
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	74/74 (100%)	73 (99%)	1 (1%)	74	90
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	74/74 (100%)	74 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	43 (98%)	1 (2%)	58	85
25	z	501/501 (100%)	498 (99%)	3 (1%)	90	96
28	C	216/216 (100%)	215 (100%)	1 (0%)	92	96
29	D	164/164 (100%)	163 (99%)	1 (1%)	90	96
30	E	165/165 (100%)	165 (100%)	0	100	100
31	F	148/148 (100%)	147 (99%)	1 (1%)	88	95
32	G	137/137 (100%)	136 (99%)	1 (1%)	88	95
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%)	102 (99%)	1 (1%)	82	93
37	L	102/102 (100%)	101 (99%)	1 (1%)	82	93
38	M	109/109 (100%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	N	100/100 (100%)	98 (98%)	2 (2%)	63	87
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%)	79 (99%)	1 (1%)	76	91
46	U	83/83 (100%)	81 (98%)	2 (2%)	57	85
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%)	54 (98%)	1 (2%)	66	88
51	Z	48/48 (100%)	48 (100%)	0	100	100
52	0	47/47 (100%)	47 (100%)	0	100	100
53	1	45/45 (100%)	45 (100%)	0	100	100
54	2	38/38 (100%)	38 (100%)	0	100	100
55	3	51/51 (100%)	51 (100%)	0	100	100
56	4	34/34 (100%)	34 (100%)	0	100	100
57	6	59/59 (100%)	59 (100%)	0	100	100
All	All	5233/5256 (100%)	5206 (100%)	27 (0%)	92	96

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	107	ARG
4	d	43	ARG
4	d	201	GLU
6	f	54	LEU
8	h	15	ASN
8	h	79	ARG
9	i	18	VAL
11	k	39	ASN
12	l	30	ARG
13	m	43	LYS
17	q	19	SER

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Mol	Chain	Res	Type
21	u	17	ARG
25	z	26	ASP
25	z	27	ARG
25	z	344	ARG
28	C	187	CYS
29	D	128	ARG
31	F	103	ILE
32	G	72	ASN
36	K	43	ILE
37	L	91	ASP
39	N	2	ARG
39	N	118	ARG
45	T	85	VAL
46	U	40	LEU
46	U	73	ASN
50	Y	58	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	23	ASN
2	b	38	HIS
3	c	175	HIS
4	d	39	GLN
4	d	99	ASN
4	d	163	GLN
7	g	27	ASN
7	g	129	ASN
9	i	80	HIS
9	i	109	GLN
10	j	35	GLN
11	k	37	GLN
11	k	39	ASN
13	m	13	HIS
16	p	79	ASN
17	q	30	HIS
19	s	68	HIS
19	s	82	HIS
20	t	12	GLN
20	t	60	GLN
25	z	11	HIS
25	z	47	GLN

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Mol	Chain	Res	Type
25	z	61	HIS
25	z	91	GLN
25	z	100	GLN
25	z	420	GLN
25	z	431	HIS
25	z	475	HIS
25	z	491	GLN
25	z	532	GLN
29	D	150	GLN
30	E	41	GLN
30	E	46	GLN
30	E	195	GLN
31	F	26	GLN
32	G	138	GLN
42	Q	43	GLN
44	S	7	HIS
44	S	15	GLN
47	V	78	GLN
52	0	5	ASN
54	2	16	HIS
54	2	26	ASN
56	4	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	187 (12%)	0
22	v	76/77 (98%)	8 (10%)	0
23	x	47/48 (97%)	23 (48%)	0
24	y	93/95 (97%)	12 (12%)	0
26	A	2898/2903 (99%)	411 (14%)	8 (0%)
27	B	119/120 (99%)	17 (14%)	0
58	w	2/3 (66%)	0	0
All	All	4770/4785 (99%)	658 (13%)	8 (0%)

All (658) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	A
1	a	9	G
1	a	22	G

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Mol	Chain	Res	Type
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	84	U
1	a	86	G
1	a	87	C
1	a	94	G
1	a	95	C
1	a	96	U
1	a	121	U
1	a	130	A
1	a	131	A
1	a	141	G
1	a	163	C
1	a	164	G
1	a	173	U
1	a	177	G
1	a	182	A
1	a	197	A
1	a	209	U
1	a	210	C
1	a	211	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	252	U
1	a	253	A
1	a	266	G
1	a	267	C
1	a	289	G
1	a	298	A
1	a	328	C
1	a	329	A
1	a	347	G
1	a	348	G
1	a	351	G
1	a	352	C
1	a	354	G

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Mol	Chain	Res	Type
1	a	356	A
1	a	367	U
1	a	372	C
1	a	373	A
1	a	388	G
1	a	406	G
1	a	411	A
1	a	414	A
1	a	429	U
1	a	439	U
1	a	467	U
1	a	481	G
1	a	482	A
1	a	495	A
1	a	497	G
1	a	505	G
1	a	511	C
1	a	518	C
1	a	519	C
1	a	521	G
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	564	C
1	a	572	A
1	a	573	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	596	A
1	a	633	G
1	a	642	A
1	a	653	U
1	a	665	A
1	a	695	A
1	a	723	U
1	a	733	G
1	a	734	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	817	C
1	a	819	A
1	a	832	G
1	a	836	G
1	a	841	C
1	a	843	U
1	a	844	G
1	a	845	A
1	a	878	A
1	a	902	G
1	a	914	A
1	a	926	G
1	a	933	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	968	A
1	a	969	A
1	a	971	G
1	a	972	C
1	a	975	A
1	a	976	G
1	a	977	A
1	a	992	U
1	a	993	G
1	a	1004	A
1	a	1020	G
1	a	1028	C
1	a	1030	U
1	a	1033	G
1	a	1034	G
1	a	1043	G
1	a	1050	G
1	a	1065	U
1	a	1085	U
1	a	1094	G

