



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Sep 5, 2017 – 06:13 AM EDT

PDB ID : 5X8P
EMDB ID: : EMD-6709
Title : Structure of the 70S chloroplast ribosome from spinach
Authors : Ahmed, T.; Shi, J.; Bhushan, S.
Deposited on : unknown
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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

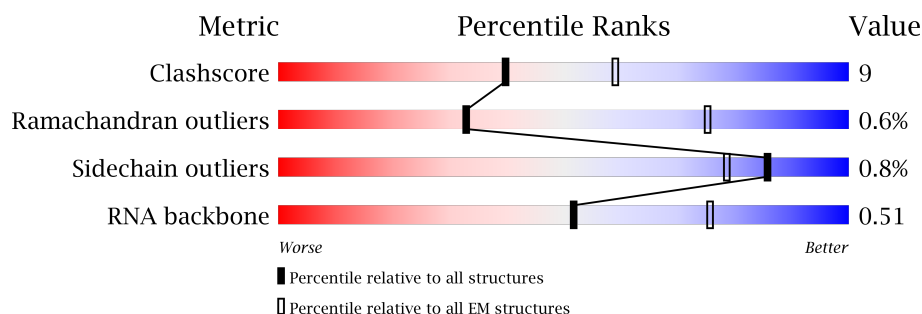
1 Overall quality at a glance i

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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

Mol	Chain	Length	Quality of chain
1	1	56	70% 13% 18%
2	2	65	58% 18% • 22%
3	3	61	72% 21% 7%
4	4	73	77% 16% • 5%
5	5	37	78% 22%
6	6	142	30% 5% 65%
7	7	116	29% 10% 60%
8	B	121	66% 23% 7% •

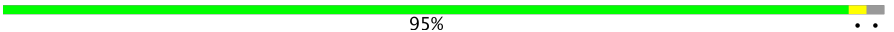


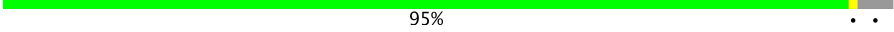
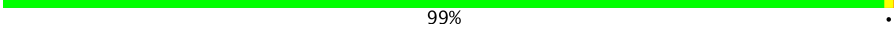



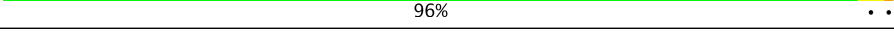

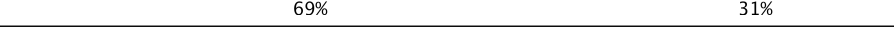
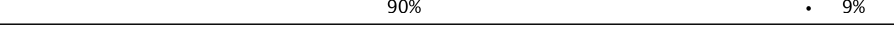
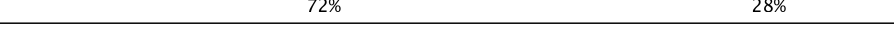


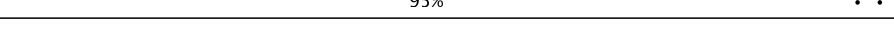









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Mol	Chain	Length	Quality of chain
9	C	271	
10	D	221	
11	E	243	
12	F	220	
13	G	182	
14	H	155	
15	K	197	
16	L	121	
17	M	192	
18	N	135	
19	O	116	
20	P	123	
21	Q	156	
22	R	127	
23	S	201	
24	T	199	
25	U	122	
26	V	145	
27	W	106	
28	X	137	
29	Y	77	
30	Z	109	
31	A	2810	
32	0	94	
33	b	236	

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Mol	Chain	Length	Quality of chain
34	c	218	
35	e	253	
36	f	146	
37	g	155	
38	h	134	
39	i	157	
40	j	122	
41	k	138	
42	l	123	
43	m	126	
44	o	90	
45	p	88	
46	q	108	
47	r	101	
48	s	92	
49	t	108	
50	u	137	
51	y	236	
52	a	1491	
53	w	121	
54	d	201	
55	v	198	
56	n	100	
57	x	47	
58	8	370	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147126 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 L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	46	Total	C	N	O	0	0
			378	250	70	58		

- Molecule 2 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	51	Total	C	N	O	S	0	0
			415	258	83	70	4		

- Molecule 3 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	57	Total	C	N	O	S	0	0
			445	268	103	71	3		

- Molecule 4 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	69	Total	C	N	O	S	0	0
			563	353	119	90	1		

- Molecule 5 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	37	Total	C	N	O	S	0	0
			304	186	70	44	4		

- Molecule 6 is a protein called protein cL37.

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

- Molecule 7 is a protein called protein cL38.

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

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	117	Total	C	N	O	P	0	0
			2500	1116	452	815	117		

- Molecule 9 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	247	Total	C	N	O	S	0	0
			1904	1181	390	327	6		

- Molecule 10 is a protein called protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	212	Total	C	N	O	S	0	0
			1620	1025	295	289	11		

- Molecule 11 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	210	Total	C	N	O	S	0	0
			1655	1052	308	292	3		

- Molecule 12 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	175	Total	C	N	O	S	0	0
			1351	862	233	248	8		

- Molecule 13 is a protein called protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	173	Total	C	N	O	S	0	0
			1353	855	249	245	4		

- Molecule 14 is a protein called protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	53	Total	C	N	O	S	0	0
			423	280	74	68	1		

- Molecule 15 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	193	Total	C	N	O	S	0	0
			1568	1000	289	274	5		

- Molecule 16 is a protein called 50S ribosomal protein L14, chloroplastic.

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

- Molecule 17 is a protein called protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	177	Total	C	N	O	S	0	0
			1342	836	264	236	6		

- Molecule 18 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	134	Total	C	N	O	S	0	0
			1067	672	217	173	5		

- Molecule 19 is a protein called protein L17.

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

- Molecule 20 is a protein called protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	120	Total	C	N	O	S	0	0
			947	589	183	170	5		

- Molecule 21 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	118	Total	C	N	O	S	0	0
			953	610	186	156	1		

- Molecule 22 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	115	Total	C	N	O	S	0	0
			996	633	208	153	2		

- Molecule 23 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	S	147	Total	C	N	O	0	0
			1171	759	202	210		

- Molecule 24 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	144	Total	C	N	O	S	0	0
			1149	731	210	200	8		

- Molecule 25 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	92	Total	C	N	O	S	0	0
			740	477	129	132	2		

- Molecule 26 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	124	Total	C	N	O	S	0	0
			993	624	187	180	2		

- Molecule 27 is a RNA chain called 4.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	102	Total	C	N	O	P	0	0
			2187	977	403	705	102		

- Molecule 28 is a protein called protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	100	Total	C	N	O	0	0
			810	511	159	140		

- Molecule 29 is a protein called protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	74	Total	C	N	O	S	0	0
			605	385	121	98	1		

- Molecule 30 is a protein called protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	90	Total	C	N	O	S	0	0
			754	470	150	131	3		

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	2809	Total	C	N	O	P	0	0
			60324	26912	11166	19437	2809		

- Molecule 32 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	0	64	Total	C	N	O	S	0	0
			521	330	89	100	2		

- Molecule 33 is a protein called 30S ribosomal protein S2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	227	Total	C	N	O	S	0	0
			1787	1127	326	321	13		

- Molecule 34 is a protein called 30S ribosomal protein S3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	213	Total	C	N	O	S	0	0
			1719	1099	310	304	6		

- Molecule 35 is a protein called 30S ribosomal protein S5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	171	Total	C	N	O	S	0	0
			1292	806	250	230	6		

- Molecule 36 is a protein called 30S ribosomal protein S6 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	111	Total	C	N	O	S	0	0
			886	566	145	171	4		

- Molecule 37 is a protein called 30S ribosomal protein S7, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	149	Total	C	N	O	S	0	0
			1161	723	231	204	3		

- Molecule 38 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	134	Total	C	N	O	S	0	0
			1088	684	211	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	133	Total	C	N	O	S	0	0
			1020	650	191	178	1		

- Molecule 40 is a protein called protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	98	Total	C	N	O	S	0	0
			796	512	142	137	5		

- Molecule 41 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	118	Total	C	N	O	S	0	0
			887	549	182	151	5		

- Molecule 42 is a protein called 30S ribosomal protein S12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	123	Total	C	N	O	S	0	0
			967	604	198	162	3		

- Molecule 43 is a protein called 30S ribosomal protein S13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	110	Total	C	N	O	S	0	0
			898	559	183	153	3		

- Molecule 44 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	62	Total	C	N	O	S	0	0
			525	339	100	85	1		

- Molecule 45 is a protein called 30S ribosomal protein S16, chloroplastic.

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

- Molecule 46 is a protein called protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	78	Total	C	N	O	S	0	0
			635	399	124	108	4		

- Molecule 47 is a protein called 30S ribosomal protein S18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	64	Total	C	N	O	S	0	0
			518	326	101	90	1		

- Molecule 48 is a protein called 30S ribosomal protein S19 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	78	Total	C	N	O	S	0	0
			627	403	118	104	2		

- Molecule 49 is a protein called protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	105	Total	C	N	O	S	0	0
			832	514	169	148	1		

- Molecule 50 is a protein called protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	44	Total	C	N	O	S	0	0
			393	238	87	66	2		

- Molecule 51 is a protein called protein plastid pY.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	108	Total	C	N	O	S	0	0
			845	521	164	159	1		

- Molecule 52 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	1480	Total	C	N	O	P	0	0
			31777	14168	5863	10266	1480		

- Molecule 53 is a protein called protein cS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	84	Total	C	N	O	S	0	0
			689	454	115	118	2		

- Molecule 54 is a protein called 30S ribosomal protein S4, chloroplastic.

