



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:29 PM BST

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 wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

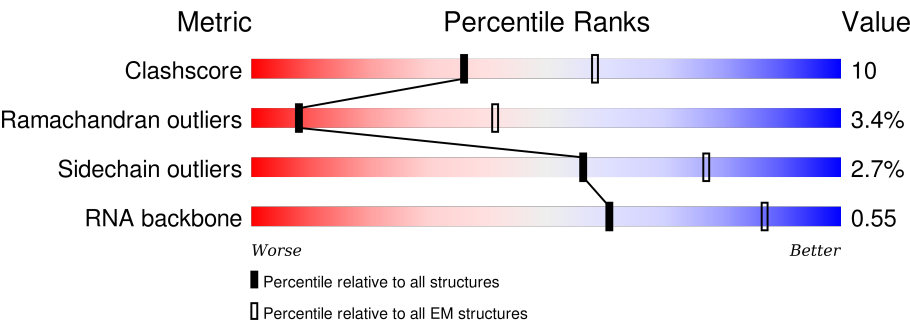
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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.















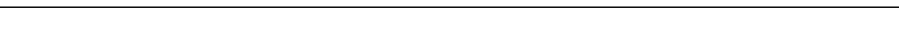

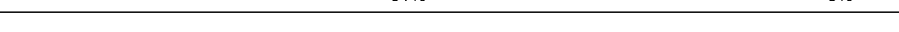

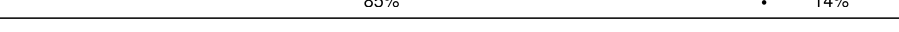








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

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


























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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	 53% 37% 9%
26	B	120	 53% 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^{fMet}.

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		
			2590	1308	640	642	0	0

- 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		

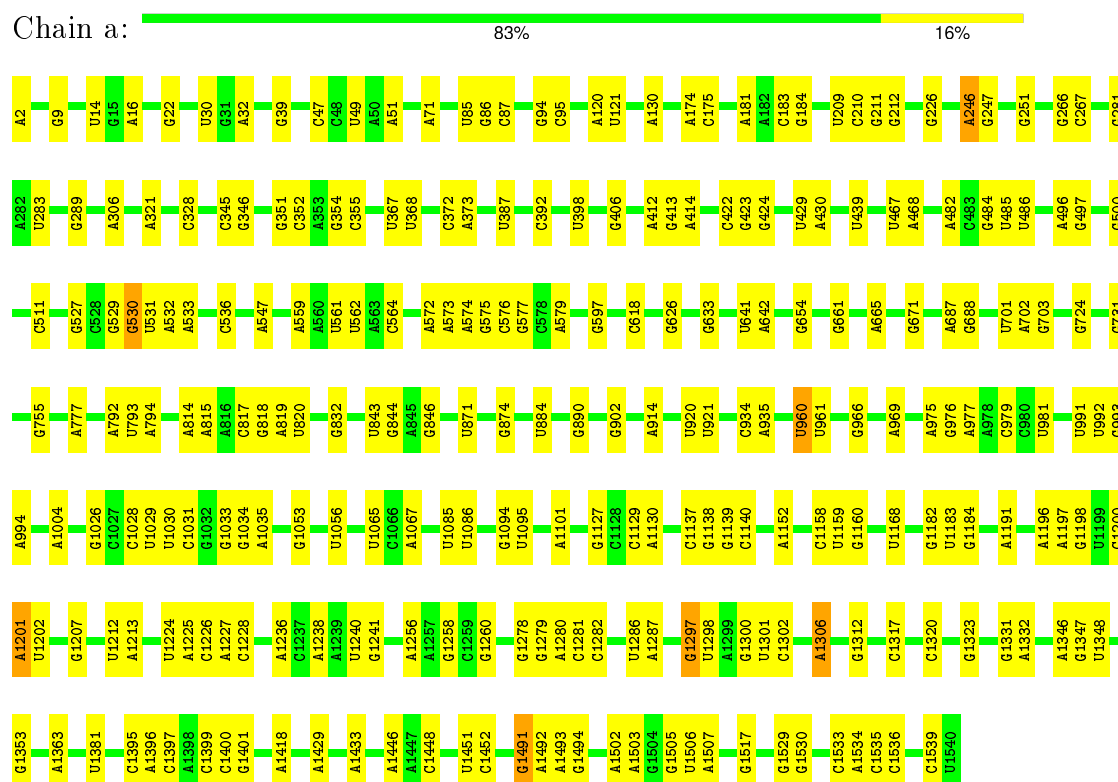
- Molecule 58 is a protein called 50S ribosomal protein L7/L12.


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

• Molecule 1: 16S ribosomal RNA



Chain e:  84% 10% 6%



- Molecule 5: 30S ribosomal protein S6

Chain f:  68% 26%




- Molecule 6: 30S ribosomal protein S8

Chain h:  96% 2%



- 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%




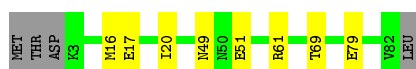
- Molecule 10: 30S ribosomal protein S16

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% .



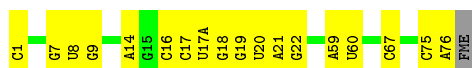
- Molecule 14: 30S ribosomal protein S21

Chain u: 82% 10% 8%



- Molecule 15: P-site fMet-tRNA^{fMet}

Chain v: 76% 23% .



- Molecule 16: mRNA

Chain x: 73% 9% 18%



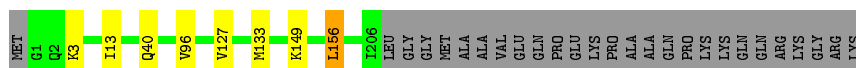
- Molecule 17: Tetracycline resistance protein TetM

Chain w: 96% .




- Molecule 18: 30S ribosomal protein S3

Chain c: 85% 12%




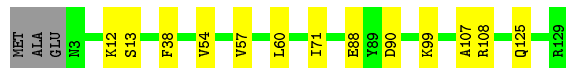
- Molecule 19: 30S ribosomal protein S7

Chain g:  78% 7% 16%




- Molecule 20: 30S ribosomal protein S9

Chain i:  88% 10% .



- Molecule 21: 30S ribosomal protein S10

Chain j:  87% 8% 5%




- Molecule 22: 30S ribosomal protein S13

Chain m:  91% 6% .




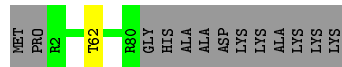
- Molecule 23: 30S ribosomal protein S14

Chain n:  90% 9% .



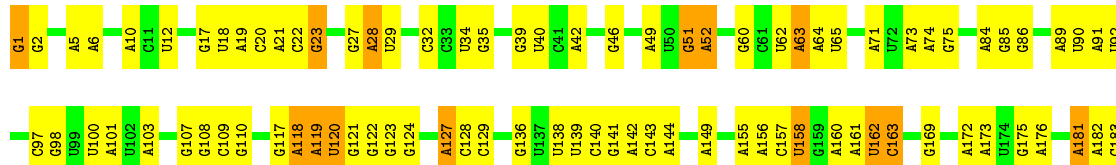
- Molecule 24: 30S ribosomal protein S19

Chain s:  85% . 14%



- Molecule 25: 23S ribosomal RNA

Chain A:  53% 37% 9%



U1534	G1432	G1331	A1247	G1139	A1067	A981	U	G805	A730	G638	U545	U360	U276	G184
A1535	A1433	G1332	G1248	G1139	G1068	C982	C	C906	C736	U639	U546	G361	G277	G185
C1536	A1434	U1340	U1249	C1140	A1069	A983	C	U807	C737	C640	U547	A454	A278	
G1537	G1435	U1141	G1250	U1141	A1070	A984		U811	C737	U641	U548	C363		G189
U1538		G1341	G1251	A1142	G1071	C985		U812	A739	U642	U549	C364	C281	A190
U1539	G1447	A1342	G1252	A1143	G1072	G989	A896	U813	C740	A643	U550	C365	A282	A191
G1448	G1343	G1343	A1253	A1151	A1073	A990	C997	U814		A644	U551	C366	C283	C192
G1454	C1345	G1345	G1256	C1152	G1075	G993	A900	C815	A743	C645	U552	G367	U284	A196
A1548	U1458	U1352	A1265	C1153	A1076	C994	C901	C816	U744	U646	U553	A460	G285	
A1549			G1266	G1160	A1077	C995	G907	C817	U745	G651	U554	C368	U286	A199
	C1461	G1361	U1267	G1179	A1078	C996	G907	C818	U746	A654	U555	G369	U287	
G1555		C1362	A1268	U1174	C1079	A996	C908	A819	C747	A655	U556	C370	U288	A204
C1558	A1469	G1363	U1269	U1175	A1080	U999	A909	G822	G748	G656	U557	U371	U289	G205
U1559	A1470	G1364	C1270	A1176	U1081		A910			G659	U558	U372	G291	U206
G1560	U1474	A1365	G1271	U1177	A1084	C1005	A911	U827	A751	G659	U559	G376	A294	C208
C1561	G1475	A1366	A1272	C1178	A1085	G1011	U919	U828	A752	A668	U560	G377	U296	A213
U1562	U1476	A1367	U1273	G1179	A1086	U1012	A920	A829	U754	U669	U561	U387	G297	G214
U1563	A1477	G1368	A1274	U1180	G1087	U1013	G923	G830	U755	A670	U562	U390	A300	A216
C1564	G1478	A1378	G1276	U1181	A1088	C1014	G924	U832	A756	G674	U563	U391	G301	A217
C1565	U1379	U1183	A1277	U1182	A1089	U1015	G924	A833	C757		U564	A480	C302	A218
A1566	G1482	G1380	G1278	U1184	A1090		G930	G834	C758		U565	A481	G303	A219
G1567	G1483		G1279	G1185	U1094	U1019	U931		G759	A677	U566	C394	G306	G220
G1568		A1383		G1186	A1095	A1020	U932	U839	A761	C678	U567	U395	U307	A222
A1569	U1486	A1384	G1283	U1187	A1096	A1021	A933	C840	C765	C679	U568	G396	G307	
U1578	U1487	U1385		U1188	A1097	G1022	U934	G841			U569	G397	A310	A227
A1579	A1490	A1386	A1287	U1189	A1098	U1023	C935	U842		G682	U570	U404	A311	C228
A1580	G1491	A1387	G1288	G1190	A1099	G1026	A936	G843	G770	A685	U571	U405		
G1581	G1492	A1395	C1289	U1191	C1102	A1027	G937	A844	G771	U686	U572	G411	U321	G232
C1585	A1493	U1396	G1292	U1199	A1103	A1028	G938	A845	C772	C687	U573	A412	A322	G242
A1495	A1495	U1397	C1293	C1200	U1105	U1033	G940	U846	G773		U574	C413	A324	U243
		C1399	G1298	U1201	G1106		A941	U847	G774	C692	U575	C414		G245
A1504	U1506	U1400	C1298	U1108	G1107	G1038	C946	A849	G775	A693	U576	C415	U328	
A1505	G1401	G1401	G1299	C1109	C1107	A1039	A947	U850	G776	U694	U577	C420	G329	G248
A1591	U1506	U1405	G1300	A1205	C1110	A1040	A948	C851	G777	C695	U578	C421	A330	G249
C1592		U1406	A1301	G1206	A1111	G1041	G949	U852	G778		U579	C422	C331	C250
A1597	G1510	U1406	A1302	G1210	U1112	C1045	G953	G857	C786		U580	C423	A332	A251
C1604	G1511	G1410	C1306	G1211	U1113	A1046	G954	G858	A781	U703	U581	C424	A334	G252
C1605	C1512	U1411		G1212	C1114	G1047	G955	G859	A782	G704	U582	C425	C335	
C1606	U1513	U1412	G1310	A1213	G1115		G956	U860	A783	A706	U583	C426	C336	A255
C1607	G1514	A1413	G1311	G1218	U1119	C1052	C957	A861	C786	G712	U584	C427	C337	A256
A1610	G1515	G1414	U1312	U1222	C1053	A1054	U958	G862	C787	G713	U585	U434		
C1611	G1516	U1415	G1313	G1223	G1124	G1055	A959	U870	A788	U714	U586	C435	A340	G259
C1612	G1517	C1417	U1314	G1223	G1125	G1056	C961	U871	A789	A715	U587	C436	C341	G260
G1612	G1524	G1418	G1317	G1235	A1126	A1057	G962	U872	C791	C717	U588	C438	A345	A265
A1613	A1525	A1419	U1318	G1236	A1127	U1058	G969	C873	A792		U589	G439	A346	G266
C1615	G1526	A1420	G1319	A1237	G1128	G1059	U970	G874	A793	A721	U590	U441		C267
A1616	A1527	C1319	C1320	G1238	A1129	U1060	G971	G875	A794	A722	U591	G442	C353	A270
A1626	G1529	G1422	A1321	G1239	U1130	U1061	A972	G879	C795	C723	U592	A443		G271
G1627	G1530	C1428		U1240	G1062	G1063	A973	G884	A800	G725	U593	G446	G356	A272
U1636	C1531	G1429	A1328	A1133	U1064	U1065	G974	C885	G801	G726	U594		U358	
	C1533	A1431	C1330	C1243	U1066	U1066	A975	A886	A802	A727	U595		G359	C275

