



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Feb 21, 2017 – 11:29 AM EST

PDB ID : 5MMM
EMDB ID: : EMD-3533
Title : Structure of the 70S chloroplast ribosome
Authors : Bieri, P.; Leibundgut, M.; Saurer, M.; Boehringer, D.; Ban, N.
Deposited on : 2016-12-11
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

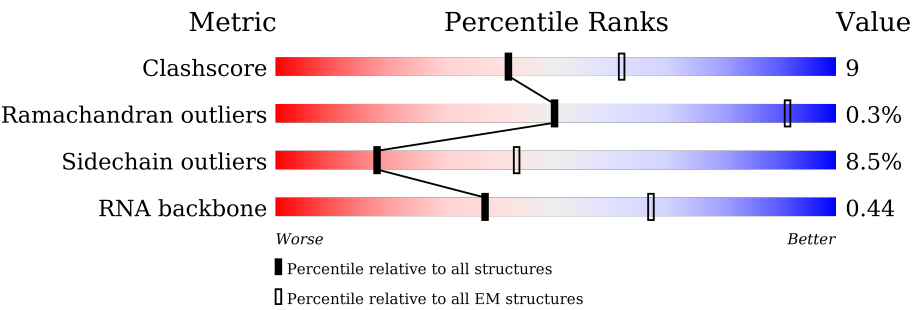
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

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








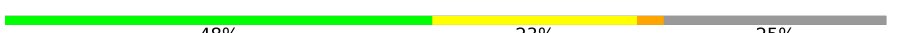



















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	0	130	<div><div>25%</div><div>23%</div><div>.</div><div>49%</div></div>
2	1	57	<div><div>58%</div><div>23%</div><div>.</div><div>16%</div></div>
3	2	66	<div><div>68%</div><div>20%</div><div>.</div><div>9%</div></div>
4	3	152	<div><div>26%</div><div>13%</div><div>.</div><div>61%</div></div>
5	4	159	<div><div>30%</div><div>13%</div><div>.</div><div>55%</div></div>
6	5	37	<div><div>59%</div><div>35%</div><div>5%</div></div>
7	6	142	<div><div>27%</div><div>6%</div><div>.</div><div>65%</div></div>
8	7	116	<div><div>26%</div><div>12%</div><div>.</div><div>60%</div></div>

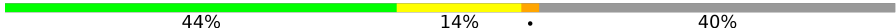

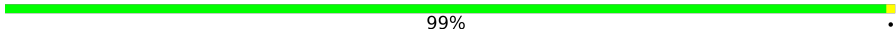


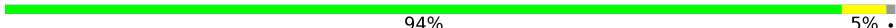



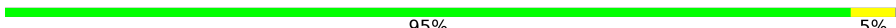


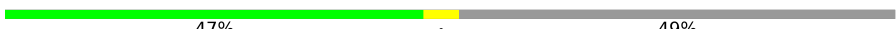












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Mol	Chain	Length	Quality of chain
9	A	2810	
10	B	121	
11	C	272	
12	D	305	
13	E	293	
14	F	258	
15	G	220	
16	H	196	
17	I	232	
18	J	224	
19	K	250	
20	L	121	
21	M	271	
22	N	135	
23	O	126	
24	P	166	
25	Q	233	
26	R	128	
27	S	256	
28	T	199	
29	U	198	
30	V	192	
31	W	106	
32	X	194	
33	Y	148	

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Mol	Chain	Length	Quality of chain
34	Z	168	
35	z	76	
36	8	174	
37	a	1491	
38	b	236	
39	c	218	
40	d	201	
41	e	308	
42	f	211	
43	g	155	
44	h	134	
45	i	208	
46	j	195	
47	k	138	
48	l	123	
49	m	172	
50	n	100	
51	o	90	
52	p	88	
53	q	165	
54	r	101	
55	s	92	
56	t	183	
57	u	180	
58	v	260	

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Mol	Chain	Length	Quality of chain
59	w	179	<div><div></div><div>46%</div><div>54%</div></div>
60	x	101	<div><div></div><div>40%</div><div>60%</div></div>
61	y	302	<div><div></div><div>37%</div><div>62%</div></div>

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 152465 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 protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	66	Total	C	N	O	S	0	0
			536	338	94	102	2		

- Molecule 2 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	48	Total	C	N	O	0	0
			396	261	75	60		

- Molecule 3 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	60	Total	C	N	O	S	0	0
			489	304	98	83	4		

- Molecule 4 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	60	Total	C	N	O	S	0	0
			467	282	107	75	3		

- Molecule 5 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	72	Total	C	N	O	S	0	0
			588	370	124	93	1		

- Molecule 6 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	37	Total	C	N	O	S	0	0
			305	186	70	45	4		

- Molecule 7 is a protein called plastid ribosomal protein cL37, PSRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	49	Total	C	N	O	S	0	0
			422	268	92	57	5		

- Molecule 8 is a protein called 50S ribosomal protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	46	Total	C	N	O	S	0	0
			368	237	71	59	1		

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	2798	Total	C	N	O	P	0	0
			60083	26804	11116	19365	2798		

- Molecule 10 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	121	Total	C	N	O	P	0	0
			2584	1154	466	843	121		

- Molecule 11 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	253	Total	C	N	O	S	0	0
			1952	1209	401	336	6		

- Molecule 12 is a protein called plastid ribosomal protein uL3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	221	Total	C	N	O	S	0	0
			1686	1066	308	301	11		

- Molecule 13 is a protein called plastid ribosomal protein uL4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	212	Total	C	N	O	S	0	0
			1676	1061	312	300	3		

- Molecule 14 is a protein called plastid ribosomal protein uL5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	193	Total	C	N	O	S	0	0
			1454	923	255	268	8		

- Molecule 15 is a protein called plastid ribosomal protein uL6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	178	Total	C	N	O	S	0	0
			1391	878	256	253	4		

- Molecule 16 is a protein called plastid ribosomal protein bL9c.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	H	48	Total	C	N	O	0	0
			382	251	69	62		

- Molecule 17 is a protein called plastid ribosomal protein uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	137	Total	C	N	O	S	0	0
			1106	711	186	203	6		

- Molecule 18 is a protein called 50S ribosomal protein L11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	133	Total	C	N	O	S	0	0
			977	624	161	186	6		

- Molecule 19 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	203	Total	C	N	O	S	0	0
			1648	1047	307	289	5		

- Molecule 20 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	121	Total	C	N	O	S	0	0
			942	588	179	170	5		

- Molecule 21 is a protein called plastid ribosomal protein uL15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	185	Total	C	N	O	S	0	0
			1410	879	280	245	6		

- Molecule 22 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	135	Total	C	N	O	S	0	0
			1075	677	218	174	6		

- Molecule 23 is a protein called plastid ribosomal protein uL14c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	116	Total	C	N	O	S	0	0
			944	592	193	155	4		

- Molecule 24 is a protein called plastid ribosomal protein uL18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	122	Total	C	N	O	S	0	0
			962	598	186	173	5		

- Molecule 25 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	118	Total	C	N	O	S	0	0
			953	611	186	155	1		

- Molecule 26 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	119	Total	C	N	O	S	0	0
			1029	652	213	162	2		

- Molecule 27 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	S	170	Total	C	N	O	0	0
			1310	844	227	239		

- Molecule 28 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	172	Total	C	N	O	S	0	0
			1395	892	257	237	9		

- Molecule 29 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	96	Total	C	N	O	S	0	0
			776	503	135	136	2		

- Molecule 30 is a protein called plastid ribosomal protein uL24c.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	134	Total	C	N	O	S	0	0
			1078	677	203	195	3		

- Molecule 31 is a RNA chain called 4.5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	106	Total	C	N	O	P	0	0
			2277	1017	423	731	106		

- Molecule 32 is a protein called plastid ribosomal protein bL27c.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	X	109	Total	C	N	O	0	0
			888	560	175	153		

- Molecule 33 is a protein called plastid ribosomal protein bL28c.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	77	Total	C	N	O	S	0	0
			634	402	128	103	1		

- Molecule 34 is a protein called plastid ribosomal protein uL29c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	101	Total	C	N	O	S	0	0
			846	529	167	147	3		

- Molecule 35 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 36 is a protein called plastid ribosomal protein bS1c.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	8	174	Total	C	N	O		0	0
			870	522	174	174			

- Molecule 37 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	1484	Total	C	N	O	P	0	0
			31868	14208	5881	10295	1484		

- Molecule 38 is a protein called 30S ribosomal protein S2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	233	Total	C	N	O	S	0	0
			1844	1163	339	329	13		

- Molecule 39 is a protein called 30S ribosomal protein S3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	216	Total	C	N	O	S	0	0
			1736	1108	313	309	6		

- Molecule 40 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	199	Total	C	N	O	S	0	0
			1633	1032	319	278	4		

- Molecule 41 is a protein called 30S ribosomal protein S5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	187	Total	C	N	O	S	0	0
			1331	826	259	240	6		

- Molecule 42 is a protein called plastid ribosomal protein bS6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	f	113	Total	C	N	O	S	0	0
			911	583	152	172	4		

- Molecule 43 is a protein called 30S ribosomal protein S7, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	154	Total	C	N	O	S	0	0
			1210	753	244	210	3		

- Molecule 44 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h	133	Total	C	N	O	S	0	0
			1079	679	210	185	5		

- Molecule 45 is a protein called plastid ribosomal protein uS9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i	144	Total	C	N	O	S	0	0
			1119	712	211	195	1		

- Molecule 46 is a protein called plastid ribosomal protein uS10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	j	99	Total	C	N	O	S	0	0
			805	517	144	139	5		

- Molecule 47 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	k	117	Total	C	N	O	S	0	0
			882	546	181	150	5		

- Molecule 48 is a protein called 30S ribosomal protein S12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	l	122	Total	C	N	O	S	0	0
			959	599	197	161	2		

- Molecule 49 is a protein called plastid ribosomal protein uS13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	m	110	Total	C	N	O	S	0	0
			904	556	182	161	5		

- Molecule 50 is a protein called 30S ribosomal protein S14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	n	99	Total	C	N	O	S	0	0
			820	507	174	136	3		

- Molecule 51 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	o	75	Total	C	N	O	S	0	0
			635	404	123	107	1		

- Molecule 52 is a protein called 30S ribosomal protein S16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	p	80	Total	C	N	O	S	0	0
			664	425	123	114	2		

- Molecule 53 is a protein called plastid ribosomal protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	q	86	Total	C	N	O	S	0	0
			693	434	136	119	4		

- Molecule 54 is a protein called 30S ribosomal protein S18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	r	60	Total	C	N	O	S	0	0
			490	308	96	85	1		

- Molecule 55 is a protein called 30S ribosomal protein S19 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	s	78	Total	C	N	O	S	0	0
			631	406	119	104	2		

- Molecule 56 is a protein called plastid ribosomal protein bS20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	t	107	Total	C	N	O	S	0	0
			853	528	173	151	1		

- Molecule 57 is a protein called plastid ribosomal protein bS21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	u	65	Total	C	N	O	S	0	0
			568	339	127	100	2		

- Molecule 58 is a protein called 30S ribosomal protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	v	80	Total	C	N	O	S	0	0
			613	388	104	121			

- Molecule 59 is a protein called 30S ribosomal protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	w	82	Total	C	N	O	S	0	0
			686	454	113	116	3		

- Molecule 60 is a protein called 30S ribosomal protein S31, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	x	40	Total	C	N	O	S	0	0
			309	192	69	48			

- Molecule 61 is a protein called Ribosome-binding factor PSRP1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	y	116	Total	C	N	O	S	0	0
			919	567	181	169	2		

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	2	1	Total	Zn	0
			1	1	
62	5	1	Total	Zn	0
			1	1	

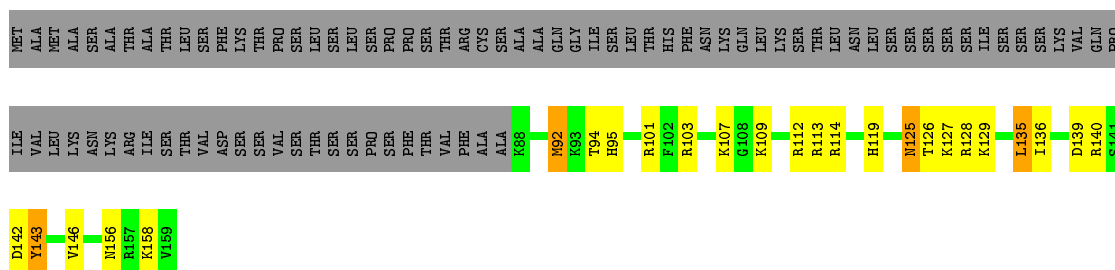
- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
63	P	1	Total Mg 1 1	0
63	B	15	Total Mg 15 15	0
63	6	1	Total Mg 1 1	0
63	W	14	Total Mg 14 14	0
63	S	1	Total Mg 1 1	0
63	k	1	Total Mg 1 1	0
63	E	1	Total Mg 1 1	0
63	V	1	Total Mg 1 1	0
63	A	511	Total Mg 511 511	0
63	n	1	Total Mg 1 1	0
63	x	1	Total Mg 1 1	0
63	R	1	Total Mg 1 1	0
63	M	2	Total Mg 2 2	0
63	D	1	Total Mg 1 1	0
63	a	219	Total Mg 219 219	0
63	4	1	Total Mg 1 1	0
63	U	1	Total Mg 1 1	0
63	H	1	Total Mg 1 1	0
63	C	1	Total Mg 1 1	0
63	7	1	Total Mg 1 1	0
63	T	1	Total Mg 1 1	0
63	l	1	Total Mg 1 1	0

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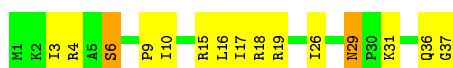
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Mol	Chain	Residues	Atoms		AltConf
63	F	1	Total	Mg	0
			1	1	



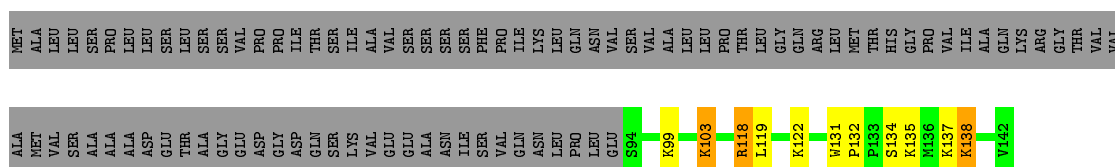
- Molecule 6: 50S ribosomal protein L36, chloroplastic

Chain 5: 59% 35% 5%



- Molecule 7: plastid ribosomal protein cL37, PSRP5

Chain 6: 27% 6% 65%



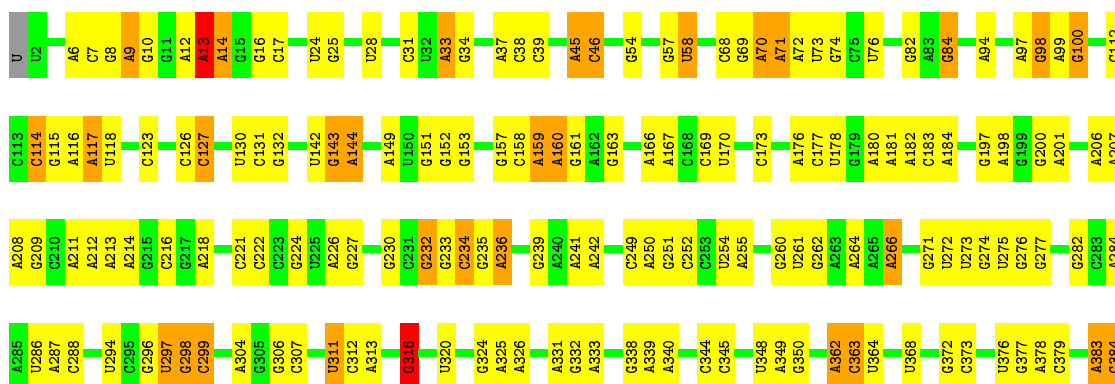
- Molecule 8: 50S ribosomal protein 6, chloroplastic

Chain 7: 26% 12% 60%

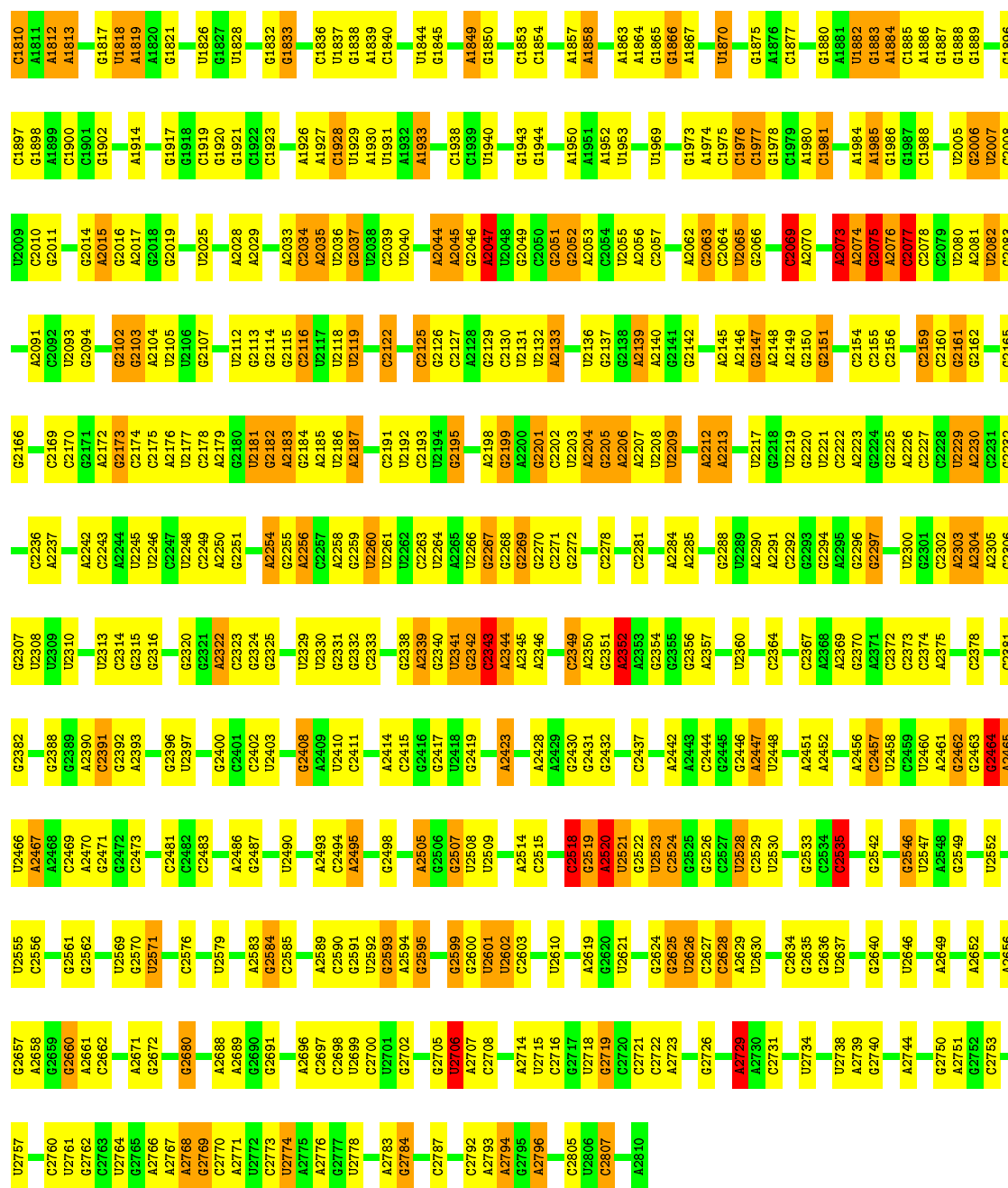


- Molecule 9: 23S ribosomal RNA

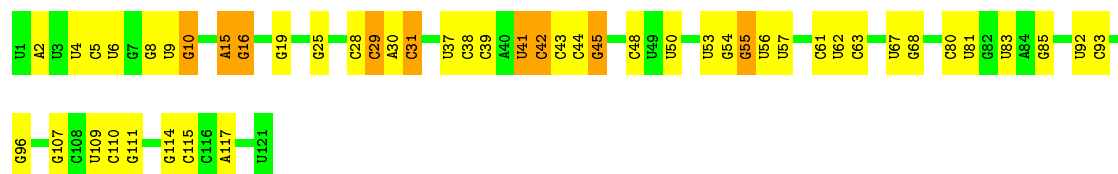
Chain A: 52% 37% 10%




A1688	C1689	A1582	G1491	A1416	U1219	U1133	A1060	G966	G885	U801	U720	A639	A555	G484	G394
C1690	A1492	A1417	A1492	U1417	U1220	G1134	G1061	C967	U886	C802	U721	G640	C556	G485	G395
A1691	C1493	U1418	G1494	U1418	C1221	A1135	U1062	G970	G887	G803	G722	G641	C557	G486	G396
C1692	A1494	C1420	A1322	G1420	U1226	U1136	U1063	U971	C988	A804	G723	G642	A588	U487	G398
U1693	A1497	U1423	U1327	U1423	G1231	G1137	G1065	G974	G889	A805	G724	A643	G559	G488	U404
C1694	G1498	A1424	U1327	U1424	G1231	A1139	G1070	G975	G890	A809	A727	A644	A560	A490	U405
U1695	G1498	C1425	U1332	C1425	A1234	G1140	C1071	C976	G894	G810	A728	A645	C561	A491	C406
A1700	A1501	U1426	U1333	U1426	A1235	C1141	U1072	G978	G894	A811	A729	G646	A492	A492	C407
C1701	A1502	U1431	U1334	U1431	G1239	G1142	G1073	G980	G895	G812	C730	G648	G565	G493	U408
G1702	G1507	U1432	C1335	U1432	G1240	U1144	A1074	G981	G	U814	U731	G650	A571	A494	G409
G1703	U1511	U1433	C1336	U1433	G1241	U1147	G1075	G982	G	A815	A732	G651	U572	A495	G410
A1704	U1512	U1434	U1337	U1434	U1241	U1147	G1078	G983	A	G816	A733	C852	U573	U411	U411
A1705	C1513	U1435	C1338	U1435	U1242	G1153	A1078	G984	G	C817	G737	A656	U576	U802	U802
C1710	C1513	U1436	A1342	U1436	U1245	G1154	A1082	G989	G902	U818	G738	U657	G577	C503	C503
A1712	U1518	U1437	U1348	U1437	G1248	A1155	G1083	G993	G902	G819	G739	A658	U578	G504	U415
A1713	A1519	U1438	C1348	U1438	G1253	U1158	G1084	C996	G906	G820	U741	A581	G511	A421	A421
A1715	A1520	U1439	U1383	U1439	U1254	G1159	A1085	C996	C907	U824	A745	U665	A582	A512	G422
G1731	A1522	A1444	A1357	G1445	U1256	A1160	G1087	G1000	A908	U666	A745	U667	A583	A513	G423
C1621	A1523	G1446	G1358	G1446	G1257	C1162	U1089	A1001	A909	C826	G749	G667	A584	A514	A424
U1620	G1524	G1447	C1359	G1447	G1258	G1163	U1090	G1002	A910	C827	A750	U668	U	C425	A425
G1629	G1526	A1448	G1363	A1448	C1259	G1166	G1091	A1003	U911	A830	C751	C669	A588	A516	C426
C1746	G1527	G1449	G1364	G1449	G1260	C1167	C1092	A1007	G915	A670	U752	C671	G589	A519	A427
G1630	U1528	U1450	U1365	U1450	A1261	C1167	C1093	A1008	G916	C590	A754	C591	C590	C520	C428
U1631	A1529	G1451	U1366	G1451	G1261	G1168	G1096	A1009	C917	U837	A754	C592	C591	C520	C429
C1632	G1530	A1452	C1366	G1452	C1264	A1169	G1097	C1010	A918	U838	U757	U675	G523	A434	A434
A1633	A1531	G1453	U1367	G1453	G1269	A1170	A1098	A1011	A919	G839	U758	U676	A524	A435	A435
C1634	G1532	G1454	C1371	G1454	C1270	G1173	G1099	A1012	C921	A840	U759	A677	A596	A525	A436
C1635	A1533	A1456	A1374	G1456	G1271	G1178	C1100	G1017	U922	C843	A761	U678	C597	A526	A436
U1636	U1534	G1457	A1375	G1457	A1272	G1178	C1101	G1017	C923	C844	A761	U679	C527	C448	C448
A1536	A1535	C1458	U1378	G1458	G1273	G1184	G1102	A1018	U924	C845	A767	G650	C605	C528	G452
G1543	G1543	A1465	C1379	A1465	A1274	G1189	A1105	U1019	G925	A846	U768	G681	A606	G529	G452
A1544	A1544	G1466	A1380	G1466	A1275	G1190	C1106	U1019	A926	U850	C768	C684	C609	U530	U453
G1546	G1546	C1467	G1381	C1467	U1276	G1191	U1109	C1023	A927	U851	G771	C688	U610	A531	G454
U1550	U1550	G1469	G1385	G1469	G1277	G1191	U1110	A1024	U931	G853	G772	U612	C536	C457	C456
G1557	G1557	A1472	A1386	A1472	A1289	G1192	U1111	A1028	G937	U856	G773	G695	U613	C457	C458
U1558	U1558	G1473	A1394	G1473	C1231	G1193	A1112	A1029	U938	G857	G774	A696	C538	G462	G462
A1559	A1559	U1474	C1397	U1474	G1282	U1195	A1113	A1038	G939	U856	A775	U637	C538	G463	G463
C1560	C1560	G1476	G1398	G1476	A1294	A1197	G1115	A1039	C940	G858	G776	U637	C538	G464	G464
G1563	A1399	G1477	A1399	G1477	A1296	A1199	A1116	U1040	C941	A859	G782	U701	G621	A540	A466
U1670	U1400	U1477	U1400	U1477	A1296	A1199	G1117	G1041	C944	G866	A785	C702	G622	A543	U468
A1673	G1401	A1480	G1401	A1480	U1299	A1202	U1118	G1045	A945	U869	G786	U705	A623	G544	A469
C1674	U1300	G1402	U1402	G1402	U1300	G1206	G1119	G1045	A946	G869	G787	G711	U628	U545	G470
A1681	G1301	G1403	G1301	G1403	G1301	C1207	C1120	U1050	A947	U878	G788	G712	G629	G546	U471
C1682	A1405	U1483	A1405	U1483	G1301	G1207	U1121	U1051	U948	C874	A791	A713	G547	A472	A472
G1683	A1406	U1485	A1406	U1485	A1307	G1208	U1122	G1052	A949	C875	G791	G714	G548	C473	C473
C1684	U1407	U1486	C1407	U1486	A1308	U1209	A1123	A1053	A950	G879	A792	G715	A633	A549	C474
G1571	C1487	A1408	A1408	C1487	U1309	A1210	U1125	U1054	C951	U880	A794	A716	G551	G551	G480
C1572	A1489	A1488	G1409	A1488	C1310	G1211	U1131	A1055	A952	U881	U795	A717	G552	G552	G481
G1573	G1573	A1489	U1415	G1573	C1311	G1218	A1131	A1056	G953	U882	G796	C719	G553	A482	A482
G1574	G1574	G1490	U1415	G1490	G1311	G1218	C1132	A1056	G954	U882	G796	C719	G554	A483	A483



- Molecule 10: 5S ribosomal RNA



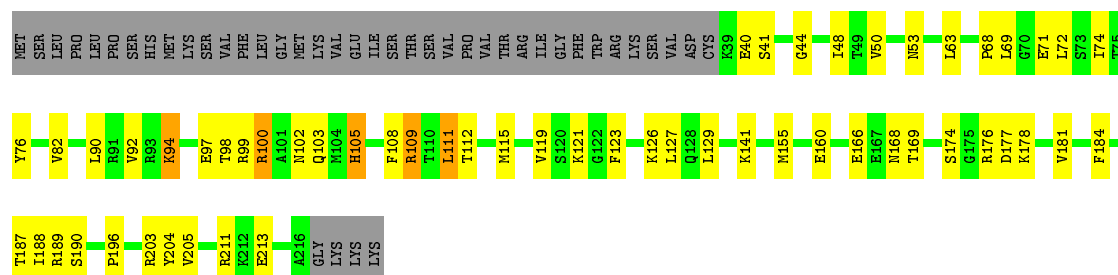
- Molecule 11: 50S ribosomal protein L2, chloroplastic

Chain F: 



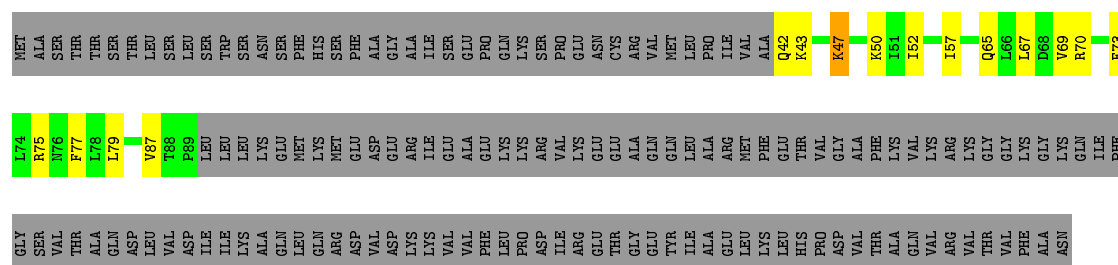
- Molecule 15: plastid ribosomal protein uL6c

Chain G: 55% 24% 19%



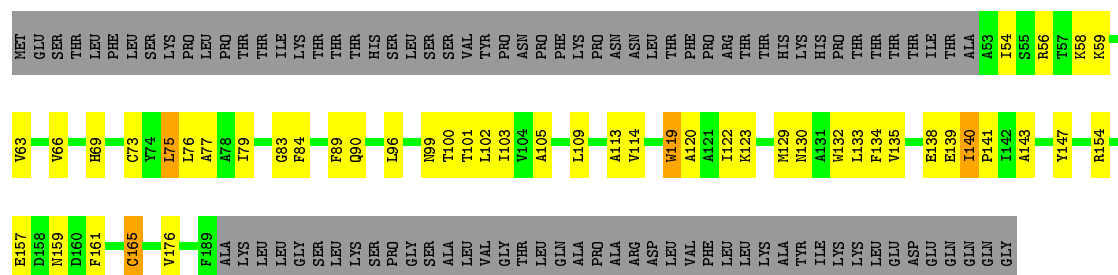
- Molecule 16: plastid ribosomal protein bL9c

