



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:22 pm GMT

PDB ID : 3J9Y  
EMDB ID: : EMD-6311  
Title : Cryo-EM structure of tetracycline resistance protein TetM bound to a translating E.coli ribosome  
Authors : Arenz, S.; Nguyen, F.; Beckmann, R.; Wilson, D.N.  
Deposited on : 2015-03-23  
Resolution : 3.90 Å(reported)  
Based on PDB ID : 5AFI

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

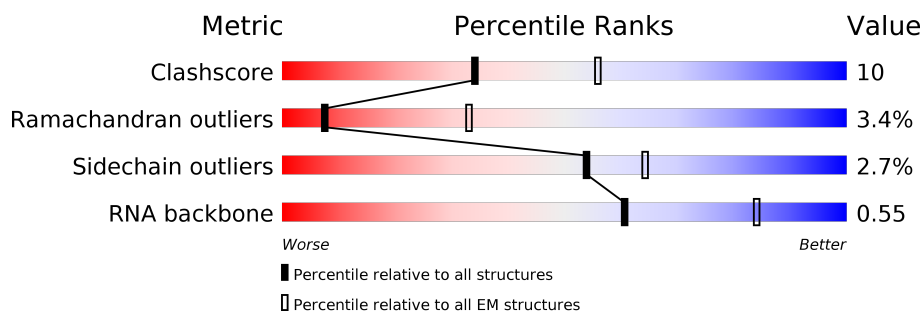
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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.











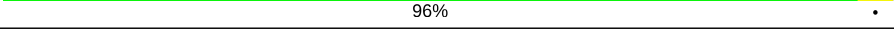







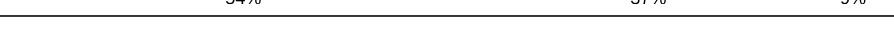

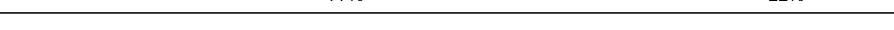
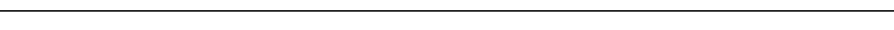
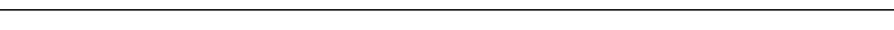
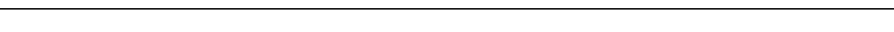
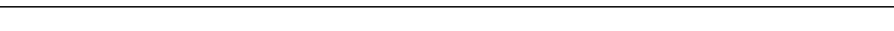
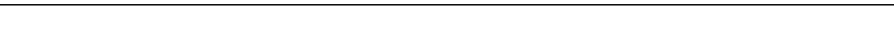

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	a	1539	83% 16%
2	b	240	85% 6% 9%
3	d	206	92% 8%
4	e	167	84% 10% 6%
5	f	135	68% 26%
6	h	130	96%
7	k	129	84% 6% 10%
8	l	124	93% 6%


























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Mol	Chain	Length	Quality of chain
9	o	89	 91% 8% .
10	p	82	 93% 7%
11	q	84	 86% 10% 5%
12	r	75	 79% 8% 13%
13	t	87	 93% 5% .
14	u	71	 82% 10% 8%
15	v	78	 76% 23% .
16	x	11	 73% 9% 18%
17	w	639	 96% .
18	c	233	 85% . 12%
19	g	179	 78% 7% 16%
20	i	130	 88% 10% .
21	j	103	 87% 8% 5%
22	m	118	 91% 6% .
23	n	102	 90% 9% .
24	s	92	 85% . 14%
25	A	2903	 54% 37% 9%
26	B	120	 54% 43% .
27	C	273	 77% 22% ..
28	D	209	 76% 22% .
29	E	201	 75% 23% .
30	F	179	 60% 34% . .
31	G	177	 80% 19% ..
32	H	149	 80% 18% .
33	I	142	 63% 33% . .

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Mol	Chain	Length	Quality of chain
34	J	142	 73% 26% .
35	K	123	 68% 28% ..
36	L	144	 64% 33% ..
37	M	136	 75% 24% .
38	N	127	 67% 27% . 6%
39	O	117	 80% 18% ..
40	P	115	 77% 21% ..
41	Q	118	 76% 23% .
42	R	103	 81% 19%
43	S	110	 70% 27% .
44	T	100	 70% 20% .. 7%
45	U	104	 73% 24% ..
46	V	94	 76% 23% .
47	W	85	 73% 15% 12%
48	X	78	 78% 19% ..
49	Y	63	 71% 27% .
50	Z	59	 80% 19% .
51	0	57	 68% 26% ..
52	1	55	 78% 13% 9%
53	2	46	 70% 30%
54	3	65	 72% 25% ..
55	4	38	 61% 39%
56	5	165	 51% 26% . 21%
57	6	70	 70% 23% . 6%
58	7	69	 99%

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 148915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 6 is a protein called 30S ribosomal protein S8.

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

- Molecule 7 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 8 is a protein called 30S ribosomal protein S12.

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

- Molecule 9 is a protein called 30S ribosomal protein S15.

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

- Molecule 10 is a protein called 30S ribosomal protein S16.

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

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 13 is a protein called 30S ribosomal protein S20.

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

- Molecule 14 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 15 is a RNA chain called P-site fMet-tRNA<sup>fMet</sup>.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	77	FME	-	FORMYLATION	GB 147949

- Molecule 16 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	x	9	Total	C	N	O	P		
			189	85	31	64	9	0	0

- Molecule 17 is a protein called Tetracycline resistance protein TetM.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	w	639	Total	C	N	O		0	0
			2590	1308	640	642			

- Molecule 18 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 19 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 20 is a protein called 30S ribosomal protein S9.

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

- Molecule 21 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 22 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 23 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	INSERTION	UNP P0AG59

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2900	Total	C	N	O	P	0	0
			62276	27788	11460	20128	2900		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
52	1	50	Total	C	N	O	0	0
			409	263	75	71		

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

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

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

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

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

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

- Molecule 56 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

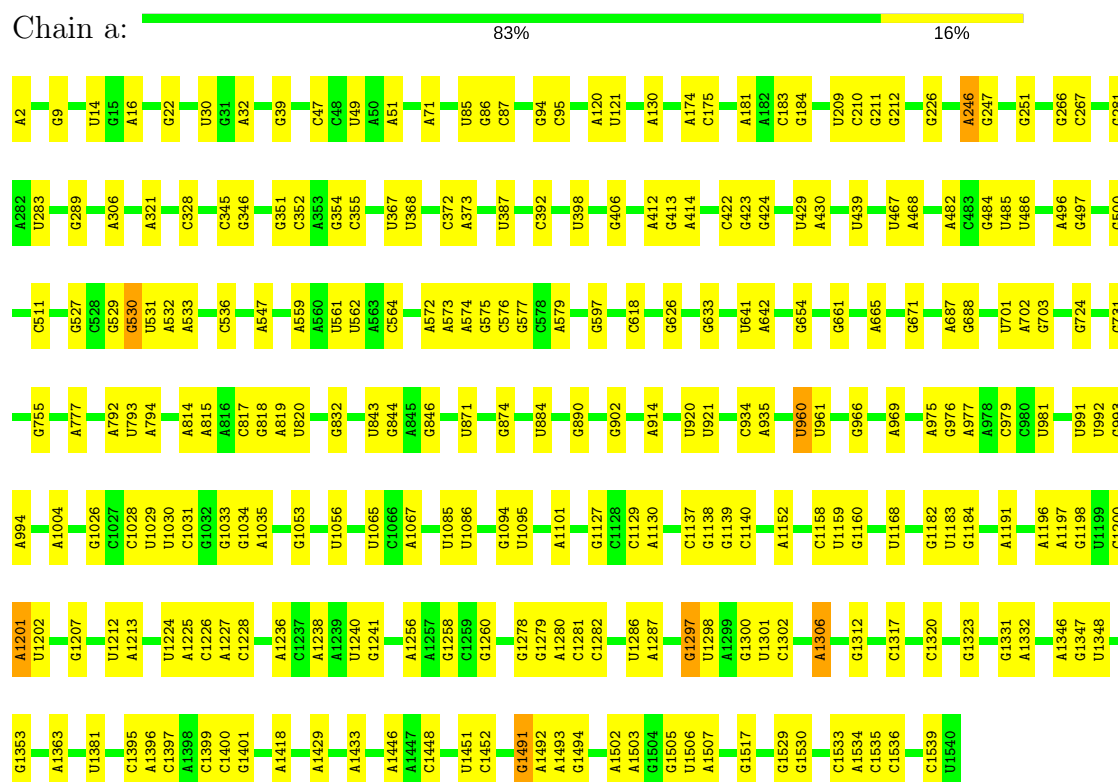
- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	7	69	Total	C	N	O	0	0
			276	138	69	69		

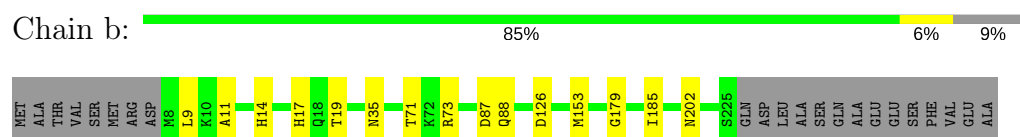
### 3 Residue-property plots

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

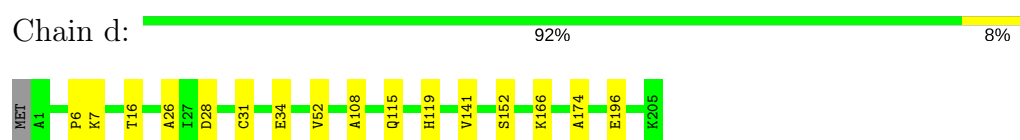
- Molecule 1: 16S ribosomal RNA




- Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5

Chain e:  84% 10% • 6%



- Molecule 5: 30S ribosomal protein S6

Chain f:  68% • • 26%




- Molecule 6: 30S ribosomal protein S8

Chain h:  96% • •



- Molecule 7: 30S ribosomal protein S11

Chain k:  84% 6% 10%



- Molecule 8: 30S ribosomal protein S12

Chain l:  93% 6% •



- Molecule 9: 30S ribosomal protein S15

Chain o:  91% 8% •




- Molecule 10: 30S ribosomal protein S16

Chain p:  93% 7%



- Molecule 11: 30S ribosomal protein S17

Chain q:  86% 10% 5%



- Molecule 12: 30S ribosomal protein S18

Chain r: 79% 8% 13%



- Molecule 13: 30S ribosomal protein S20

Chain t: 93% 5% .



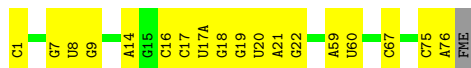
- Molecule 14: 30S ribosomal protein S21

Chain u: 82% 10% 8%



- Molecule 15: P-site fMet-tRNA<sup>fMet</sup>

Chain v: 76% 23% .



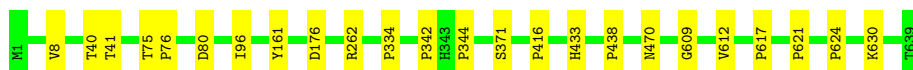
- Molecule 16: mRNA

Chain x: 73% 9% 18%



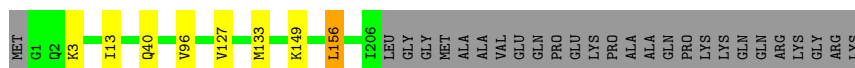
- Molecule 17: Tetracycline resistance protein TetM

Chain w: 96% .



- Molecule 18: 30S ribosomal protein S3

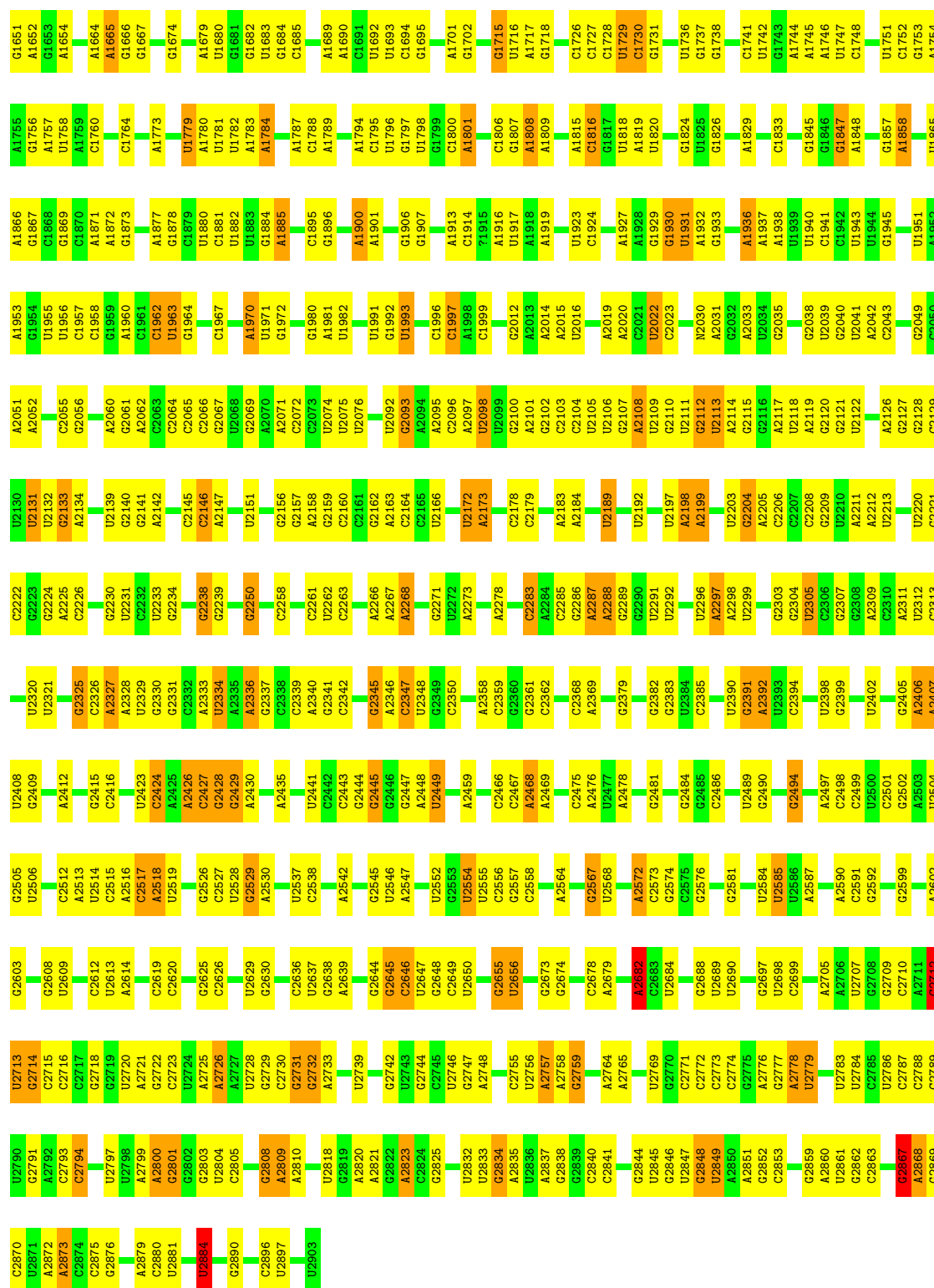
Chain c: 85% 12%







G1448	G1343	G1252	G1071	C985		U811	C737	U641	G548	C456	G363	G277	G185
G1454	U1344	A1253	C1072	G989	A896	C812	G738	U642	G549	A457	C364	A278	G189
U1458	C1345	G1256	A1073	A990	C897	U813	C740	A643	C550	G458	C365	C281	A190
C1461	U1352	A1265	C1075	G993	A900	C815	A743	G645	U554	A460	G367	A282	A191
A1469	G1361	G1266	C1076	C994	C901	C816	U744	U646	G555	C461	A368	U284	C192
A1470	C1362	U1267	A1077	C995	G907	C817	G745	G651	U562	G462	U369	G285	A196
A1475	A1268	A1268	U1078	A996	C908	A818	G746	A654	A563	U464	G370	U286	A199
U1476	G1363	U1269	A1080	U999	A909	A819	G747	A655	G465	A466	G372	U287	
A1568	A1365	G1271	U1081	C1005	A910	G822	G748	G656	U568	G467	U373	U288	A204
G1569	G1366	U1272	A1084	U1019	A911	U827	A751	G659	U569	G468	G376	U289	G205
C1561	A1367	A1273	A1085	G1011	U919	U828	A752	A658	A572	U469	G377	G291	U266
U1562	G1368		A1086	G1012	A920	A829	U754	G667	U573	G473	G386	A294	A207
U1563	A1378	A1276	G1087	U1013	A921	G830	U755	G669	A574	G474	U387	A296	C208
C1564	U1379	G1277	A1088	C1013	G923	G831	U756	A670	A575	G475	U390	G297	A213
C1565	G1380	G1278	A1089	U1014	G924	U832	U757	G674	U580	G476	A391		G215
G1566	A1383	G1279	A1090	U1015	G930	A833	G758	A677	G585			A300	A216
G1567					G931	G834	C759	C679	U589	A479	G394	G301	A217
A1568	A1384	G1283	U1094	U1019	U932		G765	G682	U590	C490	G396	G303	A219
U1578	A1385	G1284	A1095	G1026	A936	G843		A685	A591	C491	A404	U306	A221
A1579	C1386	A1287	A1096	A1027	C937	A844	G770	U686	U592	A492	G405	G307	A222
G1580	A1387	G1288	A1097	A1028	G938	A845	G771	C687	A593	G493		A310	A227
G1581	U1387	C1289	U1097	A1029	G939	U846	C772		U594	G494	G411	A311	C228
	A1395		U1101	U1033	A941	U847	U773		C595	G495	A412		
C1585	U1396	G1292	C1102	G1038	C946	C848	G774	C682		U499	C413	U321	G232
A1586	C1398	C1297	U1105	A1039	A947	U849	G775	A693	U598	G500	C414	A322	G242
G1587	C1399	G1298	G1107	A1040	C948	U850	G776	G695	G600	A501	A415	C323	U243
A1590	U1400	G1299	U1108	G1041	G949	U852	G777		C601	A502	C420	A324	A244
A1591	G1401	G1300	C1109	U1045	G953	G857	U779	U703	A602	A503	C421	U328	G245
C1592	U1406	A1302	G1110	G1046	G954	G858	G780	G704	A603	A505	A422	G329	G248
A1597	G1410	C1306	A1111	U1047	G955	G859	A783	A705	A608	G506	A423	A330	C249
C1604	U1411	G1310	U1113	G1047	U956	U860	A784	G706	A609	A507	G424	G333	G250
C1605	U1412	G1311	C1114	U1052	G957	U862	G785	G707	C610	C509	C426	C334	A251
C1606	A1413	U1312	G1115	C1053	U958	G869	G786	G712	A613	G518	U427	C335	G252
C1607	U1414	G1313	U1119	U1054	A959	G870	A787	G713	A614	U519	U434	C336	A255
A1610	U1415	C1314	U1123	G1055	A960	U871	A788	U714	U615	G527	C435	A340	A256
C1611	G1416	G1315	G1124	U1056	C961	U872	U790	A715	A616	A528	U437	C341	G260
C1612	U1417	U1316	U1125	G1057	G962	C873	C791	C717		A529	G438		
G1613	A1418	G1317	A1126	U1058	G969	G874	A792		G627	G530	U441	A346	
A1614	A1419	U1318	G1127	U1059	U970	A878	A793	A722	G630	C531	G442	C353	A285
C1615	G1421	C1319	G1128	G1060	G971	G879	C795	C723	A633	G532	G443	G356	G266
A1616	G1422	C1320	U1129	U1061	A972	U884	G801	G725	C634	G533	A443	C357	A270
G1617	C1428	A1321	U1130	U1062	A973	C885	A802	G726	G635	C542	G446	U358	G271
	U1429	U1322	G1131	G1063	G974	A886	A802	A727	G636	C544	U451	G359	A272
U1627	G1430	C1330	U1132	U1064	A975	U	G805	A730	U638	U545	A454	U360	C275
	A1431	G1331	A1134	U1065	A981	C	C806	U639	C640	A547	C455	A362	U276
A1635	G1432	G1332	C1135	U1066	C982		U807						
A1636	A1433	U1340	G1139	U1067	A984								
C1645	C1434	G1342	U1249	A1068									
C1646	U1435	A1342	C1251	A1069									
U1648			U1141	A1070									



G105  
G106  
G107  
A108  
A109  
G110  
U111  
G112  
G113  
C114  
A115  
G116  
G117  
G118  
A119  
A120

• Molecule 27: 50S ribosomal protein L2

Chain C: 77% 22% ..

MET A1 V2 F7 R12 R13 R14 V15 V16 H24 E34 K38 N43 N44 N45 I48 B51 Y61 K70 R73 E78 E81 E86 L92 L104 A105 P106 L109 L129 P130 M131 R132 V143 K149 A154 V161 Q162

A165 G168 T172 L173 R174 R175 R176 E179 M180 R181 G195 N196 M200 L201 R202 V203 L204 G205 I48 K206 W212 R216 R220 G221 T222 H231 E235 F239 V244 T245 P246 Q250 T251 K252 R257 S258 N259 K260 R261 R269 R270 S271 LYS

• Molecule 28: 50S ribosomal protein L3

Chain D: 76% 22% .

M1 L4 R13 T16 V20 V29 E30 A31 N32 R33 V34 Q36 L40 D43 G44 Y45 I48 Q49 V50 T51 T52 G53 A54 K55 H67 V73 G76 R77 W80 E81 A85 E86 G87 E88 F101 V104 T110 K114 F118 T121

T133 H134 G135 P143 Q148 N149 Q150 T151 P152 R169 R179 L188 A196 P205 A209

• Molecule 29: 50S ribosomal protein L4

Chain E: 75% 23% .

M1 E2 L3 D7 T18 F19 V31 R40 Q41 G42 T43 R49 V52 K63 G71 K74 S75 P76 S80 G81 G82 V83 T84 R88 P89 Q90 V96 N97 M100 Y101 R102 G103 A104 L105 K106 R117 V120 V121 E122 K123 A128 P129 K130 T131

L143 L144 D145 V146 L147 T148 L159 A160 A161 R162 N163 K166 V169 R170 D176 P177 V178 A182 K185 L200 A201

• Molecule 30: 50S ribosomal protein L5

Chain F: 60% 34% ..

MET A1 R2 L3 H4 D5 Y6 Y7 K8 D9 V12 M16 N20 V24 V27 P28 R29 V39 G40 E41 L48 N51 B55 L56 T67 R70 V73 I78 P83 T84 G85 G86 K87 V88 T89 I90 R91 G92 M95 V96 E97 E100 R101 L102

A106 I110 F113 L116 S120 M126 Y127 S128 M129 G130 R132 V131 E133 Q134 I136 F137 P138 E139 I140 D141 K144 R147 V148 R149 G150 I153 T156 G165 L168 D173 F174 P175 F176 R177 LYS

• Molecule 31: 50S ribosomal protein L6

Chain G: 80% 19% ..

