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

Dec 5, 2016 – 04:27 PM EST

PDB ID	:	5LZA
EMDB ID:	:	EMD-4121
Title	:	Structure of the 70S ribosome with SECIS-mRNA and P-site tRNA (Initial complex, IC)
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	:	3.60 Å(reported)

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

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

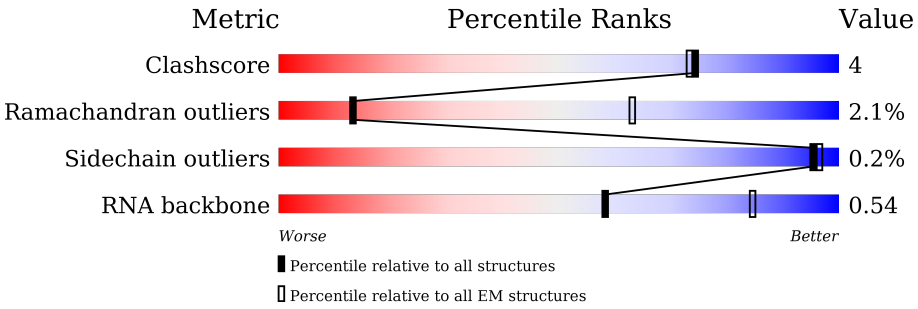
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	1539	74% 24% .
2	b	218	96% ..
3	c	206	100%
4	d	205	99% .
5	e	157	94% ..
6	f	100	93% 5% .
7	g	151	97% ..
8	h	129	98% .

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Mol	Chain	Length	Quality of chain
9	i	127	94% 6%
10	j	98	93% 5%
11	k	116	97%
12	l	123	91% 8%
13	m	114	96%
14	n	100	97%
15	o	88	98%
16	p	82	95%
17	q	80	95%
18	r	65	91% 8%
19	s	79	97%
20	t	85	100%
21	u	65	94%
22	v	77	68% 31%
23	x	48	52% 48%
24	A	2903	60% 31% 8%
25	B	120	63% 29% 7%
26	C	271	84% 16%
27	D	209	84% 16%
28	E	201	86% 14%
29	F	177	82% 18%
30	G	176	82% 15%
31	I	141	89% 10%
32	H	149	91% 9%
33	J	142	87% 13%

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Mol	Chain	Length	Quality of chain
34	K	122	77% 20%
35	L	143	85% 13%
36	M	136	85% 15%
37	N	120	89% 11%
38	O	116	92% 7%
39	P	114	84% 16%
40	Q	117	94% 5%
41	R	103	84% 16%
42	S	110	88% 12%
43	T	93	88% 12%
44	U	102	85% 13%
45	V	94	84% 16%
46	W	75	83% 17%
47	X	77	84% 16%
48	Y	63	86% 13%
49	Z	58	98%
50	0	56	89% 9%
51	1	50	76% 20%
52	2	46	83% 17%
53	3	64	88% 11%
54	4	38	87% 11%
55	6	66	79% 20%

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	-	-	-
24	G7M	A	2069	X	-	-	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 146037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1539	33119	14778	6072	10726	1543	4	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called fMet-tRNAfMet.

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

- Molecule 23 is a RNA chain called SECIS mRNA.

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

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	2900	Total	C	N	O	P	1	0
			62296	27797	11464	20134	2901		

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L11.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

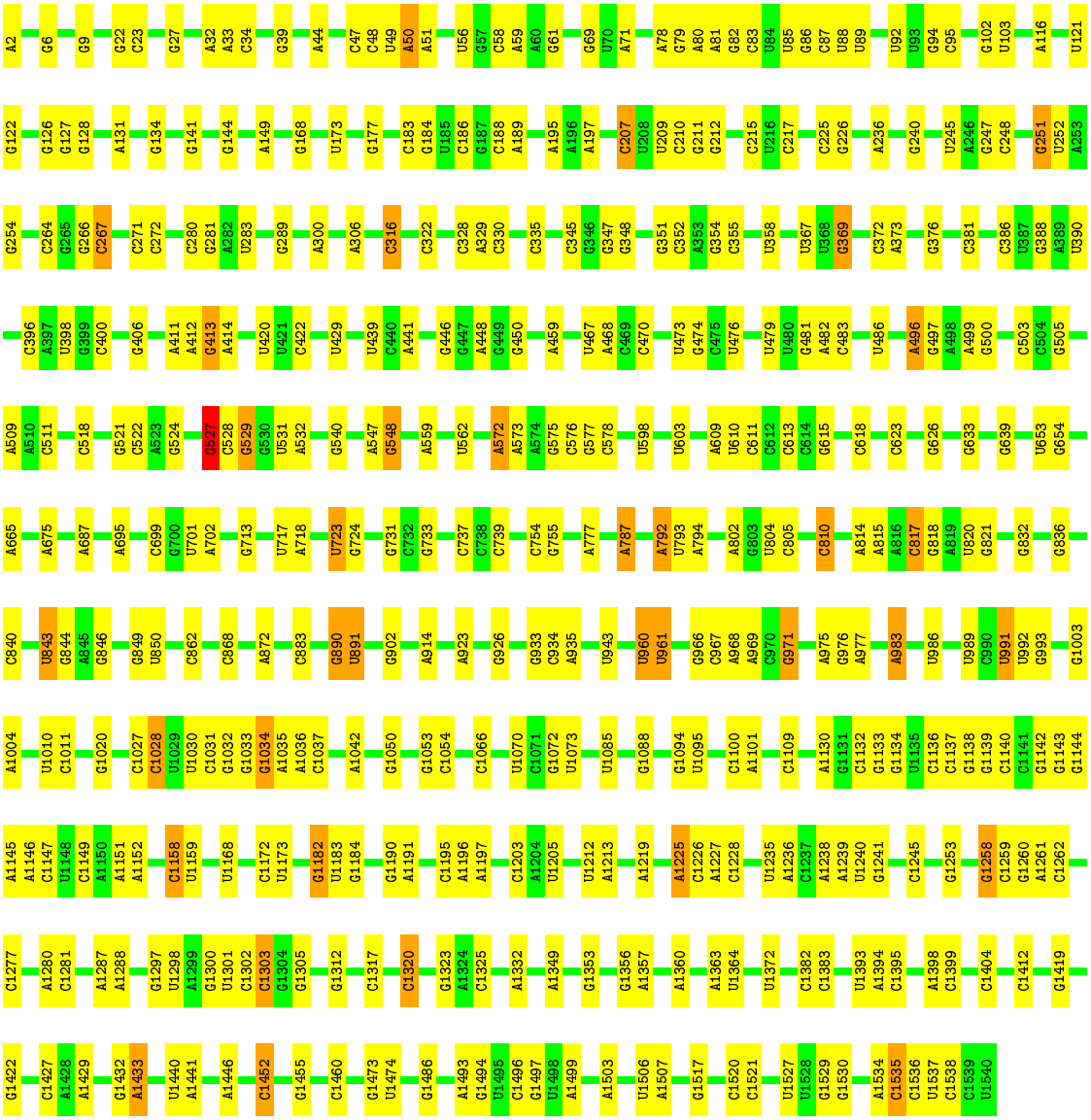
Mol	Chain	Residues	Atoms	AltConf
56	4	1	Total Zn 1 1	0
56	6	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

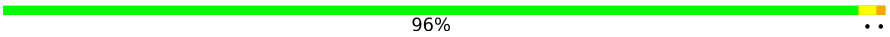
- Molecule 1: 16S ribosomal RNA

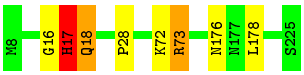
Chain a:



- Molecule 2: 30S ribosomal protein S2

Chain b:



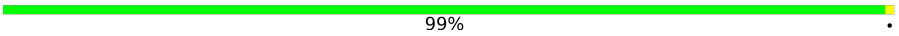


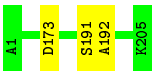
- Molecule 3: 30S ribosomal protein S3

Chain c:

- Molecule 4: 30S ribosomal protein S4

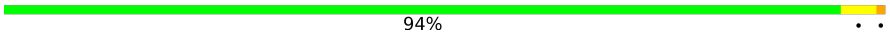
Chain d:





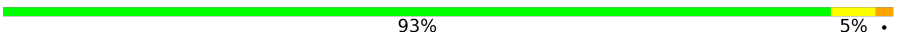
- Molecule 5: 30S ribosomal protein S5

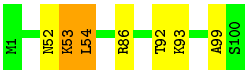
Chain e:



- Molecule 6: 30S ribosomal protein S6

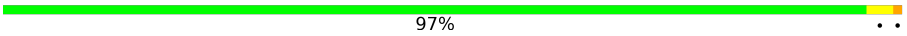
Chain f:

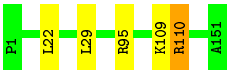




- Molecule 7: 30S ribosomal protein S7

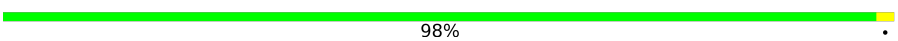
Chain g:

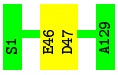




- Molecule 8: 30S ribosomal protein S8

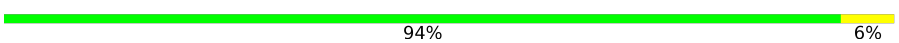
Chain h:





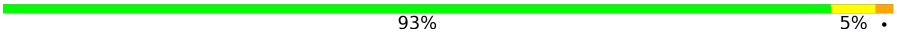
- Molecule 9: 30S ribosomal protein S9

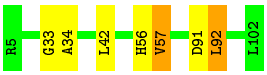
Chain i:



- Molecule 10: 30S ribosomal protein S10

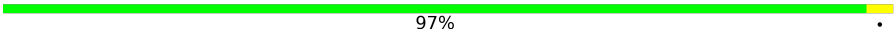
Chain j:





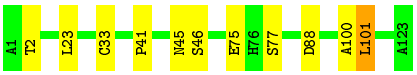
- Molecule 11: 30S ribosomal protein S11

Chain k:



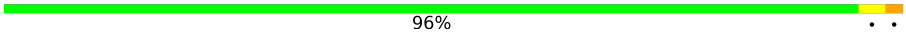
- Molecule 12: 30S ribosomal protein S12

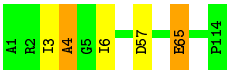
Chain l:



- Molecule 13: 30S ribosomal protein S13

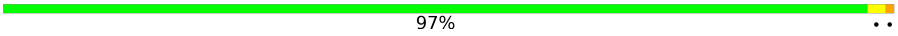
Chain m:





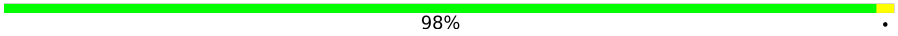
- Molecule 14: 30S ribosomal protein S14

Chain n:



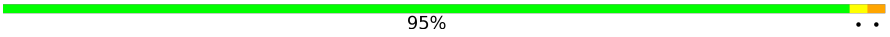
- Molecule 15: 30S ribosomal protein S15

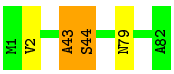
Chain o:



- Molecule 16: 30S ribosomal protein S16

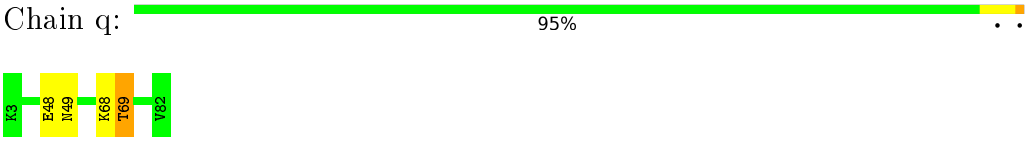
Chain p:





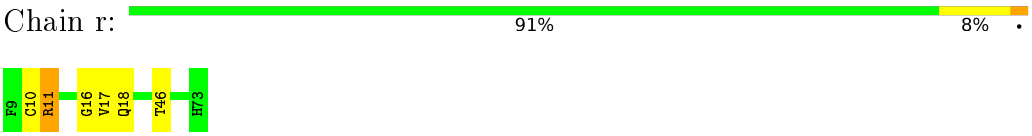
- Molecule 17: 30S ribosomal protein S17

Chain q:



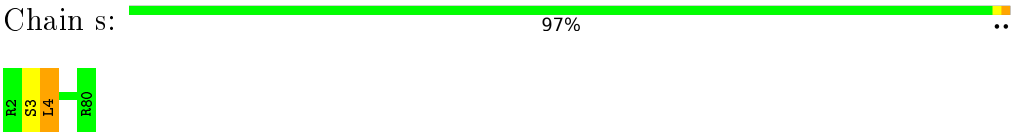
- Molecule 18: 30S ribosomal protein S18

Chain r:



- Molecule 19: 30S ribosomal protein S19

Chain s:



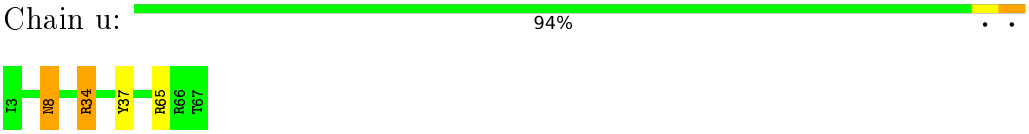
- Molecule 20: 30S ribosomal protein S20

Chain t:

There are no outlier residues recorded for this chain.

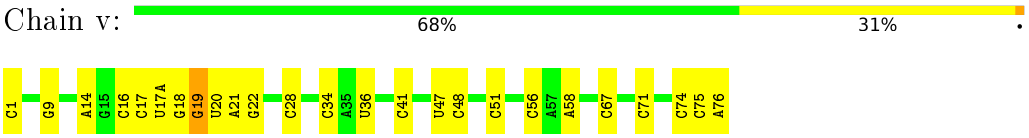
- Molecule 21: 30S ribosomal protein S21

Chain u:



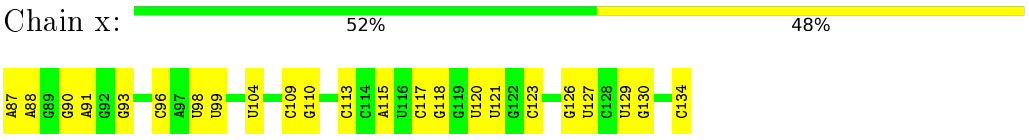
- Molecule 22: fMet-tRNAfMet

Chain v:



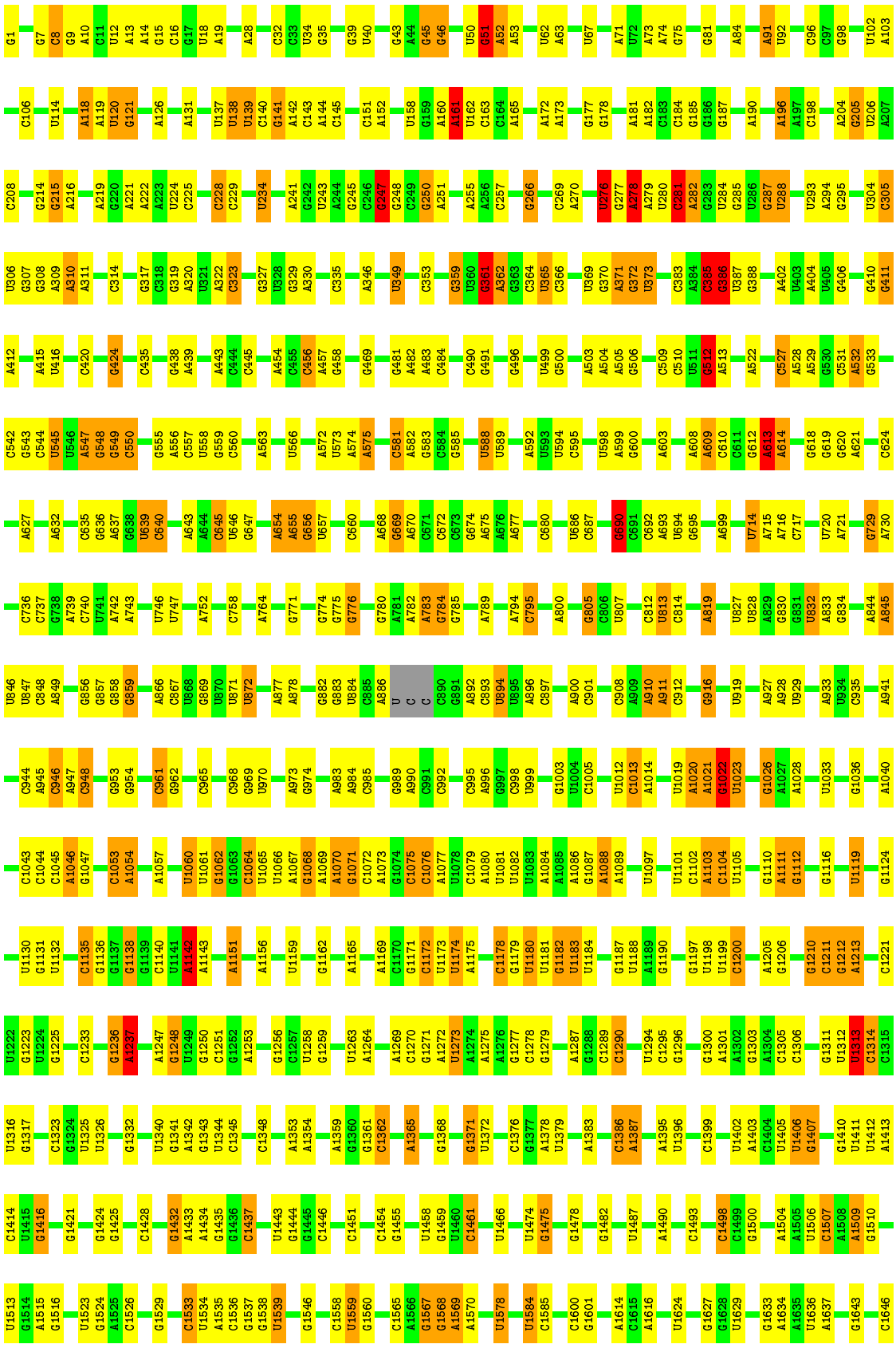
- Molecule 23: SECIS mRNA

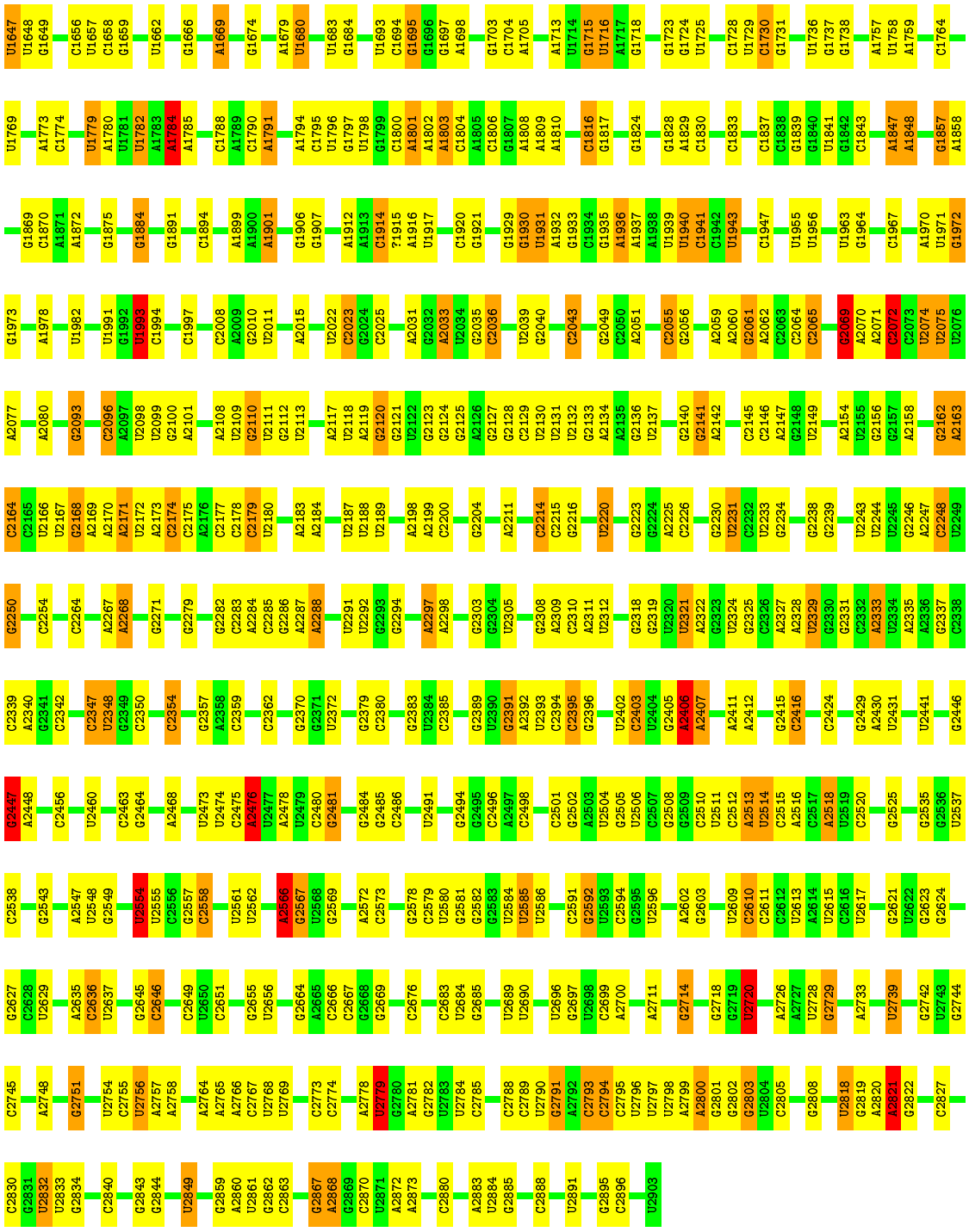
Chain x:



- Molecule 24: 23S ribosomal RNA

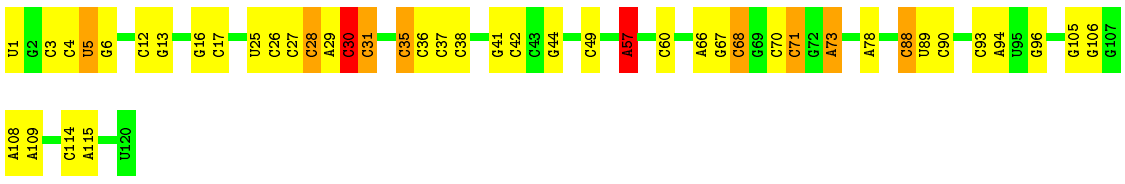
Chain A:


G1 G7 C8 G9 A10 C11 U12 A13 A14 G15 C16 G17 U18 A19 A28 C32 G33 U34 G35 G39 U40 G43 A44 G45 G46 U50 G51 A52 A53 U62 A63 U67 A71 U72 A73 A74 G75 G81 A84 A91 U92 C96 C97 G98 U102 A103
C106 U114 A118 A119 U120 G121 A126 A131 U137 U138 U139 C140 G141 A142 C143 A144 C145 C151 A152 U158 G159 A160 A161 U162 C163 C164 A165 A172 A173 G177 G178 A181 A182 C183 C184 G185 G186 G187 A190 A196 A197 C198 A204 G205 U206 A207
C208 G214 G215 A216 A219 G220 A221 A222 A223 U224 C225 C228 C229 U234 A241 G242 U243 A244 G245 G246 G247 G248 C249 G250 A251 A255 A256 C257 G266 C269 A270 U276 G277 A278 A279 U280 C281 A282 G283 U284 G285 U286 G287 U288 U293 A294 G295 U304 C305
U306 G307 G308 A309 A310 A311 C314 G317 C318 G319 A320 U321 A322 C323 G327 U328 G329 A330 C335 A346 U349 C353 G359 U360 A361 A362 G363 C364 U365 C366 U369 G370 A371 G372 U373 C383 A384 A385 G386 U387 G388 A402 U403 A404 U405 G406 G410 G411
A412 A415 U416 C420 G424 C435 G438 A439 A443 C444 C445 A454 C455 C456 A457 G458 G469 G481 A482 A483 C484 C490 G491 G496 U499 G500 A503 A504 A505 G506 C509 C510 U511 G512 A513 A522 C527 A528 A529 G530 C531 A532 G533
C542 G543 C544 U545 U546 A547 G548 G549 C550 G555 A556 C557 U558 G559 C560 A563 U566 A572 U573 A574 A575 C581 A582 G583 G584 G585 U588 U589 A592 U593 U594 C595 U598 A599 G600 A603 A608 A609 C610 C611 G612 A613 A614 G618 G619 G620 A621 C624
A627 A632 C635 G636 A637 G638 U639 C640 A643 A644 C645 U646 G647 A654 A655 G656 U657 C660 A668 G669 A670 C671 C672 G673 G674 A675 A676 A677 C680 U686 C687 G690 C691 C692 A693 U694 G695 A699 U714 A715 A716 C717 U720 A721 G729 A730
C736 C737 G738 A739 C740 U741 A742 A743 U746 U747 A752 C758 A764 G771 G774 G775 G776 G780 A781 A782 A783 G784 G785 A789 A794 C795 A800 G805 C806 U807 C812 U813 C814 A819 U827 U828 A829 G830 G831 U832 A833 G834 A844 A845
U846 U847 C848 A849 G856 G857 G858 G859 A866 C867 U868 G869 U870 U871 U872 A877 A878 G882 G883 U884 C885 A886 U C C C890 G891 A892 C893 U894 U895 A896 C897 A900 C901 C908 A909 A910 A911 C912 G916 U919 A927 A928 U929 A933 U934 C935 A941
C944 A945 C946 A947 C948 G953 G954 C961 G962 C965 C968 G969 U970 A973 G974 A983 A984 C985 G989 A990 C991 C992 C995 A996 G997 C998 U999 G1003 U1004 C1005 U1012 C1013 A1014 U1019 A1020 A1021 G1022 U1023 G1026 A1027 A1028 U1033 G1036 A1040
C1043 C1044 C1045 A1046 G1047 C1053 A1054 A1057 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 U1097 U1101 C1102 A1103 C1104 U1105 G1110 A1111 G1112 G1116 U1119 G1124
U1130 G1131 U1132 C1135 G1136 G1137 G1138 G1139 C1140 U1141 A1142 A1143 A1151 A1156 U1159 G1162 A1165 A1169 C1170 G1171 C1172 U1173 U1174 A1175 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1187 U1188 A1189 G1190 G1197 U1198 U1199 C1200 A1205 G1206 G1210 C1211 G1212 A1213 C1221
U1222 G1223 U1224 G1225 C1233 G1236 A1237 A1247 G1248 U1249 G1250 C1251 G1252 A1253 G1256 C1257 U1258 G1259 U1263 A1264 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 C1278 G1279 A1287 G1288 C1289 C1290 U1294 C1295 G1296 G1300 A1301 A1302 G1303 A1304 C1305 C1306 G1311 U1312 U1313 C1314 C1315
U1316 G1317 C1323 G1324 U1325 U1326 G1332 U1340 G1341 A1342 G1343 U1344 C1345 C1348 A1353 A1354 A1359 G1360 G1361 C1362 A1365 G1368 G1371 U1372 C1376 G1377 A1378 U1379 A1383 C1386 A1387 A1395 U1396 C1399 U1402 A1403 C1404 U1405 U1406 G1407 G1410 U1411 U1412 A1413
C1414 U1415 G1416 G1421 G1424 G1425 C1428 G1432 A1433 A1434 G1435 G1436 C1437 U1443 G1444 G1445 C1446 C1451 C1454 G1455 U1458 G1459 U1460 C1461 U1466 U1474 G1475 G1478 G1482 U1487 A1490 C1493 C1498 C1499 G1500 A1504 A1505 U1506 C1507 A1508 A1509 G1510
U1513 G1514 A1515 G1516 U1523 G1524 A1525 C1526 G1529 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1546 C1558 U1559 G1560 C1565 A1566 G1567 G1568 A1569 A1570 U1578 U1584 C1585 C1600 G1601 A1614 C1615 A1616 U1624 G1627 G1628 U1629 G1633 A1634 A1635 U1636 A1637 G1643 C1646