Chain H: 17% 7% 76%



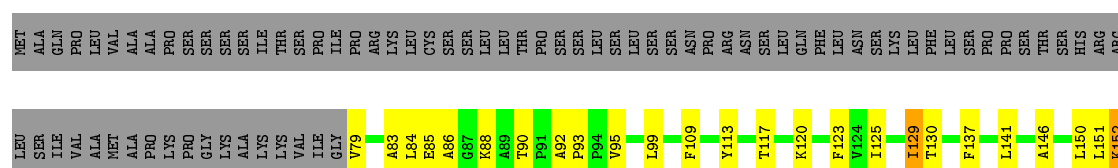
- Molecule 17: plastid ribosomal protein uL10c

Chain I: 38% 19% 41%



- Molecule 18: 50S ribosomal protein L11, chloroplastic

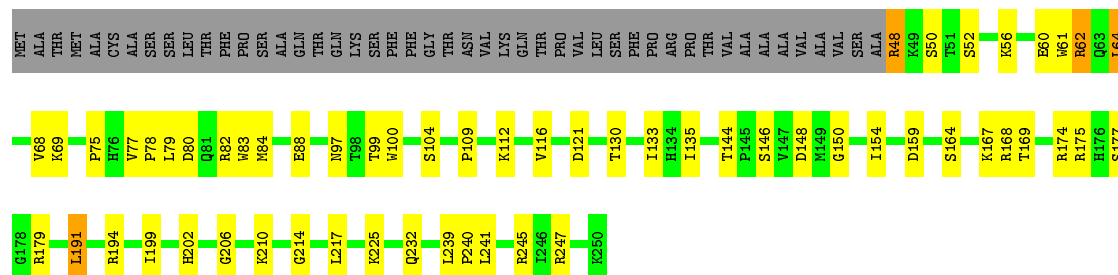
Chain J: 39% 19% 41%





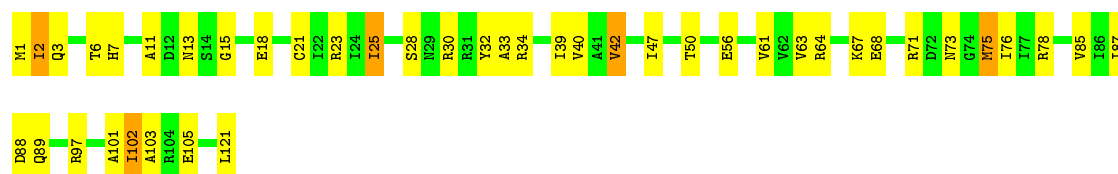
- Molecule 19: 50S ribosomal protein L13, chloroplastic

Chain K: 58% 22% 19%



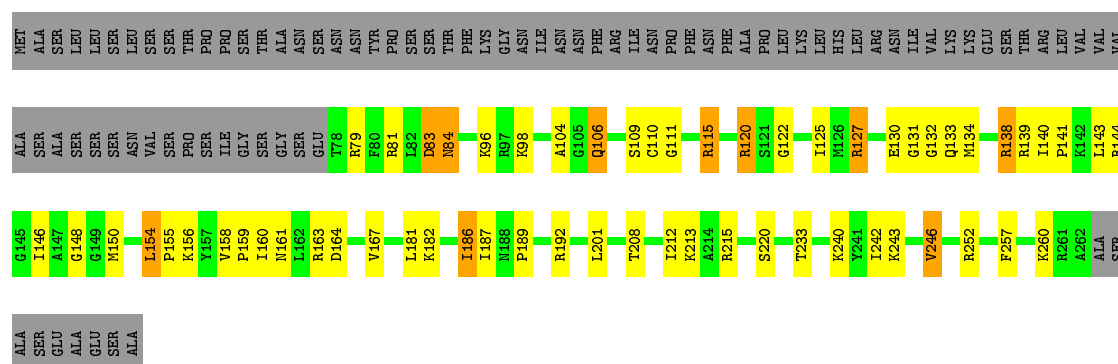
- Molecule 20: 50S ribosomal protein L14, chloroplastic

Chain L: 64% 31% 5%



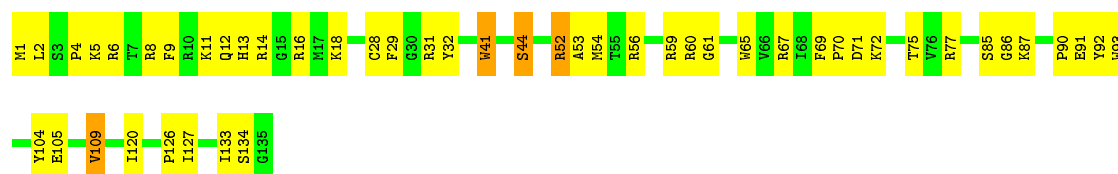
- Molecule 21: plastid ribosomal protein uL15c

Chain M: 46% 18% 32%

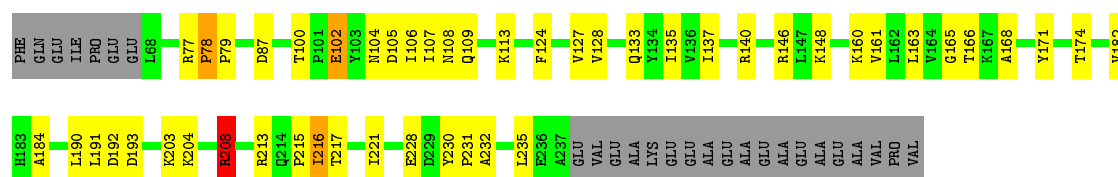


- Molecule 22: 50S ribosomal protein L16, chloroplastic

Chain N: 64% 33% 3%

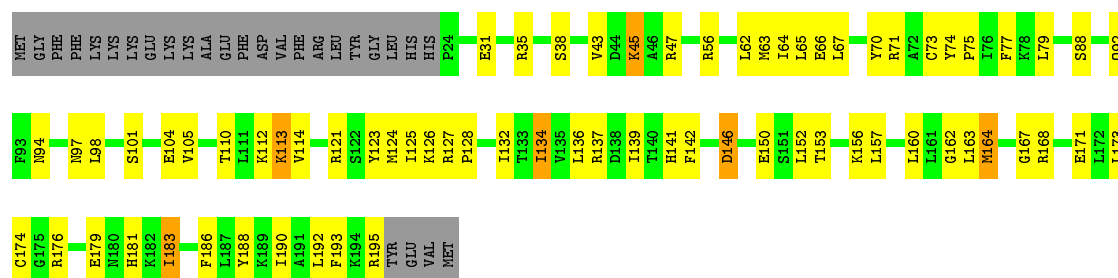


- Chain S: 47% 18% 34%



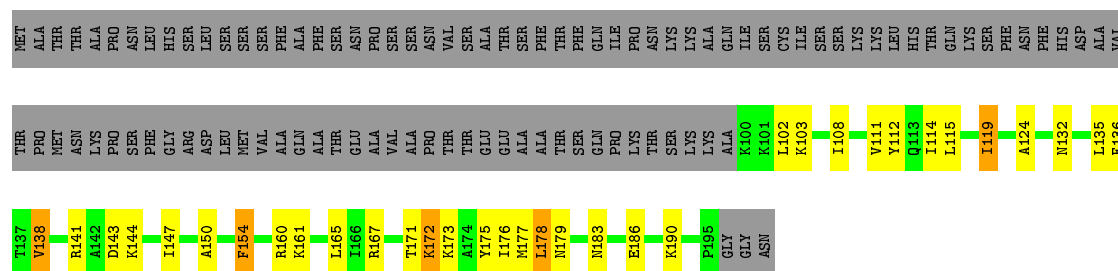
- Molecule 28: 50S ribosomal protein L22, chloroplastic

Chain T: 51% 33% 14%



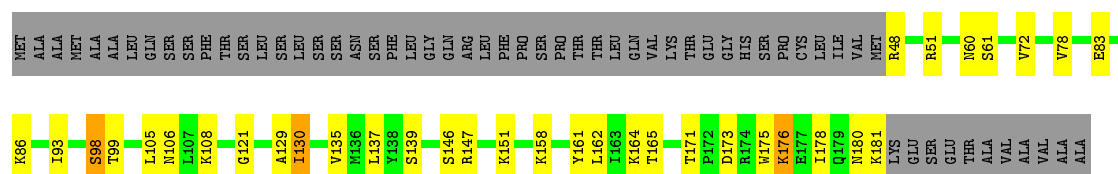
- Molecule 29: 50S ribosomal protein L23, chloroplastic

Chain U: 31% 15% 52%



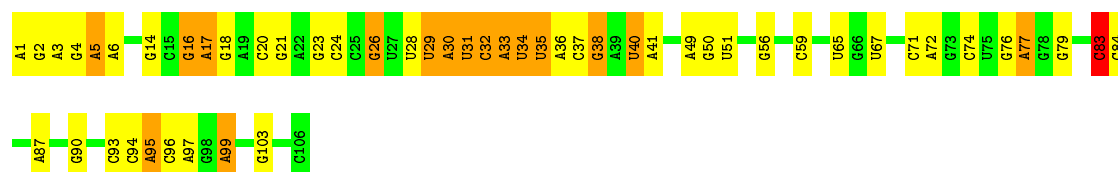
- Molecule 30: plastid ribosomal protein uL24c

Chain V: 52% 17% 30%



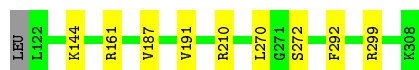
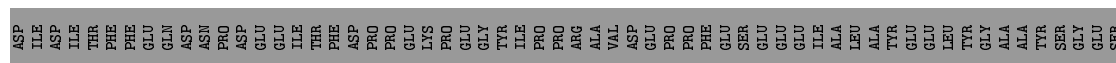
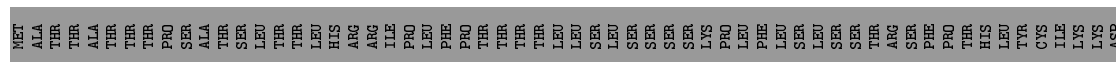
- Molecule 31: 4.5S ribosomal RNA

Chain W: 51% 33% 15%



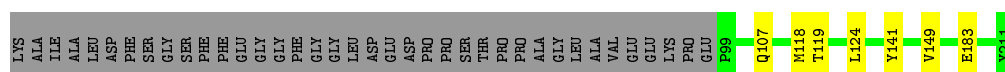
- Molecule 41: 30S ribosomal protein S5, chloroplastic

Chain e:  58% . 39%



- Molecule 42: plastid ribosomal protein bS6c

Chain f: 



- Molecule 43: 30S ribosomal protein S7, chloroplastic

Chain g:  95% 5%



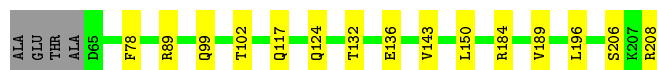
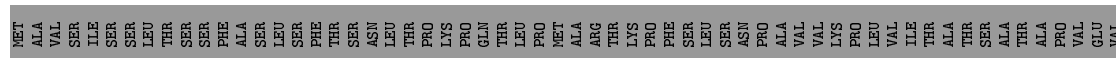
- Molecule 44: 30S ribosomal protein S8, chloroplastic

Chain h: 92% 7%



- Molecule 45: plastid ribosomal protein uS9c

Chain i:  62% 7% 31%

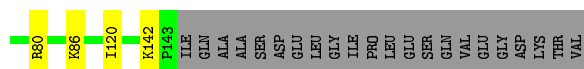
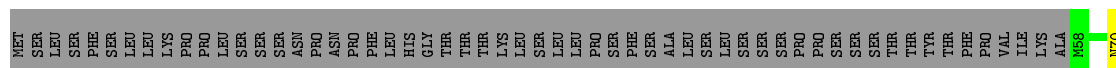


- Molecule 46: plastid ribosomal protein uS10c



- Molecule 53: plastid ribosomal protein uS17c

Chain q: 49% 48%



- Molecule 54: 30S ribosomal protein S18, chloroplastic

Chain r: 54% 5% 41%



- Molecule 55: 30S ribosomal protein S19 alpha, chloroplastic

Chain s: 80% 15%



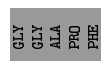
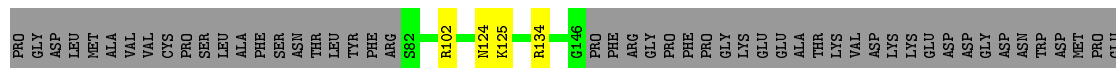
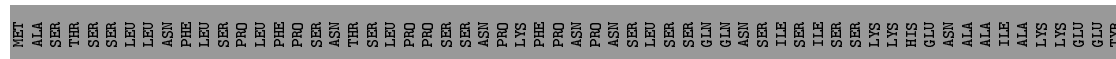
- Molecule 56: plastid ribosomal protein bS20c

Chain t: 54% 2% 42%



- Molecule 57: plastid ribosomal protein bS21c

Chain u: 34% 1% 64%



- Molecule 58: 30S ribosomal protein 2, chloroplastic

69%

- Molecule 59: 30S ribosomal protein 3, chloroplastic

54%

- Molecule 60: 30S ribosomal protein S31, chloroplastic

60%

- Molecule 61: Ribosome-binding factor PSRP1, chloroplastic

62%




4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	140583	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0	0.65	0/548	0.88	1/737 (0.1%)
10	B	0.49	0/2890	1.01	3/4503 (0.1%)
11	C	0.49	0/1986	0.69	2/2666 (0.1%)
12	D	0.54	0/1713	0.70	0/2291
13	E	0.54	0/1707	0.77	1/2298 (0.0%)
14	F	0.39	0/1475	0.60	1/1990 (0.1%)
15	G	0.39	0/1412	0.57	0/1898
16	H	0.41	0/386	0.59	0/514
17	I	0.54	0/1129	0.56	0/1521
18	J	0.56	0/992	0.58	0/1343
19	K	0.50	0/1688	0.63	0/2279
2	1	0.61	0/405	0.71	0/537
20	L	0.48	0/951	0.63	0/1282
21	M	0.50	0/1430	0.69	0/1896
22	N	0.45	0/1097	0.61	0/1471
23	O	0.55	0/959	0.72	0/1280
24	P	0.40	0/978	0.57	0/1311
25	Q	0.57	0/967	0.69	0/1299
26	R	0.60	0/1046	0.72	0/1395
27	S	0.48	0/1339	0.69	3/1826 (0.2%)
28	T	0.50	0/1420	0.63	0/1900
29	U	0.50	0/787	0.69	0/1056
3	2	0.47	0/497	0.74	1/664 (0.2%)
30	V	0.42	0/1093	0.61	0/1457
31	W	0.74	0/2551	1.18	4/3977 (0.1%)
32	X	0.45	0/905	0.60	0/1204
33	Y	0.46	0/644	0.62	0/856
34	Z	0.41	0/854	0.56	0/1131
35	z	1.35	7/1813 (0.4%)	1.93	81/2823 (2.9%)
37	a	0.57	0/35687	1.00	35/55680 (0.1%)
38	b	0.40	0/1878	0.55	0/2538
39	c	0.39	0/1763	0.58	0/2370

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
4	3	0.55	0/470	0.71	0/619
40	d	0.37	0/1661	0.57	0/2230
41	e	0.44	0/1345	0.61	0/1817
42	f	0.34	0/929	0.54	0/1255
43	g	0.37	0/1226	0.53	0/1641
44	h	0.37	0/1094	0.57	0/1467
45	i	0.37	0/1138	0.60	0/1526
46	j	0.42	0/822	0.58	0/1111
47	k	0.35	0/896	0.59	0/1206
48	l	0.45	0/975	0.60	0/1312
49	m	0.37	0/912	0.61	0/1219
5	4	0.57	0/594	0.67	0/784
50	n	0.39	0/836	0.55	0/1116
51	o	0.38	0/642	0.49	0/852
52	p	0.39	0/674	0.62	0/902
53	q	0.37	0/707	0.55	0/949
54	r	0.37	0/494	0.56	0/660
55	s	0.40	0/646	0.61	0/870
56	t	0.41	0/862	0.63	1/1151 (0.1%)
57	u	0.34	0/572	0.47	0/754
58	v	0.58	0/621	0.49	0/833
59	w	0.58	0/707	0.55	0/962
6	5	0.38	0/307	0.54	0/403
60	x	0.46	0/317	0.62	0/418
61	y	0.40	0/930	0.71	2/1243 (0.2%)
7	6	0.46	0/425	0.77	0/551
8	7	0.43	0/382	0.57	0/520
9	A	0.82	39/67297 (0.1%)	1.21	253/104984 (0.2%)
All	All	0.67	46/163471 (0.0%)	1.03	388/243348 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	E	0	1
21	M	0	1
38	b	0	1
41	e	0	1
56	t	0	2
All	All	0	6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	z	1	G	OP3-P	-10.61	1.48	1.61
9	A	1272	A	N3-C4	-8.41	1.29	1.34
9	A	1272	A	N9-C4	-7.74	1.33	1.37
9	A	727	A	N3-C4	7.72	1.39	1.34
9	A	830	A	N3-C4	-7.35	1.30	1.34
9	A	2739	A	N9-C4	-7.13	1.33	1.37
9	A	970	G	C6-N1	-7.09	1.34	1.39
9	A	1272	A	N7-C5	-6.68	1.35	1.39
9	A	772	A	N9-C4	-6.64	1.33	1.37
9	A	810	G	C6-N1	-6.25	1.35	1.39
9	A	591	C	N1-C6	-6.23	1.33	1.37
35	z	73	A	N9-C4	6.21	1.41	1.37
9	A	2044	A	N9-C4	-6.19	1.34	1.37
9	A	1399	A	N9-C4	-6.17	1.34	1.37
35	z	69	G	C6-N1	6.02	1.43	1.39
9	A	596	A	C6-N1	-5.97	1.31	1.35
9	A	727	A	N9-C4	5.91	1.41	1.37
9	A	1290	A	N3-C4	-5.90	1.31	1.34
9	A	596	A	N3-C4	-5.82	1.31	1.34
9	A	1272	A	C5-C6	-5.79	1.35	1.41
9	A	1406	A	N9-C4	-5.78	1.34	1.37
9	A	590	C	N1-C6	-5.68	1.33	1.37
9	A	180	A	N9-C4	-5.65	1.34	1.37
35	z	56	C	N1-C6	5.63	1.40	1.37
35	z	35	A	N3-C4	5.58	1.38	1.34
9	A	2051	G	C6-N1	-5.54	1.35	1.39
9	A	727	A	N1-C2	5.54	1.39	1.34
9	A	183	C	N1-C6	-5.42	1.33	1.37
9	A	805	A	N3-C4	-5.34	1.31	1.34
9	A	785	A	N3-C4	-5.34	1.31	1.34
9	A	1813	A	N9-C4	-5.33	1.34	1.37
9	A	2052	G	C5-C4	-5.30	1.34	1.38
9	A	1497	A	N9-C4	5.29	1.41	1.37
9	A	2794	A	N9-C4	-5.29	1.34	1.37
9	A	236	A	N7-C5	-5.29	1.36	1.39
9	A	469	A	N9-C4	-5.27	1.34	1.37
9	A	520	C	N1-C6	-5.23	1.34	1.37
9	A	1294	A	N9-C4	-5.22	1.34	1.37
9	A	745	A	N9-C4	-5.20	1.34	1.37
9	A	1684	C	N1-C6	-5.16	1.34	1.37
9	A	236	A	C5-C4	-5.13	1.35	1.38
35	z	69	G	N1-C2	5.11	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1374	A	N3-C4	-5.02	1.31	1.34
9	A	590	C	N3-C4	-5.01	1.30	1.33
9	A	1272	A	C6-N1	-5.01	1.32	1.35
35	z	57	G	P-OP2	-5.00	1.40	1.49