MET S1 I23 R34 N37 D38 E41 V42 V43 H44 A45 F51 G52 G53 R54 L70 L71 M74 F82 L88 R94 A95 I102 F108 D113 T126 Q127 T128 E129 I130 K133 D136 K137 Q138 V139 P153 E154 P155 K159 G160 V161



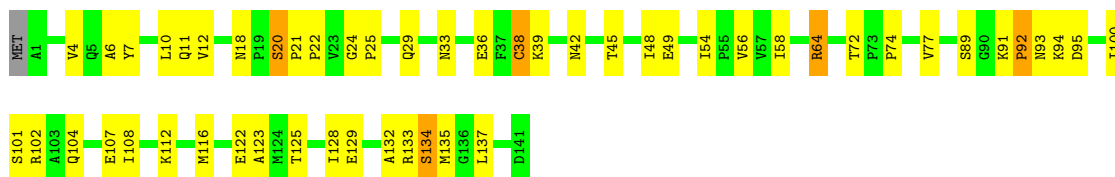
- Molecule 32: 50S ribosomal protein L9

Chain H: 80% 18%



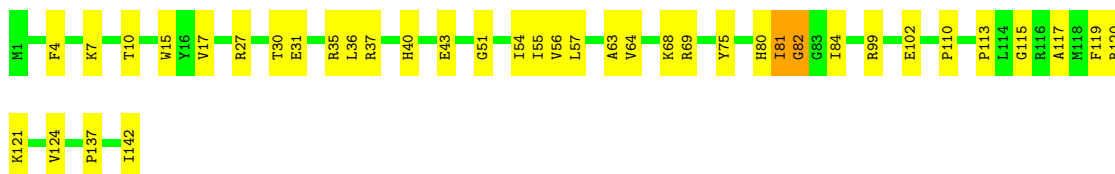
- Molecule 33: 50S ribosomal protein L11

Chain I: 63% 33%



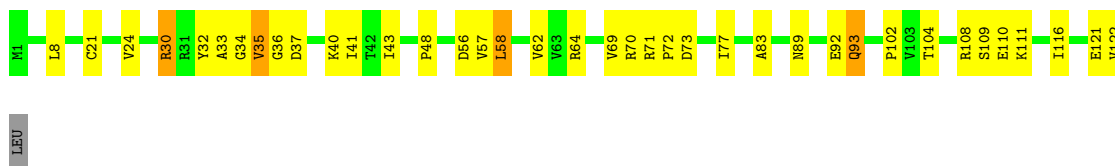
- Molecule 34: 50S ribosomal protein L13

Chain J: 73% 26%



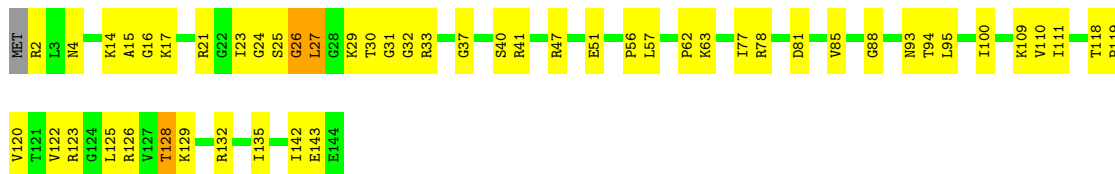
- Molecule 35: 50S ribosomal protein L14

Chain K: 68% 28%

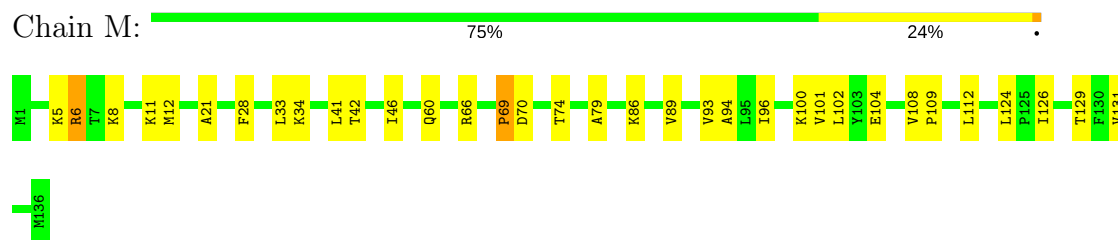


- Molecule 36: 50S ribosomal protein L15

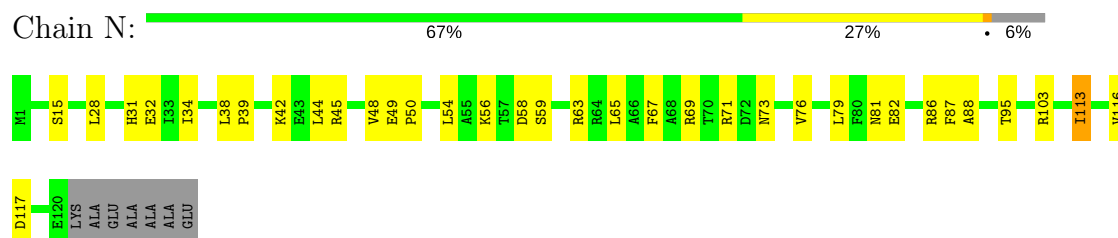
Chain L: 64% 33%



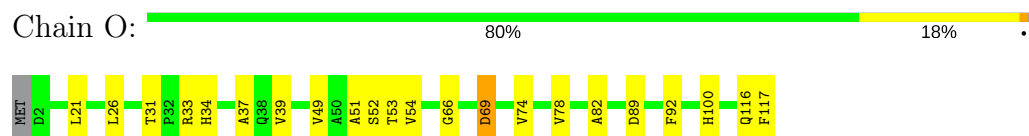
- Molecule 37: 50S ribosomal protein L16



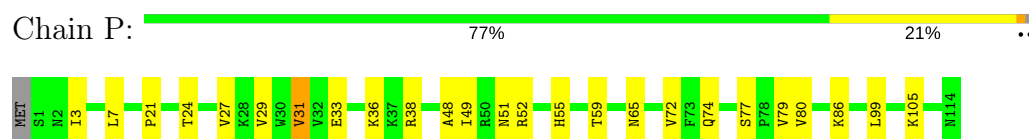
- Molecule 38: 50S ribosomal protein L17



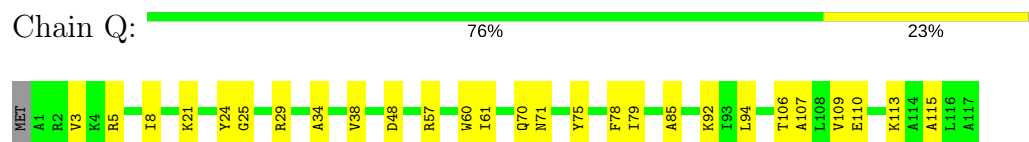
- Molecule 39: 50S ribosomal protein L18



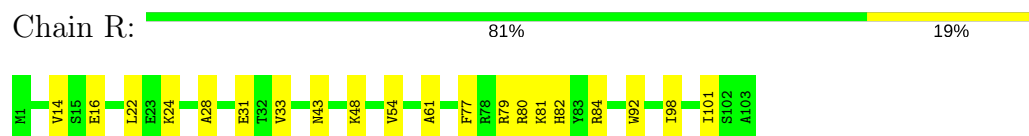
- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L22





- Molecule 44: 50S ribosomal protein L23

Chain T: 70% 20% 7%



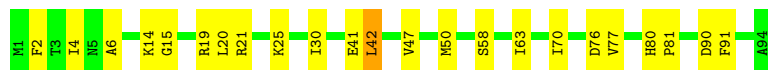
- Molecule 45: 50S ribosomal protein L24

Chain U: 73% 24%



- Molecule 46: 50S ribosomal protein L25

Chain V: 76% 23%



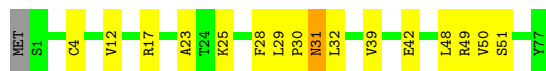
- Molecule 47: 50S ribosomal protein L27

Chain W: 73% 15% 12%



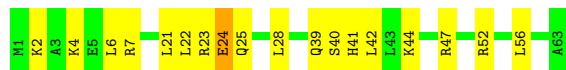
- Molecule 48: 50S ribosomal protein L28

Chain X: 78% 19%



- Molecule 49: 50S ribosomal protein L29

Chain Y: 71% 27%

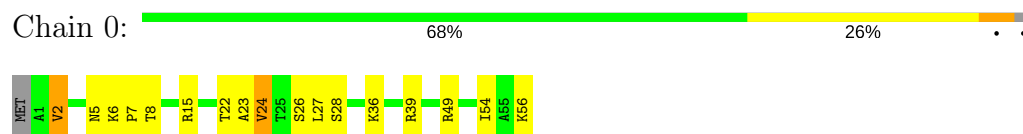


- Molecule 50: 50S ribosomal protein L30

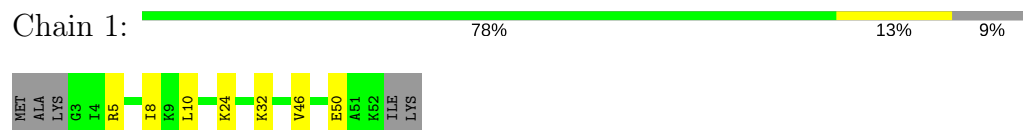
Chain Z: 80% 19%



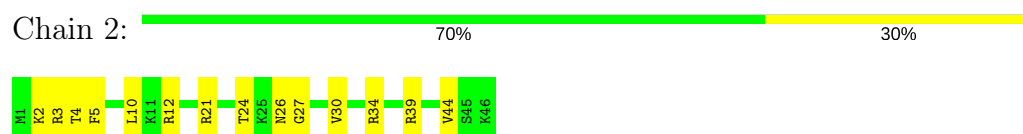
- Molecule 51: 50S ribosomal protein L32



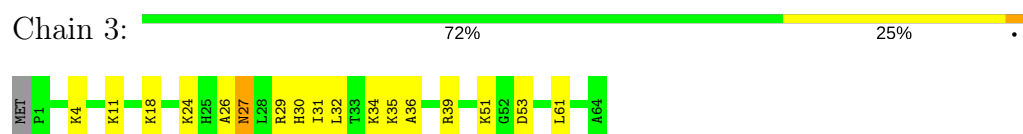
- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34



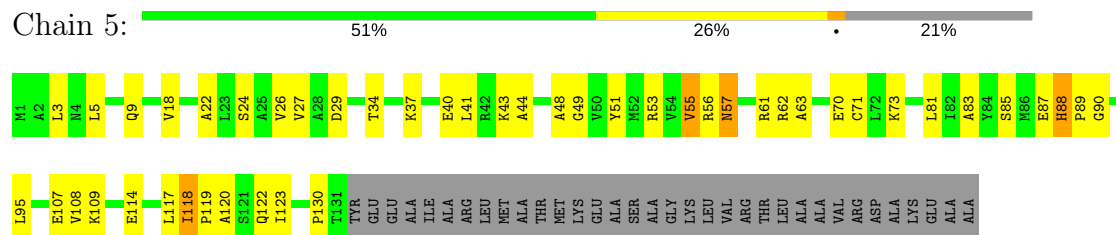
- Molecule 54: 50S ribosomal protein L35



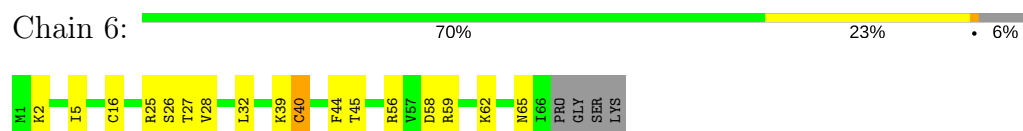
- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L10



- Molecule 57: 50S ribosomal protein L31





- Molecule 58: 50S ribosomal protein L7/L12

Chain 7:  99%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	78186	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125085	Depositor
Image detector	FEI FALCON II (4k x 4k)	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, OMG, 5MC, MA6, H2U, OMC, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 4SU, 7MG, 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	0.39	1/36701 (0.0%)	0.85	12/57246 (0.0%)
10	p	0.33	0/659	0.46	0/884
11	q	0.28	0/657	0.46	0/881
12	r	0.28	0/511	0.43	0/689
13	t	0.38	0/671	0.48	0/888
14	u	0.29	0/500	0.42	0/668
15	v	0.42	1/1747 (0.1%)	0.82	0/2721
16	x	0.58	1/210 (0.5%)	0.78	0/324
17	w	0.17	0/2594	0.35	0/3251
18	c	0.32	0/1651	0.46	0/2225
19	g	0.36	0/1195	0.50	0/1602
2	b	0.30	0/1735	0.44	0/2338
20	i	0.27	0/1034	0.45	0/1375
21	j	0.36	0/796	0.54	0/1077
22	m	0.36	0/892	0.50	0/1193
23	n	0.27	0/811	0.40	0/1081
24	s	0.28	0/652	0.44	0/877
25	A	0.47	1/69174 (0.0%)	0.90	51/107910 (0.0%)
26	B	0.38	1/2876 (0.0%)	0.86	0/4483
27	C	0.31	0/2121	0.47	0/2852
28	D	0.34	0/1586	0.48	0/2134
29	E	0.26	0/1571	0.41	0/2113
3	d	0.28	0/1665	0.44	0/2227
30	F	0.31	0/1434	0.47	0/1926
31	G	0.35	0/1343	0.47	0/1816
32	H	0.23	0/1122	0.40	0/1515
33	I	0.23	0/1046	0.44	0/1410
34	J	0.29	0/1152	0.43	0/1551
35	K	0.28	0/947	0.41	0/1268
36	L	0.26	0/1054	0.45	0/1403
37	M	0.32	0/1093	0.46	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	N	0.28	0/973	0.44	0/1301
39	O	0.33	0/902	0.44	0/1209
4	e	0.32	0/1154	0.46	0/1554
40	P	0.28	0/929	0.43	0/1242
41	Q	0.34	0/960	0.43	0/1278
42	R	0.34	0/829	0.52	0/1107
43	S	0.28	0/864	0.47	0/1156
44	T	0.29	0/744	0.45	0/994
45	U	0.35	0/787	0.44	0/1051
46	V	0.31	0/766	0.45	0/1025
47	W	0.33	0/582	0.47	0/769
48	X	0.28	0/635	0.40	0/848
49	Y	0.33	0/510	0.46	0/677
5	f	0.35	0/835	0.48	0/1128
50	Z	0.25	0/453	0.41	0/605
51	0	0.26	0/450	0.41	0/599
52	1	0.26	0/416	0.41	0/554
53	2	0.29	0/380	0.44	0/498
54	3	0.27	0/513	0.43	0/676
55	4	0.28	0/303	0.41	0/397
56	5	0.25	0/1001	0.45	0/1350
57	6	0.33	0/531	0.54	0/709
58	7	0.33	0/275	0.73	0/342
6	h	0.27	0/989	0.45	0/1326
7	k	0.28	0/885	0.48	0/1195
8	l	0.29	0/969	0.47	0/1300
9	o	0.32	0/722	0.44	0/964
All	All	0.40	5/160557 (0.0%)	0.79	63/239242 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	1	U	OP3-P	-10.61	1.48	1.61
15	v	1	C	OP3-P	-10.59	1.48	1.61
25	A	1	G	OP3-P	-10.57	1.48	1.61
1	a	2	A	OP3-P	-10.49	1.48	1.61
16	x	14	U	C1'-N1	5.54	1.57	1.48

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	974	G	N1-C6-O6	9.38	125.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1936	A	N1-C6-N6	9.08	124.05	118.60
25	A	1936	A	C2-N3-C4	-7.41	106.90	110.60
25	A	783	A	N7-C8-N9	7.26	117.43	113.80
1	a	1297	G	P-O3'-C3'	7.22	128.36	119.70
25	A	783	A	C5-N7-C8	-7.16	100.32	103.90
25	A	62	U	C2-N1-C1'	6.97	126.06	117.70
1	a	530	G	P-O5'-C5'	-6.91	109.85	120.90
25	A	974	G	C6-C5-N7	-6.75	126.35	130.40
1	a	1491	G	C4'-C3'-O3'	6.63	126.26	113.00
25	A	62	U	N1-C2-O2	6.49	127.34	122.80
25	A	984	A	C2-N3-C4	-6.48	107.36	110.60
25	A	1779	U	C5-C6-N1	-6.48	119.46	122.70
25	A	783	A	N1-C6-N6	6.47	122.48	118.60
25	A	2884	U	C2-N1-C1'	6.39	125.37	117.70
25	A	2884	U	N1-C2-O2	6.24	127.17	122.80
25	A	2076	U	C2-N1-C1'	6.08	125.00	117.70
25	A	1313	U	C2-N1-C1'	5.96	124.85	117.70
25	A	62	U	N3-C2-O2	-5.94	118.04	122.20
25	A	2682	A	C8-N9-C4	5.77	108.11	105.80
25	A	974	G	N7-C8-N9	5.71	115.96	113.10
1	a	529	G	O3'-P-O5'	-5.70	93.17	104.00
1	a	1158	C	C2-N1-C1'	5.66	125.02	118.80
25	A	2501	C	C2-N1-C1'	-5.64	112.59	118.80
25	A	2884	U	N3-C2-O2	-5.62	118.27	122.20
1	a	246	A	P-O3'-C3'	5.60	126.42	119.70
25	A	458	G	C4-N9-C1'	-5.60	119.22	126.50
25	A	2542	A	C8-N9-C4	5.60	108.04	105.80
25	A	2867	G	C6-C5-N7	5.51	133.71	130.40
25	A	2867	G	C4-N9-C1'	-5.50	119.35	126.50
25	A	2867	G	N3-C4-N9	-5.49	122.70	126.00
25	A	669	G	C8-N9-C1'	-5.49	119.86	127.00
25	A	974	G	C4-C5-N7	5.44	112.98	110.80
25	A	783	A	C8-N9-C4	-5.41	103.64	105.80
25	A	783	A	C5-C6-N1	-5.40	115.00	117.70
25	A	1142	A	OP1-P-O3'	5.38	117.05	105.20
25	A	1936	A	C4-C5-N7	5.34	113.37	110.70
25	A	752	A	P-O3'-C3'	5.33	126.09	119.70
25	A	1936	A	C5-N7-C8	-5.29	101.25	103.90
25	A	2501	C	C5-C6-N1	-5.29	118.36	121.00
25	A	669	G	C4-N9-C1'	5.26	133.34	126.50
25	A	1020	A	P-O3'-C3'	5.21	125.95	119.70
1	a	1201	A	P-O3'-C3'	5.17	125.90	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2712	C	P-O3'-C3'	5.15	125.88	119.70
25	A	271	G	OP1-P-O3'	5.15	116.53	105.20
1	a	1158	C	N1-C2-O2	5.15	121.99	118.90
25	A	783	A	C2-N3-C4	-5.15	108.03	110.60
25	A	974	G	C5-C6-O6	-5.15	125.51	128.60
25	A	2759	G	N1-C2-N3	5.12	126.97	123.90
1	a	1306	A	N7-C8-N9	5.11	116.35	113.80
25	A	1475	G	OP2-P-O3'	5.10	116.41	105.20
25	A	974	G	C5-C6-N1	-5.09	108.96	111.50
25	A	451	U	C5-C6-N1	-5.08	120.16	122.70
25	A	1652	A	C8-N9-C4	5.08	107.83	105.80
1	a	246	A	OP1-P-O3'	5.08	116.37	105.20
1	a	16	A	C8-N9-C4	5.07	107.83	105.80
25	A	458	G	O4'-C1'-N9	5.04	112.23	108.20
25	A	543	G	C5-C6-O6	-5.04	125.58	128.60
25	A	1313	U	N1-C2-O2	5.03	126.32	122.80
25	A	1936	A	C6-C5-N7	-5.02	128.79	132.30
25	A	454	A	OP2-P-O3'	5.02	116.23	105.20
25	A	2076	U	N1-C2-O2	5.01	126.31	122.80
1	a	960	U	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33029	0	16642	0	0
2	b	1704	0	1732	0	0
3	d	1643	0	1710	0	0
4	e	1141	0	1169	0	0
5	f	817	0	808	0	0
6	h	979	0	1034	0	0
7	k	869	0	878	0	0
8	l	955	0	1019	0	0
9	o	714	0	737	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	p	649	0	666	0	0
11	q	648	0	691	0	0
12	r	504	0	502	0	0
13	t	665	0	714	0	0
14	u	495	0	486	0	0
15	v	1644	0	840	0	0
16	x	189	0	96	0	0
17	w	2590	0	731	0	0
18	c	1624	0	1699	0	0
19	g	1181	0	1240	0	0
20	i	1022	0	1070	0	0
21	j	786	0	828	0	0
22	m	883	0	944	0	0
23	n	799	0	841	0	0
24	s	637	0	665	0	0
25	A	62276	0	31346	868	0
26	B	2572	0	1302	27	0
27	C	2082	0	2157	39	0
28	D	1565	0	1616	34	0
29	E	1552	0	1619	30	0
30	F	1410	0	1447	46	0
31	G	1323	0	1374	22	0
32	H	1111	0	1148	18	0
33	I	1032	0	1088	34	0
34	J	1129	0	1162	30	0
35	K	938	0	1012	24	0
36	L	1045	0	1117	35	0
37	M	1074	0	1157	20	0
38	N	960	0	1000	25	0
39	O	892	0	923	13	0
40	P	917	0	965	23	0
41	Q	947	0	1022	21	0
42	R	816	0	839	13	0
43	S	857	0	922	22	0
44	T	738	0	807	17	0
45	U	779	0	834	16	0
46	V	753	0	780	14	0
47	W	575	0	592	9	0
48	X	625	0	655	12	0
49	Y	509	0	543	10	0
50	Z	449	0	491	7	0
51	0	444	0	461	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	1	409	0	440	4	0
53	2	377	0	418	18	0
54	3	504	0	574	17	0
55	4	302	0	343	12	0
56	5	988	0	1025	33	0
57	6	522	0	524	13	0
58	7	276	0	79	0	0
All	All	148915	0	99524	1374	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 10.