U1637	U1745	U1845	U1940	U2038	U2119	U2208	U2304	U2394	U2494	U2585	U2698	U2777	C2853
U1746	U1746	U1846	U1941	U2039	U2120	U2209	U2305	U2398	U2497	U2586	U2699	U2778	U2859
C1748	U1747	U1847	U1942	U2040	U2121	U2210	U2306	U2399	U2498	U2587	C2699	A2779	A2860
U1751	U1748	A1848	U1943	U2041	U2122	A2211	U2307	U2402	C2499	A2590	A2705	U2783	A2861
C1752	U1751	G1857	U1944	C2042	A2126	U2212	U2308	U2405	C2501	A2591	G2708	U2784	C2862
G1753	C1752	A1858	G1945	C2043	G2127	U2213	U2309	U2406	C2502	A2592	G2709	C2785	C2863
U1754	G1753	U1859	U1951	G2049	G2128	U2220	U2310	G2405	G2503	G2599	C2710	U2786	U2866
G1652	U1754	U1860	U1952	C2050	C2129	U2221	U2311	A2406	A2504	G2600	C2711	C2787	G2867
G1654	G1755	A1866	U1953	A2052	U2130	C2222	C2312	A2407	U2505	G2601	C2712	C2788	A2868
U1757	U1756	G1867	U1954	U2052	U2131	G2223	C2313	U2408	U2506	A2602	C2713	C2789	G2869
U1758	A1757	C1868	U1955	C2055	U2132	G2224	U2320	G2409	U2507	G2603	U2714	U2790	C2870
U1759	U1758	G1869	U1956	G2056	U2133	A2225	U2321	U2412	C2512	G2604	C2715	A2792	U2871
A1664	U1759	C1870	U1957	G2056	A2134	C2226	G2325	U2413	A2513	U2605	C2716	A2793	U2872
A1665	C1760	A1871	U1958	A2060	U2139	G2227	C2326	G2415	U2514	U2606	C2717	C2794	A2873
G1666	U1764	A1872	U1959	A2061	G2140	U2231	C2327	C2416	U2515	U2607	G2718	U2797	C2874
G1667	U1764	G1873	U1960	A2062	G2141	U2232	A2328	U2417	A2516	U2608	G2719	U2798	C2875
G1674	U1773	A1877	U1961	C2063	A2142	U2233	U2329	U2423	C2517	A2614	U2720	U2799	G2876
U1679	U1779	C1878	U1962	C2064	U2145	U2234	G2330	C2424	U2518	C2619	A2721	A2800	A2879
U1680	U1780	G1879	U1963	C2065	C2146	G2238	C2331	A2425	U2519	C2620	G2722	G2801	C2880
G1681	U1781	U1880	U1964	C2066	C2147	U2239	A2332	C2426	G2526	U2621	U2723	G2802	G2881
U1682	U1782	C1881	C1967	C2067	U2151	G2240	U2333	C2427	C2527	G2622	U2724	G2803	U2882
G1683	U1783	U1882	U1967	U2068	U2152	G2241	A2334	G2428	U2528	C2623	A2725	U2804	U2883
G1684	U1784	U1883	A1970	C2069	U2153	G2250	A2335	G2429	G2529	G2624	A2726	U2805	U2884
C1685	A1784	G1884	U1971	A2070	G2156	C2258	A2336	A2430	U2530	U2625	A2727	C2806	G2890
U1689	U1787	A1885	U1972	A2071	G2157	C2259	G2337	U2435	U2531	G2626	U2728	G2807	U2891
A1690	U1788	C1895	U1980	C2072	G2158	C2261	C2338	A2436	U2532	U2627	U2729	A2808	U2892
U1692	A1789	C1896	U1981	C2073	G2159	U2262	U2339	U2441	U2533	C2628	U2730	A2809	U2893
U1693	U1794	G1906	U1982	U2074	G2160	C2263	G2341	C2442	U2534	G2629	G2731	U2810	U2894
C1694	U1795	G1907	U1983	U2075	C2161	U2264	C2342	C2443	U2535	U2630	U2732	U2811	U2895
G1695	U1796	C1908	U1984	U2076	C2162	A2266	G2343	G2444	U2536	U2631	U2733	U2812	U2896
A1701	U1797	G1909	U1985	U2077	C2163	A2267	A2344	U2445	U2537	G2632	U2734	U2813	U2897
G1702	U1798	C1910	U1986	U2078	C2164	A2268	C2345	G2446	U2538	U2633	U2735	U2814	U2898
U1713	U1801	A1913	C1997	C2095	U2166	G2271	C2346	U2447	U2539	U2634	U2736	U2815	U2899
U1714	U1802	C1914	U1998	C2096	U2167	U2272	C2347	U2448	U2540	U2635	U2737	U2816	U2900
G1715	U1803	A1915	C1999	C2097	U2168	A2273	C2348	U2449	U2541	U2636	U2738	U2817	U2901
U1716	U1804	U1916	U2009	C2098	C2178	A2274	C2349	A2450	U2542	U2637	U2739	U2818	U2902
A1717	U1805	A1917	U2010	U2099	C2179	G2282	G2350	U2451	U2543	U2638	U2740	U2819	U2903
G1718	U1806	A1918	G2012	A2101	C2180	C2283	C2351	U2452	U2544	U2639	U2741	U2820	U2904
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C1727	U1808	C1924	A2014	C2103	A2184	C2285	C2353	U2454	U2546	U2641	U2743	U2822	U2906
C1728	U1809	U1925	A2015	C2104	U2189	C2286	C2354	U2455	U2547	U2642	U2744	U2823	U2907
U1729	U1810	A1927	A2016	U2105	U2190	C2287	C2355	U2456	U2548	U2643	U2745	U2824	U2908
C1730	U1811	U1928	A2017	U2106	U2191	C2288	C2356	U2457	U2549	U2644	U2746	U2825	U2909
G1731	U1812	G1929	C2021	G2107	U2192	C2289	G2357	U2458	U2550	U2645	U2747	U2826	U2910
U1736	U1813	U1930	U2022	U2108	U2193	G2290	C2358	U2459	U2551	U2646	U2748	U2827	U2911
G1737	U1814	U1931	C2023	U2109	U2194	U2291	C2359	U2460	U2552	U2647	U2749	U2828	U2912
G1738	U1815	A1932	U2024	U2110	U2195	U2292	C2360	U2461	U2553	U2648	U2750	U2829	U2913
U1741	U1816	U1933	G1826	U2111	U2196	U2293	C2361	U2462	U2554	U2649	U2751	U2830	U2914
U1742	U1817	G1933	U1829	G2112	U2197	U2294	C2362	U2463	U2555	U2650	U2752	U2831	U2915
G1743	U1818	U1934	A1829	U2113	U2198	U2295	C2363	U2464	U2556	U2651	U2753	U2832	U2916
A1744	U1819	A1935	U1830	G2114	U2199	U2296	C2364	U2465	U2557	U2652	U2754	U2833	U2917
	U1820	U1936	A1831	U2115	U2200	U2297	C2365	U2466	U2558	U2653	U2755	U2834	U2918
	U1821	A1937	U1832	G2116	U2201	U2298	C2366	U2467	U2559	U2654	U2756	U2835	U2919
	U1822	A1938	A1833	U2117	U2202	U2299	C2367	U2468	U2560	U2655	U2757	U2836	U2920
	U1823	U1939	U1834	G2118	U2203	U2300	C2368	U2469	U2561	U2656	U2758	U2837	U2921
	U1824	A1940	U1835	U2119	U2204	U2301	C2369	U2470	U2562	U2657	U2759	U2838	U2922
	U1825	U1941	U1836	U2120	U2205	U2302	C2370	U2471	U2563	U2658	U2760	U2839	U2923
	U1826	A1942	U1837	U2121	U2206	U2303	C2371	U2472	U2564	U2659	U2761	U2840	U2924
	U1827	U1943	U1838	U2122	U2207	U2304	C2372	U2473	U2565	U2660	U2762	U2841	U2925
	U1828	A1944	U1839	U2123	U2208	U2305	C2373	U2474	U2566	U2661	U2763	U2842	U2926
	U1829	U1945	U1840	U2124	U2209	U2306	C2374	U2475	U2567	U2662	U2764	U2843	U2927
	U1830	A1946	U1841	U2125	U2210	U2307	C2375	U2476	U2568	U2663	U2765	U2844	U2928
	U1831	U1947	U1842	U2126	U2211	U2308	C2376	U2477	U2569	U2664	U2766	U2845	U2929
	U1832	A1948	U1843	U2127	U2212	U2309	C2377	U2478	U2570	U2665	U2767	U2846	U2930
	U1833	U1949	U1844	U2128	U2213	U2310	C2378	U2479	U2571	U2666	U2768	U2847	U2931
	U1834	A1950	U1845	U2129	U2214	U2311	C2379	U2480	U2572	U2667	U2769	U2848	U2932
	U1835	U1951	U1846	U2130	U2215	U2312	C2380	U2481	U2573	U2668	U2770	U2849	U2933
	U1836	A1952	U1847	U2131	U2216	U2313	C2381	U2482	U2574	U2669	U2771	U2850	U2934
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	U1838	A1954	U1849	U2133	U2218	U2315	C2383	U2484	U2576	U2671	U2773	U2852	U2936
	U1839	U1955	U1850	U2134	U2219	U2316	C2384	U2485	U2577	U2672	U2774	U2853	U2937
	U1840	A1956	U1851	U2135	U2220	U2317	C2385	U2486	U2578	U2673	U2775	U2854	U2938
	U1841	U1957	U1852	U2136	U2221	U2318	C2386	U2487	U2579	U2674	U2776	U2855	U2939
	U1842	A1958	U1853	U2137	U2222	U2319	C2387	U2488	U2580	U2675	U2777	U2856	U2940
	U1843	U1959	U1854	U2138	U2223	U2320	C2388	U2489	U2581	U2676	U2778	U2857	U2941
	U1844	A1960	U1855	U2139	U2224	U2321	C2389	U2490	U2582	U2677	U2779	U2858	U2942
	U1845	U1961	U1856	U2140	U2225	U2322	C2390	U2491	U2583	U2678	U2780	U2859	U2943
	U1846	A1962	U1857	U2141	U2226	U2323	C2391	U2492	U2584	U2679	U2781	U2860	U2944
	U1847	U1963	U1858	U2142	U2227	U2324	C2392	U2493	U2585	U2680	U2782	U2861	U2945
	U1848	A1964	U1859	U2143	U2228	U2325	C2393	U2494	U2586	U2681	U2783	U2862	U2946
	U1849	U1965	U1860	U2144	U2229	U2326	C2394	U2495	U2587	U2682	U2784	U2863	U2947
	U1850	A1966	U1861	U2145	U2230	U2327	C2395	U2496	U2588	U2683	U2785	U2864	U2948
	U1851	U1967	U1862	U2146	U2231	U2328	C2396	U2497	U2589	U2684	U2786	U2865	U2949
	U1852	A1968	U1863	U2147	U2232	U2329	C2397	U2498	U2590	U2685	U2787	U2866	U2950
	U1853	U1969	U1864	U2148	U2233	U2330	C2398	U2499	U2591	U2686	U2788	U2867	U2951
	U1854	A1970	U1865	U2149	U2234	U2331	C2399	U2500	U2592	U2687	U2789	U2868	U2952
	U1855	U1971	U1866	U2150	U2235	U2332	C2400	U2501	U2593	U2688	U2790	U2869	U2953
	U1856	A1972	U1867	U2151	U2236	U2333	C2401	U2502	U2594	U2689	U2791	U2870	U2954
	U1857	U1973	U1868	U2152	U2237	U2334	C2402	U2503					

A104
G105
G106
G107
A108
A109
G110
U111
G112
G113
G114
A115
G116
G117
C118
A119
A120

• Molecule 27: 50S ribosomal protein L2

Chain C: 77% 22% ..

Met A1 V2 F7 R12 R13 R14 V15 V16 E24 E34 F38 R43 R44 R45 I48 B51 Y61 F70 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 I206 W212 R216 R220 G221 T222 E231 E235 F239 V244 T245 P246 Q250 T251 R252 R257 S258 N259 R260 R261 R269 R270 S271 Lys

• Molecule 28: 50S ribosomal protein L3

Chain D: 76% 22% .

M1 L4 R13 T16 V20 V29 E30 R32 R33 R34 T35 Q36 L40 D43 G44 Y45 I48 Q49 V50 T51 T52 G53 A54 R55 H67 V73 G76 R77 W80 E81 A85 E86 G87 E88 F101 V104 T110 K114 F118 T121

T133 H134 G135 P143 Q148 M149 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 V63 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 M163 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 R8 D9 V12 M16 N20 V24 V27 P28 R29 V39 G40 E41 L48 N51 B55 L56 T67 R70 V73 I78 P83 T84 G85 G86 R87 V88 T89 R91 G92 N95 P96 E97 E100 R101 L102

A106 I110 F113 L116 S120 M126 Y127 S128 M129 G130 V131 R132 E133 Q134 I135 I136 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 R37 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



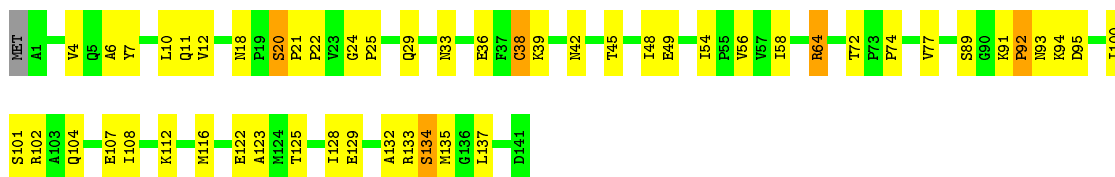
- Molecule 32: 50S ribosomal protein L9

Chain H: 80% 18%



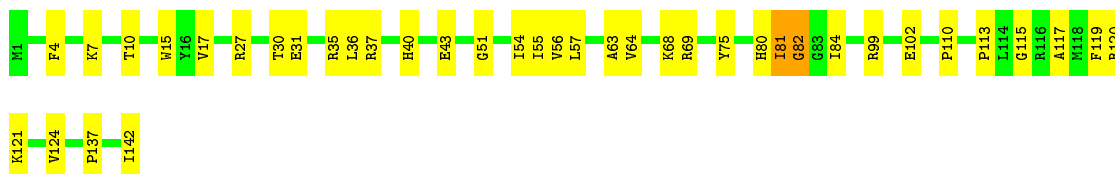
- Molecule 33: 50S ribosomal protein L11

Chain I: 63% 33%



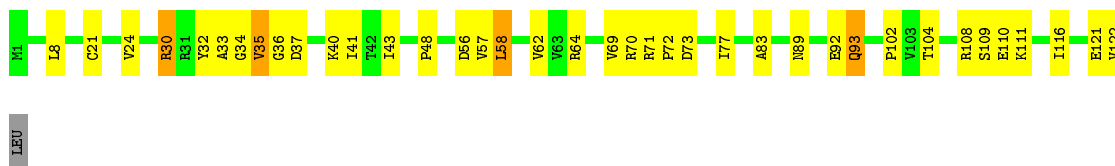
- Molecule 34: 50S ribosomal protein L13

Chain J: 73% 26%



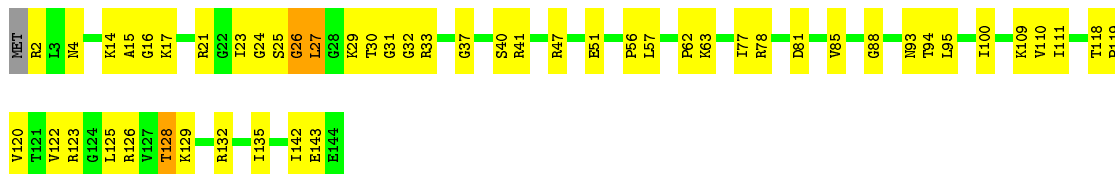
- Molecule 35: 50S ribosomal protein L14

Chain K: 68% 28%

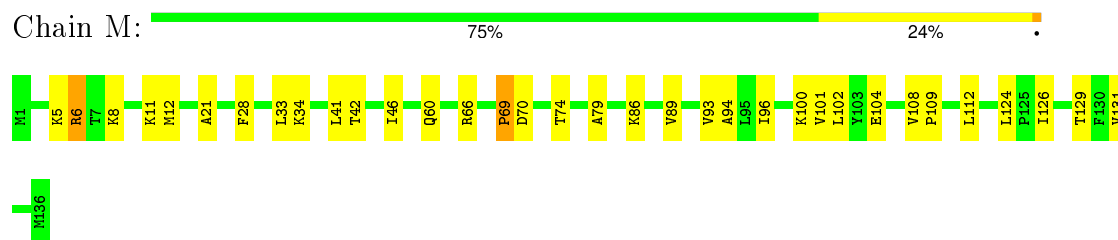


- Molecule 36: 50S ribosomal protein L15

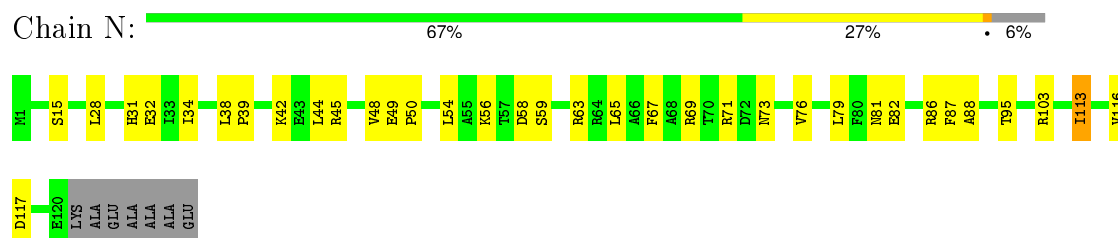
Chain L: 64% 33%



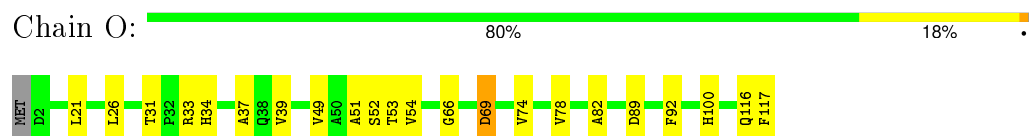
- Molecule 37: 50S ribosomal protein L16



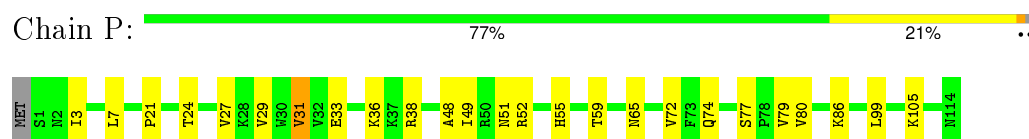
- Molecule 38: 50S ribosomal protein L17



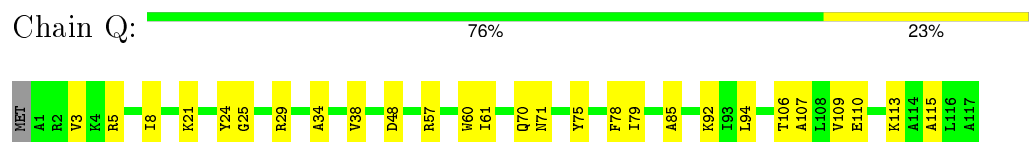
- Molecule 39: 50S ribosomal protein L18



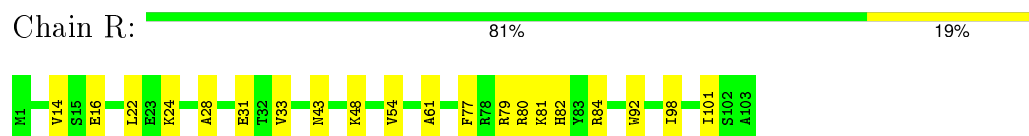
- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21



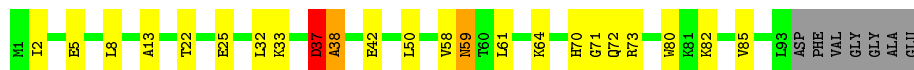
- Molecule 43: 50S ribosomal protein L22





- Molecule 44: 50S ribosomal protein L23

Chain T: 70% 20% 7%



- Molecule 45: 50S ribosomal protein L24

Chain U: 73% 24% 3%



- Molecule 46: 50S ribosomal protein L25

Chain V: 76% 23% 1%



- Molecule 47: 50S ribosomal protein L27

Chain W: 73% 15% 12%



- Molecule 48: 50S ribosomal protein L28

Chain X: 78% 19% 3%



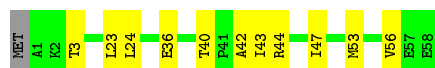
- Molecule 49: 50S ribosomal protein L29

Chain Y: 71% 27% 2%

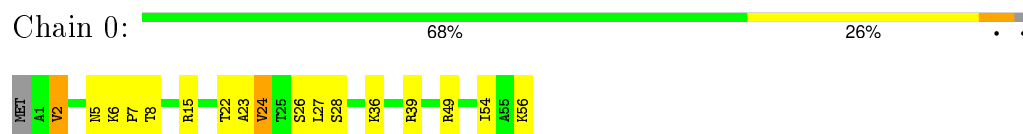


- Molecule 50: 50S ribosomal protein L30

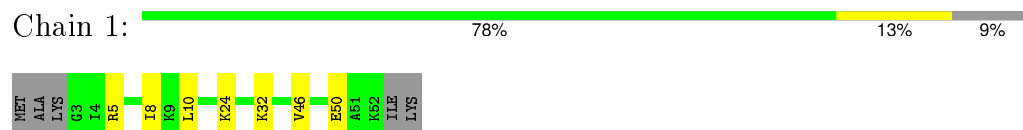
Chain Z: 80% 19% 1%



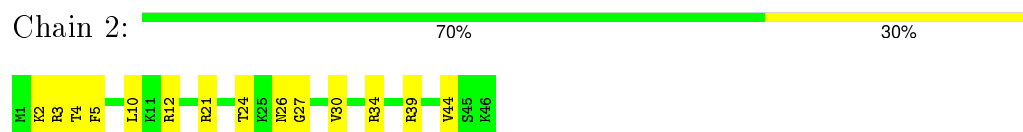
- Molecule 51: 50S ribosomal protein L32