All (388) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	727	A	N1-C2-N3	-17.96	120.32	129.30
35	z	34	G	N1-C2-N2	-13.39	104.15	116.20
9	A	1272	A	C2-N3-C4	-12.32	104.44	110.60
61	y	140	ARG	NE-CZ-NH2	-11.37	114.62	120.30
9	A	727	A	C6-N1-C2	10.68	125.01	118.60
35	z	34	G	C2-N3-C4	-10.46	106.67	111.90
35	z	33	U	C5-C4-O4	-10.35	119.69	125.90
35	z	8	U	C6-N1-C2	-10.24	114.86	121.00
35	z	7	A	C8-N9-C4	9.97	109.79	105.80
9	A	1272	A	C5-N7-C8	-9.93	98.94	103.90
9	A	2122	C	C6-N1-C2	-9.77	116.39	120.30
9	A	1272	A	N1-C2-N3	9.70	134.15	129.30
35	z	34	G	N3-C2-N2	9.61	126.63	119.90
37	a	316	C	N3-C4-C5	9.47	125.69	121.90
9	A	1272	A	N7-C8-N9	9.46	118.53	113.80
37	a	1152	A	C5-C6-N1	9.30	122.35	117.70
35	z	35	A	C8-N9-C4	9.20	109.48	105.80
35	z	46	G	C8-N9-C4	-9.20	102.72	106.40
9	A	970	G	N3-C4-C5	-9.13	124.04	128.60
9	A	1272	A	C6-C5-N7	-9.12	125.92	132.30
9	A	970	G	N1-C6-O6	-8.95	114.53	119.90
37	a	316	C	C2-N3-C4	-8.94	115.43	119.90
35	z	34	G	N1-C2-N3	8.83	129.20	123.90
9	A	901	C	C2-N1-C1'	8.79	128.47	118.80
37	a	316	C	O5'-P-OP1	-8.71	97.86	105.70
37	a	1148	C	C6-N1-C2	8.62	123.75	120.30
35	z	41	C	N3-C4-C5	-8.39	118.54	121.90
9	A	1264	C	C6-N1-C2	8.36	123.64	120.30
9	A	2706	U	N3-C2-O2	-8.16	116.49	122.20
3	2	65	LYS	CD-CE-NZ	-8.14	92.98	111.70
35	z	32	U	O5'-P-OP1	-8.12	98.39	105.70
35	z	35	A	N9-C4-C5	-8.04	102.58	105.80
35	z	18	G	C8-N9-C4	8.01	109.60	106.40
35	z	42	C	N1-C2-O2	7.98	123.69	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2518	C	C6-N1-C2	-7.96	117.11	120.30
9	A	2464	G	N3-C4-N9	7.90	130.74	126.00
35	z	56	C	C6-N1-C2	-7.89	117.14	120.30
35	z	19	G	OP2-P-O3'	7.87	122.51	105.20
35	z	19	G	N7-C8-N9	-7.85	109.17	113.10
35	z	70	G	N3-C4-C5	7.83	132.51	128.60
9	A	2036	U	C5-C6-N1	-7.74	118.83	122.70
35	z	19	G	N3-C4-C5	7.73	132.47	128.60
35	z	46	G	OP2-P-O3'	7.63	121.99	105.20
37	a	1152	A	C6-N1-C2	-7.62	114.03	118.60
9	A	1184	G	C6-C5-N7	-7.61	125.83	130.40
35	z	13	C	C6-N1-C2	7.59	123.34	120.30
9	A	1000	G	N3-C4-C5	-7.51	124.85	128.60
37	a	1302	C	C6-N1-C2	-7.48	117.31	120.30
35	z	41	C	C5-C6-N1	7.45	124.72	121.00
9	A	2635	G	C8-N9-C4	7.40	109.36	106.40
9	A	2102	G	C8-N9-C4	-7.40	103.44	106.40
35	z	3	C	C6-N1-C2	-7.40	117.34	120.30
35	z	5	G	C4-C5-N7	-7.37	107.85	110.80
9	A	596	A	N1-C6-N6	-7.37	114.18	118.60
9	A	2518	C	N3-C4-C5	-7.36	118.96	121.90
9	A	802	C	N3-C4-C5	7.34	124.83	121.90
9	A	788	G	N3-C4-C5	-7.27	124.97	128.60
35	z	69	G	N3-C4-C5	7.26	132.23	128.60
37	a	316	C	C2-N1-C1'	-7.25	110.82	118.80
35	z	19	G	C8-N9-C4	7.22	109.29	106.40
9	A	901	C	C6-N1-C2	-7.20	117.42	120.30
9	A	234	C	C6-N1-C2	7.12	123.15	120.30
37	a	316	C	C5-C4-N4	-7.11	115.22	120.20
35	z	39	U	OP2-P-O3'	7.10	120.83	105.20
9	A	1650	A	C8-N9-C4	7.08	108.63	105.80
9	A	462	G	C6-C5-N7	-7.07	126.16	130.40
9	A	2294	G	C8-N9-C4	-7.07	103.57	106.40
9	A	971	U	N3-C4-C5	-7.07	110.36	114.60
35	z	7	A	N9-C4-C5	-7.07	102.97	105.80
9	A	1211	G	C8-N9-C4	7.05	109.22	106.40
35	z	70	G	N3-C4-N9	-7.02	121.79	126.00
9	A	2102	G	N7-C8-N9	7.00	116.60	113.10
9	A	2464	G	C8-N9-C1'	-6.98	117.92	127.00
9	A	901	C	N1-C2-O2	6.97	123.08	118.90
35	z	35	A	N3-C4-N9	6.96	132.97	127.40
9	A	1272	A	C8-N9-C4	-6.96	103.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	773	U	C6-N1-C2	6.95	125.17	121.00
35	z	43	C	C6-N1-C2	-6.95	117.52	120.30
9	A	1692	C	C6-N1-C2	6.94	123.08	120.30
9	A	588	A	C8-N9-C4	6.94	108.58	105.80
9	A	1334	U	N3-C2-O2	-6.93	117.35	122.20
27	S	208	ARG	NE-CZ-NH1	6.92	123.76	120.30
9	A	2063	C	C6-N1-C2	6.86	123.04	120.30
9	A	1272	A	C5-C6-N1	-6.83	114.28	117.70
35	z	45	U	C6-N1-C2	-6.83	116.90	121.00
9	A	922	U	C5-C6-N1	-6.81	119.29	122.70
35	z	18	G	N9-C4-C5	-6.78	102.69	105.40
9	A	1272	A	C4-C5-C6	6.76	120.38	117.00
9	A	773	U	C5-C6-N1	-6.73	119.33	122.70
9	A	2706	U	N1-C2-O2	6.71	127.50	122.80
35	z	65	G	N3-C2-N2	-6.71	115.20	119.90
9	A	970	G	C6-N1-C2	-6.70	121.08	125.10
35	z	44	G	C4-C5-N7	-6.70	108.12	110.80
9	A	2016	G	C8-N9-C4	-6.64	103.75	106.40
9	A	2006	G	C8-N9-C4	6.62	109.05	106.40
13	E	112	GLY	N-CA-C	-6.62	96.56	113.10
37	a	64	C	C6-N1-C2	-6.61	117.66	120.30
9	A	462	G	C4-N9-C1'	6.60	135.08	126.50
9	A	1332	G	O4'-C1'-N9	6.59	113.47	108.20
9	A	2272	G	C4-C5-N7	6.54	113.41	110.80
9	A	540	A	C4-C5-C6	-6.53	113.73	117.00
9	A	805	A	N1-C2-N3	6.52	132.56	129.30
9	A	2760	C	C6-N1-C2	6.51	122.90	120.30
37	a	316	C	C6-N1-C2	6.48	122.89	120.30
9	A	2122	C	C2-N1-C1'	6.46	125.91	118.80
9	A	1184	G	C4-C5-N7	6.45	113.38	110.80
35	z	42	C	N3-C4-C5	6.42	124.47	121.90
9	A	1684	C	C5-C6-N1	-6.40	117.80	121.00
9	A	2352	A	C8-N9-C4	-6.40	103.24	105.80
37	a	299	C	C6-N1-C2	-6.39	117.74	120.30
9	A	772	A	C2-N3-C4	-6.38	107.41	110.60
35	z	67	C	C6-N1-C2	6.38	122.85	120.30
37	a	299	C	N1-C2-O2	6.36	122.72	118.90
9	A	843	C	C6-N1-C2	-6.33	117.77	120.30
9	A	788	G	C4-N9-C1'	6.32	134.71	126.50
9	A	2533	G	N3-C4-N9	6.32	129.79	126.00
35	z	46	G	O5'-P-OP2	-6.29	100.04	105.70
9	A	2464	G	N9-C4-C5	-6.29	102.88	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	512	A	C8-N9-C4	-6.29	103.28	105.80
9	A	523	G	O4'-C1'-N9	6.27	113.22	108.20
37	a	1106	C	N3-C2-O2	-6.25	117.53	121.90
9	A	416	C	C6-N1-C2	6.21	122.78	120.30
9	A	820	G	C5-C6-N1	6.21	114.60	111.50
9	A	2073	A	O4'-C1'-N9	6.20	113.16	108.20
9	A	462	G	C8-N9-C1'	-6.19	118.95	127.00
37	a	299	C	N3-C2-O2	-6.18	117.57	121.90
9	A	2268	G	C2-N3-C4	6.18	114.99	111.90
9	A	536	C	C5-C6-N1	-6.17	117.92	121.00
9	A	514	A	N9-C4-C5	6.16	108.27	105.80
35	z	18	G	C4-C5-N7	6.15	113.26	110.80
9	A	1902	G	N3-C4-C5	-6.12	125.54	128.60
27	S	78	PRO	N-CA-CB	6.11	110.64	103.30
35	z	15	G	P-O3'-C3'	6.11	127.03	119.70
35	z	21	A	O5'-P-OP1	-6.10	100.21	105.70
14	F	57	LEU	CA-CB-CG	-6.10	101.27	115.30
9	A	2063	C	C5-C6-N1	-6.10	117.95	121.00
9	A	1290	A	N1-C2-N3	6.09	132.34	129.30
9	A	540	A	C8-N9-C4	6.07	108.23	105.80
35	z	69	G	N3-C2-N2	-6.06	115.66	119.90
9	A	788	G	N3-C4-N9	6.06	129.63	126.00
9	A	2065	U	C2-N1-C1'	-6.05	110.43	117.70
9	A	2391	C	C5-C6-N1	-6.05	117.97	121.00
35	z	8	U	C5-C6-N1	6.05	125.73	122.70
9	A	2065	U	C5-C6-N1	-6.05	119.68	122.70
35	z	69	G	C8-N9-C4	6.04	108.81	106.40
37	a	299	C	C2-N1-C1'	6.03	125.44	118.80
35	z	19	G	N3-C4-N9	-6.03	122.38	126.00
1	0	89	LEU	CA-CB-CG	6.03	129.16	115.30
9	A	2272	G	N9-C4-C5	-6.02	102.99	105.40
9	A	2349	C	C6-N1-C2	6.02	122.71	120.30
9	A	462	G	C4-C5-C6	6.01	122.41	118.80
9	A	2628	C	C6-N1-C2	-6.01	117.89	120.30
9	A	1184	G	C4-N9-C1'	6.00	134.29	126.50
9	A	1272	A	C4-C5-N7	5.99	113.70	110.70
9	A	1661	U	C5-C6-N1	-5.99	119.70	122.70
9	A	2464	G	C4-N9-C1'	5.99	134.29	126.50
35	z	34	G	OP2-P-O3'	5.99	118.39	105.20
37	a	1106	C	C2-N1-C1'	5.99	125.39	118.80
9	A	1684	C	C6-N1-C2	5.99	122.69	120.30
9	A	2437	C	C6-N1-C2	-5.99	117.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2660	G	C8-N9-C4	-5.99	104.01	106.40
35	z	67	C	N3-C4-C5	5.99	124.29	121.90
9	A	970	G	C4-N9-C1'	5.98	134.28	126.50
9	A	1184	G	C8-N9-C1'	-5.97	119.23	127.00
35	z	42	C	C6-N1-C2	5.95	122.68	120.30
9	A	525	A	C6-N1-C2	-5.95	115.03	118.60
9	A	1277	G	C4-C5-N7	5.94	113.18	110.80
9	A	2535	C	N1-C2-O2	5.94	122.47	118.90
9	A	2272	G	C5-C6-O6	-5.93	125.04	128.60
9	A	2391	C	C6-N1-C2	5.93	122.67	120.30
9	A	727	A	C2-N3-C4	5.91	113.56	110.60
9	A	901	C	C5-C6-N1	5.91	123.95	121.00
9	A	565	G	C8-N9-C1'	-5.89	119.35	127.00
35	z	70	G	N3-C2-N2	-5.88	115.78	119.90
9	A	2523	U	P-O3'-C3'	5.88	126.75	119.70
9	A	100	G	C8-N9-C4	5.87	108.75	106.40
61	y	140	ARG	NE-CZ-NH1	5.87	123.23	120.30
9	A	2505	A	C8-N9-C4	5.87	108.15	105.80
35	z	36	A	OP2-P-O3'	5.86	118.10	105.20
9	A	1264	C	C5-C6-N1	-5.86	118.07	121.00
9	A	2523	U	C5-C6-N1	5.86	125.63	122.70
35	z	19	G	C4-N9-C1'	-5.86	118.89	126.50
9	A	565	G	N9-C4-C5	-5.85	103.06	105.40
9	A	2343	C	C5-C6-N1	5.85	123.92	121.00
35	z	69	G	N1-C2-N2	5.84	121.46	116.20
37	a	316	C	N1-C2-O2	-5.84	115.39	118.90
35	z	30	G	OP2-P-O3'	5.84	118.05	105.20
9	A	588	A	N7-C8-N9	-5.83	110.88	113.80
9	A	1299	U	C5-C6-N1	-5.82	119.79	122.70
9	A	114	C	C6-N1-C2	-5.80	117.98	120.30
9	A	970	G	N3-C4-N9	5.80	129.48	126.00
9	A	1731	G	N3-C4-N9	5.78	129.47	126.00
9	A	591	C	C5-C6-N1	-5.78	118.11	121.00
10	B	29	C	C6-N1-C2	-5.78	117.99	120.30
9	A	127	C	C6-N1-C2	-5.77	117.99	120.30
9	A	919	A	N1-C6-N6	-5.76	115.14	118.60
9	A	232	G	N3-C4-N9	5.76	129.46	126.00
9	A	486	G	C8-N9-C4	5.76	108.70	106.40
9	A	802	C	C6-N1-C2	5.76	122.60	120.30
9	A	641	C	C2-N3-C4	-5.76	117.02	119.90
35	z	40	C	C6-N1-C2	5.75	122.60	120.30
9	A	1184	G	N3-C4-N9	5.74	129.44	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2610	U	C5-C6-N1	5.74	125.57	122.70
9	A	1334	U	C2-N1-C1'	5.74	124.58	117.70
35	z	42	C	C5-C4-N4	-5.73	116.19	120.20
9	A	2634	C	N3-C4-C5	-5.70	119.62	121.90
37	a	1106	C	N1-C2-O2	5.69	122.32	118.90
37	a	1106	C	C6-N1-C2	-5.69	118.02	120.30
9	A	2592	U	N1-C2-O2	5.69	126.78	122.80
37	a	29	G	C8-N9-C4	-5.68	104.13	106.40
9	A	2035	A	C8-N9-C4	5.68	108.07	105.80
37	a	166	G	N3-C4-C5	-5.68	125.76	128.60
35	z	44	G	N3-C2-N2	-5.67	115.93	119.90
9	A	1334	U	N1-C2-O2	5.67	126.77	122.80
9	A	2343	C	C4-C5-C6	-5.67	114.57	117.40
9	A	585	A	C8-N9-C4	5.66	108.06	105.80
9	A	809	A	N1-C2-N3	5.66	132.13	129.30
9	A	1977	C	C6-N1-C2	-5.65	118.04	120.30
9	A	232	G	C8-N9-C4	5.65	108.66	106.40
37	a	298	A	N9-C4-C5	5.65	108.06	105.80
9	A	565	G	N3-C4-N9	5.63	129.38	126.00
9	A	1445	G	C8-N9-C4	-5.63	104.15	106.40
9	A	1635	C	C2-N1-C1'	5.63	124.99	118.80
9	A	2159	C	C6-N1-C2	-5.62	118.05	120.30
9	A	426	C	C6-N1-C2	5.61	122.55	120.30
9	A	311	U	C5-C6-N1	-5.61	119.90	122.70
9	A	1184	G	N9-C4-C5	-5.60	103.16	105.40
37	a	687	C	C6-N1-C2	-5.60	118.06	120.30
9	A	705	U	C6-N1-C2	5.60	124.36	121.00
9	A	2507	G	N3-C4-C5	5.60	131.40	128.60
9	A	901	C	C6-N1-C1'	-5.60	114.08	120.80
35	z	27	G	O5'-P-OP2	5.60	117.42	110.70
9	A	2805	C	C6-N1-C2	-5.59	118.06	120.30
9	A	564	U	C5-C6-N1	-5.58	119.91	122.70
27	S	79	PRO	N-CA-CB	5.57	109.98	103.30
35	z	46	G	N3-C4-C5	-5.56	125.82	128.60
9	A	1160	A	C8-N9-C4	5.55	108.02	105.80
9	A	951	C	C5-C6-N1	5.55	123.78	121.00
9	A	901	C	N3-C2-O2	-5.55	118.02	121.90
11	C	231	GLY	N-CA-C	-5.54	99.25	113.10
9	A	1713	A	C5-N7-C8	-5.53	101.14	103.90
9	A	1000	G	C4-N9-C1'	5.52	133.68	126.50
9	A	2518	C	C4-C5-C6	5.52	120.16	117.40
9	A	1309	U	C5-C4-O4	5.52	129.21	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2635	G	N9-C4-C5	-5.51	103.20	105.40
35	z	70	G	P-O3'-C3'	5.49	126.29	119.70
9	A	1684	C	C2-N3-C4	-5.49	117.16	119.90
35	z	46	G	N7-C8-N9	5.48	115.84	113.10
9	A	970	G	C5-C6-N1	5.47	114.24	111.50
35	z	70	G	N1-C2-N2	5.47	121.13	116.20
9	A	591	C	C2-N3-C4	-5.47	117.16	119.90
9	A	2007	U	N3-C2-O2	-5.46	118.38	122.20
37	a	298	A	N1-C6-N6	-5.45	115.33	118.60
37	a	1043	G	O4'-C1'-N9	5.44	112.55	108.20
35	z	34	G	N9-C4-C5	-5.44	103.22	105.40
9	A	761	A	C8-N9-C4	-5.44	103.62	105.80
9	A	1400	U	N1-C2-N3	5.44	118.16	114.90
9	A	1333	U	C5-C6-N1	-5.43	119.98	122.70
9	A	1002	G	C5-C6-O6	-5.43	125.34	128.60
9	A	25	G	N1-C6-O6	-5.43	116.64	119.90
9	A	1010	C	C6-N1-C2	5.42	122.47	120.30
9	A	772	A	C5-N7-C8	-5.41	101.19	103.90
37	a	115	C	C2-N1-C1'	5.41	124.75	118.80
11	C	144	LEU	CA-CB-CG	5.40	127.71	115.30
31	W	24	C	N3-C4-C5	5.40	124.06	121.90
9	A	2077	C	C2-N1-C1'	5.39	124.73	118.80
9	A	1272	A	N1-C6-N6	5.38	121.83	118.60
35	z	70	G	OP1-P-O3'	5.38	117.03	105.20
9	A	830	A	N1-C2-N3	5.37	131.99	129.30
9	A	801	U	C5-C6-N1	-5.37	120.02	122.70
9	A	514	A	C8-N9-C4	-5.36	103.66	105.80
9	A	646	G	C5-C6-N1	5.36	114.18	111.50
9	A	970	G	N1-C2-N3	5.36	127.11	123.90
31	W	16	G	N9-C4-C5	-5.35	103.26	105.40
9	A	1497	A	C2-N3-C4	5.35	113.28	110.60
35	z	58	A	N9-C4-C5	-5.34	103.66	105.80
9	A	524	A	N1-C2-N3	5.34	131.97	129.30
9	A	2156	C	C6-N1-C2	-5.34	118.16	120.30
35	z	65	G	C4-C5-N7	-5.34	108.66	110.80
9	A	2535	C	N3-C2-O2	-5.34	118.16	121.90
9	A	1705	A	C8-N9-C4	-5.33	103.67	105.80
9	A	2520	A	C8-N9-C4	-5.33	103.67	105.80
9	A	788	G	C8-N9-C1'	-5.33	120.08	127.00
9	A	2122	C	C5-C6-N1	5.32	123.66	121.00
35	z	47	U	C6-N1-C2	5.32	124.19	121.00
37	a	1018	C	C6-N1-C2	-5.32	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2731	C	C5-C6-N1	-5.32	118.34	121.00
9	A	2075	G	C8-N9-C4	-5.31	104.28	106.40
35	z	40	C	O5'-P-OP2	-5.31	100.92	105.70
9	A	540	A	C5-C6-N1	5.30	120.35	117.70
9	A	1523	A	C8-N9-C4	-5.30	103.68	105.80
35	z	62	C	C6-N1-C2	-5.30	118.18	120.30
9	A	406	C	N3-C4-C5	5.28	124.01	121.90
9	A	745	A	C8-N9-C4	5.28	107.91	105.80
35	z	46	G	N9-C4-C5	5.28	107.51	105.40
35	z	17	C	OP2-P-O3'	5.27	116.80	105.20
9	A	1359	G	C4-N9-C1'	5.26	133.34	126.50
9	A	2065	U	N1-C2-N3	5.26	118.05	114.90
10	B	55	G	C8-N9-C4	-5.25	104.30	106.40
31	W	83	C	N3-C2-O2	-5.25	118.22	121.90
9	A	2047	A	C6-N1-C2	-5.25	115.45	118.60
9	A	2528	U	N1-C2-N3	5.25	118.05	114.90
37	a	351	G	C8-N9-C4	-5.24	104.30	106.40
9	A	1973	G	N3-C4-C5	-5.24	125.98	128.60
9	A	13	A	O4'-C1'-N9	5.24	112.39	108.20
35	z	69	G	N3-C4-N9	-5.24	122.86	126.00
37	a	166	G	C4-N9-C1'	5.24	133.31	126.50
9	A	615	G	C8-N9-C4	5.24	108.50	106.40
9	A	2294	G	N3-C4-C5	-5.24	125.98	128.60
9	A	759	G	O4'-C1'-N9	5.23	112.39	108.20
9	A	514	A	C6-N1-C2	-5.23	115.46	118.60
9	A	1635	C	C5-C6-N1	5.21	123.61	121.00
9	A	2729	A	C2-N3-C4	5.20	113.20	110.60
35	z	29	G	N3-C4-C5	5.20	131.20	128.60
37	a	1148	C	N3-C4-C5	5.20	123.98	121.90
35	z	64	A	N9-C4-C5	-5.20	103.72	105.80
35	z	5	G	C5-N7-C8	5.19	106.90	104.30
9	A	641	C	N3-C4-C5	5.19	123.98	121.90
9	A	1184	G	C5-C6-O6	-5.19	125.48	128.60
9	A	1275	A	C6-N1-C2	-5.19	115.49	118.60
9	A	2408	G	O4'-C1'-N9	5.19	112.35	108.20
35	z	40	C	N3-C4-C5	5.19	123.97	121.90
9	A	730	C	C6-N1-C2	-5.17	118.23	120.30
9	A	316	G	N3-C4-C5	-5.17	126.01	128.60
35	z	33	U	N3-C4-C5	5.17	117.70	114.60
35	z	34	G	O3'-P-O5'	-5.17	94.18	104.00
9	A	1512	U	C2-N1-C1'	5.16	123.89	117.70
9	A	462	G	N3-C4-N9	5.16	129.09	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	571	G	C8-N9-C4	5.16	108.46	106.40
9	A	2065	U	C2-N3-C4	-5.16	123.91	127.00
9	A	2229	U	C2-N1-C1'	5.15	123.88	117.70
9	A	514	A	N1-C2-N3	5.15	131.87	129.30
9	A	1206	C	C5-C6-N1	-5.14	118.43	121.00
9	A	456	C	N1-C2-N3	5.14	122.80	119.20
9	A	173	C	C6-N1-C2	-5.14	118.25	120.30
9	A	805	A	C6-N1-C2	-5.14	115.52	118.60
9	A	2036	U	C6-N1-C2	5.14	124.08	121.00
37	a	298	A	C8-N9-C4	-5.14	103.75	105.80
9	A	2739	A	C2-N3-C4	-5.13	108.03	110.60
9	A	540	A	N1-C2-N3	-5.13	126.73	129.30
9	A	112	C	C2-N1-C1'	5.12	124.43	118.80
9	A	1184	G	N1-C6-O6	5.12	122.97	119.90
35	z	43	C	N3-C4-C5	-5.12	119.85	121.90
9	A	1635	C	N1-C2-O2	5.12	121.97	118.90
9	A	2464	G	C6-C5-N7	-5.11	127.33	130.40
9	A	1988	C	C5-C6-N1	-5.11	118.44	121.00
10	B	55	G	N7-C8-N9	5.11	115.66	113.10
9	A	2272	G	N1-C6-O6	5.11	122.97	119.90
31	W	83	C	N1-C2-O2	5.11	121.97	118.90
9	A	316	G	C4-N9-C1'	5.11	133.14	126.50
9	A	1000	G	C2-N3-C4	5.10	114.45	111.90
9	A	1000	G	C5-C6-N1	5.10	114.05	111.50
9	A	28	U	C2-N3-C4	-5.10	123.94	127.00
9	A	970	G	C8-N9-C1'	-5.09	120.38	127.00
37	a	1003	C	C2-N1-C1'	5.09	124.40	118.80
9	A	58	U	N3-C2-O2	-5.09	118.64	122.20
9	A	2451	A	N1-C6-N6	5.08	121.65	118.60
9	A	2807	C	C6-N1-C2	-5.08	118.27	120.30
37	a	478	G	N3-C4-C5	-5.08	126.06	128.60
9	A	537	U	C5-C6-N1	-5.07	120.17	122.70
9	A	538	C	N1-C2-O2	5.07	121.94	118.90
9	A	592	G	C8-N9-C4	5.07	108.43	106.40
9	A	214	A	C4-C5-N7	5.06	113.23	110.70
9	A	2593	G	C4-N9-C1'	5.06	133.08	126.50
9	A	24	U	C4-C5-C6	5.06	122.73	119.70
9	A	971	U	C6-N1-C2	-5.06	117.97	121.00
56	t	172	GLY	N-CA-C	5.06	125.74	113.10
9	A	2077	C	C6-N1-C2	-5.05	118.28	120.30
35	z	9	A	OP2-P-O3'	5.05	116.31	105.20
9	A	1919	C	N1-C2-O2	5.05	121.93	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	z	70	G	C6-C5-N7	5.05	133.43	130.40
9	A	1055	A	C8-N9-C4	5.05	107.82	105.80
9	A	1788	U	C5-C6-N1	-5.05	120.18	122.70
9	A	830	A	C6-N1-C2	-5.04	115.57	118.60
9	A	1976	C	C5-C4-N4	-5.04	116.67	120.20
9	A	970	G	N1-C2-N2	-5.04	111.67	116.20
9	A	2034	C	C5-C6-N1	-5.03	118.48	121.00
9	A	525	A	N1-C6-N6	-5.02	115.58	118.60
9	A	2360	U	C2-N1-C1'	5.02	123.73	117.70
35	z	35	A	P-O3'-C3'	5.02	125.72	119.70
9	A	2660	G	N3-C4-C5	-5.02	126.09	128.60
9	A	2344	A	C8-N9-C4	-5.02	103.79	105.80
9	A	1000	G	N3-C4-N9	5.01	129.01	126.00
9	A	1060	A	C8-N9-C4	5.01	107.81	105.80
9	A	2069	C	O4'-C1'-N1	5.01	112.21	108.20
37	a	115	C	C6-N1-C2	-5.01	118.30	120.30
9	A	2051	G	N1-C6-O6	-5.00	116.90	119.90
9	A	457	C	N1-C2-O2	-5.00	115.90	118.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	E	134	ARG	Peptide
21	M	104	ALA	Peptide
38	b	74	VAL	Peptide
41	e	144	LYS	Peptide
56	t	173	TRP	Peptide
56	t	75	LYS	Peptide

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	0	536	0	515	27	0
2	1	396	0	437	11	0
3	2	489	0	507	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	467	0	526	11	0
5	4	588	0	658	15	0
6	5	305	0	344	14	0
7	6	422	0	508	8	0
8	7	368	0	386	7	0
9	A	60083	0	30259	664	0
10	B	2584	0	1305	36	0
11	C	1952	0	2038	58	0
12	D	1686	0	1772	55	0
13	E	1676	0	1737	46	0
14	F	1454	0	1488	46	0
15	G	1391	0	1458	36	0
16	H	382	0	437	10	0
17	I	1106	0	1122	38	0
18	J	977	0	1027	33	0
19	K	1648	0	1684	44	0
20	L	942	0	996	27	0
21	M	1410	0	1495	46	0
22	N	1075	0	1134	38	0
23	O	944	0	1004	29	0
24	P	962	0	984	31	0
25	Q	953	0	1050	33	0
26	R	1029	0	1092	40	0
27	S	1310	0	1315	32	0
28	T	1395	0	1482	45	0
29	U	776	0	837	22	0
30	V	1078	0	1144	21	0
31	W	2277	0	1146	27	0
32	X	888	0	923	20	0
33	Y	634	0	684	13	0
34	Z	846	0	918	17	0
35	z	1623	0	821	0	0
36	8	870	0	184	1	0
37	a	31868	0	16050	0	0
38	b	1844	0	1887	0	0
39	c	1736	0	1819	0	0
40	d	1633	0	1730	0	0
41	e	1331	0	1312	0	0
42	f	911	0	923	0	0
43	g	1210	0	1284	0	0
44	h	1079	0	1137	0	0
45	i	1119	0	1181	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	j	805	0	849	0	0
47	k	882	0	928	0	0
48	l	959	0	1035	0	0
49	m	904	0	943	0	0
50	n	820	0	858	0	0
51	o	635	0	686	0	0
52	p	664	0	703	0	0
53	q	693	0	729	0	0
54	r	490	0	532	0	0
55	s	631	0	661	0	0
56	t	853	0	915	0	0
57	u	568	0	576	0	0
58	v	613	0	621	0	0
59	w	686	0	706	0	0
60	x	309	0	323	0	0
61	y	919	0	958	0	0
62	2	1	0	0	0	0
62	5	1	0	0	0	0
63	4	1	0	0	0	0
63	6	1	0	0	0	0
63	7	1	0	0	0	0
63	A	511	0	0	0	0
63	B	15	0	0	0	0
63	C	1	0	0	0	0
63	D	1	0	0	0	0
63	E	1	0	0	0	0
63	F	1	0	0	0	0
63	H	1	0	0	0	0
63	M	2	0	0	0	0
63	P	1	0	0	0	0
63	R	1	0	0	0	0
63	S	1	0	0	0	0
63	T	1	0	0	0	0
63	U	1	0	0	0	0
63	V	1	0	0	0	0
63	W	14	0	0	0	0
63	a	219	0	0	0	0
63	k	1	0	0	0	0
63	l	1	0	0	0	0
63	n	1	0	0	0	0
63	x	1	0	0	0	0
All	All	152465	0	104763	1383	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 9.