All (1374) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1422:G:OP1	35:K:48:PRO:HG3	96.78	1.14
25:A:1055:G:H1	25:A:1104:C:H42	1.11	0.96
48:X:17:ARG:HE	48:X:23:ALA:HB2	1.29	0.94
25:A:704:G:H2'	25:A:726:G:H22	1.30	0.93
25:A:335:C:H4'	25:A:1434:A:O4'	117.09	0.90
25:A:335:C:O2'	25:A:1433:A:N3	111.47	0.89
30:F:134:GLN:NE2	30:F:149:ARG:O	2.06	0.89
25:A:585:G:N7	41:Q:5:ARG:NH1	2.26	0.83
25:A:1432:G:H5''	40:P:105:LYS:HG2	53.17	0.83
42:R:14:VAL:HG21	42:R:98:ILE:HG13	1.61	0.82
45:U:65:GLN:HB2	45:U:68:ASN:OD1	1.80	0.81
25:A:2848:G:H2'	25:A:2867:G:N2	1.95	0.81
25:A:2333:A:H4'	25:A:2334:U:O5'	1.81	0.81
25:A:1103:A:H3'	25:A:1104:C:H5''	1.62	0.81
25:A:1060:U:H5'	25:A:1062:G:H5'	1.63	0.81
28:D:13:ARG:HH11	40:P:55:HIS:HA	1.44	0.79
25:A:1845:G:N2	25:A:1895:C:O2	2.14	0.79
25:A:1399:C:N3	25:A:1401:G:C6	6.99	0.79
25:A:1936:A:H2	25:A:1943:U:H3	1.31	0.78
25:A:2220:U:H4'	32:H:97:ARG:HH21	1.48	0.78
43:S:53:SER:O	43:S:57:ASN:HB2	1.83	0.78
34:J:80:HIS:O	34:J:82:GLY:N	2.15	0.78
25:A:335:C:H4'	25:A:1434:A:C4'	117.94	0.77
29:E:146:VAL:HG12	29:E:185:LYS:HB2	1.65	0.77
56:5:87:GLU:HG2	56:5:95:LEU:HD12	1.66	0.77
25:A:1041:G:H1	25:A:1114:C:H42	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:117:ALA:HA	34:J:120:ARG:HH21	1.49	0.76
27:C:106:PRO:HD2	27:C:109:LEU:HD22	1.66	0.76
25:A:2345:G:H4'	25:A:2346:A:H5''	1.67	0.75
28:D:35:THR:OG1	28:D:49:GLN:HG2	1.86	0.74
25:A:1532:A:H2	25:A:1539:U:H3	1.34	0.74
25:A:1022:G:H4'	25:A:1023:U:O5'	1.88	0.73
25:A:2848:G:H2'	25:A:2867:G:H22	1.50	0.72
25:A:458:G:O2'	25:A:459:U:OP2	2.06	0.72
25:A:1090:A:H61	25:A:1101:U:H3	1.35	0.72
25:A:2808:G:H4'	25:A:2809:A:O5'	1.88	0.72
49:Y:6:LEU:HD13	49:Y:56:LEU:HD22	1.72	0.72
43:S:73:LYS:HB2	43:S:106:VAL:HB	1.71	0.72
36:L:62:PRO:HB2	54:3:29:ARG:HH11	1.55	0.72
25:A:572:A:OP2	42:R:80:ARG:NH2	2.22	0.71
25:A:1059:G:H22	33:I:128:ILE:HG12	1.53	0.71
25:A:530:G:O3'	25:A:530:G:OP1	5.94	0.71
25:A:704:G:H1'	25:A:727:A:N6	2.05	0.71
33:I:91:LYS:HG3	33:I:94:LYS:HE2	1.70	0.71
52:1:8:ILE:HD13	52:1:24:LYS:HE3	1.71	0.71
30:F:3:LEU:HA	30:F:6:TYR:HB3	1.73	0.71
40:P:33:GLU:HB2	40:P:36:LYS:HB2	1.71	0.71
35:K:69:VAL:HG21	35:K:104:THR:HG21	1.72	0.71
43:S:4:ILE:HG22	43:S:106:VAL:HG22	1.71	0.71
46:V:20:LEU:HD11	46:V:41:GLU:HG3	1.72	0.71
45:U:32:LYS:HB3	45:U:63:ALA:HB1	1.73	0.70
25:A:2682:A:H61	25:A:2728:U:H1'	1.56	0.70
25:A:328:U:H4'	45:U:65:GLN:HE21	1.55	0.70
25:A:1188:U:C2'	25:A:1189:A:H5'	2.21	0.70
25:A:2644:G:C2'	25:A:2645:G:H5'	2.22	0.70
25:A:284:U:H3	25:A:356:G:H1	1.40	0.69
25:A:568:U:H1'	25:A:2030:6MZ:H9C1	1.72	0.69
25:A:1341:G:N3	44:T:59:ASN:OD1	2.25	0.69
25:A:1213:A:N6	25:A:1236:G:H1'	2.07	0.69
25:A:1432:G:C5'	40:P:105:LYS:HG2	54.12	0.69
27:C:131:MET:HE1	27:C:143:VAL:HG13	1.74	0.69
25:A:910:A:H62	37:M:12:MET:HA	1.58	0.69
25:A:2133:G:H21	25:A:2158:A:H61	1.41	0.68
53:2:12:ARG:HE	53:2:44:VAL:HG21	1.58	0.68
25:A:1046:A:H4'	56:5:61:ARG:HB3	1.75	0.68
25:A:1399:C:C4	25:A:1401:G:C6	6.85	0.68
25:A:532:A:H3'	25:A:532:A:N3	4.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:196:ASN:OD1	27:C:196:ASN:O	2.11	0.68
25:A:1422:G:OP1	35:K:48:PRO:CG	97.57	0.68
25:A:2331:G:H4'	47:W:39:THR:H	1.57	0.68
25:A:1565:C:O2'	25:A:1566:A:H8	1.77	0.68
25:A:545:U:H3	25:A:548:G:H1	1.41	0.68
25:A:776:G:H4'	25:A:777:G:O5'	1.94	0.68
25:A:107:G:H2'	25:A:108:G:H8	1.58	0.68
25:A:2339:C:H2'	25:A:2340:A:H8	1.59	0.68
25:A:1613:G:H4'	53:2:3:ARG:HE	1.58	0.67
25:A:1011:G:O2'	25:A:1013:C:H5''	1.93	0.67
25:A:703:U:H2'	25:A:704:G:O4'	1.94	0.67
25:A:1055:G:H1	25:A:1104:C:N4	1.90	0.67
25:A:1478:G:H1	25:A:1513:U:H3	1.42	0.67
25:A:2291:U:H2'	25:A:2292:U:C6	2.29	0.67
25:A:947:A:HO2'	25:A:984:A:H2	1.43	0.67
25:A:2759:G:H21	31:G:138:GLN:NE2	1.93	0.67
27:C:165:ALA:HB3	27:C:172:THR:HB	1.76	0.67
25:A:2564:A:OP1	25:A:2648:G:H4'	1.95	0.67
25:A:1999:C:H5''	25:A:2723:C:O2'	1.95	0.67
25:A:2786:U:H2'	25:A:2787:C:H6	1.60	0.66
25:A:530:G:N3	25:A:530:G:H3'	5.46	0.66
35:K:40:LYS:HE3	35:K:57:VAL:HG12	1.76	0.66
25:A:51:G:H4'	25:A:52:A:H5'	1.78	0.66
25:A:335:C:C5'	25:A:1434:A:H4'	120.29	0.66
25:A:841:G:H2'	25:A:842:U:C6	2.31	0.66
27:C:48:ILE:HD11	27:C:51:ARG:HA	1.78	0.66
25:A:1530:G:N2	25:A:1542:U:H1'	2.11	0.66
30:F:28:PRO:HB2	30:F:168:LEU:HD22	1.77	0.65
25:A:1701:A:H2'	25:A:1702:G:H5'	1.78	0.65
25:A:218:A:OP2	25:A:218:A:H8	1.79	0.65
25:A:5:A:H2'	25:A:6:A:H8	1.62	0.65
30:F:140:ILE:HG22	30:F:142:TYR:H	1.60	0.65
25:A:499:U:H5''	45:U:42:LYS:HE2	1.78	0.65
25:A:503:A:H1'	25:A:506:G:OP2	1.96	0.65
25:A:948:C:O2	25:A:984:A:O2'	2.14	0.65
34:J:17:VAL:HG23	34:J:137:PRO:HB2	1.78	0.65
46:V:21:ARG:HA	46:V:25:LYS:O	1.95	0.65
53:2:3:ARG:HG3	53:2:5:PHE:H	1.61	0.65
25:A:248:G:O5'	25:A:249:C:H5'	1.96	0.65
25:A:454:A:H4'	25:A:455:C:OP2	1.97	0.65
25:A:655:A:H4'	25:A:656:G:H5'	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2788:C:H2'	25:A:2789:C:C6	2.32	0.65
33:I:101:SER:HB3	33:I:104:GLN:OE1	1.97	0.65
25:A:2428:G:H5''	25:A:2429:G:O5'	1.96	0.65
25:A:5:A:H2'	25:A:6:A:C8	2.31	0.65
25:A:1212:G:O2'	25:A:1236:G:N2	2.29	0.65
25:A:1930:G:O2'	25:A:1931:U:P	2.55	0.65
38:N:69:ARG:O	38:N:71:ARG:N	2.28	0.65
25:A:1474:U:H4'	25:A:1701:A:N3	71.19	0.65
25:A:2131:U:O5'	25:A:2133:G:H4'	1.97	0.65
25:A:2800:A:H3'	25:A:2801:G:H5'	1.77	0.64
25:A:753:A:OP2	25:A:753:A:H8	1.79	0.64
25:A:704:G:H2'	25:A:726:G:N2	2.10	0.64
32:H:9:VAL:HB	32:H:13:GLY:HA3	1.78	0.64
34:J:117:ALA:HA	34:J:120:ARG:NH2	2.12	0.64
25:A:2537:U:H2'	25:A:2538:C:C6	2.33	0.64
51:O:54:ILE:HG13	51:O:56:LYS:HB3	1.80	0.64
25:A:2808:G:HO2'	25:A:2809:A:H8	1.46	0.64
33:I:122:GLU:O	33:I:125:THR:HB	1.97	0.64
25:A:2584:U:H3'	25:A:2585:U:H5''	1.80	0.64
25:A:189:G:H1	25:A:205:G:HO2'	1.45	0.63
25:A:1028:A:N6	25:A:1125:G:H2'	2.13	0.63
25:A:923:G:H2'	25:A:924:G:H8	1.63	0.63
25:A:1186:G:H2'	25:A:1187:G:O4'	1.99	0.63
25:A:120:U:H5''	25:A:122:G:OP2	1.98	0.63
25:A:859:G:O2'	25:A:860:U:P	2.56	0.63
25:A:2097:A:H2'	25:A:2098:U:O4'	1.98	0.63
25:A:2712:C:O2'	25:A:2713:U:H5'	1.99	0.62
26:B:94:A:OP1	46:V:19:ARG:HD3	1.99	0.62
44:T:58:VAL:HG22	44:T:85:VAL:HG13	1.80	0.62
25:A:2867:G:O2'	25:A:2868:A:H8	1.82	0.62
25:A:370:G:O2'	25:A:424:G:OP1	2.17	0.62
25:A:2394:C:H5''	36:L:63:LYS:HE3	1.81	0.62
25:A:1188:U:H2'	25:A:1189:A:H5'	1.82	0.62
25:A:404:A:H1'	25:A:406:G:C4	2.33	0.62
36:L:93:ASN:O	36:L:95:LEU:N	2.30	0.62
56:5:73:LYS:HB3	56:5:117:LEU:HD11	1.81	0.62
26:B:118:C:H2'	26:B:119:A:C8	2.35	0.62
33:I:33:ASN:HB2	33:I:64:ARG:HH22	1.64	0.62
25:A:2638:G:HO2'	25:A:2639:A:H8	1.48	0.62
25:A:1062:G:H22	33:I:134:SER:HB2	1.65	0.62
25:A:839:U:H2'	25:A:840:C:C6	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:145:ASP:HA	29:E:166:LYS:HB3	1.81	0.62
38:N:58:ASP:OD1	38:N:63:ARG:NH2	2.33	0.62
25:A:1385:A:OP1	25:A:1385:A:H4'	1.99	0.61
25:A:2786:U:H2'	25:A:2787:C:C6	2.35	0.61
25:A:1019:U:H3	25:A:1142:A:N6	1.98	0.61
25:A:2346:A:H3'	25:A:2347:C:C5'	2.31	0.61
40:P:59:THR:HG22	40:P:72:VAL:HG12	1.82	0.61
25:A:1542:U:H2'	25:A:1543:G:O4'	1.99	0.61
47:W:33:ILE:HD11	47:W:78:ILE:HD11	1.82	0.61
25:A:704:G:H1'	25:A:727:A:H61	1.64	0.61
25:A:1081:U:H4'	33:I:123:ALA:HB1	1.81	0.61
42:R:82:HIS:O	42:R:82:HIS:ND1	2.31	0.61
25:A:242:G:HO2'	25:A:243:U:P	2.23	0.61
25:A:1816:C:N4	27:C:34:GLU:OE2	2.33	0.61
55:4:36:ARG:HG2	55:4:37:GLN:H	1.66	0.61
25:A:2074:U:H2'	25:A:2075:U:C6	2.36	0.61
38:N:73:ASN:HA	38:N:76:VAL:HG12	1.80	0.61
56:5:53:ARG:HB3	56:5:55:VAL:HG13	1.82	0.60
28:D:54:ALA:HA	28:D:76:GLY:HA2	1.83	0.60
25:A:2517:C:O3'	25:A:2518:A:H3'	2.00	0.60
43:S:59:GLU:HA	43:S:64:ALA:HA	1.83	0.60
25:A:2104:C:H2'	25:A:2105:U:C6	2.36	0.60
25:A:2267:A:H5''	25:A:2268:A:H5'	1.83	0.60
25:A:2391:G:H2'	25:A:2424:C:H41	1.65	0.60
28:D:4:LEU:HD23	28:D:29:VAL:HG11	1.82	0.60
25:A:2655:G:O2'	25:A:2656:U:P	2.59	0.60
25:A:878:A:H3'	25:A:879:G:H8	1.64	0.60
37:M:21:ALA:HB1	37:M:100:LYS:HD3	1.83	0.60
25:A:372:G:O2'	25:A:373:U:P	2.60	0.60
25:A:242:G:O2'	25:A:243:U:P	2.59	0.60
25:A:144:A:H4'	44:T:2:ILE:HD11	1.83	0.60
57:6:62:LYS:C	57:6:65:ASN:HD21	2.04	0.60
25:A:221:A:N1	25:A:265:A:O2'	2.33	0.60
46:V:76:ASP:HB3	46:V:90:ASP:HB2	1.83	0.60
25:A:546:U:H2'	25:A:547:A:H4'	1.84	0.60
25:A:828:U:O4	25:A:858:G:N2	40.59	0.60
25:A:1086:A:N3	25:A:1086:A:H2'	2.17	0.59
38:N:28:LEU:HD23	38:N:48:VAL:HG21	1.82	0.59
25:A:1490:A:H62	27:C:73:ILE:HG23	1.67	0.59
25:A:1026:G:H2'	25:A:1027:A:H8	1.65	0.59
25:A:1386:C:H2'	25:A:1387:A:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Y:24:GLU:O	49:Y:28:LEU:HB2	2.01	0.59
25:A:100:U:H4'	25:A:101:A:O4'	2.01	0.59
25:A:437:U:H2'	25:A:438:G:H8	1.67	0.59
25:A:639:U:H2'	25:A:640:C:C6	2.38	0.59
25:A:1019:U:H2'	25:A:1020:A:H8	1.66	0.59
25:A:2427:C:H5'	25:A:2429:G:H5'	1.84	0.59
25:A:476:G:N1	25:A:479:A:OP2	2.36	0.59
28:D:121:THR:HG21	28:D:143:PRO:HB3	1.85	0.59
25:A:2238:G:N3	25:A:2238:G:H2'	2.17	0.59
33:I:135:MET:HB2	33:I:137:LEU:HG	1.85	0.59
46:V:4:ILE:HD13	46:V:47:VAL:HG22	1.84	0.59
25:A:2233:U:H2'	25:A:2234:G:C8	2.38	0.59
25:A:1779:U:H5	25:A:1784:A:N7	2.01	0.59
25:A:283:G:H1	25:A:357:C:H42	1.51	0.59
25:A:479:A:H4'	25:A:480:A:OP1	2.03	0.59
25:A:633:A:H2'	25:A:634:C:H5'	1.85	0.59
25:A:2267:A:H5''	25:A:2268:A:C5'	2.33	0.59
25:A:2557:G:H2'	25:A:2558:C:C6	2.38	0.59
25:A:84:A:H4'	25:A:85:G:O5'	2.03	0.59
25:A:2115:G:H4'	25:A:2166:U:O2	2.03	0.59
25:A:530:G:N3	25:A:530:G:C5'	5.89	0.59
25:A:847:U:O2	25:A:934:U:H1'	2.03	0.59
25:A:2305:U:H5''	30:F:130:GLY:HA3	1.85	0.59
33:I:102:ARG:HA	33:I:129:GLU:OE2	2.03	0.59
27:C:203:VAL:O	27:C:205:GLY:N	2.36	0.58
54:3:30:HIS:ND1	54:3:31:ILE:HG13	2.18	0.58
25:A:1432:G:O5'	40:P:105:LYS:HG3	53.43	0.58
25:A:265:A:H4'	25:A:266:G:OP1	2.03	0.58
27:C:244:VAL:HG12	27:C:250:GLN:HA	1.86	0.58
29:E:117:ARG:HH12	36:L:2:ARG:HG2	1.68	0.58
36:L:78:ARG:HB2	36:L:81:ASP:OD1	2.04	0.58
25:A:2326:C:O2'	25:A:2327:A:OP1	2.20	0.58
35:K:109:SER:O	35:K:111:LYS:N	2.35	0.58
25:A:2271:G:H5'	47:W:16:ARG:HD3	1.84	0.58
25:A:271:G:H4'	25:A:272:A:OP1	2.03	0.58
25:A:495:G:H1'	43:S:57:ASN:OD1	2.04	0.58
38:N:45:ARG:HG2	38:N:95:THR:HG21	1.86	0.58
25:A:2285:C:OP2	52:1:5:ARG:NH1	2.37	0.58
25:A:302:C:H2'	25:A:303:G:H8	1.69	0.58
25:A:466:A:OP1	53:2:34:ARG:NH1	2.37	0.58
25:A:1956:U:H2'	25:A:1957:C:H5'	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2427:C:H5''	25:A:2428:G:OP1	2.03	0.58
25:A:2554:U:H2'	25:A:2555:U:C6	2.39	0.58
25:A:434:U:O2'	25:A:436:C:N4	2.36	0.58
25:A:289:G:H2'	25:A:290:U:O4'	2.04	0.58
41:Q:70:GLN:C	41:Q:71:ASN:HD22	2.08	0.58
40:P:29:VAL:HG22	40:P:80:VAL:HA	1.85	0.57
40:P:31:VAL:HG13	40:P:38:ARG:HB3	1.86	0.57
25:A:770:G:H5''	53:2:10:LEU:HD23	1.86	0.57
31:G:41:GLU:HA	31:G:54:ARG:HH21	1.69	0.57
25:A:2391:G:H2'	25:A:2424:C:N4	2.20	0.57
29:E:148:ILE:O	29:E:169:VAL:HA	2.04	0.57
29:E:88:ARG:O	29:E:90:GLN:N	2.37	0.57
25:A:686:U:O2'	53:2:5:PHE:HA	2.05	0.57
25:A:2328:A:H2'	25:A:2329:U:C6	2.39	0.57
25:A:2591:C:H2'	25:A:2592:G:C8	2.39	0.57
25:A:1019:U:H2'	25:A:1020:A:C8	2.40	0.57
25:A:1614:A:N1	43:S:93:ALA:HB2	2.20	0.57
44:T:13:ALA:HB3	44:T:33:LYS:HD3	1.86	0.57
56:5:27:VAL:HG13	56:5:83:ALA:HB3	1.87	0.57
25:A:2776:A:H4'	25:A:2777:G:O5'	2.04	0.57
25:A:301:G:H4'	25:A:302:C:OP1	2.04	0.57
25:A:2867:G:O2'	25:A:2868:A:C8	2.57	0.57
29:E:3:LEU:HD13	29:E:120:VAL:HG21	1.85	0.57
38:N:44:LEU:HD23	38:N:113:ILE:HD13	1.87	0.57
49:Y:2:LYS:HB3	49:Y:52:ARG:HD3	1.87	0.57
25:A:2644:G:H2'	25:A:2645:G:H5'	1.86	0.57
33:I:74:PRO:HG2	33:I:77:VAL:HG22	1.87	0.57
25:A:1283:G:H1'	25:A:1329:U:O2	2.05	0.57
25:A:2518:A:N3	25:A:2518:A:H2'	2.20	0.57
25:A:281:C:N3	25:A:359:G:N2	2.53	0.57
34:J:102:GLU:HG3	34:J:119:PHE:HZ	1.69	0.57
34:J:36:LEU:O	34:J:51:GLY:HA3	2.05	0.57
43:S:3:THR:HG21	43:S:58:ALA:HB2	1.87	0.57
30:F:141:ASP:HB2	30:F:144:LYS:HD3	1.85	0.57
25:A:2297:A:N1	25:A:2321:U:H5	2.03	0.56
25:A:302:C:H2'	25:A:303:G:C8	2.39	0.56
56:5:34:THR:O	56:5:37:LYS:HB3	2.05	0.56
25:A:1689:A:H2'	25:A:1690:A:C8	2.41	0.56
25:A:204:A:H4'	25:A:205:G:OP1	2.06	0.56
25:A:2283:C:OP2	25:A:2390:U:H5	1.89	0.56
36:L:132:ARG:HG3	36:L:142:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:12:ARG:NE	53:2:44:VAL:HG21	2.19	0.56
25:A:1858:A:N6	25:A:1884:G:O2'	2.38	0.56
35:K:21:CYS:HA	35:K:41:ILE:HG22	1.87	0.56
25:A:1432:G:O3'	40:P:105:LYS:HD3	53.65	0.56
25:A:290:U:H2'	25:A:291:G:C8	2.41	0.56
25:A:368:A:H2'	25:A:369:U:O4'	2.06	0.56
25:A:394:C:H2'	25:A:395:U:O4'	2.05	0.56
25:A:630:G:N2	25:A:633:A:OP2	2.34	0.56
37:M:11:LYS:HD2	37:M:86:LYS:HG2	1.88	0.56
29:E:88:ARG:HD3	29:E:89:PRO:HD2	1.86	0.56
25:A:1199:U:H1'	41:Q:3:VAL:HG22	1.88	0.56
56:5:56:ARG:HD3	56:5:81:LEU:HD21	1.87	0.56
25:A:172:A:H2'	25:A:173:A:C8	2.40	0.56
25:A:859:G:O2'	25:A:860:U:OP2	2.23	0.56
25:A:969:G:H2'	25:A:970:U:C6	2.41	0.56
25:A:1396:U:H5''	25:A:1397:U:OP2	2.06	0.56
25:A:1869:G:H1'	25:A:1872:A:N6	2.20	0.56
25:A:2345:G:H4'	25:A:2346:A:C5'	2.36	0.56
25:A:861:A:H2'	25:A:862:G:O4'	2.05	0.56
35:K:40:LYS:NZ	35:K:89:ASN:OD1	2.38	0.56
25:A:1847:G:H21	25:A:1848:A:H62	1.54	0.56
25:A:162:U:O2'	25:A:163:C:H5'	2.06	0.55
28:D:1:MET:HG2	28:D:205:PRO:HG2	1.88	0.55
45:U:14:THR:OG1	45:U:68:ASN:ND2	2.38	0.55
25:A:1222:U:H2'	25:A:1223:G:C8	2.41	0.55
25:A:712:G:H2'	25:A:713:G:H5'	1.89	0.55
25:A:1040:A:H2	25:A:1115:G:H22	1.54	0.55
27:C:162:GLN:OE1	27:C:174:ARG:NH2	2.40	0.55
35:K:121:GLU:HG2	35:K:122:VAL:HG23	1.86	0.55
43:S:56:ALA:HA	43:S:59:GLU:HG2	1.87	0.55
46:V:42:LEU:HD13	46:V:47:VAL:HG21	1.86	0.55
53:2:24:THR:HG23	53:2:27:GLY:H	1.70	0.55
25:A:1315:C:H2'	25:A:1316:U:H6	1.71	0.55
25:A:2341:G:H2'	25:A:2342:C:O4'	2.07	0.55
36:L:14:LYS:O	36:L:16:GLY:N	2.39	0.55
25:A:1251:C:OP2	41:Q:5:ARG:HD2	2.06	0.55
25:A:1857:G:H2'	25:A:1884:G:N2	2.21	0.55
25:A:277:G:H1'	25:A:361:G:H1	1.71	0.55
26:B:118:C:H2'	26:B:119:A:H8	1.70	0.55
56:5:88:HIS:HB2	56:5:89:PRO:HD3	1.88	0.55
25:A:2339:C:H2'	25:A:2340:A:C8	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2469:A:N6	25:A:2481:G:O2'	2.40	0.55
25:A:373:U:O2'	25:A:423:A:H1'	2.07	0.55
33:I:33:ASN:HB2	33:I:64:ARG:HH12	1.72	0.55
38:N:34:ILE:HG13	38:N:113:ILE:HG23	1.88	0.55
56:5:37:LYS:HG3	56:5:41:LEU:HD12	1.88	0.55
25:A:1028:A:H61	25:A:1125:G:H2'	1.71	0.55
25:A:1434:A:H2'	25:A:1435:G:C8	2.42	0.55
27:C:154:ALA:HB2	27:C:161:VAL:HG23	1.88	0.55
30:F:116:LEU:HB2	30:F:175:PRO:HB2	1.87	0.55
25:A:2648:G:H2'	25:A:2649:C:O4'	2.06	0.55
25:A:468:G:H2'	25:A:469:G:H5'	1.88	0.55
56:5:29:ASP:HB2	56:5:56:ARG:HH12	1.72	0.55
25:A:1179:G:C4	25:A:1180:U:H1'	2.42	0.55
25:A:1434:A:H2'	25:A:1435:G:H8	1.71	0.55
25:A:1405:U:H2'	25:A:1406:U:C6	2.42	0.54
25:A:1794:A:H2'	25:A:1795:C:C6	2.42	0.54
28:D:49:GLN:HA	28:D:80:TRP:O	2.07	0.54
33:I:11:GLN:NE2	33:I:54:ILE:O	2.41	0.54
25:A:841:G:H2'	25:A:842:U:H6	1.72	0.54
37:M:74:THR:HA	37:M:89:VAL:HA	1.89	0.54
57:6:56:ARG:O	57:6:59:ARG:HB3	2.08	0.54
25:A:1330:C:O2'	25:A:1331:G:H5'	2.07	0.54
25:A:2114:A:N6	25:A:2117:A:H62	2.06	0.54
48:X:17:ARG:NE	48:X:23:ALA:HB2	2.11	0.54
25:A:1432:G:O5'	40:P:105:LYS:CG	54.12	0.54
25:A:493:G:H2'	25:A:494:G:O4'	2.07	0.54
30:F:39:VAL:HG12	30:F:85:GLY:HA2	1.90	0.54
32:H:84:ALA:HA	32:H:91:PHE:H	1.73	0.54
25:A:1565:C:O2'	25:A:1566:A:H2'	2.07	0.54
25:A:2756:U:H5''	55:4:19:ARG:HA	1.90	0.54
25:A:390:U:H4'	25:A:391:A:O5'	2.08	0.54
25:A:542:C:H3'	25:A:543:G:H5''	1.89	0.54
25:A:851:C:H2'	25:A:852:U:C6	2.42	0.54
25:A:1203:U:H1'	36:L:4:ASN:HB3	1.90	0.54
25:A:468:G:N7	53:2:39:ARG:NH2	2.56	0.54
25:A:2852:G:H2'	25:A:2853:C:O4'	2.07	0.54
55:4:37:GLN:HG3	55:4:38:GLY:H	1.72	0.53
25:A:1111:A:O2'	25:A:1112:G:OP1	2.22	0.53
25:A:1410:G:H2'	25:A:1411:U:C6	2.43	0.53
25:A:2576:G:H8	25:A:2581:G:O6	1.90	0.53
25:A:505:A:HO2'	25:A:509:C:HO2'	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:956:G:HO2'	25:A:959:A:H62	1.55	0.53
30:F:134:GLN:H	30:F:134:GLN:CD	2.12	0.53
35:K:33:ALA:HB1	35:K:37:ASP:HB2	1.90	0.53
37:M:28:PHE:HB2	37:M:104:GLU:OE1	2.08	0.53
49:Y:23:ARG:O	49:Y:25:GLN:N	2.41	0.53
25:A:1548:A:H2'	25:A:1549:A:C8	2.42	0.53
25:A:2746:U:H1'	31:G:138:GLN:HE22	1.72	0.53
25:A:549:G:O2'	25:A:550:C:OP1	2.26	0.53
25:A:1332:G:N3	25:A:1332:G:H5''	2.24	0.53
25:A:2832:U:H1'	25:A:2834:G:C4	2.43	0.53
25:A:107:G:H2'	25:A:108:G:C8	2.41	0.53
25:A:2198:A:HO2'	25:A:2199:A:H8	1.57	0.53
25:A:760:G:H2'	25:A:761:A:O4'	2.09	0.53
25:A:784:G:O2'	25:A:785:G:H5''	2.09	0.53
43:S:14:ALA:O	43:S:18:ARG:HB2	2.08	0.53
25:A:1021:A:N3	25:A:1022:G:H5''	2.22	0.53
25:A:1399:C:N3	25:A:1401:G:O6	6.65	0.53
32:H:113:SER:O	32:H:116:ARG:NH1	2.39	0.53
36:L:122:VAL:HB	36:L:142:ILE:HG23	1.89	0.53
56:5:37:LYS:O	56:5:41:LEU:HB2	2.08	0.53
25:A:1297:C:O2'	25:A:1302:A:N1	2.36	0.53
28:D:114:LYS:HE3	28:D:196:ALA:HB2	1.90	0.53
25:A:1130:U:O2'	25:A:1131:G:OP1	2.26	0.53
25:A:1177:G:H2'	25:A:1178:C:O4'	2.09	0.53
25:A:715:A:H2'	25:A:716:A:C8	3.34	0.53
25:A:743:A:OP1	28:D:135:GLY:HA2	2.08	0.53
25:A:747:5MC:CM5	25:A:2612:C:H4'	2.38	0.53
25:A:2296:U:H4'	25:A:2297:A:OP1	2.08	0.53
25:A:265:A:H1'	25:A:266:G:O4'	2.08	0.53
25:A:1565:C:O2'	25:A:1566:A:C8	2.60	0.52
29:E:31:VAL:HG21	29:E:104:ALA:HB2	1.91	0.52
51:0:54:ILE:HG23	51:0:56:LYS:H	1.74	0.52
53:2:34:ARG:HH21	53:2:39:ARG:HD3	1.74	0.52
25:A:1645:G:H5''	25:A:1646:C:H5'	1.91	0.52
25:A:2258:C:O2'	25:A:2426:A:H4'	2.09	0.52
25:A:2725:A:O2'	25:A:2726:A:O5'	2.16	0.52
25:A:2884:U:H3	51:0:39:ARG:CZ	2.22	0.52
25:A:413:C:H2'	25:A:414:C:C6	2.44	0.52
25:A:468:G:C2'	25:A:469:G:H5'	2.39	0.52
25:A:844:A:H61	25:A:934:U:H3	1.56	0.52
25:A:910:A:H2'	25:A:911:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:W:74:LYS:HD2	47:W:74:LYS:H	1.74	0.52
25:A:774:G:N2	25:A:787:C:O2'	2.41	0.52
26:B:41:G:H2'	26:B:41:G:N3	2.24	0.52
37:M:41:LEU:HD22	37:M:124:LEU:HD22	1.92	0.52
25:A:2230:G:H5''	48:X:29:LEU:HD12	1.92	0.52
25:A:530:G:N3	25:A:530:G:C3'	5.31	0.52
26:B:104:A:H2'	26:B:105:G:O4'	2.09	0.52
28:D:49:GLN:NE2	28:D:67:HIS:NE2	2.52	0.52
29:E:97:ASN:HB2	29:E:100:MET:HG3	1.92	0.52
25:A:2126:A:N1	25:A:2163:A:H1'	2.24	0.52
25:A:2406:A:H5'	25:A:2407:A:OP1	2.10	0.52
25:A:2678:C:H2'	25:A:2679:A:O4'	2.09	0.52
29:E:143:LEU:HB3	29:E:146:VAL:HG11	1.91	0.52
43:S:4:ILE:HD12	43:S:6:LYS:HE3	1.92	0.52
25:A:301:G:OP2	45:U:81:ARG:NH1	2.41	0.52
46:V:30:ILE:HD11	46:V:63:ILE:HD12	1.92	0.52
56:5:57:ASN:HB2	56:5:62:ARG:HD2	1.91	0.52
25:A:1796:U:H2'	25:A:1797:G:C8	2.44	0.52
25:A:947:A:O2'	25:A:984:A:H2	1.91	0.52
37:M:34:LYS:HE3	37:M:131:VAL:HG11	1.91	0.52
39:O:51:ALA:HB3	39:O:78:VAL:HG22	1.91	0.52
25:A:1475:G:O2'	25:A:1476:U:OP2	2.27	0.52
25:A:677:A:O2'	25:A:2071:A:H5'	2.10	0.52
40:P:48:ALA:HB3	40:P:59:THR:OG1	2.09	0.52
25:A:2346:A:H3'	25:A:2347:C:H5'	1.91	0.52
34:J:63:ALA:HA	34:J:69:ARG:HH22	1.75	0.52
39:O:69:ASP:N	39:O:69:ASP:OD1	2.42	0.52
56:5:48:ALA:HB3	56:5:51:TYR:CE2	2.45	0.52
56:5:48:ALA:HB3	56:5:51:TYR:HE2	1.75	0.52
25:A:335:C:H4'	25:A:1434:A:H4'	118.87	0.52
25:A:2303:G:H2'	25:A:2304:G:O4'	2.10	0.52
25:A:2625:G:H2'	25:A:2626:C:O4'	2.10	0.52
25:A:28:A:O2'	25:A:296:U:OP1	49.76	0.52
25:A:532:A:N3	25:A:532:A:C2'	3.12	0.52
39:O:53:THR:HG23	39:O:74:VAL:HG21	1.92	0.52
55:4:27:CYS:SG	55:4:30:GLU:N	2.79	0.52
25:A:1239:G:H2'	25:A:1240:U:O4'	2.10	0.52
25:A:2809:A:H2'	25:A:2810:A:C8	2.45	0.52
25:A:519:U:H5''	43:S:25:ARG:HH21	1.74	0.52
25:A:1682:G:C4	25:A:1757:A:H1'	2.45	0.51
25:A:32:C:N4	25:A:446:G:O2'	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:532:A:N3	25:A:532:A:C3'	4.07	0.51
25:A:722:A:H2'	25:A:723:C:O4'	2.10	0.51
32:H:70:GLU:HB2	32:H:134:VAL:HG21	1.91	0.51
44:T:70:HIS:O	44:T:72:GLN:N	2.43	0.51
47:W:33:ILE:HG22	47:W:34:VAL:HG23	1.92	0.51
30:F:110:ILE:O	30:F:113:PHE:HB2	2.10	0.51
31:G:23:ILE:HD11	31:G:42:VAL:HG11	1.93	0.51
25:A:1422:G:H5'	35:K:48:PRO:HG3	99.24	0.51
39:O:49:VAL:HG21	39:O:82:ALA:HA	1.91	0.51
56:5:114:GLU:HA	56:5:123:ILE:HB	1.90	0.51
25:A:1046:A:O2'	56:5:61:ARG:O	2.23	0.51
57:6:58:ASP:O	57:6:62:LYS:HG3	2.11	0.51
30:F:39:VAL:O	30:F:41:GLU:HG2	2.11	0.51
46:V:76:ASP:OD1	46:V:77:VAL:N	2.41	0.51
25:A:1055:G:O2'	25:A:1084:A:N6	2.36	0.51
25:A:1509:A:H2'	25:A:1510:G:C8	2.45	0.51
25:A:259:G:O2'	25:A:260:G:H5'	2.10	0.51
25:A:642:U:H2'	25:A:644:A:OP2	2.10	0.51
26:B:28:C:H2'	26:B:29:A:C8	2.45	0.51
30:F:126:ASN:OD1	30:F:156:THR:HG23	2.10	0.51
37:M:102:LEU:HD11	37:M:126:ILE:HD11	1.91	0.51
39:O:89:ASP:HA	39:O:116:GLN:O	2.10	0.51
56:5:57:ASN:HD22	56:5:63:ALA:HB2	1.74	0.51
25:A:2514:U:H2'	25:A:2515:C:C6	2.45	0.51
25:A:358:U:H2'	25:A:359:G:C8	2.88	0.51
25:A:372:G:HO2'	25:A:373:U:H6	1.58	0.51
25:A:479:A:O2'	25:A:481:G:H5''	2.11	0.51
25:A:542:C:C3'	25:A:543:G:H5''	2.40	0.51
28:D:55:LYS:HE2	28:D:77:ARG:HA	1.92	0.51
25:A:1088:A:H61	33:I:134:SER:HB3	1.75	0.51
25:A:2879:A:H8	25:A:2881:U:O4	1.92	0.51
34:J:36:LEU:HD22	34:J:121:LYS:HB2	1.93	0.51
35:K:92:GLU:O	35:K:93:GLN:O	2.29	0.51
25:A:1517:G:H1'	25:A:1919:A:O2'	100.47	0.51
25:A:884:U:H2'	25:A:885:C:O4'	2.10	0.51
25:A:1962:5MC:O2'	25:A:1964:G:OP2	2.28	0.51
25:A:270:A:N1	25:A:369:U:O2'	2.40	0.51
25:A:321:U:H5''	29:E:131:THR:HG23	1.91	0.51
25:A:948:C:H2'	25:A:949:G:C8	2.46	0.51
29:E:148:ILE:HB	29:E:169:VAL:HG22	1.92	0.51
29:E:170:ARG:NH2	29:E:176:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:W:61:GLY:HA3	47:W:79:GLU:O	2.11	0.51
25:A:962:G:H21	25:A:2250:G:H1	1.59	0.51
25:A:2515:C:H2'	25:A:2516:A:C8	2.46	0.51