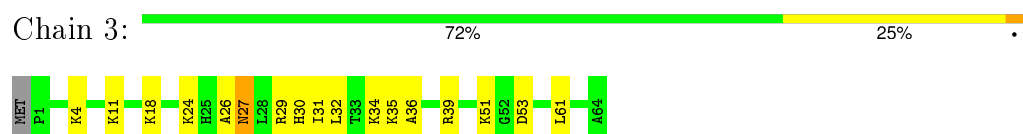
- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34



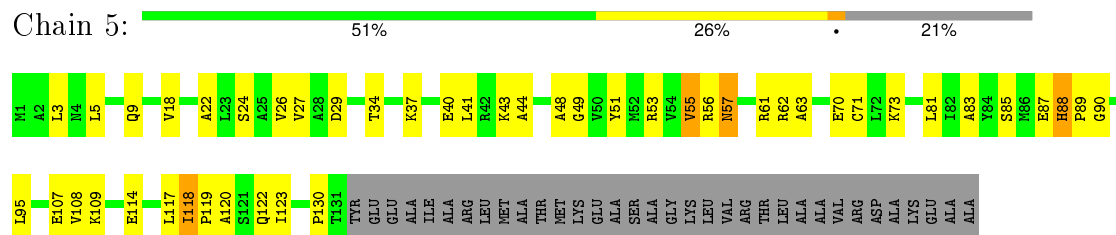
- Molecule 54: 50S ribosomal protein L35



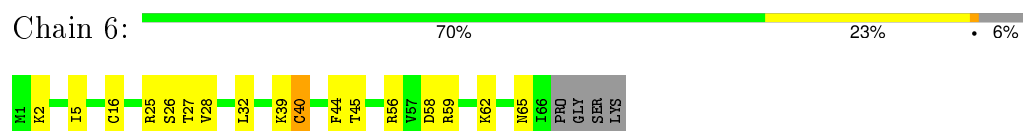
- Molecule 55: 50S ribosomal protein L36