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Mol	Chain	Res	Type
1	a	1095	U
1	a	1101	A
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1139	G
1	a	1140	C
1	a	1158	C
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1169	A
1	a	1182	G
1	a	1196	A
1	a	1197	A
1	a	1206	G
1	a	1213	A
1	a	1214	C
1	a	1227	A
1	a	1228	C
1	a	1236	A
1	a	1238	A
1	a	1256	A
1	a	1258	G
1	a	1260	G
1	a	1278	G
1	a	1280	A
1	a	1286	U
1	a	1287	A
1	a	1300	G
1	a	1301	U
1	a	1302	C
1	a	1317	C
1	a	1320	C
1	a	1346	A
1	a	1353	G
1	a	1363	A
1	a	1364	U
1	a	1370	G
1	a	1378	C
1	a	1406	U
1	a	1419	G

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Mol	Chain	Res	Type
1	a	1441	A
1	a	1487	G
1	a	1492	A
1	a	1503	A
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1538	C
1	a	1539	C
1	a	1540	U
22	v	9	G
22	v	13	C
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	54	5MU
22	v	56	C
22	v	76	A
23	x	88	A
23	x	90	G
23	x	91	A
23	x	96	C
23	x	97	A
23	x	98	U
23	x	109	C
23	x	110	G
23	x	113	C
23	x	114	C
23	x	115	A
23	x	116	U
23	x	117	C
23	x	123	C
23	x	124	A
23	x	125	G
23	x	126	G
23	x	127	U

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Mol	Chain	Res	Type
23	x	128	C
23	x	129	U
23	x	130	G
23	x	133	C
23	x	134	C
24	y	8	G
24	y	9	U
24	y	17	G
24	y	18	G
24	y	20	G
24	y	45	U
24	y	47(E)	G
24	y	47(G)	C
24	y	47(H)	A
24	y	47(I)	G
24	y	47(J)	C
24	y	49	G
26	A	10	A
26	A	14	A
26	A	34	U
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	103	A
26	A	118	A
26	A	119	A
26	A	120	U
26	A	131	A
26	A	138	U
26	A	139	U
26	A	142	A
26	A	163	C
26	A	196	A
26	A	197	A
26	A	199	A
26	A	204	A
26	A	215	G
26	A	216	A

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Mol	Chain	Res	Type
26	A	221	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	285	G
26	A	294	A
26	A	295	G
26	A	297	G
26	A	300	A
26	A	311	A
26	A	329	G
26	A	330	A
26	A	346	A
26	A	362	A
26	A	383	C
26	A	385	C
26	A	386	G
26	A	387	U
26	A	396	G
26	A	404	A
26	A	405	U
26	A	411	G
26	A	412	A
26	A	429	A
26	A	435	C
26	A	455	C
26	A	480	A
26	A	481	G
26	A	490	C
26	A	491	G
26	A	504	A
26	A	505	A
26	A	509	C
26	A	510	C
26	A	529	A
26	A	530	G
26	A	531	C

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Mol	Chain	Res	Type
26	A	532	A
26	A	547	A
26	A	549	G
26	A	563	A
26	A	568	U
26	A	573	U
26	A	575	A
26	A	586	A
26	A	588	U
26	A	603	A
26	A	613	A
26	A	614	A
26	A	615	U
26	A	616	A
26	A	622	G
26	A	637	A
26	A	645	C
26	A	646	U
26	A	647	G
26	A	653	U
26	A	655	A
26	A	678	C
26	A	685	A
26	A	686	U
26	A	717	C
26	A	730	A
26	A	747	5MU
26	A	748	G
26	A	764	A
26	A	765	C
26	A	775	G
26	A	776	G
26	A	782	A
26	A	783	A
26	A	784	G
26	A	785	G
26	A	792	A
26	A	805	G
26	A	811	U
26	A	812	C
26	A	845	A
26	A	846	U

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Mol	Chain	Res	Type
26	A	859	G
26	A	869	G
26	A	883	G
26	A	885	C
26	A	886	A
26	A	887	U
26	A	888	C
26	A	891	G
26	A	893	C
26	A	910	A
26	A	914	G
26	A	932	U
26	A	941	A
26	A	945	A
26	A	946	C
26	A	961	C
26	A	965	C
26	A	974	G
26	A	983	A
26	A	989	G
26	A	996	A
26	A	1006	C
26	A	1009	A
26	A	1012	U
26	A	1013	C
26	A	1022	G
26	A	1025	G
26	A	1026	G
26	A	1033	U
26	A	1040	A
26	A	1045	C
26	A	1046	A
26	A	1047	G
26	A	1054	A
26	A	1057	A
26	A	1060	U
26	A	1061	U
26	A	1062	G
26	A	1064	C
26	A	1065	U
26	A	1066	U
26	A	1067	A