25:A:2649:C:H2'	25:A:2650:U:C6	2.46	0.51
25:A:833:A:H2'	25:A:834:G:C8	2.45	0.51
35:K:24:VAL:HG13	35:K:33:ALA:HB2	1.93	0.51
38:N:56:LYS:NZ	38:N:87:PHE:O	2.44	0.51
55:4:11:CYS:HB3	55:4:33:HIS:CE1	2.46	0.51
25:A:1399:C:N4	25:A:1401:G:C2	8.11	0.51
25:A:2262:U:O2'	25:A:2263:C:H5'	2.10	0.51
25:A:2298:A:H2'	25:A:2299:U:O4'	2.11	0.51
25:A:52:A:H8	25:A:52:A:OP2	1.94	0.51
28:D:133:THR:HG23	28:D:134:HIS:N	2.26	0.51
32:H:33:GLN:HB2	32:H:35:LYS:HG2	1.93	0.51
25:A:1005:C:O2'	34:J:30:THR:HG21	2.11	0.51
57:6:44:PHE:HD1	57:6:45:THR:HG23	1.76	0.50
25:A:1815:A:H4'	25:A:1816:C:OP1	2.11	0.50
25:A:2101:A:H2'	25:A:2102:G:H8	1.76	0.50
25:A:2591:C:H2'	25:A:2592:G:H8	1.75	0.50
25:A:405:U:H3'	25:A:406:G:H5'	2.96	0.50
33:I:25:PRO:O	33:I:29:GLN:HB2	2.11	0.50
25:A:2845:U:H5''	40:P:51:ASN:O	2.11	0.50
25:A:1112:G:H2'	25:A:1113:U:C6	2.45	0.50
25:A:1243:C:H1'	36:L:4:ASN:O	2.11	0.50
29:E:76:PRO:HA	29:E:82:GLY:HA3	1.93	0.50
36:L:118:THR:O	36:L:120:VAL:N	2.44	0.50
41:Q:25:GLY:O	41:Q:29:ARG:NH1	2.44	0.50
45:U:36:GLU:HA	45:U:61:GLU:HG2	1.94	0.50
25:A:123:G:O2'	25:A:124:G:H5'	2.11	0.50
25:A:792:A:H1'	25:A:794:A:N7	14.55	0.50
30:F:141:ASP:O	30:F:143:ASP:N	2.44	0.50
50:Z:40:THR:HG22	50:Z:43:ILE:HG12	1.92	0.50
25:A:589:U:H2'	25:A:590:A:C8	2.46	0.50
25:A:716:A:H2'	25:A:717:C:O4'	2.11	0.50
26:B:111:U:O2'	26:B:112:G:H5'	2.12	0.50
30:F:133:GLU:HB3	30:F:135:ILE:HG13	1.94	0.50
42:R:61:ALA:HB2	42:R:98:ILE:HD13	1.94	0.50
25:A:1182:G:H2'	25:A:1183:U:O4'	2.12	0.50
25:A:28:A:H2'	25:A:29:U:O4'	2.63	0.50
25:A:1019:U:O2'	25:A:1020:A:H5'	2.11	0.50
25:A:1266:G:N2	25:A:1269:A:OP2	13.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1329:U:O5'	25:A:1330:C:H5	1.95	0.50
25:A:2101:A:H2'	25:A:2102:G:C8	2.47	0.50
25:A:2327:A:H2'	25:A:2328:A:C8	2.46	0.50
30:F:3:LEU:HD11	30:F:100:GLU:HB2	1.93	0.50
31:G:153:PRO:HA	31:G:159:LYS:O	2.12	0.50
50:Z:3:THR:HB	50:Z:36:GLU:HG2	1.94	0.50
51:O:24:VAL:HG22	51:O:26:SER:H	1.77	0.50
25:A:1210:G:O6	25:A:1237:A:H2'	2.11	0.50
25:A:1877:A:H2'	25:A:1878:G:O4'	2.12	0.50
25:A:2224:G:H4'	25:A:2226:C:C2	2.46	0.50
25:A:2391:G:O2'	25:A:2392:A:O5'	2.23	0.50
25:A:39:G:H1'	29:E:43:THR:HG21	1.93	0.50
25:A:196:A:H5''	36:L:47:ARG:HH22	1.76	0.50
38:N:79:LEU:O	38:N:81:ASN:N	2.42	0.50
25:A:795:C:H4'	25:A:1506:U:C2	82.48	0.49
25:A:530:G:C4	25:A:530:G:H5'	5.37	0.49
29:E:41:GLN:OE1	29:E:43:THR:OG1	2.29	0.49
25:A:530:G:N3	25:A:530:G:H5'	5.91	0.49
25:A:1142:A:H4'	25:A:1143:A:OP1	2.10	0.49
25:A:1399:C:N4	25:A:1401:G:N1	7.13	0.49
25:A:1701:A:C2'	25:A:1702:G:H5'	2.40	0.49
25:A:175:G:H2'	25:A:176:A:O4'	2.11	0.49
25:A:2516:A:O2'	25:A:2517:C:H5'	2.12	0.49
25:A:2698:U:H2'	25:A:2699:C:C6	2.48	0.49
25:A:2758:A:H2	31:G:34:ARG:HH21	1.59	0.49
31:G:94:ARG:HD2	31:G:127:GLN:HB3	1.94	0.49
25:A:1201:U:H2'	25:A:1202:G:H8	1.77	0.49
25:A:543:G:O6	25:A:550:C:N3	2.46	0.49
25:A:721:A:H2'	25:A:722:A:C8	2.47	0.49
35:K:43:ILE:HD12	35:K:56:ASP:HB2	1.93	0.49
25:A:473:G:O2'	25:A:474:G:H5'	2.12	0.49
30:F:67:THR:O	30:F:83:PRO:HA	2.12	0.49
25:A:2759:G:N2	31:G:138:GLN:NE2	2.59	0.49
36:L:110:VAL:HG11	36:L:135:ILE:HD11	1.93	0.49
36:L:33:ARG:HD3	36:L:40:SER:HA	1.95	0.49
40:P:74:GLN:HB2	40:P:77:SER:HB2	1.93	0.49
25:A:1586:A:C2	25:A:1587:G:H1'	2.48	0.49
25:A:1881:C:H2'	25:A:1882:U:O4'	2.13	0.49
25:A:367:G:N2	25:A:368:A:H1'	2.28	0.49
25:A:974:G:H2'	25:A:974:G:N3	2.28	0.49
26:B:1:U:H2'	26:B:2:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:T:22:THR:HA	44:T:25:GLU:HG2	1.93	0.49
46:V:80:HIS:CG	46:V:81:PRO:HD2	2.48	0.49
25:A:2134:A:N6	25:A:2156:G:H2'	2.27	0.49
25:A:2529:G:H4'	31:G:174:LYS:HE3	1.94	0.49
25:A:580:U:H2'	25:A:581:C:C6	2.48	0.49
25:A:948:C:H2'	25:A:949:G:H8	1.76	0.49
31:G:102:ILE:O	31:G:113:ASP:HA	2.12	0.49
32:H:47:PHE:HA	32:H:51:ARG:HB2	1.95	0.49
43:S:52:GLU:HA	43:S:55:ILE:HD12	1.95	0.49
25:A:1266:G:O2'	25:A:1267:U:OP2	2.30	0.49
25:A:1900:A:O4'	25:A:1970:A:H5''	2.12	0.49
25:A:2405:G:HO2'	25:A:2406:A:P	2.36	0.49
25:A:2572:A:H2'	28:D:149:ASN:HD22	1.76	0.49
25:A:2725:A:O2'	25:A:2726:A:C8	2.66	0.49
25:A:528:A:C2	25:A:2042:A:H2'	2.48	0.49
43:S:28:LYS:HE3	43:S:70:LYS:NZ	2.28	0.49
25:A:1139:G:O2'	25:A:1140:C:H5'	2.13	0.49
25:A:1715:G:HO2'	25:A:1716:U:H6	1.57	0.49
25:A:704:G:C2'	25:A:726:G:H22	2.13	0.49
30:F:134:GLN:HE22	30:F:149:ARG:N	2.11	0.49
25:A:2020:A:H5'	51:O:8:THR:HG22	1.94	0.49
25:A:1689:A:H2'	25:A:1690:A:H8	1.76	0.49
25:A:356:G:H2'	25:A:357:C:C6	2.48	0.49
25:A:395:U:H2'	25:A:396:G:C8	2.47	0.49
25:A:562:U:H2'	25:A:572:A:O4'	2.13	0.49
25:A:636:G:N7	36:L:109:LYS:HD3	2.28	0.49
25:A:974:G:C8	25:A:990:A:N6	2.76	0.49
26:B:106:G:H2'	26:B:107:G:O4'	2.13	0.49
25:A:1558:C:H4'	25:A:1559:U:O5'	2.13	0.48
25:A:2103:C:H2'	25:A:2104:C:C6	2.48	0.48
25:A:2305:U:C2	30:F:150:GLY:O	2.67	0.48
25:A:2529:G:OP2	25:A:2530:A:H5''	2.12	0.48
25:A:2861:U:H2'	25:A:2862:G:H8	1.77	0.48
25:A:437:U:H2'	25:A:438:G:C8	2.48	0.48
26:B:13:G:C8	26:B:70:C:H4'	2.48	0.48
30:F:102:LEU:HD12	30:F:106:ALA:HB3	1.95	0.48
30:F:73:VAL:HG22	30:F:78:ILE:HG12	1.95	0.48
25:A:1160:G:N7	25:A:1182:G:N2	20.72	0.48
25:A:2205:A:H2'	25:A:2206:C:C6	2.48	0.48
25:A:420:C:H2'	25:A:421:C:O4'	2.13	0.48
25:A:687:C:H1'	53:2:4:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:79:LEU:C	38:N:81:ASN:H	2.16	0.48
25:A:2120:G:H2'	25:A:2121:G:C8	2.48	0.48
25:A:2159:G:H2'	25:A:2160:C:O4'	2.13	0.48
25:A:322:A:OP2	29:E:163:ASN:HB2	2.13	0.48
34:J:15:TRP:HB3	34:J:137:PRO:HB3	1.95	0.48
48:X:39:VAL:HG12	48:X:42:GLU:H	1.78	0.48
25:A:2331:G:O2'	25:A:2336:A:N1	2.46	0.48
25:A:635:C:O2'	25:A:639:U:H5''	2.13	0.48
25:A:670:A:OP2	25:A:670:A:H8	1.95	0.48
25:A:873:C:H2'	25:A:874:G:H8	1.77	0.48
25:A:981:A:OP2	25:A:982:C:N4	2.43	0.48
27:C:7:PRO:HB3	27:C:13:ARG:HB2	1.95	0.48
35:K:102:PRO:HB3	35:K:121:GLU:HB3	1.94	0.48
38:N:49:GLU:HB2	38:N:50:PRO:HD3	1.96	0.48
25:A:2720:U:H5''	40:P:52:ARG:NH2	2.28	0.48
25:A:1106:G:H3'	25:A:1107:G:H8	1.76	0.48
25:A:335:C:C1'	25:A:1434:A:H1'	114.96	0.48
25:A:2552:OMU:H5	25:A:2556:C:H41	1.79	0.48
25:A:2875:C:O2'	25:A:2876:G:H5'	2.14	0.48
25:A:454:A:H3'	25:A:455:C:C6	2.48	0.48
27:C:15:VAL:HG22	27:C:205:GLY:HA3	1.96	0.48
31:G:136:ASP:OD2	31:G:139:VAL:HG23	2.13	0.48
25:A:127:A:H5''	25:A:128:C:C6	2.48	0.48
25:A:1900:A:H1'	25:A:1970:A:H2'	1.95	0.48
25:A:213:A:H2'	25:A:214:G:C8	2.48	0.48
25:A:2655:G:O2'	25:A:2656:U:OP2	2.31	0.48
25:A:969:G:H2'	25:A:970:U:H6	1.76	0.48
26:B:90:C:H2'	26:B:91:C:O4'	2.13	0.48
48:X:48:LEU:HB3	48:X:50:VAL:HG13	1.96	0.48
25:A:1183:U:H2'	25:A:1184:U:C6	2.49	0.48
25:A:2405:G:O2'	25:A:2406:A:OP2	2.32	0.48
25:A:2788:C:O2'	25:A:2809:A:N3	2.43	0.48
25:A:335:C:O4'	25:A:1434:A:H1'	116.30	0.48
26:B:79:G:H2'	26:B:80:U:O4'	2.13	0.48
33:I:38:CYS:SG	33:I:39:LYS:N	2.87	0.48
25:A:495:G:H5''	43:S:4:ILE:HG13	1.95	0.48
56:5:5:LEU:O	56:5:9:GLN:HB2	2.13	0.48
25:A:2178:C:H2'	25:A:2179:C:C6	2.49	0.48
30:F:89:THR:HG21	30:F:91:ARG:HH11	1.79	0.48
42:R:77:PHE:HD1	42:R:84:ARG:HB3	1.79	0.48
25:A:2071:A:H2'	25:A:2072:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2808:G:H2'	25:A:2890:G:O6	2.14	0.48
25:A:39:G:H2'	25:A:40:U:C6	2.49	0.48
28:D:32:ASN:HA	28:D:51:THR:O	2.13	0.48
25:A:831:G:H5''	36:L:37:GLY:HA2	1.95	0.48
36:L:77:ILE:O	36:L:110:VAL:O	2.32	0.48
37:M:42:THR:HG22	37:M:93:VAL:HG12	1.96	0.48
25:A:1378:A:O2'	25:A:1380:G:OP2	2.31	0.47
25:A:1590:A:H2'	25:A:1591:A:H8	1.79	0.47
25:A:2065:C:H1'	25:A:2449:H2U:HN3	1.79	0.47
25:A:2172:U:OP2	25:A:2173:A:H5'	2.14	0.47
25:A:20:C:H2'	25:A:21:A:C8	2.49	0.47
49:Y:44:LYS:HA	49:Y:47:ARG:HH22	1.79	0.47
25:A:2051:A:H8	25:A:2051:A:OP2	1.97	0.47
25:A:2467:C:H2'	25:A:2468:A:O4'	2.14	0.47
25:A:441:U:H2'	25:A:442:G:O4'	2.13	0.47
25:A:458:G:O2'	25:A:469:G:N1	2.47	0.47
25:A:934:U:H2'	25:A:935:C:C6	2.49	0.47
28:D:179:ARG:HB3	28:D:188:LEU:HD12	1.95	0.47
30:F:165:GLY:O	30:F:168:LEU:HB3	2.14	0.47
36:L:24:GLY:C	36:L:26:GLY:H	2.17	0.47
25:A:1320:C:O2'	25:A:1321:A:H5''	2.14	0.47
25:A:1310:G:H1'	25:A:1611:C:H5''	1.96	0.47
25:A:181:A:H2'	25:A:182:A:C8	2.49	0.47
25:A:2443:C:OP1	29:E:63:LYS:HD3	2.14	0.47
25:A:1052:C:H2'	25:A:1053:C:C5	2.50	0.47
25:A:435:C:H2'	25:A:436:C:H5'	1.96	0.47
35:K:34:GLY:O	35:K:36:GLY:N	2.47	0.47
36:L:122:VAL:HG21	36:L:135:ILE:HD13	1.97	0.47
36:L:128:THR:OG1	36:L:129:LYS:N	2.44	0.47
25:A:1477:A:H2'	25:A:1478:G:O4'	2.15	0.47
25:A:2714:G:O2'	25:A:2715:C:H5'	2.14	0.47
45:U:85:ARG:NH1	45:U:99:SER:OG	2.47	0.47
25:A:121:G:H4'	25:A:149:A:H5'	1.95	0.47
25:A:1538:G:H2'	25:A:1539:U:C6	2.50	0.47
25:A:2266:A:H8	25:A:2266:A:OP1	1.98	0.47
25:A:2408:U:H2'	25:A:2409:G:H8	1.80	0.47
25:A:244:A:H2'	25:A:245:G:O4'	2.15	0.47
25:A:2526:G:H2'	25:A:2527:C:C6	2.49	0.47
28:D:48:ILE:O	28:D:81:GLU:HA	2.15	0.47
29:E:52:VAL:O	29:E:74:LYS:HE3	2.14	0.47
56:5:41:LEU:O	56:5:44:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:6:28:VAL:HG11	57:6:32:LEU:HD13	1.95	0.47
25:A:1340:U:H3'	44:T:61:LEU:HD22	1.97	0.47
25:A:1857:G:H1'	25:A:1885:A:N6	2.29	0.47
25:A:1930:G:O2'	25:A:1931:U:OP2	2.26	0.47
25:A:2014:A:H2'	25:A:2015:A:C8	2.50	0.47
25:A:322:A:H5'	25:A:340:A:H1'	1.97	0.47
25:A:554:U:H2'	25:A:555:G:O4'	2.15	0.47
34:J:35:ARG:HA	34:J:40:HIS:HD2	1.79	0.47
25:A:108:G:H2'	25:A:109:C:O4'	2.15	0.47
25:A:1019:U:H3	25:A:1142:A:H62	1.62	0.47
25:A:120:U:H4'	25:A:121:G:H5''	1.96	0.47
25:A:1715:G:O2'	25:A:1716:U:H6	1.98	0.47
25:A:2771:C:H2'	25:A:2772:C:C6	2.50	0.47
26:B:50:A:H2'	26:B:51:G:O4'	2.15	0.47
26:B:75:G:H2'	26:B:76:G:O4'	2.14	0.47
36:L:30:THR:O	36:L:32:GLY:N	2.48	0.47
25:A:1430:G:H2'	25:A:1431:A:O4'	2.15	0.47
25:A:160:A:H2'	25:A:161:A:O4'	2.74	0.47
25:A:1636:U:H2'	25:A:1637:A:C8	2.50	0.47
25:A:2297:A:N1	25:A:2321:U:C5	2.83	0.47
25:A:685:A:H5''	25:A:788:A:H62	1.80	0.47
25:A:692:C:H5''	27:C:38:LYS:HB3	1.96	0.47
25:A:807:U:H1'	25:A:2445:2MG:OP1	2.15	0.47
25:A:1038:G:H2'	25:A:1039:A:C8	2.50	0.47
25:A:1109:C:N3	25:A:1110:G:N2	2.63	0.47
25:A:1418:G:H2'	25:A:1579:A:H62	1.80	0.47
25:A:1:G:H2'	25:A:2:G:H8	1.80	0.47
25:A:2405:G:H1'	25:A:2412:A:N6	2.29	0.47
25:A:871:U:H2'	25:A:872:U:C6	2.50	0.47
33:I:20:SER:HB3	33:I:21:PRO:HD3	1.97	0.47
25:A:2287:A:C2'	25:A:2288:A:O5'	2.63	0.47
25:A:251:A:H2'	25:A:252:G:O4'	2.15	0.47
25:A:404:A:H1'	25:A:406:G:N9	2.30	0.47
25:A:923:G:H2'	25:A:924:G:C8	2.48	0.47
25:A:2823:A:OP1	28:D:118:PHE:HB2	2.15	0.47
40:P:24:THR:O	40:P:86:LYS:HB2	2.15	0.47
25:A:1078:U:HO2'	25:A:1088:A:H2	1.62	0.46
25:A:1533:C:O2	25:A:1538:G:N2	2.46	0.46
25:A:1343:G:H1'	25:A:1597:A:C4	2.51	0.46
25:A:1363:C:O2'	25:A:1809:A:N3	2.47	0.46
25:A:2391:G:OP2	54:3:34:LYS:HD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2629:U:O2'	25:A:2630:G:H5''	2.15	0.46
25:A:2645:G:H4'	25:A:2732:G:H1'	1.97	0.46
25:A:2808:G:O2'	25:A:2809:A:H8	1.97	0.46
25:A:635:C:H2'	25:A:636:G:O4'	2.15	0.46
33:I:133:ARG:HA	33:I:137:LEU:O	2.15	0.46
33:I:42:ASN:HA	33:I:45:THR:HB	1.97	0.46
41:Q:85:ALA:HB2	41:Q:115:ALA:HB2	1.97	0.46
25:A:136:G:H1	25:A:143:C:H42	1.63	0.46
25:A:1432:G:P	40:P:105:LYS:CG	54.36	0.46
25:A:1454:C:H5'	38:N:63:ARG:CZ	2.45	0.46
25:A:172:A:H2'	25:A:173:A:H8	1.79	0.46
33:I:33:ASN:HB2	33:I:64:ARG:NH2	2.29	0.46
38:N:38:LEU:HB3	38:N:39:PRO:HD3	1.97	0.46
25:A:1111:A:HO2'	25:A:1112:G:P	2.37	0.46
25:A:1177:G:H2'	25:A:1178:C:C4'	2.45	0.46
25:A:1212:G:H1'	25:A:1237:A:N6	2.30	0.46
25:A:2012:G:H8	25:A:2012:G:O5'	1.98	0.46
25:A:2286:G:H4'	25:A:2287:A:O5'	2.14	0.46
25:A:242:G:O2'	25:A:243:U:OP2	2.27	0.46
25:A:2584:U:C3'	25:A:2585:U:H5''	2.44	0.46
25:A:2808:G:H2'	25:A:2890:G:C6	2.51	0.46
25:A:336:C:O2'	25:A:337:C:H5'	2.15	0.46
25:A:789:A:N1	53:2:3:ARG:NH1	2.55	0.46
31:G:41:GLU:HB3	31:G:52:GLY:O	2.15	0.46
34:J:75:TYR:HB3	34:J:84:ILE:HD11	1.95	0.46
42:R:28:ALA:HB3	42:R:31:GLU:HB2	1.97	0.46
25:A:1474:U:H4'	25:A:1701:A:C2	71.26	0.46
25:A:1728:C:O2'	25:A:1729:U:C6	2.69	0.46
25:A:1751:U:H2'	25:A:1752:C:C6	2.51	0.46
25:A:2721:A:H1'	25:A:2873:A:O2'	2.16	0.46
25:A:973:A:H5'	25:A:1188:U:H1'	1.98	0.46
35:K:41:ILE:HG13	35:K:58:LEU:O	2.15	0.46
41:Q:71:ASN:N	41:Q:71:ASN:HD22	2.12	0.46
50:Z:47:ILE:HD13	50:Z:56:VAL:HG21	1.97	0.46
25:A:2742:G:OP1	55:4:36:ARG:HD3	2.16	0.46
25:A:1951:U:H2'	25:A:1953:A:OP2	2.15	0.46
25:A:185:G:H4'	25:A:218:A:H4'	1.98	0.46
25:A:500:G:N1	25:A:503:A:OP2	2.49	0.46
25:A:549:G:HO2'	25:A:550:C:P	2.39	0.46
40:P:29:VAL:HG13	40:P:79:VAL:HG22	1.96	0.46
44:T:80:TRP:CZ3	44:T:82:LYS:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:X:17:ARG:HE	48:X:23:ALA:CB	2.15	0.46
48:X:30:PRO:O	48:X:32:LEU:N	2.49	0.46
50:Z:40:THR:HG23	50:Z:42:ALA:H	1.80	0.46
25:A:2515:C:H2'	25:A:2516:A:H8	1.81	0.46
25:A:930:G:H1'	50:Z:24:LEU:HD21	1.97	0.46
30:F:4:HIS:CD2	30:F:8:LYS:HE3	2.51	0.46
30:F:9:ASP:N	30:F:9:ASP:OD1	2.47	0.46
31:G:126:THR:HG22	31:G:128:THR:H	1.81	0.46
25:A:2528:U:H2'	25:A:2530:A:O5'	2.16	0.46
25:A:259:G:C2'	25:A:260:G:H5'	2.46	0.46
26:B:114:C:H2'	26:B:115:A:C8	2.51	0.46
32:H:64:ALA:O	32:H:67:ALA:HB3	2.15	0.46
33:I:48:ILE:HG13	33:I:49:GLU:H	1.81	0.46
43:S:72:THR:HG21	43:S:108:SER:HB3	1.98	0.46
55:4:1:MET:HE3	55:4:34:LYS:HG2	1.98	0.46
25:A:128:C:H2'	25:A:129:C:H6	1.81	0.46
25:A:1684:G:H2'	25:A:1685:C:C6	2.51	0.46
25:A:2688:G:H1'	25:A:2721:A:N6	2.31	0.46
25:A:2777:G:H1'	25:A:2779:U:H5	1.80	0.46
28:D:36:GLN:HB3	28:D:49:GLN:HB3	1.97	0.46
39:O:37:ALA:HB3	39:O:78:VAL:HG21	1.98	0.46
39:O:26:LEU:HD13	39:O:39:VAL:HG22	1.97	0.46
56:5:26:VAL:HG21	56:5:114:GLU:HG2	1.98	0.46
25:A:1069:A:N6	25:A:1073:A:C4	2.84	0.46
25:A:2862:G:H2'	25:A:2863:C:C6	2.51	0.46
25:A:287:G:H2'	25:A:288:U:C6	2.51	0.46
25:A:772:C:O2'	25:A:773:U:H5'	2.16	0.46
45:U:17:ASP:HB3	45:U:20:LYS:HD2	1.98	0.46
45:U:42:LYS:HG2	45:U:59:GLU:OE1	2.16	0.46
48:X:32:LEU:HD22	48:X:49:ARG:HG2	1.98	0.46
25:A:1085:A:H61	56:5:34:THR:HG22	1.81	0.46
25:A:1107:G:H1'	56:5:81:LEU:HD12	1.97	0.46
25:A:2183:A:H2'	25:A:2184:A:C8	2.51	0.46
25:A:2313:C:H5''	30:F:87:LYS:HD2	1.98	0.46
25:A:2705:A:O2'	25:A:2852:G:OP1	2.26	0.46
25:A:974:G:H1'	25:A:975:A:H8	1.80	0.46
26:B:87:U:H5''	26:B:88:C:OP2	2.16	0.46
30:F:12:VAL:O	30:F:16:MET:HG2	2.16	0.46
30:F:129:MET:HG3	30:F:153:ILE:HB	1.98	0.46
34:J:99:ARG:NH1	34:J:102:GLU:OE2	2.49	0.46
25:A:1287:A:H5'	38:N:103:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:U:96:LYS:O	45:U:97:SER:O	2.34	0.46
25:A:1318:U:H2'	25:A:1319:C:C6	2.51	0.45
25:A:1932:A:H2'	25:A:1933:G:O4'	2.17	0.45
25:A:1297:C:OP1	25:A:2710:C:H4'	2.16	0.45
44:T:5:GLU:HA	44:T:8:LEU:HD12	1.98	0.45
25:A:1819:A:H3'	27:C:176:ARG:HG2	1.98	0.45
25:A:2329:U:H2'	25:A:2330:G:C8	2.51	0.45
25:A:2756:U:H4'	25:A:2757:A:OP1	2.15	0.45
25:A:2379:G:H4'	39:O:21:LEU:HD11	1.98	0.45
25:A:1045:C:H1'	25:A:1047:G:C2	2.51	0.45
25:A:1103:A:H3'	25:A:1104:C:C5'	2.42	0.45
25:A:1432:G:C5'	40:P:105:LYS:CG	53.70	0.45
25:A:1798:U:OP2	27:C:270:ARG:NH2	2.49	0.45
25:A:1930:G:HO2'	25:A:1931:U:P	2.32	0.45
25:A:2019:A:H2	25:A:2035:G:H22	1.64	0.45
25:A:2444:G:OP2	29:E:63:LYS:HD2	2.16	0.45
25:A:2869:G:H2'	25:A:2870:C:O4'	2.17	0.45
25:A:811:U:N3	36:L:21:ARG:NH2	2.64	0.45
53:2:30:VAL:O	53:2:34:ARG:HG2	2.17	0.45
25:A:1604:C:H2'	25:A:1605:C:C6	2.51	0.45
25:A:335:C:H4'	25:A:1434:A:C1'	116.48	0.45
27:C:252:LYS:HE3	27:C:252:LYS:HB2	1.83	0.45
33:I:4:VAL:HA	33:I:7:TYR:CE2	2.52	0.45
49:Y:39:GLN:HB2	49:Y:41:HIS:CE1	2.52	0.45
25:A:1182:G:H4'	25:A:1183:U:O5'	4.94	0.45
25:A:1306:C:N4	25:A:1606:C:H2'	2.30	0.45
25:A:1858:A:C2	25:A:1885:A:H1'	2.51	0.45
25:A:424:G:H2'	25:A:425:G:O4'	2.36	0.45
25:A:89:A:H2'	25:A:90:U:C6	2.51	0.45
35:K:35:VAL:HG22	35:K:69:VAL:HG12	1.98	0.45
56:5:118:ILE:H	56:5:119:PRO:CD	2.29	0.45
25:A:1530:G:H22	25:A:1542:U:H1'	1.79	0.45
25:A:1692:U:O2'	25:A:1693:U:H2'	2.15	0.45
25:A:2139:U:H2'	25:A:2140:G:C8	2.51	0.45
25:A:286:U:H2'	25:A:287:G:C8	2.52	0.45
25:A:357:C:H2'	25:A:358:U:C6	2.51	0.45
28:D:31:ALA:O	28:D:33:ARG:HG2	2.17	0.45
25:A:1857:G:H2'	25:A:1884:G:H22	1.82	0.45
25:A:2141:G:N2	25:A:2151:U:H1'	2.31	0.45
25:A:2851:A:H2'	25:A:2852:G:O4'	2.17	0.45
25:A:321:U:H4'	25:A:322:A:OP2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:18:U:O2'	25:A:554:U:OP1	2.35	0.45
25:A:568:U:H2'	25:A:570:G:OP2	2.17	0.45
26:B:13:G:N7	26:B:70:C:H4'	2.31	0.45
30:F:138:PRO:HB3	57:6:32:LEU:HD11	1.97	0.45
32:H:2:GLN:HB3	32:H:39:ALA:HB3	1.99	0.45
25:A:529:A:OP2	34:J:113:PRO:HD3	2.17	0.45
25:A:1682:G:H2'	25:A:1683:U:C6	2.52	0.45
25:A:1916:A:H2'	25:A:1917:PSU:O4'	2.16	0.45
25:A:2846:G:H2'	25:A:2847:U:O4'	2.17	0.45
25:A:974:G:H1'	25:A:975:A:C8	2.52	0.45
25:A:674:G:H5''	29:E:71:GLY:H	1.81	0.45
31:G:37:ASN:OD1	31:G:38:ASP:N	2.50	0.45
31:G:70:LEU:O	31:G:74:MET:HG3	2.15	0.45
31:G:95:ALA:HB1	31:G:130:ILE:HD11	1.97	0.45
25:A:1088:A:H61	33:I:134:SER:CB	2.29	0.45
25:A:1152:C:H2'	25:A:1153:C:C6	2.51	0.45
25:A:1198:U:H2'	25:A:1199:U:C6	2.52	0.45
25:A:1315:C:H2'	25:A:1316:U:C6	2.50	0.45
25:A:2638:G:H1'	25:A:2778:A:N6	2.32	0.45
25:A:2793:C:H2'	25:A:2794:C:C6	2.52	0.45
25:A:2840:C:H2'	25:A:2841:C:C6	2.52	0.45
25:A:2861:U:H2'	25:A:2862:G:C8	2.52	0.45
28:D:40:LEU:HA	28:D:44:GLY:H	1.82	0.45
28:D:35:THR:HG22	28:D:73:VAL:HG21	1.98	0.45
25:A:1188:U:O2'	25:A:1189:A:H5'	2.16	0.45
25:A:2065:C:H2'	25:A:2066:C:C6	2.52	0.45
25:A:2100:G:H1	25:A:2189:U:H3	1.64	0.45
25:A:2512:C:H2'	25:A:2513:A:O4'	2.17	0.45
25:A:2712:C:OP1	25:A:2714:G:H4'	2.17	0.45
25:A:465:G:H2'	25:A:466:A:C8	2.51	0.45
28:D:149:ASN:CG	28:D:150:GLN:H	2.20	0.45
30:F:56:LEU:HD13	30:F:88:VAL:HG23	1.99	0.45
25:A:2514:U:H5''	34:J:81:ILE:HD11	1.99	0.45
25:A:1328:A:H2'	25:A:1330:C:C4	2.52	0.44
25:A:1328:A:H2'	25:A:1330:C:C5	2.52	0.44
25:A:155:A:H2'	25:A:156:A:C8	2.52	0.44
25:A:1590:A:H2'	25:A:1591:A:C8	2.53	0.44
25:A:1610:A:OP1	25:A:1611:C:H5	2.00	0.44
25:A:1744:A:H3'	25:A:1745:A:H8	1.81	0.44
25:A:2233:U:H2'	25:A:2234:G:H8	1.80	0.44
25:A:414:C:H2'	25:A:415:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:955:PSU:H5'	37:M:86:LYS:HD3	1.99	0.44
25:A:973:A:H5''	42:R:81:LYS:HD2	1.98	0.44
25:A:2271:G:OP1	47:W:14:ALA:HB1	2.17	0.44
55:4:22:VAL:HG11	55:4:36:ARG:HH11	1.82	0.44
25:A:1014:A:H2'	25:A:1015:U:C6	2.52	0.44
25:A:1528:A:H2'	25:A:1529:G:O4'	2.17	0.44
25:A:2146:C:H4'	25:A:2147:A:C4	2.52	0.44
25:A:2291:U:H2'	25:A:2292:U:H6	1.77	0.44
25:A:780:G:OP1	27:C:216:ARG:NH2	2.49	0.44
29:E:49:ARG:O	29:E:74:LYS:HE2	2.17	0.44
25:A:2022:U:O4	51:O:5:ASN:ND2	2.50	0.44
25:A:117:G:C6	25:A:119:A:C6	3.05	0.44
25:A:1807:G:H2'	25:A:1808:A:H5'	1.99	0.44
25:A:2093:G:OP1	32:H:24:GLY:HA3	2.18	0.44
25:A:2208:C:H2'	25:A:2209:G:C8	2.52	0.44
25:A:2221:G:H2'	25:A:2222:C:C6	2.52	0.44
25:A:2427:C:C5'	25:A:2429:G:H5'	2.46	0.44
25:A:307:G:N1	25:A:310:A:OP2	2.50	0.44
25:A:358:U:H2'	25:A:359:G:H8	2.06	0.44
25:A:651:G:H5'	54:3:18:LYS:HG3	1.99	0.44
29:E:18:THR:HA	29:E:106:LYS:HE3	1.99	0.44
33:I:18:ASN:HB2	33:I:38:CYS:HB3	1.99	0.44
34:J:63:ALA:HA	34:J:69:ARG:NH2	2.32	0.44
37:M:5:LYS:O	37:M:6:ARG:HG2	2.17	0.44
41:Q:57:ARG:HA	41:Q:60:TRP:CE3	2.53	0.44
42:R:24:LYS:HD3	42:R:92:TRP:HB3	1.99	0.44
56:5:87:GLU:OE2	56:5:95:LEU:HB2	2.17	0.44
25:A:2307:G:H8	25:A:2307:G:OP1	2.00	0.44
25:A:753:A:C8	25:A:753:A:OP2	2.67	0.44
32:H:30:LEU:HB3	32:H:36:ALA:HB3	2.00	0.44
34:J:35:ARG:HB2	34:J:54:ILE:HD11	1.98	0.44
36:L:51:GLU:OE1	36:L:56:PRO:HA	2.17	0.44
38:N:28:LEU:HD13	38:N:34:ILE:HG12	2.00	0.44
40:P:77:SER:O	40:P:80:VAL:HG22	2.18	0.44
25:A:1266:G:O2'	25:A:2012:G:N1	2.38	0.44
25:A:1525:A:H2'	25:A:1526:C:O4'	2.17	0.44
25:A:2121:G:H2'	25:A:2122:U:O4'	2.18	0.44
25:A:2197:U:O2'	25:A:2198:A:H2'	2.17	0.44
25:A:458:G:O2'	25:A:459:U:P	2.76	0.44
33:I:56:VAL:HG13	33:I:58:ILE:HD11	1.99	0.44
34:J:110:PRO:O	34:J:115:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1614:A:C2	43:S:93:ALA:HB2	2.53	0.44
50:Z:23:LEU:HD11	50:Z:53:MET:SD	2.58	0.44
25:A:1432:G:O2'	25:A:1433:A:H5'	2.18	0.44
25:A:2325:G:C6	25:A:2326:C:N4	2.86	0.44
25:A:598:U:H2'	25:A:599:A:C8	2.52	0.44
25:A:2572:A:C8	28:D:149:ASN:ND2	2.86	0.44
43:S:20:VAL:HG11	43:S:44:ALA:HA	2.00	0.44
25:A:1204:A:H4'	25:A:1205:A:H5''	1.99	0.44
25:A:1278:C:H2'	25:A:1279:G:C8	2.53	0.44
25:A:1563:U:H2'	25:A:1564:C:C6	2.53	0.44
25:A:1806:C:H1'	27:C:43:ASN:HD21	1.83	0.44
25:A:2489:U:C4	25:A:2490:G:C6	3.05	0.44
25:A:2773:C:H2'	25:A:2774:C:C6	2.53	0.44
25:A:756:A:H2'	25:A:757:G:O4'	2.17	0.44
35:K:64:ARG:HB2	35:K:83:ALA:HB3	2.00	0.44
35:K:71:ARG:HH11	35:K:77:ILE:HD11	1.83	0.44
36:L:57:LEU:HD22	54:3:53:ASP:HB3	1.98	0.44
25:A:1820:U:C2	27:C:200:MET:HB2	2.53	0.44
25:A:232:G:OP2	25:A:232:G:H8	2.01	0.44
25:A:600:G:H2'	25:A:601:C:O4'	2.17	0.44
25:A:745:1MG:HM11	25:A:745:1MG:HN21	1.67	0.44
30:F:120:SER:HB2	30:F:127:TYR:CE1	2.53	0.44
30:F:1:ALA:H1	30:F:97:GLU:HA	1.81	0.44
30:F:97:GLU:HG2	57:6:25:ARG:HB2	1.99	0.44
25:A:19:A:H5''	41:Q:21:LYS:HG2	2.00	0.44
25:A:1094:U:H2'	25:A:1096:A:N7	2.33	0.44
25:A:1361:G:H2'	25:A:1362:C:C6	2.52	0.44
25:A:1432:G:P	40:P:105:LYS:HG3	53.69	0.44
25:A:1746:A:H2'	25:A:1747:U:C6	2.53	0.44
25:A:278:A:C2	25:A:362:A:H1'	2.53	0.44
25:A:2859:G:H2'	25:A:2860:A:C8	2.53	0.44
25:A:310:A:C2'	25:A:311:A:H5''	2.48	0.44
25:A:463:G:N2	25:A:466:A:OP2	2.36	0.44
25:A:490:C:H2'	25:A:491:G:C8	9.34	0.44
25:A:971:G:H2'	25:A:972:A:O4'	2.18	0.44
25:A:2204:G:H4'	27:C:149:LYS:HD3	1.99	0.44
34:J:7:LYS:HB2	34:J:10:THR:OG1	2.18	0.44