All (1383) 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)
9:A:1857:A:HO2'	9:A:1858:A:H8	1.05	0.97
17:I:122:ILE:HD12	17:I:165:CYS:HB2	1.50	0.94
9:A:652:C:N4	9:A:657:U:O4	2.01	0.94
10:B:54:G:HO2'	10:B:55:G:H8	1.00	0.93
9:A:817:C:OP2	21:M:120:ARG:NH1	2.03	0.92
14:F:55:ASN:HA	14:F:59:THR:HB	1.52	0.89
20:L:15:GLY:HA3	20:L:50:THR:HG21	1.57	0.87
9:A:1828:U:OP2	11:C:152:ARG:NH1	2.08	0.86
9:A:540:A:H62	9:A:2055:U:H3	1.24	0.85
9:A:1086:G:H21	18:J:198:ILE:HG12	1.43	0.83
9:A:144:A:OP1	25:Q:160:ARG:NH2	157.24	0.83
9:A:1485:U:H5'	9:A:1486:U:H5'	1.60	0.83
10:B:15:A:H4'	10:B:16:G:H5''	1.60	0.83
9:A:2767:A:H3'	9:A:2768:A:H5''	1.60	0.82
2:1:6:LYS:NZ	9:A:2033:A:N7	2.29	0.81
9:A:2345:A:H2'	9:A:2346:A:C8	2.16	0.80
9:A:2456:A:H4'	9:A:2457:C:H5''	1.62	0.80
13:E:128:SER:HB2	13:E:134:ARG:HH22	1.47	0.80
17:I:139:GLU:HB3	17:I:141:PRO:HD2	1.65	0.79
3:2:49:ARG:HG3	3:2:60:ILE:HD12	1.65	0.79
9:A:1810:C:OP2	11:C:178:ARG:NH2	2.16	0.78
9:A:2142:G:H1	9:A:2174:C:H42	1.28	0.78
9:A:2122:C:O2	9:A:2195:G:N1	2.15	0.78
2:1:13:LYS:NZ	9:A:528:C:OP1	2.16	0.78
9:A:1082:A:H4'	17:I:83:GLY:HA2	1.65	0.78
9:A:844:G:H1'	21:M:130:GLU:HB3	1.66	0.77
14:F:107:ILE:HG23	14:F:118:PRO:HD2	1.66	0.77
9:A:2267:G:O6	9:A:2271:C:N4	2.17	0.77
10:B:8:G:H21	24:P:85:GLN:HE22	1.30	0.77
9:A:2310:U:H5''	24:P:143:ARG:HH12	1.50	0.77
9:A:311:U:OP2	30:V:147:ARG:NH2	2.16	0.77
9:A:2464:G:N7	9:A:2518:C:H2'	2.00	0.76
9:A:2077:C:H42	9:A:2464:G:H1	1.32	0.76
9:A:596:A:H62	9:A:1272:A:H2	1.33	0.76
19:K:97:ASN:HD21	27:S:135:ILE:H	1.31	0.76
25:Q:138:ARG:HH12	25:Q:203:ILE:HB	1.51	0.75
9:A:13:A:H2'	9:A:14:A:C8	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2105:U:OP1	16:H:47:LYS:NZ	2.16	0.75
9:A:2657:G:OP2	19:K:194:ARG:NH2	2.20	0.75
9:A:2151:G:N1	9:A:2169:C:O2	2.20	0.75
9:A:1098:A:N7	9:A:1124:A:O2'	2.20	0.75
20:L:30:ARG:HG2	20:L:32:TYR:H	1.52	0.75
7:6:118:ARG:NH1	9:A:1491:G:OP2	2.15	0.74
1:0:37:ARG:N	10:B:45:G:OP1	2.19	0.74
9:A:1693:U:H2'	9:A:1694:C:H6	1.52	0.74
9:A:2601:U:H5'	9:A:2602:U:H5'	1.69	0.74
19:K:75:PRO:HD2	19:K:88:GLU:HG2	1.68	0.74
6:5:6:SER:HB2	9:A:2483:C:H5''	1.70	0.73
20:L:2:ILE:HB	20:L:33:ALA:HB3	1.70	0.73
9:A:316:G:H22	9:A:339:A:H61	1.35	0.73
22:N:13:HIS:O	22:N:72:LYS:NZ	2.22	0.72
9:A:2726:G:OP1	23:O:28:ARG:NH1	2.22	0.72
12:D:296:LYS:HB3	12:D:302:ILE:HD11	1.71	0.72
24:P:81:HIS:HD2	24:P:100:THR:HB	1.54	0.72
9:A:2256:A:OP1	11:C:239:ARG:NH2	2.23	0.72
15:G:189:ARG:HD2	15:G:204:TYR:HE1	1.55	0.72
9:A:885:G:H1	9:A:911:U:H3	1.38	0.72
9:A:888:C:H3'	9:A:889:G:H8	1.54	0.72
6:5:19:ARG:HG2	9:A:2774:U:H5''	1.72	0.71
11:C:42:ARG:CZ	11:C:44:ILE:HD11	2.21	0.71
12:D:93:MET:H	12:D:121:ASN:HD21	1.36	0.71
10:B:44:C:O2	14:F:145:ARG:NH1	2.23	0.71
1:0:61:THR:HG22	1:0:62:GLY:H	1.56	0.71
21:M:134:MET:SD	21:M:138:ARG:NH1	2.65	0.70
14:F:211:THR:HG22	14:F:213:ALA:H	1.57	0.70
28:T:164:MET:HB2	28:T:168:ARG:HB2	1.74	0.70
9:A:2075:G:N2	9:A:2076:A:N1	2.40	0.69
9:A:1090:U:H1'	18:J:205:ASN:HD21	1.58	0.69
21:M:240:LYS:HE3	21:M:242:ILE:HD11	1.75	0.69
9:A:2125:C:O2	9:A:2161:G:N2	2.23	0.69
12:D:146:ASP:N	12:D:146:ASP:OD1	2.24	0.69
21:M:182:LYS:HE2	21:M:189:PRO:HG2	1.75	0.69
9:A:376:U:O2'	9:A:378:A:N1	2.25	0.69
1:0:60:THR:HB	14:F:52:GLU:HA	1.74	0.69
9:A:45:A:H2'	9:A:46:C:H5'	1.74	0.69
21:M:143:LEU:HB2	21:M:146:ILE:HD12	1.73	0.69
9:A:681:A:H5''	21:M:122:GLY:HA2	1.75	0.69
9:A:879:G:O3'	22:N:6:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:182:A:N6	9:A:2447:A:O2'	2.26	0.68
17:I:77:ALA:HB3	17:I:133:LEU:HB3	1.76	0.68
9:A:9:A:C2	31:W:99:A:H1'	2.28	0.68
27:S:192:ASP:OD1	27:S:193:ASP:N	2.25	0.68
9:A:1978:G:O2'	9:A:1981:C:OP2	2.09	0.68
9:A:1693:U:H2'	9:A:1694:C:C6	2.28	0.68
10:B:43:C:O2'	14:F:116:GLN:NE2	2.26	0.68
9:A:757:U:O2'	9:A:2628:C:O2'	2.12	0.68
26:R:76:TYR:OH	26:R:84:ASP:OD2	2.11	0.68
9:A:1817:G:H5'	9:A:1818:U:OP2	1.94	0.67
9:A:1106:C:O2'	9:A:1116:A:OP1	2.13	0.67
9:A:1604:A:H2'	9:A:1605:A:C8	2.29	0.67
15:G:126:LYS:HE3	15:G:205:VAL:HG11	1.76	0.67
28:T:181:HIS:HB2	28:T:183:ILE:HD11	1.76	0.67
9:A:646:G:OP2	21:M:156:LYS:NZ	2.26	0.67
9:A:1220:U:H1'	26:R:4:VAL:HG22	1.77	0.67
13:E:128:SER:HB2	13:E:134:ARG:NH2	2.09	0.67
9:A:255:A:OP2	9:A:271:G:N1	2.20	0.67
9:A:545:U:H2'	9:A:546:G:C8	2.30	0.67
19:K:100:TRP:H	26:R:99:GLN:HE22	1.42	0.66
9:A:723:G:H2'	9:A:724:G:H5''	1.77	0.66
17:I:63:VAL:HG13	17:I:113:ALA:HB2	1.78	0.66
20:L:88:ASP:OD1	20:L:89:GLN:N	2.27	0.66
9:A:1074:A:O2'	17:I:59:LYS:HD2	1.96	0.66
11:C:23:ASN:HD21	11:C:76:THR:HG21	1.60	0.66
9:A:312:C:OP1	30:V:164:LYS:NZ	2.29	0.66
17:I:56:ARG:HA	17:I:59:LYS:HE2	1.78	0.65
29:U:108:ILE:HD13	34:Z:138:LYS:HD2	1.78	0.65
34:Z:90:LEU:HD21	34:Z:104:ASP:HB3	1.77	0.65
27:S:127:VAL:HG11	27:S:182:VAL:HG21	1.77	0.65
11:C:132:PRO:O	11:C:135:THR:OG1	2.14	0.65
9:A:1075:G:N2	9:A:1138:G:O2'	2.30	0.65
5:4:107:LYS:HB2	9:A:663:A:H5'	1.79	0.65
9:A:1122:U:H1'	9:A:1125:U:H5	1.62	0.65
12:D:93:MET:H	12:D:121:ASN:ND2	1.94	0.65
13:E:104:THR:HG22	13:E:107:GLU:HG2	1.79	0.65
9:A:1494:G:H22	9:A:1550:U:H3	1.43	0.65
2:1:3:VAL:HG12	9:A:2029:A:C2	2.32	0.65
9:A:2486:A:N6	9:A:2498:G:O2'	2.30	0.64
13:E:103:LEU:HB3	13:E:107:GLU:HB2	1.78	0.64
20:L:13:ASN:HD21	20:L:97:ARG:HB3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:176:A:H2'	9:A:177:C:C6	2.32	0.64
9:A:869:G:O2'	9:A:925:G:O6	2.12	0.64
8:7:50:ARG:NH1	9:A:1055:A:O2'	2.30	0.64
9:A:555:A:N6	9:A:558:A:O2'	2.27	0.64
9:A:1092:C:H4'	18:J:161:LYS:HG2	1.79	0.64
9:A:2073:A:N6	9:A:2520:A:O5'	2.30	0.64
9:A:68:C:H2'	9:A:69:G:C8	2.86	0.64
11:C:157:VAL:HB	11:C:190:GLN:HG3	1.80	0.64
12:D:90:ILE:HD11	12:D:137:VAL:HG11	1.78	0.64
9:A:1091:G:O2'	18:J:160:SER:O	2.16	0.64
9:A:2069:C:H5'	9:A:2070:A:H5''	1.79	0.64
9:A:2077:C:N4	9:A:2464:G:H1	1.95	0.64
19:K:206:GLY:O	19:K:210:LYS:NZ	2.31	0.64
9:A:426:C:H2'	9:A:427:A:C8	2.33	0.63
9:A:1211:G:H5''	21:M:111:GLY:HA2	1.80	0.63
9:A:2719:G:OP1	23:O:83:LYS:NZ	2.32	0.63
20:L:76:ILE:HB	25:Q:195:VAL:HB	1.78	0.63
9:A:1531:A:N6	11:C:94:ASP:OD2	2.31	0.63
34:Z:81:LEU:HD11	34:Z:144:ILE:HD12	1.81	0.63
26:R:26:GLY:O	26:R:30:ARG:NH1	2.32	0.63
9:A:2628:C:H5'	9:A:2629:A:OP2	1.99	0.63
9:A:555:A:H61	9:A:558:A:HO2'	1.45	0.63
11:C:133:LEU:HD21	11:C:163:LYS:HE2	1.81	0.63
25:Q:184:ARG:HG3	25:Q:193:GLU:HG2	1.80	0.63
29:U:183:ASN:HB3	29:U:186:GLU:HG3	1.79	0.63
9:A:157:G:O2'	9:A:159:A:OP1	2.12	0.62
9:A:2290:A:H2'	9:A:2291:A:C8	2.34	0.62
9:A:394:G:H22	9:A:404:U:H3	1.46	0.62
14:F:56:ARG:O	14:F:60:ASN:HB3	1.98	0.62
9:A:2142:G:H1	9:A:2174:C:N4	1.97	0.62
9:A:757:U:HO2'	9:A:2628:C:HO2'	1.47	0.62
9:A:2047:A:O2'	9:A:2049:G:OP2	2.17	0.62
9:A:468:U:O2	9:A:471:U:O2'	2.16	0.62
23:O:89:LEU:HD22	23:O:93:VAL:HG23	1.81	0.62
14:F:160:ALA:HB1	14:F:190:VAL:HB	1.82	0.62
12:D:88:ALA:O	12:D:294:PRO:HG2	1.99	0.62
18:J:84:LEU:HD21	18:J:95:VAL:HB	1.81	0.62
9:A:701:U:O2'	9:A:791:G:OP1	2.16	0.62
25:Q:153:LEU:HD12	25:Q:165:TYR:HE2	1.62	0.62
23:O:11:MET:SD	23:O:11:MET:N	2.73	0.62
9:A:2761:U:OP2	9:A:2773:C:N4	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:577:G:O3'	21:M:115:ARG:NH2	2.32	0.62
9:A:144:A:P	25:Q:160:ARG:HH22	157.64	0.62
21:M:98:LYS:HE2	21:M:106:GLN:HG3	1.80	0.62
23:O:67:GLU:OE1	23:O:72:LYS:HE3	2.00	0.61
9:A:2807:C:HO2'	31:W:95:A:HO2'	1.43	0.61
11:C:75:VAL:HG13	11:C:76:THR:HG22	1.83	0.61
20:L:30:ARG:HD3	20:L:32:TYR:O	2.00	0.61
9:A:1271:G:H4'	9:A:1311:C:C5	67.23	0.61
9:A:635:C:H2'	9:A:636:C:C6	2.35	0.61
9:A:2767:A:H3'	9:A:2768:A:C5'	2.30	0.61
9:A:622:G:H2'	9:A:623:A:C8	6.18	0.61
13:E:104:THR:HG23	13:E:106:ALA:H	1.65	0.61
17:I:100:THR:HG21	17:I:143:ALA:HB2	1.83	0.61
13:E:230:THR:HG22	13:E:231:PRO:HD2	1.81	0.61
32:X:120:ASP:N	32:X:120:ASP:OD1	2.34	0.61
9:A:241:A:H2'	9:A:242:A:C8	2.34	0.61
29:U:119:ILE:HG13	29:U:135:LEU:HB3	1.82	0.61
9:A:2284:A:H5''	9:A:2285:A:H5'	1.82	0.61
9:A:98:G:H2'	30:V:175:TRP:CZ2	2.36	0.61
9:A:1520:A:O2'	9:A:1543:G:O6	2.13	0.61
9:A:1883:G:H2'	9:A:1884:A:O4'	2.01	0.61
9:A:2206:A:H2'	9:A:2207:A:C8	2.36	0.61
9:A:420:A:H2'	9:A:421:A:H8	1.65	0.61
13:E:243:GLU:OE1	21:M:81:ARG:NH2	2.34	0.61
13:E:60:PHE:O	13:E:196:ARG:NH1	2.33	0.61
19:K:121:ASP:O	19:K:247:ARG:NH1	2.32	0.61
32:X:93:ILE:HG22	32:X:94:ILE:HG13	1.83	0.61
20:L:68:GLU:HG3	20:L:78:ARG:HB2	1.83	0.61
4:3:99:THR:O	9:A:697:U:O2'	2.20	0.60
9:A:976:C:O2	9:A:983:G:N2	18.70	0.60
9:A:1002:G:HO2'	9:A:1147:U:H5	48.20	0.60
12:D:143:ARG:HG2	12:D:144:LEU:H	1.65	0.60
26:R:112:TYR:CZ	26:R:116:ILE:HD11	2.37	0.60
9:A:1837:U:H5'	9:A:1985:A:H5'	1.83	0.60
27:S:208:ARG:HH11	27:S:208:ARG:HG3	1.65	0.60
15:G:166:GLU:HG3	15:G:168:ASN:HB2	1.84	0.60
26:R:92:LEU:HD22	26:R:96:ILE:HG21	1.84	0.60
17:I:100:THR:HG22	17:I:135:VAL:HG12	1.84	0.59
1:0:43:PRO:HG3	14:F:111:ALA:HB1	1.84	0.59
9:A:530:U:H2'	9:A:531:A:H8	1.67	0.59
26:R:49:ASP:HA	26:R:52:ARG:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:77:HIS:CG	1:0:78:PRO:HD2	2.38	0.59
9:A:2345:A:H2'	9:A:2346:A:H8	1.62	0.59
19:K:191:LEU:HD13	19:K:199:ILE:HG13	1.85	0.59
27:S:208:ARG:HH11	27:S:208:ARG:CG	2.16	0.59
9:A:1090:U:H1'	18:J:205:ASN:ND2	2.17	0.59
9:A:944:C:H2'	9:A:945:A:H5''	5.66	0.59
24:P:129:LYS:O	24:P:133:GLU:HG2	2.01	0.59
9:A:1291:C:H5''	9:A:1292:G:H5'	1.84	0.59
9:A:1570:C:H4'	9:A:1571:G:C2	2.37	0.59
23:O:106:ARG:HH11	23:O:126:VAL:HG21	1.68	0.59
9:A:1055:A:C2	9:A:2505:A:H5'	2.38	0.59
11:C:223:PRO:HD3	11:C:230:GLY:H	1.66	0.59
30:V:176:LYS:O	30:V:180:ASN:ND2	2.36	0.59
3:2:59:THR:HG22	3:2:60:ILE:H	1.68	0.58
9:A:2269:G:H2'	9:A:2270:G:C8	2.38	0.58
9:A:474:C:O2'	13:E:118:GLN:NE2	2.36	0.58
9:A:76:U:OP1	34:Z:114:ARG:NH2	2.36	0.58
5:4:101:ARG:NH2	9:A:235:G:OP2	2.35	0.58
21:M:83:ASP:OD1	21:M:83:ASP:N	2.35	0.58
33:Y:97:ARG:HG2	33:Y:98:LEU:N	2.17	0.58
9:A:2203:U:H2'	9:A:2204:A:O4'	2.04	0.58
10:B:29:C:OP1	24:P:78:SER:OG	2.21	0.58
17:I:73:CYS:SG	17:I:134:PHE:HB3	2.44	0.58
11:C:244:THR:HG22	11:C:245:PRO:HD2	1.85	0.58
20:L:102:ILE:HG22	20:L:103:ALA:H	1.69	0.58
20:L:15:GLY:HA2	20:L:47:ILE:HD12	1.84	0.58
27:S:128:VAL:HG22	27:S:133:GLN:HG2	1.85	0.58
28:T:79:LEU:HB3	28:T:134:ILE:HD11	1.85	0.58
1:0:42:HIS:CE1	14:F:116:GLN:HE22	2.22	0.58
9:A:2340:G:C2'	9:A:2341:U:H5'	2.33	0.58
21:M:84:ASN:N	21:M:84:ASN:OD1	2.37	0.58
9:A:2198:A:H2'	9:A:2199:G:C8	2.38	0.58
9:A:296:G:H2'	9:A:297:U:C6	2.39	0.58
17:I:103:ILE:HD12	17:I:134:PHE:HE2	1.69	0.58
9:A:1689:C:O2'	23:O:19:ARG:NH2	2.37	0.58
9:A:2329:U:H5'	14:F:138:LEU:HD12	1.85	0.57
9:A:1074:A:N1	17:I:63:VAL:HG21	2.19	0.57
22:N:44:SER:HB3	22:N:70:PRO:HG3	1.85	0.57
29:U:135:LEU:HD21	29:U:175:TYR:CD2	2.39	0.57
19:K:52:SER:HB3	31:W:1:A:O4'	2.04	0.57
15:G:44:GLY:HA3	15:G:105:HIS:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:189:ARG:HD2	15:G:204:TYR:CE1	2.39	0.57
8:7:68:ALA:HB1	8:7:70:TRP:CD1	2.39	0.57
9:A:1385:G:H5''	33:Y:73:ARG:HH21	1.70	0.57
9:A:1887:G:H2'	9:A:1888:G:H8	1.69	0.57
9:A:548:G:O2'	9:A:549:A:O5'	2.23	0.57
15:G:76:TYR:OH	15:G:112:THR:HG21	2.04	0.57
6:5:17:ILE:HG22	6:5:18:ARG:H	1.68	0.57
9:A:1497:A:O2'	9:A:1498:G:H5'	2.04	0.57
9:A:1559:A:H3'	9:A:1560:C:H6	1.68	0.57
14:F:54:ILE:HG23	14:F:58:LYS:HZ2	1.69	0.57
28:T:141:HIS:O	28:T:142:PHE:HB2	2.04	0.57
12:D:273:LEU:HD13	25:Q:126:LEU:HD21	1.85	0.57
30:V:98:SER:OG	30:V:98:SER:O	2.18	0.57
28:T:62:LEU:HD22	28:T:77:PHE:CE1	2.39	0.57
9:A:1812:A:H2'	9:A:1813:A:C8	2.40	0.57
9:A:622:G:H2'	9:A:623:A:H8	5.56	0.57
27:S:208:ARG:NH1	27:S:208:ARG:HG3	2.19	0.57
9:A:531:A:H2'	9:A:532:A:C8	2.40	0.57
15:G:48:ILE:HB	15:G:90:LEU:HB2	1.87	0.57
9:A:1133:U:H2'	9:A:1134:G:H8	1.70	0.57
11:C:121:LYS:HG2	11:C:124:ASN:ND2	2.20	0.57
14:F:155:ARG:HG2	14:F:159:LEU:HD23	1.87	0.57
13:E:240:LEU:O	21:M:81:ARG:HD3	2.05	0.57
9:A:1444:A:H2'	9:A:1445:G:C8	2.40	0.56
9:A:2250:A:H2'	9:A:2251:G:C8	2.39	0.56
17:I:161:PHE:HE2	17:I:176:VAL:HG11	1.69	0.56
28:T:31:GLU:OE2	28:T:176:ARG:NH2	2.37	0.56
17:I:120:ALA:HB1	17:I:123:LYS:HE3	1.87	0.56
9:A:2352:A:N7	9:A:2354:G:C5	2.72	0.56
18:J:79:VAL:HG22	18:J:130:THR:HG23	1.87	0.56
9:A:1690:A:OP2	23:O:11:MET:HA	2.05	0.56
28:T:88:SER:O	28:T:92:GLN:HA	2.05	0.56
10:B:4:U:H2'	10:B:5:C:C6	2.41	0.56
23:O:54:MET:HE1	23:O:123:ILE:HG21	1.87	0.56
5:4:125:ASN:ND2	5:4:127:LYS:H	2.04	0.56
9:A:2546:G:H5''	9:A:2547:U:H5''	1.87	0.56
6:5:31:LYS:HE2	9:A:2495:A:H5'	1.88	0.56
9:A:1289:A:H2'	9:A:1290:A:O4'	2.06	0.56
9:A:754:A:O2'	9:A:1695:U:OP1	2.23	0.56
9:A:232:G:OP2	9:A:234:C:N4	2.36	0.56
13:E:72:LEU:HD22	13:E:259:TYR:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Z:108:MET:O	34:Z:112:VAL:HG23	2.06	0.56
1:0:37:ARG:HB3	1:0:42:HIS:HD2	1.69	0.56
13:E:238:ASP:OD1	13:E:238:ASP:N	2.38	0.56
32:X:93:ILE:HD11	32:X:117:ALA:HB2	1.87	0.56
6:5:3:ILE:HD13	9:A:2556:C:H4'	1.86	0.56
9:A:1019:U:H2'	9:A:1020:C:C6	3.08	0.56
18:J:164:GLN:NE2	18:J:204:ALA:O	2.38	0.56
31:W:32:C:H2'	31:W:33:A:H2'	1.86	0.56
9:A:1497:A:N3	9:A:1497:A:H2'	2.21	0.56
29:U:138:VAL:HG22	29:U:172:LYS:HB3	1.87	0.56
9:A:1603:A:H2'	9:A:1604:A:C8	2.41	0.56
22:N:91:GLU:HB2	22:N:92:TYR:CD1	2.40	0.56
9:A:628:A:OP1	13:E:157:ARG:HD3	2.06	0.55
33:Y:77:PHE:HD2	33:Y:137:VAL:HG12	1.71	0.55
9:A:411:U:H1'	16:H:42:GLN:HE21	1.70	0.55
12:D:186:LEU:HB2	12:D:189:GLU:HG3	1.89	0.55
29:U:138:VAL:HG21	29:U:147:ILE:HD11	1.88	0.55
9:A:1593:U:O2'	9:A:1594:A:OP1	2.23	0.55
9:A:495:A:O2'	30:V:121:GLY:HA3	2.06	0.55
9:A:953:G:H2'	9:A:954:G:H8	1.69	0.55
10:B:29:C:H2'	10:B:30:A:O4'	2.07	0.55
14:F:188:GLN:OE1	14:F:205:MET:HG3	2.07	0.55
25:Q:213:LYS:NZ	31:W:67:U:OP1	2.25	0.55
18:J:176:LEU:HB3	18:J:196:MET:HG3	1.88	0.55
26:R:96:ILE:HG23	26:R:100:ILE:HD12	1.88	0.55
9:A:1854:C:H5'	11:C:252:GLY:O	2.07	0.55
15:G:76:TYR:HE1	15:G:108:PHE:HB3	1.70	0.55
9:A:2292:C:H1'	22:N:85:SER:H	1.72	0.55
30:V:178:ILE:HA	30:V:181:LYS:HD2	1.87	0.55
9:A:543:A:H2'	9:A:543:A:N3	2.21	0.55
14:F:61:TYR:OH	14:F:82:PRO:O	2.17	0.55
9:A:2519:G:O2'	9:A:2521:U:OP2	2.25	0.55
9:A:490:A:H1'	30:V:108:LYS:HZ1	1.72	0.55
19:K:130:THR:HG21	19:K:241:LEU:HD23	1.87	0.55
21:M:159:PRO:O	21:M:160:ILE:HD13	2.07	0.55
3:2:36:GLN:HE21	9:A:2302:C:H41	1.53	0.55
9:A:1073:G:H4'	9:A:1074:A:H5''	1.89	0.55
9:A:2142:G:N3	9:A:2187:A:O2'	2.37	0.55
9:A:2715:U:H2'	9:A:2716:C:C6	2.42	0.55
9:A:670:A:O2'	9:A:671:C:H5'	3.64	0.55
14:F:187:GLU:HG2	14:F:202:ALA:HB1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:34:LEU:HB3	23:O:54:MET:SD	2.47	0.55
14:F:97:SER:HB3	14:F:137:THR:O	2.06	0.54
9:A:1111:G:N1	9:A:1114:A:OP2	2.39	0.54
9:A:420:A:H2'	9:A:421:A:C8	2.41	0.54
9:A:548:G:O2'	9:A:549:A:H8	1.89	0.54
9:A:1917:G:OP1	11:C:236:PRO:HB2	2.07	0.54
10:B:92:U:OP1	22:N:16:ARG:HG3	2.08	0.54
27:S:104:ASN:HA	27:S:107:ILE:HG22	1.89	0.54
9:A:1073:G:OP1	17:I:59:LYS:NZ	2.39	0.54
23:O:62:ILE:HG21	23:O:104:TYR:CD2	2.42	0.54
27:S:137:ILE:HG13	27:S:140:ARG:HG3	1.88	0.54
8:7:54:LYS:HE2	9:A:2473:C:O3'	2.07	0.54
9:A:2116:C:N3	9:A:2201:G:N2	2.52	0.54
18:J:179:ILE:HG22	18:J:199:ILE:HD12	1.89	0.54
9:A:211:A:H2'	9:A:212:A:C8	2.43	0.54
17:I:154:ARG:HD2	17:I:159:ASN:HB2	1.88	0.54
27:S:166:THR:HG22	27:S:168:ALA:H	1.73	0.54
29:U:165:LEU:HD23	29:U:173:LYS:HD3	1.90	0.54
10:B:31:C:OP1	24:P:49:ARG:HD2	2.07	0.54
25:Q:118:LYS:HB2	25:Q:121:ASP:OD2	2.08	0.54
9:A:1189:G:H5'	27:S:148:LYS:HE2	1.89	0.54
11:C:256:ARG:HH22	11:C:262:SER:HB2	1.71	0.54
22:N:91:GLU:HB2	22:N:92:TYR:HD1	1.73	0.54
23:O:61:MET:HG3	23:O:80:ILE:HD11	1.90	0.54
9:A:1073:G:H5''	9:A:1075:G:H5''	1.88	0.54
9:A:1452:A:H8	9:A:1480:A:HO2'	52.79	0.54
9:A:2254:A:H2'	9:A:2256:A:N7	2.23	0.54
9:A:2662:C:HO2'	9:A:2750:G:HO2'	1.55	0.54
9:A:1840:C:OP1	11:C:200:ARG:NH2	2.41	0.54
9:A:126:C:H2'	9:A:127:C:H6	1.73	0.54
9:A:2154:C:H42	9:A:2165:G:H22	1.55	0.54
9:A:2549:G:N2	9:A:2680:G:O2'	2.41	0.54
9:A:70:A:H4'	9:A:71:A:H5''	1.90	0.54
10:B:5:C:H2'	10:B:6:U:C6	2.42	0.54
14:F:161:LEU:O	14:F:164:THR:OG1	2.19	0.54
18:J:150:LEU:HD13	18:J:203:ALA:HB2	1.89	0.54
19:K:80:ASP:OD1	19:K:80:ASP:N	2.40	0.54
21:M:161:ASN:HA	21:M:201:LEU:O	2.08	0.54
9:A:1019:U:H2'	9:A:1020:C:H6	2.39	0.54
9:A:13:A:H2'	9:A:14:A:H8	1.70	0.53
26:R:17:ILE:HG23	26:R:39:LYS:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:99:LYS:O	7:6:103:LYS:HG2	2.07	0.53
9:A:1084:G:H5''	9:A:1085:A:H5'	1.89	0.53
11:C:207:LYS:HD2	11:C:212:LYS:HD3	1.89	0.53
18:J:189:CYS:SG	18:J:195:ALA:HB2	2.49	0.53
10:B:50:U:P	24:P:151:ARG:HE	2.32	0.53
9:A:1438:G:H2'	9:A:1439:U:C6	3.50	0.53
9:A:2464:G:H2'	9:A:2518:C:C5	2.43	0.53
9:A:656:A:H2'	9:A:658:A:C8	2.43	0.53
19:K:97:ASN:HD21	27:S:135:ILE:N	2.04	0.53
9:A:2154:C:N4	9:A:2165:G:H22	2.07	0.53
32:X:143:GLN:O	32:X:145:GLU:N	2.40	0.53
1:0:57:LEU:HD21	1:0:59:MET:HG2	1.90	0.53
9:A:2447:A:N3	9:A:2447:A:H2'	2.24	0.53
9:A:423:G:OP2	9:A:2423:A:O2'	2.25	0.53
31:W:29:U:H2'	31:W:83:C:H42	1.73	0.53
9:A:177:C:H2'	9:A:178:U:H5'	1.89	0.53
14:F:164:THR:HG22	14:F:165:ARG:H	1.73	0.53
24:P:46:ALA:HB1	24:P:51:GLU:OE1	2.09	0.53
30:V:60:ASN:O	30:V:61:SER:OG	2.21	0.53
9:A:1211:G:OP1	21:M:109:SER:OG	2.24	0.53
15:G:71:GLU:O	15:G:176:ARG:NH1	2.41	0.53
28:T:113:LYS:HG3	28:T:125:ILE:HB	1.91	0.53
9:A:1844:U:H5''	9:A:1845:G:H5'	1.89	0.53
9:A:2729:A:N3	9:A:2729:A:H2'	2.24	0.53
9:A:306:G:H2'	9:A:307:C:H6	1.74	0.53
18:J:129:ILE:HD11	18:J:137:PHE:HB2	1.90	0.53
20:L:13:ASN:ND2	20:L:97:ARG:HB3	2.23	0.53
22:N:126:PRO:HG2	22:N:127:ILE:HG23	1.90	0.53
23:O:20:LEU:HD13	23:O:30:LEU:HD23	1.91	0.53
9:A:2390:A:H2'	9:A:2391:C:C6	2.44	0.53
9:A:37:A:H2'	9:A:38:C:C6	2.44	0.53
12:D:170:GLU:O	12:D:291:ARG:NH2	2.41	0.53
10:B:9:U:OP1	24:P:53:ARG:NH2	2.41	0.53
1:0:53:CYS:HB3	1:0:57:LEU:HB3	1.91	0.53
9:A:58:U:H1'	9:A:72:A:H2'	1.91	0.53
17:I:76:LEU:HD22	17:I:134:PHE:HD1	1.74	0.53
20:L:71:ARG:HD3	20:L:75:MET:HE2	1.89	0.53
25:Q:138:ARG:NH1	25:Q:203:ILE:HB	2.22	0.53
9:A:2464:G:H2'	9:A:2518:C:H5	1.74	0.52
6:5:10:ILE:HG13	9:A:2494:C:N4	2.23	0.52
9:A:297:U:C5	9:A:298:G:C8	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:576:U:H2'	9:A:577:G:O4'	2.09	0.52
9:A:793:A:N7	11:C:216:VAL:HG21	2.24	0.52
12:D:214:ARG:NH1	12:D:250:MET:O	2.42	0.52
20:L:63:VAL:HG23	20:L:64:ARG:HG3	1.91	0.52
9:A:2133:A:H62	9:A:2181:U:H1'	1.73	0.52
9:A:2396:G:H2'	9:A:2397:U:C6	2.44	0.52
9:A:2470:A:H2'	9:A:2471:G:H8	1.74	0.52
9:A:640:G:H2'	9:A:641:C:C6	2.44	0.52
24:P:76:PHE:CE2	24:P:78:SER:HB3	2.45	0.52
32:X:97:ARG:HA	32:X:97:ARG:HH11	1.74	0.52
9:A:2464:G:H4'	9:A:2465:A:H5'	1.92	0.52
28:T:63:MET:HA	28:T:66:GLU:CD	2.29	0.52
9:A:1887:G:H2'	9:A:1888:G:C8	2.43	0.52
14:F:88:VAL:HG13	14:F:208:CYS:HB2	1.91	0.52
19:K:177:SER:OG	19:K:179:ARG:HG3	2.10	0.52
3:2:20:ARG:HG2	3:2:30:VAL:HG21	1.92	0.52
7:6:132:PRO:O	7:6:135:LYS:N	2.39	0.52
9:A:1408:A:H5'	9:A:1488:A:H1'	1.90	0.52
15:G:187:THR:O	15:G:190:SER:OG	2.22	0.52
23:O:64:LEU:HD23	23:O:76:ALA:HB2	1.92	0.52
24:P:84:VAL:HG21	24:P:155:LEU:HD11	1.91	0.52
26:R:31:LEU:O	26:R:35:ILE:HG13	2.09	0.52
26:R:79:SER:OG	26:R:80:LYS:N	2.41	0.52
9:A:1168:U:H4'	9:A:1169:A:O4'	2.10	0.52
10:B:114:G:H2'	10:B:115:C:C6	2.44	0.52
9:A:1813:A:OP1	11:C:257:LYS:HE3	2.10	0.52
18:J:92:ALA:HB3	18:J:93:PRO:HD3	1.92	0.52
1:0:74:SER:OG	1:0:75:GLY:N	2.43	0.52
6:5:9:PRO:HD3	6:5:16:LEU:HD21	1.91	0.52
9:A:1487:C:H5'	9:A:1488:A:OP1	2.10	0.52
9:A:815:A:H2'	9:A:817:C:C4	2.45	0.52
9:A:1195:U:H5''	9:A:1196:A:H2'	1.90	0.52
9:A:296:G:H2'	9:A:297:U:C5	2.44	0.52
20:L:21:CYS:HB2	20:L:39:ILE:HD12	1.92	0.52
9:A:984:G:OP2	22:N:14:ARG:NH1	2.43	0.52
9:A:1321:A:H4'	9:A:1322:A:H5''	1.92	0.52
9:A:1437:G:H2'	9:A:1438:G:C8	2.45	0.52
9:A:2330:U:H2'	9:A:2331:G:H8	1.74	0.52
9:A:2524:C:C2	9:A:2599:G:N2	2.78	0.52
9:A:2332:G:H2'	9:A:2333:C:C6	2.45	0.51
9:A:488:G:N2	9:A:491:A:OP2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:530:U:H2'	9:A:531:A:C8	2.45	0.51
9:A:548:G:HO2'	9:A:549:A:P	2.32	0.51
28:T:70:TYR:HB2	28:T:73:CYS:SG	2.50	0.51
9:A:1689:C:OP1	31:W:18:G:N1	2.33	0.51
9:A:1953:U:OP1	9:A:2621:U:O2'	2.27	0.51
19:K:239:LEU:HD12	19:K:240:PRO:HD2	1.91	0.51
22:N:61:GLY:HA3	22:N:109:VAL:HG13	1.92	0.51
9:A:2249:C:P	33:Y:97:ARG:HH22	2.34	0.51
9:A:261:U:H3	9:A:266:A:H61	1.58	0.51
11:C:237:ILE:HD11	11:C:242:PRO:HG3	1.92	0.51
32:X:159:ARG:HG2	32:X:163:GLU:OE2	2.10	0.51
9:A:1559:A:H5'	9:A:1560:C:OP2	2.11	0.51
9:A:843:C:H2'	9:A:844:G:C8	2.45	0.51
19:K:164:SER:O	19:K:167:LYS:HB2	2.09	0.51
22:N:77:ARG:NH2	22:N:86:GLY:O	2.37	0.51
9:A:758:U:H4'	28:T:121:ARG:HH21	1.75	0.51
5:4:113:ARG:HB2	21:M:141:PRO:HG2	1.92	0.51
28:T:152:LEU:HD22	28:T:156:LYS:HB3	1.93	0.51
13:E:206:LEU:HD11	13:E:229:LEU:HG	1.91	0.51
16:H:69:VAL:HG12	16:H:70:ARG:O	2.11	0.51
25:Q:130:ALA:HB1	25:Q:177:ILE:HD12	1.91	0.51
3:2:42:THR:O	3:2:42:THR:OG1	2.29	0.51
4:3:123:GLY:O	4:3:126:LEU:HB2	2.10	0.51
9:A:2103:G:C6	9:A:2104:A:N7	2.78	0.51
22:N:59:ARG:HG3	22:N:60:ARG:H	1.75	0.51
9:A:2528:U:H2'	9:A:2529:C:O4'	2.11	0.51
10:B:61:C:H2'	10:B:62:U:H6	1.76	0.51
24:P:71:PRO:HD2	24:P:139:VAL:HG12	1.93	0.51
27:S:106:ILE:HD13	28:T:162:GLY:HA3	1.92	0.51
28:T:167:GLY:O	28:T:171:GLU:HG2	2.10	0.51
30:V:99:THR:HB	30:V:129:ALA:HB1	1.93	0.51
9:A:2147:G:H21	9:A:2172:A:H61	1.57	0.51
9:A:2149:A:H1'	9:A:2173:G:O2'	2.11	0.51
14:F:153:LEU:HD21	14:F:226:MET:HE1	1.92	0.51
23:O:106:ARG:NH1	23:O:126:VAL:HG21	2.26	0.51
23:O:72:LYS:NZ	31:W:74:C:OP1	2.24	0.51
9:A:2078:C:C2	9:A:2464:G:N2	2.79	0.50
9:A:2381:C:H2'	9:A:2382:G:O4'	2.11	0.50
20:L:101:ALA:C	20:L:102:ILE:HG12	2.32	0.50
22:N:1:MET:HG2	22:N:44:SER:HB2	1.91	0.50
9:A:880:U:P	22:N:6:ARG:HH11	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2136:U:OP2	9:A:2183:A:O2'	2.27	0.50
11:C:138:HIS:ND1	11:C:189:GLY:O	2.26	0.50
12:D:166:ARG:NH1	31:W:26:G:OP1	2.44	0.50
12:D:193:GLU:OE2	12:D:268:LYS:HA	2.11	0.50
13:E:206:LEU:HB3	13:E:245:LEU:HD22	1.92	0.50
30:V:83:GLU:CD	30:V:106:ASN:H	2.14	0.50
9:A:1087:G:H1'	18:J:198:ILE:HG23	1.93	0.50
9:A:1273:G:H1	26:R:37:GLN:HE21	1.59	0.50
9:A:2150:G:N1	9:A:2170:C:H1'	2.26	0.50
9:A:2204:A:H3'	9:A:2205:G:H8	1.76	0.50
9:A:2066:G:H4'	12:D:237:ALA:O	2.11	0.50
13:E:167:SER:O	21:M:79:ARG:HG3	2.11	0.50
17:I:75:LEU:HD13	17:I:140:ILE:HB	1.93	0.50
22:N:54:MET:HE1	22:N:104:TYR:HB3	1.93	0.50
28:T:94:ASN:HB3	28:T:97:ASN:ND2	2.26	0.50
4:3:111:THR:O	4:3:116:LEU:HD23	2.10	0.50
9:A:1040:U:OP1	26:R:70:ARG:NH2	2.45	0.50
9:A:1363:A:O2'	9:A:1365:U:OP2	2.27	0.50
9:A:2221:U:H2'	9:A:2222:C:C6	2.47	0.50
9:A:2331:G:H5'	14:F:88:VAL:HG11	1.92	0.50
14:F:67:PRO:O	14:F:71:GLU:HG2	2.11	0.50
14:F:73:PHE:CE2	14:F:221:LYS:HD2	2.46	0.50
15:G:82:VAL:HG22	15:G:92:VAL:HG22	1.93	0.50
19:K:75:PRO:CD	19:K:88:GLU:HG2	2.39	0.50
4:3:144:PRO:HG2	4:3:149:ARG:HB2	1.94	0.50
9:A:1133:U:H2'	9:A:1134:G:C8	2.45	0.50
11:C:121:LYS:HE2	11:C:124:ASN:HD21	1.77	0.50
15:G:94:LYS:HE2	15:G:105:HIS:CE1	2.46	0.50
2:1:22:LYS:O	2:1:25:TYR:HB3	2.12	0.50
6:5:37:GLY:HA2	9:A:1153:G:H5'	1.92	0.50
12:D:237:ALA:HB3	12:D:241:PRO:HD2	1.94	0.50
17:I:154:ARG:HA	17:I:157:GLU:HB2	1.94	0.50
22:N:52:ARG:HH11	22:N:52:ARG:HB3	1.76	0.50
28:T:186:PHE:O	28:T:190:ILE:HG13	2.12	0.50
9:A:2464:G:N2	9:A:2467:A:C6	2.80	0.50
25:Q:138:ARG:HH22	25:Q:203:ILE:CG2	2.25	0.50
9:A:1635:C:OP1	29:U:144:LYS:HB2	2.12	0.50
9:A:1209:U:O2'	9:A:1210:A:H5'	2.11	0.50
9:A:2460:U:H2'	9:A:2461:A:C8	2.47	0.50
9:A:591:C:H2'	9:A:592:G:C8	2.46	0.50
19:K:159:ASP:OD1	19:K:159:ASP:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Z:89:MET:HG2	34:Z:152:LEU:HB2	1.94	0.50
9:A:1420:C:OP1	29:U:160:ARG:NH2	2.45	0.50
9:A:312:C:H2'	9:A:313:A:C8	2.47	0.49
10:B:83:U:H3	10:B:96:G:H1	1.59	0.49
9:A:740:G:C8	11:C:203:ARG:NH1	2.80	0.49
9:A:1557:G:N3	9:A:1557:G:H2'	2.26	0.49
9:A:640:G:H2'	9:A:641:C:H6	1.76	0.49
15:G:99:ARG:O	15:G:103:GLN:HG3	2.12	0.49
3:2:45:ARG:NH2	3:2:47:GLU:OE1	2.45	0.49
9:A:241:A:H2'	9:A:242:A:H8	1.77	0.49
22:N:67:ARG:NH1	22:N:105:GLU:OE1	2.43	0.49
32:X:71:ASP:CG	32:X:72:SER:H	2.15	0.49
3:2:56:TYR:O	9:A:2388:G:H4'	2.12	0.49
9:A:1466:G:H1'	9:A:1933:A:O3'	109.85	0.49
9:A:888:C:H5	9:A:908:A:H2	1.61	0.49
9:A:947:A:H2'	9:A:948:U:H5''	1.94	0.49
1:0:62:GLY:O	14:F:155:ARG:HD3	2.13	0.49
28:T:188:TYR:HE2	28:T:195:ARG:HB2	1.76	0.49
9:A:1700:A:H61	9:A:2010:C:H42	1.60	0.49
9:A:1837:U:H2'	9:A:1838:G:O4'	2.12	0.49
9:A:984:G:N7	22:N:14:ARG:NH2	2.60	0.49
25:Q:118:LYS:O	25:Q:121:ASP:HB2	2.13	0.49
33:Y:110:TRP:CE3	33:Y:113:GLY:HA3	2.47	0.49
1:0:38:LYS:HD2	1:0:41:ILE:HD13	1.95	0.49
9:A:2093:U:H2'	9:A:2094:G:O4'	2.12	0.49
16:H:69:VAL:HG13	16:H:73:PHE:HD2	1.78	0.49
17:I:54:ILE:HG23	17:I:58:LYS:HD3	1.95	0.49
21:M:140:ILE:HG23	21:M:141:PRO:HD2	1.94	0.49
5:4:95:HIS:NE2	9:A:236:A:OP1	2.46	0.49
9:A:874:G:H2'	9:A:875:C:C6	2.48	0.49
11:C:167:SER:HB2	11:C:179:LEU:HG	1.94	0.49
20:L:61:VAL:HG13	20:L:87:ILE:HD13	1.95	0.49
22:N:41:TRP:CZ2	22:N:72:LYS:HE2	2.47	0.49
22:N:8:ARG:H	22:N:8:ARG:HD2	1.76	0.49
9:A:2206:A:H2'	9:A:2207:A:H8	1.75	0.49
9:A:635:C:H2'	9:A:636:C:H6	1.76	0.49
12:D:120:GLY:HA3	12:D:141:TYR:O	2.13	0.49
17:I:140:ILE:HG12	17:I:141:PRO:HD3	1.95	0.49
9:A:2208:U:H2'	9:A:2209:U:O4'	2.13	0.49
9:A:2369:A:H2'	9:A:2370:G:O4'	2.12	0.49
14:F:46:VAL:O	14:F:56:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:135:ILE:HG22	19:K:217:LEU:HD22	1.95	0.49
9:A:1003:A:H1'	9:A:1018:A:C2	2.47	0.49
9:A:17:C:O2'	9:A:564:U:OP1	2.29	0.49
9:A:2136:U:OP1	9:A:2182:G:N2	2.46	0.49
9:A:2258:A:H2'	9:A:2259:G:C8	2.48	0.49
9:A:2075:G:H5''	9:A:2520:A:OP1	2.13	0.49
9:A:490:A:H1'	30:V:108:LYS:NZ	2.28	0.49
9:A:717:A:H2'	9:A:718:G:O4'	2.12	0.49
12:D:232:LEU:HD21	12:D:250:MET:HG2	1.94	0.49
14:F:183:VAL:HG13	14:F:185:PHE:HE1	1.77	0.49
15:G:108:PHE:HA	15:G:111:LEU:HB2	1.95	0.49
24:P:81:HIS:CD2	24:P:100:THR:HB	2.42	0.49
30:V:78:VAL:HG22	30:V:135:VAL:HG12	1.95	0.49
9:A:1394:A:H5'	9:A:2230:A:H1'	1.94	0.48
9:A:646:G:H2'	9:A:647:C:C6	2.48	0.48
9:A:881:U:H4'	22:N:69:PHE:CE2	2.48	0.48
12:D:95:THR:HG23	12:D:288:ASN:O	2.13	0.48
9:A:1348:C:H5''	28:T:71:ARG:NH2	2.28	0.48
31:W:5:A:H5'	31:W:6:A:OP2	2.13	0.48
1:O:51:VAL:HB	1:O:59:MET:HG3	1.95	0.48
6:5:9:PRO:HD3	6:5:16:LEU:HD11	1.95	0.48
9:A:1485:U:H5'	9:A:1486:U:C5'	2.38	0.48
9:A:642:G:N2	9:A:645:A:OP2	2.29	0.48
11:C:150:LEU:HD13	11:C:172:LEU:HD11	1.95	0.48
12:D:149:LEU:HD12	12:D:149:LEU:HA	1.61	0.48
9:A:1039:A:OP1	26:R:77:ASN:HB3	2.13	0.48
28:T:146:ASP:O	28:T:150:GLU:HG2	2.13	0.48
32:X:89:PRO:HD3	32:X:120:ASP:OD1	2.14	0.48
9:A:1444:A:H2'	9:A:1445:G:H8	1.76	0.48
9:A:1582:A:H2'	9:A:1583:A:C8	2.48	0.48
9:A:236:A:O5'	9:A:236:A:H8	1.96	0.48
11:C:100:ILE:HD12	11:C:101:LEU:O	2.14	0.48
14:F:111:ALA:O	14:F:115:GLY:N	2.45	0.48
17:I:100:THR:CG2	17:I:135:VAL:HG12	2.43	0.48
32:X:155:ARG:HG2	32:X:156:GLU:N	2.28	0.48
9:A:126:C:H2'	9:A:127:C:C6	2.48	0.48
9:A:824:U:H2'	9:A:825:C:C6	2.48	0.48
11:C:193:ASN:OD1	11:C:196:VAL:HG23	2.13	0.48
11:C:78:GLU:OE2	11:C:89:LEU:HB2	2.13	0.48
15:G:196:PRO:O	15:G:211:ARG:HA	2.13	0.48
17:I:119:TRP:HE1	17:I:165:CYS:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:153:LEU:HD12	25:Q:165:TYR:CE2	2.47	0.48
25:Q:170:ILE:HD11	25:Q:182:ARG:HD3	1.94	0.48
1:0:50:LYS:HG3	1:0:58:VAL:HG13	1.95	0.48
6:5:19:ARG:HG2	9:A:2774:U:C5'	2.42	0.48
9:A:2290:A:H2'	9:A:2291:A:H8	1.76	0.48
9:A:227:G:O2'	9:A:239:G:O6	2.27	0.48
4:3:135:ARG:NH2	9:A:480:G:N7	2.61	0.48
9:A:564:U:C2'	9:A:565:G:H5'	2.43	0.48
9:A:839:G:C2	9:A:840:A:N6	2.82	0.48
14:F:89:VAL:HG23	14:F:207:VAL:HG22	1.96	0.48
20:L:25:ILE:HD11	20:L:40:VAL:HG23	1.95	0.48
8:7:85:LEU:HD13	27:S:160:LYS:HE3	1.94	0.48
9:A:581:A:O2'	27:S:203:LYS:NZ	2.46	0.48
28:T:105:VAL:HG22	28:T:132:ILE:HG23	1.95	0.48
12:D:224:HIS:H	12:D:224:HIS:CD2	2.30	0.48
9:A:629:C:O3'	13:E:258:ARG:NH2	2.47	0.48
27:S:105:ASP:O	27:S:109:GLN:HG2	2.14	0.48
28:T:123:TYR:HE2	28:T:125:ILE:HD11	1.78	0.48
9:A:1408:A:H2'	9:A:1409:G:C8	2.48	0.48
9:A:2403:U:H4'	32:X:112:ASP:HA	1.96	0.48
5:4:112:ARG:O	5:4:135:LEU:HD22	2.14	0.48
9:A:1832:G:H2'	9:A:1833:G:H5''	1.96	0.48
9:A:866:G:H5''	9:A:866:G:H8	1.79	0.48
10:B:28:C:H2'	10:B:29:C:H6	1.79	0.48
10:B:56:U:O2'	14:F:77:ASN:ND2	2.35	0.48
4:3:126:LEU:HD23	4:3:129:ARG:NH2	2.29	0.48
9:A:2307:G:H2'	9:A:2308:U:O4'	2.14	0.48
9:A:612:U:O2'	9:A:614:G:O2'	2.31	0.48
9:A:880:U:OP1	22:N:6:ARG:HD3	2.14	0.48
14:F:53:THR:O	14:F:56:ARG:HB2	2.14	0.48
9:A:273:U:O2'	9:A:274:G:H5'	2.14	0.47
9:A:555:A:C6	9:A:558:A:H1'	2.49	0.47
9:A:2213:A:OP1	33:Y:107:ARG:NH2	2.46	0.47
9:A:1817:G:H8	9:A:1817:G:H5''	1.79	0.47
9:A:2339:A:C6	9:A:2350:A:N6	2.82	0.47
22:N:4:PRO:HG2	22:N:93:TRP:CZ3	2.49	0.47
10:B:117:A:H4'	24:P:102:GLN:HE21	1.78	0.47
29:U:150:ALA:O	29:U:154:PHE:HB2	2.14	0.47
9:A:1269:G:P	13:E:143:PRO:HG3	2.54	0.47
9:A:1333:U:H4'	9:A:1334:U:O5'	2.15	0.47
9:A:1337:U:H2'	9:A:1338:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:555:A:N6	9:A:558:A:HO2'	2.07	0.47
9:A:677:A:O2'	9:A:678:U:H5'	2.14	0.47
18:J:150:LEU:HD23	18:J:171:ILE:HD13	1.96	0.47
24:P:116:THR:HG22	24:P:118:GLU:H	1.79	0.47
29:U:119:ILE:HG21	29:U:167:ARG:HH22	1.79	0.47
5:4:126:THR:HA	5:4:129:LYS:HE3	1.96	0.47
9:A:1088:U:O4	18:J:205:ASN:ND2	2.37	0.47
9:A:1615:G:H2'	9:A:1616:A:C8	2.49	0.47
9:A:2691:G:H5''	20:L:30:ARG:HB2	1.97	0.47
9:A:2722:C:H2'	9:A:2723:A:O4'	2.14	0.47
27:S:171:TYR:CE2	27:S:232:ALA:HB2	2.48	0.47
1:0:53:CYS:HG	1:0:73:TRP:HE1	1.55	0.47
5:4:142:ASP:O	5:4:146:VAL:HG23	2.14	0.47
13:E:116:TYR:CZ	13:E:130:ARG:HD3	2.49	0.47
15:G:69:LEU:HD11	15:G:121:LYS:O	2.15	0.47
20:L:121:LEU:HD22	25:Q:165:TYR:HE1	1.79	0.47
21:M:141:PRO:HD3	21:M:154:LEU:HD22	24.48	0.47
28:T:112:LYS:HB3	28:T:124:MET:CE	2.43	0.47
1:0:53:CYS:SG	1:0:73:TRP:NE1	2.85	0.47
9:A:176:A:H2'	9:A:177:C:H6	1.78	0.47
26:R:109:TYR:HB3	27:S:235:LEU:HD11	1.96	0.47
8:7:53:LYS:O	8:7:58:HIS:HB2	2.15	0.47
9:A:1523:A:N3	9:A:1546:C:H4'	2.30	0.47
9:A:511:G:N1	9:A:514:A:OP2	2.46	0.47
9:A:670:A:H61	9:A:681:A:H61	28.23	0.47
13:E:207:PHE:HB2	13:E:228:LEU:HD22	1.96	0.47
21:M:154:LEU:HD12	21:M:155:PRO:HD2	1.97	0.47
31:W:34:U:O3'	31:W:35:U:H4'	2.15	0.47
12:D:148:LYS:NZ	31:W:38:G:OP2	2.47	0.47
9:A:1275:A:H5''	9:A:1276:U:H5''	1.96	0.47
9:A:1632:U:C2'	9:A:1633:A:H5'	2.45	0.47
19:K:116:VAL:HG12	19:K:154:ILE:HB	1.95	0.47
5:4:140:ARG:O	5:4:143:TYR:HB2	2.15	0.47
9:A:1074:A:C8	17:I:59:LYS:HE3	2.50	0.47
9:A:1100:C:N3	9:A:1120:C:N4	2.63	0.47
9:A:1096:G:N2	9:A:1123:A:O2'	2.48	0.47
9:A:142:U:H1'	9:A:153:G:N2	2.29	0.47
9:A:1692:C:H2'	9:A:1693:U:C6	2.49	0.47
9:A:2373:C:H2'	9:A:2374:C:O4'	2.15	0.47
9:A:2757:U:O2	9:A:2784:G:N2	2.48	0.47
9:A:407:C:O2'	33:Y:83:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:243:THR:HG22	11:C:244:THR:O	2.14	0.47
18:J:123:PHE:HE1	18:J:152:LYS:HD2	1.80	0.47
32:X:131:ASP:OD1	32:X:132:LYS:N	2.47	0.47
9:A:2039:C:H2'	9:A:2040:U:O4'	2.15	0.47
9:A:2600:G:OP2	9:A:2600:G:N2	2.39	0.47
9:A:2706:U:H2'	9:A:2706:U:O2	2.14	0.47
9:A:306:G:O3'	30:V:158:LYS:NZ	2.47	0.47
9:A:628:A:H2'	9:A:629:C:O4'	2.14	0.47
12:D:214:ARG:HA	12:D:254:MET:SD	2.55	0.47
15:G:53:ASN:HB3	15:G:68:PRO:HG3	1.97	0.47
27:S:146:ARG:HA	27:S:217:THR:OG1	2.15	0.47
9:A:2260:U:H2'	9:A:2261:U:C6	2.49	0.47
9:A:767:A:H2'	9:A:768:G:O4'	2.14	0.47
9:A:695:G:C2	9:A:805:A:C2	3.03	0.47
13:E:58:LEU:HD23	13:E:64:LYS:HA	1.97	0.47
15:G:74:ILE:HG12	15:G:115:MET:HE1	1.97	0.47
16:H:52:ILE:HD12	16:H:87:VAL:HG11	1.97	0.47
22:N:31:ARG:O	22:N:134:SER:HB2	2.15	0.47
25:Q:144:ARG:HB3	25:Q:144:ARG:HE	1.52	0.47
26:R:88:ARG:HE	26:R:118:LYS:HG3	1.80	0.47
31:W:30:A:H2'	31:W:31:U:O4'	2.14	0.47
9:A:2025:U:OP2	28:T:45:LYS:NZ	2.46	0.46
9:A:2414:A:H2'	9:A:2415:C:C6	2.49	0.46
9:A:2636:G:OP1	12:D:246:LYS:NZ	2.47	0.46
9:A:2697:C:H2'	9:A:2698:C:C6	2.50	0.46
15:G:92:VAL:HG21	15:G:109:ARG:HB2	1.96	0.46
15:G:72:LEU:HD13	15:G:115:MET:HB2	1.96	0.46
17:I:99:ASN:HB3	17:I:138:GLU:HB2	1.97	0.46
19:K:83:TRP:CG	19:K:84:MET:N	2.83	0.46