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

- Molecule 55 is a protein called protein cS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	190	Total	C	N	O	S	0	0
			1464	908	255	298	3		

- Molecule 56 is a protein called 30S ribosomal protein S14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	n	99	Total	C	N	O	S	0	0
			819	507	174	135	3		

- Molecule 57 is a protein called protein bTHXc.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	x	37	Total	C	N	O	0	0
			289	179	65	45		

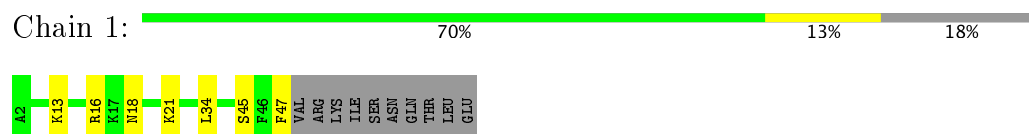
- Molecule 58 is a protein called 30S ribosomal protein S1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	8	154	Total	C	N	O	S	0	0
			1201	744	222	227	8		

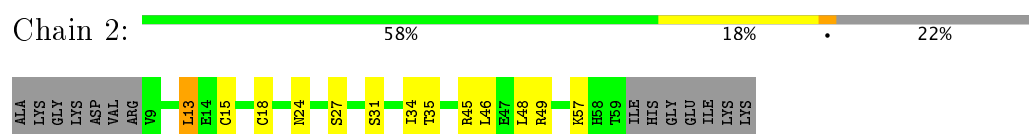
3 Residue-property plots [i](#)

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

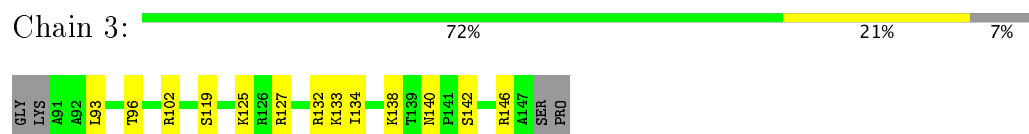
- Molecule 1: 50S ribosomal protein L32, chloroplastic



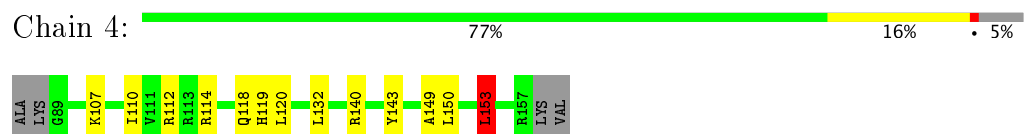
- Molecule 2: 50S ribosomal protein L33, chloroplastic



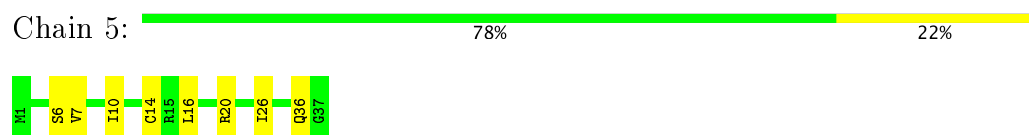
- Molecule 3: 50S ribosomal protein L34, chloroplastic



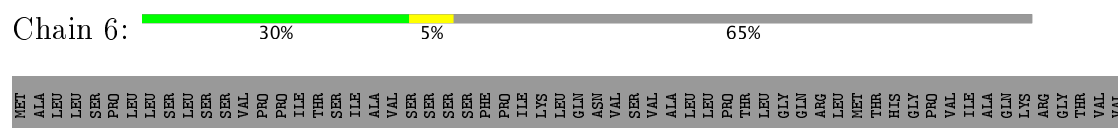
- Molecule 4: 50S ribosomal protein L35, chloroplastic

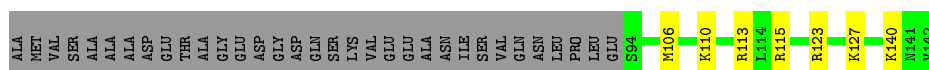


- Molecule 5: 50S ribosomal protein L36, chloroplastic

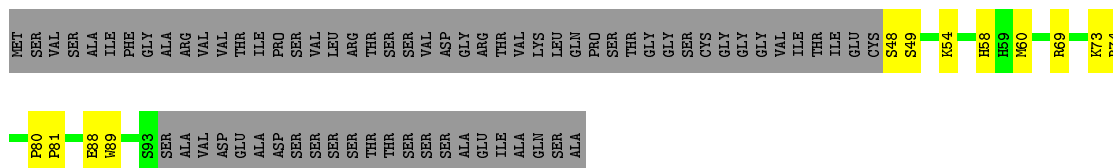


- Molecule 6: protein cL37

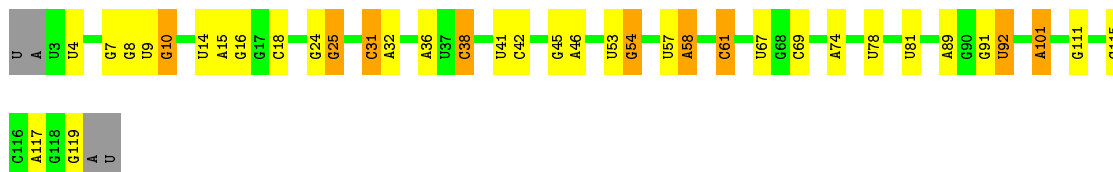




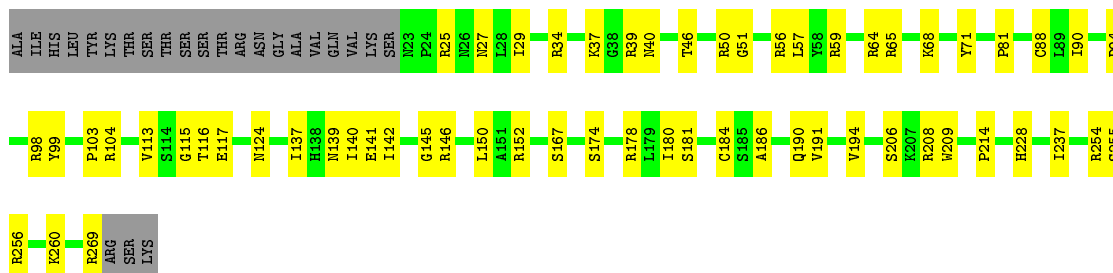
- Molecule 7: protein cL38



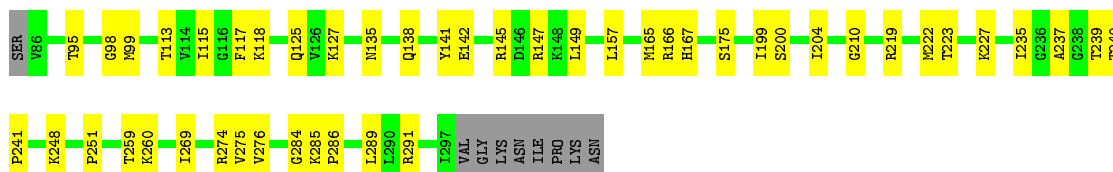
- Molecule 8: 5S rRNA



- Molecule 9: 50S ribosomal protein L2, chloroplastic

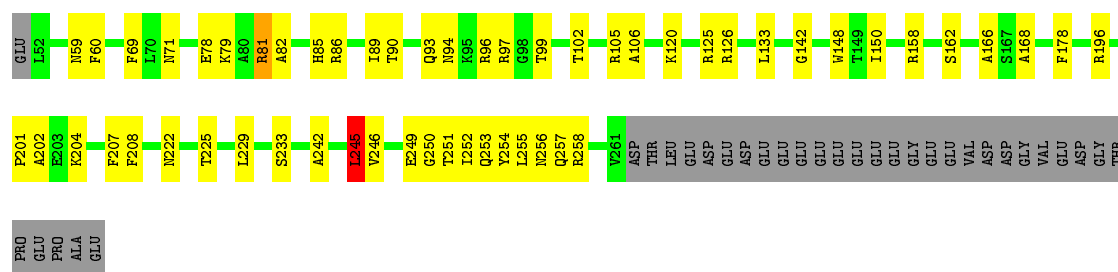


- Molecule 10: protein L3

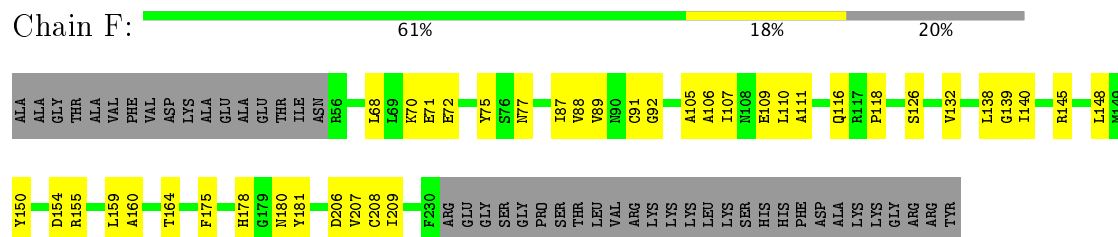


- Molecule 11: 50S ribosomal protein L4, chloroplastic

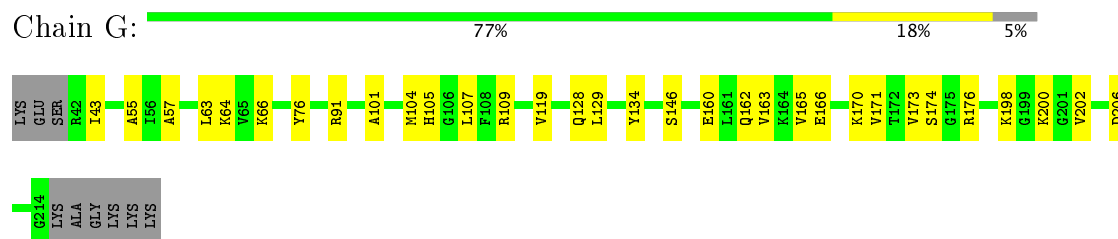




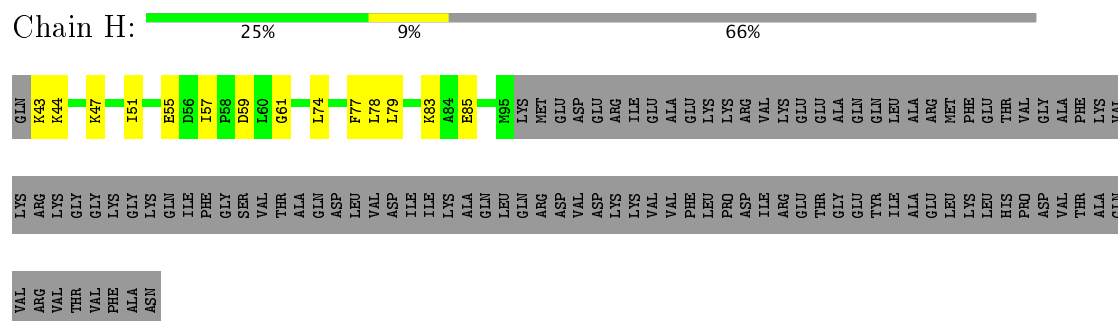
- Molecule 12: 50S ribosomal protein L5, chloroplastic



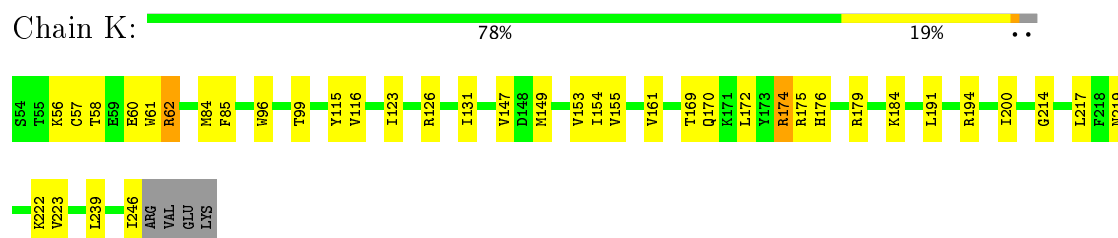
- Molecule 13: protein L6



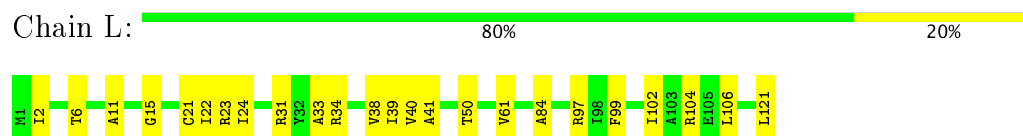
- Molecule 14: protein L9



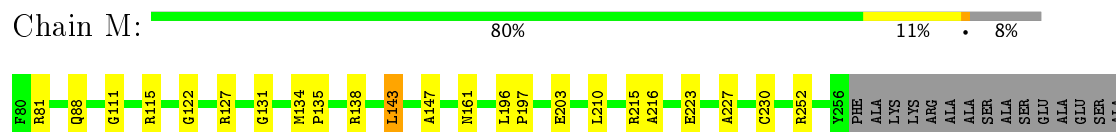
- Molecule 15: 50S ribosomal protein L13, chloroplastic