36:L:95:LEU:HD22	36:L:100:ILE:HD11	1.98	0.44
25:A:909:A:OP1	36:L:17:LYS:HD3	63.52	0.44
25:A:1866:A:H2'	25:A:1867:G:O4'	2.18	0.43
25:A:1956:U:C2'	25:A:1957:C:H5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2261:C:C6	47:W:12:SER:OG	2.71	0.43
25:A:278:A:N3	25:A:278:A:H2'	2.32	0.43
25:A:563:A:OP2	42:R:79:ARG:NH2	2.50	0.43
25:A:1127:A:H2'	25:A:1128:G:H5''	2.00	0.43
25:A:1235:G:C6	25:A:1236:G:N2	2.86	0.43
25:A:2712:C:H3'	25:A:2714:G:H5''	1.99	0.43
25:A:532:A:H2'	25:A:532:A:N3	2.47	0.43
25:A:546:U:H1'	25:A:548:G:C2	2.53	0.43
25:A:678:C:H2'	25:A:679:C:C6	2.53	0.43
27:C:149:LYS:HG3	27:C:149:LYS:O	2.91	0.43
30:F:3:LEU:HD13	30:F:96:TRP:HE3	1.83	0.43
33:I:104:GLN:O	33:I:107:GLU:HB3	2.18	0.43
33:I:104:GLN:O	33:I:108:ILE:HG13	2.17	0.43
37:M:60:GLN:NE2	37:M:108:VAL:HG12	2.33	0.43
41:Q:5:ARG:HB2	41:Q:8:ILE:HD11	2.00	0.43
50:Z:44:ARG:HD2	50:Z:47:ILE:HD12	1.99	0.43
57:6:58:ASP:N	57:6:58:ASP:OD1	2.49	0.43
25:A:1432:G:O2'	25:A:1433:A:H8	3.82	0.43
25:A:1679:A:H2'	25:A:1680:U:C6	2.54	0.43
25:A:17:G:H4'	41:Q:24:TYR:HE1	1.83	0.43
25:A:2112:G:H5'	25:A:2113:U:C5	2.53	0.43
25:A:2730:C:O2'	25:A:2731:G:H5'	2.18	0.43
25:A:2783:U:H2'	25:A:2784:U:C6	2.52	0.43
27:C:86:ARG:HD3	27:C:104:LEU:HD21	2.01	0.43
28:D:85:ALA:C	28:D:87:GLY:H	2.22	0.43
29:E:102:ARG:NH1	29:E:200:LEU:O	2.51	0.43
30:F:153:ILE:H	30:F:153:ILE:HD12	1.82	0.43
25:A:494:G:H4'	43:S:6:LYS:O	2.18	0.43
45:U:83:GLY:O	45:U:93:ARG:HA	2.19	0.43
25:A:2884:U:C6	51:0:49:ARG:HG2	2.53	0.43
54:3:27:ASN:O	54:3:35:LYS:HE2	2.18	0.43
54:3:32:LEU:HD23	54:3:35:LYS:HD2	2.00	0.43
25:A:1637:A:H5'	25:A:1760:C:O2'	2.18	0.43
25:A:1872:A:H2'	25:A:1873:G:O4'	2.18	0.43
25:A:207:A:H2'	25:A:208:C:O4'	2.19	0.43
25:A:249:C:O2	54:3:11:LYS:NZ	2.51	0.43
30:F:24:VAL:O	30:F:27:VAL:HG12	2.17	0.43
39:O:31:THR:HG22	39:O:33:ARG:H	1.84	0.43
40:P:27:VAL:HG12	40:P:29:VAL:HG23	2.01	0.43
46:V:30:ILE:HG12	46:V:91:PHE:HB2	2.00	0.43
25:A:2066:C:O2'	25:A:2067:G:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:571:U:OP1	25:A:819:A:O2'	20.54	0.43
33:I:11:GLN:NE2	33:I:56:VAL:HG12	2.34	0.43
34:J:102:GLU:HG3	34:J:119:PHE:CZ	2.52	0.43
34:J:37:ARG:NH2	34:J:110:PRO:HG3	2.33	0.43
25:A:1509:A:H2'	25:A:1510:G:H8	1.82	0.43
25:A:1996:C:H4'	25:A:1997:C:OP1	2.19	0.43
25:A:2358:A:H2'	25:A:2359:C:O4'	2.19	0.43
25:A:2646:C:H2'	25:A:2647:U:O4'	2.19	0.43
25:A:2837:A:H2'	25:A:2838:G:C8	2.54	0.43
25:A:900:A:H2'	25:A:901:C:O4'	2.19	0.43
25:A:938:G:H2'	25:A:939:G:H8	1.83	0.43
36:L:135:ILE:HB	36:L:142:ILE:HD11	2.01	0.43
55:4:30:GLU:HA	55:4:31:PRO:HD3	1.89	0.43
56:5:57:ASN:ND2	56:5:63:ALA:HB2	2.33	0.43
25:A:1980:G:O2'	25:A:1982:U:OP2	2.26	0.43
25:A:2526:G:H2'	25:A:2527:C:H6	1.83	0.43
25:A:2567:G:H2'	25:A:2568:U:C6	2.54	0.43
25:A:2590:A:H2'	25:A:2591:C:C6	2.54	0.43
25:A:63:A:H2'	25:A:64:A:C8	2.53	0.43
25:A:2884:U:C5	51:0:49:ARG:HG2	2.54	0.43
56:5:40:GLU:O	56:5:43:LYS:HB3	2.18	0.43
25:A:1378:A:C4	25:A:1380:G:N7	2.87	0.43
25:A:2286:G:H5''	25:A:2287:A:OP1	2.18	0.43
25:A:2347:C:H2'	25:A:2348:U:C6	2.54	0.43
25:A:2619:C:O2'	25:A:2620:C:H5'	2.19	0.43
25:A:723:C:H2'	25:A:724:U:O4'	2.19	0.43
28:D:16:THR:OG1	28:D:20:VAL:O	2.24	0.43
29:E:178:VAL:O	29:E:182:ALA:HB2	2.19	0.43
34:J:31:GLU:HG2	34:J:142:ILE:HG12	2.01	0.43
36:L:62:PRO:HG2	54:3:24:LYS:HB3	1.99	0.43
37:M:69:PRO:HA	37:M:94:ALA:HB2	2.00	0.43
41:Q:107:ALA:O	42:R:48:LYS:HE3	2.19	0.43
43:S:23:LEU:HD22	51:0:23:ALA:HB2	2.00	0.43
51:0:28:SER:O	51:0:36:LYS:HA	2.18	0.43
25:A:1070:A:H4'	25:A:1071:G:OP2	2.19	0.43
25:A:1386:C:H2'	25:A:1387:A:H8	1.81	0.43
25:A:2141:G:H2'	25:A:2142:A:H8	1.84	0.43
25:A:242:G:N7	54:3:4:LYS:HG2	2.34	0.43
25:A:249:C:O2'	36:L:63:LYS:NZ	2.30	0.43
25:A:2848:G:O2'	25:A:2849:U:H5'	2.18	0.43
25:A:364:C:H2'	25:A:365:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:476:G:H4'	25:A:502:A:N1	2.34	0.43
30:F:39:VAL:C	30:F:41:GLU:H	2.22	0.43
34:J:56:VAL:HB	34:J:124:VAL:HG12	1.99	0.43
51:O:6:LYS:HA	51:O:7:PRO:HD3	1.87	0.43
25:A:682:G:H5'	53:2:26:ASN:CG	2.39	0.43
54:3:26:ALA:O	54:3:27:ASN:CG	2.57	0.43
25:A:2466:C:OP1	55:4:4:ARG:HB3	2.18	0.43
57:6:39:LYS:O	57:6:40:CYS:CB	2.67	0.43
25:A:1421:G:C2	25:A:1422:G:C8	3.07	0.43
25:A:1469:A:H2'	25:A:1470:A:C8	2.54	0.43
25:A:1754:A:N1	25:A:2716:C:O2'	2.36	0.43
25:A:1788:C:O2'	25:A:1789:A:H5'	2.19	0.43
25:A:2038:G:H2'	25:A:2039:U:O4'	2.19	0.43
25:A:2728:U:H2'	25:A:2729:G:H8	1.84	0.43
28:D:35:THR:HG1	28:D:49:GLN:HG2	1.81	0.43
34:J:99:ARG:HA	34:J:102:GLU:HB3	2.01	0.43
37:M:34:LYS:HA	37:M:101:VAL:HA	2.01	0.43
38:N:81:ASN:N	38:N:81:ASN:OD1	2.52	0.43
44:T:64:LYS:HD2	44:T:64:LYS:N	2.34	0.43
46:V:6:ALA:HB2	46:V:42:LEU:HB3	2.01	0.43
25:A:1129:A:HO2'	25:A:2515:C:HO2'	1.67	0.42
25:A:1204:A:H4'	25:A:1205:A:C5'	2.49	0.42
25:A:1726:C:H2'	25:A:1727:C:C6	2.54	0.42
25:A:191:A:H2'	25:A:192:C:C6	2.54	0.42
25:A:1936:A:H2	25:A:1943:U:N3	2.09	0.42
25:A:2494:G:O2'	37:M:79:ALA:HA	2.18	0.42
26:B:53:A:N3	26:B:53:A:H2'	2.33	0.42
26:B:79:G:N7	46:V:14:LYS:NZ	2.66	0.42
33:I:112:LYS:O	33:I:116:MET:HG2	2.18	0.42
25:A:2684:U:O4'	35:K:70:ARG:NH1	2.52	0.42
48:X:4:CYS:HA	48:X:32:LEU:HD21	2.01	0.42
48:X:31:ASN:O	48:X:51:SER:HA	2.19	0.42
56:5:18:VAL:HG11	56:5:70:GLU:HB3	2.01	0.42
56:5:71:CYS:HB3	56:5:117:LEU:HD12	2.02	0.42
25:A:1022:G:N2	25:A:1142:A:C2	2.87	0.42
25:A:2361:G:O3'	54:3:27:ASN:ND2	2.49	0.42
25:A:255:A:H2'	25:A:256:A:O4'	2.19	0.42
25:A:1783:A:N1	25:A:2587:A:H2'	2.33	0.42
25:A:278:A:H2	25:A:362:A:H1'	1.83	0.42
31:G:82:PHE:O	31:G:133:LYS:HA	2.19	0.42
33:I:92:PRO:HB2	33:I:93:ASN:H	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:U:40:LEU:HD23	45:U:61:GLU:HG3	2.01	0.42
46:V:2:PHE:HA	46:V:50:MET:HE1	2.01	0.42
25:A:1028:A:N3	25:A:2486:C:O2'	2.42	0.42
25:A:1201:U:H2'	25:A:1202:G:C8	2.55	0.42
25:A:182:A:H2'	25:A:183:C:O4'	2.18	0.42
25:A:189:G:H2'	25:A:205:G:N2	2.34	0.42
25:A:2415:G:H2'	25:A:2416:C:C6	2.55	0.42
25:A:2530:A:N6	31:G:155:PRO:HG3	2.34	0.42
25:A:2682:A:H61	25:A:2728:U:C1'	2.27	0.42
25:A:297:G:N2	25:A:300:A:OP2	13.50	0.42
26:B:85:G:H2'	26:B:86:G:H8	1.84	0.42
27:C:179:GLU:HG3	27:C:269:ARG:HA	2.00	0.42
25:A:1816:C:H3'	27:C:61:TYR:CE1	2.54	0.42
25:A:2572:A:H2'	28:D:149:ASN:ND2	2.34	0.42
52:1:32:LYS:HB3	52:1:50:GLU:HB3	2.01	0.42
25:A:789:A:C6	53:2:3:ARG:NH1	2.88	0.42
25:A:158:U:O2	25:A:169:G:N2	2.52	0.42
25:A:1923:U:H2'	25:A:1924:C:C6	2.55	0.42
25:A:2128:G:H2'	25:A:2129:C:O4'	2.18	0.42
25:A:413:C:H2'	25:A:414:C:H6	1.85	0.42
25:A:751:A:HO2'	25:A:752:A:H2	1.67	0.42
25:A:816:C:H2'	25:A:817:C:C6	2.54	0.42
28:D:101:PHE:HA	28:D:104:VAL:HG22	2.02	0.42
31:G:51:PHE:CE1	31:G:71:LEU:HD22	2.54	0.42
34:J:35:ARG:HD3	34:J:40:HIS:CD2	2.54	0.42
35:K:108:ARG:NH1	35:K:116:ILE:HD13	2.34	0.42
41:Q:57:ARG:NH1	41:Q:61:ILE:HD11	2.34	0.42
42:R:33:VAL:HG23	42:R:61:ALA:HB3	2.01	0.42
44:T:38:ALA:HA	44:T:42:GLU:OE1	2.19	0.42
45:U:88:ASP:CG	45:U:89:GLY:H	2.21	0.42
25:A:118:A:H2'	25:A:120:U:O4	2.19	0.42
25:A:2362:C:P	54:3:27:ASN:ND2	2.92	0.42
25:A:2896:C:H2'	25:A:2897:U:C6	2.54	0.42
30:F:48:LEU:HA	30:F:51:ASN:ND2	2.34	0.42
41:Q:78:PHE:HE1	41:Q:109:VAL:HA	1.85	0.42
25:A:1366:A:H2'	25:A:1367:A:O4'	2.20	0.42
25:A:1486:U:O2'	25:A:1487:U:H5'	2.19	0.42
25:A:1529:G:H2'	25:A:1530:G:O4'	2.20	0.42
25:A:2398:U:H2'	25:A:2399:G:C8	2.54	0.42
25:A:783:A:H2'	25:A:784:G:H4'	2.02	0.42
30:F:92:GLY:N	30:F:95:MET:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:4:PHE:HE2	34:J:43:GLU:HB2	1.84	0.42
25:A:811:U:C4	36:L:21:ARG:NH2	2.87	0.42
43:S:84:ARG:HB2	43:S:96:ILE:HG13	2.00	0.42
44:T:33:LYS:HG2	44:T:80:TRP:CZ3	2.55	0.42
25:A:1413:A:H2'	25:A:1414:C:O4'	2.20	0.42
25:A:156:A:H2'	25:A:157:C:O4'	2.20	0.42
25:A:1796:U:H2'	25:A:1797:G:H8	1.84	0.42
25:A:17:G:H4'	41:Q:24:TYR:CE1	2.54	0.42
25:A:2016:U:H1'	51:O:2:VAL:HG13	2.01	0.42
25:A:2040:G:H2'	25:A:2041:U:O4'	2.20	0.42
25:A:2637:U:H2'	25:A:2638:G:O4'	2.19	0.42
25:A:2682:A:N6	25:A:2728:U:H1'	2.30	0.42
25:A:848:C:H2'	25:A:849:A:C8	2.55	0.42
30:F:134:GLN:OE1	30:F:147:ARG:O	2.36	0.42
32:H:114:GLU:N	32:H:114:GLU:OE1	2.51	0.42
32:H:132:PHE:HB2	32:H:140:ALA:HB3	2.02	0.42
36:L:17:LYS:HE3	36:L:27:LEU:CD2	2.50	0.42
37:M:66:ARG:HG3	37:M:101:VAL:HG12	2.02	0.42
38:N:67:PHE:O	38:N:71:ARG:HD2	2.19	0.42
42:R:16:GLU:HB2	42:R:101:ILE:HG12	2.01	0.42
25:A:1747:U:H2'	25:A:1748:C:C6	2.55	0.42
25:A:190:A:OP2	48:X:25:LYS:NZ	2.53	0.42
25:A:2648:G:N2	25:A:2673:G:H1'	2.35	0.42
25:A:2747:G:O6	25:A:2755:C:H5''	2.19	0.42
25:A:706:A:H2'	25:A:707:G:O4'	2.20	0.42
25:A:935:C:O2'	25:A:936:A:H5'	2.19	0.42
25:A:995:C:O2'	41:Q:92:LYS:HE2	2.20	0.42
25:A:779:U:P	27:C:48:ILE:HG22	2.60	0.42
31:G:41:GLU:HB2	31:G:54:ARG:HE	1.85	0.42
56:5:117:LEU:HD22	56:5:120:ALA:HA	2.02	0.42
56:5:49:GLY:H	56:5:51:TYR:HE2	1.68	0.42
25:A:1143:A:N7	34:J:27:ARG:NH1	2.67	0.42
25:A:1235:G:N1	25:A:1236:G:N2	2.68	0.42
25:A:335:C:C4'	25:A:1434:A:H4'	118.85	0.42
25:A:1511:G:H2'	25:A:1512:C:C6	2.55	0.42
25:A:2545:G:H2'	25:A:2546:U:O4'	2.20	0.42
25:A:2556:C:H2'	25:A:2557:G:O4'	2.20	0.42
25:A:813:U:H2'	25:A:814:C:C6	2.55	0.42
26:B:78:A:H2'	26:B:79:G:O4'	2.20	0.42
25:A:2287:A:O2'	25:A:2288:A:H2'	2.20	0.42
25:A:832:U:H2'	25:A:833:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:822:G:OP2	25:A:946:C:H5''	2.20	0.42
27:C:259:ASN:O	27:C:261:ARG:N	2.47	0.42
25:A:1993:U:H4'	28:D:133:THR:HG22	2.02	0.42
30:F:132:ARG:O	30:F:150:GLY:HA3	2.19	0.42
34:J:80:HIS:C	34:J:82:GLY:H	2.13	0.42
38:N:31:HIS:O	38:N:32:GLU:HB2	2.20	0.42
25:A:1265:A:H3'	51:O:15:ARG:HH11	1.85	0.41
52:1:10:LEU:HD23	52:1:50:GLU:HA	2.02	0.41
25:A:2391:G:H5''	54:3:31:ILE:HD12	2.02	0.41
25:A:1078:U:H4'	25:A:1079:C:H5''	2.02	0.41
25:A:1880:U:H2'	25:A:1881:C:C6	2.55	0.41
25:A:2572:A:OP1	25:A:2574:G:H4'	2.20	0.41
25:A:2709:G:H2'	25:A:2710:C:C6	2.55	0.41
25:A:594:U:H2'	25:A:595:C:C6	2.54	0.41
27:C:2:VAL:HG21	27:C:201:LEU:HD12	2.02	0.41
29:E:97:ASN:O	29:E:100:MET:N	2.51	0.41
32:H:84:ALA:HB2	32:H:90:LEU:HD12	2.02	0.41
33:I:72:THR:HG21	33:I:112:LYS:HB3	2.02	0.41
39:O:33:ARG:HG2	39:O:34:HIS:CD2	2.55	0.41
54:3:29:ARG:HA	54:3:29:ARG:HD3	1.76	0.41
25:A:1023:U:H4'	25:A:1123:C:OP1	2.21	0.41
25:A:1447:C:H2'	25:A:1448:G:C8	2.55	0.41
25:A:1847:G:O2'	25:A:1848:A:H8	2.03	0.41
25:A:2064:C:H2'	25:A:2065:C:C6	2.55	0.41
25:A:366:C:H2'	25:A:367:G:O4'	2.19	0.41
25:A:84:A:N7	25:A:101:A:H2	2.18	0.41
26:B:16:G:C6	26:B:17:C:C4	3.08	0.41
28:D:110:THR:HG21	28:D:169:ARG:HH11	1.85	0.41
29:E:122:GLU:HB2	29:E:123:LYS:H	1.68	0.41
30:F:139:GLU:HA	57:6:28:VAL:HG22	2.01	0.41
32:H:3:VAL:HA	32:H:38:PRO:HA	2.02	0.41
35:K:36:GLY:HA2	35:K:62:VAL:O	2.19	0.41
37:M:33:LEU:HD12	37:M:129:THR:O	2.20	0.41
56:5:43:LYS:HE2	56:5:43:LYS:HB3	1.84	0.41
25:A:1717:A:H2'	25:A:1718:G:O4'	2.19	0.41
25:A:2039:U:H2'	25:A:2040:G:C8	2.55	0.41
25:A:2287:A:C6	25:A:2289:G:C5	3.07	0.41
25:A:2746:U:H5''	31:G:137:LYS:HG2	2.01	0.41
25:A:2844:G:H2'	25:A:2845:U:O4'	2.20	0.41
25:A:426:C:H2'	25:A:427:U:H6	1.85	0.41
25:A:97:C:H2'	25:A:98:G:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Q:109:VAL:HG12	41:Q:113:LYS:HE2	2.01	0.41
45:U:52:ASN:OD1	45:U:54:PRO:HD3	2.19	0.41
56:5:24:SER:HA	56:5:85:SER:O	2.19	0.41
25:A:1752:C:H2'	25:A:1753:G:C8	2.56	0.41
25:A:507:A:H5''	25:A:508:A:H3'	2.02	0.41
26:B:13:G:O2'	26:B:15:A:H2'	2.19	0.41
28:D:151:THR:HB	28:D:152:PRO:HD3	2.01	0.41
30:F:7:TYR:OH	30:F:29:ARG:HB3	2.20	0.41
33:I:33:ASN:HB2	33:I:64:ARG:NH1	2.34	0.41
33:I:33:ASN:HB3	33:I:36:GLU:HG2	2.01	0.41
38:N:69:ARG:C	38:N:71:ARG:H	2.17	0.41
39:O:34:HIS:CB	39:O:53:THR:HG1	2.33	0.41
44:T:8:LEU:HA	44:T:50:LEU:HD21	2.01	0.41
25:A:1736:U:H2'	25:A:1737:G:O4'	2.20	0.41
25:A:1801:A:H5'	25:A:2203:U:O2'	2.20	0.41
25:A:2572:A:H5''	25:A:2574:G:H4'	2.02	0.41
25:A:2756:U:H1'	25:A:2757:A:H5''	2.02	0.41
25:A:758:C:O2	25:A:758:C:H2'	2.20	0.41
36:L:23:ILE:H	36:L:23:ILE:HD12	1.84	0.41
25:A:1287:A:H5'	38:N:103:ARG:NH1	2.36	0.41
41:Q:75:TYR:CZ	41:Q:79:ILE:HG13	2.55	0.41
43:S:34:ASP:HB3	51:O:27:LEU:HD22	2.03	0.41
54:3:36:ALA:O	54:3:39:ARG:HB2	2.20	0.41
25:A:1045:C:H5'	25:A:1046:A:C5'	2.50	0.41
25:A:1112:G:H2'	25:A:1113:U:H6	1.86	0.41
25:A:1180:U:H2'	25:A:1181:U:H5'	2.02	0.41
25:A:1789:A:OP2	27:C:220:ARG:NH2	2.46	0.41
25:A:2230:G:H2'	25:A:2231:U:C6	2.56	0.41
25:A:2283:C:OP2	25:A:2390:U:C5	2.72	0.41
25:A:329:G:OP2	45:U:68:ASN:ND2	2.54	0.41
25:A:340:A:H2'	25:A:341:C:O4'	2.21	0.41
26:B:54:G:H2'	26:B:55:U:C6	2.56	0.41
32:H:66:ASN:HB3	32:H:134:VAL:O	2.20	0.41
36:L:125:LEU:HB3	36:L:126:ARG:H	1.55	0.41
37:M:109:PRO:HD2	37:M:112:LEU:HD23	2.03	0.41
38:N:38:LEU:HG	38:N:42:LYS:HE2	2.03	0.41
40:P:3:ILE:HD12	40:P:3:ILE:H	1.86	0.41
57:6:26:SER:OG	57:6:27:THR:N	2.53	0.41
25:A:1067:A:H4'	25:A:1068:G:O5'	4.70	0.41
25:A:2599:G:C8	27:C:235:GLU:HG2	2.56	0.41
25:A:753:A:H2'	25:A:754:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:859:G:H1'	25:A:860:U:H5	1.85	0.41
27:C:24:HIS:HB3	27:C:81:GLU:OE1	2.20	0.41
36:L:123:ARG:HA	36:L:143:GLU:O	2.20	0.41
44:T:37:ASP:OD1	44:T:38:ALA:N	2.54	0.41
44:T:8:LEU:HD11	49:Y:22:LEU:HD12	2.03	0.41
25:A:2092:U:H4'	25:A:2093:G:O5'	2.20	0.41
25:A:2298:A:OP1	30:F:70:ARG:NH2	2.52	0.41
25:A:2368:C:H2'	25:A:2369:A:H8	1.86	0.41
25:A:993:G:N3	25:A:993:G:H2'	3.04	0.41
25:A:1826:G:OP1	27:C:222:THR:HG23	2.19	0.41
32:H:9:VAL:HG12	32:H:11:ASN:H	1.85	0.41
34:J:17:VAL:HG22	34:J:55:ILE:HB	2.02	0.41
39:O:92:PHE:HB2	39:O:117:PHE:CE1	2.56	0.41
53:2:21:ARG:O	53:2:27:GLY:HA3	2.21	0.41
25:A:687:C:H5''	53:2:2:LYS:NZ	2.35	0.41
25:A:1292:G:H2'	25:A:1293:C:C6	2.56	0.41
25:A:1319:C:H2'	25:A:1320:C:O4'	2.20	0.41
25:A:1591:A:H2'	25:A:1592:C:O4'	2.21	0.41
25:A:1741:C:H2'	25:A:1742:U:C6	2.56	0.41
25:A:2285:C:O2'	25:A:2287:A:H1'	2.20	0.41
25:A:456:C:C2	44:T:73:ARG:NH2	2.87	0.41
25:A:919:U:H2'	25:A:920:A:O4'	2.19	0.41
26:B:48:U:H2'	26:B:49:C:C6	2.56	0.41
25:A:1140:C:P	34:J:68:LYS:HZ2	2.44	0.41
28:D:20:VAL:HG22	35:K:72:PRO:HB2	2.03	0.41
38:N:54:LEU:HD21	38:N:65:LEU:HB3	2.02	0.41
38:N:82:GLU:O	38:N:86:ARG:HB2	2.21	0.41
43:S:14:ALA:HB1	43:S:18:ARG:HH21	1.85	0.41
44:T:8:LEU:HD13	49:Y:21:LEU:HB3	2.02	0.41
25:A:1071:G:N2	25:A:1089:A:O2'	2.54	0.41
25:A:1562:U:H2'	25:A:1563:U:O4'	2.20	0.41
25:A:1957:C:H2'	25:A:1958:C:C6	2.56	0.41
25:A:21:A:H2'	25:A:22:C:O4'	2.21	0.41
25:A:609:A:H2'	25:A:610:C:O4'	2.21	0.41
25:A:739:A:H1'	25:A:740:C:H5	1.86	0.41
25:A:857:G:H2'	25:A:858:G:O4'	2.21	0.41
27:C:78:GLU:HB3	27:C:92:LEU:O	2.21	0.41
33:I:20:SER:HA	33:I:24:GLY:HA3	2.02	0.41
54:3:51:LYS:HB2	54:3:51:LYS:HE3	1.87	0.41
55:4:7:VAL:HG22	55:4:38:GLY:HA3	2.03	0.41
25:A:1943:U:H1'	25:A:1945:G:OP2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2106:U:H2'	25:A:2107:G:C8	2.56	0.41
25:A:2697:G:H2'	25:A:2698:U:O4'	2.21	0.41
25:A:275:C:H3'	25:A:276:U:H5''	2.03	0.41
25:A:2803:G:H2'	25:A:2804:U:C6	2.56	0.41
25:A:460:A:H2'	25:A:461:C:O4'	2.20	0.41
25:A:490:C:H4'	25:A:491:G:OP2	2.21	0.41
25:A:737:C:H2'	25:A:738:G:O4'	2.21	0.41
26:B:43:C:O2'	30:F:91:ARG:HG2	2.20	0.41
28:D:148:GLN:HB2	28:D:152:PRO:HG2	2.03	0.41
29:E:128:ALA:O	29:E:130:LYS:N	2.51	0.41
39:O:52:SER:OG	39:O:54:VAL:HG12	2.21	0.41
48:X:12:VAL:HG23	48:X:28:PHE:HB2	2.03	0.41
53:2:34:ARG:HE	53:2:39:ARG:HD2	1.86	0.40
57:6:2:LYS:O	57:6:5:ILE:HG12	2.21	0.40
25:A:2030:6MZ:C2	25:A:2499:C:H5''	2.51	0.40
25:A:2475:C:O5'	25:A:2475:C:H6	2.04	0.40
25:A:306:U:H2'	25:A:307:G:O4'	2.21	0.40
25:A:608:A:H2'	25:A:609:A:O4'	2.41	0.40
27:C:104:LEU:HD23	27:C:104:LEU:HA	1.89	0.40
27:C:70:LYS:HD2	27:C:73:ILE:HD12	2.02	0.40
28:D:43:ASP:HB3	28:D:45:TYR:CE2	2.55	0.40
30:F:175:PRO:HB2	30:F:176:PHE:H	1.71	0.40
36:L:21:ARG:HD3	36:L:21:ARG:HA	1.85	0.40
47:W:21:ARG:HB2	47:W:33:ILE:HG23	2.03	0.40
49:Y:28:LEU:HD13	49:Y:42:LEU:HB3	2.03	0.40
25:A:1132:U:H3'	25:A:1132:U:OP2	2.21	0.40
25:A:1454:C:H5'	38:N:63:ARG:NH2	2.36	0.40
25:A:1730:C:O2	25:A:1731:G:N1	2.54	0.40
25:A:1884:G:H5'	25:A:1885:A:OP1	2.19	0.40
25:A:218:A:OP2	25:A:218:A:C8	2.67	0.40
25:A:2804:U:H2'	25:A:2805:C:C6	2.56	0.40
25:A:2825:G:N3	25:A:2825:G:H5''	2.36	0.40
25:A:310:A:O2'	25:A:311:A:H5''	2.20	0.40
25:A:869:G:H1'	37:M:8:LYS:HD2	2.02	0.40
25:A:844:A:N6	25:A:934:U:H3	2.19	0.40
33:I:129:GLU:O	33:I:132:ALA:HB3	2.21	0.40
46:V:30:ILE:HG21	46:V:70:ILE:HG21	2.02	0.40
55:4:5:ALA:O	55:4:38:GLY:HA2	2.21	0.40
25:A:1495:A:O5'	25:A:1495:A:H8	2.04	0.40
25:A:1418:G:N1	25:A:1579:A:OP2	2.44	0.40
25:A:1824:G:O3'	27:C:246:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2408:U:H2'	25:A:2409:G:C8	2.56	0.40
25:A:376:G:H2'	25:A:377:G:H8	1.86	0.40
25:A:443:A:OP1	29:E:40:ARG:HG2	2.21	0.40
25:A:633:A:C2'	25:A:634:C:H5'	2.50	0.40
25:A:736:C:H2'	25:A:737:C:C6	2.82	0.40
30:F:137:PHE:HA	30:F:138:PRO:HD3	1.77	0.40
31:G:88:LEU:HG	31:G:161:VAL:HG22	2.03	0.40
41:Q:71:ASN:N	41:Q:71:ASN:ND2	2.69	0.40
42:R:14:VAL:CG2	42:R:98:ILE:HG13	2.43	0.40
49:Y:4:LYS:HG2	49:Y:7:ARG:HH22	1.87	0.40
25:A:1045:C:H1'	25:A:1047:G:N3	2.36	0.40
25:A:1078:U:O2'	25:A:1088:A:H5''	2.22	0.40
25:A:1096:A:H2'	25:A:1097:U:O5'	2.22	0.40
25:A:1560:G:OP2	25:A:1560:G:H8	2.05	0.40
25:A:1665:A:H2'	25:A:1666:G:O4'	2.21	0.40
25:A:2108:A:H2'	25:A:2109:U:O4'	2.21	0.40
25:A:22:C:H2'	25:A:23:G:O4'	2.21	0.40
25:A:613:A:N3	25:A:613:A:H2'	2.36	0.40
29:E:159:LEU:C	29:E:161:ALA:H	2.25	0.40
25:A:2674:G:H5'	35:K:30:ARG:HH21	1.85	0.40
37:M:41:LEU:HG	37:M:96:ILE:HG13	2.03	0.40
41:Q:106:THR:O	41:Q:110:GLU:HG2	2.21	0.40
41:Q:34:ALA:O	41:Q:38:VAL:HG23	2.21	0.40
56:5:107:GLU:O	56:5:109:LYS:N	2.55	0.40
57:6:39:LYS:O	57:6:40:CYS:SG	2.80	0.40
25:A:335:C:C4'	25:A:1434:A:C4'	117.92	0.40
25:A:1857:G:O2'	25:A:1858:A:H8	2.04	0.40
25:A:1936:A:N6	25:A:1963:U:N3	2.69	0.40
25:A:591:U:H2'	25:A:592:A:C8	2.56	0.40
25:A:64:A:H2'	25:A:65:U:C6	2.56	0.40
26:B:17:C:H2'	26:B:18:G:O4'	2.22	0.40
27:C:16:VAL:H	27:C:203:VAL:HG22	1.84	0.40
27:C:257:ARG:NH1	27:C:259:ASN:HB2	2.37	0.40
27:C:132:ARG:NH1	32:H:93:SER:OG	2.54	0.40
38:N:56:LYS:HZ2	38:N:88:ALA:HA	1.86	0.40
40:P:21:PRO:HD3	40:P:49:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/240 (90%)	183 (85%)	23 (11%)	10 (5%)	3	30
3	d	203/206 (98%)	172 (85%)	21 (10%)	10 (5%)	2	29
4	e	155/167 (93%)	130 (84%)	16 (10%)	9 (6%)	2	26
5	f	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	2	25
6	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	7	45
7	k	114/129 (88%)	92 (81%)	16 (14%)	6 (5%)	2	28
8	l	121/124 (98%)	96 (79%)	20 (16%)	5 (4%)	3	33
9	o	86/89 (97%)	71 (83%)	10 (12%)	5 (6%)	2	26
10	p	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	6	44
11	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	1	24
12	r	63/75 (84%)	53 (84%)	5 (8%)	5 (8%)	1	18
13	t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	7	45
14	u	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1	18
17	w	637/639 (100%)	562 (88%)	51 (8%)	24 (4%)	4	35
18	c	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	18	61
19	g	149/179 (83%)	124 (83%)	15 (10%)	10 (7%)	1	23
20	i	125/130 (96%)	98 (78%)	19 (15%)	8 (6%)	1	24
21	j	96/103 (93%)	74 (77%)	16 (17%)	6 (6%)	1	24
22	m	112/118 (95%)	99 (88%)	8 (7%)	5 (4%)	3	31
23	n	99/102 (97%)	82 (83%)	12 (12%)	5 (5%)	2	28
24	s	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
27	C	269/273 (98%)	242 (90%)	22 (8%)	5 (2%)	9	50
28	D	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	18	61
29	E	199/201 (99%)	172 (86%)	20 (10%)	7 (4%)	4	38
30	F	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	4	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	G	174/177 (98%)	148 (85%)	21 (12%)	5 (3%)	5	42
32	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	6	43
33	I	139/142 (98%)	110 (79%)	20 (14%)	9 (6%)	1	24
34	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	13	55
35	K	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	6	44
36	L	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1	18
37	M	134/136 (98%)	117 (87%)	14 (10%)	3 (2%)	8	47
38	N	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	6	44
39	O	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	20	63
40	P	112/115 (97%)	93 (83%)	18 (16%)	1 (1%)	20	63
41	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
42	R	101/103 (98%)	81 (80%)	18 (18%)	2 (2%)	9	49
43	S	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	27
44	T	91/100 (91%)	77 (85%)	11 (12%)	3 (3%)	4	39
45	U	100/104 (96%)	81 (81%)	16 (16%)	3 (3%)	5	41
46	V	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	8	47
47	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	13	55
48	X	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	14	57
49	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	11	53
50	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
51	0	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	9	50
52	1	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
53	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	3	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	11	53
55	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
56	5	129/165 (78%)	100 (78%)	22 (17%)	7 (5%)	2	28
57	6	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	11	53
58	7	67/69 (97%)	58 (87%)	8 (12%)	1 (2%)	12	54
All	All	6551/6928 (95%)	5610 (86%)	716 (11%)	225 (3%)	7	39