21:M:187:ILE:O	21:M:189:PRO:HD3	2.14	0.46
29:U:136:PHE:HD2	29:U:176:ILE:HD13	1.80	0.46
9:A:2722:C:O2'	31:W:56:G:OP1	2.23	0.46
1:0:46:ARG:HG2	1:0:48:ASP:OD1	2.15	0.46
9:A:2792:C:H2'	9:A:2793:A:O4'	2.15	0.46
9:A:349:A:H2'	9:A:350:G:O4'	2.14	0.46
24:P:93:HIS:HD2	24:P:95:LEU:HD23	1.80	0.46
29:U:111:VAL:O	29:U:114:ILE:HG12	2.15	0.46
32:X:122:LEU:HD21	32:X:140:ARG:HH11	1.80	0.46
33:Y:102:ASN:O	33:Y:122:SER:HA	2.15	0.46
34:Z:85:GLY:O	34:Z:88:PHE:HB3	2.16	0.46
1:0:76:ASN:ND2	1:0:76:ASN:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1416:A:O2'	9:A:1418:U:OP2	2.33	0.46
9:A:545:U:H2'	9:A:546:G:H8	1.80	0.46
10:B:30:A:P	24:P:78:SER:HB2	2.55	0.46
23:O:111:LEU:HA	23:O:111:LEU:HD12	1.73	0.46
23:O:69:SER:OG	23:O:72:LYS:HG2	2.15	0.46
23:O:36:THR:HG21	23:O:81:TYR:H	1.80	0.46
9:A:1502:A:H8	9:A:1502:A:O5'	1.98	0.46
9:A:1764:A:N1	9:A:2734:U:O2'	2.43	0.46
9:A:2155:C:N3	9:A:2165:G:N2	2.63	0.46
9:A:702:C:O2'	11:C:39:ARG:NH2	2.48	0.46
9:A:70:A:H5''	9:A:72:A:C8	2.49	0.46
11:C:149:GLN:O	11:C:152:ARG:HG3	2.15	0.46
14:F:66:VAL:O	14:F:70:LYS:HB2	2.15	0.46
17:I:105:ALA:HB1	17:I:109:LEU:HD22	1.97	0.46
26:R:116:ILE:HA	26:R:119:GLU:OE2	2.16	0.46
26:R:58:ARG:HH12	26:R:94:ARG:NH1	2.14	0.46
28:T:79:LEU:HD13	28:T:134:ILE:HD11	1.98	0.46
33:Y:144:ASP:O	33:Y:148:GLU:HG3	2.16	0.46
9:A:927:A:N6	9:A:1308:A:N1	102.83	0.46
15:G:184:PHE:O	15:G:188:ILE:HG12	2.15	0.46
32:X:73:LYS:H	32:X:73:LYS:HG2	1.49	0.46
9:A:143:G:OP2	9:A:143:G:H8	1.99	0.46
9:A:1567:C:H5'	9:A:1568:U:OP2	2.15	0.46
9:A:2340:G:H2'	9:A:2341:U:H5'	1.97	0.46
9:A:2535:C:H5'	9:A:2535:C:O2	2.16	0.46
9:A:794:A:H2'	9:A:795:U:H4'	1.96	0.46
10:B:48:C:OP1	24:P:49:ARG:HG3	2.16	0.46
9:A:1110:U:O2'	17:I:90:GLN:NE2	2.48	0.46
24:P:103:LYS:O	24:P:107:GLU:HG2	2.15	0.46
2:1:13:LYS:HG2	2:1:14:ARG:N	2.31	0.46
9:A:1511:U:O5'	9:A:1511:U:H6	1.98	0.46
9:A:2113:G:H2'	9:A:2114:G:C8	2.51	0.46
9:A:2263:C:H2'	9:A:2264:U:C6	2.51	0.46
22:N:53:ALA:HB1	22:N:120:ILE:HG22	1.98	0.46
9:A:17:C:O3'	26:R:23:SER:HA	2.15	0.46
9:A:573:G:H21	26:R:37:GLN:HE22	1.62	0.46
34:Z:140:TRP:O	34:Z:144:ILE:HG12	2.16	0.46
9:A:1090:U:H2'	9:A:1091:G:H8	1.81	0.46
9:A:1207:G:H2'	9:A:1208:G:O4'	2.16	0.46
9:A:2463:G:H2'	9:A:2464:G:O4'	2.15	0.46
9:A:316:G:N2	9:A:339:A:H61	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:982:G:OP1	9:A:982:G:H4'	4.77	0.46
9:A:1264:C:H1'	21:M:83:ASP:O	2.16	0.46
9:A:166:A:H2'	9:A:167:A:C8	2.51	0.46
9:A:2660:G:H2'	9:A:2661:A:O4'	2.14	0.46
12:D:90:ILE:HA	12:D:90:ILE:HD13	1.69	0.46
9:A:623:A:N6	13:E:233:SER:HB3	2.31	0.46
25:Q:152:ARG:HD2	25:Q:205:GLU:OE1	2.16	0.46
9:A:1849:A:H5'	9:A:1850:G:OP2	2.16	0.46
9:A:1976:C:H4'	9:A:1977:C:C5	2.51	0.46
9:A:197:G:H2'	9:A:198:A:C8	2.51	0.46
9:A:221:C:H2'	9:A:222:C:C6	2.51	0.46
9:A:306:G:H2'	9:A:307:C:C6	2.51	0.46
26:R:88:ARG:HH22	27:S:174:THR:HG21	1.81	0.46
9:A:2714:A:H2'	9:A:2715:U:O4'	2.17	0.45
9:A:739:G:O2'	9:A:741:U:H5''	2.16	0.45
9:A:889:G:N2	9:A:907:C:O2	2.49	0.45
18:J:113:TYR:HD1	18:J:141:LEU:HD21	1.80	0.45
25:Q:119:LEU:HD22	25:Q:122:ILE:HD12	1.97	0.45
26:R:78:TYR:CZ	26:R:82:ILE:HG13	2.51	0.45
28:T:56:ARG:NH1	28:T:64:ILE:HD11	2.31	0.45
6:5:15:ARG:HH12	9:A:2771:A:H1'	1.81	0.45
9:A:1573:C:H2'	9:A:1574:G:C8	2.51	0.45
9:A:316:G:H22	9:A:339:A:N6	2.08	0.45
10:B:30:A:H2'	10:B:31:C:C6	2.51	0.45
13:E:51:GLU:HB3	13:E:69:PHE:CD1	2.51	0.45
14:F:195:LYS:O	14:F:199:VAL:HG23	2.16	0.45
32:X:87:ALA:O	32:X:120:ASP:HA	2.16	0.45
7:6:118:ARG:O	7:6:122:LYS:HG3	2.15	0.45
14:F:120:LYS:HE3	14:F:137:THR:HG21	1.98	0.45
20:L:3:GLN:O	20:L:6:THR:OG1	2.20	0.45
9:A:1689:C:H3'	23:O:12:LYS:HG2	1.98	0.45
9:A:1569:A:H2'	9:A:1569:A:N3	2.31	0.45
9:A:1704:A:O2'	9:A:1710:G:N7	2.41	0.45
9:A:539:A:H62	9:A:2056:A:H3'	1.82	0.45
9:A:947:A:H61	9:A:950:A:H61	1.64	0.45
14:F:114:THR:HG22	14:F:152:PHE:CE1	2.51	0.45
18:J:180:ALA:O	18:J:184:LEU:HB2	2.16	0.45
32:X:105:LYS:HE2	32:X:105:LYS:HB2	1.68	0.45
9:A:1105:A:H4'	9:A:1106:C:O5'	4.91	0.45
9:A:1142:G:H2'	9:A:1143:C:C6	2.51	0.45
12:D:96:LYS:HD2	12:D:282:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:204:LYS:HA	13:E:225:THR:HB	1.99	0.45
15:G:115:MET:HE3	15:G:115:MET:HB3	1.85	0.45
9:A:1880:G:N7	21:M:252:ARG:NH1	2.65	0.45
26:R:116:ILE:O	26:R:119:GLU:HG2	2.17	0.45
29:U:119:ILE:HD12	29:U:135:LEU:HD13	1.98	0.45
9:A:221:C:H2'	9:A:222:C:H6	1.82	0.45
9:A:2221:U:H2'	9:A:2222:C:H6	1.82	0.45
10:B:16:G:H2'	10:B:16:G:N3	2.30	0.45
10:B:61:C:H2'	10:B:62:U:C6	2.51	0.45
17:I:56:ARG:HA	17:I:59:LYS:CE	2.46	0.45
19:K:62:ARG:HD3	19:K:62:ARG:HA	4.40	0.45
21:M:186:ILE:H	21:M:186:ILE:HG13	1.45	0.45
26:R:24:PHE:O	26:R:29:SER:HB3	2.16	0.45
27:S:100:THR:HG22	27:S:102:GLU:H	1.81	0.45
9:A:1448:A:H4'	9:A:1449:C:O4'	2.16	0.45
9:A:144:A:H5'	25:Q:160:ARG:HH12	158.27	0.45
9:A:1592:A:H8	9:A:1592:A:OP1	1.99	0.45
9:A:1714:A:H2'	9:A:1715:A:O4'	2.17	0.45
22:N:65:TRP:HB2	22:N:105:GLU:HB2	1.99	0.45
9:A:1272:A:OP1	26:R:13:ARG:NH1	2.49	0.45
26:R:43:LEU:HA	26:R:43:LEU:HD23	1.73	0.45
26:R:88:ARG:NH1	26:R:88:ARG:O	2.50	0.45
28:T:62:LEU:HD22	28:T:77:PHE:HE1	1.79	0.45
9:A:84:G:OP2	30:V:72:VAL:N	2.50	0.45
34:Z:90:LEU:HA	34:Z:90:LEU:HD12	1.76	0.45
9:A:1801:A:OP1	11:C:207:LYS:HG3	2.17	0.45
10:B:67:U:C4	10:B:109:U:C4	3.05	0.45
18:J:176:LEU:HD11	18:J:210:ILE:HG21	1.98	0.45
21:M:257:PHE:CD1	21:M:257:PHE:N	2.84	0.45
22:N:75:THR:HA	22:N:90:PRO:HA	1.99	0.45
25:Q:138:ARG:HH22	25:Q:203:ILE:HB	1.81	0.45
27:S:230:TYR:CG	27:S:231:PRO:HD2	2.52	0.45
31:W:32:C:H5'	31:W:33:A:OP2	2.17	0.45
1:0:70:VAL:HG11	1:0:73:TRP:HB3	1.98	0.45
8:7:66:LYS:O	8:7:72:ILE:HD11	2.16	0.45
9:A:1056:A:N6	9:A:1153:G:H2'	2.32	0.45
9:A:1116:A:H2'	9:A:1116:A:N3	2.32	0.45
9:A:1116:A:N6	18:J:205:ASN:HB2	2.32	0.45
9:A:1473:G:H5'	9:A:1474:A:H5''	1.98	0.45
9:A:1870:U:H3	9:A:1896:G:H1	1.63	0.45
2:1:5:LYS:NZ	9:A:2069:C:OP1	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:101:LEU:HD23	11:C:101:LEU:HA	1.79	0.45
14:F:108:ASN:O	14:F:112:LEU:HG	2.16	0.45
4:3:96:LEU:HD23	4:3:96:LEU:HA	1.71	0.45
9:A:1886:A:H2'	9:A:1887:G:H8	1.81	0.45
9:A:213:A:N1	9:A:429:C:O2'	2.39	0.45
9:A:918:A:H2'	9:A:919:A:O4'	6.08	0.45
17:I:96:LEU:HD13	17:I:102:LEU:HB2	1.97	0.45
9:A:550:G:H5'	19:K:104:SER:HB2	1.99	0.45
26:R:28:HIS:O	26:R:35:ILE:HG12	2.17	0.45
9:A:1269:G:C5	26:R:3:ARG:HB2	2.52	0.45
9:A:556:C:H4'	9:A:557:C:OP1	2.16	0.44
15:G:177:ASP:O	15:G:181:VAL:HG12	2.17	0.44
15:G:184:PHE:CE2	15:G:188:ILE:HD11	2.52	0.44
22:N:29:PHE:CE2	22:N:67:ARG:HD3	2.53	0.44
32:X:146:ASN:HA	32:X:147:PRO:HD3	1.85	0.44
5:4:140:ARG:HD2	5:4:140:ARG:HA	1.71	0.44
9:A:1809:G:OP1	11:C:256:ARG:NH1	2.44	0.44
9:A:1921:G:N2	9:A:1938:C:H1'	2.32	0.44
9:A:2062:A:H2'	9:A:2063:C:O4'	2.17	0.44
9:A:2393:A:H8	9:A:2393:A:OP1	2.00	0.44
9:A:262:G:HO2'	9:A:264:A:H2	1.64	0.44
19:K:214:GLY:O	19:K:217:LEU:HB2	2.18	0.44
21:M:163:ARG:O	21:M:167:VAL:HG23	2.17	0.44
23:O:92:GLU:OE2	23:O:96:ARG:HD2	2.18	0.44
23:O:96:ARG:HD3	23:O:97:TYR:CE2	2.53	0.44
29:U:135:LEU:HD23	29:U:135:LEU:HA	1.54	0.44
9:A:307:C:P	30:V:158:LYS:HZ1	2.40	0.44
9:A:1078:A:N1	9:A:2769:G:C6	2.86	0.44
9:A:636:C:O2'	9:A:668:U:H5''	2.17	0.44
9:A:711:G:H2'	9:A:712:G:O4'	2.18	0.44
14:F:83:LYS:O	14:F:211:THR:HG23	2.17	0.44
18:J:109:PHE:CD1	18:J:129:ILE:HD13	2.51	0.44
20:L:73:ASN:HB2	20:L:75:MET:HB2	2.00	0.44
10:B:8:G:N2	24:P:85:GLN:HE22	2.07	0.44
28:T:74:TYR:HB3	28:T:75:PRO:HD3	1.98	0.44
12:D:119:GLU:HB2	31:W:36:A:C5	2.52	0.44
9:A:143:G:H5'	9:A:144:A:OP2	4.71	0.44
9:A:1864:A:H2'	9:A:1865:G:O4'	2.16	0.44
9:A:2236:C:H2'	9:A:2237:A:O4'	2.18	0.44
9:A:2303:A:H4'	9:A:2304:A:O4'	2.18	0.44
9:A:881:U:H2'	9:A:882:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:53:U:C4	10:B:54:G:C2	3.05	0.44
13:E:113:ARG:O	13:E:114:LYS:HG2	2.17	0.44
13:E:79:THR:O	13:E:83:VAL:HG23	2.17	0.44
19:K:202:HIS:O	19:K:202:HIS:ND1	2.51	0.44
21:M:243:LYS:O	21:M:246:VAL:HG23	2.18	0.44
1:0:50:LYS:HB3	1:0:67:ASP:OD1	2.17	0.44
1:0:46:ARG:NH1	1:0:66:LYS:HB2	2.32	0.44
1:0:79:PHE:CG	1:0:80:TYR:N	2.85	0.44
9:A:1154:A:H4'	9:A:1155:A:H5''	1.99	0.44
9:A:2250:A:H2'	9:A:2251:G:H8	1.80	0.44
9:A:2430:G:H2'	9:A:2431:G:O4'	2.17	0.44
11:C:97:LYS:O	11:C:98:ARG:HD3	2.18	0.44
19:K:61:TRP:HZ2	28:T:157:LEU:HD23	1.82	0.44
30:V:86:LYS:HD2	30:V:105:LEU:HD22	2.00	0.44
31:W:76:G:H5''	31:W:77:A:OP1	2.18	0.44
9:A:1113:A:N6	9:A:1114:A:H62	2.14	0.44
9:A:114:C:H2'	9:A:115:G:O4'	2.17	0.44
9:A:1234:A:H2'	9:A:1235:A:H4'	4.11	0.44
9:A:2112:U:H2'	9:A:2113:G:O4'	2.17	0.44
9:A:2142:G:H21	9:A:2187:A:H4'	1.82	0.44
9:A:966:G:C6	9:A:967:C:C4	3.06	0.44
11:C:46:THR:OG1	11:C:47:ALA:N	2.51	0.44
11:C:68:LYS:HD2	11:C:115:GLY:HA2	1.98	0.44
12:D:202:THR:HG22	12:D:288:ASN:HD21	1.82	0.44
9:A:684:C:OP1	13:E:105:ARG:NH1	2.51	0.44
25:Q:200:SER:HB3	25:Q:203:ILE:HG13	1.99	0.44
28:T:98:LEU:HD13	28:T:136:LEU:HD13	1.99	0.44
9:A:1169:A:H5'	19:K:245:ARG:CZ	2.47	0.44
9:A:2278:C:C2	9:A:2297:G:N2	2.86	0.44
9:A:555:A:H2	9:A:558:A:OP1	1.99	0.44
11:C:172:LEU:HD23	11:C:172:LEU:HA	1.74	0.44
9:A:2320:G:O2'	14:F:174:SER:O	2.34	0.44
22:N:32:TYR:HD1	22:N:133:ILE:HG22	1.81	0.44
22:N:71:ASP:N	22:N:71:ASP:OD1	2.41	0.44
27:S:191:LEU:HD23	27:S:215:PRO:HA	1.99	0.44
29:U:124:ALA:HB2	29:U:135:LEU:HD12	1.99	0.44
29:U:161:LYS:O	29:U:177:MET:HG2	2.18	0.44
9:A:1468:C:H2'	9:A:1469:G:C8	2.53	0.44
9:A:1488:A:H2'	9:A:1489:A:C8	2.53	0.44
9:A:169:C:H2'	9:A:170:U:C6	2.53	0.44
9:A:2624:G:H2'	9:A:2625:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:331:A:OP2	13:E:222:ASN:HB2	2.18	0.44
9:A:525:A:H2'	9:A:526:A:O4'	2.18	0.44
9:A:716:A:H2'	9:A:717:A:O4'	2.18	0.44
9:A:750:A:H1'	9:A:751:C:H5	1.82	0.44
9:A:753:G:H2'	9:A:754:A:C8	2.53	0.44
9:A:838:U:H4'	9:A:839:G:C8	2.52	0.44
14:F:221:LYS:O	14:F:225:LEU:HG	2.18	0.44
9:A:1088:U:C2	9:A:1090:U:H5'	2.52	0.44
9:A:1520:A:H4'	9:A:1521:G:OP1	2.17	0.44
9:A:362:A:H5'	9:A:363:C:OP2	2.18	0.44
9:A:540:A:C2	9:A:2037:G:C8	3.06	0.44
11:C:138:HIS:HD2	11:C:139:ASN:HB2	1.83	0.44
28:T:123:TYR:CE2	28:T:125:ILE:HD11	2.53	0.44
28:T:173:LEU:HD12	28:T:193:PHE:CE2	2.53	0.44
9:A:1226:U:O4	13:E:224:ARG:NE	2.51	0.43
9:A:1530:G:H2'	9:A:1532:G:N7	2.33	0.43
9:A:2116:C:C2	9:A:2201:G:N2	2.86	0.43
9:A:2154:C:H42	9:A:2165:G:H1	1.66	0.43
9:A:2304:A:C8	9:A:2306:G:C8	3.06	0.43
17:I:69:HIS:ND1	17:I:103:ILE:HD11	2.32	0.43
9:A:1088:U:H5	18:J:202:THR:HG23	1.83	0.43
9:A:578:U:P	21:M:115:ARG:HH21	2.41	0.43
5:4:156:ASN:OD1	5:4:158:LYS:HD3	2.19	0.43
6:5:29:ASN:HD21	6:5:31:LYS:HB2	1.84	0.43
9:A:1073:G:C5'	9:A:1075:G:H5''	2.48	0.43
9:A:2150:G:H1	9:A:2170:C:H1'	1.83	0.43
9:A:824:U:H2'	9:A:825:C:H6	1.84	0.43
9:A:845:C:H2'	9:A:846:A:H8	1.82	0.43
10:B:80:C:H2'	10:B:81:U:O4'	2.18	0.43
12:D:188:GLU:OE2	12:D:271:THR:HG23	2.18	0.43
13:E:102:THR:O	13:E:103:LEU:HD23	2.18	0.43
13:E:55:LEU:O	13:E:67:GLU:HA	2.19	0.43
16:H:42:GLN:HB2	16:H:43:LYS:H	1.59	0.43
19:K:148:ASP:OD1	19:K:150:GLY:N	2.52	0.43
9:A:1415:U:C4	9:A:1416:A:C6	3.06	0.43
9:A:1493:C:H5'	9:A:1494:G:OP2	2.19	0.43
9:A:2075:G:N2	9:A:2076:A:C6	2.86	0.43
9:A:818:U:H2'	9:A:819:G:H8	1.84	0.43
12:D:270:ASP:HB2	12:D:275:VAL:HG22	1.99	0.43
13:E:120:LYS:HG3	13:E:124:ALA:HB3	2.00	0.43
14:F:127:ILE:HD12	14:F:132:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:155:MET:SD	15:G:188:ILE:HD13	2.59	0.43
21:M:213:LYS:HD3	21:M:233:THR:HB	1.99	0.43
22:N:32:TYR:CD1	22:N:133:ILE:HG22	2.52	0.43
23:O:64:LEU:HA	23:O:64:LEU:HD12	1.67	0.43
24:P:67:THR:HB	24:P:68:PRO:HD2	2.00	0.43
28:T:114:VAL:HG22	28:T:124:MET:SD	2.58	0.43
9:A:9:A:H1'	31:W:99:A:C2	2.53	0.43
9:A:1195:U:H3'	9:A:1196:A:C8	2.53	0.43
11:C:206:SER:HA	11:C:209:TRP:CE3	2.53	0.43
9:A:2322:A:C2	14:F:204:GLY:HA3	2.53	0.43
14:F:57:LEU:HD21	14:F:154:ASP:HB2	2.01	0.43
19:K:50:SER:HA	31:W:1:A:N7	2.34	0.43
20:L:11:ALA:HB3	20:L:85:VAL:HG22	1.99	0.43
9:A:836:G:H1'	21:M:133:GLN:NE2	2.33	0.43
21:M:134:MET:O	21:M:139:ARG:NH1	2.51	0.43
23:O:56:LYS:HG2	23:O:57:TYR:CD1	2.54	0.43
24:P:61:ARG:NH2	24:P:89:ASP:OD2	2.52	0.43
25:Q:154:GLU:HA	25:Q:162:LEU:HD22	2.01	0.43
25:Q:228:ARG:HB2	25:Q:228:ARG:HH11	1.84	0.43
26:R:32:THR:OG1	26:R:33:ARG:N	2.52	0.43
28:T:112:LYS:HB3	28:T:124:MET:HE1	2.00	0.43
9:A:1142:G:C6	9:A:1143:C:N4	2.87	0.43
9:A:1320:G:O5'	9:A:1320:G:H8	2.01	0.43
9:A:1702:G:O3'	20:L:6:THR:HG23	2.19	0.43
9:A:621:G:H2'	9:A:622:G:C8	3.66	0.43
11:C:76:THR:OG1	11:C:77:ILE:N	2.51	0.43
12:D:284:GLY:HA3	12:D:288:ASN:OD1	2.18	0.43
29:U:114:ILE:HG13	29:U:115:LEU:HG	2.00	0.43
9:A:519:A:N6	28:T:38:SER:OG	2.52	0.43
11:C:23:ASN:ND2	11:C:76:THR:HG21	2.30	0.43
11:C:80:ASP:OD1	11:C:81:PRO:HD2	2.18	0.43
12:D:150:THR:OG1	12:D:152:PRO:HD2	2.19	0.43
13:E:51:GLU:HG3	13:E:53:ILE:H	1.82	0.43
30:V:151:LYS:HB2	30:V:161:TYR:CE1	2.54	0.43
6:5:17:ILE:HG22	6:5:18:ARG:N	2.32	0.43
9:A:1023:C:O2	19:K:99:THR:OG1	2.37	0.43
9:A:2028:A:H2'	9:A:2029:A:C8	2.53	0.43
9:A:2118:U:H2'	9:A:2119:U:H5''	2.00	0.43
9:A:2570:G:H2'	9:A:2571:U:O4'	2.19	0.43
9:A:2718:U:O2'	23:O:83:LYS:HE3	2.18	0.43
9:A:2764:U:H4'	15:G:178:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:649:A:H4'	9:A:650:G:O5'	2.19	0.43
9:A:675:U:H2'	9:A:676:U:C6	2.53	0.43
20:L:7:HIS:HB3	20:L:18:GLU:OE2	2.18	0.43
24:P:105:ILE:HD13	24:P:123:ILE:HG12	2.01	0.43
28:T:179:GLU:H	28:T:179:GLU:HG3	1.63	0.43
29:U:132:ASN:O	29:U:178:LEU:HD12	2.19	0.43
31:W:1:A:H2'	31:W:2:G:H8	1.83	0.43
1:0:37:ARG:HB3	1:0:42:HIS:CD2	2.52	0.43
2:1:40:THR:HG23	2:1:42:ASN:H	1.84	0.43
4:3:146:SER:HA	4:3:150:ALA:HB2	2.00	0.43
7:6:138:LYS:HB3	7:6:138:LYS:HE2	1.78	0.43
9:A:1137:C:C5	9:A:1138:G:C6	3.07	0.43
9:A:1535:A:H2'	9:A:1536:A:C8	2.54	0.43
9:A:2045:A:C6	9:A:2515:C:H1'	2.54	0.43
7:6:122:LYS:NZ	9:A:1407:C:OP1	2.34	0.43
9:A:472:A:C2	9:A:482:A:C5	3.07	0.43
9:A:980:G:H2'	9:A:981:G:O4'	2.18	0.43
12:D:184:LYS:HE2	12:D:184:LYS:HB2	1.77	0.43
15:G:112:THR:HA	15:G:115:MET:HE3	2.00	0.43
18:J:146:ALA:HB2	18:J:183:LYS:HZ2	1.83	0.43
24:P:125:GLU:HG2	24:P:162:HIS:CD2	2.54	0.43
24:P:72:ARG:NH2	24:P:87:ILE:HD12	2.34	0.43
32:X:74:GLY:O	32:X:76:ARG:NH1	2.52	0.43
9:A:2341:U:H3'	9:A:2342:G:H5'	2.01	0.43
9:A:299:C:H2'	9:A:299:C:O2	3.12	0.43
9:A:348:U:O5'	9:A:348:U:H6	2.02	0.43
11:C:239:ARG:C	11:C:241:SER:H	2.22	0.43
12:D:235:ILE:HD12	12:D:244:VAL:HG11	2.01	0.43
14:F:155:ARG:O	14:F:159:LEU:HB3	2.18	0.43
15:G:160:GLU:OE2	15:G:176:ARG:HG3	2.19	0.43
19:K:64:LEU:O	19:K:68:VAL:HG13	2.19	0.43
20:L:42:VAL:HA	20:L:56:GLU:O	2.18	0.43
9:A:645:A:H5'	21:M:156:LYS:HZ3	1.84	0.43
22:N:12:GLN:HG3	22:N:13:HIS:H	1.84	0.43
23:O:89:LEU:HD23	23:O:89:LEU:HA	1.79	0.43
27:S:190:LEU:HB2	27:S:216:ILE:HG22	2.01	0.43
1:0:46:ARG:CZ	1:0:66:LYS:HB2	2.48	0.42
9:A:2794:A:C2	9:A:2796:A:C4	3.07	0.42
9:A:976:C:H1'	9:A:1012:G:C8	2.53	0.42
11:C:49:HIS:CE1	11:C:215:VAL:HG22	2.54	0.42
12:D:229:HIS:N	12:D:229:HIS:ND1	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:62:LEU:HA	28:T:62:LEU:HD23	1.74	0.42
28:T:63:MET:HG2	28:T:63:MET:H	1.67	0.42
34:Z:86:GLU:HB3	34:Z:108:MET:HE1	1.99	0.42
5:4:114:ARG:HD3	5:4:136:ILE:CG1	2.50	0.42
9:A:1063:U:OP1	15:G:99:ARG:NH2	2.52	0.42
9:A:1090:U:H2'	9:A:1091:G:C8	2.53	0.42
9:A:1109:U:H2'	9:A:1110:U:C6	2.54	0.42
9:A:1226:U:H6	9:A:1226:U:O5'	2.02	0.42
9:A:1518:U:C5	9:A:1519:A:H2	2.37	0.42
9:A:1583:A:H2'	9:A:1584:C:C6	2.54	0.42
9:A:1882:U:C4	21:M:260:LYS:HD3	2.55	0.42
9:A:2456:A:N6	9:A:2602:U:OP1	2.52	0.42
9:A:344:C:H2'	9:A:345:C:H6	1.84	0.42
9:A:426:C:H2'	9:A:427:A:H8	1.80	0.42
9:A:564:U:H2'	9:A:565:G:H5'	2.01	0.42
9:A:910:A:H8	9:A:910:A:OP2	2.02	0.42
12:D:90:ILE:HG23	12:D:90:ILE:HD12	1.76	0.42
13:E:171:ASN:HD22	13:E:244:LYS:HD3	1.84	0.42
18:J:151:LEU:HG	18:J:206:MET:HE1	2.00	0.42
27:S:204:LYS:HD3	27:S:204:LYS:HA	1.69	0.42
33:Y:110:TRP:CE2	33:Y:145:LEU:HD12	2.54	0.42
9:A:1009:A:H5''	9:A:1010:C:OP2	2.18	0.42
9:A:1114:A:H4'	9:A:1131:A:C2	2.54	0.42
9:A:1897:C:H2'	9:A:1898:G:O4'	2.20	0.42
9:A:548:G:O2'	9:A:549:A:P	2.75	0.42
10:B:41:U:H3'	10:B:42:C:C5'	2.49	0.42
13:E:179:ALA:HB1	13:E:213:VAL:HG11	2.01	0.42
19:K:56:LYS:O	19:K:60:GLU:HG3	2.20	0.42
27:S:184:ALA:HB2	27:S:221:ILE:HD13	2.01	0.42
27:S:191:LEU:HB2	27:S:213:ARG:NH1	2.35	0.42
9:A:1348:C:H5''	28:T:71:ARG:HH22	1.85	0.42
31:W:17:A:H1'	31:W:23:G:C2	2.54	0.42
1:0:61:THR:HG22	1:0:62:GLY:N	2.29	0.42
4:3:105:ARG:NH1	4:3:149:ARG:O	2.52	0.42
9:A:1397:C:N4	9:A:1398:G:C6	2.88	0.42
9:A:1928:C:H2'	9:A:1929:U:C6	2.55	0.42
9:A:2008:C:P	12:D:222:MET:HB2	2.59	0.42
9:A:483:A:H2'	9:A:484:G:C8	2.54	0.42
9:A:984:G:OP1	22:N:87:LYS:HG3	2.19	0.42
12:D:90:ILE:HD11	12:D:173:LEU:HD11	2.01	0.42
13:E:256:ASN:O	13:E:256:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:226:MET:HE3	14:F:226:MET:HB3	1.87	0.42
9:A:1089:U:O4	18:J:83:ALA:HB2	2.19	0.42
9:A:2432:G:H5'	21:M:148:GLY:HA3	2.01	0.42
23:O:31:LEU:HA	23:O:31:LEU:HD23	1.63	0.42
27:S:124:PHE:CE1	27:S:165:GLY:HA3	2.55	0.42
30:V:137:LEU:HA	30:V:137:LEU:HD23	1.77	0.42
9:A:2561:G:H2'	9:A:2562:G:O4'	2.19	0.42
9:A:254:U:C5	9:A:272:U:C4	3.07	0.42
9:A:2656:A:C2	9:A:2796:A:C8	3.07	0.42
9:A:6:A:H2'	9:A:7:C:O4'	2.19	0.42
9:A:920:A:H8	9:A:920:A:O5'	2.01	0.42
12:D:223:THR:O	12:D:225:GLY:N	2.52	0.42
12:D:232:LEU:HD12	12:D:232:LEU:HA	1.65	0.42
15:G:98:THR:CG2	15:G:100:ARG:HB2	2.49	0.42
17:I:161:PHE:CE2	17:I:176:VAL:HG21	2.54	0.42
25:Q:119:LEU:O	25:Q:122:ILE:HB	2.19	0.42
29:U:112:TYR:O	34:Z:91:ARG:NH2	2.53	0.42
9:A:115:G:C6	9:A:117:A:N6	2.87	0.42
9:A:1632:U:O2'	9:A:1633:A:H5'	2.19	0.42
9:A:1875:G:H2'	9:A:1889:G:N2	2.34	0.42
9:A:2073:A:O2'	9:A:2074:A:P	2.78	0.42
9:A:2260:U:H2'	9:A:2261:U:H6	1.83	0.42
9:A:605:C:H2'	9:A:606:A:C8	2.54	0.42
12:D:224:HIS:CD2	12:D:224:HIS:N	2.87	0.42
25:Q:138:ARG:O	25:Q:138:ARG:HD3	2.20	0.42
25:Q:140:VAL:HA	25:Q:141:PRO:HD3	1.85	0.42
2:1:11:TYR:CD1	2:1:11:TYR:C	2.93	0.42
9:A:262:G:C2	9:A:264:A:H5''	2.54	0.42
9:A:504:G:H2'	9:A:505:G:O4'	2.20	0.42
9:A:720:U:H3	9:A:733:A:H61	1.67	0.42
9:A:880:U:H5''	22:N:6:ARG:HG3	2.01	0.42
9:A:886:U:H3	9:A:910:A:H61	1.68	0.42
9:A:926:A:H1'	9:A:931:U:O4	17.60	0.42
11:C:178:ARG:HG2	11:C:179:LEU:N	2.34	0.42
9:A:2595:G:N7	12:D:234:SER:HB2	2.33	0.42
17:I:133:LEU:HD21	17:I:143:ALA:HB1	2.02	0.42
24:P:122:LYS:HA	24:P:122:LYS:HD2	1.81	0.42
26:R:74:VAL:HB	26:R:75:TYR:CD2	2.54	0.42
26:R:84:ASP:HB3	26:R:115:ILE:CG2	2.49	0.42
9:A:151:G:H2'	9:A:152:G:O4'	2.20	0.42
9:A:2212:A:C2	16:H:77:PHE:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2461:A:H2'	9:A:2462:G:O4'	2.20	0.42
12:D:107:GLY:HA3	25:Q:202:ASN:ND2	2.35	0.42
12:D:178:ASP:OD1	12:D:178:ASP:N	2.51	0.42
17:I:130:ASN:ND2	17:I:132:TRP:HE1	2.18	0.42
19:K:130:THR:HA	19:K:133:ILE:HD12	2.01	0.42
19:K:64:LEU:HD23	19:K:64:LEU:HA	1.83	0.42
28:T:183:ILE:HG12	28:T:183:ILE:H	1.65	0.42
30:V:139:SER:HB2	30:V:162:LEU:HD12	2.01	0.42
32:X:146:ASN:HD22	32:X:149:SER:HB2	1.85	0.42
33:Y:126:LEU:O	33:Y:130:GLU:HG3	2.20	0.42
9:A:1158:U:O4	12:D:241:PRO:HA	2.20	0.42
9:A:2014:G:C2'	9:A:2015:A:H5'	2.49	0.42
12:D:92:VAL:HB	12:D:121:ASN:ND2	2.35	0.42
12:D:99:MET:HB3	12:D:99:MET:HE2	1.67	0.42
18:J:180:ALA:HB1	18:J:195:ALA:HB1	2.01	0.42
21:M:181:LEU:HB3	21:M:187:ILE:HD12	2.02	0.42
9:A:1883:G:C2	21:M:257:PHE:CE1	3.08	0.42
9:A:674:C:H5''	21:M:96:LYS:HG3	2.02	0.42
24:P:161:GLU:OE2	24:P:162:HIS:HD2	2.03	0.42
2:1:18:ASN:ND2	9:A:14:A:O3'	2.53	0.42
9:A:1300:U:H2'	9:A:1301:G:O4'	2.20	0.42
9:A:1701:A:H2'	9:A:1702:G:O4'	2.20	0.42
9:A:383:A:O2'	9:A:384:G:OP2	3.68	0.42
9:A:489:A:H2'	9:A:490:A:C8	2.54	0.42
9:A:888:C:H3'	9:A:889:G:C8	2.44	0.42
13:E:161:LEU:HD23	13:E:161:LEU:HA	1.75	0.42
18:J:171:ILE:HG12	18:J:210:ILE:HG12	2.01	0.42
26:R:58:ARG:NH1	26:R:94:ARG:HD2	2.35	0.42
28:T:45:LYS:H	28:T:45:LYS:HG2	1.58	0.42
31:W:93:C:H2'	31:W:94:C:O4'	2.19	0.42
6:5:17:ILE:HD11	6:5:26:ILE:HG12	2.02	0.41
9:A:1088:U:N1	9:A:1090:U:H5'	2.35	0.41
9:A:1135:A:H4'	17:I:129:MET:HG2	2.01	0.41
9:A:1307:A:C6	9:A:1310:C:C2	3.08	0.41
9:A:2313:U:H4'	9:A:2314:C:OP1	2.20	0.41
9:A:2391:C:H2'	9:A:2392:G:O4'	2.20	0.41
9:A:2625:G:H5''	9:A:2626:U:OP1	2.19	0.41
12:D:179:PHE:HA	12:D:183:GLN:OE1	2.19	0.41
16:H:50:LYS:HG2	16:H:67:LEU:O	2.20	0.41
9:A:984:G:P	22:N:87:LYS:HG3	2.60	0.41
28:T:79:LEU:HA	28:T:79:LEU:HD23	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Z:74:GLU:H	34:Z:74:GLU:HG3	1.41	0.41
2:1:26:TRP:O	2:1:30:LYS:HG2	2.21	0.41
5:4:136:ILE:HA	5:4:136:ILE:HD13	1.90	0.41
9:A:1557:G:C4	9:A:1559:A:C8	3.09	0.41
9:A:1853:C:H2'	9:A:1854:C:C6	2.54	0.41
9:A:2469:C:H2'	9:A:2470:A:C8	2.55	0.41
9:A:434:A:H2'	9:A:435:A:C8	2.55	0.41
9:A:722:G:C2	9:A:732:A:C6	3.08	0.41
9:A:844:G:C6	9:A:845:C:N4	2.87	0.41
10:B:54:G:H8	10:B:54:G:O5'	2.03	0.41
11:C:226:HIS:HA	11:C:227:PRO:HD3	1.92	0.41
15:G:123:PHE:O	15:G:174:SER:HA	2.20	0.41
9:A:2212:A:N3	16:H:77:PHE:HB2	2.35	0.41
19:K:109:PRO:O	19:K:112:LYS:HG3	2.20	0.41
10:B:48:C:OP2	24:P:49:ARG:NH2	2.53	0.41
26:R:106:ASN:O	26:R:110:MET:HG3	2.19	0.41
27:S:105:ASP:OD1	27:S:106:ILE:N	2.53	0.41
32:X:131:ASP:OD1	32:X:132:LYS:HG3	2.20	0.41
34:Z:76:LEU:HD22	34:Z:115:MET:CE	2.50	0.41
7:6:119:LEU:HD13	9:A:1405:A:H5'	2.03	0.41
9:A:1028:A:H2'	9:A:1029:A:C8	2.80	0.41
9:A:1269:G:OP1	13:E:143:PRO:HG3	2.20	0.41
9:A:1604:A:H2'	9:A:1605:A:H8	1.83	0.41
9:A:2705:G:N1	9:A:2738:U:OP2	2.32	0.41
9:A:881:U:O2	9:A:915:G:N2	2.35	0.41
13:E:64:LYS:HE3	13:E:66:GLY:O	2.21	0.41
17:I:76:LEU:HD22	17:I:134:PHE:CD1	2.55	0.41
25:Q:168:ILE:HB	25:Q:232:PHE:CE2	2.56	0.41
9:A:592:G:OP1	26:R:32:THR:HG21	2.20	0.41
26:R:96:ILE:HA	26:R:96:ILE:HD12	1.81	0.41
32:X:71:ASP:OD1	32:X:72:SER:N	2.53	0.41
9:A:160:A:C2	9:A:161:G:C4	3.08	0.41
9:A:1863:A:H2'	9:A:1864:A:C8	2.56	0.41
9:A:2082:U:H6	9:A:2082:U:H5'	1.85	0.41
9:A:2139:A:O2'	9:A:2187:A:N6	2.51	0.41
9:A:2410:U:H2'	9:A:2411:C:H6	1.86	0.41
13:E:159:LEU:HD12	13:E:159:LEU:HA	1.90	0.41
13:E:78:GLU:HG3	13:E:78:GLU:H	1.63	0.41
22:N:11:LYS:HB3	22:N:87:LYS:HE3	2.03	0.41
24:P:48:THR:HG22	24:P:50:ARG:HB3	2.01	0.41
27:S:127:VAL:HG12	27:S:161:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:134:SER:O	7:6:138:LYS:HG2	2.20	0.41
9:A:1454:G:H2'	9:A:1455:A:C8	2.56	0.41
9:A:2245:U:H2'	9:A:2246:U:C6	2.55	0.41
9:A:2490:U:OP1	9:A:2546:G:N2	2.50	0.41
9:A:2658:A:P	19:K:175:ARG:HH12	2.42	0.41
19:K:144:THR:HG22	19:K:146:SER:H	1.85	0.41
5:4:95:HIS:HE2	9:A:236:A:P	2.43	0.41
9:A:1804:U:H2'	9:A:1805:C:C6	2.56	0.41
9:A:1875:G:H2'	9:A:1889:G:H22	1.86	0.41
9:A:409:U:H1'	9:A:2248:U:O2'	2.20	0.41
9:A:2292:C:H2'	9:A:2292:C:H6	1.69	0.41
9:A:2584:G:H2'	9:A:2585:C:C6	2.56	0.41
9:A:724:G:H1'	9:A:729:A:H62	1.84	0.41
9:A:794:A:C5	9:A:796:G:H1'	2.56	0.41
9:A:919:A:N3	9:A:2281:C:O2'	2.43	0.41
13:E:153:ASN:HB2	13:E:156:GLU:HB2	2.03	0.41
17:I:66:VAL:HG22	17:I:103:ILE:HG21	2.01	0.41
18:J:86:ALA:HA	18:J:117:THR:HG21	2.02	0.41
19:K:100:TRP:CE3	26:R:102:ILE:HD13	2.56	0.41
20:L:13:ASN:O	20:L:15:GLY:N	2.54	0.41
22:N:16:ARG:NE	22:N:18:LYS:HE3	2.36	0.41
30:V:130:ILE:HD13	30:V:130:ILE:HG21	1.83	0.41
1:0:39:SER:O	1:0:40:ASP:HB3	2.20	0.41
9:A:1378:U:H2'	9:A:1379:C:O4'	2.20	0.41
9:A:2341:U:H3'	9:A:2342:G:C5'	2.51	0.41
9:A:926:A:H4'	9:A:926:A:OP1	3.16	0.41
10:B:62:U:H2'	10:B:63:C:C6	2.54	0.41
11:C:102:HIS:HA	11:C:103:PRO:HD3	1.91	0.41
11:C:114:SER:HB3	11:C:125:ALA:HB3	2.01	0.41
12:D:142:GLU:HB3	12:D:166:ARG:HB3	2.02	0.41
12:D:151:MET:HB3	12:D:151:MET:HE2	1.95	0.41
18:J:85:GLU:OE1	18:J:88:LYS:HD2	2.20	0.41
19:K:77:VAL:HA	19:K:78:PRO:HD3	1.90	0.41
25:Q:148:ILE:HD13	25:Q:168:ILE:HG13	2.03	0.41
25:Q:151:ILE:HG12	25:Q:206:ILE:HG13	2.01	0.41
28:T:65:LEU:HD23	28:T:65:LEU:HA	1.88	0.41
31:W:49:A:O2'	31:W:50:G:H5'	2.21	0.41
1:0:74:SER:HB3	14:F:158:ASN:HA	2.03	0.41
9:A:1023:C:OP2	26:R:54:LYS:NZ	2.54	0.41
9:A:1374:A:H2'	9:A:1375:A:C8	2.55	0.41
9:A:1690:A:N7	9:A:2019:G:N2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:96:LEU:HD21	9:A:1790:A:C4	2.55	0.41
9:A:1818:U:H3'	9:A:1819:A:C8	2.56	0.41
9:A:2410:U:H2'	9:A:2411:C:C6	2.55	0.41
9:A:372:G:H2'	9:A:373:C:C6	2.56	0.41
9:A:701:U:H5''	9:A:702:C:OP2	2.21	0.41
11:C:138:HIS:CD2	11:C:139:ASN:HB2	2.55	0.41
11:C:179:LEU:HD13	11:C:267:ILE:HD11	2.03	0.41
12:D:204:ILE:HD11	12:D:285:LYS:HD3	2.03	0.41
26:R:97:LEU:HA	26:R:97:LEU:HD23	1.73	0.41
27:S:108:ASN:ND2	27:S:113:LYS:HE3	2.35	0.41
34:Z:140:TRP:CE2	34:Z:144:ILE:HD11	2.56	0.41
2:1:6:LYS:HD3	2:1:6:LYS:HA	1.72	0.41
9:A:1195:U:H3'	9:A:1196:A:H8	1.86	0.41
9:A:1335:C:O5'	9:A:1335:C:H6	2.04	0.41
9:A:1454:G:N2	9:A:1595:C:O2	2.54	0.41
9:A:2080:U:O2'	9:A:2081:A:H5'	2.21	0.41
9:A:2356:G:C2	9:A:2357:A:C4	3.09	0.41
9:A:2467:A:OP1	9:A:2514:A:O2'	2.28	0.41
9:A:2555:U:H2'	9:A:2556:C:H6	1.85	0.41
28:T:127:ARG:HA	28:T:128:PRO:HD3	1.82	0.41
9:A:1636:U:OP1	29:U:172:LYS:HE3	2.21	0.41
9:A:2165:G:H2'	9:A:2166:G:C8	2.56	0.41
9:A:2204:A:H3'	9:A:2205:G:C8	2.55	0.41
9:A:2699:U:H2'	9:A:2700:C:C6	2.56	0.41
9:A:410:G:H21	16:H:42:GLN:NE2	2.19	0.41
9:A:457:C:O2'	9:A:458:G:H5'	2.21	0.41
9:A:481:G:H4'	13:E:120:LYS:HD2	2.03	0.41
17:I:154:ARG:CD	17:I:159:ASN:HB2	2.51	0.41
18:J:120:LYS:HD2	18:J:125:ILE:HD11	2.03	0.41
21:M:158:VAL:HA	21:M:159:PRO:HD3	1.81	0.41
33:Y:98:LEU:HA	33:Y:98:LEU:HD12	1.66	0.41
8:7:80:PRO:HA	8:7:81:PRO:HD3	1.93	0.41
9:A:1178:G:H4'	26:R:83:HIS:CD2	2.56	0.41
9:A:2225:G:H2'	9:A:2226:A:C8	2.56	0.41
9:A:2288:G:H8	9:A:2288:G:O5'	2.04	0.41
9:A:2342:G:C6	9:A:2343:C:N3	2.89	0.41
9:A:324:G:H2'	9:A:325:A:O4'	2.21	0.41
9:A:715:G:N2	9:A:737:G:C4	2.88	0.41
9:A:2256:A:P	11:C:239:ARG:NH2	2.93	0.41
19:K:217:LEU:HD23	19:K:217:LEU:HA	1.90	0.41
25:Q:219:LEU:HB3	25:Q:221:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1093:C:H1'	9:A:1102:G:N2	2.36	0.40
9:A:1407:C:H2'	9:A:1408:A:C8	2.56	0.40
9:A:552:G:OP2	19:K:69:LYS:NZ	2.36	0.40
9:A:826:C:H2'	9:A:827:C:H6	1.85	0.40
12:D:145:ARG:NH1	12:D:147:ARG:HH11	2.19	0.40
13:E:200:ASP:O	13:E:202:ALA:N	2.45	0.40
13:E:232:ARG:NH1	13:E:232:ARG:O	2.51	0.40
15:G:141:LYS:HA	15:G:141:LYS:HD3	1.88	0.40
15:G:203:ARG:HG3	15:G:204:TYR:O	2.21	0.40
9:A:1074:A:C2	17:I:63:VAL:HG21	2.56	0.40
22:N:2:LEU:HD13	22:N:69:PHE:HD1	1.86	0.40
23:O:36:THR:HG22	23:O:80:ILE:HG23	2.02	0.40
25:Q:175:ALA:O	25:Q:179:THR:N	2.53	0.40
28:T:126:LYS:O	28:T:128:PRO:HD3	2.20	0.40
31:W:40:U:H2'	31:W:41:A:C8	2.56	0.40
31:W:50:G:H2'	31:W:51:U:O4'	2.21	0.40
34:Z:101:LYS:O	34:Z:104:ASP:HB2	2.20	0.40
4:3:104:SER:O	4:3:107:SER:N	2.54	0.40
9:A:1087:G:H3'	9:A:1088:U:H2'	2.03	0.40
9:A:1168:U:C6	9:A:1168:U:H5'	2.56	0.40
9:A:1809:G:N2	11:C:150:LEU:HD22	2.35	0.40
9:A:1886:A:H2'	9:A:1887:G:C8	2.55	0.40
9:A:2113:G:N2	9:A:2204:A:H62	2.19	0.40
9:A:850:G:C6	9:A:851:U:N3	2.89	0.40
10:B:29:C:C2	10:B:30:A:C8	3.08	0.40
11:C:228:HIS:CD2	11:C:228:HIS:N	2.88	0.40
9:A:2652:A:O2'	12:D:170:GLU:OE1	2.27	0.40
14:F:54:ILE:H	14:F:54:ILE:HG13	1.41	0.40
19:K:135:ILE:O	19:K:150:GLY:HA3	2.21	0.40
19:K:164:SER:O	19:K:167:LYS:HE3	2.21	0.40
20:L:67:LYS:HG3	20:L:68:GLU:H	1.87	0.40
21:M:109:SER:O	21:M:110:CYS:HB2	2.22	0.40
21:M:130:GLU:O	21:M:132:GLY:N	2.54	0.40
19:K:97:ASN:ND2	27:S:135:ILE:H	2.09	0.40
28:T:67:LEU:HD23	28:T:67:LEU:HA	1.81	0.40
29:U:190:LYS:HE2	34:Z:156:GLN:HB3	2.02	0.40
34:Z:92:LEU:HD23	34:Z:92:LEU:HA	1.87	0.40
5:4:92:MET:HB3	5:4:92:MET:HE2	1.75	0.40
9:A:1649:G:C2	9:A:1655:G:C5	3.09	0.40
9:A:1673:A:H2'	9:A:1674:C:C6	2.56	0.40
9:A:378:A:N3	9:A:378:A:H2'	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:675:U:H2'	9:A:676:U:H6	1.87	0.40
12:D:145:ARG:CZ	12:D:147:ARG:HD3	2.51	0.40
12:D:198:ASP:OD1	12:D:262:ARG:HA	2.22	0.40
13:E:94:ASN:OD1	13:E:149:THR:HA	2.21	0.40
15:G:72:LEU:HD12	15:G:119:VAL:HG13	2.02	0.40
15:G:94:LYS:HB2	15:G:97:GLU:OE2	2.22	0.40
19:K:48:ARG:NH2	31:W:2:G:N7	2.70	0.40
9:A:2051:G:H2'	9:A:2052:G:C8	2.56	0.40
9:A:33:A:O2'	9:A:466:A:N3	2.52	0.40
9:A:771:G:H2'	9:A:772:A:O4'	2.22	0.40
9:A:888:C:C4	9:A:909:A:C5	3.09	0.40
10:B:10:G:OP1	24:P:57:HIS:NE2	2.53	0.40
11:C:110:ASP:OD1	11:C:111:THR:N	2.53	0.40
11:C:256:ARG:NH2	11:C:262:SER:HB2	2.35	0.40
12:D:181:PRO:O	12:D:182:SER:HB3	2.21	0.40
21:M:127:ARG:HD2	21:M:127:ARG:HA	1.85	0.40
21:M:154:LEU:HD12	21:M:154:LEU:HA	1.83	0.40
31:W:40:U:C4	31:W:87:A:N6	2.89	0.40
36:8:1131:UNK:CB	36:8:1219:UNK:HA	2.51	0.40
9:A:1192:A:H2'	9:A:1193:U:C6	2.56	0.40
9:A:16:G:H2'	9:A:17:C:C6	2.57	0.40
9:A:1866:G:H5''	9:A:1867:A:OP2	2.21	0.40
3:2:30:VAL:HG23	9:A:2417:G:H4'	2.04	0.40
9:A:491:A:C2	9:A:492:A:C5	3.10	0.40
9:A:826:C:H2'	9:A:827:C:C6	2.57	0.40
9:A:940:C:H2'	9:A:941:C:C6	2.57	0.40
11:C:237:ILE:HG21	11:C:237:ILE:HD13	1.82	0.40
15:G:44:GLY:HA3	15:G:105:HIS:NE2	2.35	0.40
9:A:1086:G:N2	18:J:198:ILE:HG12	2.22	0.40
19:K:225:LYS:HB2	19:K:225:LYS:HE3	1.63	0.40
9:A:2432:G:C5'	21:M:148:GLY:HA3	2.51	0.40
23:O:20:LEU:O	23:O:22:ARG:HG2	2.21	0.40
10:B:10:G:O5'	24:P:61:ARG:NH1	2.54	0.40
33:Y:96:LYS:HD3	33:Y:96:LYS:HA	1.83	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	
1	0	64/130 (49%)	56 (88%)	5 (8%)	3 (5%)	3	26
2	1	46/57 (81%)	45 (98%)	1 (2%)	0	100	100
3	2	58/66 (88%)	53 (91%)	5 (9%)	0	100	100
4	3	58/152 (38%)	54 (93%)	4 (7%)	0	100	100
5	4	70/159 (44%)	66 (94%)	4 (6%)	0	100	100
6	5	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
7	6	47/142 (33%)	46 (98%)	0	1 (2%)	9	47
8	7	44/116 (38%)	41 (93%)	3 (7%)	0	100	100
11	C	251/272 (92%)	235 (94%)	15 (6%)	1 (0%)	39	79
12	D	219/305 (72%)	206 (94%)	12 (6%)	1 (0%)	34	75
13	E	210/293 (72%)	196 (93%)	14 (7%)	0	100	100
14	F	191/258 (74%)	178 (93%)	13 (7%)	0	100	100
15	G	176/220 (80%)	165 (94%)	11 (6%)	0	100	100
16	H	46/196 (24%)	43 (94%)	3 (6%)	0	100	100
17	I	135/232 (58%)	132 (98%)	3 (2%)	0	100	100
18	J	131/224 (58%)	126 (96%)	5 (4%)	0	100	100
19	K	201/250 (80%)	193 (96%)	8 (4%)	0	100	100
20	L	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
21	M	183/271 (68%)	168 (92%)	13 (7%)	2 (1%)	17	61
22	N	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
23	O	114/126 (90%)	108 (95%)	6 (5%)	0	100	100
24	P	120/166 (72%)	113 (94%)	7 (6%)	0	100	100
25	Q	116/233 (50%)	114 (98%)	2 (2%)	0	100	100
26	R	117/128 (91%)	110 (94%)	7 (6%)	0	100	100
27	S	168/256 (66%)	158 (94%)	8 (5%)	2 (1%)	16	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	T	170/199 (85%)	162 (95%)	7 (4%)	1 (1%)	30	72
29	U	94/198 (48%)	89 (95%)	5 (5%)	0	100	100
30	V	132/192 (69%)	123 (93%)	9 (7%)	0	100	100
32	X	107/194 (55%)	96 (90%)	11 (10%)	0	100	100
33	Y	75/148 (51%)	73 (97%)	2 (3%)	0	100	100
34	Z	99/168 (59%)	95 (96%)	3 (3%)	1 (1%)	19	63
38	b	231/236 (98%)	221 (96%)	10 (4%)	0	100	100
39	c	214/218 (98%)	201 (94%)	13 (6%)	0	100	100
40	d	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
41	e	185/308 (60%)	182 (98%)	3 (2%)	0	100	100
42	f	111/211 (53%)	106 (96%)	4 (4%)	1 (1%)	21	65
43	g	152/155 (98%)	146 (96%)	6 (4%)	0	100	100
44	h	131/134 (98%)	127 (97%)	2 (2%)	2 (2%)	13	54
45	i	142/208 (68%)	136 (96%)	6 (4%)	0	100	100
46	j	97/195 (50%)	93 (96%)	3 (3%)	1 (1%)	19	63
47	k	115/138 (83%)	108 (94%)	7 (6%)	0	100	100
48	l	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
49	m	108/172 (63%)	101 (94%)	6 (6%)	1 (1%)	21	65
50	n	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
51	o	73/90 (81%)	72 (99%)	1 (1%)	0	100	100
52	p	78/88 (89%)	74 (95%)	4 (5%)	0	100	100
53	q	84/165 (51%)	78 (93%)	6 (7%)	0	100	100
54	r	58/101 (57%)	55 (95%)	3 (5%)	0	100	100
55	s	76/92 (83%)	75 (99%)	1 (1%)	0	100	100
56	t	105/183 (57%)	100 (95%)	3 (3%)	2 (2%)	10	49
57	u	63/180 (35%)	62 (98%)	1 (2%)	0	100	100
58	v	78/260 (30%)	76 (97%)	2 (3%)	0	100	100
59	w	80/179 (45%)	78 (98%)	2 (2%)	0	100	100
60	x	38/101 (38%)	37 (97%)	1 (3%)	0	100	100
61	y	114/302 (38%)	106 (93%)	8 (7%)	0	100	100
All	All	6476/9784 (66%)	6138 (95%)	319 (5%)	19 (0%)	50	82