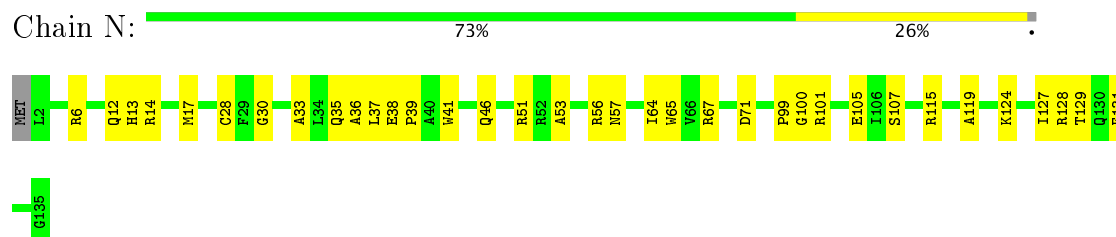
- Molecule 16: 50S ribosomal protein L14, chloroplastic



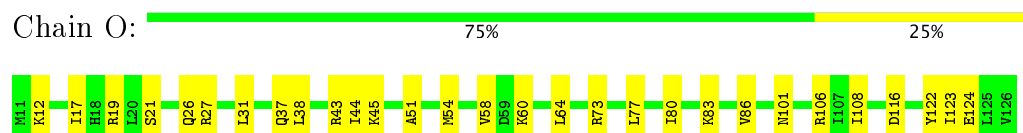
- Molecule 17: protein L15



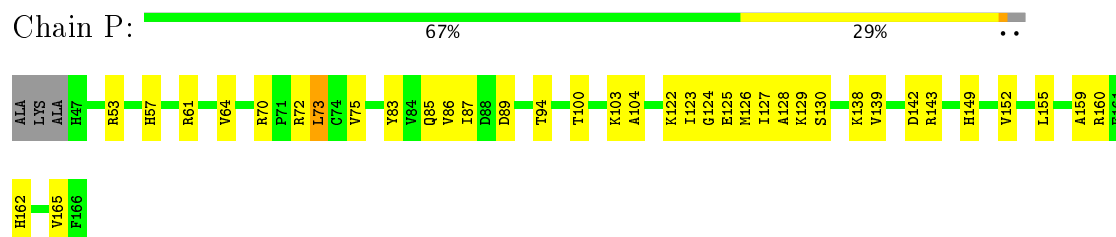
- Molecule 18: 50S ribosomal protein L16, chloroplastic



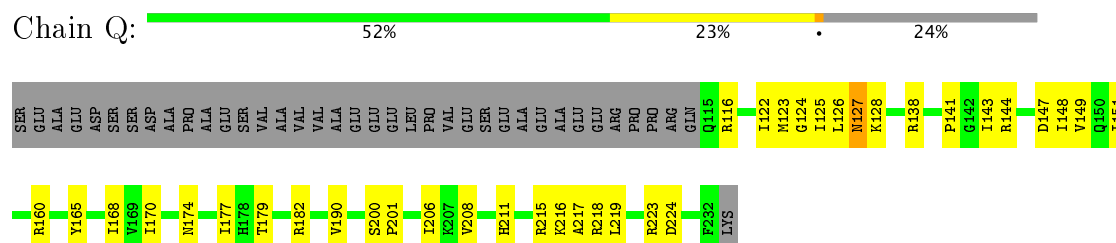
- Molecule 19: protein L17



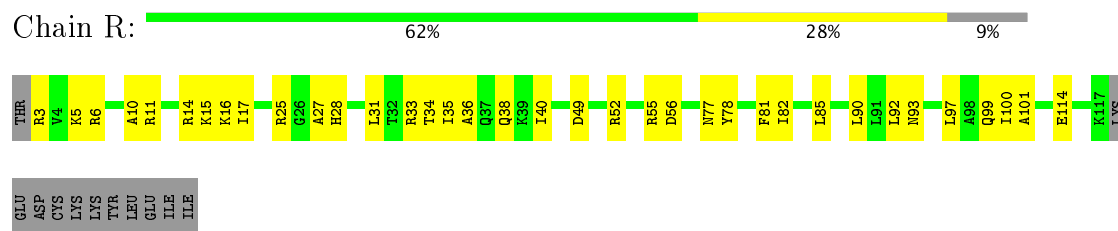
- Molecule 20: protein L18



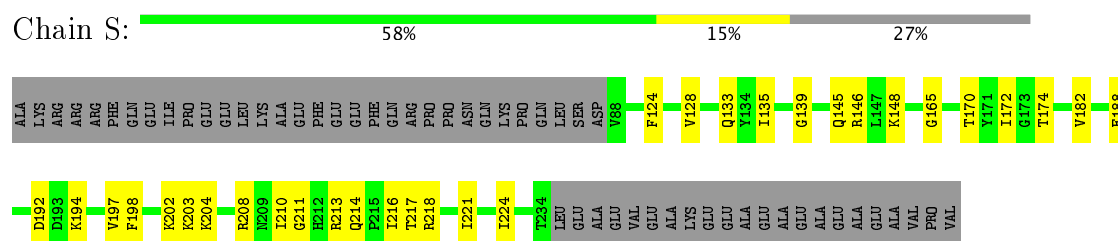
- Molecule 21: 50S ribosomal protein L19, chloroplastic



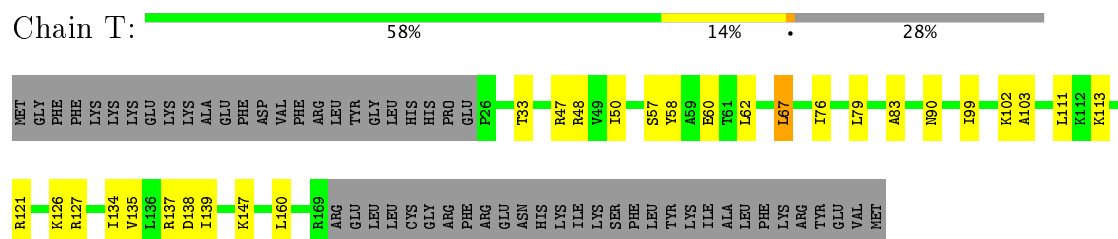
- Molecule 22: 50S ribosomal protein L20, chloroplastic



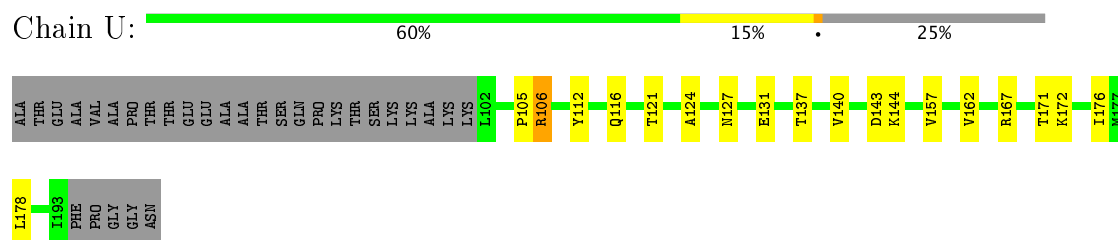
- Molecule 23: 50S ribosomal protein L21, chloroplastic



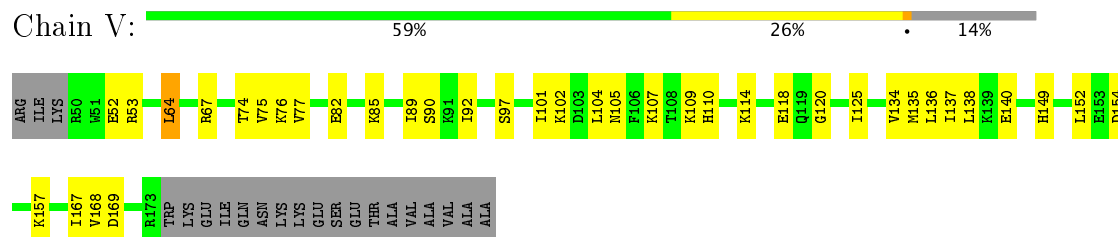
- Molecule 24: 50S ribosomal protein L22, chloroplastic



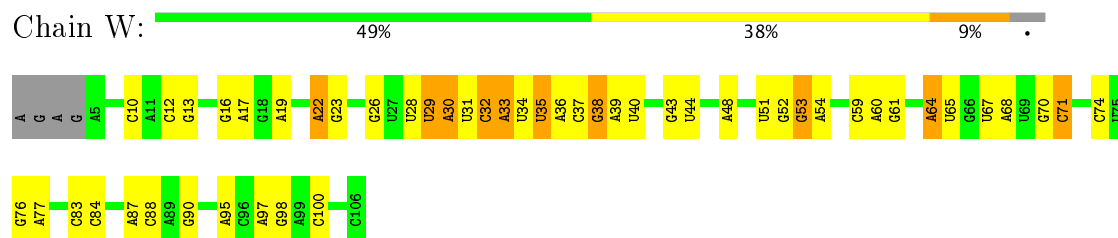
- Molecule 25: 50S ribosomal protein L23, chloroplastic



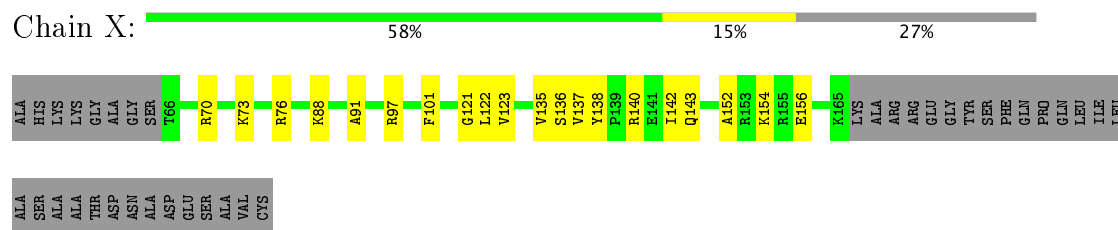
- Molecule 26: 50S ribosomal protein L24, chloroplastic