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	e	122	VAL
5	f	63	ASN
10	p	8	ARG
11	q	79	GLU
12	r	17	VAL
17	w	76	PRO
17	w	80	ASP
17	w	176	ASP
17	w	334	PRO
17	w	342	PRO
17	w	344	PRO
17	w	416	PRO
17	w	433	HIS
17	w	438	PRO
17	w	612	VAL
17	w	617	PRO
17	w	624	PRO
18	c	156	LEU
20	i	12	LYS
20	i	71	ILE
21	j	57	VAL
21	j	75	ASP
21	j	89	ARG
27	C	204	LEU
30	F	175	PRO
31	G	108	PHE
34	J	81	ILE
35	K	93	GLN
36	L	15	ALA
36	L	85	VAL
36	L	128	THR
43	S	67	ASP
45	U	6	ARG
45	U	97	SER
48	X	31	ASN
54	3	27	ASN
2	b	17	HIS
2	b	19	THR
2	b	179	GLY
3	d	26	ALA
3	d	108	ALA
4	e	23	THR
4	e	93	VAL

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Mol	Chain	Res	Type
6	h	66	GLN
7	k	76	TYR
7	k	77	GLY
7	k	88	PRO
8	l	75	GLU
9	o	21	THR
9	o	45	HIS
11	q	17	GLU
11	q	49	ASN
12	r	46	THR
13	t	68	LYS
14	u	12	ASP
17	w	41	THR
17	w	96	ILE
18	c	13	ILE
19	g	16	LYS
19	g	56	SER
19	g	63	VAL
19	g	112	ASP
19	g	145	GLU
20	i	57	VAL
21	j	29	ALA
21	j	77	VAL
22	m	104	ASN
23	n	54	ASP
27	C	195	GLY
27	C	231	HIS
32	H	9	VAL
33	I	89	SER
33	I	92	PRO
35	K	35	VAL
35	K	110	GLU
36	L	29	LYS
36	L	31	GLY
36	L	111	ILE
37	M	70	ASP
39	O	66	GLY
40	P	65	ASN
42	R	43	ASN
42	R	54	VAL
43	S	2	GLU
43	S	3	THR