- 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 images	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:1059:G:H22	33:I:128:ILE:HG12	1.53	0.71
25:A:572:A:OP2	42:R:80:ARG:NH2	2.22	0.71
25:A:530:G:OP1	25:A:530:G:O3'	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
43:S:4:ILE:HG22	43:S:106:VAL:HG22	1.71	0.71
35:K:69:VAL:HG21	35:K:104:THR:HG21	1.72	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:1432:G:C5'	40:P:105:LYS:HG2	54.12	0.69
25:A:1213:A:N6	25:A:1236:G:H1'	2.07	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:545:U:H3	25:A:548:G:H1	1.41	0.68
25:A:1565:C:O2'	25:A:1566:A:H8	1.77	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:2759:G:H21	31:G:138:GLN:NE2	1.93	0.67
25:A:947:A:HO2'	25:A:984:A:H2	1.43	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
27:C:165:ALA:HB3	27:C:172:THR:HB	1.76	0.67
25:A:1999:C:H5''	25:A:2723:C:O2'	1.95	0.67
25:A:2564:A:OP1	25:A:2648:G:H4'	1.95	0.67
25:A:2786:U:H2'	25:A:2787:C:H6	1.60	0.66
25:A:530:G:H3'	25:A:530:G:N3	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
27:C:48:ILE:HD11	27:C:51:ARG:HA	1.78	0.66
25:A:841:G:H2'	25:A:842:U:C6	2.31	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
30:F:140:ILE:HG22	30:F:142:TYR:H	1.60	0.65
25:A:218:A:H8	25:A:218:A:OP2	1.79	0.65
25:A:5:A:H2'	25:A:6:A:H8	1.62	0.65
25:A:499:U:H5''	45:U:42:LYS:HE2	1.78	0.65
46:V:21:ARG:HA	46:V:25:LYS:O	1.95	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
25:A:454:A:H4'	25:A:455:C:OP2	1.97	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: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:5:A:H2'	25:A:6:A:C8	2.31	0.65
25:A:2428:G:H5''	25:A:2429:G:O5'	1.96	0.65
25:A:1212:G:O2'	25:A:1236:G:N2	2.29	0.65
38:N:69:ARG:O	38:N:71:ARG:N	2.28	0.65
25:A:1930:G:O2'	25:A:1931:U:P	2.55	0.65
25:A:2131:U:O5'	25:A:2133:G:H4'	1.97	0.65
25:A:1474:U:H4'	25:A:1701:A:N3	71.19	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
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
51:O:54:ILE:HG13	51:O:56:LYS:HB3	1.80	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:2394:C:H5''	36:L:63:LYS:HE3	1.81	0.62
25:A:370:G:O2'	25:A:424:G:OP1	2.17	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
33:I:33:ASN:HB2	33:I:64:ARG:HH22	1.64	0.62
26:B:118:C:H2'	26:B:119:A:C8	2.35	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
38:N:58:ASP:OD1	38:N:63:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:839:U:H2'	25:A:840:C:C6	2.34	0.62
29:E:145:ASP:HA	29:E:166:LYS:HB3	1.81	0.62
25:A:2786:U:H2'	25:A:2787:C:C6	2.35	0.61
25:A:1385:A:OP1	25:A:1385:A:H4'	1.99	0.61
25:A:2346:A:H3'	25:A:2347:C:C5'	2.31	0.61
25:A:1019:U:H3	25:A:1142:A:N6	1.98	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:1081:U:H4'	33:I:123:ALA:HB1	1.81	0.61
25:A:704:G:H1'	25:A:727:A:H61	1.64	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
38:N:73:ASN:HA	38:N:76:VAL:HG12	1.80	0.61
25:A:2074:U:H2'	25:A:2075:U:C6	2.36	0.61
55:4:36:ARG:HG2	55:4:37:GLN:H	1.66	0.61
28:D:54:ALA:HA	28:D:76:GLY:HA2	1.83	0.60
56:5:53:ARG:HB3	56:5:55:VAL:HG13	1.82	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:2267:A:H5''	25:A:2268:A:H5'	1.83	0.60
28:D:4:LEU:HD23	28:D:29:VAL:HG11	1.82	0.60
25:A:2391:G:H2'	25:A:2424:C:H41	1.65	0.60
25:A:2104:C:H2'	25:A:2105:U:C6	2.36	0.60
37:M:21:ALA:HB1	37:M:100:LYS:HD3	1.83	0.60
25:A:878:A:H3'	25:A:879:G:H8	1.64	0.60
25:A:2655:G:O2'	25:A:2656:U:P	2.59	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:H2'	25:A:1086:A:N3	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
49:Y:24:GLU:O	49:Y:28:LEU:HB2	2.01	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)
25:A:1026:G:H2'	25:A:1027:A:H8	1.65	0.59
25:A:639:U:H2'	25:A:640:C:C6	2.38	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:1019:U:H2'	25:A:1020:A:H8	1.66	0.59
25:A:476:G:N1	25:A:479:A:OP2	2.36	0.59
25:A:2427:C:H5'	25:A:2429:G:H5'	1.84	0.59
28:D:121:THR:HG21	28:D:143:PRO:HB3	1.85	0.59
46:V:4:ILE:HD13	46:V:47:VAL:HG22	1.84	0.59
33:I:135:MET:HB2	33:I:137:LEU:HG	1.85	0.59
25:A:2238:G:N3	25:A:2238:G:H2'	2.17	0.59
25:A:2233:U:H2'	25:A:2234:G:C8	2.38	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:1779:U:H5	25:A:1784:A:N7	2.01	0.59
25:A:2267:A:H5''	25:A:2268:A:C5'	2.33	0.59
25:A:84:A:H4'	25:A:85:G:O5'	2.03	0.59
25:A:2557:G:H2'	25:A:2558:C:C6	2.38	0.59
25:A:530:G:C5'	25:A:530:G:N3	5.89	0.59
25:A:2115:G:H4'	25:A:2166:U:O2	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
25:A:847:U:O2	25:A:934:U:H1'	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
36:L:78:ARG:HB2	36:L:81:ASP:OD1	2.04	0.58
25:A:265:A:H4'	25:A:266:G:OP1	2.03	0.58
29:E:117:ARG:HH12	36:L:2:ARG:HG2	1.68	0.58
27:C:244:VAL:HG12	27:C:250:GLN:HA	1.86	0.58
35:K:109:SER:O	35:K:111:LYS:N	2.35	0.58
25:A:2326:C:O2'	25:A:2327:A:OP1	2.20	0.58
25:A:2271:G:H5'	47:W:16:ARG:HD3	1.84	0.58
25:A:495:G:H1'	43:S:57:ASN:OD1	2.04	0.58
25:A:271:G:H4'	25:A:272:A:OP1	2.03	0.58
38:N:45:ARG:HG2	38:N:95:THR:HG21	1.86	0.58
25:A:466:A:OP1	53:2:34:ARG:NH1	2.37	0.58
25:A:302:C:H2'	25:A:303:G:H8	1.69	0.58
25:A:2285:C:OP2	52:1:5:ARG:NH1	2.37	0.58
25:A:2427:C:H5''	25:A:2428:G:OP1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1956:U:H2'	25:A:1957:C:H5'	1.86	0.58
41:Q:70:GLN:C	41:Q:71:ASN:HD22	2.08	0.58
25:A:289:G:H2'	25:A:290:U:O4'	2.04	0.58
40:P:31:VAL:HG13	40:P:38:ARG:HB3	1.86	0.57
40:P:29:VAL:HG22	40:P:80:VAL:HA	1.85	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:88:ARG:O	29:E:90:GLN:N	2.37	0.57
29:E:148:ILE:O	29:E:169:VAL:HA	2.04	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
44:T:13:ALA:HB3	44:T:33:LYS:HD3	1.86	0.57
25:A:1614:A:N1	43:S:93:ALA:HB2	2.20	0.57
25:A:301:G:H4'	25:A:302:C:OP1	2.04	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:2867:G:O2'	25:A:2868:A:C8	2.57	0.57
38:N:44:LEU:HD23	38:N:113:ILE:HD13	1.87	0.57
29:E:3:LEU:HD13	29:E:120:VAL:HG21	1.85	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:36:LEU:O	34:J:51:GLY:HA3	2.05	0.57
34:J:102:GLU:HG3	34:J:119:PHE:HZ	1.69	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:302:C:H2'	25:A:303:G:C8	2.39	0.56
25:A:2297:A:N1	25:A:2321:U:H5	2.03	0.56
25:A:204:A:H4'	25:A:205:G:OP1	2.06	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: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)
25:A:1432:G:O3'	40:P:105:LYS:HD3	53.65	0.56
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:630:G:N2	25:A:633:A:OP2	2.34	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
37:M:11:LYS:HD2	37:M:86:LYS:HG2	1.88	0.56
25:A:394:C:H2'	25:A:395:U:O4'	2.05	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
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
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:1396:U:H5''	25:A:1397:U:OP2	2.06	0.56
25:A:2345:G:H4'	25:A:2346:A:C5'	2.36	0.56
35:K:40:LYS:NZ	35:K:89:ASN:OD1	2.38	0.56
25:A:861:A:H2'	25:A:862:G:O4'	2.05	0.56
25:A:1869:G:H1'	25:A:1872:A:N6	2.20	0.56
25:A:1847:G:H21	25:A:1848:A:H62	1.54	0.56
45:U:14:THR:OG1	45:U:68:ASN:ND2	2.38	0.55
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
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
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
25:A:1040:A:H2	25:A:1115:G:H22	1.54	0.55
35:K:121:GLU:HG2	35:K:122:VAL:HG23	1.86	0.55
27:C:162:GLN:OE1	27:C:174:ARG:NH2	2.40	0.55
25:A:1251:C:OP2	41:Q:5:ARG:HD2	2.06	0.55
53:2:24:THR:HG23	53:2:27:GLY:H	1.70	0.55
25:A:2341:G:H2'	25:A:2342:C:O4'	2.07	0.55
25:A:1315:C:H2'	25:A:1316:U:H6	1.71	0.55
36:L:14:LYS:O	36:L:16:GLY:N	2.39	0.55
26:B:118:C:H2'	26:B:119:A:H8	1.70	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
33:I:33:ASN:HB2	33:I:64:ARG:HH12	1.72	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:373:U:O2'	25:A:423:A:H1'	2.07	0.55
38:N:34:ILE:HG13	38:N:113:ILE:HG23	1.88	0.55
56:5:88:HIS:HB2	56:5:89:PRO:HD3	1.88	0.55
25:A:2469:A:N6	25:A:2481:G:O2'	2.40	0.55
25:A:1434:A:H2'	25:A:1435:G:C8	2.42	0.55
25:A:1028:A:H61	25:A:1125:G:H2'	1.71	0.55
56:5:37:LYS:HG3	56:5:41:LEU:HD12	1.88	0.55
30:F:116:LEU:HB2	30:F:175:PRO:HB2	1.87	0.55
27:C:154:ALA:HB2	27:C:161:VAL:HG23	1.88	0.55
25:A:468:G:H2'	25:A:469:G:H5'	1.88	0.55
25:A:2648:G:H2'	25:A:2649:C:O4'	2.06	0.55
25:A:1434:A:H2'	25:A:1435:G:H8	1.71	0.55
25:A:1179:G:C4	25:A:1180:U:H1'	2.42	0.55
56:5:29:ASP:HB2	56:5:56:ARG:HH12	1.72	0.55
25:A:1405:U:H2'	25:A:1406:U:C6	2.42	0.54
28:D:49:GLN:HA	28:D:80:TRP:O	2.07	0.54
25:A:1794:A:H2'	25:A:1795:C:C6	2.42	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
48:X:17:ARG:NE	48:X:23:ALA:HB2	2.11	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
25:A:1432:G:O5'	40:P:105:LYS:CG	54.12	0.54
32:H:84:ALA:HA	32:H:91:PHE:H	1.73	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
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:1203:U:H1'	36:L:4:ASN:HB3	1.90	0.54
25:A:542:C:H3'	25:A:543:G:H5''	1.89	0.54
25:A:390:U:H4'	25:A:391:A:O5'	2.08	0.54
25:A:851:C:H2'	25:A:852:U:C6	2.42	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
30:F:134:GLN:H	30:F:134:GLN:CD	2.12	0.53
37:M:28:PHE:HB2	37:M:104:GLU:OE1	2.08	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:505:A:HO2'	25:A:509:C:HO2'	1.56	0.53
35:K:33:ALA:HB1	35:K:37:ASP:HB2	1.90	0.53
49:Y:23:ARG:O	49:Y:25:GLN:N	2.41	0.53
25:A:2576:G:H8	25:A:2581:G:O6	1.90	0.53
25:A:956:G:HO2'	25:A:959:A:H62	1.55	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:1548:A:H2'	25:A:1549:A:C8	2.42	0.53
25:A:2832:U:H1'	25:A:2834:G:C4	2.43	0.53
25:A:1332:G:N3	25:A:1332:G:H5''	2.24	0.53
25:A:107:G:H2'	25:A:108:G:C8	2.41	0.53
43:S:14:ALA:O	43:S:18:ARG:HB2	2.08	0.53
25:A:784:G:O2'	25:A:785:G:H5''	2.09	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:1399:C:N3	25:A:1401:G:O6	6.65	0.53
25:A:1021:A:N3	25:A:1022:G:H5''	2.22	0.53
36:L:122:VAL:HB	36:L:142:ILE:HG23	1.89	0.53
32:H:113:SER:O	32:H:116:ARG:NH1	2.39	0.53
25:A:1297:C:O2'	25:A:1302:A:N1	2.36	0.53
56:5:37:LYS:O	56:5:41:LEU:HB2	2.08	0.53
28:D:114:LYS:HE3	28:D:196:ALA:HB2	1.90	0.53
25:A:715:A:H2'	25:A:716:A:C8	3.34	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: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:265:A:H1'	25:A:266:G:O4'	2.08	0.53
25:A:2296:U:H4'	25:A:2297:A:OP1	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
53:2:34:ARG:HH21	53:2:39:ARG:HD3	1.74	0.52
25:A:468:G:C2'	25:A:469:G:H5'	2.39	0.52
25:A:910:A:H2'	25:A:911:A:C8	2.45	0.52
51:0:54:ILE:HG23	51:0:56:LYS:H	1.74	0.52
25:A:844:A:H61	25:A:934:U:H3	1.56	0.52
25:A:413:C:H2'	25:A:414:C:C6	2.44	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:1645:G:H5''	25:A:1646:C:H5'	1.91	0.52
25:A:2884:U:H3	51:0:39:ARG:CZ	2.22	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
26:B:41:G:H2'	26:B:41:G:N3	2.24	0.52
25:A:774:G:N2	25:A:787:C:O2'	2.41	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:C3'	25:A:530:G:N3	5.31	0.52
28:D:49:GLN:NE2	28:D:67:HIS:NE2	2.52	0.52
26:B:104:A:H2'	26:B:105:G:O4'	2.09	0.52
29:E:97:ASN:HB2	29:E:100:MET:HG3	1.92	0.52
43:S:4:ILE:HD12	43:S:6:LYS:HE3	1.92	0.52
29:E:143:LEU:HB3	29:E:146:VAL:HG11	1.91	0.52
46:V:30:ILE:HD11	46:V:63:ILE:HD12	1.92	0.52
25:A:301:G:OP2	45:U:81:ARG:NH1	2.41	0.52
25:A:2678:C:H2'	25:A:2679:A:O4'	2.09	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:947:A:O2'	25:A:984:A:H2	1.91	0.52
39:O:51:ALA:HB3	39:O:78:VAL:HG22	1.91	0.52
25:A:1796:U:H2'	25:A:1797:G:C8	2.44	0.52
37:M:34:LYS:HE3	37:M:131:VAL:HG11	1.91	0.52
56:5:57:ASN:HB2	56:5:62:ARG:HD2	1.91	0.52
40:P:48:ALA:HB3	40:P:59:THR:OG1	2.09	0.52
25:A:677:A:O2'	25:A:2071:A:H5'	2.10	0.52
25:A:1475:G:O2'	25:A:1476:U:OP2	2.27	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
25:A:335:C:H4'	25:A:1434:A:H4'	118.87	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
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:2303:G:H2'	25:A:2304:G:O4'	2.10	0.52
56:5:48:ALA:HB3	56:5:51:TYR:HE2	1.75	0.52
56:5:48:ALA:HB3	56:5:51:TYR:CE2	2.45	0.52
25:A:2809:A:H2'	25:A:2810:A:C8	2.45	0.52
25:A:1239:G:H2'	25:A:1240:U:O4'	2.10	0.52
25:A:519:U:H5''	43:S:25:ARG:HH21	1.74	0.52
55:4:27:CYS:SG	55:4:30:GLU:N	2.79	0.52
25:A:532:A:N3	25:A:532:A:C3'	4.07	0.51
47:W:33:ILE:HG22	47:W:34:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:T:70:HIS:O	44:T:72:GLN:N	2.43	0.51
32:H:70:GLU:HB2	32:H:134:VAL:HG21	1.91	0.51
25:A:32:C:N4	25:A:446:G:O2'	2.43	0.51
25:A:722:A:H2'	25:A:723:C:O4'	2.10	0.51
25:A:1682:G:C4	25:A:1757:A:H1'	2.45	0.51
25:A:1422:G:H5'	35:K:48:PRO:HG3	99.24	0.51
31:G:23:ILE:HD11	31:G:42:VAL:HG11	1.93	0.51
30:F:110:ILE:O	30:F:113:PHE:HB2	2.10	0.51
39:O:49:VAL:HG21	39:O:82:ALA:HA	1.91	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
46:V:76:ASP:OD1	46:V:77:VAL:N	2.41	0.51
30:F:39:VAL:O	30:F:41:GLU:HG2	2.11	0.51
56:5:114:GLU:HA	56:5:123:ILE:HB	1.90	0.51
25:A:1055:G:O2'	25:A:1084:A:N6	2.36	0.51
37:M:102:LEU:HD11	37:M:126:ILE:HD11	1.91	0.51
25:A:1509:A:H2'	25:A:1510:G:C8	2.45	0.51
39:O:89:ASP:HA	39:O:116:GLN:O	2.10	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
28:D:55:LYS:HE2	28:D:77:ARG:HA	1.92	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: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
25:A:372:G:HO2'	25:A:373:U:H6	1.58	0.51
56:5:57:ASN:HD22	56:5:63:ALA:HB2	1.74	0.51
25:A:1088:A:H61	33:I:134:SER:HB3	1.75	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:2879:A:H8	25:A:2881:U:O4	1.92	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: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
25:A:270:A:N1	25:A:369:U:O2'	2.40	0.51
25:A:1962:5MC:O2'	25:A:1964:G:OP2	2.28	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: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
38:N:56:LYS:NZ	38:N:87:PHE:O	2.44	0.51
35:K:24:VAL:HG13	35:K:33:ALA:HB2	1.93	0.51
25:A:962:G:H21	25:A:2250:G:H1	1.59	0.51
25:A:833:A:H2'	25:A:834:G:C8	2.45	0.51
25:A:1399:C:N4	25:A:1401:G:C2	8.11	0.51
25:A:52:A:H8	25:A:52:A:OP2	1.94	0.51
25:A:2298:A:H2'	25:A:2299:U:O4'	2.11	0.51
25:A:1005:C:O2'	34:J:30:THR:HG21	2.11	0.51
25:A:2262:U:O2'	25:A:2263:C:H5'	2.10	0.51
55:4:11:CYS:HB3	55:4:33:HIS:CE1	2.46	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
33:I:25:PRO:O	33:I:29:GLN:HB2	2.11	0.50
25:A:405:U:H3'	25:A:406:G:H5'	2.96	0.50
25:A:1815:A:H4'	25:A:1816:C:OP1	2.11	0.50
25:A:2591:C:H2'	25:A:2592:G:H8	1.75	0.50
25:A:2845:U:H5''	40:P:51:ASN:O	2.11	0.50
25:A:2101:A:H2'	25:A:2102:G:H8	1.76	0.50
57:6:44:PHE:HD1	57:6:45:THR:HG23	1.76	0.50
25:A:1243:C:H1'	36:L:4:ASN:O	2.11	0.50
25:A:1112:G:H2'	25:A:1113:U:C6	2.45	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
45:U:36:GLU:HA	45:U:61:GLU:HG2	1.94	0.50
41:Q:25:GLY:O	41:Q:29:ARG:NH1	2.44	0.50
30:F:141:ASP:O	30:F:143:ASP:N	2.44	0.50
25:A:792:A:H1'	25:A:794:A:N7	14.55	0.50
25:A:123:G:O2'	25:A:124:G:H5'	2.11	0.50
50:Z:40:THR:HG22	50:Z:43:ILE:HG12	1.92	0.50
25:A:716:A:H2'	25:A:717:C:O4'	2.11	0.50
42:R:61:ALA:HB2	42:R:98:ILE:HD13	1.94	0.50
26:B:111:U:O2'	26:B:112:G:H5'	2.12	0.50
25:A:589:U:H2'	25:A:590:A:C8	2.46	0.50
30:F:133:GLU:HB3	30:F:135:ILE:HG13	1.94	0.50
25:A:28:A:H2'	25:A:29:U:O4'	2.63	0.50
25:A:1182:G:H2'	25:A:1183:U:O4'	2.12	0.50
25:A:1329:U:O5'	25:A:1330:C:H5	1.95	0.50
25:A:1019:U:O2'	25:A:1020:A:H5'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:3:LEU:HD11	30:F:100:GLU:HB2	1.93	0.50
25:A:2327:A:H2'	25:A:2328:A:C8	2.46	0.50
25:A:2101:A:H2'	25:A:2102:G:C8	2.47	0.50
25:A:1266:G:N2	25:A:1269:A:OP2	13.16	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
25:A:1210:G:O6	25:A:1237:A:H2'	2.11	0.50
25:A:2391:G:O2'	25:A:2392:A:O5'	2.23	0.50
38:N:79:LEU:O	38:N:81:ASN:N	2.42	0.50
25:A:1877:A:H2'	25:A:1878:G:O4'	2.12	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
51:O:24:VAL:HG22	51:O:26:SER:H	1.77	0.50
25:A:2224:G:H4'	25:A:2226:C:C2	2.46	0.50
25:A:530:G:C4	25:A:530:G:H5'	5.37	0.49
25:A:795:C:H4'	25:A:1506:U:C2	82.48	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:1399:C:N4	25:A:1401:G:N1	7.13	0.49
25:A:175:G:H2'	25:A:176:A:O4'	2.11	0.49
25:A:1142:A:H4'	25:A:1143:A:OP1	2.10	0.49
25:A:2516:A:O2'	25:A:2517:C:H5'	2.12	0.49
25:A:1701:A:C2'	25:A:1702:G:H5'	2.40	0.49
31:G:94:ARG:HD2	31:G:127:GLN:HB3	1.94	0.49
25:A:2758:A:H2	31:G:34:ARG:HH21	1.59	0.49
25:A:2698:U:H2'	25:A:2699:C:C6	2.48	0.49
25:A:543:G:O6	25:A:550:C:N3	2.46	0.49
25:A:1201:U:H2'	25:A:1202:G:H8	1.77	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
36:L:33:ARG:HD3	36:L:40:SER:HA	1.95	0.49
25:A:2759:G:N2	31:G:138:GLN:NE2	2.59	0.49
30:F:67:THR:O	30:F:83:PRO:HA	2.12	0.49
40:P:74:GLN:HB2	40:P:77:SER:HB2	1.93	0.49
36:L:110:VAL:HG11	36:L:135:ILE:HD11	1.93	0.49
25:A:473:G:O2'	25:A:474:G:H5'	2.12	0.49
44:T:22:THR:HA	44:T:25:GLU:HG2	1.93	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
25:A:1881:C:H2'	25:A:1882:U:O4'	2.13	0.49
46:V:80:HIS:CG	46:V:81:PRO:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1586:A:C2	25:A:1587:G:H1'	2.48	0.49
26:B:1:U:H2'	26:B:2:G:C8	2.47	0.49
25:A:948:C:H2'	25:A:949:G:H8	1.76	0.49
43:S:52:GLU:HA	43:S:55:ILE:HD12	1.95	0.49
25:A:2529:G:H4'	31:G:174:LYS:HE3	1.94	0.49
31:G:102:ILE:O	31:G:113:ASP:HA	2.12	0.49
25:A:2134:A:N6	25:A:2156:G:H2'	2.27	0.49
32:H:47:PHE:HA	32:H:51:ARG:HB2	1.95	0.49
25:A:580:U:H2'	25:A:581:C:C6	2.48	0.49
25:A:2725:A:O2'	25:A:2726:A:C8	2.66	0.49
25:A:2405:G:HO2'	25:A:2406:A:P	2.36	0.49
25:A:1266:G:O2'	25:A:1267:U:OP2	2.30	0.49
43:S:28:LYS:HE3	43:S:70:LYS:NZ	2.28	0.49
25:A:1900:A:O4'	25:A:1970:A:H5''	2.12	0.49
25:A:2572:A:H2'	28:D:149:ASN:HD22	1.76	0.49
25:A:528:A:C2	25:A:2042:A:H2'	2.48	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: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:562:U:H2'	25:A:572:A:O4'	2.13	0.49
25:A:356:G:H2'	25:A:357:C:C6	2.48	0.49
25:A:636:G:N7	36:L:109:LYS:HD3	2.28	0.49
26:B:106:G:H2'	26:B:107:G:O4'	2.13	0.49
25:A:1689:A:H2'	25:A:1690:A:H8	1.76	0.49
25:A:395:U:H2'	25:A:396:G:C8	2.47	0.49
25:A:974:G:C8	25:A:990:A:N6	2.76	0.49
25:A:2020:A:H5'	51:O:8:THR:HG22	1.94	0.49
26:B:13:G:C8	26:B:70:C:H4'	2.48	0.48
30:F:73:VAL:HG22	30:F:78:ILE:HG12	1.95	0.48
25:A:2103:C:H2'	25:A:2104:C:C6	2.48	0.48
25:A:437:U:H2'	25:A:438:G:C8	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
30:F:102:LEU:HD12	30:F:106:ALA:HB3	1.95	0.48
25:A:1558:C:H4'	25:A:1559:U:O5'	2.13	0.48
25:A:2861:U:H2'	25:A:2862:G:H8	1.77	0.48
25:A:687:C:H1'	53:2:4:THR:HG22	1.95	0.48
25:A:1160:G:N7	25:A:1182:G:N2	20.72	0.48
38:N:79:LEU:C	38:N:81:ASN:H	2.16	0.48
25:A:420:C:H2'	25:A:421:C:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2205:A:H2'	25:A:2206:C:C6	2.48	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:2159:G:H2'	25:A:2160:C:O4'	2.13	0.48
25:A:2120:G:H2'	25:A:2121:G:C8	2.48	0.48
25:A:635:C:O2'	25:A:639:U:H5''	2.13	0.48
38:N:49:GLU:HB2	38:N:50:PRO:HD3	1.96	0.48
25:A:2331:G:O2'	25:A:2336:A:N1	2.46	0.48
35:K:102:PRO:HB3	35:K:121:GLU:HB3	1.94	0.48
25:A:981:A:OP2	25:A:982:C:N4	2.43	0.48
25:A:873:C:H2'	25:A:874:G:H8	1.77	0.48
27:C:7:PRO:HB3	27:C:13:ARG:HB2	1.95	0.48
25:A:2720:U:H5''	40:P:52:ARG:NH2	2.28	0.48
25:A:670:A:OP2	25:A:670:A:H8	1.95	0.48
25:A:335:C:C1'	25:A:1434:A:H1'	114.96	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
25:A:2552:OMU:H5	25:A:2556:C:H41	1.79	0.48
25:A:1106:G:H3'	25:A:1107:G:H8	1.76	0.48
31:G:136:ASP:OD2	31:G:139:VAL:HG23	2.13	0.48
25:A:2875:C:O2'	25:A:2876:G:H5'	2.14	0.48
25:A:127:A:H5''	25:A:128:C:C6	2.48	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
25:A:1900:A:H1'	25:A:1970:A:H2'	1.95	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:335:C:O4'	25:A:1434:A:H1'	116.30	0.48
33:I:38:CYS:SG	33:I:39:LYS:N	2.87	0.48
25:A:2788:C:O2'	25:A:2809:A:N3	2.43	0.48
26:B:79:G:H2'	26:B:80:U:O4'	2.13	0.48
25:A:2405:G:O2'	25:A:2406:A:OP2	2.32	0.48
25:A:1183:U:H2'	25:A:1184:U:C6	2.49	0.48
25:A:495:G:H5''	43:S:4:ILE:HG13	1.95	0.48
30:F:89:THR:HG21	30:F:91:ARG:HH11	1.79	0.48
25:A:2178:C:H2'	25:A:2179:C:C6	2.49	0.48
42:R:77:PHE:HD1	42:R:84:ARG:HB3	1.79	0.48
56:5:5:LEU:O	56:5:9:GLN:HB2	2.13	0.48
25:A:2808:G:H2'	25:A:2890:G:O6	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:77:ILE:O	36:L:110:VAL:O	2.32	0.48
25:A:2071:A:H2'	25:A:2072:C:C6	2.49	0.48
28:D:32:ASN:HA	28:D:51:THR:O	2.13	0.48
25:A:39:G:H2'	25:A:40:U:C6	2.49	0.48
37:M:42:THR:HG22	37:M:93:VAL:HG12	1.96	0.48
25:A:831:G:H5''	36:L:37:GLY:HA2	1.95	0.48
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
25:A:2065:C:H1'	25:A:2449:H2U:HN3	1.79	0.47