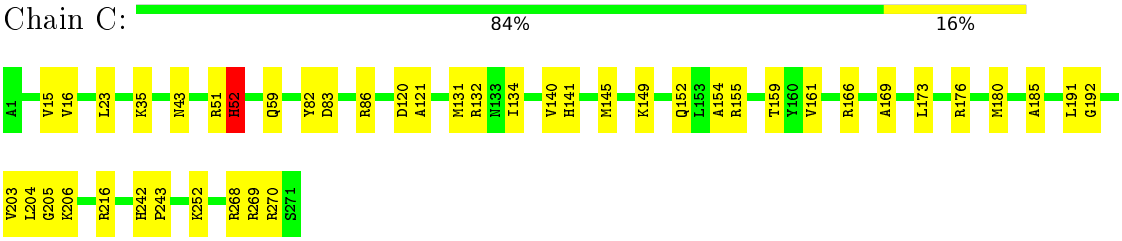
• Molecule 25: 5S ribosomal RNA

Chain B:



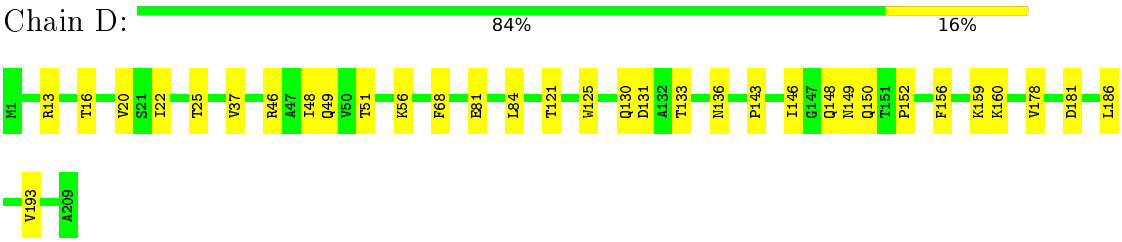
- Molecule 26: 50S ribosomal protein L2

Chain C:



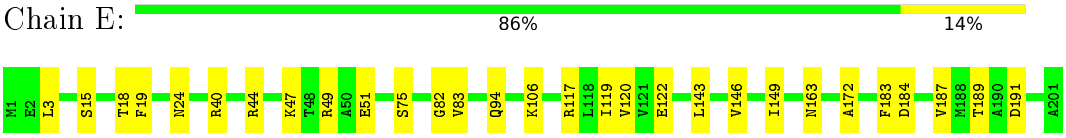
- Molecule 27: 50S ribosomal protein L3

Chain D:



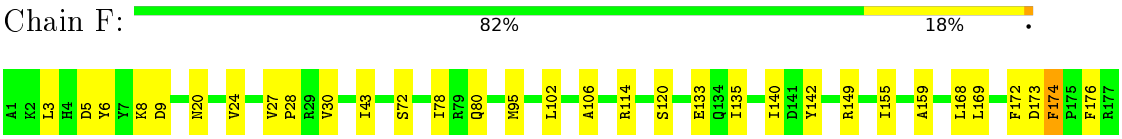
- Molecule 28: 50S ribosomal protein L4

Chain E:



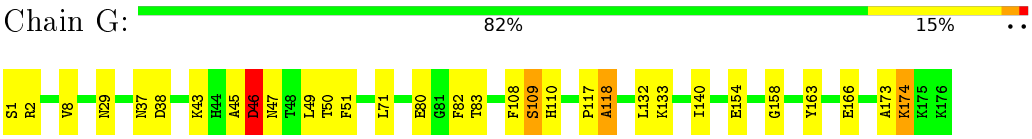
- Molecule 29: 50S ribosomal protein L5

Chain F:



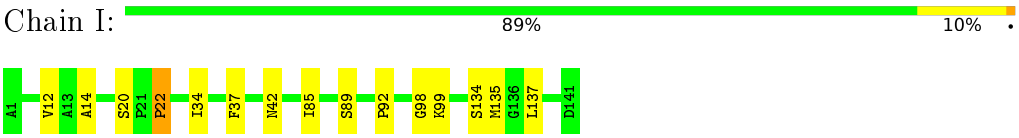
- Molecule 30: 50S ribosomal protein L6

Chain G:



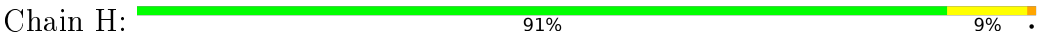
- Molecule 31: 50S ribosomal protein L11

Chain I:



- Molecule 32: 50S ribosomal protein L9

Chain H:

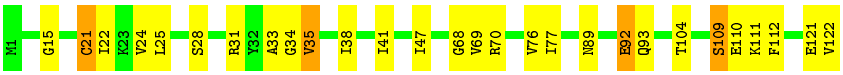


• Molecule 33: 50S ribosomal protein L13

Chain J:

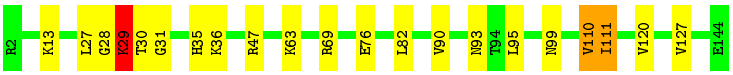
• Molecule 34: 50S ribosomal protein L14

Chain K:



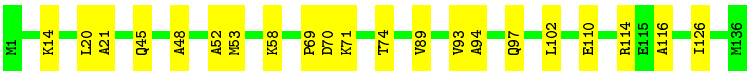
• Molecule 35: 50S ribosomal protein L15

Chain L:



• Molecule 36: 50S ribosomal protein L16

Chain M:

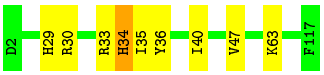


• Molecule 37: 50S ribosomal protein L17

Chain N:

• Molecule 38: 50S ribosomal protein L18

Chain O:

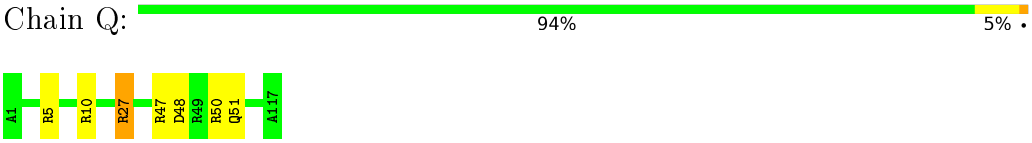


• Molecule 39: 50S ribosomal protein L19

Chain P:

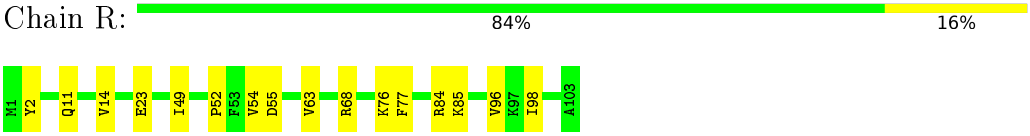
• Molecule 40: 50S ribosomal protein L20

Chain Q:



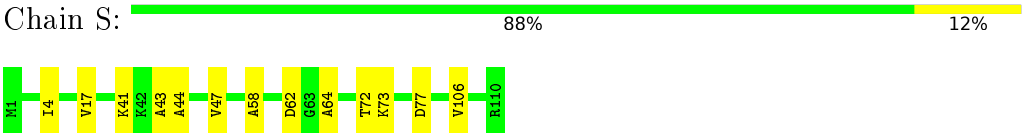
• Molecule 41: 50S ribosomal protein L21

Chain R:



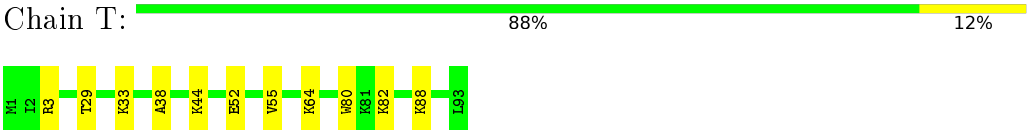
• Molecule 42: 50S ribosomal protein L22

Chain S:



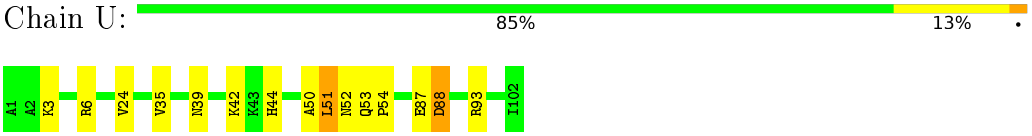
• Molecule 43: 50S ribosomal protein L23

Chain T:



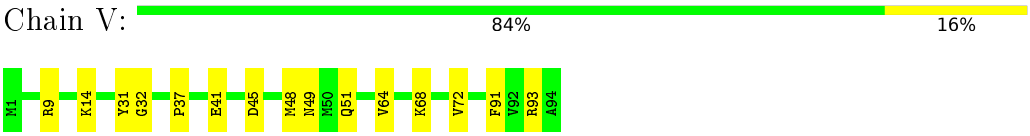
• Molecule 44: 50S ribosomal protein L24

Chain U:



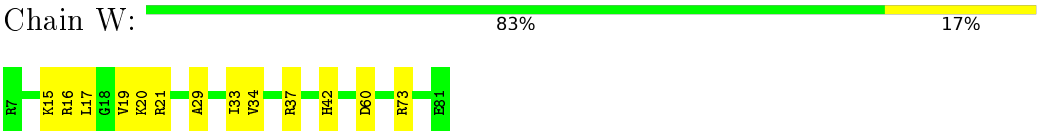
• Molecule 45: 50S ribosomal protein L25

Chain V:



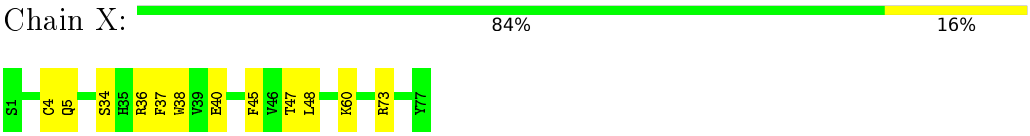
• Molecule 46: 50S ribosomal protein L27

Chain W:



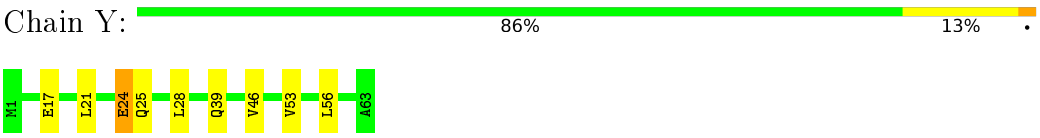
• Molecule 47: 50S ribosomal protein L28

Chain X:



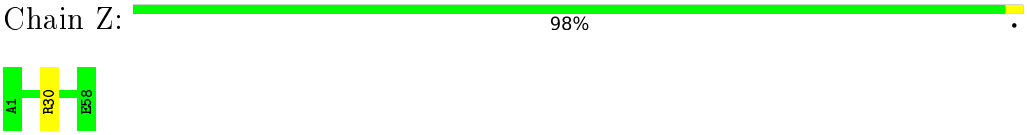
- Molecule 48: 50S ribosomal protein L29

Chain Y:



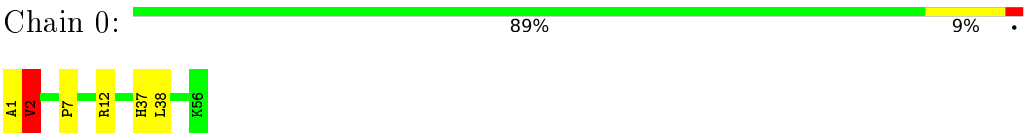
- Molecule 49: 50S ribosomal protein L30

Chain Z:



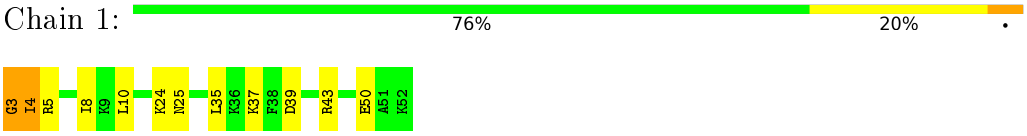
- Molecule 50: 50S ribosomal protein L32

Chain 0:



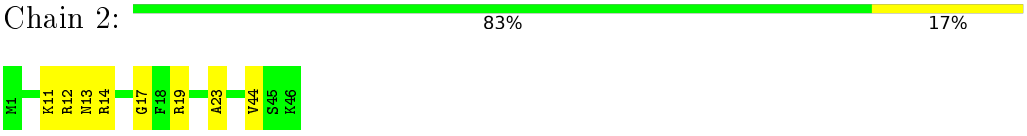
- Molecule 51: 50S ribosomal protein L33

Chain 1:



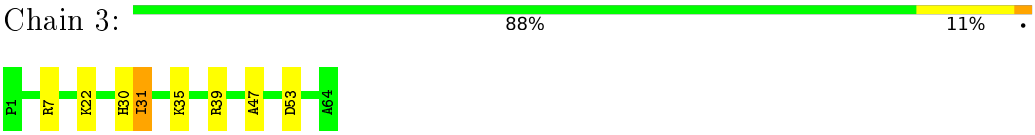
- Molecule 52: 50S ribosomal protein L34

Chain 2:



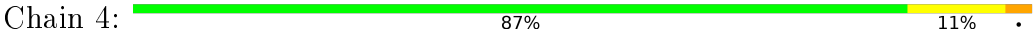
- Molecule 53: 50S ribosomal protein L35

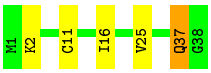
Chain 3:



- Molecule 54: 50S ribosomal protein L36

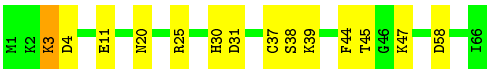
Chain 4:





- Molecule 55: 50S ribosomal protein L31

Chain 6:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	75176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	a	0.61	4/36803 (0.0%)	1.26	322/57406 (0.6%)
10	j	0.37	0/797	0.74	0/1077
11	k	0.40	0/886	0.71	0/1195
12	l	0.43	0/969	0.82	2/1300 (0.2%)
13	m	0.46	0/893	0.78	3/1193 (0.3%)
14	n	0.45	0/806	0.66	1/1074 (0.1%)
15	o	0.40	0/722	0.61	0/964
16	p	0.45	0/659	0.70	1/884 (0.1%)
17	q	0.45	0/658	0.78	1/881 (0.1%)
18	r	0.42	0/512	0.70	0/689
19	s	0.41	0/653	0.75	1/877 (0.1%)
2	b	0.43	0/1736	0.66	3/2338 (0.1%)
20	t	0.42	0/671	0.60	0/888
21	u	0.53	0/501	0.84	1/668 (0.1%)
22	v	0.55	1/1747 (0.1%)	1.29	19/2721 (0.7%)
23	x	0.58	1/1145 (0.1%)	1.09	1/1781 (0.1%)
24	A	0.66	9/69196 (0.0%)	1.26	616/107943 (0.6%)
25	B	0.59	1/2873 (0.0%)	1.25	29/4478 (0.6%)
26	C	0.48	0/2122	0.73	1/2852 (0.0%)
27	D	0.44	0/1586	0.67	0/2134
28	E	0.43	0/1571	0.63	0/2113
29	F	0.43	0/1435	0.71	2/1926 (0.1%)
3	c	0.40	0/1652	0.60	0/2225
30	G	0.42	0/1343	0.67	4/1816 (0.2%)
31	I	0.38	0/1046	0.61	0/1410
32	H	0.38	0/1122	0.63	0/1515
33	J	0.46	0/1152	0.61	0/1551
34	K	0.46	0/948	0.69	0/1268
35	L	0.44	0/1054	0.74	1/1403 (0.1%)
36	M	0.46	0/1093	0.72	1/1460 (0.1%)
37	N	0.44	0/974	0.65	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
38	O	0.42	0/902	0.59	0/1209
39	P	0.45	0/929	0.67	0/1242
4	d	0.43	0/1665	0.62	0/2227
40	Q	0.47	0/960	0.60	1/1278 (0.1%)
41	R	0.45	0/829	0.72	0/1107
42	S	0.40	0/864	0.62	0/1156
43	T	0.40	0/745	0.63	0/994
44	U	0.44	0/788	0.78	2/1051 (0.2%)
45	V	0.40	0/766	0.60	0/1025
46	W	0.41	0/582	0.62	0/769
47	X	0.38	0/635	0.59	0/848
48	Y	0.42	0/510	0.64	0/677
49	Z	0.40	0/453	0.60	0/605
5	e	0.44	0/1170	0.80	2/1573 (0.1%)
50	0	0.41	0/450	0.72	0/599
51	1	0.42	0/417	0.84	1/554 (0.2%)
52	2	0.41	0/380	0.67	0/498
53	3	0.47	0/513	0.65	0/676
54	4	0.67	1/303 (0.3%)	0.78	0/397
55	6	0.42	0/532	0.62	0/709
6	f	0.49	0/836	0.83	2/1128 (0.2%)
7	g	0.43	0/1196	0.70	3/1602 (0.2%)
8	h	0.42	0/989	0.66	0/1326
9	i	0.41	0/1034	0.69	0/1375
All	All	0.59	17/157773 (0.0%)	1.14	1020/235956 (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	5
12	l	0	1
13	m	0	1
16	p	0	1
17	q	0	2
18	r	0	3
19	s	0	1
2	b	0	4
21	u	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	A	2	0
26	C	0	1
28	E	0	1
30	G	0	3
32	H	0	2
34	K	0	3
35	L	0	4
42	S	0	1
44	U	0	3
48	Y	0	1
5	e	0	4
50	0	0	2
51	1	0	1
53	3	0	1
6	f	0	1
7	g	0	2
8	h	0	1
9	i	0	1
All	All	4	51

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	x	87	A	OP3-P	-10.73	1.48	1.61
24	A	1	G	OP3-P	-10.59	1.48	1.61
25	B	1	U	OP3-P	-10.53	1.48	1.61
22	v	1	C	OP3-P	-10.52	1.48	1.61
1	a	2	A	OP3-P	-10.51	1.48	1.61
24	A	776	G	N7-C5	-7.66	1.34	1.39
24	A	1784	A	N7-C5	-7.38	1.34	1.39
54	4	11	CYS	CB-SG	-7.14	1.70	1.82
24	A	1779	U	C5-C6	-5.86	1.28	1.34
24	A	800	A	N9-C4	-5.79	1.34	1.37
1	a	89	U	C4-C5	-5.54	1.38	1.43
24	A	1803	A	N9-C4	-5.52	1.34	1.37
24	A	984	A	N9-C4	-5.30	1.34	1.37
24	A	2868	A	N9-C8	-5.26	1.33	1.37
24	A	613	A	N9-C4	5.21	1.41	1.37
1	a	792	A	N7-C5	-5.15	1.36	1.39
1	a	2	A	N7-C5	-5.12	1.36	1.39