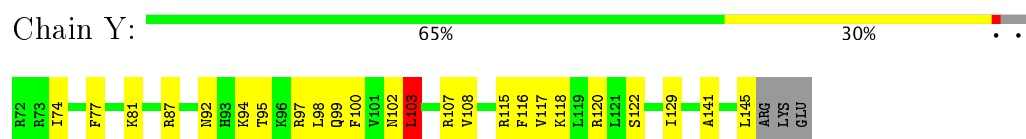
- Molecule 27: 4.8S rRNA



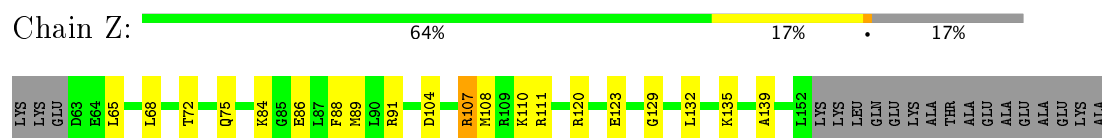
• Molecule 28: protein L27



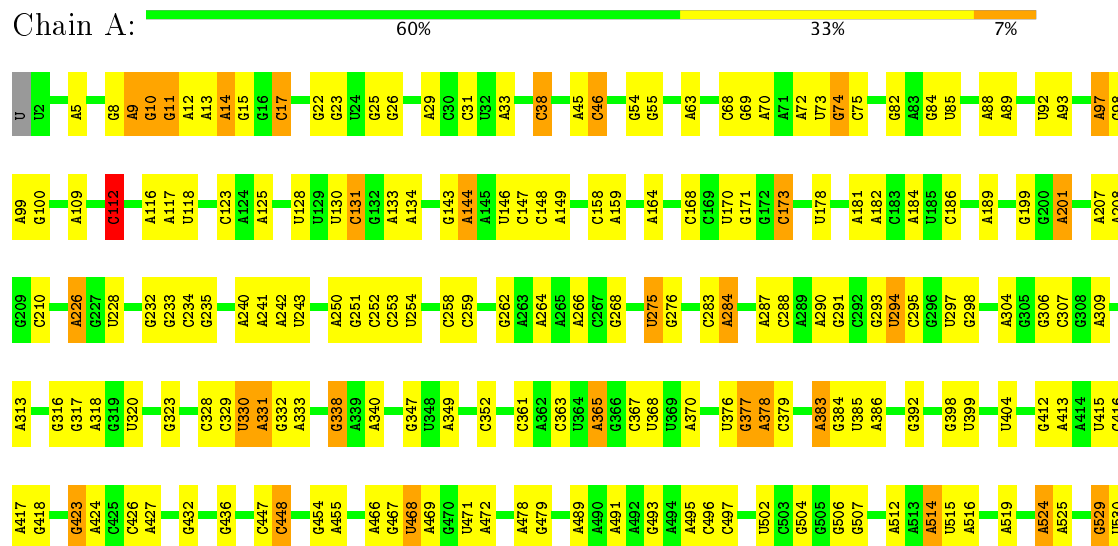
• Molecule 29: protein L28



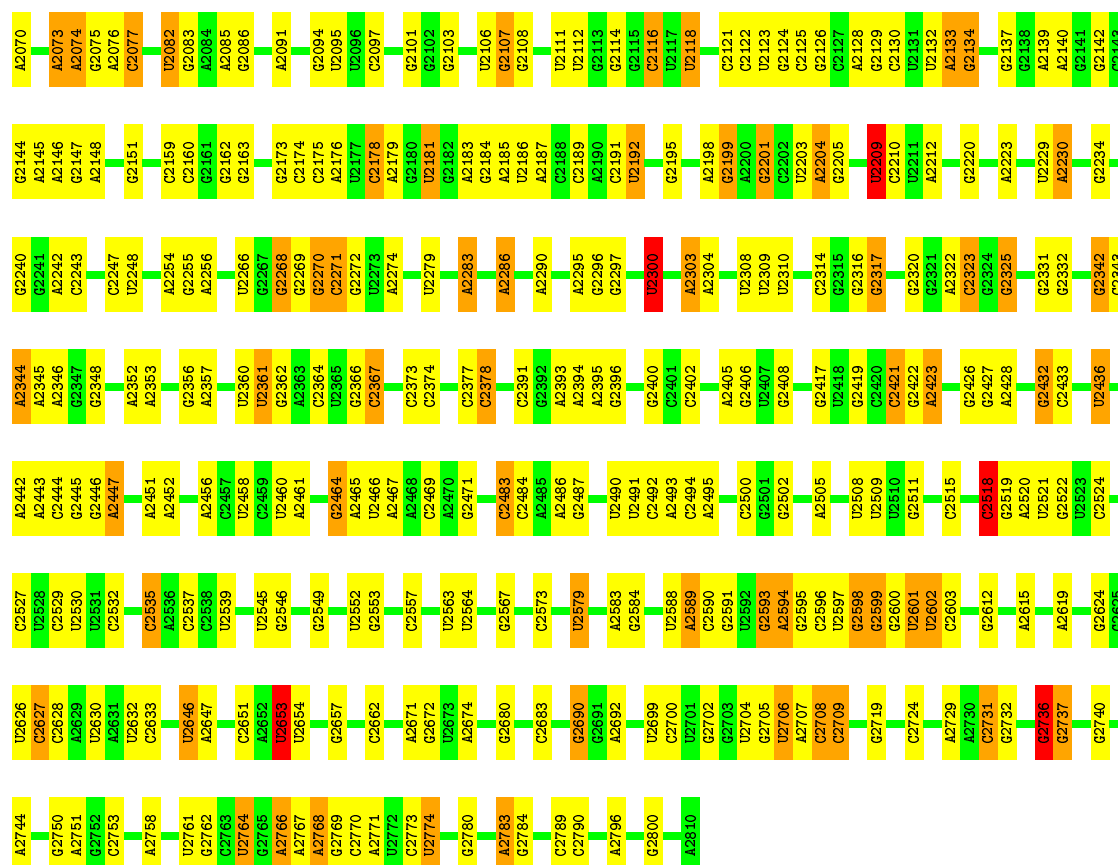
• Molecule 30: protein L29



• Molecule 31: 23S rRNA

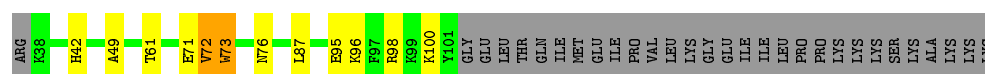


U1957	A1839	U1749	A1616	A1519	G1437	G1344	G1253	C1149	G1075	G981	G887	A804	C702	G614	A531
G1962	C1843	C1750	U1620	A1520	G1438	G1345	U1254	G1150	A1076	G982	C888	A805	C703	G615	A540
U1968	U1844	C1752	C1621	G1521	U1439	U1346	U1255	A1154	C1077	G983	G889	A811	U705	G621	A541
U1969	G1845	A1753	A1622	A1522	G1443	C1348	G1257	A1155	A1078	G984	G890	G812	G706	A621	C542
U1970	C1854	A1755	A1628	A1523	G1444	C1349	G1258	A1156	C1081	G985	G891	G813		A622	A543
C1971		G1756	G1445	G1524	G1446	C1354	C1259	A1157	G1084	U986	C893		C709	A623	C544
	G1859	G1757		G1525	G1448	G1355	A1261	U1158	G1087	A987	G894	G816		A624	C545
	G1860	G1758	C1635	U1528	C1449	C1366	G1269	U1159	G1087	A988	C895	C817	G715	C630	C546
			U1636	A1529	C1450	C1367	G1270	A1160		G989	C896	U818		G631	
	U1871	G1762	C1640	G1530	G1451	C1368	C1271	A1161	C1092	U992	G898	U819	U721	G632	G554
	G1872	G1763		A1531	A1452	C1371	A1272	G1162	G1097	C993	A897	G820	G722	A633	A555
	G1873		G1643	G1532	G1453	C1372	C1273	A1170	A1098	A1001	A898		G723	C634	C556
	U1874	G1766	A1644	A1533	G1454	U1373	A1274	G1163	G1099	G900	G899	G823	G724	U638	C557
	G1875		A1645		G1455	A1374	A1275	A1169	A1097	C901	A897	U824		A639	A558
	A1876	C1770	C1647	A1544	G1456	C1379	G1276	U1175	G1100	A1008	G904	C826	G730	G641	A560
		G1774		G1545	C1458		G1277	C1176	A1101	A1009	U904	G827	G731	C642	
	U1882		A1650	C1546	G1459	G1384	U1278	U1177	G1102	A1011	A905	C828	A732	A643	C563
	G1883	G1778		G1547	A1460	G1385		U1178	G1103	A1012	C906		A733	A644	U564
	A1884		A1662	A1548	G1461	G1386	G1281	A1183	C1104	C1013	A908	U833	G734	A645	C568
	C1885	A1783		U1550	G1462	A1387	U1282	G1189	A1105	C1014	U911	G834		C646	C569
	G1886	C1784	U1665	G1555	G1463	A1388	U1283	U1189	C1106	G1015	G915		G737	C647	C570
	G1887		A1666		G1464		U1284	A1196	C1107	G1016	G916	U838		A649	C571
	G1888	U1769		A1556	C1467	C1391	G1285	A1197	G1108	G1017	G915	G841	G740	G650	U572
	G1889	A1790	C1682	A1557	C1468	U1392	A1286	A1198	G1111	A1018	G916	G842	U741	U651	C573
	C1901	G1791	G1683	U1558	G1472	U1393	C1291	A1199	A1112	U1019	A919	C843		C652	
		C1792	C1684	A1559	A1475		G1292	A1201	A1113	C1020	A920	G844	G744	A656	U577
	G1906	A1793	G1685		G1476	C1397	C1293	G1206	A1114	A1021	A920	C845	A745	U657	U578
	C1907	U1794		U1568	G1477	A1399	A1294	U1209	G1115	A1024	U924	A846		U579	U580
		A1795	C1689	A1569	G1478	U1400	A1295	U1209	A1116	A1028	G925		G756	A663	A581
	A1914	A1796		C1570	U1480	G1401	A1296	U1209	G1117	A1028	A926	U856	G758	A664	A582
	A1915		C1692	G1571	U1481	G1402	C1297	G1211	U1118	A1037	A927	U857	G759	U665	C583
		A1801	C1696	G1572		A1403	A1298	G1211	G1119	A1037	U928	G858	A763	U666	A584
	G1920			C1573	G1484	C1404	A1298	U1219	G1120	U1040	A932	A859		G667	A585
		C1808		G1574	U1485	A1405	A1305	U1219	G1121	U1040	A932	A861	G770	U668	U586
	G1923	G1809	A1704		U1486	A1406	A1308	U1220	A1122	G1041	A933			C669	C587
		C1810	C1706	A1578	U1487	C1407	A1308	U1220	A1123		U937	U864	U773	G680	C591
	A1926	A1811			U1488	A1408	U1309	G1225	G1124	G1050	A946	A865	G774	A681	C592
	C1927	U1707	U1707	C1584	A1489	A1408	C1310	U1226	A1125	G1051	A947	A866	A775	C682	C593
	C1928	A1813	C1708		G1490		C1311	U1227	A1126	G1052	U938	G867	G776	C683	C594
	U1929	G1814	G1709	A1592	G1491	A1413	C1311	U1227	A1126	G1053	A938	G868		C684	A596
	A1930	U1815		U1593	C1493	A1416	G1315	A1228	C1130	U1054	U946	A869	U782	G685	C599
		C1710	C1711	A1594	G1494	U1417	C1316	A1234	A1131	G1055	A947	U870	G783	A686	A600
	U1931		A1712		C1495	U1418	C1317	A1235	G1132	A1056	A947	A871	U783	A687	
		U1818		A1600	A1497	C1419	A1321	G1238	G1134	A1057	G962	A872		C688	
	C1934	A1819		A1603	G1501	U1423	A1322	C1239	C1137	A1060	G966		G786		C605
	G2046	U1825	G1732	A1604	A1502	A1424	G1330	U1240	G1138	G1061	U877	C877	G787	G693	A606
	G2047	U1826	G1733	A1605	C1505	A1427	G1331	U1241	A1139	G1062	U970	U878	G788	A607	G607
	A2048	G1935	A1734	A1606	C1506		G1332	U1245	G1140	U1063	A971	U880		A696	U608
		U1827		G1607	C1507	C1431	G1333	U1245	G1141	A1064	A972		A793	A697	G609
	G2052	A1829	G1739	C1608	U1511	C1432	U1334	G1248	G1142	G1065	A973		A794	C698	C610
		U1830	G1740		U1512	U1433	C1335	C1249	G1143		A974	C883	U795	U699	C611
	U2065			G1611	C1513	U1434	C1336	C1250	U1147	A1072	A975	G884		A700	U612
		G1836	C1746	A1612	U1514	U1435	A1342	G1251			C976	G885	C802	U701	U613
	C2063	U1837		G1615	G1515	U1436	A1343	C1252	G1148		G977	U886			
	C2069	G1838	C1748												