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	92	ASP
27	S	78	PRO
49	m	53	VAL
56	t	174	TYR
11	C	232	GLU
34	Z	151	SER
46	j	150	VAL
21	M	144	ARG
44	h	68	ASN
44	h	69	LYS
56	t	79	ALA
21	M	131	GLY
28	T	146	ASP
1	0	91	ALA
12	D	212	ILE
42	f	149	VAL
1	0	72	VAL
7	6	131	TRP
27	S	77	ARG

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	
1	0	57/117 (49%)	54 (95%)	3 (5%)	28	67
2	1	41/50 (82%)	37 (90%)	4 (10%)	10	40
3	2	56/60 (93%)	50 (89%)	6 (11%)	8	35
4	3	50/125 (40%)	42 (84%)	8 (16%)	3	16
5	4	62/140 (44%)	52 (84%)	10 (16%)	3	16
6	5	34/34 (100%)	30 (88%)	4 (12%)	6	29
7	6	46/124 (37%)	42 (91%)	4 (9%)	13	47
8	7	40/96 (42%)	33 (82%)	7 (18%)	2	13
11	C	201/217 (93%)	185 (92%)	16 (8%)	15	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	D	182/259 (70%)	164 (90%)	18 (10%)	10	39
13	E	179/255 (70%)	158 (88%)	21 (12%)	7	30
14	F	152/214 (71%)	140 (92%)	12 (8%)	15	52
15	G	151/190 (80%)	137 (91%)	14 (9%)	11	42
16	H	42/170 (25%)	37 (88%)	5 (12%)	6	29
17	I	119/204 (58%)	109 (92%)	10 (8%)	14	49
18	J	106/189 (56%)	101 (95%)	5 (5%)	32	72
19	K	176/213 (83%)	166 (94%)	10 (6%)	25	65
20	L	101/101 (100%)	91 (90%)	10 (10%)	10	39
21	M	141/215 (66%)	123 (87%)	18 (13%)	5	26
22	N	108/108 (100%)	100 (93%)	8 (7%)	17	55
23	O	96/103 (93%)	81 (84%)	15 (16%)	3	18
24	P	100/139 (72%)	90 (90%)	10 (10%)	9	38
25	Q	104/207 (50%)	94 (90%)	10 (10%)	10	40
26	R	106/115 (92%)	93 (88%)	13 (12%)	6	28
27	S	137/223 (61%)	131 (96%)	6 (4%)	35	73
28	T	152/176 (86%)	134 (88%)	18 (12%)	6	29
29	U	85/171 (50%)	74 (87%)	11 (13%)	5	26
30	V	121/169 (72%)	111 (92%)	10 (8%)	14	49
32	X	92/163 (56%)	76 (83%)	16 (17%)	2	13
33	Y	67/130 (52%)	59 (88%)	8 (12%)	6	29
34	Z	93/153 (61%)	84 (90%)	9 (10%)	10	40
38	b	198/201 (98%)	184 (93%)	14 (7%)	18	58
39	c	186/188 (99%)	175 (94%)	11 (6%)	24	64
40	d	178/180 (99%)	164 (92%)	14 (8%)	15	52
41	e	121/255 (48%)	113 (93%)	8 (7%)	21	61
42	f	100/186 (54%)	94 (94%)	6 (6%)	24	64
43	g	125/126 (99%)	118 (94%)	7 (6%)	26	66
44	h	116/117 (99%)	108 (93%)	8 (7%)	19	59
45	i	114/169 (68%)	99 (87%)	15 (13%)	5	25
46	j	91/173 (53%)	85 (93%)	6 (7%)	21	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	k	91/109 (84%)	83 (91%)	8 (9%)	12	46
48	l	105/106 (99%)	98 (93%)	7 (7%)	20	60
49	m	99/151 (66%)	92 (93%)	7 (7%)	18	58
50	n	89/90 (99%)	81 (91%)	8 (9%)	12	45
51	o	70/85 (82%)	68 (97%)	2 (3%)	50	82
52	p	71/79 (90%)	63 (89%)	8 (11%)	7	32
53	q	77/149 (52%)	72 (94%)	5 (6%)	21	61
54	r	56/96 (58%)	51 (91%)	5 (9%)	12	45
55	s	68/81 (84%)	64 (94%)	4 (6%)	24	64
56	t	89/156 (57%)	84 (94%)	5 (6%)	26	66
57	u	59/160 (37%)	55 (93%)	4 (7%)	20	60
58	v	67/225 (30%)	67 (100%)	0	100	100
59	w	76/162 (47%)	76 (100%)	0	100	100
60	x	30/85 (35%)	30 (100%)	0	100	100
61	y	104/275 (38%)	99 (95%)	5 (5%)	31	71
All	All	5577/8434 (66%)	5101 (92%)	476 (8%)	18	48