All (1020) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1313	U	N3-C2-O2	-14.71	111.90	122.20
24	A	2072	C	C6-N1-C2	-14.04	114.69	120.30
1	a	89	U	C5-C4-O4	-13.94	117.53	125.90
1	a	529	G	C5-C6-O6	-13.71	120.38	128.60
24	A	62	U	N1-C2-O2	13.14	132.00	122.80
24	A	893	C	C6-N1-C2	-13.07	115.07	120.30
24	A	1313	U	N1-C2-O2	12.96	131.87	122.80
24	A	137	U	N3-C2-O2	-12.35	113.56	122.20
24	A	2297	A	C6-N1-C2	12.25	125.95	118.60
24	A	2072	C	C5-C6-N1	12.25	127.12	121.00
24	A	2868	A	N7-C8-N9	12.13	119.86	113.80
24	A	2297	A	N1-C2-N3	-11.50	123.55	129.30
1	a	529	G	N1-C6-O6	11.49	126.80	119.90
24	A	2321	U	C4-C5-C6	11.37	126.52	119.70
24	A	62	U	N3-C2-O2	-11.36	114.25	122.20
24	A	548	G	N7-C8-N9	11.29	118.74	113.10
24	A	1112	G	N3-C2-N2	-11.13	112.11	119.90
19	s	4	LEU	CA-CB-CG	10.99	140.57	115.30
1	a	737	C	C5-C6-N1	10.92	126.46	121.00
1	a	737	C	C6-N1-C2	-10.91	115.94	120.30
1	a	215	C	N1-C2-O2	10.80	125.38	118.90
24	A	548	G	C8-N9-C4	-10.66	102.14	106.40
24	A	1313	U	C2-N1-C1'	10.60	130.42	117.70
5	e	77	ASN	N-CA-CB	-10.46	91.77	110.60
1	a	1027	C	C5-C6-N1	10.40	126.20	121.00
24	A	783	A	C8-N9-C4	-10.22	101.71	105.80
1	a	89	U	N3-C4-O4	10.19	126.53	119.40
24	A	776	G	N3-C4-C5	-10.18	123.51	128.60
24	A	883	G	N1-C6-O6	-9.95	113.93	119.90
24	A	62	U	C2-N1-C1'	9.89	129.56	117.70
1	a	413	G	C5-N7-C8	9.82	109.21	104.30
24	A	1451	C	N1-C2-O2	-9.82	113.01	118.90
24	A	2416	C	C6-N1-C2	-9.77	116.39	120.30
13	m	65	GLU	N-CA-CB	-9.73	93.08	110.60
24	A	1498	C	N1-C2-O2	9.60	124.66	118.90
1	a	503	C	C6-N1-C2	-9.41	116.54	120.30
24	A	2447	G	P-O3'-C3'	9.32	130.89	119.70
24	A	2481	G	C6-N1-C2	9.28	130.67	125.10
24	A	893	C	N3-C2-O2	-9.27	115.41	121.90
24	A	795	C	C5-C6-N1	9.26	125.63	121.00
24	A	783	A	N7-C8-N9	9.23	118.41	113.80
24	A	1314	C	C6-N1-C2	-9.21	116.62	120.30
24	A	2884	U	N3-C2-O2	-9.20	115.76	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	792	A	C5-N7-C8	9.17	108.48	103.90
24	A	1784	A	C5-N7-C8	9.13	108.47	103.90
24	A	2868	A	C8-N9-C4	-9.09	102.17	105.80
24	A	866	A	C5-C6-N6	-9.01	116.49	123.70
24	A	669	G	C2-N3-C4	8.97	116.38	111.90
1	a	1134	G	N3-C2-N2	-8.94	113.64	119.90
1	a	1028	C	C5-C6-N1	8.93	125.47	121.00
1	a	1003	G	N3-C2-N2	-8.88	113.69	119.90
1	a	891	U	C5-C6-N1	8.87	127.13	122.70
22	v	74	C	N1-C2-O2	8.85	124.21	118.90
1	a	1149	C	N1-C2-O2	8.82	124.19	118.90
24	A	2407	A	O5'-P-OP2	-8.81	97.77	105.70
24	A	2226	C	N1-C2-O2	8.76	124.16	118.90
1	a	1027	C	C6-N1-C2	-8.75	116.80	120.30
24	A	581	C	C5-C6-N1	8.71	125.35	121.00
24	A	1081	U	N3-C2-O2	-8.65	116.15	122.20
24	A	613	A	C2-N3-C4	8.64	114.92	110.60
16	p	44	SER	N-CA-CB	-8.62	97.58	110.50
24	A	1362	C	C6-N1-C2	-8.61	116.85	120.30
24	A	385	C	OP2-P-O3'	8.60	124.11	105.20
24	A	1716	U	C5-C6-N1	8.57	126.99	122.70
24	A	278	A	C2-N3-C4	8.51	114.85	110.60
1	a	943	U	N3-C2-O2	-8.45	116.28	122.20
24	A	67	U	C5-C4-O4	-8.45	120.83	125.90
24	A	1105	U	N3-C2-O2	-8.45	116.29	122.20
24	A	1451	C	C2-N3-C4	-8.38	115.71	119.90
25	B	31	C	C6-N1-C2	-8.38	116.95	120.30
24	A	1779	U	C4-C5-C6	8.37	124.72	119.70
24	A	893	C	C5-C6-N1	8.33	125.16	121.00
2	b	73	ARG	N-CA-CB	-8.31	95.64	110.60
1	a	168	G	C5-C6-O6	-8.28	123.63	128.60
24	A	2884	U	N1-C2-O2	8.27	128.59	122.80
24	A	1101	U	N3-C2-O2	-8.24	116.43	122.20
1	a	529	G	C4-C5-N7	8.22	114.09	110.80
24	A	67	U	N3-C4-O4	8.22	125.15	119.40
24	A	484	C	C5-C6-N1	8.18	125.09	121.00
44	U	51	LEU	N-CA-CB	-8.15	94.11	110.40
24	A	687	C	N1-C2-O2	8.13	123.78	118.90
24	A	281	C	C6-N1-C2	-8.09	117.06	120.30
24	A	2406	A	O5'-P-OP2	-8.07	98.44	105.70
24	A	1498	C	C6-N1-C2	-8.07	117.07	120.30
24	A	2473	U	N3-C2-O2	-8.06	116.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	34	C	N1-C2-O2	8.05	123.73	118.90
24	A	2226	C	N3-C2-O2	-8.03	116.28	121.90
1	a	522	C	C5-C4-N4	8.01	125.81	120.20
1	a	413	G	N7-C8-N9	-8.01	109.10	113.10
1	a	754	C	C2-N1-C1'	8.01	127.61	118.80
24	A	948	C	C5-C6-N1	8.00	125.00	121.00
24	A	1416	G	N3-C2-N2	-7.99	114.30	119.90
1	a	1158	C	C2-N1-C1'	7.95	127.55	118.80
24	A	1387	A	N7-C8-N9	7.95	117.78	113.80
24	A	1104	C	N1-C2-O2	7.94	123.66	118.90
24	A	1237	A	N7-C8-N9	7.92	117.76	113.80
24	A	1183	U	N3-C2-O2	-7.92	116.66	122.20
24	A	1507	C	C6-N1-C2	-7.89	117.14	120.30
1	a	1427	C	C6-N1-C2	-7.88	117.15	120.30
24	A	137	U	N1-C2-O2	7.87	128.31	122.80
24	A	1941	C	N1-C2-O2	7.86	123.62	118.90
24	A	1005	C	C6-N1-C2	-7.85	117.16	120.30
1	a	923	A	N7-C8-N9	7.83	117.72	113.80
24	A	1498	C	N3-C2-O2	-7.83	116.42	121.90
1	a	413	G	N1-C6-O6	-7.82	115.21	119.90
24	A	2791	G	N3-C2-N2	-7.79	114.44	119.90
24	A	2131	U	N3-C2-O2	-7.79	116.75	122.20
24	A	2069	G7M	P-O3'-C3'	7.78	129.03	119.70
24	A	1461	C	C6-N1-C2	-7.75	117.20	120.30
24	A	1680	U	N3-C2-O2	-7.75	116.78	122.20
24	A	281	C	C5-C6-N1	7.72	124.86	121.00
24	A	912	C	N1-C2-O2	7.71	123.53	118.90
24	A	2473	U	N1-C2-O2	7.71	128.20	122.80
17	q	69	THR	N-CA-CB	-7.70	95.68	110.30
22	v	19	G	N1-C6-O6	-7.69	115.29	119.90
12	l	101	LEU	N-CA-CB	-7.67	95.06	110.40
24	A	948	C	C6-N1-C2	-7.65	117.24	120.30
24	A	2758	A	N1-C6-N6	-7.65	114.01	118.60
7	g	110	ARG	N-CA-CB	-7.64	96.85	110.60
24	A	999	U	N3-C2-O2	-7.62	116.87	122.20
24	A	2868	A	C5-N7-C8	-7.62	100.09	103.90
1	a	413	G	OP2-P-O3'	7.58	121.88	105.20
24	A	795	C	C6-N1-C2	-7.58	117.27	120.30
1	a	87	C	C5-C6-N1	7.58	124.79	121.00
24	A	2424	C	N3-C4-C5	7.57	124.93	121.90
1	a	1028	C	C6-N1-C2	-7.57	117.27	120.30
24	A	141	G	C2-N3-C4	7.57	115.69	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	581	C	C6-N1-C2	-7.57	117.27	120.30
24	A	1843	C	C6-N1-C2	-7.57	117.27	120.30
1	a	1205	U	N3-C2-O2	-7.56	116.91	122.20
24	A	1402	U	N3-C2-O2	-7.55	116.91	122.20
1	a	422	C	N1-C2-O2	7.55	123.43	118.90
24	A	1539	U	C5-C6-N1	7.50	126.45	122.70
24	A	893	C	N1-C2-O2	7.50	123.40	118.90
24	A	2796	U	N3-C2-O2	-7.48	116.96	122.20
24	A	2074	U	N3-C2-O2	-7.48	116.97	122.20
1	a	1158	C	C6-N1-C2	-7.47	117.31	120.30
1	a	87	C	C6-N1-C2	-7.46	117.32	120.30
22	v	56	C	N1-C2-O2	7.46	123.37	118.90
1	a	754	C	N1-C2-O2	7.44	123.36	118.90
24	A	776	G	C4-N9-C1'	7.43	136.16	126.50
1	a	1197	A	O5'-P-OP2	-7.42	99.02	105.70
24	A	1507	C	C5-C6-N1	7.42	124.71	121.00
24	A	373	U	N3-C2-O2	-7.42	117.01	122.20
24	A	654	A	C2-N3-C4	7.41	114.31	110.60
25	B	26	C	N1-C2-O2	7.41	123.35	118.90
24	A	1314	C	C5-C6-N1	7.41	124.70	121.00
24	A	1005	C	N1-C2-O2	7.39	123.34	118.90
25	B	30	C	C6-N1-C2	-7.38	117.35	120.30
24	A	2243	U	O5'-P-OP1	-7.38	99.06	105.70
1	a	868	C	C6-N1-C2	-7.37	117.35	120.30
24	A	1774	C	N3-C2-O2	-7.36	116.75	121.90
1	a	1393	U	N3-C2-O2	-7.35	117.06	122.20
1	a	1497	G	N1-C6-O6	-7.35	115.49	119.90
24	A	2179	C	C5-C6-N1	7.34	124.67	121.00
24	A	198	C	C5-C6-N1	7.34	124.67	121.00
24	A	12	U	N3-C2-O2	-7.33	117.07	122.20
6	f	53	LYS	N-CA-CB	7.32	123.78	110.60
24	A	548	G	C5-N7-C8	-7.32	100.64	104.30
24	A	776	G	N3-C4-N9	7.31	130.39	126.00
1	a	529	G	N9-C4-C5	-7.31	102.48	105.40
1	a	1149	C	N3-C2-O2	-7.31	116.78	121.90
24	A	361	G	C5-C6-O6	-7.30	124.22	128.60
24	A	867	C	N1-C2-O2	7.30	123.28	118.90
24	A	484	C	C6-N1-C2	-7.30	117.38	120.30
1	a	215	C	N3-C4-N4	7.30	123.11	118.00
1	a	623	C	C6-N1-C2	-7.30	117.38	120.30
1	a	1132	C	N3-C2-O2	-7.29	116.80	121.90
24	A	1313	U	C6-N1-C2	-7.28	116.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1225	A	C2-N3-C4	7.27	114.24	110.60
30	G	46	ASP	N-CA-CB	-7.27	97.51	110.60
1	a	215	C	N3-C2-O2	-7.24	116.83	121.90
24	A	2827	C	C6-N1-C2	-7.23	117.41	120.30
24	A	1237	A	C8-N9-C4	-7.21	102.92	105.80
24	A	1081	U	N1-C2-O2	7.21	127.84	122.80
24	A	1843	C	C5-C6-N1	7.20	124.60	121.00
1	a	225	C	C6-N1-C2	-7.20	117.42	120.30
26	C	83	ASP	CB-CG-OD1	7.20	124.78	118.30
1	a	1395	C	N1-C2-O2	7.18	123.21	118.90
24	A	139	U	N3-C2-O2	-7.16	117.19	122.20
1	a	522	C	N3-C4-C5	-7.16	119.04	121.90
24	A	2179	C	C6-N1-C2	-7.16	117.44	120.30
25	B	26	C	N3-C2-O2	-7.15	116.89	121.90
24	A	1340	U	N3-C2-O2	-7.13	117.21	122.20
1	a	168	G	N1-C6-O6	7.12	124.17	119.90
24	A	1387	A	C8-N9-C4	-7.10	102.96	105.80
24	A	2250	G	N3-C4-C5	7.09	132.14	128.60
1	a	1277	C	N3-C2-O2	-7.08	116.94	121.90
1	a	225	C	C5-C6-N1	7.07	124.53	121.00
24	A	883	G	C5-C6-O6	7.06	132.84	128.60
1	a	1195	C	N1-C2-O2	7.06	123.14	118.90
24	A	669	G	N3-C4-C5	-7.06	125.07	128.60
24	A	1183	U	N1-C2-O2	7.05	127.74	122.80
24	A	776	G	C4-C5-C6	7.05	123.03	118.80
24	A	2610	C	P-O3'-C3'	7.03	128.14	119.70
1	a	177	G	C2-N3-C4	7.03	115.41	111.90
1	a	264	C	C5-C6-N1	7.03	124.51	121.00
24	A	32	C	C6-N1-C2	-7.02	117.49	120.30
24	A	2476	A	N1-C2-N3	7.02	132.81	129.30
1	a	450	G	N1-C6-O6	-7.00	115.70	119.90
24	A	1848	A	N7-C8-N9	7.00	117.30	113.80
22	v	56	C	N3-C2-O2	-6.98	117.01	121.90
24	A	2840	C	C5-C6-N1	6.98	124.49	121.00
24	A	2821	A	O5'-P-OP1	-6.98	99.42	105.70
24	A	1076	C	C6-N1-C2	-6.97	117.51	120.30
24	A	1841	U	N3-C2-O2	-6.97	117.32	122.20
1	a	739	C	C6-N1-C2	-6.97	117.51	120.30
1	a	1132	C	N1-C2-O2	6.97	123.08	118.90
24	A	1212	G	P-O3'-C3'	6.97	128.06	119.70
1	a	236	A	N7-C8-N9	6.94	117.27	113.80
24	A	1211	C	OP2-P-O3'	6.94	120.47	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1914	C	C4-C5-C6	6.93	120.86	117.40
24	A	645	C	N1-C2-O2	6.90	123.04	118.90
24	A	1044	C	N3-C4-N4	-6.90	113.17	118.00
24	A	2162	G	OP2-P-O3'	6.89	120.36	105.20
24	A	228	C	P-O3'-C3'	6.89	127.97	119.70
29	F	173	ASP	CB-CG-OD1	6.89	124.50	118.30
1	a	623	C	N1-C2-O2	6.88	123.03	118.90
1	a	1412	C	C6-N1-C2	-6.87	117.55	120.30
24	A	2416	C	C5-C6-N1	6.87	124.44	121.00
1	a	1395	C	N3-C2-O2	-6.87	117.09	121.90
1	a	1520	C	C6-N1-C2	-6.87	117.55	120.30
24	A	2822	G	O5'-P-OP1	-6.87	99.52	105.70
24	A	2131	U	N1-C2-O2	6.86	127.60	122.80
1	a	267	C	N1-C2-O2	6.85	123.01	118.90
1	a	78	A	N1-C2-N3	-6.85	125.88	129.30
24	A	2793	C	N3-C4-N4	-6.85	113.21	118.00
24	A	2474	U	N3-C2-O2	-6.84	117.41	122.20
1	a	186	C	C6-N1-C2	-6.83	117.57	120.30
1	a	1455	G	N1-C6-O6	6.83	124.00	119.90
1	a	1173	U	C5-C6-N1	6.82	126.11	122.70
1	a	960	U	P-O3'-C3'	6.81	127.87	119.70
1	a	598	U	N3-C2-O2	-6.80	117.44	122.20
1	a	1433	A	N7-C8-N9	6.80	117.20	113.80
24	A	2888	C	C6-N1-C2	-6.80	117.58	120.30
1	a	527	G7M	P-O3'-C3'	6.80	127.86	119.70
24	A	205	G	O4'-C1'-N9	6.79	113.64	108.20
1	a	1143	G	N3-C2-N2	-6.79	115.15	119.90
24	A	2011	U	N3-C2-O2	-6.79	117.45	122.20
1	a	1297	G	P-O3'-C3'	6.79	127.85	119.70
24	A	1290	C	C5-C6-N1	6.79	124.39	121.00
1	a	960	U	N1-C2-O2	6.78	127.55	122.80
24	A	257	C	N1-C2-O2	6.78	122.97	118.90
24	A	1305	C	C6-N1-C2	-6.78	117.59	120.30
24	A	2248	C	N1-C2-O2	6.78	122.97	118.90
24	A	867	C	N3-C2-O2	-6.77	117.16	121.90
1	a	1496	C	C6-N1-C2	-6.77	117.59	120.30
25	B	68	C	C6-N1-C2	-6.74	117.60	120.30
24	A	1362	C	C5-C6-N1	6.74	124.37	121.00
24	A	1600	C	C6-N1-C2	-6.72	117.61	120.30
1	a	754	C	N3-C2-O2	-6.72	117.20	121.90
24	A	866	A	N1-C6-N6	6.72	122.63	118.60
1	a	422	C	N3-C2-O2	-6.71	117.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	755	G	O5'-P-OP2	-6.70	99.67	105.70
24	A	327	G	N3-C2-N2	-6.70	115.21	119.90
24	A	1371	G	N3-C4-N9	-6.70	121.98	126.00
24	A	365	U	C5-C6-N1	6.70	126.05	122.70
1	a	522	C	C6-N1-C2	-6.70	117.62	120.30
24	A	1399	C	C5-C6-N1	6.70	124.35	121.00
24	A	2745	C	N1-C2-O2	6.70	122.92	118.90
24	A	2561	U	N1-C2-N3	6.69	118.92	114.90
24	A	847	U	N3-C2-O2	-6.69	117.52	122.20
24	A	1578	U	N3-C2-O2	-6.69	117.52	122.20
24	A	12	U	N1-C2-O2	6.68	127.48	122.80
24	A	758	C	N3-C2-O2	-6.68	117.22	121.90
24	A	2617	U	N3-C2-O2	-6.68	117.52	122.20
24	A	2554	U	O5'-P-OP1	-6.68	99.69	105.70
24	A	1498	C	C2-N1-C1'	6.68	126.15	118.80
1	a	1455	G	C6-C5-N7	-6.68	126.39	130.40
24	A	912	C	C2-N1-C1'	6.67	126.14	118.80
1	a	1404	C	C6-N1-C2	-6.67	117.63	120.30
1	a	264	C	C6-N1-C2	-6.66	117.64	120.30
1	a	252	U	N3-C2-O2	-6.65	117.55	122.20
24	A	1624	U	N3-C2-O2	-6.65	117.55	122.20
24	A	1022	G	N3-C2-N2	-6.64	115.25	119.90
1	a	529	G	C6-C5-N7	-6.64	126.42	130.40
1	a	817	C	N1-C2-O2	6.62	122.87	118.90
1	a	623	C	C5-C6-N1	6.61	124.31	121.00
24	A	2649	C	C5-C6-N1	6.61	124.31	121.00
24	A	361	G	N1-C6-O6	6.61	123.87	119.90
24	A	373	U	N1-C2-O2	6.61	127.42	122.80
1	a	386	C	C6-N1-C2	-6.60	117.66	120.30
24	A	2354	C	C6-N1-C2	-6.60	117.66	120.30
24	A	2774	C	C6-N1-C2	-6.60	117.66	120.30
24	A	1365	A	C2-N3-C4	6.59	113.90	110.60
24	A	143	C	C6-N1-C2	-6.59	117.66	120.30
24	A	1005	C	N3-C2-O2	-6.58	117.29	121.90
24	A	2036	C	C6-N1-C2	-6.58	117.67	120.30
24	A	2796	U	N1-C2-N3	6.57	118.84	114.90
24	A	1294	U	N3-C2-O2	-6.57	117.60	122.20
24	A	62	U	C5-C6-N1	6.55	125.98	122.70
1	a	792	A	N7-C8-N9	-6.54	110.53	113.80
1	a	1027	C	C2-N3-C4	6.53	123.16	119.90
24	A	714	U	N3-C2-O2	-6.53	117.63	122.20
24	A	2403	C	C6-N1-C2	-6.52	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	783	A	C5-N7-C8	-6.51	100.64	103.90
24	A	528	A	N7-C8-N9	6.51	117.05	113.80
24	A	91	A	P-O3'-C3'	6.51	127.51	119.70
1	a	1372	U	N3-C2-O2	-6.50	117.65	122.20
24	A	687	C	N3-C2-O2	-6.50	117.35	121.90
1	a	400	C	C5-C6-N1	6.49	124.25	121.00
24	A	550	C	C5-C6-N1	6.49	124.25	121.00
1	a	1172	C	C6-N1-C2	-6.48	117.71	120.30
1	a	217	C	C5-C6-N1	6.47	124.23	121.00
24	A	1658	C	C6-N1-C2	-6.47	117.71	120.30
24	A	1947	C	C6-N1-C2	-6.47	117.71	120.30
24	A	758	C	C6-N1-C2	-6.46	117.71	120.30
13	m	4	ALA	N-CA-CB	-6.46	101.05	110.10
25	B	42	C	N1-C2-O2	6.46	122.78	118.90
1	a	1494[A]	G	C8-N9-C4	-6.44	103.82	106.40
1	a	1494[C]	G	C8-N9-C4	-6.44	103.82	106.40
24	A	2561	U	C2-N3-C4	-6.44	123.13	127.00
1	a	983	A	C2-N3-C4	6.44	113.82	110.60
24	A	62	U	C2-N3-C4	6.44	130.86	127.00
1	a	1225	A	N3-C4-N9	6.43	132.54	127.40
24	A	807	U	N3-C2-O2	-6.43	117.70	122.20
24	A	2424	C	C5-C4-N4	-6.43	115.70	120.20
24	A	121	G	N1-C6-O6	6.42	123.75	119.90
24	A	1994	C	N3-C2-O2	-6.41	117.41	121.90
25	B	60	C	C5-C6-N1	6.41	124.21	121.00
24	A	1348	C	N1-C2-O2	6.41	122.75	118.90
24	A	386	G	O5'-P-OP2	-6.41	99.93	105.70
24	A	2321	U	N3-C4-O4	6.41	123.88	119.40
25	B	17	C	N1-C2-O2	6.41	122.74	118.90
2	b	17	HIS	N-CA-CB	-6.40	99.07	110.60
24	A	2870	C	C6-N1-C2	-6.40	117.74	120.30
1	a	610	U	N3-C2-O2	-6.40	117.72	122.20
24	A	2372	U	N3-C2-O2	-6.40	117.72	122.20
24	A	2481	G	C5-C6-N1	-6.40	108.30	111.50
1	a	1205	U	N1-C2-O2	6.39	127.28	122.80
24	A	2312	U	C5-C6-N1	6.39	125.90	122.70
24	A	807	U	N1-C2-O2	6.39	127.27	122.80
22	v	74	C	N3-C2-O2	-6.39	117.43	121.90
1	a	810	C	C5-C6-N1	6.38	124.19	121.00
1	a	923	A	C8-N9-C4	-6.38	103.25	105.80
24	A	919	U	N1-C2-O2	6.37	127.26	122.80
24	A	866	A	C5-C6-N1	6.36	120.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1804	C	C6-N1-C2	-6.36	117.76	120.30
24	A	1848	A	C8-N9-C4	-6.35	103.26	105.80
24	A	2168	G	N3-C4-C5	-6.33	125.43	128.60
24	A	999	U	N1-C2-O2	6.33	127.23	122.80
1	a	413	G	C2-N3-C4	6.33	115.06	111.90
22	v	67	C	N1-C2-O2	6.33	122.70	118.90
24	A	2168	G	C2-N3-C4	6.33	115.06	111.90
1	a	207	C	N3-C2-O2	-6.33	117.47	121.90
24	A	894	U	N3-C2-O2	-6.32	117.77	122.20
24	A	512	G	O4'-C1'-N9	6.32	113.25	108.20
24	A	547	A	C2-N3-C4	6.31	113.75	110.60
1	a	618	C	N1-C2-O2	6.31	122.68	118.90
1	a	1011	C	C5-C6-N1	6.31	124.15	121.00
24	A	1669	A	C2-N3-C4	6.31	113.75	110.60
25	B	12	C	N3-C2-O2	-6.31	117.48	121.90
24	A	454	A	OP2-P-O3'	6.30	119.06	105.20
1	a	960	U	N3-C2-O2	-6.29	117.79	122.20
24	A	1314	C	C2-N1-C1'	6.29	125.72	118.80
24	A	1567	G	P-O3'-C3'	6.29	127.25	119.70
24	A	2755	C	N1-C2-O2	6.29	122.67	118.90
1	a	413	G	C4-C5-N7	-6.29	108.29	110.80
1	a	483	C	C6-N1-C2	-6.28	117.79	120.30
24	A	2025	C	C6-N1-C2	-6.28	117.79	120.30
24	A	2250	G	N3-C4-N9	-6.28	122.23	126.00
24	A	366	C	C6-N1-C2	-6.28	117.79	120.30
25	B	37	C	N1-C2-O2	6.26	122.66	118.90
1	a	1538	C	C6-N1-C2	-6.26	117.80	120.30
24	A	2220	U	C5-C6-N1	6.26	125.83	122.70
1	a	1258	G	N1-C6-O6	-6.25	116.15	119.90
24	A	1784	A	N7-C8-N9	-6.24	110.68	113.80
1	a	33	A	N7-C8-N9	6.24	116.92	113.80
24	A	314	C	C6-N1-C2	-6.24	117.80	120.30
1	a	1011	C	C6-N1-C2	-6.24	117.81	120.30
1	a	80	A	N1-C2-N3	6.24	132.42	129.30
1	a	369	G	C6-C5-N7	-6.21	126.67	130.40
1	a	186	C	N1-C2-O2	6.21	122.62	118.90
25	B	37	C	N3-C2-O2	-6.20	117.56	121.90
24	A	16	C	C6-N1-C2	-6.20	117.82	120.30
24	A	205	G	OP2-P-O3'	6.20	118.83	105.20
24	A	581	C	O5'-P-OP1	-6.19	100.13	105.70
1	a	500	G	N1-C6-O6	6.19	123.61	119.90
24	A	1920	C	C6-N1-C2	-6.18	117.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	276	U	N1-C2-O2	6.17	127.12	122.80
24	A	287	G	C6-N1-C2	-6.17	121.40	125.10
24	A	1081	U	N3-C4-C5	6.17	118.30	114.60
24	A	2794	C	C6-N1-C2	-6.17	117.83	120.30
1	a	810	C	C6-N1-C2	-6.17	117.83	120.30
1	a	1320	C	N1-C2-O2	6.17	122.60	118.90
24	A	1399	C	C6-N1-C2	-6.17	117.83	120.30
24	A	2782	G	C6-C5-N7	-6.17	126.70	130.40
1	a	207	C	N1-C2-O2	6.16	122.60	118.90
22	v	56	C	C6-N1-C2	-6.16	117.83	120.30
24	A	2561	U	N3-C2-O2	-6.16	117.89	122.20
24	A	1044	C	C5-C4-N4	6.16	124.51	120.20
24	A	2405	G	OP2-P-O3'	6.16	118.75	105.20
1	a	1432	G	P-O3'-C3'	6.15	127.08	119.70
24	A	198	C	N1-C2-O2	6.15	122.59	118.90
1	a	316	C	N1-C2-O2	6.14	122.59	118.90
1	a	754	C	OP1-P-O3'	6.14	118.72	105.20
1	a	1134	G	C6-N1-C2	-6.14	121.41	125.10
24	A	805	G	N9-C4-C5	-6.14	102.94	105.40
25	B	68	C	C5-C6-N1	6.14	124.07	121.00
1	a	1383	C	N1-C2-O2	6.13	122.58	118.90
24	A	2742	G	C4-C5-N7	6.13	113.25	110.80
1	a	1301	U	P-O3'-C3'	6.12	127.05	119.70
24	A	106	C	C6-N1-C2	-6.12	117.85	120.30
1	a	1497	G	N3-C2-N2	-6.12	115.62	119.90
1	a	961	U	N3-C2-O2	-6.12	117.92	122.20
24	A	512	G	OP2-P-O3'	6.11	118.63	105.20
1	a	890	G	P-O3'-C3'	6.10	127.02	119.70
1	a	1262	C	N1-C2-O2	6.10	122.56	118.90
24	A	832	U	N1-C2-N3	6.10	118.56	114.90
25	B	38	C	C5-C4-N4	-6.10	115.93	120.20
24	A	1584	U	C5-C6-N1	6.10	125.75	122.70
24	A	1716	U	C2-N1-C1'	6.10	125.02	117.70
25	B	28	C	C6-N1-C2	-6.09	117.86	120.30
1	a	1277	C	C6-N1-C2	-6.09	117.86	120.30
24	A	2566	A	P-O3'-C3'	6.09	127.00	119.70
24	A	2683	C	N3-C2-O2	-6.08	117.64	121.90
1	a	840	C	N3-C4-N4	-6.08	113.74	118.00
1	a	272	C	C6-N1-C2	-6.07	117.87	120.30
1	a	578	C	C6-N1-C2	-6.07	117.87	120.30
24	A	353	C	C6-N1-C2	-6.07	117.87	120.30
1	a	548	G	N1-C6-O6	6.06	123.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	847	U	N1-C2-O2	6.06	127.04	122.80
1	a	1357	A	N7-C8-N9	6.05	116.83	113.80
1	a	991	U	N1-C2-O2	6.05	127.04	122.80
1	a	1303	C	N1-C2-O2	6.05	122.53	118.90
24	A	1994	C	C6-N1-C2	-6.05	117.88	120.30
24	A	2074	U	N1-C2-O2	6.04	127.03	122.80
24	A	385	C	P-O3'-C3'	6.04	126.95	119.70
1	a	503	C	C5-C6-N1	6.04	124.02	121.00
24	A	349	U	N1-C2-O2	6.03	127.02	122.80
24	A	2244	U	C5-C4-O4	-6.03	122.28	125.90
24	A	2141	G	N7-C8-N9	6.03	116.12	113.10
25	B	27	C	N1-C2-O2	6.03	122.52	118.90
1	a	883	C	N1-C2-O2	6.02	122.51	118.90
24	A	214	G	N3-C4-C5	-6.02	125.59	128.60
40	Q	27	ARG	NE-CZ-NH1	-6.02	117.29	120.30
5	e	122	VAL	N-CA-CB	-6.02	98.26	111.50
24	A	935	C	C6-N1-C2	-6.02	117.89	120.30
1	a	215	C	C2-N1-C1'	6.01	125.42	118.80
24	A	672	C	C6-N1-C2	-6.01	117.89	120.30
24	A	1894	C	N1-C2-O2	6.01	122.51	118.90
24	A	2061	G	P-O3'-C3'	6.01	126.92	119.70
1	a	626	G	C6-C5-N7	-6.01	126.79	130.40
24	A	2496	C	N1-C2-O2	6.01	122.50	118.90
1	a	1494[A]	G	N7-C8-N9	6.00	116.10	113.10
1	a	1494[C]	G	N7-C8-N9	6.00	116.10	113.10
24	A	1340	U	N1-C2-O2	6.00	127.00	122.80
24	A	2720	U	N3-C2-O2	-6.00	118.00	122.20
24	A	1784	A	C4-C5-C6	6.00	120.00	117.00
24	A	2558	C	C5-C6-N1	6.00	124.00	121.00
24	A	366	C	C5-C6-N1	5.99	124.00	121.00
1	a	248	C	C6-N1-C2	-5.99	117.90	120.30
24	A	2379	G	N1-C6-O6	5.99	123.49	119.90
24	A	543	G	N1-C6-O6	5.99	123.49	119.90
24	A	284	U	N3-C2-O2	-5.99	118.01	122.20
24	A	284	U	N1-C2-O2	5.98	126.99	122.80
24	A	528	A	C5-N7-C8	-5.98	100.91	103.90
24	A	1023	U	N1-C2-O2	5.98	126.99	122.80
24	A	62	U	C6-N1-C1'	-5.98	112.83	121.20
24	A	528	A	C8-N9-C4	-5.98	103.41	105.80
1	a	1147	C	N1-C2-O2	5.97	122.48	118.90
24	A	2463	C	C5-C6-N1	5.97	123.99	121.00
1	a	50	A	C2-N3-C4	5.97	113.58	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1578	U	N1-C2-O2	5.97	126.98	122.80
24	A	2711	A	O5'-P-OP2	5.97	117.86	110.70
24	A	1313	U	C6-N1-C1'	-5.97	112.85	121.20
1	a	943	U	N1-C2-O2	5.96	126.97	122.80
24	A	2329	U	C5-C6-N1	5.96	125.68	122.70
29	F	172	PHE	C-N-CA	5.96	136.59	121.70
1	a	1140	C	N1-C2-O2	5.96	122.47	118.90
1	a	626	G	N3-C4-N9	5.94	129.56	126.00
24	A	2518	A	C2-N3-C4	5.94	113.57	110.60
22	v	36	U	N3-C2-O2	-5.94	118.04	122.20
24	A	919	U	N3-C2-O2	-5.94	118.04	122.20
24	A	2254	C	N1-C2-O2	5.94	122.46	118.90
30	G	174	LYS	N-CA-CB	5.94	121.29	110.60
24	A	81	G	N3-C2-N2	-5.93	115.75	119.90
24	A	866	A	N9-C4-C5	-5.93	103.43	105.80
1	a	1037	C	C6-N1-C2	-5.92	117.93	120.30
1	a	1455	G	N3-C4-N9	5.92	129.56	126.00
24	A	62	U	C6-N1-C2	-5.92	117.45	121.00
1	a	56	U	C5-C4-O4	-5.92	122.35	125.90
1	a	1228	C	C6-N1-C2	-5.91	117.94	120.30
24	A	1782	U	O5'-P-OP1	-5.91	100.38	105.70
24	A	456	C	O5'-P-OP2	-5.90	100.39	105.70
1	a	1109	C	C6-N1-C2	-5.90	117.94	120.30
24	A	1020	A	P-O3'-C3'	5.90	126.78	119.70
24	A	1112	G	N3-C4-N9	-5.90	122.46	126.00
24	A	140	C	C6-N1-C2	-5.90	117.94	120.30
25	B	49	C	C6-N1-C2	-5.89	117.94	120.30
1	a	322	C	C5-C6-N1	5.89	123.95	121.00
24	A	51	G	P-O3'-C3'	5.89	126.77	119.70
1	a	369	G	N1-C6-O6	5.89	123.43	119.90
24	A	758	C	N1-C2-O2	5.89	122.43	118.90
24	A	1020	A	OP2-P-O3'	5.89	118.16	105.20
1	a	217	C	C6-N1-C2	-5.88	117.95	120.30
24	A	1994	C	N1-C2-O2	5.88	122.42	118.90
25	B	42	C	N3-C2-O2	-5.87	117.79	121.90
24	A	141	G	N3-C4-C5	-5.87	125.67	128.60
25	B	12	C	N1-C2-O2	5.87	122.42	118.90
25	B	38	C	N3-C4-N4	5.87	122.11	118.00
24	A	1830	C	N1-C2-O2	5.87	122.42	118.90
1	a	1535	C	C5-C6-N1	5.87	123.93	121.00
24	A	435	C	C6-N1-C2	-5.86	117.95	120.30
24	A	1054	A	N1-C2-N3	-5.86	126.37	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	2782	G	N3-C4-N9	5.86	129.52	126.00
24	A	1810	A	C8-N9-C4	-5.85	103.46	105.80
24	A	2036	C	C5-C6-N1	5.85	123.93	121.00
24	A	2867	G	N9-C4-C5	-5.85	103.06	105.40
24	A	2282	G	N1-C6-O6	-5.85	116.39	119.90