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Mol	Chain	Res	Type
44	T	37	ASP
44	T	38	ALA
44	T	71	GLY
49	Y	24	GLU
56	5	55	VAL
2	b	73	ARG
2	b	87	ASP
2	b	153	MET
3	d	7	LYS
3	d	31	CYS
3	d	152	SER
3	d	166	LYS
3	d	174	ALA
4	e	98	ALA
4	e	99	SER
4	e	121	ASN
5	f	54	LEU
5	f	92	THR
6	h	74	ILE
7	k	14	GLN
8	l	2	THR
8	l	46	SER
9	o	2	LEU
9	o	13	GLU
10	p	49	GLY
11	q	16	MET
13	t	76	ALA
14	u	29	ALA
14	u	32	ARG
14	u	34	ARG
17	w	8	VAL
17	w	371	SER
19	g	64	ALA
19	g	95	ARG
20	i	90	ASP
20	i	107	ALA
20	i	125	GLN
21	j	35	GLN
22	m	6	ILE
22	m	7	ASN
22	m	113	LYS
23	n	22	LYS

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Mol	Chain	Res	Type
23	n	38	ASP
23	n	55	SER
27	C	239	PHE
29	E	89	PRO
29	E	122	GLU
31	G	44	HIS
31	G	45	ALA
32	H	15	LEU
33	I	12	VAL
33	I	64	ARG
36	L	88	GLY
37	M	6	ARG
38	N	59	SER
43	S	62	ASP
56	5	88	HIS
56	5	118	ILE
57	6	40	CYS
2	b	11	ALA
2	b	88	GLN
2	b	126	ASP
4	e	100	GLU
4	e	102	THR
5	f	56	LYS
5	f	86	ARG
5	f	99	ALA
6	h	22	ALA
7	k	92	ARG
8	l	23	LEU
9	o	75	ALA
12	r	18	GLN
12	r	71	ASP
17	w	40	THR
17	w	262	ARG
17	w	470	ASN
19	g	29	LEU
20	i	99	LYS
28	D	32	ASN
29	E	80	SER
29	E	160	ALA
30	F	20	ASN
30	F	142	TYR
30	F	173	ASP

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Mol	Chain	Res	Type
30	F	176	PHE
32	H	2	GLN
33	I	6	ALA
33	I	20	SER
36	L	25	SER
38	N	117	ASP
43	S	65	ASP
46	V	58	SER
47	W	8	ASN
51	0	2	VAL
56	5	22	ALA
56	5	90	GLY
56	5	130	PRO
58	7	72	VAL
2	b	14	HIS
3	d	34	GLU
12	r	70	THR
17	w	161	TYR
17	w	609	GLY
17	w	630	LYS
23	n	2	LYS
29	E	84	THR
30	F	174	PHE
31	G	70	LEU
32	H	3	VAL
33	I	22	PRO
33	I	100	ILE
34	J	82	GLY
36	L	94	THR
3	d	6	PRO
3	d	28	ASP
20	i	13	SER
28	D	148	GLN
29	E	83	VAL
33	I	38	CYS
36	L	119	PRO
43	S	101	SER
7	k	119	GLY
8	l	44	PRO
17	w	75	THR
27	C	168	GLY
36	L	26	GLY

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Mol	Chain	Res	Type
37	M	69	PRO
38	N	116	VAL
11	q	20	ILE
14	u	9	GLU
45	U	38	ILE
19	g	5	VAL
29	E	129	PRO
46	V	15	GLY
56	5	108	VAL
17	w	621	PRO
19	g	28	ILE
4	e	26	GLY
22	m	9	PRO
31	G	155	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/198 (91%)	175 (97%)	5 (3%)	49	76
3	d	172/173 (99%)	166 (96%)	6 (4%)	41	72
4	e	114/126 (90%)	105 (92%)	9 (8%)	14	50
5	f	87/116 (75%)	83 (95%)	4 (5%)	31	66
6	h	104/105 (99%)	103 (99%)	1 (1%)	80	90
7	k	89/99 (90%)	87 (98%)	2 (2%)	57	81
8	l	103/104 (99%)	100 (97%)	3 (3%)	48	75
9	o	76/77 (99%)	74 (97%)	2 (3%)	51	78
10	p	65/65 (100%)	61 (94%)	4 (6%)	21	58
11	q	74/78 (95%)	71 (96%)	3 (4%)	35	69
12	r	48/65 (74%)	47 (98%)	1 (2%)	59	82
13	t	65/66 (98%)	63 (97%)	2 (3%)	45	74
14	u	44/61 (72%)	42 (96%)	2 (4%)	32	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	w	6/576 (1%)	6 (100%)	0	100	100
18	c	170/190 (90%)	163 (96%)	7 (4%)	35	69
19	g	124/147 (84%)	122 (98%)	2 (2%)	68	86
20	i	105/107 (98%)	100 (95%)	5 (5%)	30	65
21	j	86/90 (96%)	84 (98%)	2 (2%)	56	80
22	m	92/96 (96%)	90 (98%)	2 (2%)	57	81
23	n	79/84 (94%)	75 (95%)	4 (5%)	28	63
24	s	70/79 (89%)	69 (99%)	1 (1%)	71	87
27	C	216/218 (99%)	208 (96%)	8 (4%)	39	71
28	D	164/164 (100%)	161 (98%)	3 (2%)	64	85
29	E	165/165 (100%)	160 (97%)	5 (3%)	46	75
30	F	148/150 (99%)	141 (95%)	7 (5%)	30	65
31	G	137/138 (99%)	137 (100%)	0	100	100
32	H	114/114 (100%)	114 (100%)	0	100	100
33	I	109/110 (99%)	106 (97%)	3 (3%)	49	76
34	J	116/116 (100%)	114 (98%)	2 (2%)	66	86
35	K	103/104 (99%)	98 (95%)	5 (5%)	29	64
36	L	102/103 (99%)	100 (98%)	2 (2%)	60	83
37	M	109/109 (100%)	108 (99%)	1 (1%)	82	92
38	N	100/103 (97%)	98 (98%)	2 (2%)	60	83
39	O	86/87 (99%)	84 (98%)	2 (2%)	56	80
40	P	99/100 (99%)	96 (97%)	3 (3%)	46	75
41	Q	89/90 (99%)	87 (98%)	2 (2%)	57	81
42	R	84/84 (100%)	83 (99%)	1 (1%)	75	89
43	S	93/93 (100%)	90 (97%)	3 (3%)	44	74
44	T	80/84 (95%)	77 (96%)	3 (4%)	38	70
45	U	83/85 (98%)	82 (99%)	1 (1%)	75	89
46	V	78/78 (100%)	77 (99%)	1 (1%)	73	88
47	W	57/63 (90%)	56 (98%)	1 (2%)	64	85
48	X	67/68 (98%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	54 (98%)	1 (2%)	64	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	Z	48/49 (98%)	48 (100%)	0	100	100
51	0	47/48 (98%)	45 (96%)	2 (4%)	33	68
52	1	45/49 (92%)	44 (98%)	1 (2%)	57	81
53	2	38/38 (100%)	38 (100%)	0	100	100
54	3	51/52 (98%)	50 (98%)	1 (2%)	60	83
55	4	34/34 (100%)	34 (100%)	0	100	100
56	5	100/123 (81%)	97 (97%)	3 (3%)	46	75
57	6	59/62 (95%)	58 (98%)	1 (2%)	66	86
All	All	4829/5638 (86%)	4698 (97%)	131 (3%)	54	77

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	9	LEU
2	b	35	ASN
2	b	71	THR
2	b	185	ILE
2	b	202	ASN
3	d	16	THR
3	d	52	VAL
3	d	115	GLN
3	d	119	HIS
3	d	141	VAL
3	d	196	GLU
4	e	10	LEU
4	e	11	GLN
4	e	45	VAL
4	e	51	LYS
4	e	75	LEU
4	e	122	VAL
4	e	140	ILE
4	e	156	ARG
4	e	158	LYS
5	f	54	LEU
5	f	74	LEU
5	f	86	ARG
5	f	89	VAL
6	h	58	LEU
7	k	30	ILE

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Mol	Chain	Res	Type
7	k	39	ASN
8	l	20	VAL
8	l	28	GLN
8	l	63	THR
9	o	44	GLU
9	o	86	LEU
10	p	19	VAL
10	p	26	ASN
10	p	34	GLU
10	p	70	ARG
11	q	51	GLU
11	q	61	ARG
11	q	69	THR
12	r	24	ASP
13	t	22	SER
13	t	26	MET
14	u	19	LYS
14	u	23	GLU
18	c	3	LYS
18	c	40	GLN
18	c	96	VAL
18	c	127	VAL
18	c	133	MET
18	c	149	LYS
18	c	156	LEU
19	g	58	LEU
19	g	83	THR
20	i	38	PHE
20	i	54	VAL
20	i	60	LEU
20	i	88	GLU
20	i	108	ARG
21	j	10	LEU
21	j	64	GLN
22	m	15	VAL
22	m	99	GLN
23	n	26	LEU
23	n	33	VAL
23	n	49	GLN
23	n	60	GLN
24	s	62	THR
27	C	12	ARG

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Mol	Chain	Res	Type
27	C	13	ARG
27	C	45	ASN
27	C	129	LEU
27	C	181	ARG
27	C	206	LYS
27	C	212	TRP
27	C	257	ARG
28	D	33	ARG
28	D	52	THR
28	D	88	GLU
29	E	7	ASP
29	E	19	PHE
29	E	40	ARG
29	E	41	GLN
29	E	96	VAL
30	F	3	LEU
30	F	5	ASP
30	F	9	ASP
30	F	55	ASP
30	F	95	MET
30	F	129	MET
30	F	134	GLN
33	I	10	LEU
33	I	95	ASP
33	I	134	SER
34	J	57	LEU
34	J	64	VAL
35	K	8	LEU
35	K	30	ARG
35	K	32	TYR
35	K	58	LEU
35	K	73	ASP
36	L	27	LEU
36	L	41	ARG
37	M	46	ILE
38	N	15	SER
38	N	113	ILE
39	O	69	ASP
39	O	100	HIS
40	P	7	LEU
40	P	31	VAL
40	P	99	LEU

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Mol	Chain	Res	Type
41	Q	48	ASP
41	Q	94	LEU
42	R	22	LEU
43	S	25	ARG
43	S	62	ASP
43	S	77	ASP
44	T	32	LEU
44	T	37	ASP
44	T	59	ASN
45	U	82	VAL
46	V	42	LEU
47	W	67	VAL
49	Y	40	SER
51	0	22	THR
51	0	24	VAL
52	1	46	VAL
54	3	61	LEU
56	5	3	LEU
56	5	57	ASN
56	5	122	GLN
57	6	16	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	202	ASN
3	d	70	GLN
3	d	119	HIS
3	d	135	GLN
5	f	11	HIS
7	k	39	ASN
8	l	76	HIS
9	o	45	HIS
10	p	26	ASN
11	q	30	HIS
12	r	51	GLN
18	c	40	GLN
19	g	141	HIS
21	j	64	GLN
21	j	70	HIS
22	m	90	HIS
23	n	49	GLN

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Mol	Chain	Res	Type
24	s	51	HIS
24	s	56	HIS
27	C	196	ASN
28	D	49	GLN
28	D	149	ASN
30	F	134	GLN
31	G	103	ASN
31	G	138	GLN
34	J	40	HIS
41	Q	71	ASN
43	S	61	ASN
45	U	65	GLN
51	0	5	ASN
57	6	65	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	254 (16%)	0
15	v	76/78 (97%)	17 (22%)	0
16	x	8/11 (72%)	0	0
25	A	2894/2903 (99%)	542 (18%)	0
26	B	119/120 (99%)	17 (14%)	0
All	All	4632/4651 (99%)	830 (17%)	0

All (830) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	14	U
1	a	22	G
1	a	30	U
1	a	32	A
1	a	39	G
1	a	47	C
1	a	49	U
1	a	51	A
1	a	71	A
1	a	85	U
1	a	86	G
1	a	87	C

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Mol	Chain	Res	Type
1	a	94	G
1	a	95	C
1	a	120	A
1	a	121	U
1	a	130	A
1	a	174	A
1	a	175	C
1	a	181	A
1	a	183	C
1	a	184	G
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	246	A
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	283	U
1	a	289	G
1	a	306	A
1	a	321	A
1	a	328	C
1	a	345	C
1	a	346	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	355	C
1	a	367	U
1	a	368	U
1	a	372	C
1	a	373	A
1	a	387	U
1	a	392	C
1	a	398	U
1	a	406	G
1	a	412	A
1	a	413	G

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Mol	Chain	Res	Type
1	a	414	A
1	a	422	C
1	a	423	G
1	a	424	G
1	a	429	U
1	a	430	A
1	a	439	U
1	a	467	U
1	a	468	A
1	a	482	A
1	a	484	G
1	a	485	U
1	a	486	U
1	a	496	A
1	a	497	G
1	a	500	G
1	a	511	C
1	a	527	7MG
1	a	530	G
1	a	531	U
1	a	532	A
1	a	533	A
1	a	536	C
1	a	547	A
1	a	559	A
1	a	561	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	574	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	579	A
1	a	597	G
1	a	618	C
1	a	626	G
1	a	633	G
1	a	641	U
1	a	642	A
1	a	654	G

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Mol	Chain	Res	Type
1	a	661	G
1	a	665	A
1	a	671	G
1	a	687	A
1	a	688	G
1	a	701	U
1	a	702	A
1	a	703	G
1	a	724	G
1	a	731	G
1	a	755	G
1	a	777	A
1	a	792	A
1	a	793	U
1	a	794	A
1	a	814	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	832	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	871	U
1	a	874	G
1	a	884	U
1	a	890	G
1	a	902	G
1	a	914	A
1	a	920	U
1	a	921	U
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A

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Mol	Chain	Res	Type
1	a	979	C
1	a	981	U
1	a	991	U
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1004	A
1	a	1026	G
1	a	1028	C
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1053	G
1	a	1056	U
1	a	1065	U
1	a	1067	A
1	a	1085	U
1	a	1086	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1127	G
1	a	1129	C
1	a	1130	A
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1152	A
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1182	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1198	G

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Mol	Chain	Res	Type
1	a	1200	C
1	a	1201	A
1	a	1202	U
1	a	1207	2MG
1	a	1212	U
1	a	1213	A
1	a	1224	U
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1228	C
1	a	1236	A
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1256	A
1	a	1258	G
1	a	1260	G
1	a	1278	G
1	a	1279	G
1	a	1280	A
1	a	1281	C
1	a	1282	C
1	a	1286	U
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1301	U
1	a	1302	C
1	a	1306	A
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1331	G
1	a	1332	A
1	a	1346	A
1	a	1347	G
1	a	1348	U
1	a	1353	G
1	a	1363	A

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Mol	Chain	Res	Type
1	a	1381	U
1	a	1395	C
1	a	1396	A
1	a	1397	C
1	a	1399	C
1	a	1400	C
1	a	1401	G
1	a	1418	A
1	a	1429	A
1	a	1433	A
1	a	1446	A
1	a	1448	C
1	a	1451	U
1	a	1452	C
1	a	1491	G
1	a	1492	A
1	a	1493	A
1	a	1494	G
1	a	1502	A
1	a	1503	A
1	a	1505	G
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1539	C
15	v	7	G
15	v	8	4SU
15	v	9	G
15	v	14	A
15	v	16	C
15	v	17	C
15	v	17(A)	U
15	v	18	G
15	v	19	G
15	v	20	H2U
15	v	21	A

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Mol	Chain	Res	Type
15	v	22	G
15	v	59	A
15	v	60	U
15	v	67	C
15	v	75	C
15	v	76	A
25	A	10	A
25	A	12	U
25	A	23	G
25	A	27	G
25	A	28	A
25	A	34	U
25	A	35	G
25	A	42	A
25	A	46	G
25	A	49	A
25	A	51	G
25	A	52	A
25	A	60	G
25	A	63	A
25	A	71	A
25	A	73	A
25	A	74	A
25	A	75	G
25	A	91	A
25	A	92	U
25	A	103	A
25	A	110	G
25	A	118	A
25	A	119	A
25	A	120	U
25	A	127	A
25	A	138	U
25	A	139	U
25	A	140	C
25	A	141	G
25	A	142	A
25	A	158	U
25	A	162	U
25	A	163	C
25	A	181	A
25	A	196	A

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Mol	Chain	Res	Type
25	A	199	A
25	A	204	A
25	A	205	G
25	A	215	G
25	A	216	A
25	A	218	A
25	A	219	A
25	A	221	A
25	A	222	A
25	A	227	A
25	A	228	C
25	A	242	G
25	A	243	U
25	A	248	G
25	A	249	C
25	A	255	A
25	A	265	A
25	A	266	G
25	A	267	C
25	A	272	A
25	A	276	U
25	A	278	A
25	A	281	C
25	A	294	A
25	A	301	G
25	A	302	C
25	A	311	A
25	A	321	U
25	A	322	A
25	A	323	C
25	A	324	A
25	A	329	G
25	A	330	A
25	A	333	G
25	A	334	C
25	A	346	A
25	A	353	C
25	A	361	G
25	A	362	A
25	A	370	G
25	A	371	A
25	A	372	G

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Mol	Chain	Res	Type
25	A	373	U
25	A	386	G
25	A	387	U
25	A	390	U
25	A	391	A
25	A	404	A
25	A	405	U
25	A	406	G
25	A	411	G
25	A	422	A
25	A	424	G
25	A	442	G
25	A	446	G
25	A	454	A
25	A	455	C
25	A	457	A
25	A	458	G
25	A	459	U
25	A	467	G
25	A	480	A
25	A	481	G
25	A	490	C
25	A	491	G
25	A	504	A
25	A	505	A
25	A	506	G
25	A	508	A
25	A	518	G
25	A	527	C
25	A	529	A
25	A	530	G
25	A	532	A
25	A	533	G
25	A	542	C
25	A	543	G
25	A	545	U
25	A	547	A
25	A	550	C
25	A	555	G
25	A	563	A
25	A	572	A
25	A	573	U

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Mol	Chain	Res	Type
25	A	575	A
25	A	603	A
25	A	614	A
25	A	616	A
25	A	627	A
25	A	637	A
25	A	645	C
25	A	646	U
25	A	654	A
25	A	655	A
25	A	659	G
25	A	668	A
25	A	669	G
25	A	670	A
25	A	677	A
25	A	685	A
25	A	686	U
25	A	687	C
25	A	694	U
25	A	695	G
25	A	717	C
25	A	726	G
25	A	730	A
25	A	740	C
25	A	747	5MC
25	A	748	G
25	A	752	A
25	A	753	A
25	A	765	C
25	A	772	C
25	A	775	G
25	A	776	G
25	A	777	G
25	A	782	A
25	A	784	G
25	A	785	G
25	A	789	A
25	A	791	C
25	A	801	G
25	A	802	A
25	A	805	G
25	A	806	C

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Mol	Chain	Res	Type
25	A	812	C
25	A	819	A
25	A	822	G
25	A	827	U
25	A	828	U
25	A	830	G
25	A	831	G
25	A	845	A
25	A	846	U
25	A	847	U
25	A	858	G
25	A	859	G
25	A	860	U
25	A	878	A
25	A	896	A
25	A	897	C
25	A	907	G
25	A	910	A
25	A	932	U
25	A	941	A
25	A	946	C
25	A	953	G
25	A	958	U
25	A	961	C
25	A	974	G
25	A	975	A
25	A	982	C
25	A	983	A
25	A	985	C
25	A	989	G
25	A	990	A
25	A	995	C
25	A	996	A
25	A	999	U
25	A	1011	G
25	A	1012	U
25	A	1013	C
25	A	1021	A
25	A	1022	G
25	A	1023	U
25	A	1026	G
25	A	1033	U

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Mol	Chain	Res	Type
25	A	1046	A
25	A	1053	C
25	A	1054	A
25	A	1057	A
25	A	1060	U
25	A	1061	U
25	A	1062	G
25	A	1064	C
25	A	1065	U
25	A	1066	U
25	A	1068	G
25	A	1069	A
25	A	1070	A
25	A	1071	G
25	A	1072	C
25	A	1075	C
25	A	1076	C
25	A	1079	C
25	A	1084	A
25	A	1088	A
25	A	1089	A
25	A	1090	A
25	A	1104	C
25	A	1111	A
25	A	1112	G
25	A	1119	U
25	A	1130	U
25	A	1131	G
25	A	1132	U
25	A	1134	A
25	A	1135	C
25	A	1142	A
25	A	1143	A
25	A	1151	A
25	A	1174	U
25	A	1175	A
25	A	1176	U
25	A	1179	G
25	A	1180	U
25	A	1206	G
25	A	1212	G
25	A	1213	A

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Mol	Chain	Res	Type
25	A	1218	G
25	A	1237	A
25	A	1238	G
25	A	1247	A
25	A	1248	G
25	A	1250	G
25	A	1251	C
25	A	1253	A
25	A	1256	G
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1276	A
25	A	1289	C
25	A	1298	C
25	A	1300	G
25	A	1301	A
25	A	1302	A
25	A	1311	G
25	A	1315	C
25	A	1321	A
25	A	1329	U
25	A	1330	C
25	A	1332	G
25	A	1341	G
25	A	1345	C
25	A	1352	U
25	A	1365	A
25	A	1368	G
25	A	1378	A
25	A	1379	U
25	A	1380	G
25	A	1383	A
25	A	1385	A
25	A	1395	A
25	A	1397	U
25	A	1416	G
25	A	1419	A
25	A	1420	A
25	A	1428	C
25	A	1454	C
25	A	1458	U

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Mol	Chain	Res	Type
25	A	1461	C
25	A	1482	G
25	A	1483	G
25	A	1490	A
25	A	1491	G
25	A	1493	C
25	A	1504	A
25	A	1515	A
25	A	1524	G
25	A	1533	C
25	A	1535	A
25	A	1536	C
25	A	1537	G
25	A	1555	G
25	A	1559	U
25	A	1560	G
25	A	1567	G
25	A	1569	A
25	A	1578	U
25	A	1581	G
25	A	1585	C
25	A	1607	C
25	A	1611	C
25	A	1616	A
25	A	1627	G
25	A	1647	U
25	A	1648	U
25	A	1651	G
25	A	1654	A
25	A	1664	A
25	A	1665	A
25	A	1667	G
25	A	1674	G
25	A	1694	C
25	A	1695	G
25	A	1715	G
25	A	1729	U
25	A	1730	C
25	A	1738	G
25	A	1756	G
25	A	1758	U
25	A	1764	C

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Mol	Chain	Res	Type
25	A	1773	A
25	A	1780	A
25	A	1781	U
25	A	1782	U
25	A	1784	A
25	A	1787	A
25	A	1800	C
25	A	1801	A
25	A	1808	A
25	A	1816	C
25	A	1818	U
25	A	1829	A
25	A	1833	C
25	A	1847	G
25	A	1858	A
25	A	1865	U
25	A	1871	A
25	A	1885	A
25	A	1896	G
25	A	1900	A
25	A	1901	A
25	A	1906	G
25	A	1907	G
25	A	1913	A
25	A	1914	C
25	A	1927	A
25	A	1929	G
25	A	1930	G
25	A	1931	U
25	A	1937	A
25	A	1938	A
25	A	1940	U
25	A	1941	C
25	A	1955	U
25	A	1960	A
25	A	1962	5MC
25	A	1963	U
25	A	1967	C
25	A	1970	A
25	A	1971	U
25	A	1972	G
25	A	1981	A

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Mol	Chain	Res	Type
25	A	1991	U
25	A	1992	G
25	A	1993	U
25	A	1997	C
25	A	2022	U
25	A	2023	C
25	A	2031	A
25	A	2033	A
25	A	2043	C
25	A	2049	G
25	A	2052	A
25	A	2055	C
25	A	2056	G
25	A	2060	A
25	A	2061	G
25	A	2062	A
25	A	2069	7MG
25	A	2093	G
25	A	2095	A
25	A	2096	C
25	A	2098	U
25	A	2108	A
25	A	2110	G
25	A	2111	U
25	A	2112	G
25	A	2113	U
25	A	2118	U
25	A	2119	A
25	A	2127	G
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2145	C
25	A	2146	C
25	A	2157	G
25	A	2162	G
25	A	2164	C
25	A	2172	U
25	A	2173	A
25	A	2189	U
25	A	2192	U
25	A	2198	A

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Mol	Chain	Res	Type
25	A	2199	A
25	A	2204	G
25	A	2211	A
25	A	2212	A
25	A	2213	U
25	A	2225	A
25	A	2238	G
25	A	2239	G
25	A	2250	G
25	A	2268	A
25	A	2273	A
25	A	2278	A
25	A	2283	C
25	A	2287	A
25	A	2288	A
25	A	2297	A
25	A	2305	U
25	A	2309	A
25	A	2311	A
25	A	2312	U
25	A	2320	U
25	A	2325	G
25	A	2327	A
25	A	2334	U
25	A	2336	A
25	A	2337	G
25	A	2345	G
25	A	2347	C
25	A	2350	C
25	A	2382	G
25	A	2383	G
25	A	2385	C
25	A	2391	G
25	A	2392	A
25	A	2402	U
25	A	2406	A
25	A	2407	A
25	A	2423	U
25	A	2424	C
25	A	2426	A
25	A	2427	C
25	A	2428	G

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Mol	Chain	Res	Type
25	A	2429	G
25	A	2430	A
25	A	2435	A
25	A	2441	U
25	A	2445	2MG
25	A	2447	G
25	A	2448	A
25	A	2449	H2U
25	A	2459	A
25	A	2468	A
25	A	2476	A
25	A	2478	A
25	A	2484	G
25	A	2494	G
25	A	2497	A
25	A	2498	OMC
25	A	2502	G
25	A	2504	PSU
25	A	2505	G
25	A	2506	U
25	A	2517	C
25	A	2518	A
25	A	2519	U
25	A	2529	G
25	A	2547	A
25	A	2554	U
25	A	2567	G
25	A	2572	A
25	A	2573	C
25	A	2585	U
25	A	2602	A
25	A	2603	G
25	A	2608	G
25	A	2609	U
25	A	2613	U
25	A	2614	A
25	A	2636	C
25	A	2645	G
25	A	2646	C
25	A	2655	G
25	A	2656	U
25	A	2682	A

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Mol	Chain	Res	Type
25	A	2689	U
25	A	2690	U
25	A	2707	U
25	A	2712	C
25	A	2713	U
25	A	2714	G
25	A	2718	G
25	A	2722	G
25	A	2726	A
25	A	2731	G
25	A	2732	G
25	A	2733	A
25	A	2739	U
25	A	2744	G
25	A	2748	A
25	A	2757	A
25	A	2764	A
25	A	2765	A
25	A	2769	U
25	A	2778	A
25	A	2779	U
25	A	2791	G
25	A	2794	C
25	A	2797	U
25	A	2799	A
25	A	2800	A
25	A	2801	G
25	A	2808	G
25	A	2809	A
25	A	2818	U
25	A	2820	A
25	A	2821	A
25	A	2823	A
25	A	2833	U
25	A	2834	G
25	A	2835	A
25	A	2848	G
25	A	2849	U
25	A	2867	G
25	A	2868	A
25	A	2872	A
25	A	2873	A

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Mol	Chain	Res	Type
25	A	2880	C
25	A	2884	U
26	B	4	C
26	B	12	C
26	B	13	G
26	B	24	G
26	B	25	U
26	B	35	C
26	B	40	U
26	B	44	G
26	B	45	A
26	B	56	G
26	B	67	G
26	B	88	C
26	B	89	U
26	B	91	C
26	B	108	A
26	B	109	A
26	B	116	G

There are no RNA pucker outliers to report.