49:Y:44:LYS:HA	49:Y:47:ARG:HH22	1.79	0.47
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:458:G:O2'	25:A:469:G:N1	2.47	0.47
30:F:165:GLY:O	30:F:168:LEU:HB3	2.14	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
36:L:24:GLY:C	36:L:26:GLY:H	2.17	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:2051:A:H8	25:A:2051:A:OP2	1.97	0.47
25:A:1320:C:O2'	25:A:1321:A:H5''	2.14	0.47
25:A:2443:C:OP1	29:E:63:LYS:HD3	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:435:C:H2'	25:A:436:C:H5'	1.96	0.47
36:L:122:VAL:HG21	36:L:135:ILE:HD13	1.97	0.47
25:A:1052:C:H2'	25:A:1053:C:C5	2.50	0.47
35:K:34:GLY:O	35:K:36:GLY:N	2.47	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
29:E:52:VAL:O	29:E:74:LYS:HE3	2.14	0.47
25:A:1538:G:H2'	25:A:1539:U:C6	2.50	0.47
25:A:244:A:H2'	25:A:245:G:O4'	2.15	0.47
28:D:48:ILE:O	28:D:81:GLU:HA	2.15	0.47
25:A:2526:G:H2'	25:A:2527:C:C6	2.49	0.47
25:A:2408:U:H2'	25:A:2409:G:H8	1.80	0.47
25:A:2266:A:OP1	25:A:2266:A:H8	1.98	0.47
25:A:120:U:H4'	25:A:121:G:H5''	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:554:U:H2'	25:A:555:G:O4'	2.15	0.47
25:A:322:A:H5'	25:A:340:A:H1'	1.97	0.47
25:A:1019:U:H3	25:A:1142:A:H62	1.62	0.47
25:A:108:G:H2'	25:A:109:C:O4'	2.15	0.47
34:J:35:ARG:HA	34:J:40:HIS:HD2	1.79	0.47
25:A:1930:G:O2'	25:A:1931:U:OP2	2.26	0.47
56:5:41:LEU:O	56:5:44:ALA:HB3	2.15	0.47
25:A:1857:G:H1'	25:A:1885:A:N6	2.29	0.47
25:A:1340:U:H3'	44:T:61:LEU:HD22	1.97	0.47
25:A:1715:G:O2'	25:A:1716:U:H6	1.98	0.47
25:A:2014:A:H2'	25:A:2015:A:C8	2.50	0.47
57:6:28:VAL:HG11	57:6:32:LEU:HD13	1.95	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: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
25:A:692:C:H5''	27:C:38:LYS:HB3	1.96	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:807:U:H1'	25:A:2445:2MG:OP1	2.15	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
33:I:20:SER:HB3	33:I:21:PRO:HD3	1.97	0.47
25:A:1038:G:H2'	25:A:1039:A:C8	2.50	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
25:A:1:G:H2'	25:A:2:G:H8	1.80	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:923:G:H2'	25:A:924:G:C8	2.48	0.47
25:A:404:A:H1'	25:A:406:G:N9	2.30	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: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:2808:G:O2'	25:A:2809:A:H8	1.97	0.46
25:A:2645:G:H4'	25:A:2732:G:H1'	1.97	0.46
25:A:635:C:H2'	25:A:636:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1343:G:H1'	25:A:1597:A:C4	2.51	0.46
25:A:2391:G:OP2	54:3:34:LYS:HD2	2.14	0.46
33:I:133:ARG:HA	33:I:137:LEU:O	2.15	0.46
25:A:2629:U:O2'	25:A:2630:G:H5''	2.15	0.46
33:I:42:ASN:HA	33:I:45:THR:HB	1.97	0.46
25:A:1363:C:O2'	25:A:1809:A:N3	2.47	0.46
41:Q:85:ALA:HB2	41:Q:115:ALA:HB2	1.97	0.46
25:A:1432:G:P	40:P:105:LYS:CG	54.36	0.46
33:I:33:ASN:HB2	33:I:64:ARG:NH2	2.29	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
25:A:136:G:H1	25:A:143:C:H42	1.63	0.46
38:N:38:LEU:HB3	38:N:39:PRO:HD3	1.97	0.46
34:J:75:TYR:HB3	34:J:84:ILE:HD11	1.95	0.46
25:A:2808:G:H2'	25:A:2890:G:C6	2.51	0.46
25:A:1212:G:H1'	25:A:1237:A:N6	2.30	0.46
25:A:789:A:N1	53:2:3:ARG:NH1	2.55	0.46
25:A:336:C:O2'	25:A:337:C:H5'	2.15	0.46
25:A:1177:G:H2'	25:A:1178:C:C4'	2.45	0.46
25:A:2584:U:C3'	25:A:2585:U:H5''	2.44	0.46
25:A:242:G:O2'	25:A:243:U:OP2	2.27	0.46
25:A:2286:G:H4'	25:A:2287:A:O5'	2.14	0.46
31:G:41:GLU:HB3	31:G:52:GLY:O	2.15	0.46
25:A:1111:A:HO2'	25:A:1112:G:P	2.37	0.46
25:A:2012:G:O5'	25:A:2012:G:H8	1.98	0.46
42:R:28:ALA:HB3	42:R:31:GLU:HB2	1.97	0.46
25:A:973:A:H5'	25:A:1188:U:H1'	1.98	0.46
25:A:1474:U:H4'	25:A:1701:A:C2	71.26	0.46
41:Q:71:ASN:N	41:Q:71:ASN:HD22	2.12	0.46
35:K:41:ILE:HG13	35:K:58:LEU:O	2.15	0.46
25:A:2721:A:H1'	25:A:2873:A:O2'	2.16	0.46
25:A:1728:C:O2'	25:A:1729:U:C6	2.69	0.46
50:Z:47:ILE:HD13	50:Z:56:VAL:HG21	1.97	0.46
25:A:1751:U:H2'	25:A:1752:C:C6	2.51	0.46
48:X:17:ARG:HE	48:X:23:ALA:CB	2.15	0.46
44:T:80:TRP:CZ3	44:T:82:LYS:HB3	2.50	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
25:A:185:G:H4'	25:A:218:A:H4'	1.98	0.46
25:A:2742:G:OP1	55:4:36:ARG:HD3	2.16	0.46
40:P:29:VAL:HG13	40:P:79:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Z:40:THR:HG23	50:Z:42:ALA:H	1.80	0.46
48:X:30:PRO:O	48:X:32:LEU:N	2.49	0.46
25:A:1951:U:H2'	25:A:1953:A:OP2	2.15	0.46
25:A:2515:C:H2'	25:A:2516:A:H8	1.81	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: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
43:S:72:THR:HG21	43:S:108:SER:HB3	1.98	0.46
26:B:114:C:H2'	26:B:115:A:C8	2.51	0.46
25:A:259:G:C2'	25:A:260:G:H5'	2.46	0.46
33:I:48:ILE:HG13	33:I:49:GLU:H	1.81	0.46
25:A:2528:U:H2'	25:A:2530:A:O5'	2.16	0.46
32:H:64:ALA:O	32:H:67:ALA:HB3	2.15	0.46
25:A:128:C:H2'	25:A:129:C:H6	1.81	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
25:A:2777:G:H1'	25:A:2779:U:H5	1.80	0.46
25:A:2688:G:H1'	25:A:2721:A:N6	2.31	0.46
55:4:1:MET:HE3	55:4:34:LYS:HG2	1.98	0.46
25:A:1684:G:H2'	25:A:1685:C:C6	2.51	0.46
39:O:26:LEU:HD13	39:O:39:VAL:HG22	1.97	0.46
45:U:42:LYS:HG2	45:U:59:GLU:OE1	2.16	0.46
56:5:26:VAL:HG21	56:5:114:GLU:HG2	1.98	0.46
25:A:2862:G:H2'	25:A:2863:C:C6	2.51	0.46
48:X:32:LEU:HD22	48:X:49:ARG:HG2	1.98	0.46
25:A:1069:A:N6	25:A:1073:A:C4	2.84	0.46
45:U:17:ASP:HB3	45:U:20:LYS:HD2	1.98	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
30:F:12:VAL:O	30:F:16:MET:HG2	2.16	0.46
34:J:99:ARG:NH1	34:J:102:GLU:OE2	2.49	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: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
25:A:2183:A:H2'	25:A:2184:A:C8	2.51	0.46
45:U:96:LYS:O	45:U:97:SER:O	2.34	0.46
25:A:1287:A:H5'	38:N:103:ARG:HH11	1.80	0.46
25:A:2313:C:H5''	30:F:87:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:129:MET:HG3	30:F:153:ILE:HB	1.98	0.46
25:A:1297:C:OP1	25:A:2710:C:H4'	2.16	0.45
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
44:T:5:GLU:HA	44:T:8:LEU:HD12	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:1819:A:H3'	27:C:176:ARG:HG2	1.98	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:1045:C:H1'	25:A:1047:G:C2	2.51	0.45
25:A:1930:G:HO2'	25:A:1931:U:P	2.32	0.45
25:A:2444:G:OP2	29:E:63:LYS:HD2	2.16	0.45
25:A:811:U:N3	36:L:21:ARG:NH2	2.64	0.45
25:A:1798:U:OP2	27:C:270:ARG:NH2	2.49	0.45
25:A:2019:A:H2	25:A:2035:G:H22	1.64	0.45
25:A:2869:G:H2'	25:A:2870:C:O4'	2.17	0.45
25:A:335:C:H4'	25:A:1434:A:C1'	116.48	0.45
53:2:30:VAL:O	53:2:34:ARG:HG2	2.17	0.45
33:I:4:VAL:HA	33:I:7:TYR:CE2	2.52	0.45
25:A:1604:C:H2'	25:A:1605:C:C6	2.51	0.45
49:Y:39:GLN:HB2	49:Y:41:HIS:CE1	2.52	0.45
27:C:252:LYS:HE3	27:C:252:LYS:HB2	1.83	0.45
25:A:1306:C:N4	25:A:1606:C:H2'	2.30	0.45
35:K:35:VAL:HG22	35:K:69:VAL:HG12	1.98	0.45
25:A:424:G:H2'	25:A:425:G:O4'	2.36	0.45
25:A:1858:A:C2	25:A:1885:A:H1'	2.51	0.45
25:A:1182:G:H4'	25:A:1183:U:O5'	4.94	0.45
25:A:89:A:H2'	25:A:90:U:C6	2.51	0.45
25:A:357:C:H2'	25:A:358:U:C6	2.51	0.45
25:A:1530:G:H22	25:A:1542:U:H1'	1.79	0.45
25:A:286:U:H2'	25:A:287:G:C8	2.52	0.45
28:D:31:ALA:O	28:D:33:ARG:HG2	2.17	0.45
56:5:118:ILE:H	56:5:119:PRO:CD	2.29	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:529:A:OP2	34:J:113:PRO:HD3	2.17	0.45
25:A:18:U:O2'	25:A:554:U:OP1	2.35	0.45
25:A:321:U:H4'	25:A:322:A:OP2	2.14	0.45
25:A:568:U:H2'	25:A:570:G:OP2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:13:G:N7	26:B:70:C:H4'	2.31	0.45
25:A:1857:G:H2'	25:A:1884:G:H22	1.82	0.45
25:A:2851:A:H2'	25:A:2852:G:O4'	2.17	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:2141:G:N2	25:A:2151:U:H1'	2.31	0.45
25:A:1682:G:H2'	25:A:1683:U:C6	2.52	0.45
25:A:974:G:H1'	25:A:975:A:C8	2.52	0.45
31:G:95:ALA:HB1	31:G:130:ILE:HD11	1.97	0.45
25:A:2846:G:H2'	25:A:2847:U:O4'	2.17	0.45
31:G:37:ASN:OD1	31:G:38:ASP:N	2.50	0.45
25:A:1916:A:H2'	25:A:1917:PSU:O4'	2.16	0.45
25:A:674:G:H5''	29:E:71:GLY:H	1.81	0.45
31:G:70:LEU:O	31:G:74:MET:HG3	2.15	0.45
25:A:1088:A:H61	33:I:134:SER:CB	2.29	0.45
28:D:35:THR:HG22	28:D:73:VAL:HG21	1.98	0.45
25:A:2638:G:H1'	25:A:2778:A:N6	2.32	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:1152:C:H2'	25:A:1153:C:C6	2.51	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
25:A:2840:C:H2'	25:A:2841:C:C6	2.52	0.45
25:A:2793:C:H2'	25:A:2794:C:C6	2.52	0.45
25:A:2514:U:H5''	34:J:81:ILE:HD11	1.99	0.45
25:A:465:G:H2'	25:A:466:A:C8	2.51	0.45
25:A:1188:U:O2'	25:A:1189:A:H5'	2.16	0.45
30:F:56:LEU:HD13	30:F:88:VAL:HG23	1.99	0.45
25:A:2712:C:OP1	25:A:2714:G:H4'	2.17	0.45
28:D:149:ASN:CG	28:D:150:GLN:H	2.20	0.45
25:A:2065:C:H2'	25:A:2066:C:C6	2.52	0.45
25:A:2512:C:H2'	25:A:2513:A:O4'	2.17	0.45
25:A:2100:G:H1	25:A:2189:U:H3	1.64	0.45
25:A:1328:A:H2'	25:A:1330:C:C5	2.52	0.44
25:A:1328:A:H2'	25:A:1330:C:C4	2.52	0.44
25:A:973:A:H5''	42:R:81:LYS:HD2	1.98	0.44
25:A:2233:U:H2'	25:A:2234:G:H8	1.80	0.44
25:A:2271:G:OP1	47:W:14:ALA:HB1	2.17	0.44
25:A:955:PSU:H5'	37:M:86:LYS:HD3	1.99	0.44
25:A:414:C:H2'	25:A:415:A:C8	2.52	0.44
25:A:1590:A:H2'	25:A:1591:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1610:A:OP1	25:A:1611:C:H5	2.00	0.44
25:A:155:A:H2'	25:A:156:A:C8	2.52	0.44
25:A:1744:A:H3'	25:A:1745:A:H8	1.81	0.44
29:E:49:ARG:O	29:E:74:LYS:HE2	2.17	0.44
25:A:780:G:OP1	27:C:216:ARG:NH2	2.49	0.44
25:A:2291:U:H2'	25:A:2292:U:H6	1.77	0.44
25:A:1528:A:H2'	25:A:1529:G:O4'	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:2146:C:H4'	25:A:2147:A:C4	2.52	0.44
25:A:307:G:N1	25:A:310:A:OP2	2.50	0.44
33:I:18:ASN:HB2	33:I:38:CYS:HB3	1.99	0.44
25:A:358:U:H2'	25:A:359:G:H8	2.06	0.44
25:A:117:G:C6	25:A:119:A:C6	3.05	0.44
25:A:2427:C:C5'	25:A:2429:G:H5'	2.46	0.44
41:Q:57:ARG:HA	41:Q:60:TRP:CE3	2.53	0.44
34:J:63:ALA:HA	34:J:69:ARG:NH2	2.32	0.44
29:E:18:THR:HA	29:E:106:LYS:HE3	1.99	0.44
25:A:2093:G:OP1	32:H:24:GLY:HA3	2.18	0.44
25:A:1807:G:H2'	25:A:1808:A:H5'	1.99	0.44
25:A:2208:C:H2'	25:A:2209:G:C8	2.52	0.44
25:A:2022:U:O4	51:0:5:ASN:ND2	2.50	0.44
37:M:5:LYS:O	37:M:6:ARG:HG2	2.17	0.44
25:A:651:G:H5'	54:3:18:LYS:HG3	1.99	0.44
25:A:2221:G:H2'	25:A:2222:C:C6	2.52	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
34:J:35:ARG:HB2	34:J:54:ILE:HD11	1.98	0.44
25:A:753:A:C8	25:A:753:A:OP2	2.67	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
36:L:51:GLU:OE1	36:L:56:PRO:HA	2.17	0.44
32:H:30:LEU:HB3	32:H:36:ALA:HB3	2.00	0.44
25:A:2307:G:H8	25:A:2307:G:OP1	2.00	0.44
34:J:110:PRO:O	34:J:115:GLY:HA3	2.17	0.44
25:A:458:G:O2'	25:A:459:U:P	2.76	0.44
25:A:1614:A:C2	43:S:93:ALA:HB2	2.53	0.44
33:I:56:VAL:HG13	33:I:58:ILE:HD11	1.99	0.44
25:A:2197:U:O2'	25:A:2198:A:H2'	2.17	0.44
25:A:1266:G:O2'	25:A:2012:G:N1	2.38	0.44
25:A:2121:G:H2'	25:A:2122:U:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1525:A:H2'	25:A:1526:C:O4'	2.17	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
43:S:20:VAL:HG11	43:S:44:ALA:HA	2.00	0.44
25:A:2572:A:C8	28:D:149:ASN:ND2	2.86	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
25:A:1806:C:H1'	27:C:43:ASN:HD21	1.83	0.44
25:A:1278:C:H2'	25:A:1279:G:C8	2.53	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:1563:U:H2'	25:A:1564:C:C6	2.53	0.44
25:A:756:A:H2'	25:A:757:G:O4'	2.17	0.44
25:A:1204:A:H4'	25:A:1205:A:H5''	1.99	0.44
25:A:19:A:H5''	41:Q:21:LYS:HG2	2.00	0.44
25:A:600:G:H2'	25:A:601:C:O4'	2.17	0.44
25:A:1820:U:C2	27:C:200:MET:HB2	2.53	0.44
36:L:57:LEU:HD22	54:3:53:ASP:HB3	1.98	0.44
30:F:97:GLU:HG2	57:6:25:ARG:HB2	1.99	0.44
30:F:1:ALA:H1	30:F:97:GLU:HA	1.81	0.44
30:F:120:SER:HB2	30:F:127:TYR:CE1	2.53	0.44
25:A:232:G:OP2	25:A:232:G:H8	2.01	0.44
25:A:745:1MG:HM11	25:A:745:1MG:HN21	1.67	0.44
25:A:310:A:C2'	25:A:311:A:H5''	2.48	0.44
25:A:1432:G:P	40:P:105:LYS:HG3	53.69	0.44
34:J:7:LYS:HB2	34:J:10:THR:OG1	2.18	0.44
25:A:463:G:N2	25:A:466:A:OP2	2.36	0.44
25:A:909:A:OP1	36:L:17:LYS:HD3	63.52	0.44
25:A:971:G:H2'	25:A:972:A:O4'	2.18	0.44
36:L:95:LEU:HD22	36:L:100:ILE:HD11	1.98	0.44
25:A:1361:G:H2'	25:A:1362:C:C6	2.52	0.44
25:A:278:A:C2	25:A:362:A:H1'	2.53	0.44
25:A:1094:U:H2'	25:A:1096:A:N7	2.33	0.44
25:A:2204:G:H4'	27:C:149:LYS:HD3	1.99	0.44
25:A:2859:G:H2'	25:A:2860:A:C8	2.53	0.44
25:A:1746:A:H2'	25:A:1747:U:C6	2.53	0.44
25:A:490:C:H2'	25:A:491:G:C8	9.34	0.44
25:A:1956:U:C2'	25:A:1957:C:H5'	2.48	0.43
25:A:278:A:N3	25:A:278:A:H2'	2.32	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:1866:A:H2'	25:A:1867:G:O4'	2.18	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:532:A:H2'	25:A:532:A:N3	2.47	0.43
41:Q:5:ARG:HB2	41:Q:8:ILE:HD11	2.00	0.43
30:F:3:LEU:HD13	30:F:96:TRP:HE3	1.83	0.43
25:A:1235:G:C6	25:A:1236:G:N2	2.86	0.43
25:A:546:U:H1'	25:A:548:G:C2	2.53	0.43
33:I:104:GLN:O	33:I:108:ILE:HG13	2.17	0.43
33:I:104:GLN:O	33:I:107:GLU:HB3	2.18	0.43
25:A:2712:C:H3'	25:A:2714:G:H5''	1.99	0.43
50:Z:44:ARG:HD2	50:Z:47:ILE:HD12	1.99	0.43
27:C:149:LYS:HG3	27:C:149:LYS:O	2.91	0.43
37:M:60:GLN:NE2	37:M:108:VAL:HG12	2.33	0.43
25:A:678:C:H2'	25:A:679:C:C6	2.53	0.43
25:A:17:G:H4'	41:Q:24:TYR:HE1	1.83	0.43
25:A:1432:G:O2'	25:A:1433:A:H8	3.82	0.43
25:A:494:G:H4'	43:S:6:LYS:O	2.18	0.43
57:6:58:ASP:OD1	57:6:58:ASP:N	2.49	0.43
28:D:85:ALA:C	28:D:87:GLY:H	2.22	0.43
30:F:153:ILE:H	30:F:153:ILE:HD12	1.82	0.43
27:C:86:ARG:HD3	27:C:104:LEU:HD21	2.01	0.43
45:U:83:GLY:O	45:U:93:ARG:HA	2.19	0.43
25:A:2730:C:O2'	25:A:2731:G:H5'	2.18	0.43
29:E:102:ARG:NH1	29:E:200:LEU:O	2.51	0.43
25:A:2112:G:H5'	25:A:2113:U:C5	2.53	0.43
25:A:1679:A:H2'	25:A:1680:U:C6	2.54	0.43
25:A:2783:U:H2'	25:A:2784:U:C6	2.52	0.43
30:F:24:VAL:O	30:F:27:VAL:HG12	2.17	0.43
46:V:30:ILE:HG12	46:V:91:PHE:HB2	2.00	0.43
25:A:249:C:O2	54:3:11:LYS:NZ	2.51	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
25:A:1872:A:H2'	25:A:1873:G:O4'	2.18	0.43
25:A:2884:U:C6	51:0:49:ARG:HG2	2.53	0.43
25:A:1637:A:H5'	25:A:1760:C:O2'	2.18	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:207:A:H2'	25:A:208:C:O4'	2.19	0.43
34:J:37:ARG:NH2	34:J:110:PRO:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:102:GLU:HG3	34:J:119:PHE:CZ	2.52	0.43
33:I:11:GLN:NE2	33:I:56:VAL:HG12	2.34	0.43
25:A:2066:C:O2'	25:A:2067:G:H5'	2.18	0.43
25:A:571:U:OP1	25:A:819:A:O2'	20.54	0.43
36:L:135:ILE:HB	36:L:142:ILE:HD11	2.01	0.43
25:A:1509:A:H2'	25:A:1510:G:H8	1.82	0.43
25:A:900:A:H2'	25:A:901:C:O4'	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:1996:C:H4'	25:A:1997:C:OP1	2.19	0.43
25:A:2837:A:H2'	25:A:2838:G:C8	2.54	0.43
25:A:938:G:H2'	25:A:939:G:H8	1.83	0.43
25:A:2590:A:H2'	25:A:2591:C:C6	2.54	0.43
56:5:57:ASN:ND2	56:5:63:ALA:HB2	2.33	0.43
55:4:30:GLU:HA	55:4:31:PRO:HD3	1.89	0.43
25:A:63:A:H2'	25:A:64:A:C8	2.53	0.43
25:A:2526:G:H2'	25:A:2527:C:H6	1.83	0.43
25:A:1980:G:O2'	25:A:1982:U:OP2	2.26	0.43
25:A:2567:G:H2'	25:A:2568:U:C6	2.54	0.43
25:A:2347:C:H2'	25:A:2348:U:C6	2.54	0.43
36:L:62:PRO:HG2	54:3:24:LYS:HB3	1.99	0.43
25:A:2286:G:H5''	25:A:2287:A:OP1	2.18	0.43
43:S:23:LEU:HD22	51:0:23:ALA:HB2	2.00	0.43
25:A:2884:U:C5	51:0:49:ARG:HG2	2.54	0.43
25:A:723:C:H2'	25:A:724:U:O4'	2.19	0.43
25:A:1378:A:C4	25:A:1380:G:N7	2.87	0.43
28:D:16:THR:OG1	28:D:20:VAL:O	2.24	0.43
25:A:2619:C:O2'	25:A:2620:C:H5'	2.19	0.43
29:E:178:VAL:O	29:E:182:ALA:HB2	2.19	0.43
41:Q:107:ALA:O	42:R:48:LYS:HE3	2.19	0.43
56:5:40:GLU:O	56:5:43:LYS:HB3	2.18	0.43
37:M:69:PRO:HA	37:M:94:ALA:HB2	2.00	0.43
34:J:31:GLU:HG2	34:J:142:ILE:HG12	2.01	0.43
25:A:2848:G:O2'	25:A:2849:U:H5'	2.18	0.43
25:A:476:G:H4'	25:A:502:A:N1	2.34	0.43
25:A:249:C:O2'	36:L:63:LYS:NZ	2.30	0.43
25:A:242:G:N7	54:3:4:LYS:HG2	2.34	0.43
25:A:1386:C:H2'	25:A:1387:A:H8	1.81	0.43
30:F:39:VAL:C	30:F:41:GLU:H	2.22	0.43
25:A:2141:G:H2'	25:A:2142:A:H8	1.84	0.43
25:A:1070:A:H4'	25:A:1071:G:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:56:VAL:HB	34:J:124:VAL:HG12	1.99	0.43
25:A:364:C:H2'	25:A:365:U:C6	2.54	0.43
51:O:28:SER:O	51:O:36:LYS:HA	2.18	0.43
25:A:1421:G:C2	25:A:1422:G:C8	3.07	0.43
28:D:35:THR:HG1	28:D:49:GLN:HG2	1.81	0.43
25:A:2728:U:H2'	25:A:2729:G:H8	1.84	0.43
46:V:6:ALA:HB2	46:V:42:LEU:HB3	2.01	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
57:6:39:LYS:O	57:6:40:CYS:CB	2.67	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:1788:C:O2'	25:A:1789:A:H5'	2.19	0.43
25:A:2466:C:OP1	55:4:4:ARG:HB3	2.18	0.43
25:A:1469:A:H2'	25:A:1470:A:C8	2.54	0.43
51:O:6:LYS:HA	51:O:7:PRO:HD3	1.87	0.43
25:A:2038:G:H2'	25:A:2039:U:O4'	2.19	0.43
25:A:1754:A:N1	25:A:2716:C:O2'	2.36	0.43
44:T:64:LYS:HD2	44:T:64:LYS:N	2.34	0.43
25:A:1936:A:H2	25:A:1943:U:N3	2.09	0.42
25:A:1129:A:HO2'	25:A:2515:C:HO2'	1.67	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
48:X:4:CYS:HA	48:X:32:LEU:HD21	2.01	0.42
25:A:191:A:H2'	25:A:192:C:C6	2.54	0.42
25:A:1204:A:H4'	25:A:1205:A:C5'	2.49	0.42
48:X:31:ASN:O	48:X:51:SER:HA	2.19	0.42
25:A:1726:C:H2'	25:A:1727:C:C6	2.54	0.42
25:A:2684:U:O4'	35:K:70:ARG:NH1	2.52	0.42
25:A:2494:G:O2'	37:M:79:ALA:HA	2.18	0.42
25:A:1022:G:N2	25:A:1142:A:C2	2.87	0.42
45:U:40:LEU:HD23	45:U:61:GLU:HG3	2.01	0.42
56:5:71:CYS:HB3	56:5:117:LEU:HD12	2.02	0.42
33:I:92:PRO:HB2	33:I:93:ASN:H	1.73	0.42
46:V:2:PHE:HA	46:V:50:MET:HE1	2.01	0.42
25:A:278:A:H2	25:A:362:A:H1'	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:5:18:VAL:HG11	56:5:70:GLU:HB3	2.01	0.42
31:G:82:PHE:O	31:G:133:LYS:HA	2.19	0.42
25:A:2682:A:H61	25:A:2728:U:C1'	2.27	0.42
25:A:189:G:H2'	25:A:205:G:N2	2.34	0.42
25:A:1028:A:N3	25:A:2486:C:O2'	2.42	0.42
25:A:1816:C:H3'	27:C:61:TYR:CE1	2.54	0.42
27:C:179:GLU:HG3	27:C:269:ARG:HA	2.00	0.42
25:A:1201:U:H2'	25:A:1202:G:C8	2.55	0.42
25:A:2530:A:N6	31:G:155:PRO:HG3	2.34	0.42
25:A:2572:A:H2'	28:D:149:ASN:ND2	2.34	0.42
25:A:297:G:N2	25:A:300:A:OP2	13.50	0.42
25:A:182:A:H2'	25:A:183:C:O4'	2.18	0.42
26:B:85:G:H2'	26:B:86:G:H8	1.84	0.42
25:A:2415:G:H2'	25:A:2416:C:C6	2.55	0.42
42:R:33:VAL:HG23	42:R:61:ALA:HB3	2.01	0.42
25:A:789:A:C6	53:2:3:ARG:NH1	2.88	0.42
34:J:35:ARG:HD3	34:J:40:HIS:CD2	2.54	0.42
41:Q:57:ARG:NH1	41:Q:61:ILE:HD11	2.34	0.42
28:D:101:PHE:HA	28:D:104:VAL:HG22	2.02	0.42
25:A:413:C:H2'	25:A:414:C:H6	1.85	0.42
25:A:158:U:O2	25:A:169:G:N2	2.52	0.42
35:K:108:ARG:NH1	35:K:116:ILE:HD13	2.34	0.42
25:A:751:A:HO2'	25:A:752:A:H2	1.67	0.42
52:1:32:LYS:HB3	52:1:50:GLU:HB3	2.01	0.42
45:U:88:ASP:CG	45:U:89:GLY:H	2.21	0.42
25:A:816:C:H2'	25:A:817:C:C6	2.54	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
31:G:51:PHE:CE1	31:G:71:LEU:HD22	2.54	0.42
44:T:38:ALA:HA	44:T:42:GLU:OE1	2.19	0.42
25:A:118:A:H2'	25:A:120:U:O4	2.19	0.42
30:F:48:LEU:HA	30:F:51:ASN:ND2	2.34	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
41:Q:78:PHE:HE1	41:Q:109:VAL:HA	1.85	0.42
30:F:92:GLY:N	30:F:95:MET:HG2	2.34	0.42
44:T:33:LYS:HG2	44:T:80:TRP:CZ3	2.55	0.42
25:A:1529:G:H2'	25:A:1530:G:O4'	2.20	0.42
25:A:811:U:C4	36:L:21:ARG:NH2	2.87	0.42
25:A:783:A:H2'	25:A:784:G:H4'	2.02	0.42
25:A:1366:A:H2'	25:A:1367:A:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S:84:ARG:HB2	43:S:96:ILE:HG13	2.00	0.42
34:J:4:PHE:HE2	34:J:43:GLU:HB2	1.84	0.42
25:A:2398:U:H2'	25:A:2399:G:C8	2.54	0.42
25:A:1486:U:O2'	25:A:1487:U:H5'	2.19	0.42
25:A:17:G:H4'	41:Q:24:TYR:CE1	2.54	0.42
30:F:134:GLN:OE1	30:F:147:ARG:O	2.36	0.42
25:A:2682:A:N6	25:A:2728:U:H1'	2.30	0.42
36:L:17:LYS:HE3	36:L:27:LEU:CD2	2.50	0.42
38:N:67:PHE:O	38:N:71:ARG:HD2	2.19	0.42
25:A:2637:U:H2'	25:A:2638:G:O4'	2.19	0.42
25:A:1796:U:H2'	25:A:1797:G:H8	1.84	0.42
37:M:66:ARG:HG3	37:M:101:VAL:HG12	2.02	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:2040:G:H2'	25:A:2041:U:O4'	2.20	0.42
42:R:16:GLU:HB2	42:R:101:ILE:HG12	2.01	0.42
32:H:132:PHE:HB2	32:H:140:ALA:HB3	2.02	0.42
25:A:2016:U:H1'	51:O:2:VAL:HG13	2.01	0.42
25:A:848:C:H2'	25:A:849:A:C8	2.55	0.42
32:H:114:GLU:OE1	32:H:114:GLU:N	2.51	0.42
25:A:2648:G:N2	25:A:2673:G:H1'	2.35	0.42
25:A:779:U:P	27:C:48:ILE:HG22	2.60	0.42
25:A:190:A:OP2	48:X:25:LYS:NZ	2.53	0.42
25:A:935:C:O2'	25:A:936:A:H5'	2.19	0.42
31:G:41:GLU:HB2	31:G:54:ARG:HE	1.85	0.42
25:A:1747:U:H2'	25:A:1748:C:C6	2.55	0.42
25:A:706:A:H2'	25:A:707:G:O4'	2.20	0.42
25:A:995:C:O2'	41:Q:92:LYS:HE2	2.20	0.42
25:A:2747:G:O6	25:A:2755:C:H5''	2.19	0.42
25:A:335:C:C4'	25:A:1434:A:H4'	118.85	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:1511:G:H2'	25:A:1512:C:C6	2.55	0.42
26:B:78:A:H2'	26:B:79:G:O4'	2.20	0.42
56:5:117:LEU:HD22	56:5:120:ALA:HA	2.02	0.42
25:A:2556:C:H2'	25:A:2557:G:O4'	2.20	0.42
56:5:49:GLY:H	56:5:51:TYR:HE2	1.68	0.42
25:A:2545:G:H2'	25:A:2546:U:O4'	2.20	0.42
25:A:813:U:H2'	25:A:814:C:C6	2.55	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