24	A	2794	C	C2-N1-C1'	5.84	125.23	118.80
25	B	5	U	N3-C2-O2	-5.84	118.11	122.20
1	a	723	U	C5-C6-N1	5.84	125.62	122.70
24	A	1455	G	N3-C4-N9	5.84	129.50	126.00
1	a	1433	A	C8-N9-C4	-5.83	103.47	105.80
24	A	288	U	C5-C6-N1	5.83	125.62	122.70
24	A	2354	C	C5-C6-N1	5.83	123.92	121.00
24	A	776	G	C8-N9-C1'	-5.82	119.43	127.00
24	A	2096	C	O5'-P-OP2	-5.82	100.46	105.70
24	A	2773	C	C6-N1-C2	-5.82	117.97	120.30
1	a	850	U	C5-C6-N1	5.81	125.61	122.70
24	A	2683	C	N1-C2-O2	5.81	122.39	118.90
24	A	2581	G	N3-C4-N9	5.81	129.49	126.00
24	A	805	G	N3-C4-N9	5.80	129.48	126.00
25	B	12	C	C6-N1-C2	-5.80	117.98	120.30
24	A	965	C	C6-N1-C2	-5.80	117.98	120.30
24	A	305	C	C5-C6-N1	5.80	123.90	121.00
24	A	2180	U	C2-N3-C4	5.79	130.48	127.00
24	A	1135	C	OP1-P-O3'	5.79	117.93	105.20
1	a	1190	G	P-O3'-C3'	5.78	126.64	119.70
22	v	34	C	C5-C4-N4	-5.78	116.16	120.20
1	a	1245	C	C5-C6-N1	5.78	123.89	121.00
25	B	31	C	N3-C2-O2	-5.78	117.86	121.90
24	A	866	A	C4-C5-N7	5.77	113.58	110.70
1	a	1538	C	C5-C6-N1	5.76	123.88	121.00
24	A	2072	C	C2-N1-C1'	5.76	125.14	118.80
24	A	714	U	N1-C2-O2	5.76	126.83	122.80
24	A	893	C	N3-C4-C5	-5.76	119.60	121.90
24	A	2739	U	N1-C2-O2	5.76	126.83	122.80
24	A	1180	U	C5-C4-O4	-5.75	122.45	125.90
1	a	188	C	N1-C2-O2	5.75	122.35	118.90
13	m	57	ASP	CB-CG-OD1	5.75	123.48	118.30
24	A	1105	U	C2-N3-C4	-5.75	123.55	127.00
24	A	1213	A	C2-N3-C4	5.75	113.48	110.60
24	A	1769	U	N3-C2-O2	-5.75	118.17	122.20
24	A	1305	C	C5-C6-N1	5.75	123.88	121.00
1	a	316	C	N3-C2-O2	-5.75	117.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1539	U	C2-N3-C4	5.74	130.45	127.00
24	A	8	C	C5-C6-N1	5.74	123.87	121.00
24	A	984	A	C2-N3-C4	-5.74	107.73	110.60
1	a	186	C	C5-C6-N1	5.74	123.87	121.00
24	A	1159	U	N1-C2-O2	5.74	126.81	122.80
24	A	2370	G	C6-N1-C2	-5.74	121.66	125.10
30	G	174	LYS	N-CA-C	-5.73	95.52	111.00
24	A	1930	G	O4'-C1'-N9	5.73	112.79	108.20
24	A	91	A	OP2-P-O3'	5.73	117.81	105.20
24	A	2803	G	C6-C5-N7	-5.73	126.96	130.40
24	A	1940	U	P-O3'-C3'	5.73	126.57	119.70
24	A	1416	G	C6-N1-C2	-5.73	121.67	125.10
24	A	1920	C	C5-C6-N1	5.73	123.86	121.00
1	a	215	C	C5-C4-N4	-5.72	116.19	120.20
1	a	1182	G	P-O3'-C3'	5.72	126.57	119.70
24	A	383	C	N1-C2-O2	5.72	122.33	118.90
24	A	1159	U	N3-C2-O2	-5.72	118.20	122.20
24	A	1303	G	N1-C6-O6	5.72	123.33	119.90
1	a	611	C	N1-C2-O2	5.72	122.33	118.90
1	a	623	C	N3-C4-N4	5.72	122.00	118.00
1	a	1320	C	N3-C2-O2	-5.72	117.90	121.90
22	v	34	C	C2-N1-C1'	5.71	125.08	118.80
24	A	1728	C	N1-C2-O2	-5.71	115.47	118.90
24	A	205	G	C8-N9-C4	5.71	108.68	106.40
24	A	2649	C	C6-N1-C2	-5.71	118.02	120.30
24	A	2321	U	N3-C4-C5	-5.70	111.18	114.60
24	A	2594	C	C6-N1-C2	-5.70	118.02	120.30
24	A	1533	C	N3-C4-N4	-5.70	114.01	118.00
24	A	1461	C	C5-C6-N1	5.70	123.85	121.00
24	A	2226	C	C6-N1-C2	-5.70	118.02	120.30
24	A	2827	C	C5-C6-N1	5.70	123.85	121.00
24	A	2370	G	N3-C4-C5	-5.70	125.75	128.60
24	A	640	C	C6-N1-C2	-5.69	118.02	120.30
24	A	2403	C	N1-C2-O2	5.69	122.31	118.90
24	A	2405	G	P-O3'-C3'	5.69	126.53	119.70
24	A	557	C	N1-C2-O2	5.69	122.31	118.90
1	a	572	A	P-O3'-C3'	5.68	126.52	119.70
24	A	2867	G	C8-N9-C4	5.68	108.67	106.40
1	a	369	G	N3-C4-N9	5.68	129.41	126.00
1	a	470	C	C6-N1-C2	-5.68	118.03	120.30
24	A	1730	C	C6-N1-C2	-5.67	118.03	120.30
7	g	22	LEU	CA-CB-CG	5.67	128.34	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	101	LEU	CA-CB-CG	5.67	128.33	115.30
1	a	1034	G	N1-C6-O6	-5.67	116.50	119.90
1	a	717	U	N1-C2-O2	5.66	126.76	122.80
1	a	891	U	C6-N1-C2	-5.66	117.60	121.00
24	A	1021	A	C2-N3-C4	5.66	113.43	110.60
1	a	1158	C	N3-C2-O2	-5.66	117.94	121.90
24	A	2174	C	N1-C2-O2	5.65	122.29	118.90
1	a	883	C	C6-N1-C2	-5.65	118.04	120.30
22	v	34	C	N3-C4-N4	5.65	121.95	118.00
24	A	1314	C	N1-C2-O2	5.65	122.29	118.90
35	L	29	LYS	N-CA-CB	-5.65	100.43	110.60
24	A	349	U	N3-C2-O2	-5.64	118.25	122.20
24	A	1662	U	N3-C2-O2	-5.64	118.25	122.20
1	a	348	G	N1-C6-O6	5.64	123.28	119.90
1	a	1356	G	N3-C2-N2	5.64	123.85	119.90
24	A	961	C	C6-N1-C2	-5.64	118.04	120.30
24	A	1043	C	C6-N1-C2	-5.64	118.04	120.30
24	A	2884	U	C2-N1-C1'	5.64	124.47	117.70
24	A	645	C	N3-C2-O2	-5.64	117.95	121.90
24	A	1816	C	N1-C2-O2	5.64	122.28	118.90
1	a	613	C	C6-N1-C2	-5.64	118.05	120.30
24	A	2244	U	N3-C4-O4	5.64	123.35	119.40
1	a	754	C	C6-N1-C1'	-5.63	114.04	120.80
24	A	1142	A	C2-N3-C4	-5.63	107.78	110.60
1	a	1303	C	N3-C2-O2	-5.63	117.96	121.90
1	a	1455	G	C5-C6-O6	-5.63	125.22	128.60
24	A	1963	U	C5-C6-N1	5.63	125.51	122.70
24	A	2162	G	OP1-P-OP2	-5.63	111.16	119.60
24	A	1290	C	C6-N1-C2	-5.63	118.05	120.30
24	A	805	G	C4-C5-N7	5.62	113.05	110.80
24	A	1680	U	N1-C2-O2	5.62	126.74	122.80
1	a	1382	C	N1-C2-O2	5.62	122.27	118.90
24	A	484	C	N1-C2-O2	5.62	122.27	118.90
24	A	1585	C	N1-C2-O2	5.62	122.27	118.90
24	A	2474	U	N1-C2-O2	5.62	126.73	122.80
24	A	2795	C	C6-N1-C2	-5.62	118.05	120.30
1	a	961	U	N1-C2-O2	5.62	126.73	122.80
24	A	542	C	N3-C4-N4	-5.61	114.07	118.00
24	A	901	C	N1-C2-O2	5.61	122.27	118.90
1	a	413	G	C8-N9-C4	5.61	108.64	106.40
1	a	1149	C	C6-N1-C2	-5.61	118.06	120.30
24	A	1323	C	N3-C2-O2	-5.60	117.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	348	G	C6-C5-N7	-5.59	127.05	130.40
24	A	2496	C	N3-C2-O2	-5.59	117.99	121.90
24	A	2796	U	C2-N3-C4	-5.59	123.65	127.00
1	a	413	G	N3-C4-N9	5.59	129.35	126.00
1	a	251	G	O4'-C1'-N9	-5.58	103.73	108.20
1	a	1173	U	C5-C4-O4	-5.58	122.55	125.90
22	v	71	C	C6-N1-C2	-5.58	118.07	120.30
24	A	1839	G	C2-N3-C4	5.58	114.69	111.90
24	A	1105	U	N1-C2-O2	5.58	126.70	122.80
24	A	872	U	C5-C6-N1	5.58	125.49	122.70
24	A	912	C	N3-C2-O2	-5.58	118.00	121.90
24	A	1526	C	C6-N1-C2	-5.58	118.07	120.30
24	A	1104	C	N3-C4-N4	5.57	121.90	118.00
30	G	46	ASP	N-CA-C	5.57	126.04	111.00
24	A	1269	A	N1-C2-N3	-5.57	126.52	129.30
24	A	1407	G	C4-C5-N7	5.57	113.03	110.80
24	A	1371	G	N3-C4-C5	5.56	131.38	128.60
24	A	2312	U	C6-N1-C2	-5.56	117.66	121.00
24	A	1081	U	C2-N3-C4	-5.56	123.67	127.00
1	a	316	C	C2-N1-C1'	5.56	124.91	118.80
1	a	986	U	C5-C6-N1	5.56	125.48	122.70
24	A	2562	U	N3-C2-O2	-5.56	118.31	122.20
1	a	1261	A	C2-N3-C4	5.55	113.38	110.60
24	A	1005	C	C2-N1-C1'	5.55	124.91	118.80
24	A	1500	G	N1-C6-O6	5.55	123.23	119.90
24	A	198	C	C6-N1-C2	-5.55	118.08	120.30
24	A	1402	U	N1-C2-O2	5.55	126.69	122.80
24	A	2562	U	N1-C2-O2	5.55	126.69	122.80
24	A	205	G	P-O3'-C3'	5.55	126.36	119.70
1	a	814	A	C2-N3-C4	5.55	113.37	110.60
1	a	1003	G	N1-C2-N2	5.55	121.19	116.20
1	a	1277	C	N1-C2-O2	5.55	122.23	118.90
24	A	2782	G	N1-C6-O6	5.55	123.23	119.90
24	A	2863	C	C6-N1-C2	-5.54	118.08	120.30
24	A	1731	G	C8-N9-C4	-5.54	104.18	106.40
24	A	2818	U	N1-C2-O2	5.54	126.68	122.80
1	a	843	U	C5-C6-N1	5.54	125.47	122.70
24	A	2739	U	N3-C2-O2	-5.54	118.32	122.20
1	a	322	C	C6-N1-C2	-5.54	118.09	120.30
24	A	1102	C	N3-C2-O2	-5.54	118.03	121.90
24	A	1941	C	N3-C2-O2	-5.54	118.03	121.90
24	A	1930	G	P-O3'-C3'	5.53	126.34	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	935	C	C5-C6-N1	5.53	123.76	121.00
1	a	991	U	N3-C2-O2	-5.53	118.33	122.20
44	U	88	ASP	N-CA-CB	-5.52	100.66	110.60
24	A	2751	G	O5'-P-OP2	5.52	117.33	110.70
1	a	1195	C	N3-C2-O2	-5.52	118.04	121.90
1	a	737	C	C2-N3-C4	5.52	122.66	119.90
24	A	1138	G	N1-C6-O6	-5.51	116.59	119.90
24	A	2456	C	C6-N1-C2	-5.51	118.10	120.30
24	A	257	C	N3-C2-O2	-5.51	118.05	121.90
24	A	1111	A	P-O3'-C3'	5.50	126.30	119.70
1	a	1486	G	N3-C4-C5	-5.50	125.85	128.60
1	a	102	G	N1-C6-O6	-5.50	116.60	119.90
1	a	717	U	N3-C2-O2	-5.50	118.35	122.20
24	A	2168	G	N3-C4-N9	5.50	129.30	126.00
1	a	618	C	N3-C2-O2	-5.50	118.05	121.90
24	A	776	G	C8-N9-C4	-5.50	104.20	106.40
24	A	845	A	N1-C2-N3	-5.50	126.55	129.30
24	A	933	A	C2-N3-C4	5.50	113.35	110.60
1	a	34	C	C5-C6-N1	5.49	123.75	121.00
1	a	804	U	N3-C2-O2	-5.49	118.36	122.20
24	A	1210	G	C2-N3-C4	5.49	114.65	111.90
24	A	2782	G	N9-C4-C5	-5.49	103.20	105.40
1	a	168	G	N3-C4-N9	5.49	129.29	126.00
1	a	1288	A	N7-C8-N9	5.49	116.55	113.80
24	A	1982	U	N1-C2-O2	5.49	126.64	122.80
24	A	916	G	C4-C5-N7	5.49	112.99	110.80
24	A	1498	C	C5-C6-N1	5.49	123.74	121.00
1	a	1372	U	N1-C2-O2	5.48	126.64	122.80
24	A	2023	C	N1-C2-O2	5.48	122.19	118.90
22	v	71	C	N3-C2-O2	-5.47	118.07	121.90
24	A	208	C	C6-N1-C2	-5.47	118.11	120.30
25	B	88	C	N1-C2-O2	5.47	122.18	118.90
1	a	1452	C	C6-N1-C2	-5.46	118.11	120.30
14	n	33	VAL	C-N-CA	5.46	135.36	121.70
24	A	314	C	C5-C6-N1	5.46	123.73	121.00
1	a	1088	G	N9-C4-C5	-5.46	103.22	105.40
24	A	2514	U	C5-C6-N1	5.46	125.43	122.70
1	a	1010	U	N3-C2-O2	-5.46	118.38	122.20
24	A	2867	G	P-O3'-C3'	5.46	126.25	119.70
1	a	1034	G	C5-C6-N1	5.45	114.22	111.50
1	a	1173	U	N3-C4-O4	5.45	123.22	119.40
24	A	789	A	OP2-P-O3'	5.45	117.18	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	613	A	N3-C4-C5	-5.45	122.99	126.80
1	a	1297	G	O5'-P-OP2	-5.44	100.80	105.70
24	A	383	C	N3-C2-O2	-5.44	118.09	121.90
1	a	1134	G	N1-C2-N2	5.44	121.10	116.20
1	a	188	C	C6-N1-C2	-5.44	118.12	120.30
24	A	1343	G	C4-N9-C1'	5.44	133.57	126.50
24	A	2510	C	C6-N1-C2	-5.44	118.13	120.30
1	a	890	G	OP2-P-O3'	5.43	117.16	105.20
24	A	1839	G	N3-C4-C5	-5.43	125.89	128.60
24	A	690	G	C4-N9-C1'	5.43	133.55	126.50
1	a	609	A	C2-N3-C4	5.42	113.31	110.60
24	A	215	G	OP1-P-O3'	5.42	117.13	105.20
24	A	435	C	N1-C2-O2	5.42	122.16	118.90
24	A	894	U	N1-C2-O2	5.42	126.60	122.80
24	A	2567	G	C4-N9-C1'	5.42	133.54	126.50
1	a	358	U	N3-C2-O2	-5.42	118.41	122.20
24	A	161	A	OP1-P-O3'	5.41	117.11	105.20
24	A	813	U	N3-C2-O2	-5.41	118.41	122.20
1	a	413	G	N3-C4-C5	-5.41	125.90	128.60
24	A	177	G	C4-N9-C1'	5.41	133.53	126.50
24	A	2754	U	N1-C2-O2	5.41	126.58	122.80
51	1	39	ASP	CB-CG-OD1	5.41	123.17	118.30
24	A	2793	C	N3-C2-O2	-5.40	118.12	121.90
24	A	609	A	C8-N9-C4	-5.40	103.64	105.80
1	a	1219	A	N7-C8-N9	5.40	116.50	113.80
1	a	1493[A]	A	P-O3'-C3'	5.40	126.18	119.70
1	a	1493[C]	A	P-O3'-C3'	5.40	126.18	119.70
1	a	335	C	C6-N1-C2	-5.40	118.14	120.30
24	A	32	C	C5-C6-N1	5.40	123.70	121.00
24	A	1875	G	OP2-P-O3'	5.40	117.07	105.20
24	A	2008	C	C6-N1-C2	-5.40	118.14	120.30
24	A	1112	G	C5-C6-O6	5.39	131.84	128.60
24	A	2581	G	C2-N3-C4	5.39	114.60	111.90
1	a	355	C	C6-N1-C2	-5.39	118.14	120.30
24	A	276	U	N3-C2-O2	-5.39	118.43	122.20
24	A	287	G	N3-C2-N2	-5.39	116.13	119.90
24	A	669	G	C4-N9-C1'	5.39	133.50	126.50
24	A	278	A	N3-C4-C5	-5.39	123.03	126.80
24	A	137	U	N1-C2-N3	5.38	118.13	114.90
1	a	1182	G	OP2-P-O3'	5.38	117.03	105.20
1	a	787	A	C2-N3-C4	5.38	113.29	110.60
1	a	58	C	N3-C4-N4	-5.38	114.24	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	623	C	C2-N1-C1'	5.38	124.71	118.80
1	a	1383	C	N3-C2-O2	-5.38	118.14	121.90
1	a	891	U	C2-N1-C1'	5.37	124.15	117.70
24	A	1104	C	C2-N1-C1'	5.37	124.71	118.80
24	A	2896	C	C5-C6-N1	5.37	123.69	121.00
24	A	1993	U	N1-C2-O2	5.37	126.56	122.80
1	a	500	G	C6-C5-N7	-5.37	127.18	130.40
1	a	1225	A	N1-C2-N3	-5.37	126.62	129.30
1	a	1432	G	OP2-P-O3'	5.37	117.01	105.20
1	a	603	U	C5-C6-N1	5.36	125.38	122.70
1	a	1399	C	N1-C2-O2	-5.36	115.68	118.90
24	A	2460	U	N1-C2-O2	5.36	126.56	122.80
24	A	672	C	C5-C6-N1	5.36	123.68	121.00
24	A	1956	U	N3-C2-O2	-5.35	118.45	122.20
24	A	2372	U	N1-C2-O2	5.35	126.55	122.80
24	A	2109	U	C5-C6-N1	5.35	125.38	122.70
24	A	2666	C	N1-C2-O2	5.35	122.11	118.90
24	A	2311	A	C5-N7-C8	5.35	106.57	103.90
1	a	1073	U	N3-C2-O2	-5.34	118.46	122.20
24	A	1407	G	C6-C5-N7	-5.34	127.19	130.40
24	A	1993	U	N3-C2-O2	-5.34	118.46	122.20
24	A	445	C	C6-N1-C2	-5.34	118.16	120.30
24	A	1026	G	C2-N3-C4	5.33	114.57	111.90
1	a	390	U	N3-C4-O4	5.33	123.13	119.40
24	A	2025	C	N1-C2-O2	5.33	122.10	118.90
24	A	456	C	C6-N1-C2	-5.33	118.17	120.30
24	A	335	C	C6-N1-C2	-5.33	118.17	120.30
24	A	1982	U	N3-C2-O2	-5.33	118.47	122.20
1	a	983	A	N3-C4-C5	-5.33	123.07	126.80
24	A	1102	C	N1-C2-O2	5.33	122.09	118.90
1	a	805	C	N1-C2-O2	5.32	122.09	118.90
1	a	1460	C	N1-C2-O2	5.32	122.09	118.90
24	A	1104	C	C2-N3-C4	5.32	122.56	119.90
1	a	23	C	C6-N1-C2	-5.32	118.17	120.30
1	a	1527	U	O5'-P-OP2	-5.32	100.92	105.70
24	A	2669	G	N1-C6-O6	-5.32	116.71	119.90
24	A	639	U	N3-C2-O2	-5.31	118.48	122.20
1	a	56	U	C5-C6-N1	5.31	125.36	122.70
1	a	540	G	C8-N9-C4	-5.31	104.28	106.40
1	a	1262	C	N3-C2-O2	-5.31	118.19	121.90
1	a	983	A	N3-C4-N9	5.31	131.65	127.40
1	a	883	C	N3-C2-O2	-5.30	118.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1371	G	C4-N9-C1'	-5.30	119.61	126.50
24	A	2220	U	N1-C2-O2	5.30	126.51	122.80
24	A	2794	C	C5-C6-N1	5.30	123.65	121.00
25	B	26	C	C6-N1-C2	-5.30	118.18	120.30
1	a	470	C	C5-C6-N1	5.29	123.64	121.00
1	a	529	G	OP2-P-O3'	5.29	116.84	105.20
24	A	1658	C	C5-C6-N1	5.29	123.65	121.00
1	a	1184	G	N3-C4-C5	-5.29	125.95	128.60
24	A	929	U	N3-C2-O2	-5.29	118.50	122.20
1	a	575	G	N3-C2-N2	-5.29	116.20	119.90
1	a	675	A	N7-C8-N9	5.29	116.44	113.80
22	v	41	C	C6-N1-C2	-5.29	118.19	120.30
24	A	1406	U	C5-C6-N1	5.29	125.34	122.70
24	A	1212	G	OP2-P-O3'	5.28	116.82	105.20
1	a	473	U	N3-C2-O2	-5.28	118.50	122.20
24	A	121	G	C6-C5-N7	-5.28	127.23	130.40
24	A	2075	U	C5-C6-N1	5.28	125.34	122.70
24	A	143	C	N1-C2-O2	5.28	122.07	118.90
1	a	78	A	N9-C4-C5	-5.28	103.69	105.80
24	A	327	G	C6-N1-C2	-5.28	121.93	125.10
24	A	2832	U	P-O3'-C3'	5.28	126.03	119.70
24	A	2337	G	N3-C4-C5	-5.28	125.96	128.60
1	a	27	G	C5-C6-O6	-5.27	125.44	128.60
7	g	110	ARG	N-CA-C	5.27	125.24	111.00
24	A	362	A	C2-N3-C4	5.27	113.24	110.60
1	a	188	C	N3-C2-O2	-5.27	118.21	121.90
24	A	2888	C	N3-C2-O2	-5.26	118.22	121.90
1	a	450	G	N3-C2-N2	-5.26	116.22	119.90
24	A	366	C	N1-C2-O2	5.25	122.05	118.90
24	A	998	C	C5-C6-N1	5.25	123.63	121.00
1	a	862	C	C6-N1-C2	-5.25	118.20	120.30
24	A	1830	C	C6-N1-C2	-5.25	118.20	120.30
24	A	2581	G	N3-C4-C5	-5.25	125.98	128.60
25	B	31	C	C2-N1-C1'	5.25	124.57	118.80
24	A	2645	G	C4-N9-C1'	5.25	133.32	126.50
25	B	73	A	C2-N3-C4	5.25	113.22	110.60
24	A	445	C	N3-C2-O2	-5.25	118.23	121.90
24	A	776	G	C6-C5-N7	-5.25	127.25	130.40
24	A	1894	C	N3-C2-O2	-5.24	118.23	121.90
1	a	971	G	C8-N9-C4	5.24	108.50	106.40
24	A	2093	G	C5-N7-C8	5.24	106.92	104.30
24	A	1921	G	N1-C6-O6	5.24	123.05	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	420	U	C5-C6-N1	5.24	125.32	122.70
24	A	2254	C	N3-C2-O2	-5.23	118.24	121.90
24	A	1200	C	C6-N1-C2	-5.23	118.21	120.30
24	A	1043	C	C5-C6-N1	5.22	123.61	121.00
24	A	1716	U	C6-N1-C2	-5.22	117.86	121.00
25	B	27	C	N3-C2-O2	-5.22	118.24	121.90
24	A	1782	U	C5-C6-N1	5.22	125.31	122.70
24	A	1151	A	N1-C2-N3	-5.22	126.69	129.30
1	a	810	C	C2-N1-C1'	5.22	124.54	118.80
24	A	1666	G	N1-C6-O6	-5.22	116.77	119.90
1	a	923	A	C5-N7-C8	-5.21	101.29	103.90
24	A	1788	C	C6-N1-C2	-5.21	118.21	120.30
24	A	2380	C	C6-N1-C2	-5.21	118.22	120.30
24	A	2395	C	C5-C6-N1	5.21	123.61	121.00
24	A	2558	C	C6-N1-C2	-5.21	118.21	120.30
24	A	1180	U	C2-N1-C1'	5.21	123.96	117.70
24	A	2592	G	C6-C5-N7	-5.21	127.27	130.40
6	f	54	LEU	CB-CG-CD1	5.21	119.85	111.00
24	A	2321	U	C5-C6-N1	-5.21	120.10	122.70
24	A	2818	U	N3-C2-O2	-5.21	118.56	122.20
24	A	2248	C	C5-C6-N1	5.20	123.60	121.00
1	a	236	A	C8-N9-C4	-5.20	103.72	105.80
1	a	496	A	C2-N3-C4	5.20	113.20	110.60
25	B	57	A	C8-N9-C4	-5.20	103.72	105.80
1	a	1349	A	O5'-P-OP1	-5.20	101.03	105.70
24	A	2200	C	N1-C2-O2	5.20	122.02	118.90
24	A	992	C	C6-N1-C2	-5.19	118.22	120.30
24	A	2870	C	C5-C6-N1	5.19	123.60	121.00
24	A	2779	U	O5'-P-OP2	-5.19	101.03	105.70
1	a	1245	C	C6-N1-C2	-5.19	118.22	120.30
1	a	1142	G	N3-C2-N2	5.19	123.53	119.90
24	A	139	U	C6-N1-C2	-5.19	117.89	121.00
24	A	1725	U	N3-C2-O2	-5.19	118.57	122.20
24	A	2348	U	N3-C2-O2	-5.19	118.57	122.20
24	A	2128	G	N1-C6-O6	5.18	123.01	119.90
1	a	1497	G	C6-C5-N7	5.18	133.51	130.40
22	v	51	C	C6-N1-C2	-5.18	118.23	120.30
24	A	121	G	N9-C4-C5	-5.18	103.33	105.40
24	A	1023	U	N3-C2-O2	-5.18	118.58	122.20
24	A	1103	A	OP1-P-O3'	5.18	116.59	105.20
1	a	1190	G	OP2-P-O3'	5.17	116.58	105.20
24	A	247	G	C5-N7-C8	5.17	106.89	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	27	G	N1-C6-O6	5.17	123.00	119.90
1	a	1142	G	C6-C5-N7	-5.17	127.30	130.40
1	a	1144	G	C8-N9-C4	-5.17	104.33	106.40
24	A	543	G	C5-C6-O6	-5.17	125.50	128.60
1	a	610	U	N1-C2-O2	5.17	126.42	122.80
1	a	1203	C	O5'-P-OP2	-5.17	101.05	105.70
24	A	435	C	N3-C2-O2	-5.17	118.28	121.90
24	A	2214	C	C6-N1-C2	-5.17	118.23	120.30
2	b	18	GLN	N-CA-CB	-5.17	101.30	110.60
24	A	1455	G	C6-C5-N7	-5.16	127.30	130.40
24	A	2101	A	N7-C8-N9	5.16	116.38	113.80
24	A	1461	C	N1-C2-O2	5.16	122.00	118.90
24	A	1935	G	OP2-P-O3'	5.16	116.55	105.20
1	a	1474	U	C5-C6-N1	5.16	125.28	122.70
25	B	71	C	C6-N1-C2	-5.16	118.24	120.30
1	a	1228	C	C5-C6-N1	5.15	123.58	121.00
24	A	293	U	N3-C2-O2	-5.15	118.59	122.20
24	A	2805	C	C6-N1-C2	-5.15	118.24	120.30
24	A	2636	C	N1-C2-O2	5.15	121.99	118.90
24	A	2669	G	N3-C2-N2	-5.15	116.29	119.90
24	A	1303	G	C6-C5-N7	-5.15	127.31	130.40
1	a	1147	C	N3-C2-O2	-5.15	118.30	121.90
24	A	2297	A	C2-N3-C4	5.15	113.17	110.60
24	A	2596	U	N3-C2-O2	-5.15	118.60	122.20
24	A	908	C	C6-N1-C2	-5.14	118.24	120.30
24	A	1487	U	N3-C2-O2	-5.14	118.60	122.20
24	A	2141	G	C8-N9-C4	-5.14	104.34	106.40
24	A	2231	U	C5-C6-N1	5.14	125.27	122.70
24	A	2667	C	N1-C2-O2	5.14	121.99	118.90
22	v	56	C	C2-N1-C1'	5.14	124.45	118.80
24	A	1233	C	C6-N1-C2	-5.14	118.24	120.30
24	A	543	G	C6-C5-N7	-5.14	127.32	130.40
1	a	1486	G	N3-C4-N9	5.14	129.08	126.00
24	A	2214	C	N1-C2-O2	5.14	121.98	118.90
24	A	2720	U	N1-C2-O2	5.13	126.39	122.80
1	a	381	C	C6-N1-C2	-5.13	118.25	120.30
1	a	450	G	N9-C4-C5	5.13	107.45	105.40
24	A	1236	G	P-O3'-C3'	5.13	125.86	119.70
1	a	476	U	N3-C2-O2	-5.13	118.61	122.20
1	a	737	C	N3-C4-N4	5.13	121.59	118.00
23	x	123	C	N1-C2-O2	5.13	121.98	118.90
24	A	639	U	N1-C2-O2	5.13	126.39	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1325	C	C6-N1-C2	-5.12	118.25	120.30
24	A	51	G	C8-N9-C4	-5.12	104.35	106.40
1	a	355	C	N1-C2-O2	5.12	121.97	118.90
1	a	524	G	C6-C5-N7	-5.12	127.33	130.40
24	A	1022	G	N3-C4-N9	-5.12	122.93	126.00
24	A	1348	C	N3-C2-O2	-5.12	118.31	121.90
1	a	1382	C	N3-C2-O2	-5.12	118.31	121.90
1	a	1521	C	C6-N1-C2	-5.12	118.25	120.30
24	A	2802	G	C6-N1-C2	-5.12	122.03	125.10
24	A	1323	C	C6-N1-C2	-5.12	118.25	120.30
24	A	610	C	N1-C2-O2	5.11	121.97	118.90
24	A	2025	C	C5-C6-N1	5.11	123.56	121.00
24	A	2867	G	OP2-P-O3'	5.11	116.45	105.20
24	A	420	C	C6-N1-C2	-5.11	118.26	120.30
1	a	1259	C	N1-C2-O2	5.11	121.97	118.90
24	A	2342	C	C5-C6-N1	5.11	123.55	121.00
1	a	316	C	C6-N1-C2	-5.10	118.26	120.30
1	a	386	C	N3-C2-O2	-5.10	118.33	121.90
24	A	1695	G	N3-C4-N9	5.10	129.06	126.00
1	a	1003	G	C6-N1-C2	-5.10	122.04	125.10
22	v	51	C	N1-C2-O2	5.10	121.96	118.90
24	A	1303	G	N3-C4-N9	5.10	129.06	126.00
24	A	2065	C	C5-C6-N1	5.10	123.55	121.00
24	A	484	C	C2-N3-C4	5.09	122.45	119.90
24	A	2395	C	C6-N1-C2	-5.09	118.26	120.30
24	A	266	G	N3-C4-N9	5.09	129.06	126.00
24	A	1446	C	C6-N1-C2	-5.09	118.26	120.30
1	a	390	U	C5-C4-O4	-5.09	122.85	125.90
24	A	1053	C	C5-C6-N1	5.09	123.55	121.00
24	A	2637	U	N1-C2-O2	5.09	126.36	122.80
24	A	1376	C	N1-C2-O2	5.09	121.95	118.90
1	a	1493[A]	A	OP2-P-O3'	5.08	116.39	105.20
1	a	1493[C]	A	OP2-P-O3'	5.08	116.39	105.20
24	A	669	G	C8-N9-C4	-5.08	104.37	106.40
1	a	413	G	C6-C5-N7	5.08	133.45	130.40
1	a	1225	A	N3-C4-C5	-5.08	123.24	126.80
24	A	2774	C	N1-C2-O2	5.08	121.95	118.90
1	a	396	C	C6-N1-C2	-5.07	118.27	120.30
1	a	1235	U	C5-C4-O4	-5.07	122.86	125.90
24	A	2782	G	C4-C5-N7	5.07	112.83	110.80
24	A	1627	G	N3-C4-N9	5.07	129.04	126.00
24	A	2043	C	C6-N1-C2	-5.07	118.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1134	G	C5-C6-O6	-5.07	125.56	128.60
24	A	911	A	N7-C8-N9	5.07	116.33	113.80
22	v	28	C	N1-C2-O2	5.06	121.94	118.90
24	A	234	U	N3-C2-O2	-5.06	118.66	122.20
24	A	1629	U	N1-C2-N3	5.06	117.94	114.90
24	A	2651	C	C6-N1-C2	-5.06	118.28	120.30
24	A	717	C	C6-N1-C2	-5.06	118.28	120.30
24	A	1313	U	C5-C6-N1	5.06	125.23	122.70
1	a	496	A	C8-N9-C4	-5.06	103.78	105.80
24	A	946	C	N1-C2-O2	5.05	121.93	118.90
24	A	2755	C	N3-C2-O2	-5.05	118.36	121.90
24	A	2756	U	OP1-P-O3'	5.05	116.31	105.20
1	a	459	A	N1-C2-N3	-5.05	126.78	129.30
1	a	699	C	C6-N1-C2	-5.05	118.28	120.30
24	A	2456	C	C5-C6-N1	5.05	123.52	121.00
24	A	1931	U	C2-N1-C1'	5.05	123.75	117.70
1	a	89	U	C2-N1-C1'	5.04	123.75	117.70
1	a	1072	G	N3-C2-N2	5.04	123.43	119.90
1	a	87	C	C2-N3-C4	5.04	122.42	119.90
1	a	1473	G	N1-C6-O6	-5.04	116.88	119.90
24	A	2888	C	N1-C2-O2	5.04	121.92	118.90
36	M	20	LEU	CA-CB-CG	5.04	126.89	115.30
24	A	177	G	C8-N9-C4	-5.04	104.38	106.40
24	A	158	U	N1-C2-O2	5.04	126.33	122.80
24	A	2149	U	N1-C2-O2	5.04	126.33	122.80
24	A	2297	A	C5-C6-N1	-5.03	115.18	117.70
1	a	254	G	O5'-P-OP1	-5.03	101.17	105.70
1	a	1144	G	N7-C8-N9	5.03	115.61	113.10
24	A	512	G	O5'-P-OP2	-5.03	101.17	105.70
24	A	1314	C	N3-C4-N4	5.03	121.52	118.00
24	A	2579	C	C5-C6-N1	5.03	123.52	121.00
24	A	2782	G	C5-C6-O6	-5.03	125.58	128.60
24	A	618	G	N3-C4-C5	-5.03	126.08	128.60
24	A	2074	U	C6-N1-C2	-5.03	117.98	121.00
24	A	2177	C	C5-C6-N1	5.03	123.51	121.00
1	a	103	U	N3-C2-O2	-5.03	118.68	122.20
21	u	34	ARG	NE-CZ-NH1	5.03	122.81	120.30
24	A	2180	U	C5-C6-N1	5.02	125.21	122.70
1	a	283	U	N1-C2-O2	5.02	126.31	122.80
1	a	1184	G	C2-N3-C4	5.02	114.41	111.90
1	a	271	C	C5-C6-N1	5.02	123.51	121.00
24	A	359	G	N3-C2-N2	-5.02	116.39	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	2129	C	C6-N1-C2	-5.02	118.29	120.30
24	A	1774	C	C6-N1-C2	-5.02	118.29	120.30
24	A	2745	C	N3-C2-O2	-5.02	118.39	121.90
24	A	1169	A	C5-C6-N1	5.01	120.21	117.70
24	A	2767	C	N1-C2-O2	5.01	121.91	118.90
1	a	754	C	C6-N1-C2	-5.01	118.30	120.30
24	A	2393	U	N3-C2-O2	-5.01	118.69	122.20
24	A	2645	G	O4'-C1'-N9	5.00	112.20	108.20
24	A	2391	G	P-O3'-C3'	5.00	125.70	119.70
1	a	1356	G	N9-C4-C5	-5.00	103.40	105.40
24	A	640	C	C5-C6-N1	5.00	123.50	121.00