• Molecule 32: 50S ribosomal protein L31

Chain 0: 55% 11% 32%



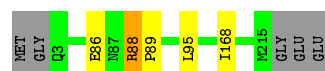
• Molecule 33: 30S ribosomal protein S2, chloroplastic

Chain b: 91%



• Molecule 34: 30S ribosomal protein S3, chloroplastic

Chain c: 95%



• Molecule 35: 30S ribosomal protein S5, chloroplastic

Chain e: 65% 32%

CYS ILE LYS LYS ASP ASP ILE ASP THR PHE PHE GLU GLN ASP ASP ASN PRO LYS ASP GLU GLU ILE THR PHE ASP PRO PRO LYS LYS PRO GLU GLY TYR ILE PRO PRO PRO ARG ALA VAL ASP GLU PRO PRO PHE GLU SER SER GLU GLU ILE ALA LEU ALA TYR GLU GLU LEU TYR GLY ALA ALA

TYR SER GLY GLU SER LEU LEU GLY ASN VAL TYR ALA MET ASP SER LYS ILE LYS LYS ALA THR G138 K144 K147 I148 L266 P302 K303 E304 E305 K308

- Molecule 36: 30S ribosomal protein S6 alpha, chloroplastic

Chain f:  75% 24%

ASP PHE SER GLY SER PHE PHE GLY GLY PHE PHE GLY GLY LEU ASP ASP ASP PRO PRO SER THR PRO PRO ALA GLY LEU VAL VAL GLU GLU LYS P97 P102 K207 LYS ARG LYS TYR

- Molecule 37: 30S ribosomal protein S7, chloroplastic

Chain g:  95% ..


MET SER ARG R4 E8 E9 A152 HIS PHE ARG

- Molecule 38: 30S ribosomal protein S8, chloroplastic

Chain h:  99% ..


M1 R67 L79 W134

- Molecule 39: 30S ribosomal protein S9, chloroplastic

Chain i:  82% 15%

THR SER ALA THR ALA PRO VAL VAL VAL ALA THR ASP LEU GLU LYS PHE VAL LYS SER ARG L63 R78 T96 A159 R176 S195 LYS ARG

- Molecule 40: protein S10

Chain j:  80% 20%

SER PHE GLU ASP THR GLY SER GLU THR SER LYS ILE ILE ILE ALA ALA ASP ASP ASP GLN MET ALA PRO LYS GLN K38 L135 L195

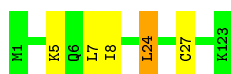
- Molecule 41: 30S ribosomal protein S11, chloroplastic

Chain k:  86% 14%

MET ALA LYS PRO PRO ILE PRO LYS ILE GLY SER ARG ARG ASN GLY ARG ILE ILE SER SER ARG LYS S21 V138

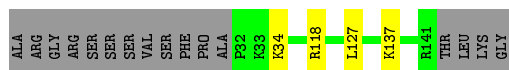
- Molecule 42: 30S ribosomal protein S12, chloroplastic

Chain l:  96% ..



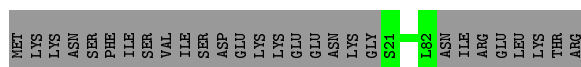
- Molecule 43: 30S ribosomal protein S13, chloroplastic

Chain m: 84% 13%



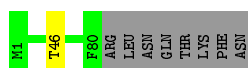
- Molecule 44: 30S ribosomal protein S15, chloroplastic

Chain o: 69% 31%



- Molecule 45: 30S ribosomal protein S16, chloroplastic

Chain p: 90% 9%



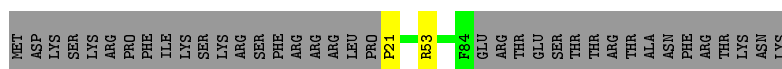
- Molecule 46: protein S17

Chain q: 72% 28%



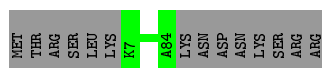
- Molecule 47: 30S ribosomal protein S18, chloroplastic