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Mol	Chain	Res	Type
26	A	1068	G
26	A	1070	A
26	A	1073	A
26	A	1076	C
26	A	1077	A
26	A	1078	U
26	A	1079	C
26	A	1082	U
26	A	1084	A
26	A	1088	A
26	A	1101	U
26	A	1108	U
26	A	1110	G
26	A	1112	G
26	A	1132	U
26	A	1133	A
26	A	1134	A
26	A	1135	C
26	A	1141	U
26	A	1142	A
26	A	1143	A
26	A	1155	A
26	A	1171	G
26	A	1175	A
26	A	1178	C
26	A	1179	G
26	A	1180	U
26	A	1181	U
26	A	1206	G
26	A	1210	G
26	A	1211	C
26	A	1241	A
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	1325	U

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Mol	Chain	Res	Type
26	A	1329	U
26	A	1332	G
26	A	1345	C
26	A	1359	A
26	A	1365	A
26	A	1368	G
26	A	1379	U
26	A	1383	A
26	A	1392	A
26	A	1395	A
26	A	1416	G
26	A	1417	C
26	A	1420	A
26	A	1428	C
26	A	1452	G
26	A	1458	U
26	A	1468	U
26	A	1476	U
26	A	1482	G
26	A	1493	C
26	A	1497	U
26	A	1498	C
26	A	1499	C
26	A	1515	A
26	A	1516	G
26	A	1535	A
26	A	1537	G
26	A	1538	G
26	A	1566	A
26	A	1569	A
26	A	1578	U
26	A	1607	C
26	A	1608	A
26	A	1609	A
26	A	1619	G
26	A	1648	U
26	A	1649	G
26	A	1651	G
26	A	1654	A
26	A	1674	G
26	A	1675	C
26	A	1715	G

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Mol	Chain	Res	Type
26	A	1732	C
26	A	1738	G
26	A	1758	U
26	A	1764	C
26	A	1773	A
26	A	1784	A
26	A	1786	A
26	A	1799	G
26	A	1800	C
26	A	1801	A
26	A	1808	A
26	A	1811	G
26	A	1816	C
26	A	1829	A
26	A	1847	A
26	A	1870	C
26	A	1884	G
26	A	1906	G
26	A	1913	A
26	A	1918	A
26	A	1929	G
26	A	1930	G
26	A	1936	A
26	A	1937	A
26	A	1942	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	1970	A
26	A	1971	U
26	A	1972	G
26	A	1982	U
26	A	1991	U
26	A	1993	U
26	A	2021	C
26	A	2022	U
26	A	2023	C
26	A	2031	A
26	A	2032	G

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Mol	Chain	Res	Type
26	A	2033	A
26	A	2043	C
26	A	2055	C
26	A	2056	G
26	A	2060	A
26	A	2061	G
26	A	2062	A
26	A	2068	U
26	A	2069	G7M
26	A	2070	A
26	A	2080	A
26	A	2093	G
26	A	2105	U
26	A	2107	G
26	A	2110	G
26	A	2111	U
26	A	2112	G
26	A	2113	U
26	A	2116	G
26	A	2118	U
26	A	2119	A
26	A	2120	G
26	A	2125	G
26	A	2127	G
26	A	2128	G
26	A	2129	C
26	A	2131	U
26	A	2132	U
26	A	2133	G
26	A	2134	A
26	A	2145	C
26	A	2146	C
26	A	2147	A
26	A	2149	U
26	A	2157	G
26	A	2158	A
26	A	2159	G
26	A	2160	C
26	A	2162	G
26	A	2164	C
26	A	2168	G
26	A	2172	U

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Mol	Chain	Res	Type
26	A	2173	A
26	A	2174	C
26	A	2177	C
26	A	2178	C
26	A	2179	C
26	A	2198	A
26	A	2204	G
26	A	2211	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	2273	A
26	A	2278	A
26	A	2283	C
26	A	2287	A
26	A	2288	A
26	A	2308	G
26	A	2310	C
26	A	2322	A
26	A	2325	G
26	A	2333	A
26	A	2335	A
26	A	2342	C
26	A	2345	G
26	A	2347	C
26	A	2350	C
26	A	2354	C
26	A	2361	G
26	A	2383	G
26	A	2385	C
26	A	2389	G
26	A	2402	U
26	A	2403	C
26	A	2406	A
26	A	2424	C
26	A	2429	G
26	A	2430	A
26	A	2434	A
26	A	2436	G

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Mol	Chain	Res	Type
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	2484	G
26	A	2502	G
26	A	2504	PSU
26	A	2505	G
26	A	2506	U
26	A	2513	A
26	A	2518	A
26	A	2520	C
26	A	2529	G
26	A	2547	A
26	A	2566	A
26	A	2567	G
26	A	2573	C
26	A	2602	A
26	A	2609	U
26	A	2613	U
26	A	2615	U
26	A	2629	U
26	A	2630	G
26	A	2689	U
26	A	2690	U
26	A	2714	G
26	A	2716	C
26	A	2726	A
26	A	2733	A
26	A	2739	U
26	A	2744	G
26	A	2748	A
26	A	2750	A
26	A	2755	C
26	A	2757	A
26	A	2765	A
26	A	2778	A
26	A	2791	G
26	A	2794	C
26	A	2797	U