All (4) chirality outliers are listed below:

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

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	0	1	ALA	Mainchain,Peptide
51	1	3	GLY	Mainchain
53	3	30	HIS	Peptide
26	C	120	ASP	Peptide
28	E	82	GLY	Peptide
30	G	117	PRO	Mainchain
30	G	118	ALA	Mainchain
30	G	173	ALA	Mainchain
32	H	2	GLN	Peptide
32	H	8	LYS	Peptide
34	K	34	GLY	Peptide
34	K	89	ASN	Mainchain
34	K	92	GLU	Mainchain
35	L	110	VAL	Mainchain
35	L	28	GLY	Mainchain
35	L	29	LYS	Mainchain
35	L	35	HIS	Mainchain
42	S	64	ALA	Mainchain
44	U	50	ALA	Peptide
44	U	87	GLU	Mainchain,Peptide
48	Y	24	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain,Peptide
2	b	72	LYS	Peptide
5	e	121	ASN	Peptide
5	e	76	ASN	Peptide
5	e	88	HIS	Peptide
5	e	92	ARG	Peptide
6	f	52	ASN	Mainchain
7	g	109	LYS	Mainchain,Peptide
8	h	46	GLU	Mainchain
9	i	56	MET	Peptide
10	j	33	GLY	Peptide
10	j	56	HIS	Mainchain
10	j	57	VAL	Mainchain
10	j	91	ASP	Mainchain
10	j	92	LEU	Mainchain
12	l	100	ALA	Peptide
13	m	3	ILE	Peptide
16	p	43	ALA	Peptide
17	q	48	GLU	Mainchain
17	q	68	LYS	Peptide
18	r	10	CYS	Peptide
18	r	11	ARG	Mainchain
18	r	16	GLY	Peptide
19	s	3	SER	Peptide
21	u	8	ASN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33119	0	16685	0	0
2	b	1705	0	1732	0	0
3	c	1625	0	1699	0	0
4	d	1643	0	1710	0	0
5	e	1157	0	1199	0	0
6	f	818	0	808	0	0
7	g	1182	0	1240	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	787	0	828	0	0
11	k	870	0	878	0	0
12	l	955	0	1019	0	0
13	m	884	0	944	0	0
14	n	794	0	836	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	649	0	691	0	0
18	r	505	0	502	0	0
19	s	638	0	665	0	0
20	t	665	0	714	0	0
21	u	496	0	486	0	0
22	v	1644	0	840	0	0
23	x	1025	0	518	0	0
24	A	62296	0	31354	341	0
25	B	2570	0	1301	10	0
26	C	2083	0	2157	28	0
27	D	1565	0	1616	24	0
28	E	1552	0	1619	18	0
29	F	1411	0	1447	17	0
30	G	1323	0	1374	14	0
31	I	1032	0	1088	7	0
32	H	1111	0	1148	5	0
33	J	1129	0	1162	13	0
34	K	939	0	1012	15	0
35	L	1045	0	1117	16	0
36	M	1074	0	1157	9	0
37	N	961	0	1000	8	0
38	O	892	0	923	4	0
39	P	917	0	965	11	0
40	Q	947	0	1022	7	0
41	R	816	0	839	10	0
42	S	857	0	922	7	0
43	T	739	0	807	5	0
44	U	780	0	834	5	0
45	V	753	0	780	9	0
46	W	575	0	592	8	0
47	X	625	0	655	9	0
48	Y	509	0	543	6	0
49	Z	449	0	491	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	0	444	0	461	4	0
51	1	410	0	440	9	0
52	2	377	0	418	6	0
53	3	504	0	574	5	0
54	4	302	0	341	3	0
55	6	523	0	522	8	0
56	4	1	0	0	0	0
56	6	1	0	0	0	0
All	All	146037	0	98182	563	0