Chain r: 61% 37%



- Molecule 48: 30S ribosomal protein S19 alpha, chloroplastic

Chain s: 85% 15%



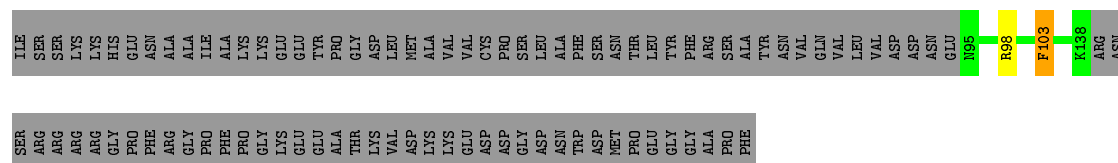
- Molecule 49: protein S20

Chain t: 95% 5%



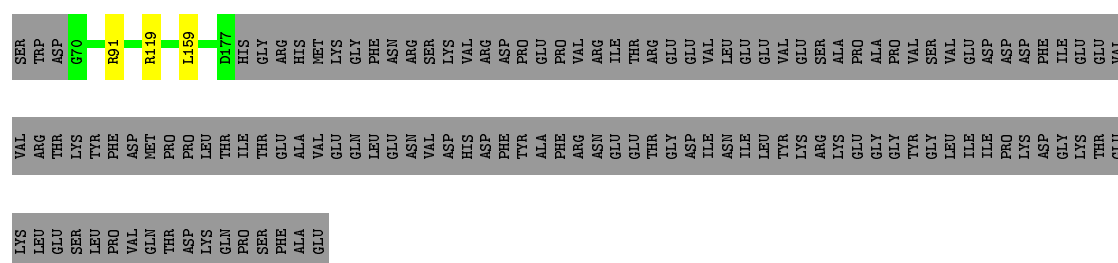
- Molecule 50: protein S21

Chain u:  31% .. 68%



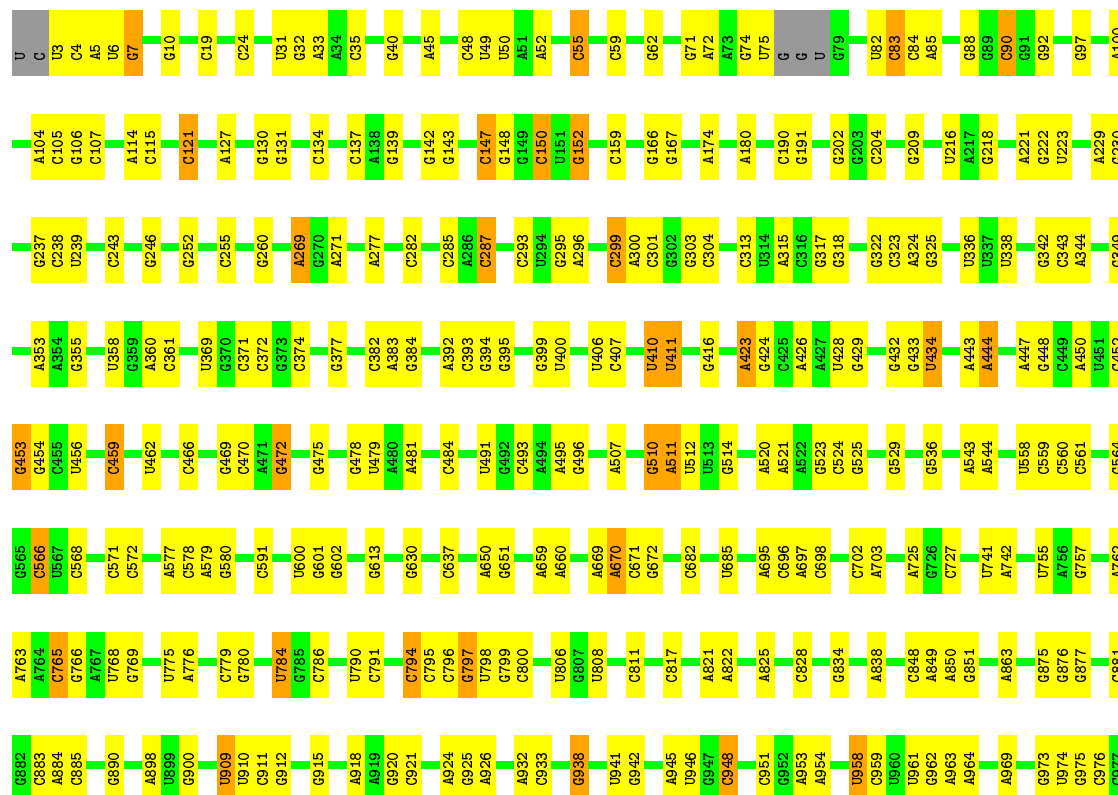
- Molecule 51: protein plastid pY

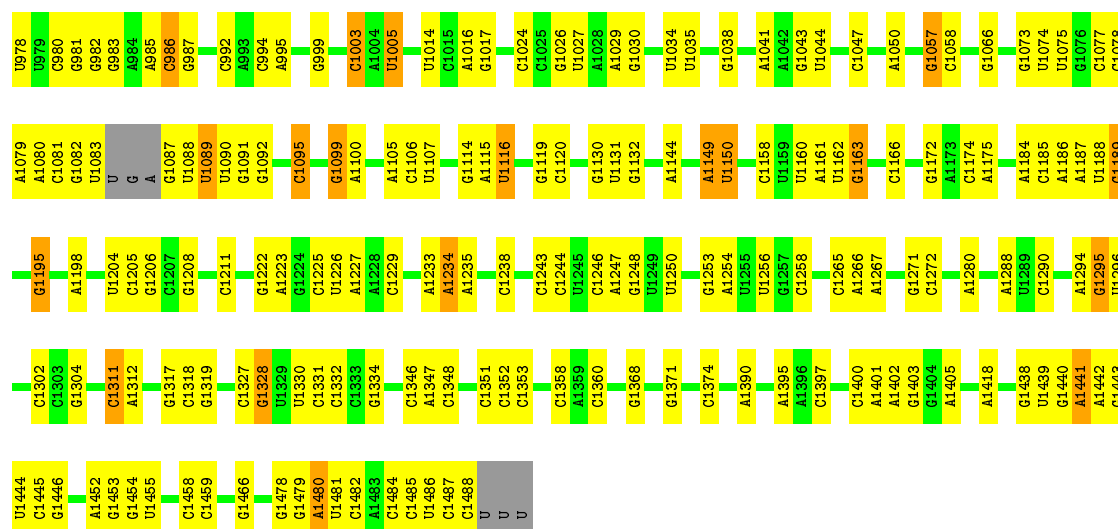
Chain y:  44% . 54%



- Molecule 52: 16S rRNA

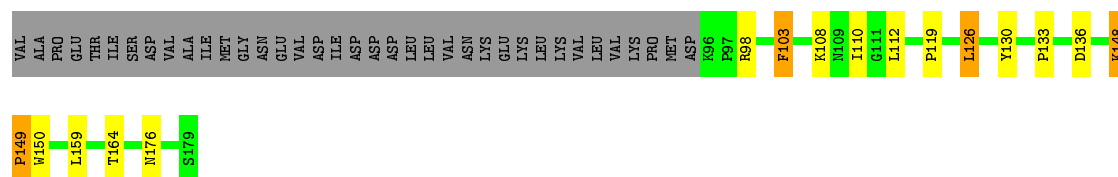
Chain a: 67% 29% .





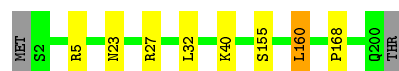
• Molecule 53: protein cS23

Chain w: 56% 10% 31%



• Molecule 54: 30S ribosomal protein S4, chloroplastic

Chain d: 95%



• Molecule 55: protein cS22

Chain v: 81% 12%



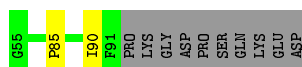
• Molecule 56: 30S ribosomal protein S14, chloroplastic

Chain n: 99%



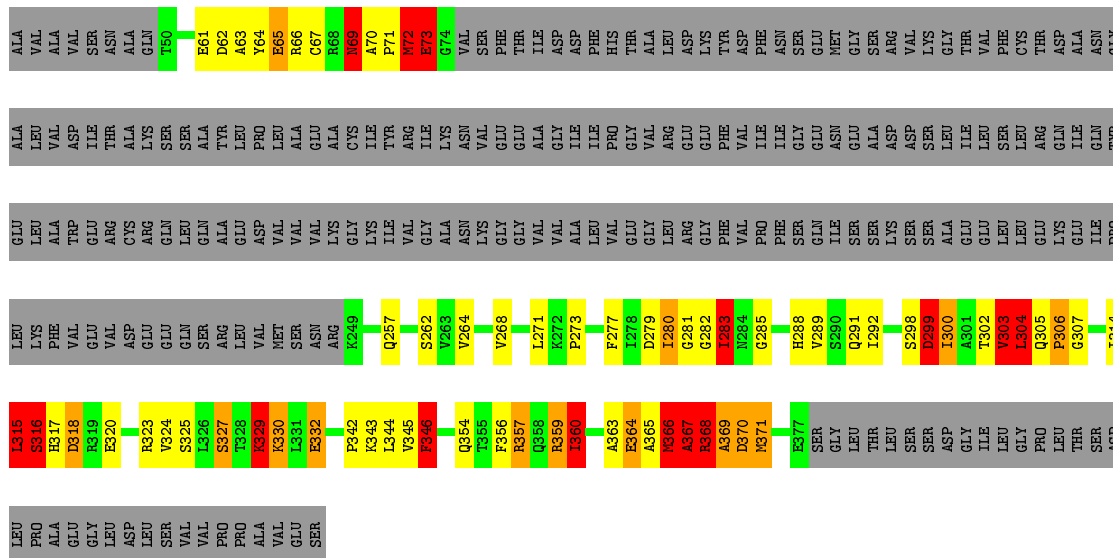
• Molecule 57: protein bTHXc

Chain x: 74% 21%



- Molecule 58: 30S ribosomal protein S1, chloroplastic

Chain 8:  23% 11% . . 58%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	81305	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	133333	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1	0.27	0/387	0.51	0/513
10	D	0.31	0/1646	0.65	0/2201
11	E	0.30	0/1687	0.65	1/2271 (0.0%)
12	F	0.28	0/1372	0.61	0/1848
13	G	0.26	0/1374	0.55	1/1849 (0.1%)
14	H	0.26	0/427	0.59	0/568
15	K	0.28	0/1608	0.57	2/2174 (0.1%)
16	L	0.31	0/951	0.59	0/1282
17	M	0.28	0/1361	0.53	0/1806
18	N	0.31	0/1089	0.61	0/1461
19	O	0.28	0/959	0.61	0/1280
2	2	0.32	0/422	0.75	1/564 (0.2%)
20	P	0.26	0/963	0.55	1/1293 (0.1%)
21	Q	0.31	0/967	0.71	2/1300 (0.2%)
22	R	0.33	0/1013	0.61	0/1351
23	S	0.31	0/1199	0.61	0/1633
24	T	0.29	0/1168	0.60	1/1566 (0.1%)
25	U	0.27	0/749	0.58	0/1006
26	V	0.27	0/1006	0.64	1/1343 (0.1%)
27	W	0.35	0/2449	1.07	10/3817 (0.3%)
28	X	0.30	0/825	0.57	0/1099
29	Y	0.28	0/615	0.65	2/819 (0.2%)
3	3	0.27	0/447	0.66	1/588 (0.2%)
30	Z	0.27	0/762	0.57	0/1012
31	A	0.35	1/67572 (0.0%)	1.05	315/105421 (0.3%)
32	0	0.29	0/533	0.66	1/718 (0.1%)
33	b	0.75	8/1819 (0.4%)	0.96	8/2458 (0.3%)
34	c	0.48	0/1746	0.72	1/2348 (0.0%)
35	e	0.61	0/1307	0.77	2/1754 (0.1%)
36	f	0.44	0/904	0.69	0/1225
37	g	0.36	0/1175	0.62	0/1574
38	h	0.88	5/1103 (0.5%)	1.69	6/1477 (0.4%)
39	i	0.43	0/1038	0.70	0/1397
4	4	0.31	0/569	0.66	1/752 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	j	0.51	0/813	0.70	1/1099 (0.1%)
41	k	0.40	0/901	0.63	0/1214
42	l	0.62	0/983	0.80	4/1323 (0.3%)
43	m	0.45	0/909	0.75	2/1209 (0.2%)
44	o	0.42	0/532	0.65	0/707
45	p	0.52	0/674	0.71	0/902
46	q	0.50	0/647	0.64	0/867
47	r	0.49	0/522	0.76	2/697 (0.3%)
48	s	0.44	0/642	0.70	0/866
49	t	0.46	0/842	0.68	0/1127
5	5	0.30	0/306	0.67	0/403
50	u	1.10	3/396 (0.8%)	0.94	3/518 (0.6%)
51	y	0.45	0/852	0.70	0/1139
52	a	1.13	32/35582 (0.1%)	1.39	473/55510 (0.9%)
53	w	0.80	2/709 (0.3%)	1.23	11/965 (1.1%)
54	d	0.40	0/1661	0.72	2/2230 (0.1%)
55	v	1.49	16/1481 (1.1%)	1.24	13/1991 (0.7%)
56	n	0.37	0/835	0.62	0/1116
57	x	0.55	0/296	0.74	1/390 (0.3%)
58	8	0.87	5/1216 (0.4%)	1.61	28/1631 (1.7%)
6	6	0.25	0/425	0.46	0/551
7	7	0.28	0/382	0.54	0/520
8	B	0.31	0/2796	1.05	12/4357 (0.3%)
9	C	0.29	0/1938	0.64	0/2603
All	All	0.65	72/159552 (0.0%)	1.08	909/237703 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	M	0	1
21	Q	0	1
23	S	0	1
32	0	0	1
33	b	0	2
34	c	0	3
35	e	0	1
36	f	0	1
37	g	0	1
39	i	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	j	0	1
42	l	0	3
43	m	0	2
50	u	0	1
53	w	0	7
54	d	0	2
55	v	0	15
58	8	0	17
All	All	0	62