All (476) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	51	VAL
1	0	57	LEU
1	0	59	MET
2	1	6	LYS
2	1	7	ARG
2	1	11	TYR
2	1	46	PHE
3	2	6	ASP
3	2	19	VAL
3	2	28	ARG
3	2	34	ILE
3	2	42	THR
3	2	60	ILE
4	3	97	CYS
4	3	98	LEU
4	3	115	ARG
4	3	118	MET

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Mol	Chain	Res	Type
4	3	126	LEU
4	3	127	LEU
4	3	129	ARG
4	3	142	THR
5	4	92	MET
5	4	94	THR
5	4	103	ARG
5	4	109	LYS
5	4	119	HIS
5	4	125	ASN
5	4	128	ARG
5	4	135	LEU
5	4	139	ASP
5	4	143	TYR
6	5	4	ARG
6	5	6	SER
6	5	29	ASN
6	5	36	GLN
7	6	103	LYS
7	6	118	ARG
7	6	137	LYS
7	6	138	LYS
8	7	54	LYS
8	7	62	THR
8	7	65	LYS
8	7	66	LYS
8	7	69	ARG
8	7	74	ARG
8	7	88	GLU
11	C	19	GLN
11	C	71	TYR
11	C	78	GLU
11	C	100	ILE
11	C	126	LEU
11	C	142	ILE
11	C	152	ARG
11	C	167	SER
11	C	178	ARG
11	C	188	VAL
11	C	196	VAL
11	C	203	ARG
11	C	224	VAL

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Mol	Chain	Res	Type
11	C	228	HIS
11	C	244	THR
11	C	270	ARG
12	D	109	VAL
12	D	132	ASP
12	D	137	VAL
12	D	146	ASP
12	D	174	VAL
12	D	178	ASP
12	D	193	GLU
12	D	213	LYS
12	D	221	LEU
12	D	222	MET
12	D	229	HIS
12	D	240	THR
12	D	260	LYS
12	D	262	ARG
12	D	273	LEU
12	D	288	ASN
12	D	292	LEU
12	D	298	VAL
13	E	52	LEU
13	E	61	SER
13	E	68	THR
13	E	78	GLU
13	E	97	ARG
13	E	113	ARG
13	E	120	LYS
13	E	130	ARG
13	E	147	ASP
13	E	152	MET
13	E	157	ARG
13	E	161	LEU
13	E	209	LEU
13	E	211	ASP
13	E	213	VAL
13	E	223	ILE
13	E	226	LEU
13	E	230	THR
13	E	238	ASP
13	E	245	LEU
13	E	261	VAL

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Mol	Chain	Res	Type
14	F	56	ARG
14	F	59	THR
14	F	78	ILE
14	F	88	VAL
14	F	110	LEU
14	F	119	VAL
14	F	122	LYS
14	F	127	ILE
14	F	155	ARG
14	F	164	THR
14	F	188	GLN
14	F	190	VAL
15	G	40	GLU
15	G	41	SER
15	G	50	VAL
15	G	63	LEU
15	G	94	LYS
15	G	100	ARG
15	G	102	ASN
15	G	105	HIS
15	G	109	ARG
15	G	111	LEU
15	G	127	LEU
15	G	129	LEU
15	G	169	THR
15	G	213	GLU
16	H	47	LYS
16	H	57	ILE
16	H	65	GLN
16	H	75	ARG
16	H	79	LEU
17	I	75	LEU
17	I	79	ILE
17	I	84	PHE
17	I	89	PHE
17	I	101	THR
17	I	114	VAL
17	I	119	TRP
17	I	140	ILE
17	I	147	TYR
17	I	165	CYS
18	J	90	THR

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Mol	Chain	Res	Type
18	J	99	LEU
18	J	129	ILE
18	J	152	LYS
18	J	171	ILE
19	K	48	ARG
19	K	62	ARG
19	K	64	LEU
19	K	79	LEU
19	K	82	ARG
19	K	168	ARG
19	K	169	THR
19	K	174	ARG
19	K	191	LEU
19	K	232	GLN
20	L	1	MET
20	L	2	ILE
20	L	23	ARG
20	L	25	ILE
20	L	28	SER
20	L	34	ARG
20	L	42	VAL
20	L	75	MET
20	L	102	ILE
20	L	105	GLU
21	M	83	ASP
21	M	84	ASN
21	M	106	GLN
21	M	115	ARG
21	M	120	ARG
21	M	125	ILE
21	M	127	ARG
21	M	138	ARG
21	M	150	MET
21	M	154	LEU
21	M	164	ASP
21	M	186	ILE
21	M	192	ARG
21	M	208	THR
21	M	212	ILE
21	M	215	ARG
21	M	220	SER
21	M	246	VAL

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Mol	Chain	Res	Type
22	N	5	LYS
22	N	9	PHE
22	N	28	CYS
22	N	41	TRP
22	N	44	SER
22	N	52	ARG
22	N	56	ARG
22	N	109	VAL
23	O	11	MET
23	O	19	ARG
23	O	22	ARG
23	O	27	ARG
23	O	28	ARG
23	O	36	THR
23	O	48	ARG
23	O	56	LYS
23	O	73	ARG
23	O	74	ARG
23	O	89	LEU
23	O	105	THR
23	O	111	LEU
23	O	123	ILE
23	O	126	VAL
24	P	49	ARG
24	P	52	ASP
24	P	53	ARG
24	P	59	ARG
24	P	70	ARG
24	P	87	ILE
24	P	127	ILE
24	P	143	ARG
24	P	151	ARG
24	P	161	GLU
25	Q	138	ARG
25	Q	161	ARG
25	Q	185	ARG
25	Q	198	LEU
25	Q	203	ILE
25	Q	206	ILE
25	Q	212	ARG
25	Q	215	ARG
25	Q	219	LEU

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Mol	Chain	Res	Type
25	Q	228	ARG
26	R	6	ARG
26	R	11	ARG
26	R	31	LEU
26	R	48	ARG
26	R	59	ARG
26	R	70	ARG
26	R	76	TYR
26	R	85	LEU
26	R	96	ILE
26	R	100	ILE
26	R	108	ILE
26	R	109	TYR
26	R	113	ASN
27	S	87	ASP
27	S	102	GLU
27	S	163	LEU
27	S	208	ARG
27	S	216	ILE
27	S	228	GLU
28	T	35	ARG
28	T	43	VAL
28	T	45	LYS
28	T	47	ARG
28	T	101	SER
28	T	104	GLU
28	T	110	THR
28	T	113	LYS
28	T	134	ILE
28	T	137	ARG
28	T	139	ILE
28	T	153	THR
28	T	160	LEU
28	T	163	LEU
28	T	164	MET
28	T	174	CYS
28	T	183	ILE
28	T	192	LEU
29	U	102	LEU
29	U	103	LYS
29	U	119	ILE
29	U	138	VAL

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Mol	Chain	Res	Type
29	U	141	ARG
29	U	143	ASP
29	U	154	PHE
29	U	171	THR
29	U	172	LYS
29	U	178	LEU
29	U	179	ASN
30	V	48	ARG
30	V	51	ARG
30	V	93	ILE
30	V	98	SER
30	V	130	ILE
30	V	146	SER
30	V	165	THR
30	V	171	THR
30	V	173	ASP
30	V	176	LYS
32	X	73	LYS
32	X	77	LEU
32	X	81	ILE
32	X	85	GLN
32	X	86	VAL
32	X	97	ARG
32	X	105	LYS
32	X	109	ILE
32	X	111	LYS
32	X	120	ASP
32	X	123	VAL
32	X	135	VAL
32	X	142	ILE
32	X	151	ARG
32	X	155	ARG
32	X	156	GLU
33	Y	72	ARG
33	Y	83	ASN
33	Y	87	ARG
33	Y	91	SER
33	Y	92	ASN
33	Y	98	LEU
33	Y	126	LEU
33	Y	144	ASP
34	Z	65	LEU