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

All (563) 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)
30:G:83:THR:HA	30:G:132:LEU:O	1.83	0.79
39:P:88:ARG:HE	39:P:112:ARG:HH21	1.32	0.76
30:G:132:LEU:HB3	30:G:140:ILE:HD11	1.69	0.74
24:A:243:U:OP2	53:3:7:ARG:NH1	2.20	0.73
39:P:59:THR:HG22	39:P:72:VAL:HG12	1.70	0.72
24:A:1646:C:H5'	24:A:1647:U:H5"	1.70	0.72
24:A:2406:A:N3	35:L:69:ARG:NH2	2.38	0.72
24:A:1171:G:N2	24:A:1178:C:O2	2.24	0.70
24:A:1466:U:HO2'	24:A:1546:G:HO2'	1.37	0.70
26:C:86:ARG:HH12	26:C:155:ARG:HH21	1.40	0.69
24:A:1601:G:OP1	43:T:64:LYS:NZ	2.25	0.69
55:6:11:GLU:HA	55:6:25:ARG:HA	1.75	0.69
24:A:1312:U:H4'	24:A:1313:U:H5'	1.75	0.69
24:A:660:C:O2'	35:L:13:LYS:NZ	2.26	0.69
24:A:2728:U:HO2'	24:A:2729:G:H8	1.42	0.68
24:A:585:G:N7	40:Q:5:ARG:NH1	2.42	0.68
52:2:12:ARG:HE	52:2:44:VAL:HG21	1.59	0.67
24:A:1568:G:H5'	26:C:59:GLN:HA	1.76	0.67
41:R:14:VAL:HG21	41:R:98:ILE:HG13	1.77	0.67
24:A:621:A:OP2	35:L:99:ASN:ND2	2.29	0.66
26:C:141:HIS:ND1	26:C:192:GLY:O	2.24	0.66
24:A:28:A:O2'	40:Q:10:ARG:NH2	2.28	0.65
45:V:48:MET:SD	45:V:51:GLN:NE2	2.69	0.65
24:A:2478:A:OP2	54:4:2:LYS:NZ	2.30	0.65
27:D:148:GLN:HB2	27:D:152:PRO:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:G:82:PHE:O	30:G:133:LYS:HA	1.97	0.64
51:1:3:GLY:O	51:1:5:ARG:N	2.29	0.64
24:A:1386:C:H2'	24:A:1387:A:C8	2.33	0.63
32:H:76:GLU:HB3	32:H:142:VAL:HG22	1.81	0.62
24:A:1064:C:O2'	24:A:1075:C:O2	2.16	0.62
24:A:2635:A:O2'	27:D:49:GLN:NE2	2.31	0.62
26:C:169:ALA:O	26:C:185:ALA:N	2.30	0.62
24:A:2512:C:O2'	27:D:159:LYS:NZ	2.32	0.61
45:V:45:ASP:O	45:V:49:ASN:ND2	2.33	0.60
24:A:877:A:O2'	24:A:900:A:N6	2.34	0.60
24:A:1273:U:O2'	24:A:1275:A:OP1	2.19	0.60
26:C:140:VAL:HG12	26:C:191:LEU:HD23	1.83	0.60
24:A:2333:A:OP2	46:W:73:ARG:NH2	2.33	0.59
24:A:1817:G:OP1	26:C:86:ARG:NH2	2.35	0.59
24:A:187:G:N2	24:A:190:A:N7	13.29	0.59
30:G:46:ASP:OD1	30:G:47:ASN:N	2.29	0.59
24:A:45:G:H5'	24:A:46:G:H5'	1.83	0.59
24:A:674:G:H2'	24:A:675:A:C8	4.86	0.59
35:L:110:VAL:HG21	35:L:127:VAL:HG22	1.85	0.58
24:A:2566:A:H61	34:K:28:SER:HB2	1.68	0.58
24:A:1342:A:O2'	24:A:1344:U:OP2	2.20	0.58
24:A:674:G:H2'	24:A:675:A:H8	4.51	0.58
24:A:1071:G:H21	24:A:1089:A:HO2'	1.52	0.58
30:G:8:VAL:HB	30:G:49:LEU:HB2	1.84	0.58
24:A:2676:C:OP1	34:K:31:ARG:NH2	2.37	0.58
24:A:833:A:H2'	24:A:834:G:C8	2.40	0.57
31:I:98:GLY:HA3	31:I:137:LEU:HD22	1.86	0.57
24:A:1140:C:OP2	33:J:68:LYS:NZ	2.37	0.57
34:K:121:GLU:HG2	34:K:122:VAL:HG23	1.86	0.57
30:G:29:ASN:ND2	30:G:80:GLU:O	2.38	0.57
24:A:320:A:N3	28:E:163:ASN:ND2	2.52	0.57
24:A:1801:A:OP2	26:C:149:LYS:NZ	2.38	0.57
24:A:270:A:N1	24:A:369:U:O2'	2.36	0.57
28:E:119:ILE:O	28:E:187:VAL:HA	2.05	0.57
24:A:1019:U:H3	24:A:1142:A:H62	1.53	0.57
24:A:547:A:O2'	24:A:548:G:N7	2.38	0.57
47:X:5:GLN:O	47:X:73:ARG:NH2	2.38	0.56
24:A:2720:U:OP1	39:P:52:ARG:NH2	2.38	0.56
24:A:600:G:OP1	28:E:24:ASN:ND2	2.37	0.56
35:L:29:LYS:HG2	35:L:30:THR:HG23	1.88	0.56
35:L:82:LEU:HD11	35:L:90:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1068:G:O2'	24:A:1070:A:N6	2.38	0.56
24:A:2140:G:H2'	24:A:2141:G:C8	2.41	0.56
24:A:1432:G:H2'	24:A:1433:A:C8	2.41	0.56
35:L:93:ASN:O	35:L:95:LEU:N	2.39	0.56
24:A:281:C:H2'	24:A:282:A:H8	1.71	0.56
24:A:668:A:H2'	24:A:670:A:H62	1.71	0.56
26:C:159:THR:HG23	26:C:176:ARG:HG2	1.87	0.56
24:A:1796:U:H2'	24:A:1797:G:H8	1.70	0.56
24:A:1124:G:O2'	54:4:37:GLN:OE1	2.23	0.55
27:D:181:ASP:HB2	27:D:186:LEU:HB2	1.88	0.55
24:A:2394:C:H5"	35:L:63:LYS:HE3	1.87	0.55
47:X:37:PHE:O	47:X:45:PHE:HA	2.07	0.55
24:A:1086:A:O2'	24:A:1103:A:N1	2.38	0.55
24:A:819:A:OP2	24:A:1187:G:N2	2.37	0.55
24:A:833:A:H2'	24:A:834:G:H8	1.71	0.55
26:C:23:LEU:HD21	26:C:82:TYR:HB2	1.89	0.55
34:K:21:CYS:HA	34:K:41:ILE:HG22	1.87	0.55
24:A:1236:G:HO2'	24:A:1237:A:H8	1.52	0.55
24:A:2327:A:H2'	24:A:2328:A:C8	2.41	0.55
24:A:598:U:H2'	24:A:599:A:H8	1.71	0.55
24:A:1798:U:OP1	26:C:269:ARG:NH2	2.40	0.55
24:A:269:C:H2'	24:A:270:A:C8	2.83	0.54
35:L:111:ILE:HD12	35:L:111:ILE:H	1.71	0.54
27:D:121:THR:HG21	27:D:143:PRO:HB3	1.89	0.54
24:A:13:A:O2'	24:A:15:G:N7	2.40	0.54
34:K:24:VAL:HG13	34:K:33:ALA:HB2	1.88	0.54
48:Y:24:GLU:HB3	48:Y:46:VAL:HG21	1.90	0.54
36:M:110:GLU:OE2	36:M:114:ARG:NH1	2.40	0.54
26:C:16:VAL:HB	26:C:203:VAL:HG22	1.90	0.54
24:A:1936:A:H2	24:A:1943:U:H3	1.54	0.53
29:F:28:PRO:HB2	29:F:168:LEU:HD22	1.89	0.53
24:A:2297:A:N1	24:A:2321:U:H5	2.06	0.53
24:A:613:A:H4'	24:A:614:A:C8	2.44	0.53
24:A:1915:3TD:H10B	24:A:1916:A:C6	2.44	0.53
29:F:43:ILE:HG21	29:F:78:ILE:HG22	1.90	0.53
24:A:2849:U:OP1	39:P:92:ARG:NH2	2.41	0.53
24:A:2359:C:O2'	53:3:53:ASP:OD2	2.24	0.53
24:A:371:A:N6	24:A:402:A:OP2	2.41	0.53
24:A:1901:A:H4'	26:C:252:LYS:HD3	1.91	0.53
41:R:2:TYR:HA	41:R:14:VAL:O	2.08	0.53
24:A:1386:C:H2'	24:A:1387:A:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1434:A:H2'	24:A:1435:G:C8	2.44	0.53
24:A:680:C:O2'	26:C:268:ARG:NH2	60.47	0.53
24:A:2318:G:O2'	24:A:2321:U:O4	2.27	0.52
27:D:25:THR:HG21	27:D:193:VAL:HG22	1.90	0.52
39:P:25:VAL:HG22	39:P:85:VAL:HG22	1.91	0.52
24:A:743:A:O2'	24:A:1659:G:OP1	2.28	0.52
24:A:1791:A:N6	24:A:1828:G:O2'	2.40	0.52
29:F:9:ASP:N	29:F:9:ASP:OD1	2.42	0.52
25:B:78:A:OP2	45:V:14:LYS:NZ	2.40	0.52
24:A:1798:U:OP2	26:C:270:ARG:NH2	2.42	0.52
55:6:37:CYS:SG	55:6:38:SER:N	2.83	0.52
32:H:32:PRO:HA	47:X:38:TRP:CD1	2.45	0.52
35:L:76:GLU:HB2	35:L:111:ILE:HD13	1.92	0.52
33:J:18:VAL:HG11	33:J:28:LEU:HD11	1.92	0.51
24:A:1405:U:H2'	24:A:1406:U:C6	2.46	0.51
24:A:2511:U:H1'	27:D:130:GLN:HE21	1.76	0.51
33:J:13:ARG:HE	33:J:121:LYS:HZ1	1.59	0.51
24:A:1045:C:H5"	24:A:1046:A:H5"	1.93	0.51
24:A:219:A:N3	24:A:234:U:O2'	2.35	0.51
24:A:1162:G:O2'	41:R:23:GLU:OE2	2.17	0.51
24:A:1912:A:H62	24:A:1917:PSU:HN3	1.59	0.51
24:A:1796:U:H2'	24:A:1797:G:C8	2.46	0.51
24:A:2120:G:H2'	24:A:2121:G:C8	2.46	0.51
26:C:131:MET:HG2	26:C:134:ILE:HD12	1.93	0.51
36:M:53:MET:HG3	36:M:116:ALA:HB1	1.93	0.51
24:A:2120:G:H2'	24:A:2121:G:H8	1.76	0.50
29:F:30:VAL:HG22	29:F:95:MET:HE1	1.92	0.50
24:A:276:U:H1'	24:A:278:A:H62	1.76	0.50
24:A:771:G:OP2	52:2:11:LYS:NZ	2.44	0.50
24:A:9:G:O2'	24:A:2800:A:N6	2.44	0.50
35:L:90:VAL:HG13	35:L:95:LEU:HD21	1.92	0.50
39:P:74:GLN:HB2	39:P:77:SER:HB2	1.94	0.50
29:F:114:ARG:HD2	55:6:47:LYS:HG2	1.93	0.50
46:W:33:ILE:HG22	46:W:34:VAL:HG23	1.92	0.50
24:A:594:U:H2'	24:A:595:C:C6	2.47	0.50
30:G:109:SER:OG	30:G:110:HIS:N	2.37	0.50
24:A:2136:G:O6	24:A:2156:G:N2	2.45	0.50
24:A:2291:U:H2'	24:A:2292:U:C6	2.47	0.50
24:A:52:A:H2'	24:A:53:A:C8	2.47	0.50
24:A:832:U:H2'	24:A:833:A:H8	1.77	0.50
26:C:145:MET:HG2	26:C:152:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2515:C:H2'	24:A:2516:A:H8	1.76	0.50
34:K:38:ILE:HD11	34:K:112:PHE:HZ	1.77	0.50
24:A:598:U:H2'	24:A:599:A:C8	2.47	0.50
38:O:40:ILE:HG12	38:O:47:VAL:HG12	1.94	0.50
24:A:1558:C:H4'	24:A:1559:U:H5"	1.92	0.49
24:A:1636:U:H2'	24:A:1637:A:H8	1.77	0.49
24:A:1779:U:H5	24:A:1784:A:N7	2.10	0.49
27:D:13:ARG:HH11	39:P:55:HIS:HA	1.77	0.49
47:X:36:ARG:HG2	47:X:45:PHE:HB3	1.94	0.49
24:A:51:G:N2	24:A:118:A:H62	2.11	0.49
30:G:43:LYS:HB2	30:G:50:THR:HB	1.93	0.49
38:O:30:ARG:HA	38:O:35:ILE:HD12	1.93	0.49
24:A:1036:G:H1	24:A:1119:U:H3	1.61	0.49
24:A:612:G:N2	24:A:614:A:O2'	2.46	0.49
24:A:583:G:P	40:Q:10:ARG:HH12	2.35	0.49
42:S:58:ALA:O	42:S:62:ASP:HB2	2.11	0.49
24:A:910:A:N3	24:A:2264:C:O2'	2.46	0.49
28:E:3:LEU:HD13	28:E:120:VAL:HG21	1.94	0.49
34:K:69:VAL:HG21	34:K:104:THR:HG21	1.93	0.49
24:A:1173:U:C4	24:A:1174:U:H1'	2.48	0.49
24:A:2362:C:OP1	53:3:39:ARG:NH1	2.35	0.49
24:A:1088:A:H61	31:I:134:SER:HB2	1.77	0.49
24:A:1869:G:N2	24:A:1872:A:OP2	2.46	0.49
24:A:269:C:H2'	24:A:270:A:H8	2.14	0.49
24:A:736:C:H2'	24:A:737:C:H6	2.09	0.49
24:A:181:A:H2'	24:A:182:A:C8	2.48	0.49
24:A:196:A:OP2	35:L:47:ARG:NH1	2.43	0.49
24:A:2537:U:H2'	24:A:2538:C:C6	2.48	0.49
24:A:371:A:O3'	47:X:60:LYS:NZ	2.44	0.49
24:A:2508:G:H1	24:A:2580:PSU:HN3	1.61	0.48
44:U:24:VAL:HA	44:U:35:VAL:HG22	1.95	0.48
46:W:19:VAL:HG22	46:W:34:VAL:HG22	1.94	0.48
24:A:500:G:N1	24:A:503:A:OP2	2.46	0.48
24:A:882:G:H1	24:A:894:U:H3	1.61	0.48
48:Y:24:GLU:O	48:Y:28:LEU:HB2	2.12	0.48
50:0:37:HIS:ND1	50:0:38:LEU:O	2.32	0.48
24:A:1071:G:N2	24:A:1089:A:HO2'	2.12	0.48
24:A:160:A:H2'	24:A:161:A:O4'	2.78	0.48
24:A:814:C:H1'	24:A:1225:G:H21	1.77	0.48
24:A:18:U:H2'	24:A:19:A:C8	2.49	0.48
30:G:1:SER:OG	30:G:2:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2328:A:H2'	24:A:2329:U:C6	2.48	0.48
24:A:736:C:H2'	24:A:737:C:C6	2.74	0.48
26:C:154:ALA:HB2	26:C:161:VAL:HG23	1.95	0.48
24:A:2071:A:H2'	24:A:2072:C:C6	2.49	0.48
24:A:582:A:H2'	24:A:583:G:H8	1.78	0.48
24:A:832:U:H2'	24:A:833:A:C8	2.49	0.48
30:G:163:TYR:HB2	30:G:166:GLU:HB2	1.96	0.48
36:M:71:LYS:HB3	36:M:93:VAL:O	2.14	0.48
24:A:1013:C:H2'	24:A:1014:A:H8	1.78	0.48
27:D:37:VAL:HG22	27:D:48:ILE:HG22	1.95	0.48
24:A:1434:A:H2'	24:A:1435:G:H8	1.78	0.48
28:E:49:ARG:HE	28:E:75:SER:HA	1.77	0.48
29:F:24:VAL:O	29:F:27:VAL:HG12	2.14	0.48
39:P:29:VAL:HG12	39:P:80:VAL:HG12	1.96	0.48
24:A:2123:G:N2	24:A:2175:C:N3	2.61	0.48
24:A:690:G:O2'	24:A:780:G:OP1	2.32	0.48
40:Q:48:ASP:HA	40:Q:51:GLN:HB2	1.95	0.48
24:A:581:C:H2'	24:A:582:A:C8	2.48	0.47
30:G:51:PHE:HZ	30:G:71:LEU:HD22	1.79	0.47
55:6:58:ASP:OD1	55:6:58:ASP:N	2.47	0.47
26:C:15:VAL:HG22	26:C:205:GLY:HA3	1.96	0.47
24:A:224:U:H2'	24:A:225:C:C6	3.82	0.47
24:A:410:G:H5"	24:A:411:G:H5'	1.95	0.47
24:A:813:U:H2'	24:A:814:C:C6	2.50	0.47
29:F:169:LEU:HB3	29:F:174:PHE:CD2	2.49	0.47
31:I:14:ALA:O	31:I:42:ASN:ND2	2.47	0.47
24:A:1509:A:H2'	24:A:1510:G:C8	2.49	0.47
24:A:2247:A:H2'	24:A:2248:C:H6	1.80	0.47
27:D:125:TRP:CD1	27:D:160:LYS:HB3	2.49	0.47
41:R:76:LYS:HG3	41:R:85:LYS:HE2	1.96	0.47
24:A:1197:G:H2'	24:A:1198:U:H6	1.79	0.47
29:F:5:ASP:O	29:F:8:LYS:N	2.47	0.47
43:T:29:THR:O	43:T:33:LYS:HB2	13.68	0.47
24:A:1062:G:H22	24:A:1088:A:H62	1.63	0.47
24:A:18:U:H2'	24:A:19:A:H8	1.78	0.47
29:F:133:GLU:HB3	29:F:135:ILE:HG13	1.97	0.47
29:F:5:ASP:OD1	29:F:6:TYR:N	2.48	0.47
39:P:21:PRO:HD3	39:P:49:ILE:HD12	1.96	0.47
24:A:1181:U:H2'	24:A:1182:G:C8	2.50	0.47
24:A:1506:U:H2'	24:A:1507:C:C6	2.50	0.47
24:A:1858:A:N6	24:A:1884:G:O2'	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2285:C:OP2	51:1:5:ARG:NH1	2.48	0.47
24:A:281:C:H2'	24:A:282:A:C8	2.48	0.47
25:B:70:C:H2'	25:B:71:C:H6	1.80	0.47
27:D:22:ILE:HG21	27:D:178:VAL:HG21	1.97	0.47
24:A:1857:G:HO2'	24:A:1858:A:H8	1.60	0.47
24:A:2554:U:H2'	24:A:2555:U:C6	2.50	0.47
24:A:1263:U:H5"	50:0:12:ARG:HD3	1.97	0.47
24:A:1509:A:H2'	24:A:1510:G:H8	1.79	0.47
46:W:29:ALA:N	46:W:60:ASP:OD1	2.48	0.47
27:D:156:PHE:CG	33:J:81:ILE:HD12	2.50	0.47
24:A:2339:C:H2'	24:A:2340:A:C8	2.50	0.46
28:E:117:ARG:NH2	28:E:183:PHE:O	2.47	0.46
24:A:1156:A:C8	40:Q:50:ARG:HD3	2.50	0.46
24:A:2051:A:H4'	27:D:146:ILE:HG12	1.96	0.46
27:D:125:TRP:CG	27:D:160:LYS:HB3	2.50	0.46
29:F:30:VAL:HG23	29:F:155:ILE:HG23	1.97	0.46
30:G:37:ASN:OD1	30:G:38:ASP:N	2.49	0.46
24:A:532:A:H5'	40:Q:27:ARG:HH12	1.79	0.46
26:C:132:ARG:O	26:C:166:ARG:NH1	2.48	0.46
28:E:47:LYS:HB2	28:E:51:GLU:HG2	1.96	0.46
24:A:1071:G:N2	24:A:1089:A:O2'	2.39	0.46
24:A:1697:G:H4'	24:A:1978:A:H5"	1.97	0.46
24:A:927:A:H2'	24:A:928:A:C8	2.50	0.46
24:A:947:A:H2'	24:A:948:C:C6	2.49	0.46
38:O:33:ARG:HG2	38:O:34:HIS:CD2	2.51	0.46
24:A:1223:G:OP1	41:R:68:ARG:NH2	2.49	0.46
24:A:783:A:H2'	24:A:784:G:H5'	1.98	0.46
24:A:856:G:H2'	24:A:857:G:C8	2.50	0.46
24:A:968:C:H2'	24:A:969:G:H8	1.80	0.46
27:D:46:ARG:HB3	27:D:84:LEU:HD12	1.97	0.46
24:A:1287:A:H5'	37:N:103:ARG:NH1	2.31	0.46
24:A:2110:G:N2	24:A:2179:C:N3	2.53	0.46
24:A:2591:C:H2'	24:A:2592:G:C8	2.51	0.46
24:A:624:C:O2'	24:A:657:U:H5"	2.16	0.46
36:M:21:ALA:HB2	36:M:97:GLN:HB2	1.98	0.46
24:A:1806:C:H1'	26:C:43:ASN:HD21	1.81	0.46
24:A:2098:U:H2'	24:A:2099:U:O4'	2.16	0.46
24:A:2271:G:H5'	46:W:16:ARG:HG2	1.98	0.46
29:F:102:LEU:O	29:F:106:ALA:HB3	2.15	0.46
24:A:1171:G:N1	24:A:1178:C:N3	2.64	0.46
24:A:1790:C:H2'	24:A:1791:A:C5	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:250:G:H2'	24:A:251:A:C8	2.51	0.46
25:B:28:C:H2'	25:B:29:A:C8	2.51	0.46
34:K:76:VAL:H	39:P:72:VAL:HG22	1.80	0.46
48:Y:17:GLU:HB2	48:Y:53:VAL:HG11	1.98	0.46
24:A:2187:U:H2'	24:A:2188:U:C6	2.51	0.46
24:A:1759:A:HO2'	24:A:2714:G:HO2'	1.64	0.46
35:L:29:LYS:O	35:L:31:GLY:N	2.49	0.46
38:O:29:HIS:HB3	38:O:36:TYR:HB2	1.98	0.46
24:A:1022:G:H22	24:A:1142:A:H2	1.65	0.45
24:A:1847:A:O2'	24:A:1848:A:H8	1.98	0.45
28:E:18:THR:HA	28:E:106:LYS:HE3	1.98	0.45
33:J:36:LEU:HD22	33:J:121:LYS:HB2	1.98	0.45
24:A:279:A:N6	24:A:361:G:H1'	2.31	0.45
24:A:608:A:H2'	24:A:609:A:C8	2.52	0.45
24:A:1569:A:H2'	24:A:1570:A:C8	2.51	0.45
24:A:2230:G:H2'	24:A:2231:U:C6	2.51	0.45
24:A:2768:U:O2'	33:J:95:ARG:NH2	2.49	0.45
24:A:581:C:H2'	24:A:582:A:H8	1.81	0.45
24:A:969:G:H2'	24:A:970:U:C6	2.52	0.45
33:J:109:LEU:HD13	33:J:118:MET:HG3	1.98	0.45
24:A:2788:C:H2'	24:A:2789:C:C6	2.51	0.45
32:H:114:GLU:HG2	32:H:134:VAL:HG12	1.98	0.45
43:T:80:TRP:CZ3	43:T:82:LYS:HB3	2.52	0.45
24:A:848:C:H2'	24:A:849:A:C8	2.51	0.45
26:C:52:HIS:O	26:C:216:ARG:N	2.45	0.45
36:M:102:LEU:HD11	36:M:126:ILE:HD11	1.99	0.45
24:A:1736:U:H2'	24:A:1737:G:O4'	2.17	0.45
24:A:28:A:N6	24:A:512:G:H1'	2.31	0.45
24:A:910:A:H2'	24:A:911:A:C8	2.51	0.45
29:F:140:ILE:HG22	29:F:142:TYR:H	1.80	0.45
24:A:126:A:H5'	52:2:19:ARG:HG3	1.97	0.45
24:A:151:C:H2'	24:A:152:A:H8	1.80	0.45
31:I:85:ILE:HD11	31:I:99:LYS:H	1.82	0.45
34:K:109:SER:O	34:K:111:LYS:N	2.50	0.45
24:A:1060:U:N3	24:A:1088:A:N7	2.56	0.45
24:A:247:G:O2'	24:A:386:G:N1	2.49	0.45
24:A:385:C:HO2'	24:A:386:G:P	2.40	0.45
51:1:8:ILE:HD13	51:1:24:LYS:HE3	1.98	0.45
24:A:1047:G:H2'	24:A:1110:G:C2	2.52	0.45
24:A:635:C:H2'	24:A:636:G:O4'	2.16	0.45
24:A:859:G:O2'	24:A:916:G:O6	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1932:A:H2'	24:A:1933:G:O4'	2.17	0.44
24:A:575:A:OP2	24:A:2055:C:N4	2.49	0.44
28:E:15:SER:HB2	28:E:18:THR:HB	1.99	0.44
47:X:38:TRP:NE1	47:X:40:GLU:OE1	2.50	0.44
52:2:12:ARG:NE	52:2:44:VAL:HG21	2.29	0.44
55:6:30:HIS:ND1	55:6:31:ASP:OD1	2.41	0.44
24:A:1433:A:H2'	24:A:1434:A:C8	2.53	0.44
24:A:715:A:H2'	24:A:716:A:C8	2.67	0.44
28:E:143:LEU:HB3	28:E:146:VAL:HG11	1.99	0.44
31:I:89:SER:HB2	31:I:135:MET:O	2.18	0.44
36:M:69:PRO:HA	36:M:94:ALA:HB2	1.98	0.44
24:A:2415:G:H2'	24:A:2416:C:C6	2.53	0.44
24:A:2655:G:O2'	24:A:2664:G:O6	2.27	0.44
24:A:482:A:N6	24:A:506:G:O2'	2.50	0.44
24:A:1802:A:H2'	24:A:1803:A:C8	2.53	0.44
24:A:2140:G:H2'	24:A:2141:G:H8	1.83	0.44
24:A:2859:G:H2'	24:A:2860:A:C8	2.53	0.44
48:Y:39:GLN:OE1	48:Y:39:GLN:N	2.50	0.44
51:1:35:LEU:HD13	51:1:37:LYS:HE2	2.00	0.44
24:A:582:A:H2'	24:A:583:G:C8	2.53	0.44
26:C:161:VAL:HG11	26:C:173:LEU:HD13	1.98	0.44
28:E:149:ILE:HD11	28:E:172:ALA:HA	1.99	0.44
44:U:52:ASN:OD1	44:U:53:GLN:N	2.51	0.44
24:A:1172:C:H2'	24:A:1173:U:C6	2.82	0.44
24:A:1723:G:H2'	24:A:1724:G:O4'	2.18	0.44
24:A:2395:C:H2'	24:A:2396:G:O4'	2.18	0.44
24:A:968:C:H2'	24:A:969:G:C8	2.53	0.44
41:R:63:VAL:HG22	41:R:96:VAL:HG12	2.00	0.44
24:A:1443:U:H2'	24:A:1444:G:H8	1.82	0.44
24:A:2015:A:C6	50:0:2:VAL:HG23	2.53	0.44
24:A:443:A:C4	28:E:40:ARG:HD3	2.53	0.44
25:B:114:C:H2'	25:B:115:A:H8	1.83	0.44
29:F:3:LEU:O	29:F:6:TYR:HB3	2.18	0.44
55:6:3:LYS:HB3	55:6:4:ASP:H	1.62	0.43
24:A:742:A:H2'	24:A:743:A:C8	2.53	0.43
24:A:871:U:H2'	24:A:872:U:C6	2.52	0.43
29:F:72:SER:OG	29:F:80:GLN:N	2.50	0.43
33:J:43:GLU:OE1	33:J:43:GLU:N	2.49	0.43
24:A:1316:U:H2'	24:A:1317:G:H8	1.83	0.43
24:A:370:G:O2'	24:A:424:G:OP1	2.36	0.43
28:E:94:GLN:OE1	28:E:94:GLN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:N:10:LEU:O	37:N:12:ARG:HG3	2.19	0.43
24:A:1289:C:H2'	24:A:1290:C:C6	2.53	0.43
24:A:2584:U:H2'	24:A:2585:U:H5"	2.00	0.43
24:A:2623:G:H2'	24:A:2624:G:H8	1.84	0.43
24:A:2699:C:H2'	24:A:2700:A:H8	1.83	0.43
24:A:588:U:H2'	24:A:589:U:C6	2.53	0.43
34:K:15:GLY:O	34:K:47:ILE:HG12	2.17	0.43
46:W:20:LYS:O	46:W:21:ARG:NH1	2.50	0.43
24:A:1412:U:H2'	24:A:1413:A:H8	1.84	0.43
24:A:1474:U:O4	24:A:1475:G:N2	2.52	0.43
24:A:2543:G:H21	24:A:2646:C:H5"	1.83	0.43
24:A:7:G:H2'	24:A:8:C:C6	2.54	0.43
54:4:16:ILE:HD13	54:4:25:VAL:HG22	2.01	0.43
24:A:2324:U:H5"	24:A:2325:G:H5"	2.01	0.43
24:A:2347:C:H2'	24:A:2348:U:C6	2.53	0.43
24:A:304:U:H2'	24:A:305:C:C6	2.53	0.43
33:J:49:ASP:HB2	33:J:114:LEU:HD11	2.00	0.43
42:S:4:ILE:HG22	42:S:106:VAL:HG22	2.01	0.43
24:A:2411:A:H2'	24:A:2412:A:C8	2.54	0.43
24:A:2557:G:H2'	24:A:2558:C:C6	2.53	0.43
24:A:287:G:H2'	24:A:288:U:C6	2.53	0.43
25:B:105:G:H2'	25:B:106:G:H8	1.84	0.43
24:A:2830:C:H5"	27:D:56:LYS:NZ	2.34	0.43
31:I:34:ILE:HA	31:I:37:PHE:HD2	1.84	0.43
53:3:22:LYS:HA	53:3:47:ALA:O	2.18	0.43
24:A:483:A:C8	44:U:44:HIS:HD2	2.37	0.43
24:A:566:U:H5"	35:L:29:LYS:HE3	2.01	0.43
24:A:1138:G:N2	33:J:108:MET:SD	2.77	0.43
24:A:1353:A:H2'	24:A:1354:A:C8	2.53	0.43
24:A:1412:U:H2'	24:A:1413:A:C8	2.54	0.43
24:A:1478:G:H1	24:A:1513:U:H3	1.66	0.43
24:A:2074:U:H2'	24:A:2075:U:C6	2.54	0.43
24:A:2485:G:H5"	36:M:45:GLN:HE21	1.84	0.43
24:A:2784:U:H2'	24:A:2785:C:H6	1.84	0.43
24:A:319:G:H22	24:A:323:C:H5	1.65	0.43
24:A:364:C:H2'	24:A:365:U:C6	2.53	0.43
34:K:21:CYS:SG	34:K:22:ILE:N	2.91	0.43
24:A:771:G:OP1	52:2:14:ARG:NH2	2.52	0.43
24:A:1082:U:O2	24:A:1086:A:N6	2.52	0.43
24:A:1184:U:OP2	49:Z:30:ARG:NH1	2.52	0.43
24:A:1258:U:H2'	24:A:1259:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1264:A:H5'	50:0:7:PRO:HG2	2.00	0.43
24:A:308:G:H2'	24:A:309:A:C8	2.54	0.43
24:A:1248:G:P	28:E:44:ARG:HH12	2.42	0.43
33:J:68:LYS:HZ3	33:J:72:LYS:HD2	1.83	0.43
33:J:95:ARG:HG2	33:J:96:ARG:HG2	2.00	0.43
44:U:3:LYS:O	44:U:93:ARG:NH2	2.48	0.43
45:V:9:ARG:HG2	45:V:41:GLU:HB2	2.00	0.43
48:Y:21:LEU:HA	48:Y:25:GLN:HB3	2.00	0.43
24:A:1326:U:O2'	24:A:2010:G:O2'	2.34	0.43
24:A:2033:A:O2'	24:A:2035:G:OP2	2.31	0.43
37:N:78:LYS:O	37:N:82:GLU:HB2	2.19	0.43
55:6:44:PHE:CD1	55:6:45:THR:HG23	2.53	0.42
24:A:1437:C:HO2'	24:A:1516:G:HO2'	1.62	0.42
24:A:1683:U:H2'	24:A:1684:G:C8	2.53	0.42
24:A:1704:C:H2'	24:A:1705:A:C8	2.54	0.42
24:A:2513:A:H2'	24:A:2514:U:C6	2.54	0.42
24:A:848:C:H2'	24:A:849:A:H8	1.84	0.42
26:C:242:HIS:HA	26:C:243:PRO:HD3	1.90	0.42
42:S:44:ALA:HA	42:S:47:VAL:HG12	2.01	0.42
24:A:1679:A:H2'	24:A:1680:U:H6	1.84	0.42
24:A:1693:U:OP2	24:A:1694:C:N4	2.48	0.42
24:A:172:A:H2'	24:A:173:A:H8	1.84	0.42
24:A:2800:A:C2	24:A:2895:G:H1'	2.54	0.42
24:A:560:C:O2'	40:Q:47:ARG:NH2	2.49	0.42
34:K:35:VAL:HG13	34:K:69:VAL:HG11	2.00	0.42
37:N:45:ARG:HG2	37:N:95:THR:HG21	1.99	0.42
45:V:32:GLY:H	45:V:93:ARG:HH21	1.67	0.42
24:A:1443:U:H2'	24:A:1444:G:C8	2.55	0.42
24:A:2861:U:H2'	24:A:2862:G:H8	1.84	0.42
27:D:131:ASP:O	27:D:136:ASN:ND2	2.52	0.42
36:M:74:THR:HA	36:M:89:VAL:HA	2.01	0.42
41:R:77:PHE:HD1	41:R:84:ARG:HB3	1.85	0.42
47:X:34:SER:HA	47:X:48:LEU:O	2.18	0.42
24:A:1636:U:H2'	24:A:1637:A:C8	2.54	0.42
27:D:48:ILE:O	27:D:81:GLU:HA	2.19	0.42
28:E:3:LEU:HD21	28:E:19:PHE:HE2	1.85	0.42
41:R:49:ILE:HD12	41:R:52:PRO:HA	2.01	0.42
42:S:41:LYS:H	42:S:41:LYS:HG2	1.63	0.42
47:X:36:ARG:HG3	47:X:47:THR:OG1	2.19	0.42
24:A:2627:G:O2'	24:A:2781:A:N1	2.43	0.42
24:A:739:A:H1'	24:A:740:C:H5	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:4:ILE:H	51:1:4:ILE:HG13	1.61	0.42
24:A:172:A:H2'	24:A:173:A:C8	2.55	0.42
24:A:2233:U:H2'	24:A:2234:G:C8	2.54	0.42
24:A:2446:G:H2'	24:A:2447:G:H5"	2.01	0.42
24:A:306:U:H2'	24:A:307:G:O4'	2.19	0.42
24:A:639:U:H2'	24:A:640:C:C6	2.55	0.42
25:B:30:C:H2'	25:B:31:C:H5'	2.02	0.42
27:D:84:LEU:HD23	27:D:84:LEU:HA	1.85	0.42
24:A:2684:U:O4'	34:K:70:ARG:NH1	2.53	0.42
24:A:1410:G:H2'	24:A:1411:U:H6	1.83	0.42
24:A:1837:C:H2'	24:A:1899:A:H61	1.84	0.42
24:A:549:G:H2'	24:A:550:C:C6	2.54	0.42
28:E:143:LEU:HD13	28:E:146:VAL:HG11	2.01	0.42
37:N:30:ARG:HG2	37:N:31:HIS:CD2	2.55	0.42
24:A:1371:G:H2'	24:A:1372:U:C6	3.16	0.42
24:A:619:G:OP2	24:A:620:G:N2	2.50	0.42
25:B:35:C:H2'	25:B:36:C:O4'	2.19	0.42
27:D:13:ARG:HA	27:D:22:ILE:O	2.19	0.42
53:3:31:ILE:O	53:3:35:LYS:NZ	2.33	0.42
24:A:1199:U:H2'	24:A:1200:C:C6	2.54	0.42
24:A:144:A:H2'	24:A:145:C:C6	2.55	0.42
24:A:1683:U:H2'	24:A:1684:G:H8	1.84	0.42
24:A:2164:C:H41	24:A:2171:A:H61	1.68	0.42
24:A:2124:G:O6	24:A:2174:C:N4	2.53	0.42
24:A:2696:U:H2'	24:A:2697:G:C8	2.55	0.42
24:A:527:C:C4	24:A:2779:U:H2'	2.54	0.42
28:E:189:THR:HG22	28:E:191:ASP:H	1.85	0.42
24:A:2303:G:O2'	29:F:120:SER:O	2.30	0.42
24:A:1669:A:O3'	24:A:2549:G:H5'	2.19	0.42
32:H:11:ASN:CG	32:H:12:LEU:H	2.23	0.42
35:L:82:LEU:HD21	35:L:120:VAL:HG11	2.02	0.42
37:N:103:ARG:NH2	37:N:110:MET:SD	2.93	0.42
45:V:31:TYR:HB3	45:V:37:PRO:HB3	2.02	0.42
24:A:372:G:P	47:X:60:LYS:HZ1	2.42	0.42
55:6:20:ASN:HD22	55:6:39:LYS:HE2	1.84	0.41
24:A:1424:G:H2'	24:A:1425:G:O4'	2.20	0.41
24:A:1478:G:N2	24:A:1513:U:O2	2.38	0.41
24:A:1794:A:H2'	24:A:1795:C:C6	2.55	0.41
24:A:692:C:H2'	24:A:693:A:C8	2.55	0.41
25:B:5:U:H2'	25:B:6:G:H8	1.86	0.41
25:B:93:C:H2'	25:B:94:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D:51:THR:HG21	27:D:68:PHE:HE1	1.85	0.41
41:R:76:LYS:HB2	41:R:85:LYS:HB3	2.02	0.41
24:A:1197:G:H2'	24:A:1198:U:C6	2.55	0.41
24:A:2394:C:OP1	35:L:63:LYS:HG2	2.20	0.41
24:A:415:A:H2'	24:A:416:U:C6	2.55	0.41
24:A:438:G:H2'	24:A:439:A:C8	2.54	0.41
24:A:660:C:OP1	28:E:94:GLN:HB2	2.21	0.41
26:C:86:ARG:NH1	26:C:155:ARG:HH21	2.14	0.41
24:A:280:U:H2'	24:A:281:C:C6	2.55	0.41
24:A:574:A:H2	27:D:150:GLN:HE22	1.68	0.41
42:S:72:THR:OG1	42:S:73:LYS:N	2.53	0.41
24:A:1857:G:N2	24:A:1884:G:H2'	2.36	0.41
24:A:2039:U:H2'	24:A:2040:G:C8	2.55	0.41
24:A:2233:U:H2'	24:A:2234:G:H8	1.86	0.41
24:A:2246:G:H2'	24:A:2247:A:C8	2.55	0.41
24:A:458:G:O2'	24:A:469:G:O6	2.37	0.41
32:H:108:VAL:HG12	32:H:110:VAL:H	1.85	0.41
31:I:12:VAL:HG11	31:I:22:PRO:HB2	2.01	0.41
37:N:55:ALA:HA	37:N:80:PHE:CE1	2.55	0.41
41:R:11:GLN:OE1	41:R:11:GLN:N	2.53	0.41
24:A:184:C:H2'	24:A:185:G:C8	2.56	0.41
24:A:794:A:H2'	24:A:795:C:C6	2.56	0.41
29:F:28:PRO:HB3	29:F:159:ALA:HB2	2.02	0.41
45:V:72:VAL:HG12	45:V:93:ARG:HA	2.02	0.41
24:A:499:U:H5"	44:U:42:LYS:HE2	2.03	0.41
24:A:310:A:O2'	24:A:311:A:H2'	2.20	0.41
25:B:30:C:H1'	25:B:57:A:H61	1.85	0.41
43:T:44:LYS:HG3	43:T:55:VAL:HG11	2.01	0.41
24:A:545:U:O2	24:A:548:G:N2	2.46	0.41
24:A:814:C:H1'	24:A:1225:G:N2	2.36	0.41
24:A:1824:G:H5"	26:C:51:ARG:HH21	1.86	0.41
34:K:25:LEU:HD12	34:K:38:ILE:HG22	2.03	0.41
34:K:68:GLY:HA2	34:K:77:ILE:O	2.21	0.41
24:A:1028:A:N3	24:A:2486:C:O2'	2.46	0.41
24:A:1993:U:H4'	27:D:133:THR:CG2	2.51	0.41
24:A:2843:G:H2'	24:A:2844:G:O4'	2.21	0.41
26:C:180:MET:HB2	26:C:268:ARG:H	1.86	0.41
36:M:48:ALA:O	36:M:52:ALA:HB2	2.20	0.41
24:A:2064:C:H2'	24:A:2065:C:C6	2.56	0.41
27:D:16:THR:OG1	27:D:20:VAL:O	2.35	0.41
42:S:17:VAL:HA	42:S:43:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2285:C:P	51:1:25:ASN:HD22	2.44	0.41
52:2:13:ASN:O	52:2:17:GLY:HA3	2.21	0.41
24:A:1057:A:N6	24:A:1080:A:H61	2.19	0.41
24:A:1062:G:H22	24:A:1088:A:N6	2.19	0.41
24:A:120:U:H4'	24:A:121:G:H5"	2.03	0.41
24:A:2284:A:HO2'	24:A:2288:A:N6	2.19	0.41
24:A:2476:A:H2	24:A:2481:G:H1	1.67	0.41
24:A:39:G:H2'	24:A:40:U:C6	2.56	0.41
24:A:655:A:H4'	24:A:656:G:H5'	2.02	0.41
26:C:35:LYS:HB2	26:C:35:LYS:HE3	1.82	0.41
30:G:2:ARG:HA	30:G:2:ARG:HD3	4.70	0.41
33:J:17:VAL:HG23	33:J:137:PRO:HB2	2.02	0.41
45:V:72:VAL:HG21	45:V:91:PHE:HB3	2.02	0.41
46:W:15:LYS:HB2	46:W:37:ARG:HH22	1.86	0.41
24:A:1278:C:H2'	24:A:1279:G:H8	1.87	0.40
24:A:1715:G:HO2'	24:A:1716:U:H6	1.64	0.40
24:A:1972:G:H2'	24:A:1973:G:H8	1.86	0.40
24:A:2183:A:H2'	24:A:2184:A:C8	2.56	0.40
24:A:558:U:H2'	24:A:559:G:C8	2.56	0.40
24:A:720:U:H2'	24:A:721:A:C8	2.56	0.40
24:A:1361:G:H2'	24:A:1362:C:C6	2.57	0.40
24:A:1538:G:H2'	24:A:1539:U:C6	2.56	0.40
24:A:2141:G:H2'	24:A:2142:A:H8	1.86	0.40
51:1:5:ARG:NH1	51:1:25:ASN:HB2	2.36	0.40
24:A:973:A:H5'	24:A:1188:U:H1'	2.03	0.40
24:A:1295:C:H2'	24:A:1296:G:H8	1.87	0.40
24:A:2163:A:H2'	24:A:2164:C:H5'	2.02	0.40
24:A:2267:A:H5"	24:A:2268:A:H5"	2.02	0.40
24:A:953:G:H2'	24:A:954:G:O4'	2.90	0.40
30:G:154:GLU:O	30:G:158:GLY:N	2.54	0.40
24:A:1277:G:H4'	37:N:20:MET:HE3	2.03	0.40
42:S:77:ASP:N	42:S:77:ASP:OD1	2.38	0.40
46:W:42:HIS:NE2	46:W:73:ARG:HD3	2.37	0.40
51:1:10:LEU:HD23	51:1:50:GLU:HA	2.02	0.40
24:A:643:A:H1'	51:1:43:ARG:NH2	2.37	0.40
24:A:1289:C:H2'	24:A:1290:C:H6	1.86	0.40
24:A:1316:U:H2'	24:A:1317:G:C8	2.57	0.40
24:A:1656:C:H2'	24:A:1657:U:H6	1.86	0.40
24:A:2215:C:H2'	24:A:2216:G:H8	1.87	0.40
24:A:2819:G:H2'	24:A:2821:A:N7	2.36	0.40
24:A:138:U:C4	43:T:3:ARG:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:V:64:VAL:HA	45:V:68:LYS:O	2.21	0.40
48:Y:56:LEU:HA	48:Y:56:LEU:HD23	1.89	0.40
24:A:385:C:HO2'	24:A:388:G:H22	1.69	0.40
24:A:729:G:C5	26:C:206:LYS:HB2	2.56	0.40
39:P:91:VAL:HG21	39:P:96:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/218 (99%)	189 (88%)	23 (11%)	4 (2%)	10	53
3	c	204/206 (99%)	190 (93%)	13 (6%)	1 (0%)	34	77
4	d	203/205 (99%)	187 (92%)	14 (7%)	2 (1%)	19	66
5	e	155/157 (99%)	134 (86%)	16 (10%)	5 (3%)	5	42
6	f	98/100 (98%)	82 (84%)	10 (10%)	6 (6%)	2	24
7	g	149/151 (99%)	135 (91%)	11 (7%)	3 (2%)	9	53
8	h	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	24	69
9	i	125/127 (98%)	104 (83%)	15 (12%)	6 (5%)	3	30
10	j	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3	33
11	k	114/116 (98%)	100 (88%)	11 (10%)	3 (3%)	7	46
12	l	121/123 (98%)	98 (81%)	14 (12%)	9 (7%)	1	18
13	m	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	6	46
14	n	98/100 (98%)	83 (85%)	13 (13%)	2 (2%)	9	53
15	o	86/88 (98%)	73 (85%)	11 (13%)	2 (2%)	8	50
16	p	80/82 (98%)	71 (89%)	6 (8%)	3 (4%)	4	37
17	q	78/80 (98%)	66 (85%)	10 (13%)	2 (3%)	7	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	r	63/65 (97%)	57 (90%)	2 (3%)	4 (6%)	2 23
19	s	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	15 60
20	t	83/85 (98%)	77 (93%)	6 (7%)	0	100 100
21	u	63/65 (97%)	50 (79%)	9 (14%)	4 (6%)	2 23
26	C	269/271 (99%)	246 (91%)	20 (7%)	3 (1%)	17 64
27	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	34 77
28	E	199/201 (99%)	184 (92%)	12 (6%)	3 (2%)	13 57
29	F	175/177 (99%)	158 (90%)	13 (7%)	4 (2%)	8 50
30	G	174/176 (99%)	157 (90%)	11 (6%)	6 (3%)	5 41
31	I	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	8 51
32	H	147/149 (99%)	129 (88%)	14 (10%)	4 (3%)	6 46
33	J	140/142 (99%)	136 (97%)	4 (3%)	0	100 100
34	K	120/122 (98%)	105 (88%)	10 (8%)	5 (4%)	3 33
35	L	141/143 (99%)	129 (92%)	9 (6%)	3 (2%)	9 52
36	M	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	8 51
37	N	118/120 (98%)	106 (90%)	12 (10%)	0	100 100
38	O	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	11 54
39	P	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	21 67
40	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100 100
41	R	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	9 53
42	S	108/110 (98%)	102 (94%)	6 (6%)	0	100 100
43	T	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	5 41
44	U	100/102 (98%)	89 (89%)	6 (6%)	5 (5%)	3 29
45	V	92/94 (98%)	90 (98%)	2 (2%)	0	100 100
46	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	14 59
47	X	75/77 (97%)	71 (95%)	4 (5%)	0	100 100
48	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100 100
49	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100 100
50	0	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	10 53
51	1	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	9 52
52	2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	12 56
54	4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	6 45
55	6	64/66 (97%)	59 (92%)	4 (6%)	1 (2%)	12 56
All	All	5717/5817 (98%)	5150 (90%)	447 (8%)	120 (2%)	13 52