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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
30:F:132:ARG:O	30:F:150:GLY:HA3	2.19	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
25:A:1993:U:H4'	28:D:133:THR:HG22	2.02	0.42
27:C:259:ASN:O	27:C:261:ARG:N	2.47	0.42
25:A:1078:U:H4'	25:A:1079:C:H5''	2.02	0.41
32:H:84:ALA:HB2	32:H:90:LEU:HD12	2.02	0.41
25:A:2709:G:H2'	25:A:2710:C:C6	2.55	0.41
27:C:2:VAL:HG21	27:C:201:LEU:HD12	2.02	0.41
39:O:33:ARG:HG2	39:O:34:HIS:CD2	2.55	0.41
25:A:2391:G:H5''	54:3:31:ILE:HD12	2.02	0.41
29:E:97:ASN:O	29:E:100:MET:N	2.51	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
33:I:72:THR:HG21	33:I:112:LYS:HB3	2.02	0.41
52:1:10:LEU:HD23	52:1:50:GLU:HA	2.02	0.41
25:A:1265:A:H3'	51:0:15:ARG:HH11	1.85	0.41
25:A:594:U:H2'	25:A:595:C:C6	2.54	0.41
25:A:1447:C:H2'	25:A:1448:G:C8	2.55	0.41
25:A:1023:U:H4'	25:A:1123:C:OP1	2.21	0.41
54:3:29:ARG:HA	54:3:29:ARG:HD3	1.76	0.41
29:E:122:GLU:HB2	29:E:123:LYS:H	1.68	0.41
25:A:84:A:N7	25:A:101:A:H2	2.18	0.41
28:D:110:THR:HG21	28:D:169:ARG:HH11	1.85	0.41
26:B:16:G:C6	26:B:17:C:C4	3.08	0.41
25:A:366:C:H2'	25:A:367:G:O4'	2.19	0.41
25:A:1847:G:O2'	25:A:1848:A:H8	2.03	0.41
37:M:33:LEU:HD12	37:M:129:THR:O	2.20	0.41
25:A:2064:C:H2'	25:A:2065:C:C6	2.55	0.41
35:K:36:GLY:HA2	35:K:62:VAL:O	2.19	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
25:A:2746:U:H5''	31:G:137:LYS:HG2	2.01	0.41
25:A:2287:A:C6	25:A:2289:G:C5	3.07	0.41
25:A:2844:G:H2'	25:A:2845:U:O4'	2.20	0.41
56:5:43:LYS:HE2	56:5:43:LYS:HB3	1.84	0.41
25:A:2039:U:H2'	25:A:2040:G:C8	2.55	0.41
41:Q:109:VAL:HG12	41:Q:113:LYS:HE2	2.01	0.41
25:A:97:C:H2'	25:A:98:G:O4'	2.19	0.41
25:A:426:C:H2'	25:A:427:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1717:A:H2'	25:A:1718:G:O4'	2.19	0.41
45:U:52:ASN:OD1	45:U:54:PRO:HD3	2.19	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
26:B:13:G:O2'	26:B:15:A:H2'	2.19	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
25:A:507:A:H5''	25:A:508:A:H3'	2.02	0.41
25:A:1752:C:H2'	25:A:1753:G:C8	2.56	0.41
44:T:8:LEU:HA	44:T:50:LEU:HD21	2.01	0.41
30:F:7:TYR:OH	30:F:29:ARG:HB3	2.20	0.41
56:5:24:SER:HA	56:5:85:SER:O	2.19	0.41
28:D:151:THR:HB	28:D:152:PRO:HD3	2.01	0.41
25:A:2756:U:H1'	25:A:2757:A:H5''	2.02	0.41
25:A:1736:U:H2'	25:A:1737:G:O4'	2.20	0.41
25:A:2572:A:H5''	25:A:2574:G:H4'	2.02	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
25:A:1801:A:H5'	25:A:2203:U:O2'	2.20	0.41
36:L:23:ILE:H	36:L:23:ILE:HD12	1.84	0.41
25:A:758:C:O2	25:A:758:C:H2'	2.20	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
25:A:1045:C:H5'	25:A:1046:A:C5'	2.50	0.41
25:A:1180:U:H2'	25:A:1181:U:H5'	2.02	0.41
25:A:2283:C:OP2	25:A:2390:U:C5	2.72	0.41
25:A:1112:G:H2'	25:A:1113:U:H6	1.86	0.41
25:A:2230:G:H2'	25:A:2231:U:C6	2.56	0.41
32:H:66:ASN:HB3	32:H:134:VAL:O	2.20	0.41
38:N:38:LEU:HG	38:N:42:LYS:HE2	2.03	0.41
43:S:34:ASP:HB3	51:O:27:LEU:HD22	2.03	0.41
25:A:1789:A:OP2	27:C:220:ARG:NH2	2.46	0.41
54:3:36:ALA:O	54:3:39:ARG:HB2	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
26:B:54:G:H2'	26:B:55:U:C6	2.56	0.41
40:P:3:ILE:HD12	40:P:3:ILE:H	1.86	0.41
25:A:753:A:H2'	25:A:754:U:C6	2.56	0.41
25:A:859:G:H1'	25:A:860:U:H5	1.85	0.41
44:T:8:LEU:HD11	49:Y:22:LEU:HD12	2.03	0.41
27:C:24:HIS:HB3	27:C:81:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:T:37:ASP:OD1	44:T:38:ALA:N	2.54	0.41
25:A:1067:A:H4'	25:A:1068:G:O5'	4.70	0.41
57:6:26:SER:OG	57:6:27:THR:N	2.53	0.41
25:A:2599:G:C8	27:C:235:GLU:HG2	2.56	0.41
36:L:123:ARG:HA	36:L:143:GLU:O	2.20	0.41
34:J:17:VAL:HG22	34:J:55:ILE:HB	2.02	0.41
32:H:9:VAL:HG12	32:H:11:ASN:H	1.85	0.41
25:A:2298:A:OP1	30:F:70:ARG:NH2	2.52	0.41
25:A:2092:U:H4'	25:A:2093:G:O5'	2.20	0.41
39:O:92:PHE:HB2	39:O:117:PHE:CE1	2.56	0.41
25:A:2368:C:H2'	25:A:2369:A:H8	1.86	0.41
25:A:1826:G:OP1	27:C:222:THR:HG23	2.19	0.41
25:A:993:G:N3	25:A:993:G:H2'	3.04	0.41
25:A:919:U:H2'	25:A:920:A:O4'	2.19	0.41
25:A:1140:C:P	34:J:68:LYS:HZ2	2.44	0.41
25:A:456:C:C2	44:T:73:ARG:NH2	2.87	0.41
25:A:687:C:H5''	53:2:2:LYS:NZ	2.35	0.41
38:N:54:LEU:HD21	38:N:65:LEU:HB3	2.02	0.41
33:I:20:SER:HA	33:I:24:GLY:HA3	2.02	0.41
25:A:1319:C:H2'	25:A:1320:C:O4'	2.20	0.41
25:A:857:G:H2'	25:A:858:G:O4'	2.21	0.41
25:A:2285:C:O2'	25:A:2287:A:H1'	2.20	0.41
25:A:1957:C:H2'	25:A:1958:C:C6	2.56	0.41
43:S:14:ALA:HB1	43:S:18:ARG:HH21	1.85	0.41
53:2:21:ARG:O	53:2:27:GLY:HA3	2.21	0.41
26:B:48:U:H2'	26:B:49:C:C6	2.56	0.41
25:A:1591:A:H2'	25:A:1592:C:O4'	2.21	0.41
25:A:21:A:H2'	25:A:22:C:O4'	2.21	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
27:C:78:GLU:HB3	27:C:92:LEU:O	2.21	0.41
28:D:20:VAL:HG22	35:K:72:PRO:HB2	2.03	0.41
38:N:82:GLU:O	38:N:86:ARG:HB2	2.21	0.41
25:A:1741:C:H2'	25:A:1742:U:C6	2.56	0.41
25:A:1292:G:H2'	25:A:1293:C:C6	2.56	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:1943:U:H1'	25:A:1945:G:OP2	2.20	0.41
26:B:43:C:O2'	30:F:91:ARG:HG2	2.20	0.41
39:O:52:SER:OG	39:O:54:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4:7:VAL:HG22	55:4:38:GLY:HA3	2.03	0.41
25:A:2697:G:H2'	25:A:2698:U:O4'	2.21	0.41
25:A:490:C:H4'	25:A:491:G:OP2	2.21	0.41
28:D:148:GLN:HB2	28:D:152:PRO:HG2	2.03	0.41
25:A:2803:G:H2'	25:A:2804:U:C6	2.56	0.41
48:X:12:VAL:HG23	48:X:28:PHE:HB2	2.03	0.41
25:A:2106:U:H2'	25:A:2107:G:C8	2.56	0.41
25:A:275:C:H3'	25:A:276:U:H5''	2.03	0.41
25:A:737:C:H2'	25:A:738:G:O4'	2.21	0.41
25:A:460:A:H2'	25:A:461:C:O4'	2.20	0.41
29:E:128:ALA:O	29:E:130:LYS:N	2.51	0.41
54:3:51:LYS:HB2	54:3:51:LYS:HE3	1.87	0.41
25:A:306:U:H2'	25:A:307:G:O4'	2.21	0.40
53:2:34:ARG:HE	53:2:39:ARG:HD2	1.86	0.40
25:A:2030:6MZ:C2	25:A:2499:C:H5''	2.51	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
27:C:70:LYS:HD2	27:C:73:ILE:HD12	2.02	0.40
49:Y:28:LEU:HD13	49:Y:42:LEU:HB3	2.03	0.40
30:F:175:PRO:HB2	30:F:176:PHE:H	1.71	0.40
27:C:104:LEU:HD23	27:C:104:LEU:HA	1.89	0.40
25:A:608:A:H2'	25:A:609:A:O4'	2.41	0.40
28:D:43:ASP:HB3	28:D:45:TYR:CE2	2.55	0.40
57:6:2:LYS:O	57:6:5:ILE:HG12	2.21	0.40
25:A:2475:C:O5'	25:A:2475:C:H6	2.04	0.40
25:A:310:A:O2'	25:A:311:A:H5''	2.20	0.40
46:V:30:ILE:HG21	46:V:70:ILE:HG21	2.02	0.40
25:A:218:A:OP2	25:A:218:A:C8	2.67	0.40
25:A:1454:C:H5'	38:N:63:ARG:NH2	2.36	0.40
33:I:129:GLU:O	33:I:132:ALA:HB3	2.21	0.40
25:A:844:A:N6	25:A:934:U:H3	2.19	0.40
25:A:1884:G:H5'	25:A:1885:A:OP1	2.19	0.40
25:A:869:G:H1'	37:M:8:LYS:HD2	2.02	0.40
25:A:2804:U:H2'	25:A:2805:C:C6	2.56	0.40
25:A:1730:C:O2	25:A:1731:G:N1	2.54	0.40
25:A:1132:U:H3'	25:A:1132:U:OP2	2.21	0.40
25:A:2825:G:N3	25:A:2825:G:H5''	2.36	0.40
42:R:14:VAL:CG2	42:R:98:ILE:HG13	2.43	0.40
55:4:5:ALA:O	55:4:38:GLY:HA2	2.21	0.40
25:A:633:A:C2'	25:A:634:C:H5'	2.50	0.40
41:Q:71:ASN:N	41:Q:71:ASN:ND2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2408:U:H2'	25:A:2409:G:C8	2.56	0.40
30:F:137:PHE:HA	30:F:138:PRO:HD3	1.77	0.40
25:A:1418:G:N1	25:A:1579:A:OP2	2.44	0.40
25:A:736:C:H2'	25:A:737:C:C6	2.82	0.40
31:G:88:LEU:HG	31:G:161:VAL:HG22	2.03	0.40
25:A:1824:G:O3'	27:C:246:PRO:HD3	2.21	0.40
49:Y:4:LYS:HG2	49:Y:7:ARG:HH22	1.87	0.40
25:A:1495:A:O5'	25:A:1495:A:H8	2.04	0.40
25:A:1078:U:O2'	25:A:1088:A:H5''	2.22	0.40
25:A:1045:C:H1'	25:A:1047:G:N3	2.36	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
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
25:A:1096:A:H2'	25:A:1097:U:O5'	2.22	0.40
29:E:159:LEU:C	29:E:161:ALA:H	2.25	0.40
41:Q:34:ALA:O	41:Q:38:VAL:HG23	2.21	0.40
41:Q:106:THR:O	41:Q:110:GLU:HG2	2.21	0.40
25:A:2108:A:H2'	25:A:2109:U:O4'	2.21	0.40
25:A:1665:A:H2'	25:A:1666:G:O4'	2.21	0.40
25:A:1560:G:OP2	25:A:1560:G:H8	2.05	0.40
25:A:335:C:C4'	25:A:1434:A:C4'	117.92	0.40
25:A:1936:A:N6	25:A:1963:U:N3	2.69	0.40
38:N:56:LYS:HZ2	38:N:88:ALA:HA	1.86	0.40
27:C:16:VAL:H	27:C:203:VAL:HG22	1.84	0.40
26:B:17:C:H2'	26:B:18:G:O4'	2.22	0.40
25:A:1857:G:O2'	25:A:1858:A:H8	2.04	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
40:P:21:PRO:HD3	40:P:49:ILE:HD12	2.04	0.40
57:6:39:LYS:O	57:6:40:CYS:SG	2.80	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
56:5:107:GLU:O	56:5:109:LYS:N	2.55	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	33
3	d	203/206 (98%)	172 (85%)	21 (10%)	10 (5%)	3	32
4	e	155/167 (93%)	130 (84%)	16 (10%)	9 (6%)	2	28
5	f	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	2	27
6	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	7	49
7	k	114/129 (88%)	92 (81%)	16 (14%)	6 (5%)	2	30
8	l	121/124 (98%)	96 (79%)	20 (16%)	5 (4%)	3	36
9	o	86/89 (97%)	71 (83%)	10 (12%)	5 (6%)	2	28
10	p	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	7	48
11	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	2	26
12	r	63/75 (84%)	53 (84%)	5 (8%)	5 (8%)	1	19
13	t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	7	49
14	u	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1	19
17	w	637/639 (100%)	562 (88%)	51 (8%)	24 (4%)	4	38
18	c	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	19	64
19	g	149/179 (83%)	124 (83%)	15 (10%)	10 (7%)	1	25
20	i	125/130 (96%)	98 (78%)	19 (15%)	8 (6%)	2	26
21	j	96/103 (93%)	74 (77%)	16 (17%)	6 (6%)	2	26
22	m	112/118 (95%)	99 (88%)	8 (7%)	5 (4%)	3	33
23	n	99/102 (97%)	82 (83%)	12 (12%)	5 (5%)	2	31
24	s	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
27	C	269/273 (98%)	242 (90%)	22 (8%)	5 (2%)	10	53
28	D	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	19	64
29	E	199/201 (99%)	172 (86%)	20 (10%)	7 (4%)	4	41
30	F	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	5	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	G	174/177 (98%)	148 (85%)	21 (12%)	5 (3%)	6	45
32	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	6	46
33	I	139/142 (98%)	110 (79%)	20 (14%)	9 (6%)	1	26
34	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	14	58
35	K	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	7	48
36	L	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1	20
37	M	134/136 (98%)	117 (87%)	14 (10%)	3 (2%)	8	50
38	N	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	7	48
39	O	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	21	65
40	P	112/115 (97%)	93 (83%)	18 (16%)	1 (1%)	21	65
41	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
42	R	101/103 (98%)	81 (80%)	18 (18%)	2 (2%)	9	52
43	S	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	29
44	T	91/100 (91%)	77 (85%)	11 (12%)	3 (3%)	5	42
45	U	100/104 (96%)	81 (81%)	16 (16%)	3 (3%)	5	44
46	V	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	8	50
47	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	14	58
48	X	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	15	59
49	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	12	56
50	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
51	0	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	10	53
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%)	12	56
55	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
56	5	129/165 (78%)	100 (78%)	22 (17%)	7 (5%)	2	30
57	6	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	12	56
58	7	67/69 (97%)	58 (87%)	8 (12%)	1 (2%)	13	57
All	All	6551/6928 (95%)	5610 (86%)	716 (11%)	225 (3%)	8	42