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	142	PHE	CE1-CZ	-18.97	1.01	1.37
55	v	142	PHE	CE2-CZ	-17.85	1.03	1.37
55	v	142	PHE	CG-CD2	-15.89	1.15	1.38
38	h	67	ARG	CZ-NH2	-15.34	1.13	1.33
55	v	165	PHE	CE2-CZ	-14.94	1.08	1.37
55	v	142	PHE	CG-CD1	-14.77	1.16	1.38
38	h	67	ARG	CB-CG	-14.59	1.13	1.52
55	v	168	VAL	CB-CG1	-14.33	1.22	1.52
55	v	195	VAL	CB-CG2	-13.41	1.24	1.52
55	v	194	ARG	CG-CD	-12.82	1.19	1.51
50	u	103	PHE	CD1-CE1	-11.76	1.15	1.39
55	v	165	PHE	CG-CD2	-10.85	1.22	1.38
50	u	103	PHE	CD2-CE2	-10.60	1.18	1.39
55	v	26	VAL	CB-CG1	-9.95	1.31	1.52
33	b	7	ASN	CG-ND2	-9.61	1.08	1.32
50	u	103	PHE	CB-CG	-9.12	1.35	1.51
33	b	201	ASP	CB-CG	9.03	1.70	1.51
55	v	142	PHE	CD2-CE2	7.99	1.55	1.39
55	v	142	PHE	CD1-CE1	7.72	1.54	1.39
53	w	149	PRO	CG-CD	-7.71	1.25	1.50
52	a	7	G	C2-N3	-7.63	1.26	1.32
38	h	67	ARG	CZ-NH1	-7.51	1.23	1.33
33	b	209	ASP	CG-OD2	-7.19	1.08	1.25
52	a	4	C	C4-C5	-6.92	1.37	1.43
53	w	164	THR	CB-CG2	-6.82	1.29	1.52
52	a	1081	C	N3-C4	6.76	1.38	1.33
52	a	1087	G	C6-N1	-6.71	1.34	1.39
52	a	900	G	C6-N1	-6.71	1.34	1.39
55	v	193	ILE	CB-CG2	-6.67	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	1480	A	N9-C8	-6.61	1.32	1.37
52	a	147	C	N3-C4	-6.49	1.29	1.33
55	v	79	VAL	CB-CG1	-6.48	1.39	1.52
52	a	4	C	C5-C6	-6.41	1.29	1.34
52	a	786	C	N3-C4	-6.40	1.29	1.33
52	a	107	C	N3-C4	-6.37	1.29	1.33
52	a	150	C	N3-C4	-6.30	1.29	1.33
52	a	881	C	N3-C4	-6.28	1.29	1.33
38	h	67	ARG	CG-CD	-6.17	1.36	1.51
52	a	1441	A	N1-C2	-6.03	1.28	1.34
38	h	67	ARG	CA-CB	-6.02	1.40	1.53
52	a	1482	C	C5-C6	-5.97	1.29	1.34
52	a	7	G	C5-C4	-5.94	1.34	1.38
33	b	20	PHE	CE2-CZ	-5.88	1.26	1.37
58	8	289	VAL	CB-CG1	-5.88	1.40	1.52
52	a	951	C	N3-C4	-5.75	1.29	1.33
52	a	448	G	C6-N1	-5.69	1.35	1.39
52	a	1440	G	N3-C4	-5.68	1.31	1.35
33	b	56	GLU	CD-OE2	-5.66	1.19	1.25
52	a	1029	A	N7-C5	-5.61	1.35	1.39
52	a	450	A	C6-N1	-5.58	1.31	1.35
52	a	1016	A	N9-C4	-5.53	1.34	1.37
58	8	327	SER	CB-OG	-5.53	1.35	1.42
55	v	95	VAL	CB-CG2	-5.50	1.41	1.52
58	8	368	ARG	CB-CG	5.45	1.67	1.52
52	a	74	G	O3'-P	-5.41	1.54	1.61
33	b	40	LYS	CD-CE	-5.40	1.37	1.51
52	a	269	A	N9-C4	-5.40	1.34	1.37
52	a	361	C	N3-C4	-5.38	1.30	1.33
58	8	65	GLU	CB-CG	-5.28	1.42	1.52
52	a	7	G	N3-C4	-5.28	1.31	1.35
31	A	2447	A	N9-C4	5.19	1.41	1.37
52	a	898	A	N7-C5	-5.19	1.36	1.39
33	b	112	GLU	CD-OE2	-5.19	1.20	1.25
52	a	1358	C	C2-O2	-5.14	1.19	1.24
52	a	885	C	N3-C4	-5.13	1.30	1.33
52	a	371	C	N3-C4	-5.12	1.30	1.33
33	b	7	ASN	CB-CG	-5.10	1.39	1.51
52	a	271	A	N7-C5	-5.10	1.36	1.39
55	v	195	VAL	CB-CG1	-5.08	1.42	1.52
52	a	510	G	N9-C4	-5.07	1.33	1.38
58	8	332	GLU	CB-CG	-5.04	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	428	U	C2-N3	-5.03	1.34	1.37