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Mol	Chain	Res	Type
26	A	2798	U
26	A	2818	U
26	A	2821	A
26	A	2848	G
26	A	2849	U
26	A	2850	A
26	A	2873	A
26	A	2884	U
27	B	13	G
27	B	24	G
27	B	25	U
27	B	27	C
27	B	30	C
27	B	35	C
27	B	38	C
27	B	42	C
27	B	43	C
27	B	51	G
27	B	57	A
27	B	67	G
27	B	87	U
27	B	89	U
27	B	90	C
27	B	108	A
27	B	109	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	885	C
26	A	886	A
26	A	890	C
26	A	960	A
26	A	1536	C
26	A	2211	A
26	A	2250	G
26	A	2430	A

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	1.06	1 (5%)	15,36,39	2.61	2 (13%)
26	2MG	A	1835	26	18,26,27	1.07	2 (11%)	21,38,41	2.32	6 (28%)
26	PSU	A	1911	26	15,21,22	1.25	3 (20%)	16,30,33	2.02	3 (18%)
26	3TD	A	1915	26	15,22,23	3.18	5 (33%)	17,32,35	1.97	3 (17%)
26	PSU	A	1917	26	15,21,22	1.30	3 (20%)	16,30,33	2.55	2 (12%)
26	5MU	A	1939	26	13,22,23	0.74	1 (7%)	16,32,35	2.26	2 (12%)
26	5MC	A	1962	26	14,22,23	1.05	1 (7%)	17,32,35	2.05	5 (29%)
26	6MZ	A	2030	26	17,25,26	1.11	1 (5%)	15,36,39	1.69	3 (20%)
26	G7M	A	2069	26	18,26,27	1.16	2 (11%)	21,39,42	2.69	9 (42%)
26	OMG	A	2251	26,22	18,26,27	1.07	2 (11%)	21,38,41	1.82	4 (19%)
26	2MG	A	2445	26	18,26,27	1.06	2 (11%)	21,38,41	2.25	5 (23%)
26	H2U	A	2449	26	17,21,22	1.30	4 (23%)	23,30,33	2.10	2 (8%)
26	PSU	A	2457	26	15,21,22	1.58	2 (13%)	16,30,33	2.32	4 (25%)
26	OMC	A	2498	26	15,22,23	0.74	0	20,31,34	1.31	2 (10%)
26	2MA	A	2503	26	17,25,26	1.55	3 (17%)	18,37,40	3.59	3 (16%)
26	PSU	A	2504	26	15,21,22	1.23	2 (13%)	16,30,33	2.55	3 (18%)
26	OMU	A	2552	26	14,22,23	0.71	0	19,31,34	1.74	1 (5%)
26	PSU	A	2580	26	15,21,22	1.50	3 (20%)	16,30,33	2.55	5 (31%)
26	PSU	A	2604	26	15,21,22	1.29	2 (13%)	16,30,33	2.42	4 (25%)
26	PSU	A	2605	26	15,21,22	1.20	2 (13%)	16,30,33	2.24	4 (25%)
26	1MG	A	745	26	17,26,27	1.51	2 (11%)	19,39,42	1.41	2 (10%)
26	PSU	A	746	26	15,21,22	1.61	3 (20%)	16,30,33	2.17	3 (18%)
26	5MU	A	747	26	13,22,23	0.67	1 (7%)	16,32,35	2.74	2 (12%)
26	PSU	A	955	26	15,21,22	1.47	4 (26%)	16,30,33	2.47	4 (25%)
1	2MG	a	1207	1	18,26,27	1.13	2 (11%)	21,38,41	2.22	7 (33%)
1	4OC	a	1402	1	15,23,24	0.67	0	21,32,35	1.96	4 (19%)
1	5MC	a	1407	1	14,22,23	1.18	1 (7%)	17,32,35	0.97	1 (5%)
1	UR3	a	1498	1	13,22,23	0.62	0	18,32,35	0.91	1 (5%)
1	2MG	a	1516	1	18,26,27	1.09	2 (11%)	21,38,41	2.27	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	a	1518	1	18,26,27	0.96	1 (5%)	15,38,41	2.71	5 (33%)
1	MA6	a	1519	1	18,26,27	0.94	1 (5%)	15,38,41	2.28	3 (20%)
1	PSU	a	516	1	15,21,22	1.38	1 (6%)	16,30,33	2.23	3 (18%)
1	G7M	a	527	1	18,26,27	1.23	2 (11%)	21,39,42	2.71	8 (38%)
1	2MG	a	966	1	18,26,27	1.17	2 (11%)	21,38,41	2.47	5 (23%)
1	5MC	a	967	1	14,22,23	1.45	1 (7%)	17,32,35	1.08	1 (5%)
22	H2U	v	20	22	17,21,22	1.08	2 (11%)	23,30,33	1.93	3 (13%)
22	5MU	v	54	22	13,22,23	0.59	0	16,32,35	2.80	2 (12%)
22	PSU	v	55	22	15,21,22	1.17	2 (13%)	16,30,33	2.24	3 (18%)
22	4SU	v	8	22	12,21,22	0.75	0	15,30,33	0.87	1 (6%)
24	H2U	y	19	24	17,21,22	1.07	2 (11%)	23,30,33	2.24	4 (17%)
24	6IA	y	37	24	20,29,30	0.83	1 (5%)	22,41,44	2.42	3 (13%)
24	5MU	y	54	24	13,22,23	0.56	0	16,32,35	2.82	2 (12%)
24	PSU	y	55	24	15,21,22	1.04	2 (13%)	16,30,33	2.27	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	6MZ	A	1618	26	-	0/5/27/28	0/3/3/3
26	2MG	A	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
26	3TD	A	1915	26	-	0/7/25/26	0/2/2/2
26	PSU	A	1917	26	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/3/25/26	0/2/2/2
26	5MC	A	1962	26	-	0/3/25/26	0/2/2/2
26	6MZ	A	2030	26	-	0/5/27/28	0/3/3/3
26	G7M	A	2069	26	2/2/5/5	0/3/25/26	0/3/3/3
26	OMG	A	2251	26,22	-	0/5/27/28	0/3/3/3