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%)	51	79
3	d	172/173 (99%)	166 (96%)	6 (4%)	43	76
4	e	114/126 (90%)	105 (92%)	9 (8%)	15	54
5	f	87/116 (75%)	83 (95%)	4 (5%)	33	70
6	h	104/105 (99%)	103 (99%)	1 (1%)	82	91
7	k	89/99 (90%)	87 (98%)	2 (2%)	60	84
8	l	103/104 (99%)	100 (97%)	3 (3%)	50	79
9	o	76/77 (99%)	74 (97%)	2 (3%)	54	81
10	p	65/65 (100%)	61 (94%)	4 (6%)	23	62
11	q	74/78 (95%)	71 (96%)	3 (4%)	37	73
12	r	48/65 (74%)	47 (98%)	1 (2%)	61	85
13	t	65/66 (98%)	63 (97%)	2 (3%)	47	78
14	u	44/61 (72%)	42 (96%)	2 (4%)	34	71

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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%)	37	73
19	g	124/147 (84%)	122 (98%)	2 (2%)	70	88
20	i	105/107 (98%)	100 (95%)	5 (5%)	31	69
21	j	86/90 (96%)	84 (98%)	2 (2%)	58	83
22	m	92/96 (96%)	90 (98%)	2 (2%)	60	84
23	n	79/84 (94%)	75 (95%)	4 (5%)	29	68
24	s	70/79 (89%)	69 (99%)	1 (1%)	74	89
27	C	216/218 (99%)	208 (96%)	8 (4%)	41	75
28	D	164/164 (100%)	161 (98%)	3 (2%)	66	87
29	E	165/165 (100%)	160 (97%)	5 (3%)	48	78
30	F	148/150 (99%)	141 (95%)	7 (5%)	32	70
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%)	51	79
34	J	116/116 (100%)	114 (98%)	2 (2%)	68	88
35	K	103/104 (99%)	98 (95%)	5 (5%)	31	69
36	L	102/103 (99%)	100 (98%)	2 (2%)	63	86
37	M	109/109 (100%)	108 (99%)	1 (1%)	84	92
38	N	100/103 (97%)	98 (98%)	2 (2%)	63	86
39	O	86/87 (99%)	84 (98%)	2 (2%)	58	83
40	P	99/100 (99%)	96 (97%)	3 (3%)	48	78
41	Q	89/90 (99%)	87 (98%)	2 (2%)	60	84
42	R	84/84 (100%)	83 (99%)	1 (1%)	78	90
43	S	93/93 (100%)	90 (97%)	3 (3%)	46	78
44	T	80/84 (95%)	77 (96%)	3 (4%)	40	74
45	U	83/85 (98%)	82 (99%)	1 (1%)	78	90
46	V	78/78 (100%)	77 (99%)	1 (1%)	76	89
47	W	57/63 (90%)	56 (98%)	1 (2%)	66	87
48	X	67/68 (98%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	54 (98%)	1 (2%)	66	87

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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%)	35	72
52	1	45/49 (92%)	44 (98%)	1 (2%)	60	84
53	2	38/38 (100%)	38 (100%)	0	100	100
54	3	51/52 (98%)	50 (98%)	1 (2%)	63	86
55	4	34/34 (100%)	34 (100%)	0	100	100
56	5	100/123 (81%)	97 (97%)	3 (3%)	48	78
57	6	59/62 (95%)	58 (98%)	1 (2%)	68	88
All	All	4829/5638 (86%)	4698 (97%)	131 (3%)	56	80

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%)	91 (3%)
26	B	119/120 (99%)	17 (14%)	4 (3%)
All	All	4632/4651 (99%)	830 (17%)	95 (2%)

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

All (95) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	51	G
25	A	86	G
25	A	204	A
25	A	227	A
25	A	242	G
25	A	265	A
25	A	271	G
25	A	301	G
25	A	311	A
25	A	321	U
25	A	332	A
25	A	345	A
25	A	372	G
25	A	386	G
25	A	390	U
25	A	446	G
25	A	454	A
25	A	458	G
25	A	479	A

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Mol	Chain	Res	Type
25	A	480	A
25	A	490	C
25	A	503	A
25	A	530	G
25	A	549	G
25	A	571	U
25	A	637	A
25	A	685	A
25	A	686	U
25	A	747	5MC
25	A	752	A
25	A	774	G
25	A	776	G
25	A	800	A
25	A	830	G
25	A	858	G
25	A	859	G
25	A	974	G
25	A	1012	U
25	A	1020	A
25	A	1022	G
25	A	1070	A
25	A	1089	A
25	A	1111	A
25	A	1124	G
25	A	1130	U
25	A	1133	A
25	A	1134	A
25	A	1141	U
25	A	1142	A
25	A	1182	G
25	A	1190	G
25	A	1210	G
25	A	1212	G
25	A	1275	A
25	A	1288	G
25	A	1300	G
25	A	1331	G
25	A	1378	A
25	A	1399	C
25	A	1432	G
25	A	1626	A

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Mol	Chain	Res	Type
25	A	1693	U
25	A	1713	A
25	A	1783	A
25	A	1799	G
25	A	1857	G
25	A	1930	G
25	A	1940	U
25	A	2060	A
25	A	2092	U
25	A	2197	U
25	A	2210	U
25	A	2282	G
25	A	2286	G
25	A	2296	U
25	A	2326	C
25	A	2333	A
25	A	2391	G
25	A	2405	G
25	A	2406	A
25	A	2517	C
25	A	2518	A
25	A	2566	A
25	A	2614	A
25	A	2655	G
25	A	2712	C
25	A	2756	U
25	A	2798	U
25	A	2808	G
25	A	2820	A
25	A	2866	U
26	B	24	G
26	B	56	G
26	B	66	A
26	B	88	C