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Mol	Chain	Res	Type
34	Z	74	GLU
34	Z	76	LEU
34	Z	81	LEU
34	Z	87	LEU
34	Z	104	ASP
34	Z	132	LEU
34	Z	133	SER
34	Z	146	VAL
38	b	7	ASN
38	b	8	ILE
38	b	30	ARG
38	b	53	PHE
38	b	77	LYS
38	b	79	LYS
38	b	83	SER
38	b	114	ARG
38	b	119	ARG
38	b	163	ASP
38	b	175	THR
38	b	194	ASN
38	b	218	LEU
38	b	232	TYR
39	c	4	LYS
39	c	5	ILE
39	c	24	SER
39	c	42	CYS
39	c	58	GLU
39	c	78	MET
39	c	83	LEU
39	c	103	LEU
39	c	107	ASN
39	c	116	ARG
39	c	209	ILE
40	d	8	ARG
40	d	9	PHE
40	d	12	ILE
40	d	15	LEU
40	d	23	ASN
40	d	96	PHE
40	d	97	ARG
40	d	104	ILE
40	d	109	GLN

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Mol	Chain	Res	Type
40	d	112	ASN
40	d	134	ASP
40	d	152	LEU
40	d	179	ILE
40	d	189	ASN
41	e	161	ARG
41	e	187	VAL
41	e	191	VAL
41	e	210	ARG
41	e	270	LEU
41	e	272	SER
41	e	292	PHE
41	e	299	ARG
42	f	107	GLN
42	f	118	MET
42	f	119	THR
42	f	124	LEU
42	f	141	TYR
42	f	183	GLU
43	g	6	THR
43	g	10	LYS
43	g	15	ASP
43	g	25	MET
43	g	36	LYS
43	g	63	ARG
43	g	72	ASP
44	h	20	ARG
44	h	28	SER
44	h	45	ILE
44	h	46	GLU
44	h	60	VAL
44	h	76	THR
44	h	79	LEU
44	h	84	ARG
45	i	78	PHE
45	i	89	ARG
45	i	99	GLN
45	i	102	THR
45	i	117	GLN
45	i	124	GLN
45	i	132	THR
45	i	136	GLU

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Mol	Chain	Res	Type
45	i	143	VAL
45	i	150	LEU
45	i	184	ARG
45	i	189	VAL
45	i	196	LEU
45	i	206	SER
45	i	208	ARG
46	j	101	ILE
46	j	104	ARG
46	j	107	TRP
46	j	115	CYS
46	j	143	CYS
46	j	153	ASP
47	k	42	THR
47	k	45	ASP
47	k	49	ARG
47	k	51	VAL
47	k	62	ARG
47	k	102	ARG
47	k	114	ILE
47	k	122	VAL
48	l	11	THR
48	l	24	LEU
48	l	31	ARG
48	l	54	ARG
48	l	78	SER
48	l	82	VAL
48	l	101	THR
49	m	98	LEU
49	m	110	ILE
49	m	113	ASP
49	m	118	ASN
49	m	142	CYS
49	m	151	CYS
49	m	152	ARG
50	n	3	ARG
50	n	5	SER
50	n	35	THR
50	n	37	LEU
50	n	49	SER
50	n	59	LEU
50	n	68	ARG

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Mol	Chain	Res	Type
50	n	92	LEU
51	o	35	ARG
51	o	40	LEU
52	p	11	ARG
52	p	22	ILE
52	p	26	SER
52	p	28	ARG
52	p	29	GLU
52	p	33	LEU
52	p	50	VAL
52	p	66	THR
53	q	70	ASN
53	q	80	ARG
53	q	86	LYS
53	q	120	ILE
53	q	142	LYS
54	r	22	ILE
54	r	28	ILE
54	r	31	ARG
54	r	32	ASN
54	r	71	ILE
55	s	30	ILE
55	s	53	ASN
55	s	77	THR
55	s	81	ARG
56	t	99	GLU
56	t	121	SER
56	t	151	ASN
56	t	168	GLU
56	t	173	TRP
57	u	102	ARG
57	u	124	ASN
57	u	125	LYS
57	u	134	ARG
61	y	82	ARG
61	y	119	ARG
61	y	122	ASP
61	y	140	ARG
61	y	181	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	42	HIS
3	2	36	GLN
4	3	143	ASN
11	C	23	ASN
11	C	149	GLN
12	D	121	ASN
12	D	215	HIS
12	D	224	HIS
12	D	288	ASN
13	E	91	HIS
13	E	118	GLN
13	E	171	ASN
14	F	60	ASN
15	G	183	GLN
16	H	42	GLN
17	I	90	GLN
17	I	130	ASN
19	K	97	ASN
20	L	92	ASN
21	M	133	GLN
23	O	18	HIS
23	O	87	HIS
24	P	81	HIS
24	P	85	GLN
24	P	93	HIS
24	P	162	HIS
26	R	37	GLN
26	R	83	HIS
26	R	99	GLN
26	R	113	ASN
27	S	108	ASN
27	S	189	GLN
28	T	97	ASN
29	U	153	ASN
30	V	180	ASN
33	Y	99	GLN
38	b	170	GLN
38	b	194	ASN
39	c	125	ASN
40	d	57	HIS
40	d	112	ASN
40	d	149	GLN
41	e	225	HIS

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Mol	Chain	Res	Type
42	f	160	ASN
43	g	20	ASN
43	g	148	ASN
44	h	19	ASN
44	h	30	ASN
45	i	81	GLN
45	i	138	ASN
46	j	117	GLN
46	j	149	HIS
46	j	151	HIS
48	l	111	GLN
49	m	52	ASN
49	m	58	ASN
49	m	66	GLN
49	m	87	ASN
49	m	145	GLN
50	n	48	GLN
50	n	53	ASN
50	n	60	HIS
50	n	81	HIS
51	o	39	HIS
51	o	43	HIS
52	p	13	GLN
53	q	98	GLN
54	r	23	GLN
54	r	79	ASN
55	s	47	HIS
55	s	69	HIS
57	u	140	ASN
58	v	258	ASN
59	w	162	GLN
59	w	168	ASN
61	y	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	120/121 (99%)	20 (16%)	0
31	W	105/106 (99%)	34 (32%)	1 (0%)
35	z	75/76 (98%)	22 (29%)	0
37	a	1483/1491 (99%)	349 (23%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	A	2794/2810 (99%)	658 (23%)	8 (0%)
All	All	4577/4604 (99%)	1083 (23%)	9 (0%)

All (1083) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	8	G
9	A	9	A
9	A	10	G
9	A	12	A
9	A	13	A
9	A	14	A
9	A	31	C
9	A	33	A
9	A	34	G
9	A	39	C
9	A	45	A
9	A	46	C
9	A	54	G
9	A	57	G
9	A	70	A
9	A	71	A
9	A	73	U
9	A	74	G
9	A	82	G
9	A	84	G
9	A	94	A
9	A	97	A
9	A	98	G
9	A	99	A
9	A	100	G
9	A	116	A
9	A	117	A
9	A	118	U
9	A	123	C
9	A	130	U
9	A	131	C
9	A	132	G
9	A	143	G
9	A	144	A
9	A	149	A
9	A	158	C

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Mol	Chain	Res	Type
9	A	159	A
9	A	160	A
9	A	163	G
9	A	181	A
9	A	184	A
9	A	200	G
9	A	201	A
9	A	206	A
9	A	207	A
9	A	208	A
9	A	209	G
9	A	216	C
9	A	218	A
9	A	224	G
9	A	226	A
9	A	230	G
9	A	233	G
9	A	249	C
9	A	250	A
9	A	251	G
9	A	252	C
9	A	260	G
9	A	266	A
9	A	275	U
9	A	276	G
9	A	277	G
9	A	282	G
9	A	284	A
9	A	286	U
9	A	287	A
9	A	288	C
9	A	294	U
9	A	297	U
9	A	298	G
9	A	299	C
9	A	304	A
9	A	316	G
9	A	320	U
9	A	326	A
9	A	332	G
9	A	333	A
9	A	338	G

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Mol	Chain	Res	Type
9	A	340	A
9	A	362	A
9	A	363	C
9	A	364	U
9	A	368	U
9	A	377	G
9	A	379	C
9	A	383	A
9	A	384	G
9	A	398	G
9	A	415	U
9	A	416	C
9	A	417	A
9	A	418	G
9	A	423	G
9	A	424	A
9	A	436	G
9	A	448	C
9	A	452	G
9	A	453	U
9	A	454	G
9	A	467	G
9	A	468	U
9	A	469	A
9	A	480	G
9	A	485	G
9	A	487	U
9	A	491	A
9	A	492	A
9	A	493	G
9	A	502	U
9	A	507	G
9	A	519	A
9	A	520	C
9	A	529	G
9	A	539	A
9	A	540	A
9	A	541	G
9	A	542	C
9	A	543	A
9	A	544	G
9	A	549	A

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Mol	Chain	Res	Type
9	A	554	G
9	A	557	C
9	A	558	A
9	A	559	G
9	A	560	A
9	A	561	C
9	A	565	G
9	A	573	G
9	A	582	A
9	A	583	G
9	A	585	A
9	A	593	G
9	A	597	C
9	A	609	G
9	A	610	G
9	A	612	U
9	A	613	U
9	A	614	G
9	A	623	A
9	A	630	C
9	A	632	G
9	A	633	A
9	A	635	C
9	A	639	A
9	A	643	A
9	A	645	A
9	A	646	G
9	A	649	A
9	A	657	U
9	A	658	A
9	A	664	A
9	A	665	U
9	A	667	G
9	A	675	U
9	A	680	G
9	A	681	A
9	A	688	C
9	A	696	A
9	A	697	U
9	A	701	U
9	A	713	A
9	A	722	G

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Mol	Chain	Res	Type
9	A	724	G
9	A	727	A
9	A	728	A
9	A	729	A
9	A	730	C
9	A	731	U
9	A	734	G
9	A	740	G
9	A	741	U
9	A	749	G
9	A	758	U
9	A	759	G
9	A	760	A
9	A	768	G
9	A	775	A
9	A	776	G
9	A	782	G
9	A	786	G
9	A	787	G
9	A	788	G
9	A	793	A
9	A	795	U
9	A	803	G
9	A	811	A
9	A	813	C
9	A	816	G
9	A	817	C
9	A	823	C
9	A	838	U
9	A	839	G
9	A	853	G
9	A	856	U
9	A	857	G
9	A	858	G
9	A	859	A
9	A	866	G
9	A	869	G
9	A	879	G
9	A	880	U
9	A	888	C
9	A	890	G
9	A	893	C

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Mol	Chain	Res	Type
9	A	894	G
9	A	902	G
9	A	905	A
9	A	906	C
9	A	907	C
9	A	910	A
9	A	916	G
9	A	919	A
9	A	924	U
9	A	937	U
9	A	938	G
9	A	946	A
9	A	947	A
9	A	948	U
9	A	974	G
9	A	981	G
9	A	989	G
9	A	993	C
9	A	996	C
9	A	1001	A
9	A	1002	G
9	A	1007	A
9	A	1009	A
9	A	1011	A
9	A	1017	G
9	A	1018	A
9	A	1024	A
9	A	1038	A
9	A	1039	A
9	A	1040	U
9	A	1041	G
9	A	1045	G
9	A	1050	G
9	A	1051	U
9	A	1052	G
9	A	1054	U
9	A	1055	A
9	A	1061	G
9	A	1062	G
9	A	1065	G
9	A	1070	G
9	A	1071	C

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Mol	Chain	Res	Type
9	A	1072	A
9	A	1075	G
9	A	1098	A
9	A	1099	G
9	A	1116	A
9	A	1118	U
9	A	1138	G
9	A	1140	G
9	A	1143	C
9	A	1144	U
9	A	1147	U
9	A	1155	A
9	A	1160	A
9	A	1162	C
9	A	1163	G
9	A	1166	G
9	A	1169	A
9	A	1170	A
9	A	1173	G
9	A	1190	G
9	A	1196	A
9	A	1197	A
9	A	1198	A
9	A	1199	A
9	A	1202	A
9	A	1218	G
9	A	1221	C
9	A	1226	U
9	A	1231	G
9	A	1239	C
9	A	1240	G
9	A	1241	U
9	A	1245	U
9	A	1248	G
9	A	1253	G
9	A	1254	U
9	A	1255	U
9	A	1257	G
9	A	1259	C
9	A	1261	A
9	A	1271	G
9	A	1273	G

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Mol	Chain	Res	Type
9	A	1274	A
9	A	1277	G
9	A	1289	A
9	A	1292	G
9	A	1293	C
9	A	1295	A
9	A	1296	A
9	A	1301	G
9	A	1310	C
9	A	1315	G
9	A	1321	A
9	A	1322	A
9	A	1327	U
9	A	1333	U
9	A	1334	U
9	A	1342	A
9	A	1353	A
9	A	1357	A
9	A	1359	G
9	A	1366	C
9	A	1371	C
9	A	1380	A
9	A	1381	G
9	A	1386	A
9	A	1399	A
9	A	1400	U
9	A	1402	G
9	A	1405	A
9	A	1416	A
9	A	1417	U
9	A	1423	U
9	A	1424	A
9	A	1426	U
9	A	1431	C
9	A	1432	U
9	A	1433	U
9	A	1435	U
9	A	1436	U
9	A	1437	G
9	A	1444	A
9	A	1446	G
9	A	1449	C

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Mol	Chain	Res	Type
9	A	1450	G
9	A	1456	G
9	A	1458	C
9	A	1465	A
9	A	1472	A
9	A	1476	G
9	A	1477	G
9	A	1480	A
9	A	1483	G
9	A	1484	G
9	A	1485	U
9	A	1488	A
9	A	1493	C
9	A	1494	G
9	A	1497	A
9	A	1501	G
9	A	1507	G
9	A	1513	C
9	A	1519	A
9	A	1520	A
9	A	1521	G
9	A	1523	A
9	A	1524	G
9	A	1526	G
9	A	1527	G
9	A	1528	U
9	A	1533	A
9	A	1544	A
9	A	1557	G
9	A	1558	U
9	A	1559	A
9	A	1563	G
9	A	1566	G
9	A	1568	U
9	A	1570	C
9	A	1571	G
9	A	1588	U
9	A	1594	A
9	A	1600	A
9	A	1603	A
9	A	1612	A
9	A	1620	U

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Mol	Chain	Res	Type
9	A	1621	C
9	A	1629	G
9	A	1630	G
9	A	1632	U
9	A	1633	A
9	A	1634	C
9	A	1635	C
9	A	1642	C
9	A	1643	G
9	A	1644	A
9	A	1645	A
9	A	1649	G
9	A	1666	A
9	A	1670	A
9	A	1682	C
9	A	1683	G
9	A	1684	C
9	A	1685	G
9	A	1687	G
9	A	1710	G
9	A	1711	C
9	A	1734	A
9	A	1746	C
9	A	1750	C
9	A	1760	G
9	A	1762	C
9	A	1774	G
9	A	1778	G
9	A	1783	A
9	A	1791	C
9	A	1801	A
9	A	1810	C
9	A	1812	A
9	A	1818	U
9	A	1819	A
9	A	1821	G
9	A	1826	U
9	A	1833	G
9	A	1836	C
9	A	1839	A
9	A	1849	A
9	A	1858	A

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Mol	Chain	Res	Type
9	A	1866	G
9	A	1870	U
9	A	1877	C
9	A	1882	U
9	A	1883	G
9	A	1884	A
9	A	1885	C
9	A	1900	C
9	A	1914	A
9	A	1920	G
9	A	1923	C
9	A	1926	A
9	A	1927	A
9	A	1928	C
9	A	1930	A
9	A	1931	U
9	A	1933	A
9	A	1940	U
9	A	1943	G
9	A	1944	G
9	A	1950	A
9	A	1952	A
9	A	1969	U
9	A	1974	A
9	A	1975	C
9	A	1980	A
9	A	1981	C
9	A	1984	A
9	A	1985	A
9	A	1986	G
9	A	2005	U
9	A	2006	G
9	A	2007	U
9	A	2011	G
9	A	2015	A
9	A	2017	A
9	A	2034	C
9	A	2035	A
9	A	2037	G
9	A	2044	A
9	A	2045	A
9	A	2046	G

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Mol	Chain	Res	Type
9	A	2047	A
9	A	2053	A
9	A	2057	C
9	A	2064	C
9	A	2065	U
9	A	2069	C
9	A	2073	A
9	A	2074	A
9	A	2075	G
9	A	2076	A
9	A	2077	C
9	A	2082	U
9	A	2083	G
9	A	2091	A
9	A	2102	G
9	A	2103	G
9	A	2107	G
9	A	2115	G
9	A	2116	C
9	A	2119	U
9	A	2125	C
9	A	2126	G
9	A	2127	C
9	A	2129	G
9	A	2130	C
9	A	2131	U
9	A	2132	U
9	A	2133	A
9	A	2137	G
9	A	2139	A
9	A	2140	A
9	A	2145	A
9	A	2146	A
9	A	2147	G
9	A	2148	A
9	A	2151	G
9	A	2159	C
9	A	2160	C
9	A	2161	G
9	A	2162	G
9	A	2173	G
9	A	2175	C

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Mol	Chain	Res	Type
9	A	2176	A
9	A	2177	U
9	A	2178	C
9	A	2179	A
9	A	2181	U
9	A	2182	G
9	A	2183	A
9	A	2184	G
9	A	2185	A
9	A	2186	U
9	A	2187	A
9	A	2191	C
9	A	2192	U
9	A	2193	C
9	A	2195	G
9	A	2199	G
9	A	2201	G
9	A	2202	C
9	A	2204	A
9	A	2205	G
9	A	2206	A
9	A	2209	U
9	A	2212	A
9	A	2213	A
9	A	2217	U
9	A	2219	U
9	A	2220	G
9	A	2223	A
9	A	2227	C
9	A	2229	U
9	A	2230	A
9	A	2232	G
9	A	2242	A
9	A	2243	C
9	A	2254	A
9	A	2255	G
9	A	2256	A
9	A	2260	U
9	A	2266	U
9	A	2267	G
9	A	2269	G
9	A	2296	G

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Mol	Chain	Res	Type
9	A	2297	G
9	A	2300	U
9	A	2303	A
9	A	2304	A
9	A	2305	A
9	A	2315	G
9	A	2316	G
9	A	2322	A
9	A	2323	C
9	A	2324	G
9	A	2325	G
9	A	2338	G
9	A	2339	A
9	A	2341	U
9	A	2342	G
9	A	2343	C
9	A	2344	A
9	A	2349	C
9	A	2351	G
9	A	2352	A
9	A	2364	C
9	A	2367	C
9	A	2372	C
9	A	2375	A
9	A	2378	C
9	A	2400	G
9	A	2402	C
9	A	2408	G
9	A	2419	G
9	A	2423	A
9	A	2428	A
9	A	2442	A
9	A	2444	C
9	A	2446	G
9	A	2447	A
9	A	2448	U
9	A	2452	A
9	A	2457	C
9	A	2458	U
9	A	2462	G
9	A	2464	G
9	A	2465	A

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Mol	Chain	Res	Type
9	A	2466	U
9	A	2467	A
9	A	2481	C
9	A	2487	G
9	A	2493	A
9	A	2495	A
9	A	2507	G
9	A	2508	U
9	A	2509	U
9	A	2518	C
9	A	2519	G
9	A	2520	A
9	A	2521	U
9	A	2522	G
9	A	2523	U
9	A	2524	C
9	A	2526	G
9	A	2530	U
9	A	2535	C
9	A	2542	G
9	A	2546	G
9	A	2552	U
9	A	2569	U
9	A	2571	U
9	A	2576	C
9	A	2579	U
9	A	2583	A
9	A	2584	G
9	A	2589	A
9	A	2590	C
9	A	2591	G
9	A	2593	G
9	A	2594	A
9	A	2595	G
9	A	2599	G
9	A	2601	U
9	A	2602	U
9	A	2603	C
9	A	2619	A
9	A	2625	G
9	A	2626	U
9	A	2627	C

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Mol	Chain	Res	Type
9	A	2630	U
9	A	2637	U
9	A	2640	G
9	A	2646	U
9	A	2649	A
9	A	2671	A
9	A	2672	G
9	A	2680	G
9	A	2688	A
9	A	2689	A
9	A	2696	A
9	A	2702	G
9	A	2706	U
9	A	2707	A
9	A	2708	C
9	A	2719	G
9	A	2721	C
9	A	2729	A
9	A	2740	G
9	A	2744	A
9	A	2751	A
9	A	2753	C
9	A	2762	G
9	A	2766	A
9	A	2768	A
9	A	2769	G
9	A	2770	C
9	A	2774	U
9	A	2776	A
9	A	2778	U
9	A	2783	A
9	A	2784	G
9	A	2787	C
9	A	2796	A
10	B	2	A
10	B	10	G
10	B	15	A
10	B	16	G
10	B	19	G
10	B	25	G
10	B	31	C
10	B	37	U

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Mol	Chain	Res	Type
10	B	38	C
10	B	39	C
10	B	41	U
10	B	42	C
10	B	45	G
10	B	57	U
10	B	68	G
10	B	85	G
10	B	93	C
10	B	107	G
10	B	110	C
10	B	111	G
31	W	3	A
31	W	4	G
31	W	5	A
31	W	14	G
31	W	16	G
31	W	17	A
31	W	20	C
31	W	21	G
31	W	26	G
31	W	28	U
31	W	29	U
31	W	30	A
31	W	31	U
31	W	32	C
31	W	33	A
31	W	34	U
31	W	35	U
31	W	37	C
31	W	38	G
31	W	40	U
31	W	59	C
31	W	65	U
31	W	71	C
31	W	72	A
31	W	77	A
31	W	79	G
31	W	83	C
31	W	84	C
31	W	90	G
31	W	95	A

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Mol	Chain	Res	Type
31	W	96	C
31	W	97	A
31	W	99	A
31	W	103	G
35	z	3	C
35	z	16	U
35	z	19	G
35	z	20	U
35	z	21	A
35	z	25	C
35	z	31	A
35	z	32	U
35	z	33	U
35	z	34	G
35	z	36	A
35	z	37	A
35	z	40	C
35	z	41	C
35	z	42	C
35	z	52	G
35	z	59	U
35	z	70	G
35	z	71	G
35	z	73	A
35	z	75	C
35	z	76	A
37	a	2	C
37	a	3	U
37	a	5	A
37	a	6	U
37	a	7	G
37	a	8	G
37	a	10	G
37	a	14	U
37	a	20	C
37	a	23	G
37	a	31	U
37	a	32	G
37	a	33	A
37	a	39	G
37	a	40	G
37	a	45	A

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Mol	Chain	Res	Type
37	a	48	C
37	a	49	U
37	a	50	U
37	a	52	A
37	a	53	C
37	a	55	C
37	a	60	A
37	a	70	G
37	a	72	A
37	a	73	A
37	a	74	G
37	a	76	G
37	a	77	G
37	a	78	U
37	a	82	U
37	a	83	C
37	a	85	A
37	a	88	G
37	a	90	C
37	a	103	A
37	a	104	A
37	a	105	C
37	a	106	G
37	a	113	A
37	a	114	A
37	a	115	C
37	a	127	A
37	a	130	G
37	a	135	A
37	a	142	G
37	a	147	C
37	a	152	G
37	a	166	G
37	a	167	G
37	a	174	A
37	a	179	A
37	a	180	A
37	a	183	A
37	a	188	U
37	a	191	G
37	a	196	A
37	a	211	C

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Mol	Chain	Res	Type
37	a	216	U
37	a	218	G
37	a	222	G
37	a	230	G
37	a	233	A
37	a	237	G
37	a	238	C
37	a	252	G
37	a	260	G
37	a	264	G
37	a	269	A
37	a	289	G
37	a	292	A
37	a	299	C
37	a	300	A
37	a	303	G
37	a	315	A
37	a	317	G
37	a	323	C
37	a	324	A
37	a	325	G
37	a	327	A
37	a	338	U
37	a	339	U
37	a	343	C
37	a	344	A
37	a	349	G
37	a	355	G
37	a	358	U
37	a	361	C
37	a	363	G
37	a	364	A
37	a	368	A
37	a	377	G
37	a	382	C
37	a	383	A
37	a	384	G
37	a	392	A
37	a	393	C
37	a	398	C
37	a	399	G
37	a	400	U

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Mol	Chain	Res	Type
37	a	411	U
37	a	415	G
37	a	416	G
37	a	417	A
37	a	423	A
37	a	424	G
37	a	425	C
37	a	426	A
37	a	429	G
37	a	432	G
37	a	433	G
37	a	434	U
37	a	439	G
37	a	443	A
37	a	444	A
37	a	453	G
37	a	454	G
37	a	457	A
37	a	459	C
37	a	462	U
37	a	464	U
37	a	469	G
37	a	472	G
37	a	475	G
37	a	478	G
37	a	479	U
37	a	481	A
37	a	494	A
37	a	495	A
37	a	507	A
37	a	510	G
37	a	511	A
37	a	512	U
37	a	520	A
37	a	521	A
37	a	524	C
37	a	525	G
37	a	527	C
37	a	534	U
37	a	544	A
37	a	545	G
37	a	555	A

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Mol	Chain	Res	Type
37	a	579	A
37	a	597	A
37	a	598	G
37	a	600	U
37	a	613	G
37	a	623	A
37	a	634	G
37	a	635	A
37	a	637	C
37	a	658	G
37	a	659	A
37	a	660	A
37	a	670	A
37	a	671	C
37	a	672	G
37	a	690	G
37	a	696	C
37	a	697	A
37	a	703	A
37	a	708	G
37	a	725	A
37	a	735	A
37	a	741	U
37	a	742	A
37	a	757	G
37	a	762	A
37	a	763	A
37	a	765	C
37	a	767	A
37	a	768	U
37	a	775	U
37	a	776	A
37	a	780	G
37	a	784	U
37	a	791	C
37	a	792	G
37	a	793	A
37	a	794	C
37	a	796	C
37	a	797	G
37	a	798	U
37	a	799	G

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Mol	Chain	Res	Type
37	a	821	A
37	a	844	U
37	a	863	A
37	a	875	G
37	a	876	G
37	a	883	C
37	a	891	G
37	a	909	U
37	a	915	G
37	a	918	A
37	a	920	G
37	a	921	C
37	a	924	A
37	a	925	G
37	a	926	A
37	a	941	U
37	a	942	G
37	a	943	A
37	a	944	C
37	a	945	A
37	a	948	C
37	a	953	A
37	a	958	U
37	a	961	U
37	a	963	A
37	a	966	G
37	a	969	A
37	a	972	G
37	a	973	G
37	a	974	U
37	a	975	G
37	a	976	C
37	a	978	U
37	a	979	U
37	a	980	C
37	a	981	G
37	a	982	G
37	a	985	A
37	a	986	C
37	a	992	C
37	a	1002	G
37	a	1003	C

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Mol	Chain	Res	Type
37	a	1004	A
37	a	1014	U
37	a	1019	U
37	a	1033	G
37	a	1034	U
37	a	1041	A
37	a	1043	G
37	a	1044	U
37	a	1050	A
37	a	1066	G
37	a	1073	G
37	a	1075	U
37	a	1077	C
37	a	1078	C
37	a	1079	A
37	a	1080	A
37	a	1081	C
37	a	1082	G
37	a	1084	U
37	a	1085	G
37	a	1086	A
37	a	1088	U
37	a	1089	U
37	a	1091	G
37	a	1092	G
37	a	1095	C
37	a	1099	G
37	a	1100	A
37	a	1107	U
37	a	1114	G
37	a	1115	A
37	a	1116	U
37	a	1119	G
37	a	1131	U
37	a	1132	G
37	a	1134	G
37	a	1137	U
37	a	1144	A
37	a	1145	A
37	a	1149	A
37	a	1150	U
37	a	1151	C

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Mol	Chain	Res	Type
37	a	1160	U
37	a	1161	A
37	a	1162	U
37	a	1163	G
37	a	1169	G
37	a	1174	C
37	a	1175	A
37	a	1184	A
37	a	1186	A
37	a	1187	A
37	a	1188	U
37	a	1189	G
37	a	1198	A
37	a	1204	U
37	a	1205	C
37	a	1206	G
37	a	1208	G
37	a	1217	A
37	a	1223	A
37	a	1227	A
37	a	1228	A
37	a	1229	C
37	a	1233	A
37	a	1235	A
37	a	1242	U
37	a	1244	C
37	a	1245	U
37	a	1246	C
37	a	1247	A
37	a	1248	G
37	a	1249	U
37	a	1250	U
37	a	1253	G
37	a	1265	C
37	a	1266	A
37	a	1267	A
37	a	1268	C
37	a	1270	C
37	a	1271	G
37	a	1279	G
37	a	1280	A
37	a	1301	G

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Mol	Chain	Res	Type
37	a	1311	C
37	a	1312	A
37	a	1317	G
37	a	1319	G
37	a	1322	G
37	a	1328	G
37	a	1330	U
37	a	1346	C
37	a	1347	A
37	a	1363	U
37	a	1368	G
37	a	1371	G
37	a	1378	C
37	a	1390	A
37	a	1391	C
37	a	1395	A
37	a	1400	C
37	a	1401	A
37	a	1402	A
37	a	1403	G
37	a	1404	G
37	a	1405	A
37	a	1406	G
37	a	1416	G
37	a	1417	A
37	a	1418	A
37	a	1419	G
37	a	1436	G
37	a	1440	G
37	a	1441	A
37	a	1446	G
37	a	1454	G
37	a	1455	U
37	a	1456	A
37	a	1466	G
37	a	1469	G
37	a	1478	G
37	a	1479	G
37	a	1482	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	486	G
9	A	548	G
9	A	556	C
9	A	795	U
9	A	1520	A
9	A	2035	A
9	A	2447	A
9	A	2602	U
31	W	77	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 781 ligands modelled in this entry, 781 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	8	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8	1068:UNK	C	1101:UNK	N	66.30
1	8	1143:UNK	C	1201:UNK	N	11.98