26	2MG	A	2445	26	-	0/5/27/28	0/3/3/3
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
26	OMC	A	2498	26	-	0/5/27/28	0/2/2/2
26	2MA	A	2503	26	-	0/3/25/26	0/3/3/3
26	PSU	A	2504	26	-	0/7/25/26	0/2/2/2
26	OMU	A	2552	26	-	0/5/27/28	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
26	1MG	A	745	26	-	0/3/25/26	0/3/3/3
26	PSU	A	746	26	-	0/7/25/26	0/2/2/2
26	5MU	A	747	26	-	0/3/25/26	0/2/2/2
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	0/3/25/26	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/3/25/26	0/2/2/2
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
22	5MU	v	54	22	-	0/3/25/26	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/3/25/26	0/2/2/2
24	H2U	y	19	24	-	0/7/38/39	0/2/2/2
24	6IA	y	37	24	-	0/9/31/32	0/3/3/3
24	5MU	y	54	24	-	0/3/25/26	0/2/2/2
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	746	PSU	C5-C1'	-5.00	1.47	1.52
26	A	2457	PSU	C5-C1'	-4.87	1.48	1.52
26	A	2580	PSU	C5-C1'	-4.32	1.48	1.52
26	A	955	PSU	C5-C1'	-3.97	1.48	1.52
1	a	516	PSU	C5-C1'	-3.66	1.49	1.52
26	A	2604	PSU	C5-C1'	-3.48	1.49	1.52
26	A	2605	PSU	C5-C1'	-3.29	1.49	1.52
26	A	1911	PSU	C5-C1'	-3.15	1.49	1.52
26	A	1917	PSU	C5-C1'	-3.10	1.49	1.52
26	A	2504	PSU	C5-C1'	-3.01	1.49	1.52
26	A	1915	3TD	O4-C4	-2.92	1.17	1.24
26	A	2449	H2U	C4-N3	-2.80	1.33	1.37
26	A	2449	H2U	C2-N3	-2.79	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	55	PSU	C5-C1'	-2.78	1.49	1.52
22	v	20	H2U	C2-N3	-2.75	1.32	1.38
24	y	19	H2U	C4-N3	-2.70	1.33	1.37
22	v	20	H2U	C4-N3	-2.70	1.33	1.37
1	a	527	G7M	O2'-C2'	-2.70	1.36	1.43
24	y	19	H2U	C2-N3	-2.63	1.33	1.38
26	A	2069	G7M	O2'-C2'	-2.50	1.37	1.43
26	A	2449	H2U	C2-N1	-2.47	1.31	1.35
22	v	55	PSU	C2-N3	-2.41	1.33	1.38
26	A	2580	PSU	O4'-C1'	-2.32	1.40	1.44
26	A	1917	PSU	C2-N1	-2.28	1.33	1.38
26	A	2604	PSU	C2-N3	-2.28	1.33	1.38
26	A	2504	PSU	C2-N3	-2.24	1.33	1.38
26	A	2449	H2U	C6-N1	-2.23	1.44	1.47
26	A	1939	5MU	C2-N3	-2.18	1.33	1.38
26	A	2457	PSU	C2-N3	-2.18	1.33	1.38
26	A	955	PSU	C2-N3	-2.16	1.33	1.38
26	A	1917	PSU	C2-N3	-2.14	1.33	1.38
26	A	746	PSU	O4'-C1'	-2.12	1.41	1.44
26	A	955	PSU	O4'-C1'	-2.12	1.41	1.44
26	A	747	5MU	C2-N3	-2.10	1.33	1.38
24	y	55	PSU	C2-N1	-2.05	1.33	1.38
26	A	2605	PSU	C2-N3	-2.04	1.33	1.38
26	A	2580	PSU	C2-N3	-2.04	1.33	1.38
24	y	55	PSU	C5-C1'	-2.03	1.50	1.52
26	A	1911	PSU	C2-N1	-2.02	1.34	1.38
26	A	1911	PSU	C2-N3	-2.02	1.34	1.38
26	A	746	PSU	C2-N3	-2.02	1.34	1.38
26	A	955	PSU	C2-N1	-2.00	1.34	1.38
26	A	2503	2MA	C6-N6	2.44	1.33	1.29
26	A	2445	2MG	C5-C4	2.68	1.46	1.40
24	y	37	6IA	C5-C4	2.75	1.46	1.40
1	a	1516	2MG	C5-C4	2.78	1.46	1.40
26	A	1835	2MG	C5-C4	2.83	1.46	1.40
26	A	2251	OMG	C5-C4	2.93	1.47	1.40
1	a	1207	2MG	C5-C4	3.05	1.47	1.40
26	A	2251	OMG	C6-C5	3.16	1.47	1.41
26	A	2445	2MG	C6-C5	3.17	1.47	1.41
1	a	1516	2MG	C6-C5	3.27	1.47	1.41
1	a	1519	MA6	C5-C4	3.28	1.47	1.40
26	A	2069	G7M	C6-C5	3.29	1.48	1.41
26	A	1835	2MG	C6-C5	3.32	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2503	2MA	C5-C4	3.33	1.48	1.40
1	a	1207	2MG	C6-C5	3.34	1.48	1.41
1	a	966	2MG	C5-C4	3.37	1.48	1.40
26	A	1962	5MC	C5-C4	3.45	1.46	1.41
1	a	966	2MG	C6-C5	3.46	1.48	1.41
1	a	1518	MA6	C5-C4	3.47	1.48	1.40
26	A	2030	6MZ	C5-C4	3.57	1.48	1.40
1	a	527	G7M	C6-C5	3.62	1.48	1.41
26	A	745	1MG	C5-C4	3.65	1.48	1.40
26	A	1618	6MZ	C5-C4	3.69	1.48	1.40
1	a	1407	5MC	C5-C4	3.90	1.47	1.41
26	A	745	1MG	C6-C5	4.22	1.49	1.40
26	A	2503	2MA	C6-C5	4.49	1.49	1.40
1	a	967	5MC	C5-C4	4.85	1.49	1.41
26	A	1915	3TD	C4-N3	5.01	1.45	1.38
26	A	1915	3TD	C2-N1	5.04	1.48	1.38
26	A	1915	3TD	C6-N1	5.29	1.45	1.34
26	A	1915	3TD	C6-C5	7.56	1.49	1.38