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	6MZ	A	1618	25	17,25,26	1.11	1 (5%)	15,36,39	2.55	2 (13%)
25	2MG	A	1835	25	18,26,27	0.91	2 (11%)	21,38,41	2.08	6 (28%)
25	PSU	A	1911	25	15,21,22	1.45	1 (6%)	16,30,33	2.11	4 (25%)
25	3TD	A	1915	25	15,22,23	1.29	3 (20%)	17,32,35	1.57	3 (17%)
25	PSU	A	1917	25	15,21,22	1.42	1 (6%)	16,30,33	2.30	4 (25%)
25	5MU	A	1939	25	13,22,23	0.72	1 (7%)	16,32,35	2.33	2 (12%)
25	5MC	A	1962	25	14,22,23	1.33	1 (7%)	17,32,35	0.99	1 (5%)
25	6MZ	A	2030	25	17,25,26	1.03	1 (5%)	15,36,39	2.87	3 (20%)
25	7MG	A	2069	25	20,26,27	1.17	2 (10%)	23,39,42	3.18	6 (26%)
25	OMG	A	2251	25,15	18,26,27	0.94	2 (11%)	21,38,41	2.09	4 (19%)
25	2MG	A	2445	25	18,26,27	0.88	2 (11%)	21,38,41	2.34	7 (33%)
25	H2U	A	2449	25	17,21,22	0.96	2 (11%)	23,30,33	2.05	5 (21%)
25	PSU	A	2457	25	15,21,22	1.80	1 (6%)	16,30,33	2.20	4 (25%)
25	OMC	A	2498	25	15,22,23	0.78	1 (6%)	20,31,34	1.44	1 (5%)
25	2MA	A	2503	25	17,25,26	1.58	3 (17%)	18,37,40	2.71	1 (5%)
25	PSU	A	2504	25	15,21,22	1.52	1 (6%)	16,30,33	2.41	4 (25%)
25	OMU	A	2552	25	14,22,23	0.69	0	19,31,34	1.49	1 (5%)
25	PSU	A	2580	25	15,21,22	1.68	2 (13%)	16,30,33	2.20	3 (18%)
25	PSU	A	2604	25	15,21,22	1.60	2 (13%)	16,30,33	2.47	4 (25%)
25	PSU	A	2605	25	15,21,22	1.26	2 (13%)	16,30,33	2.38	4 (25%)
25	1MG	A	745	25	17,26,27	1.50	3 (17%)	19,39,42	0.84	0
25	PSU	A	746	25	15,21,22	1.38	1 (6%)	16,30,33	2.11	3 (18%)
25	5MC	A	747	25	14,22,23	1.36	1 (7%)	17,32,35	1.36	3 (17%)
25	PSU	A	955	25	15,21,22	1.62	4 (26%)	16,30,33	2.27	4 (25%)
1	2MG	a	1207	1	18,26,27	1.19	2 (11%)	21,38,41	2.22	6 (28%)
1	4OC	a	1402	1	15,23,24	1.74	4 (26%)	21,32,35	2.79	10 (47%)
1	5MC	a	1407	1	14,22,23	1.27	1 (7%)	17,32,35	1.00	1 (5%)
1	UR3	a	1498	1	13,22,23	0.68	0	18,32,35	0.75	0
1	2MG	a	1516	1	18,26,27	1.22	2 (11%)	21,38,41	2.28	6 (28%)
1	MA6	a	1518	1	18,26,27	1.11	1 (5%)	15,38,41	2.45	2 (13%)
1	MA6	a	1519	1	18,26,27	0.91	1 (5%)	15,38,41	2.68	4 (26%)
1	PSU	a	516	1	15,21,22	1.48	3 (20%)	16,30,33	2.08	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	7MG	a	527	1	20,26,27	1.25	2 (10%)	23,39,42	3.12	6 (26%)
1	2MG	a	966	1	18,26,27	1.14	2 (11%)	21,38,41	2.21	6 (28%)
1	5MC	a	967	1	14,22,23	1.20	1 (7%)	17,32,35	1.08	1 (5%)
15	H2U	v	20	15	17,21,22	0.95	2 (11%)	23,30,33	1.93	4 (17%)
15	5MU	v	54	15	13,22,23	0.57	0	16,32,35	2.40	2 (12%)
15	PSU	v	55	15	15,21,22	1.14	1 (6%)	16,30,33	2.25	4 (25%)
15	4SU	v	8	15	12,21,22	0.69	0	15,30,33	1.07	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2457	PSU	C5-C1'	-6.04	1.47	1.52
25	A	2580	PSU	C5-C1'	-5.38	1.47	1.52
25	A	2604	PSU	C5-C1'	-5.12	1.47	1.52
25	A	955	PSU	C5-C1'	-4.93	1.47	1.52
25	A	2504	PSU	C5-C1'	-4.84	1.48	1.52
25	A	1911	PSU	C5-C1'	-4.50	1.48	1.52
25	A	1917	PSU	C5-C1'	-4.37	1.48	1.52
1	a	516	PSU	C5-C1'	-4.33	1.48	1.52
25	A	746	PSU	C5-C1'	-4.20	1.48	1.52
25	A	2605	PSU	C5-C1'	-3.34	1.49	1.52
15	v	55	PSU	C5-C1'	-3.12	1.49	1.52
25	A	2605	PSU	C2-N3	-2.43	1.33	1.38
25	A	2604	PSU	C2-N3	-2.40	1.33	1.38
25	A	2449	H2U	C4-N3	-2.38	1.33	1.37
15	v	20	H2U	C2-N3	-2.38	1.33	1.38
1	a	516	PSU	O4'-C1'	-2.36	1.40	1.44
15	v	20	H2U	C4-N3	-2.33	1.33	1.37
25	A	2449	H2U	C2-N3	-2.33	1.33	1.38
1	a	516	PSU	C2-N3	-2.22	1.33	1.38
25	A	955	PSU	C2-N3	-2.21	1.33	1.38
25	A	1939	5MU	C2-N3	-2.19	1.33	1.38
25	A	2498	OMC	C6-N1	-2.17	1.33	1.35
25	A	955	PSU	C2-N1	-2.15	1.33	1.38
25	A	1915	3TD	C6-C5	-2.12	1.35	1.38
25	A	2580	PSU	O4'-C1'	-2.11	1.41	1.44
25	A	1915	3TD	C4-N3	-2.10	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	955	PSU	O4'-C1'	-2.04	1.41	1.44
25	A	2445	2MG	C6-C5	2.02	1.45	1.41
1	a	1402	4OC	C2'-C1'	2.05	1.58	1.53
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	2251	OMG	C6-C5	2.56	1.46	1.41
25	A	2251	OMG	C5-C4	2.64	1.46	1.40
25	A	1835	2MG	C6-C5	2.65	1.46	1.41
1	a	1402	4OC	O4'-C1'	2.65	1.45	1.41
25	A	1915	3TD	C10-N3	2.66	1.53	1.47
25	A	2069	7MG	C5-C4	2.69	1.46	1.39
1	a	1402	4OC	C6-C5	2.70	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
1	a	527	7MG	C5-C4	2.98	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
1	a	1516	2MG	C6-C5	3.43	1.48	1.41
1	a	1207	2MG	C6-C5	3.46	1.48	1.41
1	a	966	2MG	C6-C5	3.52	1.48	1.41
25	A	2069	7MG	C6-C5	3.53	1.46	1.41
25	A	2030	6MZ	C5-C4	3.59	1.48	1.40
1	a	527	7MG	C6-C5	3.63	1.46	1.41
25	A	2503	2MA	C6-N6	3.88	1.36	1.29
25	A	1618	6MZ	C5-C4	3.91	1.49	1.40
25	A	2503	2MA	C6-C5	4.01	1.48	1.40
1	a	967	5MC	C5-C4	4.26	1.48	1.41
1	a	1402	4OC	O3'-C3'	4.34	1.53	1.43
25	A	747	5MC	C5-C4	4.35	1.48	1.41
1	a	1407	5MC	C5-C4	4.39	1.48	1.41
25	A	745	1MG	C6-C5	4.46	1.49	1.40
25	A	1962	5MC	C5-C4	4.46	1.48	1.41

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1519	MA6	N3-C2-N1	-8.21	122.42	128.87
1	a	527	7MG	C5-C4-N3	-7.87	118.72	126.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2069	7MG	C5-C4-N3	-7.73	118.86	126.74
1	a	1518	MA6	N3-C2-N1	-7.36	123.09	128.87
25	A	1939	5MU	C5-C4-N3	-6.92	119.54	125.35
15	v	54	5MU	C5-C4-N3	-6.82	119.63	125.35
25	A	1618	6MZ	N3-C2-N1	-6.30	123.92	128.87
25	A	2030	6MZ	N3-C2-N1	-5.99	124.17	128.87
25	A	2449	H2U	C5-C6-N1	-5.94	104.25	110.76
25	A	2604	PSU	C5-C1'-C2'	-5.69	105.77	115.44
25	A	2069	7MG	C5-C6-N1	-5.64	115.00	123.39
25	A	2449	H2U	C4-N3-C2	-5.50	120.78	125.77
1	a	527	7MG	C5-C6-N1	-5.34	115.44	123.39
15	v	20	H2U	C4-N3-C2	-5.29	120.97	125.77
1	a	1402	4OC	C6-N1-C2	-5.23	112.80	121.33
15	v	20	H2U	C5-C6-N1	-5.12	105.15	110.76
25	A	2251	OMG	C5-C6-N1	-5.03	116.94	123.52
25	A	955	PSU	C5-C1'-C2'	-4.91	107.10	115.44
25	A	2445	2MG	C5-C6-N1	-4.47	117.68	123.52
25	A	2604	PSU	C5-C6-N1	-4.39	118.25	124.38
1	a	1516	2MG	C5-C6-N1	-4.37	117.81	123.52
25	A	2580	PSU	C5-C6-N1	-4.31	118.36	124.38
25	A	2605	PSU	C5-C1'-C2'	-4.25	108.22	115.44
25	A	2504	PSU	C5-C1'-C2'	-4.17	108.34	115.44
25	A	2457	PSU	C5-C6-N1	-4.17	118.56	124.38
1	a	1207	2MG	C5-C6-N1	-4.11	118.14	123.52
25	A	1915	3TD	C5-C1'-C2'	-4.01	108.63	115.44
1	a	516	PSU	C5-C6-N1	-4.00	118.80	124.38
25	A	746	PSU	C5-C6-N1	-3.96	118.86	124.38
1	a	966	2MG	C5-C6-N1	-3.91	118.42	123.52
25	A	955	PSU	C5-C6-N1	-3.89	118.95	124.38
25	A	1911	PSU	C5-C6-N1	-3.88	118.97	124.38
25	A	1835	2MG	C5-C6-N1	-3.58	118.84	123.52
25	A	2504	PSU	C5-C6-N1	-3.57	119.40	124.38
25	A	2445	2MG	C6-C5-C4	-3.52	116.84	120.86
25	A	2457	PSU	C5-C1'-C2'	-3.41	109.65	115.44
25	A	1917	PSU	C5-C6-N1	-3.39	119.65	124.38
25	A	1917	PSU	C5-C1'-C2'	-3.36	109.73	115.44
1	a	1402	4OC	CM4-N4-C4	-3.34	120.05	122.87
15	v	8	4SU	C5-C4-N3	-3.34	120.03	123.56
15	v	55	PSU	C5-C6-N1	-3.29	119.79	124.38
25	A	746	PSU	C5-C1'-C2'	-3.28	109.86	115.44
25	A	2251	OMG	N3-C2-N1	-3.24	123.15	127.56
25	A	2605	PSU	C5-C6-N1	-3.23	119.88	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1516	2MG	C6-C5-C4	-3.19	117.21	120.86
1	a	1402	4OC	O4'-C1'-C2'	-3.15	100.94	106.60
25	A	1915	3TD	C5-C6-N1	-3.11	120.04	124.38
25	A	1835	2MG	CM2-N2-C2	-3.06	119.59	123.03
25	A	2030	6MZ	C1'-N9-C4	-3.03	123.43	126.81
1	a	966	2MG	C6-C5-C4	-3.02	117.40	120.86
25	A	2445	2MG	N3-C2-N1	-2.98	121.74	126.19
15	v	55	PSU	C5-C1'-C2'	-2.91	110.49	115.44
1	a	966	2MG	CM2-N2-C2	-2.90	119.78	123.03
25	A	1835	2MG	C6-C5-C4	-2.88	117.56	120.86
25	A	2445	2MG	CM2-N2-C2	-2.88	119.80	123.03
1	a	1516	2MG	CM2-N2-C2	-2.85	119.83	123.03
1	a	1207	2MG	C6-C5-C4	-2.83	117.63	120.86
1	a	527	7MG	C8-N9-C1'	-2.82	113.98	122.43
1	a	1519	MA6	C10-N6-C9	-2.79	106.86	115.96
25	A	2251	OMG	C6-C5-C4	-2.74	117.73	120.86
1	a	1207	2MG	CM2-N2-C2	-2.65	120.05	123.03
25	A	2069	7MG	C8-N9-C1'	-2.63	114.54	122.43
1	a	1519	MA6	C1'-N9-C4	-2.61	123.89	126.81
25	A	1911	PSU	C5-C1'-C2'	-2.57	111.06	115.44
1	a	1516	2MG	N3-C2-N1	-2.46	122.51	126.19
1	a	966	2MG	N3-C2-N1	-2.24	122.84	126.19
1	a	1207	2MG	N3-C2-N1	-2.19	122.91	126.19
25	A	2069	7MG	C5-C4-N9	-2.12	102.82	106.25
25	A	1835	2MG	N3-C2-N1	-2.06	123.10	126.19
1	a	527	7MG	C5-C4-N9	-2.00	103.01	106.25
25	A	2445	2MG	N2-C2-N3	2.04	119.31	116.94
25	A	747	5MC	C4'-O4'-C1'	2.07	111.84	109.64
25	A	2449	H2U	N3-C2-N1	2.13	118.62	116.64
25	A	2449	H2U	O4-C4-N3	2.22	123.93	120.46
25	A	955	PSU	O4'-C1'-C2'	2.25	107.12	104.69
25	A	747	5MC	O4'-C1'-N1	2.28	112.44	108.10
1	a	1402	4OC	C2'-C1'-N1	2.43	120.43	113.48
15	v	20	H2U	N3-C2-N1	2.43	118.90	116.64
25	A	2457	PSU	O4'-C1'-C2'	2.46	107.35	104.69
25	A	2605	PSU	O4'-C1'-C2'	2.47	107.36	104.69
25	A	2604	PSU	O4'-C1'-C2'	2.52	107.42	104.69
25	A	2504	PSU	O4'-C1'-C2'	2.52	107.42	104.69
25	A	1917	PSU	O4'-C1'-C2'	2.68	107.59	104.69
1	a	1407	5MC	N4-C4-N3	2.70	120.88	116.92
25	A	1911	PSU	O4'-C1'-C2'	2.70	107.61	104.69
25	A	1915	3TD	O4'-C1'-C2'	2.80	107.71	104.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	747	5MC	N4-C4-N3	2.83	121.07	116.92
15	v	55	PSU	O4'-C1'-C2'	2.84	107.76	104.69
25	A	2580	PSU	O4'-C1'-C2'	2.93	107.86	104.69
25	A	1962	5MC	N4-C4-N3	2.95	121.24	116.92
1	a	1402	4OC	O3'-C3'-C4'	3.12	120.33	111.01
1	a	1402	4OC	C4'-O4'-C1'	3.23	113.07	109.64
25	A	2449	H2U	C6-N1-C2	3.29	127.25	122.16
1	a	967	5MC	N4-C4-N3	3.29	121.75	116.92
15	v	20	H2U	C6-N1-C2	3.36	127.36	122.16
1	a	516	PSU	O4'-C1'-C2'	3.44	108.41	104.69
1	a	1402	4OC	C3'-C2'-C1'	3.79	109.88	102.63
1	a	1402	4OC	O4'-C1'-N1	3.92	115.56	108.10
25	A	1835	2MG	C6-N1-C2	4.37	121.50	115.24
25	A	2445	2MG	C2-N3-C4	4.44	119.86	114.99
1	a	1402	4OC	C2-N3-C4	4.47	121.12	115.43
1	a	966	2MG	C6-N1-C2	4.67	121.92	115.24
1	a	1519	MA6	C2-N1-C6	4.70	122.73	111.64
1	a	1207	2MG	C6-N1-C2	4.77	122.08	115.24
1	a	1518	MA6	C2-N1-C6	4.83	123.03	111.64
1	a	1516	2MG	C6-N1-C2	5.22	122.72	115.24
1	a	1402	4OC	O3'-C3'-C2'	5.24	126.26	111.13
25	A	2552	OMU	C4-N3-C2	5.31	119.81	114.21
1	a	1516	2MG	C2-N3-C4	5.37	120.87	114.99
25	A	2498	OMC	C6-C5-C4	5.39	119.55	117.44
25	A	1835	2MG	C2-N3-C4	5.43	120.95	114.99
1	a	516	PSU	C4-N3-C2	5.70	119.92	115.16
25	A	1939	5MU	C4-N3-C2	5.75	119.96	115.16
25	A	2445	2MG	C6-N1-C2	5.80	123.55	115.24
25	A	955	PSU	C4-N3-C2	5.83	120.02	115.16
1	a	1207	2MG	C2-N3-C4	5.83	121.39	114.99
25	A	2604	PSU	C4-N3-C2	5.88	120.06	115.16
1	a	966	2MG	C2-N3-C4	5.91	121.47	114.99
25	A	2457	PSU	C4-N3-C2	6.09	120.24	115.16
25	A	1911	PSU	C4-N3-C2	6.10	120.25	115.16
1	a	527	7MG	C6-N1-C2	6.16	123.10	115.88
15	v	54	5MU	C4-N3-C2	6.26	120.38	115.16
25	A	2251	OMG	C6-N1-C2	6.33	123.29	115.88
25	A	746	PSU	C4-N3-C2	6.36	120.46	115.16
25	A	2069	7MG	C6-N1-C2	6.62	123.63	115.88
25	A	2580	PSU	C4-N3-C2	6.80	120.83	115.16
15	v	55	PSU	C4-N3-C2	6.87	120.89	115.16
25	A	1917	PSU	C4-N3-C2	7.04	121.03	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2605	PSU	C4-N3-C2	7.09	121.07	115.16
25	A	2504	PSU	C4-N3-C2	7.20	121.17	115.16
25	A	1618	6MZ	C2-N1-C6	7.36	121.76	116.47
1	a	527	7MG	N3-C4-N9	8.72	138.26	126.98
25	A	2030	6MZ	C2-N1-C6	8.74	122.75	116.47
25	A	2069	7MG	N3-C4-N9	8.75	138.30	126.98
25	A	2503	2MA	C2-N3-C4	10.98	120.58	115.29

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 ⓘ

There are no chain breaks in this entry.