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	17	HIS
2	b	18	GLN
2	b	73	ARG
4	d	192	ALA
5	e	77	ASN
5	e	89	THR
5	e	122	VAL
5	e	158	LYS
6	f	53	LYS
6	f	54	LEU
6	f	86	ARG
7	g	110	ARG
8	h	47	ASP
9	i	90	ASP
10	j	34	ALA
10	j	57	VAL
10	j	92	LEU
11	k	92	ARG
12	l	101	LEU
13	m	65	GLU
15	o	46	LYS
16	p	44	SER
16	p	79	ASN
17	q	49	ASN
17	q	69	THR
18	r	11	ARG
18	r	17	VAL
19	s	4	LEU
21	u	8	ASN
21	u	34	ARG
21	u	37	TYR
26	C	121	ALA
26	C	204	LEU

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Mol	Chain	Res	Type
28	E	83	VAL
29	F	174	PHE
30	G	46	ASP
30	G	108	PHE
30	G	118	ALA
30	G	174	LYS
32	H	9	VAL
34	K	92	GLU
35	L	29	LYS
35	L	36	LYS
35	L	111	ILE
38	O	63	LYS
44	U	6	ARG
44	U	51	LEU
44	U	88	ASP
50	0	2	VAL
51	1	4	ILE
53	3	31	ILE
5	e	93	VAL
7	g	29	LEU
7	g	95	ARG
9	i	57	VAL
9	i	125	GLN
10	j	42	LEU
11	k	88	PRO
12	l	75	GLU
13	m	4	ALA
13	m	6	ILE
14	n	2	LYS
29	F	20	ASN
30	G	45	ALA
32	H	3	VAL
32	H	11	ASN
32	H	41	LYS
34	K	35	VAL
34	K	110	GLU
36	M	58	LYS
36	M	70	ASP
41	R	54	VAL
41	R	55	ASP
43	T	38	ALA
43	T	52	GLU

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Mol	Chain	Res	Type
55	6	3	LYS
9	i	12	LYS
9	i	122	ARG
14	n	34	ASN
16	p	43	ALA
18	r	18	GLN
26	C	52	HIS
27	D	149	ASN
28	E	184	ASP
31	I	22	PRO
36	M	14	LYS
43	T	88	LYS
44	U	39	ASN
46	W	17	LEU
54	4	37	GLN
3	c	96	VAL
4	d	191	SER
6	f	92	THR
6	f	99	ALA
12	l	2	THR
12	l	23	LEU
12	l	45	ASN
12	l	46	SER
12	l	77	SER
12	l	88	ASP
15	o	27	GLN
18	r	46	THR
21	u	65	ARG
29	F	149	ARG
29	F	176	PHE
34	K	109	SER
6	f	93	LYS
28	E	122	GLU
30	G	109	SER
31	I	20	SER
38	O	34	HIS
39	P	86	LYS
52	2	23	ALA
34	K	93	GLN
9	i	71	ILE
44	U	54	PRO
11	k	90	PRO

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Mol	Chain	Res	Type
12	l	41	PRO
2	b	28	PRO
31	I	92	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	b	180/180 (100%)	178 (99%)	2 (1%)	80 92
3	c	170/170 (100%)	170 (100%)	0	100 100
4	d	172/172 (100%)	171 (99%)	1 (1%)	90 97
5	e	119/119 (100%)	119 (100%)	0	100 100
6	f	87/87 (100%)	87 (100%)	0	100 100
7	g	124/124 (100%)	124 (100%)	0	100 100
8	h	104/104 (100%)	104 (100%)	0	100 100
9	i	105/105 (100%)	105 (100%)	0	100 100
10	j	86/86 (100%)	86 (100%)	0	100 100
11	k	89/89 (100%)	89 (100%)	0	100 100
12	l	103/103 (100%)	102 (99%)	1 (1%)	82 93
13	m	92/92 (100%)	92 (100%)	0	100 100
14	n	79/83 (95%)	78 (99%)	1 (1%)	76 91
15	o	76/76 (100%)	76 (100%)	0	100 100
16	p	65/65 (100%)	64 (98%)	1 (2%)	72 90
17	q	74/74 (100%)	74 (100%)	0	100 100
18	r	48/56 (86%)	48 (100%)	0	100 100
19	s	70/70 (100%)	70 (100%)	0	100 100
20	t	65/65 (100%)	65 (100%)	0	100 100
21	u	44/55 (80%)	44 (100%)	0	100 100
26	C	216/216 (100%)	215 (100%)	1 (0%)	92 97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	D	164/164 (100%)	164 (100%)	0	100	100
28	E	165/165 (100%)	165 (100%)	0	100	100
29	F	148/148 (100%)	148 (100%)	0	100	100
30	G	137/137 (100%)	137 (100%)	0	100	100
31	I	109/109 (100%)	109 (100%)	0	100	100
32	H	114/114 (100%)	114 (100%)	0	100	100
33	J	116/116 (100%)	116 (100%)	0	100	100
34	K	103/103 (100%)	102 (99%)	1 (1%)	82	93
35	L	102/102 (100%)	101 (99%)	1 (1%)	82	93
36	M	109/109 (100%)	109 (100%)	0	100	100
37	N	100/100 (100%)	100 (100%)	0	100	100
38	O	86/86 (100%)	86 (100%)	0	100	100
39	P	99/99 (100%)	99 (100%)	0	100	100
40	Q	89/89 (100%)	89 (100%)	0	100	100
41	R	84/84 (100%)	84 (100%)	0	100	100
42	S	93/93 (100%)	93 (100%)	0	100	100
43	T	80/80 (100%)	80 (100%)	0	100	100
44	U	83/83 (100%)	83 (100%)	0	100	100
45	V	78/78 (100%)	78 (100%)	0	100	100
46	W	57/57 (100%)	57 (100%)	0	100	100
47	X	67/67 (100%)	66 (98%)	1 (2%)	72	90
48	Y	55/55 (100%)	55 (100%)	0	100	100
49	Z	48/48 (100%)	48 (100%)	0	100	100
50	0	47/47 (100%)	46 (98%)	1 (2%)	61	87
51	1	45/45 (100%)	45 (100%)	0	100	100
52	2	38/38 (100%)	38 (100%)	0	100	100
53	3	51/51 (100%)	51 (100%)	0	100	100
54	4	34/34 (100%)	34 (100%)	0	100	100
55	6	59/59 (100%)	59 (100%)	0	100	100
All	All	4728/4751 (100%)	4717 (100%)	11 (0%)	95	99

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	176	ASN
2	b	178	LEU
4	d	173	ASP
12	l	33	CYS
14	n	34	ASN
16	p	2	VAL
26	C	52	HIS
34	K	21	CYS
35	L	27	LEU
47	X	4	CYS
50	0	2	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	40	GLN
3	c	122	GLN
8	h	20	ASN
9	i	31	GLN
12	l	72	ASN
16	p	26	ASN
20	t	12	GLN
26	C	44	ASN
27	D	49	GLN
30	G	21	GLN
35	L	38	GLN
35	L	99	ASN
37	N	62	ASN
37	N	81	ASN
44	U	39	ASN
54	4	35	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1531/1539 (99%)	260 (16%)	0
22	v	76/77 (98%)	15 (19%)	0
23	x	47/48 (97%)	21 (44%)	0
24	A	2893/2903 (99%)	540 (18%)	34 (1%)
25	B	119/120 (99%)	17 (14%)	3 (2%)
All	All	4666/4687 (99%)	853 (18%)	37 (0%)

All (853) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	44	A
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	59	A
1	a	61	G
1	a	69	G
1	a	71	A
1	a	79	G
1	a	81	A
1	a	82	G
1	a	83	C
1	a	85	U
1	a	86	G
1	a	88	U
1	a	92	U
1	a	94	G
1	a	95	C
1	a	116	A
1	a	121	U
1	a	122	G
1	a	126	G
1	a	127	G
1	a	128	G
1	a	131	A
1	a	134	G
1	a	141	G
1	a	144	G
1	a	149	A
1	a	173	U
1	a	183	C
1	a	184	G
1	a	189	A
1	a	195	A
1	a	197	A

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Mol	Chain	Res	Type
1	a	207	C
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	280	C
1	a	281	G
1	a	289	G
1	a	300	A
1	a	306	A
1	a	316	C
1	a	328	C
1	a	329	A
1	a	330	C
1	a	345	C
1	a	347	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	369	G
1	a	372	C
1	a	373	A
1	a	376	G
1	a	388	G
1	a	398	U
1	a	406	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	429	U
1	a	439	U
1	a	441	A
1	a	446	G

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Mol	Chain	Res	Type
1	a	448	A
1	a	467	U
1	a	468	A
1	a	474	G
1	a	479	U
1	a	481	G
1	a	482	A
1	a	486	U
1	a	496	A
1	a	497	G
1	a	499	A
1	a	505	G
1	a	509	A
1	a	511	C
1	a	518	C
1	a	521	G
1	a	527	G7M
1	a	528	C
1	a	529	G
1	a	531	U
1	a	532	A
1	a	547	A
1	a	548	G
1	a	559	A
1	a	562	U
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	615	G
1	a	633	G
1	a	639	G
1	a	653	U
1	a	654	G
1	a	665	A
1	a	687	A
1	a	695	A
1	a	701	U
1	a	702	A
1	a	713	G
1	a	718	A
1	a	723	U

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Mol	Chain	Res	Type
1	a	724	G
1	a	731	G
1	a	733	G
1	a	777	A
1	a	787	A
1	a	792	A
1	a	793	U
1	a	794	A
1	a	802	A
1	a	810	C
1	a	815	A
1	a	817	C
1	a	818	G
1	a	820	U
1	a	821	G
1	a	832	G
1	a	836	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	849	G
1	a	872	A
1	a	890	G
1	a	891	U
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	967	5MC
1	a	968	A
1	a	969	A
1	a	971	G
1	a	975	A
1	a	976	G
1	a	977	A
1	a	983	A
1	a	989	U

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Mol	Chain	Res	Type
1	a	991	U
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	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1036	A
1	a	1042	A
1	a	1050	G
1	a	1053	G
1	a	1054	C
1	a	1066	C
1	a	1070	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1100	C
1	a	1101	A
1	a	1130	A
1	a	1133	G
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1145	A
1	a	1146	A
1	a	1151	A
1	a	1152	A
1	a	1158	C
1	a	1159	U
1	a	1168	U
1	a	1182	G
1	a	1183	U
1	a	1191	A
1	a	1196	A
1	a	1212	U

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Mol	Chain	Res	Type
1	a	1213	A
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1236	A
1	a	1238	A
1	a	1239	A
1	a	1240	U
1	a	1241	G
1	a	1253	G
1	a	1258	G
1	a	1260	G
1	a	1280	A
1	a	1281	C
1	a	1287	A
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1303	C
1	a	1305	G
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1332	A
1	a	1353	G
1	a	1360	A
1	a	1363	A
1	a	1364	U
1	a	1394	A
1	a	1398	A
1	a	1419	G
1	a	1422	G
1	a	1429	A
1	a	1433	A
1	a	1440	U
1	a	1441	A
1	a	1446	A
1	a	1452	C
1	a	1499	A
1	a	1503	A
1	a	1506	U

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Mol	Chain	Res	Type
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1537	U
22	v	9	G
22	v	14	A
22	v	16	C
22	v	17	C
22	v	17(A)	U
22	v	18	G
22	v	19	G
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	47	U
22	v	48	C
22	v	58	A
22	v	75	C
22	v	76	A
23	x	88	A
23	x	90	G
23	x	91	A
23	x	93	G
23	x	96	C
23	x	98	U
23	x	99	U
23	x	104	U
23	x	109	C
23	x	110	G
23	x	113	C
23	x	115	A
23	x	117	C
23	x	118	G
23	x	120	U
23	x	121	U
23	x	126	G
23	x	127	U
23	x	129	U

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Mol	Chain	Res	Type
23	x	130	G
23	x	134	C
24	A	10	A
24	A	14	A
24	A	34	U
24	A	35	G
24	A	43	G
24	A	45	G
24	A	46	G
24	A	50	U
24	A	51	G
24	A	52	A
24	A	63	A
24	A	71	A
24	A	73	A
24	A	74	A
24	A	75	G
24	A	84	A
24	A	92	U
24	A	96	C
24	A	98	G
24	A	102	U
24	A	103	A
24	A	114	U
24	A	118	A
24	A	119	A
24	A	120	U
24	A	131	A
24	A	138	U
24	A	139	U
24	A	141	G
24	A	142	A
24	A	161	A
24	A	162	U
24	A	163	C
24	A	165	A
24	A	178	G
24	A	196	A
24	A	204	A
24	A	205	G
24	A	206	U
24	A	215	G

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Mol	Chain	Res	Type
24	A	216	A
24	A	221	A
24	A	222	A
24	A	228	C
24	A	229	C
24	A	241	A
24	A	245	G
24	A	247	G
24	A	248	G
24	A	250	G
24	A	255	A
24	A	266	G
24	A	276	U
24	A	277	G
24	A	278	A
24	A	281	C
24	A	282	A
24	A	285	G
24	A	294	A
24	A	295	G
24	A	310	A
24	A	317	G
24	A	322	A
24	A	323	C
24	A	329	G
24	A	330	A
24	A	346	A
24	A	349	U
24	A	359	G
24	A	361	G
24	A	362	A
24	A	371	A
24	A	372	G
24	A	373	U
24	A	386	G
24	A	387	U
24	A	404	A
24	A	406	G
24	A	411	G
24	A	412	A
24	A	424	G
24	A	456	C

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Mol	Chain	Res	Type
24	A	457	A
24	A	481	G
24	A	490	C
24	A	491	G
24	A	496	G
24	A	504	A
24	A	505	A
24	A	509	C
24	A	510	C
24	A	513	A
24	A	522	A
24	A	527	C
24	A	529	A
24	A	531	C
24	A	532	A
24	A	533	G
24	A	544	C
24	A	545	U
24	A	549	G
24	A	556	A
24	A	563	A
24	A	573	U
24	A	575	A
24	A	588	U
24	A	592	A
24	A	603	A
24	A	613	A
24	A	614	A
24	A	627	A
24	A	632	A
24	A	637	A
24	A	645	C
24	A	646	U
24	A	647	G
24	A	654	A
24	A	655	A
24	A	656	G
24	A	669	G
24	A	677	A
24	A	686	U
24	A	690	G
24	A	694	U

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Mol	Chain	Res	Type
24	A	695	G
24	A	699	A
24	A	714	U
24	A	729	G
24	A	730	A
24	A	746	PSU
24	A	747	5MU
24	A	752	A
24	A	764	A
24	A	774	G
24	A	775	G
24	A	776	G
24	A	782	A
24	A	784	G
24	A	785	G
24	A	805	G
24	A	812	C
24	A	819	A
24	A	827	U
24	A	828	U
24	A	844	A
24	A	845	A
24	A	846	U
24	A	858	G
24	A	859	G
24	A	869	G
24	A	878	A
24	A	884	U
24	A	886	A
24	A	892	A
24	A	896	A
24	A	897	C
24	A	910	A
24	A	941	A
24	A	944	C
24	A	945	A
24	A	946	C
24	A	961	C
24	A	962	G
24	A	974	G
24	A	983	A
24	A	985	C

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Mol	Chain	Res	Type
24	A	990	A
24	A	995	C
24	A	996	A
24	A	1003	G
24	A	1012	U
24	A	1013	C
24	A	1021	A
24	A	1022	G
24	A	1023	U
24	A	1026	G
24	A	1033	U
24	A	1040	A
24	A	1046	A
24	A	1053	C
24	A	1054	A
24	A	1060	U
24	A	1061	U
24	A	1062	G
24	A	1064	C
24	A	1065	U
24	A	1066	U
24	A	1067	A
24	A	1068	G
24	A	1069	A
24	A	1070	A
24	A	1071	G
24	A	1072	C
24	A	1073	A
24	A	1075	C
24	A	1076	C
24	A	1077	A
24	A	1079	C
24	A	1084	A
24	A	1087	G
24	A	1088	A
24	A	1097	U
24	A	1104	C
24	A	1111	A
24	A	1112	G
24	A	1116	G
24	A	1119	U
24	A	1130	U

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Mol	Chain	Res	Type
24	A	1131	G
24	A	1132	U
24	A	1135	C
24	A	1136	G
24	A	1142	A
24	A	1143	A
24	A	1151	A
24	A	1165	A
24	A	1172	C
24	A	1174	U
24	A	1175	A
24	A	1178	C
24	A	1179	G
24	A	1180	U
24	A	1183	U
24	A	1205	A
24	A	1206	G
24	A	1210	G
24	A	1212	G
24	A	1213	A
24	A	1221	C
24	A	1237	A
24	A	1247	A
24	A	1248	G
24	A	1250	G
24	A	1251	C
24	A	1253	A
24	A	1256	G
24	A	1270	C
24	A	1271	G
24	A	1272	A
24	A	1273	U
24	A	1300	G
24	A	1301	A
24	A	1306	C
24	A	1311	G
24	A	1313	U
24	A	1314	C
24	A	1325	U
24	A	1332	G
24	A	1341	G
24	A	1345	C

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Mol	Chain	Res	Type
24	A	1359	A
24	A	1365	A
24	A	1368	G
24	A	1378	A
24	A	1379	U
24	A	1383	A
24	A	1386	C
24	A	1395	A
24	A	1396	U
24	A	1403	A
24	A	1407	G
24	A	1414	C
24	A	1416	G
24	A	1421	G
24	A	1428	C
24	A	1437	C
24	A	1454	C
24	A	1458	U
24	A	1459	G
24	A	1461	C
24	A	1475	G
24	A	1482	G
24	A	1490	A
24	A	1493	C
24	A	1498	C
24	A	1504	A
24	A	1509	A
24	A	1515	A
24	A	1523	U
24	A	1524	G
24	A	1529	G
24	A	1533	C
24	A	1534	U
24	A	1535	A
24	A	1536	C
24	A	1537	G
24	A	1559	U
24	A	1560	G
24	A	1565	C
24	A	1568	G
24	A	1569	A
24	A	1578	U

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Mol	Chain	Res	Type
24	A	1584	U
24	A	1614	A
24	A	1616	A
24	A	1633	G
24	A	1634	A
24	A	1643	G
24	A	1647	U
24	A	1648	U
24	A	1649	G
24	A	1674	G
24	A	1695	G
24	A	1698	A
24	A	1703	G
24	A	1713	A
24	A	1715	G
24	A	1718	G
24	A	1729	U
24	A	1730	C
24	A	1738	G
24	A	1757	A
24	A	1758	U
24	A	1764	C
24	A	1773	A
24	A	1780	A
24	A	1782	U
24	A	1784	A
24	A	1785	A
24	A	1791	A
24	A	1800	C
24	A	1801	A
24	A	1808	A
24	A	1809	A
24	A	1816	C
24	A	1829	A
24	A	1833	C
24	A	1847	A
24	A	1857	G
24	A	1870	C
24	A	1884	G
24	A	1891	G
24	A	1901	A
24	A	1906	G