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2449	H2U	C4-N3-C2	-8.59	117.98	125.77
24	y	54	5MU	C5-C4-N3	-8.12	118.53	125.35
26	A	747	5MU	C5-C4-N3	-8.09	118.56	125.35
22	v	54	5MU	C5-C4-N3	-7.68	118.90	125.35
1	a	1518	MA6	N3-C2-N1	-7.48	123.00	128.87
24	y	37	6IA	N3-C2-N1	-7.08	123.31	128.87
22	v	20	H2U	C4-N3-C2	-6.88	119.53	125.77
26	A	1939	5MU	C5-C4-N3	-6.76	119.67	125.35
26	A	1618	6MZ	N3-C2-N1	-6.32	123.91	128.87
26	A	1915	3TD	C5-C1'-C2'	-6.22	104.88	115.44
1	a	1519	MA6	N3-C2-N1	-6.13	124.05	128.87
26	A	2069	G7M	C5-C6-N1	-5.71	116.06	123.52
24	y	19	H2U	C4-N3-C2	-5.64	120.66	125.77
26	A	2504	PSU	C5-C1'-C2'	-5.44	106.20	115.44
26	A	955	PSU	C5-C1'-C2'	-5.38	106.30	115.44
1	a	527	G7M	C5-C6-N1	-5.37	116.50	123.52
24	y	37	6IA	C12-N6-C6	-4.90	117.79	123.46
26	A	2457	PSU	C5-C1'-C2'	-4.39	107.99	115.44
1	a	966	2MG	C5-C6-N1	-4.31	117.89	123.52
26	A	746	PSU	C5-C6-N1	-4.24	118.47	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2445	2MG	CM2-N2-C2	-4.23	118.28	123.03
26	A	2251	OMG	C5-C6-N1	-4.18	118.06	123.52
1	a	1207	2MG	C5-C6-N1	-4.16	118.08	123.52
26	A	2030	6MZ	N3-C2-N1	-4.16	125.60	128.87
1	a	1516	2MG	C5-C6-N1	-4.13	118.13	123.52
26	A	2445	2MG	C5-C6-N1	-4.10	118.16	123.52
1	a	1402	4OC	CM4-N4-C4	-4.09	119.42	122.87
26	A	2604	PSU	C5-C1'-C2'	-4.02	108.60	115.44
26	A	2457	PSU	C5-C6-N1	-3.95	118.88	124.38
26	A	2605	PSU	C5-C1'-C2'	-3.88	108.85	115.44
26	A	1835	2MG	C5-C6-N1	-3.85	118.49	123.52
26	A	745	1MG	C1'-N9-C4	-3.75	122.62	126.81
26	A	745	1MG	C6-C5-C4	-3.63	117.33	119.93
26	A	1835	2MG	CM2-N2-C2	-3.57	119.02	123.03
26	A	2580	PSU	C5-C6-N1	-3.50	119.49	124.38
26	A	2605	PSU	C5-C6-N1	-3.38	119.66	124.38
26	A	746	PSU	C5-C1'-C2'	-3.38	109.70	115.44
1	a	1518	MA6	C10-N6-C9	-3.30	105.19	115.96
26	A	955	PSU	C5-C6-N1	-3.27	119.83	124.38
26	A	2604	PSU	C5-C6-N1	-3.24	119.86	124.38
26	A	1915	3TD	C5-C6-N1	-3.23	119.87	124.38
26	A	2251	OMG	N3-C2-N1	-3.23	123.16	127.56
22	v	55	PSU	C5-C6-N1	-3.19	119.93	124.38
24	y	19	H2U	C5-C6-N1	-3.17	107.29	110.76
1	a	1516	2MG	C6-C5-C4	-3.16	117.25	120.86
1	a	1519	MA6	C10-N6-C9	-3.12	105.78	115.96
26	A	1911	PSU	C5-C6-N1	-2.98	120.23	124.38
26	A	2504	PSU	C5-C6-N1	-2.97	120.24	124.38
1	a	1516	2MG	CM2-N2-C2	-2.94	119.72	123.03
1	a	516	PSU	C5-C6-N1	-2.93	120.30	124.38
22	v	20	H2U	C5-C6-N1	-2.91	107.58	110.76
26	A	2445	2MG	C6-C5-C4	-2.89	117.56	120.86
1	a	527	G7M	N3-C2-N1	-2.83	123.71	127.56
22	v	8	4SU	C5-C4-N3	-2.77	120.62	123.56
26	A	1835	2MG	C6-C5-C4	-2.75	117.71	120.86
26	A	1962	5MC	CM5-C5-C4	-2.74	118.57	121.47
26	A	2069	G7M	N3-C2-N1	-2.68	123.91	127.56
26	A	2069	G7M	C4'-O4'-C1'	-2.55	106.94	109.64
1	a	1207	2MG	C6-C5-C4	-2.54	117.95	120.86
26	A	2503	2MA	C1'-N9-C4	-2.52	124.00	126.81
26	A	1962	5MC	C5-C4-N3	-2.42	117.14	121.26
24	y	55	PSU	C5-C1'-C2'	-2.39	111.38	115.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2498	OMC	CM2-O2'-C2'	-2.37	107.95	114.58
1	a	527	G7M	C4'-O4'-C1'	-2.33	107.18	109.64
1	a	1207	2MG	CM2-N2-C2	-2.33	120.42	123.03
1	a	1402	4OC	C6-N1-C2	-2.28	117.61	121.33
26	A	1835	2MG	N3-C2-N1	-2.25	122.83	126.19
1	a	1516	2MG	C1'-N9-C4	-2.22	124.32	126.81
26	A	2251	OMG	C6-C5-C4	-2.22	118.32	120.86
24	y	55	PSU	C5-C6-N1	-2.21	121.30	124.38
1	a	1516	2MG	N3-C2-N1	-2.12	123.02	126.19
26	A	2580	PSU	O2'-C2'-C1'	-2.06	107.45	111.93
26	A	2503	2MA	N3-C2-N1	-2.01	121.65	125.60
26	A	1962	5MC	CM5-C5-C6	2.01	122.71	118.63