## 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
25	6MZ	A	1618	25	18,25,26	1.13	1 (5%)	16,36,39	2.88	4 (25%)
25	2MG	A	1835	25	19,26,27	0.99	2 (10%)	20,38,41	2.11	7 (35%)
25	PSU	A	1911	25	16,21,22	1.49	1 (6%)	20,30,33	3.40	6 (30%)
25	3TD	A	1915	25	16,22,23	1.34	3 (18%)	19,32,35	1.68	5 (26%)
25	PSU	A	1917	25	16,21,22	1.45	1 (6%)	20,30,33	3.60	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	5MU	A	1939	25	14,22,23	0.80	1 (7%)	16,32,35	2.15	3 (18%)
25	5MC	A	1962	25	15,22,23	1.42	1 (6%)	17,32,35	1.07	1 (5%)
25	6MZ	A	2030	25	18,25,26	1.06	1 (5%)	16,36,39	3.18	4 (25%)
25	7MG	A	2069	25	20,26,27	1.32	2 (10%)	22,39,42	2.80	5 (22%)
25	OMG	A	2251	25,15	18,26,27	1.01	2 (11%)	22,38,41	2.05	6 (27%)
25	2MG	A	2445	25	19,26,27	1.06	4 (21%)	20,38,41	2.30	8 (40%)
25	H2U	A	2449	25	17,21,22	0.99	2 (11%)	21,30,33	2.08	3 (14%)
25	PSU	A	2457	25	16,21,22	1.81	2 (12%)	20,30,33	3.51	6 (30%)
25	OMC	A	2498	25	15,22,23	0.87	1 (6%)	19,31,34	0.83	0
25	2MA	A	2503	25	18,25,26	1.56	3 (16%)	17,37,40	1.77	2 (11%)
25	PSU	A	2504	25	16,21,22	1.57	1 (6%)	20,30,33	3.72	6 (30%)
25	OMU	A	2552	25	14,22,23	0.85	0	18,31,34	1.78	1 (5%)
25	PSU	A	2580	25	16,21,22	1.73	5 (31%)	20,30,33	3.60	6 (30%)
25	PSU	A	2604	25	16,21,22	1.63	2 (12%)	20,30,33	3.60	6 (30%)
25	PSU	A	2605	25	16,21,22	1.32	2 (12%)	20,30,33	3.54	6 (30%)
25	1MG	A	745	25	18,26,27	1.52	3 (16%)	18,39,42	1.70	2 (11%)
25	PSU	A	746	25	16,21,22	1.41	2 (12%)	20,30,33	3.52	6 (30%)
25	5MC	A	747	25	15,22,23	1.43	1 (6%)	17,32,35	1.38	3 (17%)
25	PSU	A	955	25	16,21,22	1.67	4 (25%)	20,30,33	3.44	6 (30%)
1	2MG	a	1207	1	19,26,27	1.36	3 (15%)	20,38,41	2.24	7 (35%)
1	4OC	a	1402	1	16,23,24	1.66	3 (18%)	19,32,35	2.71	8 (42%)
1	5MC	a	1407	1	15,22,23	1.36	1 (6%)	17,32,35	1.14	2 (11%)
1	UR3	a	1498	1	14,22,23	0.77	0	16,32,35	0.79	0
1	2MG	a	1516	1	19,26,27	1.31	2 (10%)	20,38,41	2.28	8 (40%)
1	MA6	a	1518	1	16,26,27	1.12	1 (6%)	18,38,41	2.59	6 (33%)
1	MA6	a	1519	1	16,26,27	0.93	1 (6%)	18,38,41	2.66	7 (38%)
1	PSU	a	516	1	16,21,22	1.52	3 (18%)	20,30,33	3.32	7 (35%)
1	7MG	a	527	1	20,26,27	1.40	2 (10%)	22,39,42	2.72	5 (22%)
1	2MG	a	966	1	19,26,27	1.22	2 (10%)	20,38,41	2.25	7 (35%)
1	5MC	a	967	1	15,22,23	1.29	1 (6%)	17,32,35	1.15	1 (5%)
15	H2U	v	20	15	17,21,22	0.99	2 (11%)	21,30,33	1.92	3 (14%)
15	5MU	v	54	15	14,22,23	0.73	0	16,32,35	2.16	3 (18%)
15	PSU	v	55	15	16,21,22	1.20	1 (6%)	20,30,33	3.56	8 (40%)
15	4SU	v	8	15	14,21,22	1.30	1 (7%)	15,30,33	1.38	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	6MZ	A	1618	25	-	0/5/27/28	0/3/3/3
25	2MG	A	1835	25	-	0/5/27/28	0/3/3/3
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	3TD	A	1915	25	-	0/7/25/26	0/2/2/2
25	PSU	A	1917	25	-	0/7/25/26	0/2/2/2
25	5MU	A	1939	25	-	0/3/25/26	0/2/2/2
25	5MC	A	1962	25	-	0/3/25/26	0/2/2/2
25	6MZ	A	2030	25	-	0/5/27/28	0/3/3/3
25	7MG	A	2069	25	-	0/7/37/38	0/3/3/3
25	OMG	A	2251	25,15	-	0/5/27/28	0/3/3/3
25	2MG	A	2445	25	-	0/5/27/28	0/3/3/3
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	OMC	A	2498	25	-	0/5/27/28	0/2/2/2
25	2MA	A	2503	25	-	0/3/25/26	0/3/3/3
25	PSU	A	2504	25	-	0/7/25/26	0/2/2/2
25	OMU	A	2552	25	-	0/5/27/28	0/2/2/2
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	1MG	A	745	25	-	0/3/25/26	0/3/3/3
25	PSU	A	746	25	-	0/7/25/26	0/2/2/2
25	5MC	A	747	25	-	0/3/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	7MG	a	527	1	-	0/7/37/38	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
15	H2U	v	20	15	-	0/7/38/39	0/2/2/2
15	5MU	v	54	15	-	0/3/25/26	0/2/2/2
15	PSU	v	55	15	-	0/7/25/26	0/2/2/2
15	4SU	v	8	15	-	0/3/25/26	0/2/2/2

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2457	PSU	C5-C1'	-6.07	1.47	1.52
25	A	2580	PSU	C5-C1'	-5.42	1.47	1.52
25	A	2604	PSU	C5-C1'	-5.15	1.47	1.52
25	A	955	PSU	C5-C1'	-4.96	1.47	1.52
25	A	2504	PSU	C5-C1'	-4.87	1.48	1.52
25	A	1911	PSU	C5-C1'	-4.52	1.48	1.52
25	A	1917	PSU	C5-C1'	-4.40	1.48	1.52
1	a	516	PSU	C5-C1'	-4.36	1.48	1.52
25	A	746	PSU	C5-C1'	-4.23	1.48	1.52
15	v	8	4SU	C4-S4	-3.93	1.60	1.67
25	A	2605	PSU	C5-C1'	-3.37	1.49	1.52
15	v	55	PSU	C5-C1'	-3.14	1.49	1.52
1	a	1207	2MG	O5'-C5'	-2.55	1.41	1.44
25	A	2605	PSU	C2-N3	-2.55	1.33	1.38
25	A	2604	PSU	C2-N3	-2.52	1.33	1.38
15	v	20	H2U	C2-N3	-2.44	1.33	1.38
25	A	2449	H2U	C4-N3	-2.42	1.33	1.37
1	a	516	PSU	O4'-C1'	-2.42	1.40	1.44
25	A	2449	H2U	C2-N3	-2.39	1.33	1.38
15	v	20	H2U	C4-N3	-2.37	1.33	1.37
1	a	516	PSU	C2-N3	-2.33	1.33	1.38
25	A	955	PSU	C2-N3	-2.32	1.33	1.38
25	A	1939	5MU	C2-N3	-2.30	1.33	1.38
25	A	955	PSU	C2-N1	-2.26	1.33	1.38
25	A	1915	3TD	C6-C5	-2.22	1.35	1.38
25	A	2580	PSU	O4'-C1'	-2.17	1.41	1.44
25	A	2445	2MG	O5'-C5'	-2.17	1.41	1.44
25	A	955	PSU	O4'-C1'	-2.10	1.41	1.44
25	A	1915	3TD	C4-N3	-2.10	1.35	1.38
25	A	2457	PSU	C2-N1	-2.10	1.34	1.38
25	A	2498	OMC	C6-N1	-2.07	1.33	1.35
25	A	2580	PSU	C2-N1	-2.06	1.34	1.38
25	A	2580	PSU	O5'-C5'	-2.03	1.41	1.44
25	A	2580	PSU	C2-N3	-2.03	1.34	1.38
25	A	746	PSU	C2-N3	-2.01	1.34	1.38
25	A	2445	2MG	C2-N2	2.07	1.35	1.34
25	A	2445	2MG	C6-C5	2.10	1.45	1.41
25	A	745	1MG	C6-N1	2.15	1.41	1.38
25	A	2445	2MG	C5-C4	2.22	1.45	1.40
25	A	1835	2MG	C5-C4	2.50	1.46	1.40
25	A	2069	7MG	C5-C4	2.60	1.46	1.39
25	A	2251	OMG	C5-C4	2.64	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2251	OMG	C6-C5	2.68	1.46	1.41
25	A	1915	3TD	C10-N3	2.69	1.53	1.47
1	a	1402	4OC	O4'-C1'	2.73	1.45	1.41
1	a	1402	4OC	C6-C5	2.74	1.44	1.38
25	A	2503	2MA	C5-C4	2.76	1.46	1.40
1	a	1519	MA6	C5-C4	2.78	1.46	1.40
25	A	1835	2MG	C6-C5	2.78	1.46	1.41
1	a	527	7MG	C5-C4	2.88	1.47	1.39
1	a	966	2MG	C5-C4	3.04	1.47	1.40
25	A	745	1MG	C5-C4	3.15	1.47	1.40
1	a	1207	2MG	C5-C4	3.20	1.47	1.40
1	a	1516	2MG	C5-C4	3.26	1.47	1.40
1	a	1518	MA6	C5-C4	3.40	1.48	1.40
25	A	2030	6MZ	C5-C4	3.59	1.48	1.40
1	a	1516	2MG	C6-C5	3.62	1.48	1.41
1	a	1207	2MG	C6-C5	3.65	1.48	1.41
1	a	966	2MG	C6-C5	3.71	1.48	1.41
25	A	2503	2MA	C6-N6	3.72	1.36	1.27
25	A	1618	6MZ	C5-C4	3.91	1.49	1.40
25	A	2503	2MA	C6-C5	4.12	1.48	1.41
25	A	2069	7MG	C6-C5	4.33	1.46	1.41
1	a	1402	4OC	O3'-C3'	4.44	1.53	1.43
1	a	527	7MG	C6-C5	4.46	1.46	1.41
1	a	967	5MC	C5-C4	4.55	1.48	1.41
25	A	745	1MG	C6-C5	4.64	1.49	1.41
25	A	747	5MC	C5-C4	4.64	1.48	1.41
1	a	1407	5MC	C5-C4	4.68	1.48	1.41
25	A	1962	5MC	C5-C4	4.76	1.48	1.41

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2580	PSU	C5-C4-N3	-10.15	117.10	125.43
25	A	746	PSU	N1-C2-N3	-9.55	121.53	128.40
15	v	55	PSU	N1-C2-N3	-9.46	121.60	128.40
25	A	2504	PSU	N1-C2-N3	-9.33	121.69	128.40
25	A	2605	PSU	N1-C2-N3	-9.32	121.70	128.40
25	A	2604	PSU	N1-C2-N3	-9.24	121.75	128.40
25	A	2504	PSU	C5-C4-N3	-9.24	117.85	125.43
25	A	1917	PSU	C5-C4-N3	-9.09	117.97	125.43
25	A	1917	PSU	N1-C2-N3	-9.02	121.91	128.40
25	A	2457	PSU	C5-C4-N3	-9.01	118.04	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1911	PSU	N1-C2-N3	-8.87	122.02	128.40
25	A	955	PSU	N1-C2-N3	-8.65	122.18	128.40
25	A	2457	PSU	N1-C2-N3	-8.47	122.31	128.40
1	a	516	PSU	C5-C4-N3	-8.35	118.58	125.43
25	A	2580	PSU	N1-C2-N3	-8.21	122.49	128.40
25	A	1911	PSU	C5-C4-N3	-8.12	118.77	125.43
15	v	55	PSU	C5-C4-N3	-8.08	118.80	125.43
25	A	955	PSU	C5-C4-N3	-7.92	118.93	125.43
25	A	2605	PSU	C5-C4-N3	-7.89	118.95	125.43
25	A	746	PSU	C5-C4-N3	-7.89	118.96	125.43
1	a	516	PSU	N1-C2-N3	-7.84	122.76	128.40
1	a	1519	MA6	N3-C2-N1	-7.39	122.42	128.86
25	A	2604	PSU	C5-C4-N3	-7.38	119.38	125.43
1	a	1518	MA6	N3-C2-N1	-6.62	123.09	128.86
25	A	2449	H2U	C5-C6-N1	-6.21	104.25	110.70
25	A	2449	H2U	C4-N3-C2	-5.87	120.78	125.81
25	A	2604	PSU	C5-C1'-C2'	-5.67	105.77	115.55
25	A	1618	6MZ	N3-C2-N1	-5.66	123.92	128.86
15	v	20	H2U	C4-N3-C2	-5.64	120.97	125.81
25	A	2030	6MZ	N3-C2-N1	-5.38	124.17	128.86
15	v	20	H2U	C5-C6-N1	-5.34	105.15	110.70
25	A	2069	7MG	C5-C6-N1	-5.34	115.00	123.37
1	a	1402	4OC	C6-N1-C2	-5.24	112.80	121.28
25	A	1939	5MU	C5-C4-N3	-5.17	119.54	125.24
15	v	54	5MU	C5-C4-N3	-5.09	119.63	125.24
1	a	527	7MG	C5-C6-N1	-5.06	115.44	123.37
25	A	1618	6MZ	C9-N6-C6	-5.04	118.53	122.85
25	A	2030	6MZ	C9-N6-C6	-4.90	118.65	122.85
25	A	955	PSU	C5-C1'-C2'	-4.90	107.10	115.55
25	A	2604	PSU	C5-C6-N1	-4.73	118.25	124.39
25	A	2580	PSU	C5-C6-N1	-4.65	118.36	124.39
1	a	527	7MG	C5-C4-N3	-4.64	118.72	126.47
25	A	2251	OMG	C5-C6-N1	-4.59	116.94	123.48
25	A	2069	7MG	C5-C4-N3	-4.56	118.86	126.47
25	A	2457	PSU	C5-C6-N1	-4.50	118.56	124.39
1	a	1518	MA6	C10-N6-C6	-4.45	106.05	119.51
1	a	516	PSU	C5-C6-N1	-4.31	118.80	124.39
25	A	746	PSU	C5-C6-N1	-4.26	118.86	124.39
25	A	2605	PSU	C5-C1'-C2'	-4.25	108.22	115.55
25	A	955	PSU	C5-C6-N1	-4.20	118.95	124.39
25	A	1911	PSU	C5-C6-N1	-4.18	118.97	124.39
25	A	2504	PSU	C5-C1'-C2'	-4.18	108.34	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2445	2MG	C5-C6-N1	-4.08	117.68	123.48
25	A	2445	2MG	C6-C5-C4	-4.03	116.84	120.84
25	A	1915	3TD	C5-C1'-C2'	-4.01	108.63	115.55
1	a	1516	2MG	C5-C6-N1	-3.99	117.81	123.48
25	A	2504	PSU	C5-C6-N1	-3.85	119.40	124.39
1	a	1207	2MG	C5-C6-N1	-3.75	118.14	123.48
25	A	1917	PSU	C5-C6-N1	-3.66	119.65	124.39
1	a	1516	2MG	C6-C5-C4	-3.66	117.21	120.84
1	a	966	2MG	C5-C6-N1	-3.56	118.42	123.48
15	v	55	PSU	C5-C6-N1	-3.55	119.79	124.39
25	A	2605	PSU	C5-C6-N1	-3.48	119.88	124.39
1	a	966	2MG	C6-C5-C4	-3.46	117.40	120.84
1	a	1519	MA6	C10-N6-C6	-3.44	109.11	119.51
25	A	2457	PSU	C5-C1'-C2'	-3.42	109.65	115.55
25	A	1917	PSU	C5-C1'-C2'	-3.37	109.73	115.55
1	a	1519	MA6	C9-N6-C6	-3.37	109.30	119.51
25	A	1915	3TD	C5-C6-N1	-3.36	120.04	124.39
1	a	1402	4OC	CM4-N4-C4	-3.35	120.05	122.94
25	A	1939	5MU	C5-C6-N1	-3.33	118.55	122.15
25	A	1835	2MG	CM2-N2-C2	-3.32	119.59	123.63
25	A	1835	2MG	C6-C5-C4	-3.30	117.56	120.84
25	A	746	PSU	C5-C1'-C2'	-3.29	109.86	115.55
25	A	1835	2MG	C5-C6-N1	-3.26	118.84	123.48
1	a	1207	2MG	C6-C5-C4	-3.24	117.63	120.84
1	a	1402	4OC	O4'-C1'-C2'	-3.23	100.94	106.59
25	A	2030	6MZ	C4-C5-N7	-3.19	106.33	109.41
1	a	966	2MG	CM2-N2-C2	-3.17	119.78	123.63
1	a	516	PSU	O4'-C1'-C5	-3.15	105.05	109.93
25	A	2445	2MG	CM2-N2-C2	-3.15	119.80	123.63
25	A	2251	OMG	C6-C5-C4	-3.14	117.73	120.84
1	a	1516	2MG	CM2-N2-C2	-3.12	119.83	123.63
1	a	1518	MA6	C9-N6-C6	-3.09	110.16	119.51
25	A	745	1MG	C4-C5-N7	-3.08	106.44	109.41
25	A	2445	2MG	N3-C2-N1	-2.97	121.74	126.23
25	A	2251	OMG	N3-C2-N1	-2.95	123.15	127.46
1	a	1207	2MG	CM2-N2-C2	-2.94	120.05	123.63
15	v	8	4SU	C5-C4-N3	-2.93	120.03	123.73
15	v	55	PSU	C5-C1'-C2'	-2.93	110.49	115.55
1	a	1519	MA6	C10-N6-C9	-2.83	106.86	116.03
25	A	2503	2MA	C4-C5-N7	-2.76	106.74	109.41
1	a	1519	MA6	C4-C5-N7	-2.73	106.78	109.41
25	A	1618	6MZ	C4-C5-N7	-2.71	106.80	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	C4-C5-N7	-2.70	106.80	109.41
25	A	1911	PSU	C5-C1'-C2'	-2.60	111.06	115.55
1	a	1207	2MG	C4-C5-N7	-2.56	106.94	109.41
15	v	54	5MU	C5-C6-N1	-2.50	119.44	122.15
1	a	1516	2MG	N3-C2-N1	-2.46	122.51	126.23
25	A	2069	7MG	C5-C4-N9	-2.40	102.82	106.31
25	A	1835	2MG	C4-C5-N7	-2.37	107.12	109.41
25	A	2251	OMG	C4-C5-N7	-2.36	107.13	109.41
1	a	1407	5MC	C5-C6-N1	-2.28	119.68	122.15
1	a	527	7MG	C5-C4-N9	-2.27	103.01	106.31
1	a	1516	2MG	C4-C5-N7	-2.25	107.24	109.41
1	a	966	2MG	N3-C2-N1	-2.24	122.84	126.23
1	a	1207	2MG	N3-C2-N1	-2.20	122.91	126.23
25	A	747	5MC	C5-C6-N1	-2.18	119.79	122.15
1	a	1518	MA6	C4-C5-N7	-2.10	107.38	109.41
25	A	1835	2MG	N3-C2-N1	-2.07	123.10	126.23
25	A	1915	3TD	O4'-C1'-C2'	2.03	107.71	104.45
25	A	2445	2MG	N2-C2-N1	2.06	118.95	116.95
15	v	55	PSU	O4'-C1'-C2'	2.06	107.76	104.45
25	A	2580	PSU	O4'-C1'-C2'	2.12	107.86	104.45
25	A	1915	3TD	O4'-C1'-C5	2.15	113.26	109.93
15	v	20	H2U	N3-C2-N1	2.17	118.90	116.73
25	A	747	5MC	O4'-C1'-N1	2.18	112.44	108.08
1	a	1516	2MG	N2-C2-N1	2.18	119.08	116.95
25	A	2449	H2U	O4-C4-N3	2.30	123.93	120.41
15	v	55	PSU	O4'-C1'-C5	2.42	113.67	109.93
25	A	2445	2MG	N2-C2-N3	2.43	119.31	116.95
1	a	516	PSU	O4'-C1'-C2'	2.46	108.41	104.45
1	a	1407	5MC	N4-C4-N3	2.62	120.88	117.00
25	A	747	5MC	N4-C4-N3	2.75	121.07	117.00
25	A	1962	5MC	N4-C4-N3	2.87	121.24	117.00
25	A	1915	3TD	C6-N1-C2	3.05	120.24	115.36
1	a	1519	MA6	N1-C6-N6	3.06	120.25	117.00
1	a	1402	4OC	C4'-O4'-C1'	3.10	113.07	109.77
1	a	1402	4OC	O3'-C3'-C4'	3.16	120.33	111.09
1	a	967	5MC	N4-C4-N3	3.21	121.75	117.00
25	A	1835	2MG	C6-N1-C2	3.53	121.50	115.18
1	a	1518	MA6	N1-C6-N6	3.63	120.85	117.00
1	a	1402	4OC	C3'-C2'-C1'	3.65	109.88	102.75
25	A	2251	OMG	C2-N3-C4	3.71	119.50	115.16
1	a	1402	4OC	O4'-C1'-N1	3.73	115.56	108.08
1	a	966	2MG	C6-N1-C2	3.77	121.92	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	v	8	4SU	C2-N3-C4	3.77	120.67	115.11
1	a	1207	2MG	C6-N1-C2	3.85	122.08	115.18
25	A	2580	PSU	C6-N1-C2	3.99	121.75	115.36
25	A	2605	PSU	C6-N1-C2	4.00	121.77	115.36
25	A	1917	PSU	C6-N1-C2	4.02	121.79	115.36
25	A	2504	PSU	C6-N1-C2	4.09	121.91	115.36
1	a	516	PSU	C6-N1-C2	4.15	122.00	115.36
25	A	2445	2MG	C2-N3-C4	4.16	119.86	115.11
15	v	55	PSU	C6-N1-C2	4.21	122.09	115.36
1	a	1516	2MG	C6-N1-C2	4.21	122.72	115.18
25	A	2457	PSU	C6-N1-C2	4.30	122.24	115.36
25	A	1911	PSU	C6-N1-C2	4.33	122.29	115.36
25	A	955	PSU	C6-N1-C2	4.35	122.32	115.36
1	a	1519	MA6	C2-N1-C6	4.45	122.73	111.82
25	A	746	PSU	C6-N1-C2	4.56	122.66	115.36
1	a	1518	MA6	C2-N1-C6	4.57	123.03	111.82
25	A	2445	2MG	C6-N1-C2	4.67	123.55	115.18
25	A	2604	PSU	C6-N1-C2	4.76	122.97	115.36
1	a	527	7MG	C6-N1-C2	4.89	123.10	116.06
25	A	2251	OMG	C6-N1-C2	5.03	123.29	116.06
1	a	1516	2MG	C2-N3-C4	5.05	120.87	115.11
25	A	1835	2MG	C2-N3-C4	5.12	120.95	115.11
25	A	2069	7MG	C6-N1-C2	5.27	123.63	116.06
1	a	1402	4OC	O3'-C3'-C2'	5.30	126.26	111.18
1	a	516	PSU	C4-N3-C2	5.44	119.92	115.16
25	A	1939	5MU	C4-N3-C2	5.48	119.96	115.16
1	a	1207	2MG	C2-N3-C4	5.50	121.39	115.11
25	A	955	PSU	C4-N3-C2	5.56	120.02	115.16
1	a	966	2MG	C2-N3-C4	5.58	121.47	115.11
25	A	2604	PSU	C4-N3-C2	5.61	120.06	115.16
25	A	745	1MG	C2-N3-C4	5.64	121.75	115.16
25	A	2457	PSU	C4-N3-C2	5.81	120.24	115.16
25	A	1911	PSU	C4-N3-C2	5.82	120.25	115.16
15	v	54	5MU	C4-N3-C2	5.96	120.38	115.16
25	A	2503	2MA	C2-N3-C4	5.98	120.58	115.41
25	A	746	PSU	C4-N3-C2	6.06	120.46	115.16
25	A	2580	PSU	C4-N3-C2	6.48	120.83	115.16
15	v	55	PSU	C4-N3-C2	6.55	120.89	115.16
25	A	2552	OMU	C4-N3-C2	6.61	119.81	114.13
25	A	1917	PSU	C4-N3-C2	6.71	121.03	115.16
25	A	2605	PSU	C4-N3-C2	6.76	121.07	115.16
25	A	2504	PSU	C4-N3-C2	6.87	121.17	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1618	6MZ	C2-N1-C6	8.03	121.76	116.53
1	a	527	7MG	N3-C4-N9	8.83	138.26	126.98
25	A	2069	7MG	N3-C4-N9	8.86	138.30	126.98
25	A	2030	6MZ	C2-N1-C6	9.55	122.75	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1917	PSU	1	0
25	A	1962	5MC	1	0
25	A	2030	6MZ	2	0
25	A	2445	2MG	1	0
25	A	2449	H2U	1	0
25	A	2552	OMU	1	0
25	A	745	1MG	1	0
25	A	747	5MC	1	0
25	A	955	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.