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Mol	Chain	Res	Type
24	A	1907	G
24	A	1914	C
24	A	1929	G
24	A	1930	G
24	A	1931	U
24	A	1936	A
24	A	1937	A
24	A	1939	5MU
24	A	1940	U
24	A	1941	C
24	A	1943	U
24	A	1955	U
24	A	1964	G
24	A	1967	C
24	A	1970	A
24	A	1971	U
24	A	1972	G
24	A	1991	U
24	A	1993	U
24	A	1997	C
24	A	2022	U
24	A	2023	C
24	A	2031	A
24	A	2033	A
24	A	2036	C
24	A	2043	C
24	A	2049	G
24	A	2055	C
24	A	2056	G
24	A	2059	A
24	A	2060	A
24	A	2061	G
24	A	2062	A
24	A	2069	G7M
24	A	2070	A
24	A	2072	C
24	A	2077	A
24	A	2080	A
24	A	2093	G
24	A	2096	C
24	A	2100	G
24	A	2108	A

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Mol	Chain	Res	Type
24	A	2110	G
24	A	2111	U
24	A	2112	G
24	A	2113	U
24	A	2117	A
24	A	2118	U
24	A	2119	A
24	A	2120	G
24	A	2125	G
24	A	2127	G
24	A	2130	U
24	A	2132	U
24	A	2133	G
24	A	2134	A
24	A	2137	U
24	A	2145	C
24	A	2146	C
24	A	2147	A
24	A	2154	A
24	A	2158	A
24	A	2162	G
24	A	2163	A
24	A	2164	C
24	A	2166	U
24	A	2167	U
24	A	2168	G
24	A	2169	A
24	A	2170	A
24	A	2171	A
24	A	2172	U
24	A	2173	A
24	A	2178	C
24	A	2189	U
24	A	2198	A
24	A	2199	A
24	A	2204	G
24	A	2211	A
24	A	2214	C
24	A	2220	U
24	A	2223	G
24	A	2225	A
24	A	2238	G

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Mol	Chain	Res	Type
24	A	2239	G
24	A	2250	G
24	A	2268	A
24	A	2279	G
24	A	2283	C
24	A	2286	G
24	A	2287	A
24	A	2288	A
24	A	2294	G
24	A	2298	A
24	A	2305	U
24	A	2309	A
24	A	2310	C
24	A	2319	G
24	A	2322	A
24	A	2331	G
24	A	2333	A
24	A	2335	A
24	A	2347	C
24	A	2350	C
24	A	2354	C
24	A	2357	G
24	A	2383	G
24	A	2385	C
24	A	2389	G
24	A	2392	A
24	A	2402	U
24	A	2403	C
24	A	2406	A
24	A	2407	A
24	A	2429	G
24	A	2430	A
24	A	2431	U
24	A	2441	U
24	A	2448	A
24	A	2464	G
24	A	2468	A
24	A	2475	C
24	A	2476	A
24	A	2480	C
24	A	2484	G
24	A	2491	U

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Mol	Chain	Res	Type
24	A	2494	G
24	A	2498	OMC
24	A	2501	C
24	A	2502	G
24	A	2504	PSU
24	A	2505	G
24	A	2506	U
24	A	2513	A
24	A	2518	A
24	A	2520	C
24	A	2525	G
24	A	2535	G
24	A	2547	A
24	A	2548	U
24	A	2554	U
24	A	2567	G
24	A	2569	G
24	A	2572	A
24	A	2573	C
24	A	2578	G
24	A	2582	G
24	A	2585	U
24	A	2586	U
24	A	2602	A
24	A	2603	G
24	A	2609	U
24	A	2610	C
24	A	2611	C
24	A	2613	U
24	A	2615	U
24	A	2621	G
24	A	2629	U
24	A	2636	C
24	A	2646	C
24	A	2656	U
24	A	2685	G
24	A	2689	U
24	A	2690	U
24	A	2714	G
24	A	2718	G
24	A	2720	U
24	A	2726	A

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Mol	Chain	Res	Type
24	A	2729	G
24	A	2733	A
24	A	2739	U
24	A	2744	G
24	A	2748	A
24	A	2751	G
24	A	2757	A
24	A	2764	A
24	A	2765	A
24	A	2766	A
24	A	2769	U
24	A	2778	A
24	A	2779	U
24	A	2790	U
24	A	2791	G
24	A	2793	C
24	A	2794	C
24	A	2797	U
24	A	2798	U
24	A	2799	A
24	A	2800	A
24	A	2801	G
24	A	2803	G
24	A	2808	G
24	A	2818	U
24	A	2820	A
24	A	2821	A
24	A	2833	U
24	A	2834	G
24	A	2849	U
24	A	2867	G
24	A	2868	A
24	A	2872	A
24	A	2873	A
24	A	2880	C
24	A	2883	A
24	A	2885	G
24	A	2891	U
25	B	4	C
25	B	13	G
25	B	16	G
25	B	25	U

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Mol	Chain	Res	Type
25	B	30	C
25	B	35	C
25	B	41	G
25	B	44	G
25	B	57	A
25	B	67	G
25	B	68	C
25	B	73	A
25	B	89	U
25	B	90	C
25	B	96	G
25	B	108	A
25	B	109	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	51	G
24	A	91	A
24	A	205	G
24	A	228	C
24	A	385	C
24	A	512	G
24	A	555	G
24	A	572	A
24	A	774	G
24	A	830	G
24	A	989	G
24	A	1020	A
24	A	1070	A
24	A	1111	A
24	A	1182	G
24	A	1190	G
24	A	1211	C
24	A	1212	G
24	A	1251	C
24	A	1432	G
24	A	1458	U
24	A	1567	G
24	A	1930	G
24	A	1940	U
24	A	2061	G

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Mol	Chain	Res	Type
24	A	2308	G
24	A	2391	G
24	A	2447	G
24	A	2566	A
24	A	2610	C
24	A	2756	U
24	A	2820	A
24	A	2832	U
24	A	2867	G
25	B	3	C
25	B	66	A
25	B	88	C

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

39 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	$\#\|Z\|>2$
24	6MZ	A	1618	24	17,25,26	1.03	1 (5%)	15,36,39	2.69	2 (13%)
24	2MG	A	1835	24	18,26,27	1.10	2 (11%)	21,38,41	2.51	7 (33%)
24	PSU	A	1911	24	15,21,22	1.45	2 (13%)	16,30,33	2.39	4 (25%)
24	3TD	A	1915	24	15,22,23	3.26	6 (40%)	17,32,35	1.59	3 (17%)
24	PSU	A	1917	24	15,21,22	1.39	2 (13%)	16,30,33	2.16	4 (25%)
24	5MU	A	1939	24	13,22,23	0.74	1 (7%)	16,32,35	2.37	2 (12%)
24	5MC	A	1962	24	14,22,23	1.14	1 (7%)	17,32,35	1.70	3 (17%)
24	6MZ	A	2030	24	17,25,26	1.05	1 (5%)	15,36,39	2.64	2 (13%)
24	G7M	A	2069	24	18,26,27	1.18	2 (11%)	21,39,42	2.50	6 (28%)
24	OMG	A	2251	24,22	18,26,27	1.08	2 (11%)	21,38,41	1.72	4 (19%)
24	2MG	A	2445	24	18,26,27	1.04	2 (11%)	21,38,41	2.27	5 (23%)
24	H2U	A	2449	24	17,21,22	1.11	2 (11%)	23,30,33	2.19	5 (21%)
24	PSU	A	2457	24	15,21,22	1.77	4 (26%)	16,30,33	2.45	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	OMC	A	2498	24	15,22,23	0.69	0	20,31,34	1.58	1 (5%)
24	2MA	A	2503	24	17,25,26	1.52	3 (17%)	18,37,40	3.16	1 (5%)
24	PSU	A	2504	24	15,21,22	1.31	1 (6%)	16,30,33	2.42	4 (25%)
24	OMU	A	2552	24	14,22,23	0.69	1 (7%)	19,31,34	1.67	1 (5%)
24	PSU	A	2580	24	15,21,22	1.53	3 (20%)	16,30,33	2.21	3 (18%)
24	PSU	A	2604	24	15,21,22	1.36	2 (13%)	16,30,33	2.41	4 (25%)
24	PSU	A	2605	24	15,21,22	1.30	2 (13%)	16,30,33	2.06	3 (18%)
24	1MG	A	745	24	17,26,27	1.49	3 (17%)	19,39,42	1.15	2 (10%)
24	PSU	A	746	24	15,21,22	1.25	1 (6%)	16,30,33	2.27	4 (25%)
24	5MU	A	747	24	13,22,23	0.58	0	16,32,35	2.74	2 (12%)
24	PSU	A	955	24	15,21,22	1.71	3 (20%)	16,30,33	2.16	4 (25%)
1	2MG	a	1207	1	18,26,27	1.14	2 (11%)	21,38,41	2.15	6 (28%)
1	4OC	a	1402	1	15,23,24	0.60	0	21,32,35	1.74	3 (14%)
1	5MC	a	1407	1	14,22,23	1.29	1 (7%)	17,32,35	0.85	1 (5%)
1	UR3	a	1498	1	13,22,23	0.63	0	18,32,35	0.83	0
1	2MG	a	1516	1	18,26,27	1.06	2 (11%)	21,38,41	2.27	6 (28%)
1	MA6	a	1518	1	18,26,27	0.96	1 (5%)	15,38,41	2.39	3 (20%)
1	MA6	a	1519	1	18,26,27	0.90	1 (5%)	15,38,41	2.51	4 (26%)
1	PSU	a	516	1	15,21,22	1.37	2 (13%)	16,30,33	2.14	3 (18%)
1	G7M	a	527	1	18,26,27	1.52	2 (11%)	21,39,42	3.06	11 (52%)
1	2MG	a	966	1	18,26,27	1.13	2 (11%)	21,38,41	2.28	6 (28%)
1	5MC	a	967	1	14,22,23	1.25	1 (7%)	17,32,35	0.93	1 (5%)
22	H2U	v	20	22	17,21,22	0.96	2 (11%)	23,30,33	1.71	4 (17%)
22	5MU	v	54	22	13,22,23	0.57	0	16,32,35	2.59	2 (12%)
22	PSU	v	55	22	15,21,22	1.10	2 (13%)	16,30,33	2.24	4 (25%)
22	4SU	v	8	22	12,21,22	0.70	0	15,30,33	0.96	1 (6%)

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
24	6MZ	A	1618	24	-	0/5/27/28	0/3/3/3
24	2MG	A	1835	24	-	0/5/27/28	0/3/3/3
24	PSU	A	1911	24	-	0/7/25/26	0/2/2/2
24	3TD	A	1915	24	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	A	1917	24	-	0/7/25/26	0/2/2/2
24	5MU	A	1939	24	-	0/3/25/26	0/2/2/2
24	5MC	A	1962	24	-	0/3/25/26	0/2/2/2
24	6MZ	A	2030	24	-	0/5/27/28	0/3/3/3
24	G7M	A	2069	24	2/2/5/5	0/3/25/26	0/3/3/3
24	OMG	A	2251	24,22	-	0/5/27/28	0/3/3/3
24	2MG	A	2445	24	-	0/5/27/28	0/3/3/3
24	H2U	A	2449	24	-	0/7/38/39	0/2/2/2
24	PSU	A	2457	24	-	0/7/25/26	0/2/2/2
24	OMC	A	2498	24	-	0/5/27/28	0/2/2/2
24	2MA	A	2503	24	-	0/3/25/26	0/3/3/3
24	PSU	A	2504	24	-	0/7/25/26	0/2/2/2
24	OMU	A	2552	24	-	0/5/27/28	0/2/2/2
24	PSU	A	2580	24	-	0/7/25/26	0/2/2/2
24	PSU	A	2604	24	-	0/7/25/26	0/2/2/2
24	PSU	A	2605	24	-	0/7/25/26	0/2/2/2
24	1MG	A	745	24	-	0/3/25/26	0/3/3/3
24	PSU	A	746	24	-	0/7/25/26	0/2/2/2
24	5MU	A	747	24	-	0/3/25/26	0/2/2/2
24	PSU	A	955	24	-	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

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	2457	PSU	C5-C1'	-5.55	1.47	1.52
24	A	955	PSU	C5-C1'	-5.34	1.47	1.52
24	A	2580	PSU	C5-C1'	-4.59	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1911	PSU	C5-C1'	-4.43	1.48	1.52
1	a	516	PSU	C5-C1'	-3.91	1.48	1.52
24	A	1917	PSU	C5-C1'	-3.90	1.48	1.52
24	A	2504	PSU	C5-C1'	-3.84	1.48	1.52
24	A	2604	PSU	C5-C1'	-3.57	1.49	1.52
24	A	746	PSU	C5-C1'	-3.51	1.49	1.52
24	A	2605	PSU	C5-C1'	-3.38	1.49	1.52
22	v	55	PSU	C5-C1'	-2.76	1.49	1.52
24	A	2449	H2U	C4-N3	-2.76	1.33	1.37
24	A	1915	3TD	O4-C4	-2.58	1.18	1.24
24	A	2449	H2U	C2-N3	-2.57	1.33	1.38
24	A	2604	PSU	C2-N3	-2.45	1.33	1.38
22	v	20	H2U	C2-N3	-2.35	1.33	1.38
24	A	2069	G7M	O2'-C2'	-2.23	1.37	1.43
24	A	1939	5MU	C2-N3	-2.22	1.33	1.38
24	A	2605	PSU	C2-N3	-2.20	1.33	1.38
24	A	2457	PSU	C2-N3	-2.18	1.33	1.38
24	A	2580	PSU	O4'-C1'	-2.18	1.41	1.44
24	A	1911	PSU	C2-N3	-2.17	1.33	1.38
24	A	955	PSU	O4'-C1'	-2.16	1.41	1.44
22	v	20	H2U	C4-N3	-2.16	1.34	1.37
24	A	2457	PSU	O4'-C1'	-2.15	1.41	1.44
22	v	55	PSU	C2-N3	-2.13	1.33	1.38
1	a	527	G7M	O2'-C2'	-2.07	1.38	1.43
1	a	516	PSU	C2-N3	-2.07	1.33	1.38
24	A	2580	PSU	C2-N3	-2.07	1.33	1.38
24	A	955	PSU	C2-N1	-2.07	1.33	1.38
24	A	1917	PSU	O4'-C1'	-2.04	1.41	1.44
24	A	2552	OMU	C2-N3	-2.03	1.33	1.38
24	A	2457	PSU	C2-N1	-2.03	1.34	1.38
24	A	745	1MG	C6-N1	2.00	1.41	1.38
24	A	1915	3TD	C5-C1'	2.05	1.54	1.52
24	A	2445	2MG	C5-C4	2.59	1.46	1.40
1	a	1516	2MG	C5-C4	2.68	1.46	1.40
24	A	1835	2MG	C5-C4	2.71	1.46	1.40
24	A	2503	2MA	C5-C4	2.85	1.46	1.40
1	a	966	2MG	C5-C4	2.88	1.47	1.40
24	A	2251	OMG	C5-C4	2.90	1.47	1.40
1	a	1207	2MG	C5-C4	3.01	1.47	1.40
1	a	1519	MA6	C5-C4	3.01	1.47	1.40
24	A	2445	2MG	C6-C5	3.23	1.47	1.41
1	a	1516	2MG	C6-C5	3.24	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	2251	OMG	C6-C5	3.25	1.47	1.41
1	a	1518	MA6	C5-C4	3.32	1.48	1.40
1	a	1207	2MG	C6-C5	3.37	1.48	1.41
24	A	1835	2MG	C6-C5	3.45	1.48	1.41
24	A	2069	G7M	C6-C5	3.46	1.48	1.41
1	a	966	2MG	C6-C5	3.55	1.48	1.41
24	A	1618	6MZ	C5-C4	3.59	1.48	1.40
24	A	745	1MG	C5-C4	3.63	1.48	1.40
24	A	1962	5MC	C5-C4	3.65	1.47	1.41
24	A	2030	6MZ	C5-C4	3.70	1.48	1.40
24	A	2503	2MA	C6-N6	3.72	1.35	1.29
24	A	2503	2MA	C6-C5	3.84	1.47	1.40
24	A	745	1MG	C6-C5	4.25	1.49	1.40
1	a	967	5MC	C5-C4	4.36	1.48	1.41
1	a	1407	5MC	C5-C4	4.37	1.48	1.41
24	A	1915	3TD	C2-N1	5.13	1.48	1.38
1	a	527	G7M	C6-C5	5.22	1.51	1.41
24	A	1915	3TD	C6-N1	5.34	1.45	1.34
24	A	1915	3TD	C4-N3	5.55	1.46	1.38
24	A	1915	3TD	C6-C5	7.56	1.49	1.38

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	747	5MU	C5-C4-N3	-8.10	118.55	125.35
1	a	527	G7M	C5-C6-N1	-7.93	113.16	123.52
22	v	54	5MU	C5-C4-N3	-7.48	119.07	125.35
1	a	1519	MA6	N3-C2-N1	-7.23	123.19	128.87
24	A	2449	H2U	C5-C6-N1	-6.90	103.21	110.76
1	a	1518	MA6	N3-C2-N1	-6.87	123.47	128.87
24	A	1939	5MU	C5-C4-N3	-6.72	119.70	125.35
24	A	2030	6MZ	N3-C2-N1	-6.26	123.95	128.87
24	A	2449	H2U	C4-N3-C2	-5.97	120.36	125.77
24	A	1618	6MZ	N3-C2-N1	-5.95	124.20	128.87
22	v	20	H2U	C5-C6-N1	-5.72	104.50	110.76
24	A	2457	PSU	C5-C1'-C2'	-5.42	106.23	115.44
24	A	2069	G7M	C5-C6-N1	-5.34	116.54	123.52
1	a	1402	4OC	CM4-N4-C4	-5.25	118.44	122.87
24	A	1962	5MC	CM5-C5-C4	-4.91	116.27	121.47
24	A	2504	PSU	C5-C1'-C2'	-4.66	107.52	115.44
24	A	1911	PSU	C5-C1'-C2'	-4.49	107.81	115.44
24	A	1915	3TD	C5-C1'-C2'	-4.38	108.00	115.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	2445	2MG	C5-C6-N1	-4.21	118.01	123.52
24	A	2604	PSU	C5-C1'-C2'	-4.19	108.32	115.44
24	A	2445	2MG	CM2-N2-C2	-4.08	118.45	123.03
1	a	1207	2MG	C5-C6-N1	-4.07	118.20	123.52
24	A	2251	OMG	C5-C6-N1	-4.07	118.20	123.52
1	a	1516	2MG	C5-C6-N1	-4.04	118.24	123.52
24	A	2457	PSU	C5-C6-N1	-3.98	118.83	124.38
1	a	966	2MG	C5-C6-N1	-3.78	118.58	123.52
24	A	1835	2MG	CM2-N2-C2	-3.75	118.81	123.03
24	A	1835	2MG	C6-C5-C4	-3.68	116.65	120.86
24	A	1835	2MG	C5-C6-N1	-3.59	118.83	123.52
24	A	2504	PSU	C5-C6-N1	-3.49	119.51	124.38
1	a	516	PSU	C5-C6-N1	-3.48	119.52	124.38
24	A	1911	PSU	C5-C6-N1	-3.47	119.53	124.38
24	A	955	PSU	C5-C6-N1	-3.45	119.57	124.38
24	A	2605	PSU	C5-C6-N1	-3.41	119.62	124.38
24	A	1917	PSU	C5-C6-N1	-3.36	119.70	124.38
24	A	2580	PSU	C5-C6-N1	-3.36	119.70	124.38
24	A	745	1MG	C6-C5-C4	-3.34	117.54	119.93
24	A	2604	PSU	C5-C6-N1	-3.34	119.72	124.38
1	a	1516	2MG	C6-C5-C4	-3.31	117.08	120.86
22	v	20	H2U	C4-N3-C2	-3.28	122.79	125.77
22	v	55	PSU	C5-C6-N1	-3.26	119.84	124.38
1	a	1207	2MG	C6-C5-C4	-3.25	117.14	120.86
24	A	746	PSU	C5-C6-N1	-3.15	119.99	124.38
1	a	966	2MG	C6-C5-C4	-3.14	117.27	120.86
24	A	2069	G7M	N3-C2-N1	-3.14	123.29	127.56
24	A	746	PSU	C5-C1'-C2'	-3.02	110.31	115.44
22	v	8	4SU	C5-C4-N3	-3.00	120.39	123.56
24	A	1915	3TD	C5-C6-N1	-2.97	120.23	124.38
24	A	2251	OMG	N3-C2-N1	-2.96	123.52	127.56
24	A	2445	2MG	C6-C5-C4	-2.87	117.58	120.86
1	a	1519	MA6	C10-N6-C9	-2.86	106.61	115.96
24	A	745	1MG	C1'-N9-C4	-2.64	123.86	126.81
24	A	1835	2MG	N3-C2-N1	-2.63	122.26	126.19
1	a	1518	MA6	C10-N6-C9	-2.55	107.62	115.96
1	a	527	G7M	C4'-O4'-C1'	-2.54	106.95	109.64
1	a	966	2MG	N3-C2-N1	-2.51	122.44	126.19
24	A	2251	OMG	C6-C5-C4	-2.47	118.03	120.86
1	a	1516	2MG	N3-C2-N1	-2.45	122.53	126.19
24	A	2605	PSU	C5-C1'-C2'	-2.41	111.34	115.44
1	a	1519	MA6	C1'-N9-C4	-2.37	124.16	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	527	G7M	N3-C2-N1	-2.36	124.34	127.56
1	a	1516	2MG	CM2-N2-C2	-2.33	120.41	123.03
22	v	55	PSU	C5-C1'-C2'	-2.30	111.54	115.44
1	a	966	2MG	CM2-N2-C2	-2.17	120.60	123.03
24	A	955	PSU	C5-C1'-C2'	-2.16	111.77	115.44
1	a	1207	2MG	N3-C2-N1	-2.13	123.00	126.19
24	A	1917	PSU	C5-C1'-C2'	-2.07	111.92	115.44
1	a	527	G7M	O2'-C2'-C3'	2.02	118.37	111.86
22	v	20	H2U	C6-N1-C2	2.02	125.28	122.16
24	A	2449	H2U	C1'-N1-C2	2.04	121.05	118.19
1	a	527	G7M	O2'-C2'-C1'	2.06	118.05	111.61
24	A	2069	G7M	N7-C8-N9	2.10	111.78	108.67
24	A	2449	H2U	O4-C4-N3	2.17	123.84	120.46
24	A	2604	PSU	O4'-C1'-C2'	2.18	107.04	104.69
1	a	1407	5MC	N4-C4-N3	2.19	120.13	116.92
22	v	20	H2U	C5-C4-N3	2.31	119.06	116.62
24	A	1915	3TD	O4'-C1'-C2'	2.32	107.20	104.69
1	a	1207	2MG	N2-C2-N3	2.33	119.65	116.94
1	a	527	G7M	C5'-C4'-C3'	2.35	124.30	115.20
24	A	746	PSU	O4'-C1'-C2'	2.39	107.27	104.69
1	a	967	5MC	N4-C4-N3	2.43	120.48	116.92
24	A	2449	H2U	C6-N1-C2	2.45	125.94	122.16
24	A	1962	5MC	CM5-C5-C6	2.51	123.71	118.63
24	A	1911	PSU	O4'-C1'-C2'	2.54	107.44	104.69
24	A	1917	PSU	O4'-C1'-C2'	2.54	107.44	104.69
24	A	2504	PSU	O4'-C1'-C2'	2.57	107.47	104.69
24	A	2457	PSU	O4'-C1'-C2'	2.70	107.61	104.69
24	A	2580	PSU	O4'-C1'-C2'	2.85	107.77	104.69
22	v	55	PSU	O4'-C1'-C2'	2.87	107.80	104.69
1	a	1402	4OC	C6-C5-C4	2.91	118.56	117.42
24	A	955	PSU	O4'-C1'-C2'	2.93	107.86	104.69
24	A	1962	5MC	N4-C4-N3	3.03	121.36	116.92
1	a	527	G7M	N7-C8-N9	3.06	113.19	108.67
1	a	516	PSU	O4'-C1'-C2'	3.11	108.05	104.69
1	a	527	G7M	O3'-C3'-C2'	3.30	122.51	111.86
1	a	527	G7M	O3'-C3'-C4'	3.43	121.25	111.01
24	A	1835	2MG	N2-C2-N1	3.49	120.99	116.94
1	a	527	G7M	C1'-N9-C4	3.56	130.78	126.81
24	A	2069	G7M	O3'-C3'-C4'	3.88	122.61	111.01
24	A	2069	G7M	C1'-N9-C4	4.10	131.38	126.81
1	a	1402	4OC	C2-N3-C4	4.47	121.12	115.43
24	A	2445	2MG	C6-N1-C2	4.48	121.65	115.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1835	2MG	C6-N1-C2	4.54	121.74	115.24
1	a	966	2MG	C6-N1-C2	4.73	122.02	115.24
24	A	2251	OMG	C6-N1-C2	4.82	121.53	115.88
1	a	1516	2MG	C6-N1-C2	4.85	122.19	115.24
1	a	1207	2MG	C6-N1-C2	4.91	122.28	115.24
1	a	1518	MA6	C2-N1-C6	4.91	123.23	111.64
1	a	1519	MA6	C2-N1-C6	5.04	123.52	111.64
1	a	1207	2MG	C2-N3-C4	5.34	120.84	114.99
1	a	1516	2MG	C2-N3-C4	5.69	121.23	114.99
24	A	2069	G7M	C6-N1-C2	5.78	122.65	115.88
24	A	2445	2MG	C2-N3-C4	5.81	121.36	114.99
24	A	2457	PSU	C4-N3-C2	6.08	120.23	115.16
24	A	2498	OMC	C6-C5-C4	6.20	119.86	117.44
24	A	1939	5MU	C4-N3-C2	6.20	120.33	115.16
24	A	2605	PSU	C4-N3-C2	6.23	120.35	115.16
24	A	2552	OMU	C4-N3-C2	6.47	121.03	114.21
1	a	966	2MG	C2-N3-C4	6.55	122.17	114.99
24	A	955	PSU	C4-N3-C2	6.69	120.74	115.16
24	A	1911	PSU	C4-N3-C2	6.78	120.82	115.16
22	v	54	5MU	C4-N3-C2	6.79	120.82	115.16
1	a	516	PSU	C4-N3-C2	6.80	120.83	115.16
22	v	55	PSU	C4-N3-C2	6.84	120.87	115.16
24	A	1917	PSU	C4-N3-C2	6.95	120.95	115.16
24	A	1835	2MG	C2-N3-C4	6.96	122.62	114.99
24	A	2504	PSU	C4-N3-C2	6.99	120.99	115.16
24	A	747	5MU	C4-N3-C2	7.03	121.03	115.16
24	A	2604	PSU	C4-N3-C2	7.23	121.19	115.16
24	A	746	PSU	C4-N3-C2	7.25	121.21	115.16
24	A	2580	PSU	C4-N3-C2	7.26	121.21	115.16
1	a	527	G7M	C6-N1-C2	7.36	124.50	115.88
24	A	2030	6MZ	C2-N1-C6	7.82	122.09	116.47
24	A	1618	6MZ	C2-N1-C6	8.10	122.29	116.47
24	A	2503	2MA	C2-N3-C4	13.00	121.55	115.29

All (4) chirality outliers are listed below:

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

All (1) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1915	3TD	1	0
24	A	1917	PSU	1	0
24	A	2580	PSU	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.