26	A	2604	PSU	O4'-C1'-C2'	2.03	106.89	104.69
26	A	1915	3TD	O4'-C1'-C2'	2.10	106.96	104.69
1	a	1207	2MG	N2-C2-N3	2.11	119.39	116.94
1	a	1498	UR3	C3U-N3-C4	2.12	121.18	118.21
1	a	1518	MA6	O4'-C1'-N9	2.15	112.16	108.11
26	A	2069	G7M	C5'-C4'-C3'	2.23	123.81	115.20
26	A	955	PSU	O4'-C1'-C2'	2.24	107.12	104.69
24	y	55	PSU	O4'-C1'-C2'	2.29	107.17	104.69
1	a	1518	MA6	C1'-N9-C4	2.39	129.47	126.81
26	A	2605	PSU	O4'-C1'-C2'	2.40	107.28	104.69
26	A	2457	PSU	O4'-C1'-C2'	2.49	107.38	104.69
1	a	1407	5MC	N4-C4-N3	2.54	120.65	116.92
24	y	19	H2U	O2-C2-N1	2.55	126.52	123.17
26	A	1911	PSU	O4'-C1'-C2'	2.60	107.50	104.69
1	a	1207	2MG	C1'-N9-C4	2.62	129.73	126.81
26	A	1962	5MC	O4'-C1'-N1	2.63	113.10	108.10
26	A	2030	6MZ	C2-N1-C6	2.64	118.37	116.47
26	A	2069	G7M	O3'-C3'-C2'	2.64	120.40	111.86
22	v	55	PSU	O4'-C1'-C2'	2.84	107.76	104.69
26	A	2449	H2U	C1'-N1-C2	2.98	122.36	118.19
1	a	527	G7M	O3'-C3'-C2'	3.12	121.94	111.86
1	a	527	G7M	O3'-C3'-C4'	3.13	120.36	111.01
1	a	967	5MC	CM5-C5-C4	3.15	124.80	121.47
22	v	20	H2U	C1'-N1-C2	3.15	122.60	118.19
1	a	516	PSU	O4'-C1'-C2'	3.41	108.38	104.69
26	A	2069	G7M	O3'-C3'-C4'	3.48	121.39	111.01
1	a	527	G7M	N7-C8-N9	3.54	113.90	108.67
26	A	2030	6MZ	C1'-N9-C4	3.68	130.92	126.81
26	A	2580	PSU	O4'-C1'-C2'	3.75	108.75	104.69
1	a	966	2MG	N2-C2-N3	3.88	121.44	116.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2069	G7M	N7-C8-N9	4.11	114.74	108.67
1	a	1402	4OC	C2-N3-C4	4.21	120.78	115.43
26	A	2498	OMC	C6-C5-C4	4.27	119.11	117.44
26	A	1917	PSU	C4-C5-C1'	4.32	128.49	121.22
26	A	1835	2MG	C6-N1-C2	4.51	121.69	115.24
26	A	2445	2MG	C6-N1-C2	4.56	121.76	115.24
1	a	966	2MG	C6-N1-C2	4.70	121.97	115.24
1	a	1207	2MG	C6-N1-C2	4.70	121.97	115.24
1	a	1516	2MG	C6-N1-C2	4.72	122.00	115.24
26	A	2069	G7M	C1'-N9-C4	4.79	132.16	126.81
1	a	966	2MG	C1'-N9-C4	4.80	132.16	126.81
26	A	2580	PSU	C5-C1'-C2'	4.92	123.79	115.44
1	a	1519	MA6	C2-N1-C6	4.94	123.29	111.64
26	A	2251	OMG	C6-N1-C2	5.01	121.75	115.88
1	a	1518	MA6	C2-N1-C6	5.06	123.58	111.64
1	a	1516	2MG	C2-N3-C4	5.44	120.95	114.99
26	A	2445	2MG	C2-N3-C4	5.51	121.03	114.99
26	A	1939	5MU	C4-N3-C2	5.57	119.81	115.16
1	a	1207	2MG	C2-N3-C4	5.58	121.11	114.99
1	a	527	G7M	C6-N1-C2	5.60	122.45	115.88
1	a	966	2MG	C2-N3-C4	5.67	121.21	114.99
1	a	527	G7M	C1'-N9-C4	5.70	133.17	126.81
26	A	2069	G7M	C6-N1-C2	5.78	122.65	115.88
1	a	1402	4OC	C6-C5-C4	5.78	119.69	117.42
26	A	1962	5MC	N4-C4-N3	5.96	125.66	116.92
26	A	2457	PSU	C4-N3-C2	6.22	120.34	115.16
26	A	1911	PSU	C4-N3-C2	6.25	120.37	115.16
26	A	746	PSU	C4-N3-C2	6.36	120.46	115.16
26	A	2605	PSU	C4-N3-C2	6.46	120.54	115.16
26	A	1835	2MG	C2-N3-C4	6.46	122.07	114.99
26	A	2580	PSU	C4-N3-C2	6.70	120.75	115.16
26	A	2552	OMU	C4-N3-C2	6.74	121.31	114.21
26	A	955	PSU	C4-N3-C2	6.86	120.88	115.16
24	y	37	6IA	C2-N1-C6	6.87	121.41	116.47
1	a	516	PSU	C4-N3-C2	6.92	120.93	115.16
22	v	55	PSU	C4-N3-C2	7.04	121.03	115.16
26	A	747	5MU	C4-N3-C2	7.13	121.10	115.16
26	A	2604	PSU	C4-N3-C2	7.15	121.12	115.16
24	y	19	H2U	C1'-N1-C2	7.19	128.26	118.19
26	A	2504	PSU	C4-N3-C2	7.45	121.37	115.16
24	y	54	5MU	C4-N3-C2	7.53	121.44	115.16
24	y	55	PSU	C4-N3-C2	7.61	121.51	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1618	6MZ	C2-N1-C6	7.67	121.98	116.47
22	v	54	5MU	C4-N3-C2	7.80	121.66	115.16
26	A	1917	PSU	C4-N3-C2	8.39	122.16	115.16
26	A	2503	2MA	C2-N3-C4	14.49	122.27	115.29

All (4) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	745	1MG	4	0
26	A	746	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 153 ligands modelled in this entry, 150 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
61	FME	v	101	22	8,9,10	0.86	0	5,9,11	1.78	1 (20%)
62	SEC	y	701	24	1,5,6	0.79	0	1,5,7	2.20	1 (100%)
63	GNP	z	701	60	29,34,34	2.59	7 (24%)	28,54,54	1.55	4 (14%)

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
61	FME	v	101	22	-	1/6/9/11	0/0/0/0
62	SEC	y	701	24	-	0/0/4/6	0/0/0/0
63	GNP	z	701	60	-	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)
63	z	701	GNP	C4-N9	-10.39	1.33	1.47
63	z	701	GNP	C8-N9	-3.98	1.34	1.47
63	z	701	GNP	C5-C6	-2.81	1.47	1.53
63	z	701	GNP	C2-N1	-2.25	1.34	1.44
63	z	701	GNP	PG-N3B	3.39	1.72	1.63
63	z	701	GNP	C1'-N9	3.65	1.49	1.42
63	z	701	GNP	PB-N3B	3.69	1.73	1.63

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	701	GNP	PA-O3A-PB	-4.93	114.82	132.71
61	v	101	FME	O-C-CA	-3.45	116.26	125.69
63	z	701	GNP	O3G-PG-O1G	-2.31	107.51	113.58
62	y	701	SEC	O-C-CA	-2.20	119.81	125.72
63	z	701	GNP	C8-N9-C4	2.66	107.81	104.78
63	z	701	GNP	C4-C5-N7	2.76	106.97	102.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.