All (909) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	h	67	ARG	NE-CZ-NH1	50.54	145.57	120.30
33	b	201	ASP	CB-CG-OD2	20.66	136.90	118.30
52	a	1440	G	N3-C2-N2	-20.49	105.56	119.90
52	a	7	G	C2-N3-C4	20.20	122.00	111.90
52	a	1441	A	N1-C2-N3	20.05	139.32	129.30
52	a	1439	U	C5-C6-N1	18.99	132.19	122.70
38	h	67	ARG	NH1-CZ-NH2	-16.53	101.21	119.40
52	a	147	C	N1-C2-O2	16.52	128.81	118.90
52	a	976	C	N1-C2-O2	16.12	128.57	118.90
52	a	150	C	N1-C2-O2	16.09	128.55	118.90
52	a	1488	C	C5-C6-N1	15.36	128.68	121.00
38	h	67	ARG	NE-CZ-NH2	-15.35	112.62	120.30
52	a	4	C	C6-N1-C2	-15.01	114.30	120.30
52	a	1480	A	N7-C8-N9	14.64	121.12	113.80
52	a	881	C	N1-C2-O2	14.50	127.60	118.90
38	h	67	ARG	CD-NE-CZ	14.42	143.78	123.60
52	a	786	C	N1-C2-O2	14.14	127.38	118.90
52	a	1077	C	N1-C2-O2	13.21	126.83	118.90
52	a	1445	C	C5-C6-N1	13.13	127.56	121.00
52	a	1487	C	C5-C6-N1	12.95	127.48	121.00
52	a	1485	C	C5-C6-N1	12.60	127.30	121.00
38	h	67	ARG	CB-CG-CD	12.09	143.04	111.60
52	a	1195	G	N1-C6-O6	11.53	126.82	119.90
52	a	147	C	N3-C2-O2	-11.49	113.86	121.90
52	a	107	C	N1-C2-O2	11.48	125.79	118.90
52	a	1440	G	N1-C2-N2	11.43	126.49	116.20
52	a	1195	G	C5-C6-O6	-11.39	121.77	128.60
52	a	1486	U	C5-C6-N1	11.28	128.34	122.70
52	a	1488	C	C6-N1-C2	-11.22	115.81	120.30
52	a	976	C	N3-C4-N4	11.18	125.82	118.00
31	A	2077	C	N1-C2-O2	11.07	125.54	118.90
52	a	1238	C	N3-C2-O2	-10.94	114.24	121.90
33	b	209	ASP	CB-CG-OD1	10.94	128.14	118.30
52	a	147	C	C2-N3-C4	10.88	125.34	119.90
52	a	976	C	N3-C2-O2	-10.87	114.29	121.90
52	a	951	C	N1-C2-O2	10.85	125.41	118.90
58	8	304	LEU	CA-CB-CG	10.83	140.21	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	8	344	LEU	CB-CG-CD2	-10.83	92.59	111.00
52	a	1445	C	C6-N1-C2	-10.81	115.97	120.30
55	v	142	PHE	CB-CG-CD1	10.79	128.35	120.80
52	a	1087	G	N3-C2-N2	10.70	127.39	119.90
52	a	4	C	C5-C6-N1	10.68	126.34	121.00
31	A	2077	C	C2-N1-C1'	10.66	130.53	118.80
52	a	147	C	N3-C4-N4	10.57	125.40	118.00
52	a	881	C	N3-C2-O2	-10.50	114.55	121.90
52	a	1484	C	C5-C6-N1	10.49	126.25	121.00
52	a	786	C	N3-C4-N4	10.43	125.30	118.00
52	a	1441	A	C2-N3-C4	-10.41	105.39	110.60
52	a	976	C	C2-N3-C4	10.39	125.09	119.90
52	a	786	C	N3-C2-O2	-10.37	114.64	121.90
52	a	150	C	N3-C2-O2	-10.30	114.69	121.90
52	a	1480	A	C5-N7-C8	-10.22	98.79	103.90
52	a	1090	U	N3-C2-O2	-10.22	115.05	122.20
52	a	1256	U	C2-N3-C4	10.16	133.09	127.00
53	w	103	PHE	CB-CG-CD2	-10.12	113.71	120.80
52	a	1441	A	C6-N1-C2	-10.10	112.54	118.60
52	a	1440	G	C6-N1-C2	-10.06	119.06	125.10
52	a	150	C	C2-N3-C4	10.06	124.93	119.90
58	8	318	ASP	CB-CG-OD1	9.99	127.29	118.30
52	a	7	G	N3-C4-C5	-9.96	123.62	128.60
31	A	1747	C	N3-C2-O2	-9.95	114.94	121.90
52	a	285	C	N1-C2-O2	9.95	124.87	118.90
52	a	983	G	N1-C6-O6	-9.94	113.93	119.90
52	a	83	C	N1-C2-O2	9.92	124.85	118.90
52	a	448	G	N1-C6-O6	9.90	125.84	119.90
52	a	1116	U	N1-C2-O2	9.88	129.72	122.80
31	A	2314	C	C2-N1-C1'	9.82	129.60	118.80
52	a	1081	C	N1-C2-O2	-9.66	113.11	118.90
52	a	1480	A	C8-N9-C4	-9.59	101.96	105.80
52	a	786	C	C2-N3-C4	9.56	124.68	119.90
52	a	1439	U	C6-N1-C2	-9.55	115.27	121.00
31	A	2314	C	N1-C2-O2	9.54	124.62	118.90
58	8	72	MET	N-CA-C	-9.53	85.27	111.00
52	a	147	C	N3-C4-C5	-9.48	118.11	121.90
52	a	786	C	N3-C4-C5	-9.41	118.13	121.90
52	a	1090	U	N1-C2-O2	9.37	129.36	122.80
52	a	794	C	N1-C2-O2	9.37	124.52	118.90
31	A	2662	C	N1-C2-O2	9.35	124.51	118.90
55	v	194	ARG	NE-CZ-NH2	-9.34	115.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	881	C	N3-C4-N4	9.29	124.50	118.00
52	a	1487	C	C6-N1-C2	-9.21	116.61	120.30
52	a	572	C	N1-C2-O2	9.21	124.43	118.90
31	A	2077	C	C6-N1-C2	-9.17	116.63	120.30
52	a	255	C	N1-C2-O2	9.15	124.39	118.90
53	w	103	PHE	CB-CG-CD1	9.15	127.20	120.80
52	a	107	C	N3-C2-O2	-9.13	115.51	121.90
52	a	976	C	N3-C4-C5	-9.11	118.26	121.90
31	A	2077	C	N3-C2-O2	-9.10	115.53	121.90
52	a	1116	U	N3-C2-O2	-9.10	115.83	122.20
52	a	285	C	N3-C2-O2	-9.04	115.58	121.90
52	a	951	C	N3-C2-O2	-9.02	115.58	121.90
52	a	948	C	C5-C6-N1	9.01	125.51	121.00
52	a	885	C	N1-C2-O2	8.95	124.27	118.90
52	a	142	G	N1-C6-O6	-8.94	114.54	119.90
52	a	1374	C	C6-N1-C2	-8.91	116.73	120.30
31	A	2268	G	C4-N9-C1'	8.90	138.07	126.50
52	a	1238	C	N1-C2-O2	8.89	124.23	118.90
52	a	1485	C	C6-N1-C2	-8.85	116.76	120.30
31	A	294	U	N1-C2-O2	8.85	128.99	122.80
31	A	1334	U	C2-N1-C1'	8.84	128.31	117.70
52	a	1166	C	O5'-P-OP1	-8.75	97.83	105.70
58	8	73	GLU	N-CA-C	-8.74	87.39	111.00
31	A	2314	C	C6-N1-C2	-8.71	116.81	120.30
52	a	1439	U	C4-C5-C6	-8.71	114.48	119.70
33	b	201	ASP	OD1-CG-OD2	-8.70	106.77	123.30
52	a	948	C	C6-N1-C2	-8.69	116.83	120.30
33	b	201	ASP	CB-CG-OD1	-8.68	110.49	118.30
55	v	165	PHE	CB-CG-CD1	8.68	126.88	120.80
31	A	1334	U	N1-C2-O2	8.67	128.87	122.80
31	A	897	A	C5-C6-N6	-8.67	116.76	123.70
31	A	900	G	N7-C8-N9	8.66	117.43	113.10
52	a	1077	C	C2-N3-C4	8.63	124.22	119.90
35	e	266	LEU	CA-CB-CG	8.60	135.08	115.30
52	a	301	C	N1-C2-O2	8.58	124.05	118.90
31	A	46	C	N1-C2-O2	8.55	124.03	118.90
52	a	150	C	N3-C4-N4	8.54	123.98	118.00
52	a	786	C	C6-N1-C2	-8.53	116.89	120.30
52	a	1081	C	C5-C4-N4	-8.53	114.23	120.20
52	a	1003	C	N1-C2-O2	8.49	124.00	118.90
52	a	1077	C	N3-C2-O2	-8.49	115.95	121.90
8	B	61	C	N1-C2-O2	8.48	123.99	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	2662	C	C2-N1-C1'	8.47	128.12	118.80
52	a	1003	C	N3-C2-O2	-8.47	115.97	121.90
52	a	1481	U	C5-C6-N1	8.47	126.94	122.70
52	a	797	G	N1-C6-O6	-8.41	114.86	119.90
33	b	40	LYS	CD-CE-NZ	-8.39	92.39	111.70
58	8	304	LEU	CB-CG-CD1	8.38	125.25	111.00
52	a	987	G	N1-C6-O6	-8.38	114.87	119.90
52	a	1081	C	C2-N3-C4	-8.38	115.71	119.90
31	A	1784	C	N3-C2-O2	-8.32	116.08	121.90
31	A	2709	C	N3-C2-O2	-8.32	116.08	121.90
31	A	294	U	N3-C2-O2	-8.30	116.39	122.20
31	A	1923	C	N3-C2-O2	-8.27	116.11	121.90
52	a	159	C	N1-C2-O2	8.26	123.86	118.90
31	A	899	A	N7-C8-N9	8.25	117.92	113.80
52	a	1358	C	C6-N1-C2	-8.24	117.00	120.30
52	a	1488	C	C4-C5-C6	-8.17	113.32	117.40
31	A	1843	C	N3-C2-O2	-8.16	116.19	121.90
55	v	142	PHE	CD1-CG-CD2	-8.14	107.71	118.30
29	Y	103	LEU	CA-CB-CG	8.12	133.98	115.30
31	A	1334	U	N3-C2-O2	-8.11	116.52	122.20
58	8	315	LEU	CB-CG-CD1	8.11	124.79	111.00
52	a	1244	C	N1-C2-O2	8.11	123.76	118.90
58	8	299	ASP	N-CA-C	-8.11	89.11	111.00
52	a	1225	C	N1-C2-O2	8.09	123.76	118.90
58	8	367	ALA	N-CA-CB	8.09	121.43	110.10
31	A	1283	U	N3-C2-O2	-8.08	116.54	122.20
52	a	881	C	C6-N1-C2	-8.06	117.08	120.30
31	A	1970	U	N1-C2-O2	8.05	128.44	122.80
21	Q	224	ASP	CB-CG-OD1	8.04	125.53	118.30
31	A	294	U	C2-N1-C1'	8.03	127.33	117.70
52	a	1440	G	C8-N9-C4	-8.00	103.20	106.40
52	a	7	G	N1-C2-N3	-8.00	119.10	123.90
52	a	1244	C	N3-C2-O2	-7.99	116.31	121.90
31	A	1970	U	N3-C2-O2	-7.97	116.62	122.20
53	w	148	LYS	C-N-CD	-7.95	103.10	120.60
52	a	881	C	C2-N3-C4	7.90	123.85	119.90
58	8	368	ARG	CB-CG-CD	7.89	132.11	111.60
31	A	112	C	N1-C2-O2	7.88	123.63	118.90
31	A	2268	G	C8-N9-C1'	-7.84	116.81	127.00
52	a	794	C	C2-N1-C1'	7.82	127.41	118.80
52	a	4	C	N3-C4-C5	-7.80	118.78	121.90
52	a	84	C	N1-C2-O2	7.79	123.58	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	2314	C	N3-C2-O2	-7.70	116.51	121.90
52	a	1106	C	C2-N1-C1'	7.70	127.27	118.80
52	a	1484	C	C6-N1-C2	-7.67	117.23	120.30
52	a	987	G	N3-C2-N2	-7.67	114.53	119.90
52	a	139	G	N1-C6-O6	-7.63	115.32	119.90
52	a	1116	U	C2-N1-C1'	7.63	126.86	117.70
58	8	360	ILE	N-CA-C	-7.62	90.42	111.00
31	A	1784	C	N1-C2-O2	7.61	123.46	118.90
31	A	1818	U	C2-N1-C1'	7.61	126.83	117.70
8	B	69	C	N1-C2-O2	7.60	123.46	118.90
31	A	448	C	N1-C2-O2	7.58	123.45	118.90
52	a	1258	C	N1-C2-O2	7.58	123.45	118.90
52	a	361	C	N1-C2-O2	7.58	123.45	118.90
52	a	1163	G	N1-C6-O6	7.57	124.44	119.90
58	8	279	ASP	CB-CG-OD1	7.57	125.11	118.30
31	A	1013	C	N1-C2-O2	7.56	123.44	118.90
52	a	881	C	C2-N1-C1'	7.55	127.10	118.80
52	a	1077	C	C2-N1-C1'	7.54	127.10	118.80
52	a	1087	G	N1-C2-N2	-7.53	109.43	116.20
52	a	147	C	C6-N1-C2	-7.50	117.30	120.30
58	8	73	GLU	CB-CA-C	7.46	125.33	110.40
31	A	2683	C	N1-C2-O2	7.45	123.37	118.90
31	A	168	C	N1-C2-O2	7.44	123.36	118.90
52	a	1095	C	N1-C2-O2	7.42	123.35	118.90
52	a	150	C	N3-C4-C5	-7.41	118.94	121.90
54	d	32	LEU	CA-CB-CG	7.41	132.34	115.30
52	a	794	C	N3-C2-O2	-7.40	116.72	121.90
52	a	1089	U	C5-C6-N1	7.40	126.40	122.70
31	A	1107	C	N1-C2-O2	7.40	123.34	118.90
31	A	38	C	N1-C2-O2	7.38	123.33	118.90
58	8	62	ASP	CB-CG-OD2	-7.37	111.66	118.30
52	a	1453	G	N1-C6-O6	7.37	124.32	119.90
52	a	959	C	N1-C2-O2	7.36	123.31	118.90
52	a	1158	C	N1-C2-O2	7.33	123.30	118.90
52	a	1272	C	N1-C2-O2	7.33	123.30	118.90
4	4	153	LEU	CA-CB-CG	7.32	132.13	115.30
31	A	2662	C	N3-C2-O2	-7.31	116.78	121.90
52	a	7	G	C5-C6-N1	7.31	115.15	111.50
52	a	295	G	C8-N9-C4	-7.30	103.48	106.40
26	V	64	LEU	CA-CB-CG	7.30	132.10	115.30
31	A	46	C	C6-N1-C2	-7.29	117.38	120.30
52	a	881	C	N3-C4-C5	-7.29	118.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	572	C	N3-C2-O2	-7.28	116.81	121.90
52	a	951	C	C6-N1-C2	-7.27	117.39	120.30
52	a	1003	C	C6-N1-C2	-7.27	117.39	120.30
52	a	139	G	N3-C2-N2	-7.26	114.82	119.90
52	a	951	C	N3-C4-N4	7.26	123.08	118.00
52	a	1003	C	C2-N1-C1'	7.25	126.78	118.80
52	a	1077	C	N3-C4-N4	7.23	123.06	118.00
52	a	1077	C	C6-N1-C2	-7.23	117.41	120.30
52	a	910	U	N3-C2-O2	-7.22	117.15	122.20
52	a	1358	C	N3-C2-O2	-7.22	116.85	121.90
52	a	885	C	N3-C2-O2	-7.21	116.85	121.90
52	a	794	C	C6-N1-C2	-7.21	117.42	120.30
52	a	1083	U	C5-C6-N1	7.21	126.30	122.70
31	A	1283	U	N1-C2-O2	7.21	127.84	122.80
31	A	2121	C	N1-C2-O2	7.21	123.22	118.90
52	a	951	C	N3-C4-C5	-7.20	119.02	121.90
52	a	1120	C	N3-C2-O2	-7.19	116.86	121.90
31	A	1432	U	N3-C2-O2	-7.19	117.17	122.20
52	a	951	C	C2-N3-C4	7.19	123.49	119.90
31	A	2314	C	C5-C6-N1	7.18	124.59	121.00
31	A	2077	C	C5-C6-N1	7.17	124.59	121.00
31	A	1595	C	N1-C2-O2	7.16	123.20	118.90
52	a	1290	C	N1-C2-O2	7.15	123.19	118.90
31	A	1459	U	N1-C2-O2	7.15	127.80	122.80
50	u	98	ARG	NE-CZ-NH1	-7.14	116.73	120.30
52	a	361	C	C6-N1-C2	-7.13	117.45	120.30
52	a	428	U	N3-C2-O2	-7.13	117.21	122.20
58	8	357	ARG	NE-CZ-NH1	-7.13	116.74	120.30
52	a	434	U	C2-N1-C1'	7.11	126.24	117.70
52	a	670	A	C2-N3-C4	7.11	114.16	110.60
55	v	165	PHE	CZ-CE2-CD2	7.11	128.63	120.10
31	A	1432	U	C2-N1-C1'	7.10	126.22	117.70
52	a	1030	G	N1-C6-O6	7.09	124.15	119.90
52	a	976	C	C6-N1-C2	-7.08	117.47	120.30
31	A	112	C	C2-N1-C1'	7.07	126.58	118.80
52	a	83	C	N3-C2-O2	-7.05	116.96	121.90
31	A	900	G	C8-N9-C4	-7.05	103.58	106.40
31	A	1432	U	N1-C2-O2	7.04	127.73	122.80
31	A	2268	G	N3-C4-N9	7.04	130.22	126.00
58	8	70	ALA	N-CA-CB	7.01	119.92	110.10
52	a	1485	C	C4-C5-C6	-7.00	113.90	117.40
52	a	1087	G	C6-N1-C2	7.00	129.30	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1335	C	C2-N1-C1'	7.00	126.50	118.80
52	a	877	G	C6-C5-N7	-6.99	126.20	130.40
58	8	318	ASP	CB-CG-OD2	-6.99	112.01	118.30
52	a	1445	C	C4-C5-C6	-6.99	113.91	117.40
31	A	2518	C	C6-N1-C2	-6.98	117.51	120.30
52	a	84	C	N3-C2-O2	-6.98	117.02	121.90
31	A	1818	U	N1-C2-O2	6.97	127.68	122.80
33	b	201	ASP	N-CA-CB	6.97	123.14	110.60
31	A	688	C	C2-N1-C1'	6.96	126.45	118.80
31	A	2209	U	N3-C2-O2	-6.96	117.33	122.20
31	A	2268	G	N3-C4-C5	-6.96	125.12	128.60
52	a	1328	G	N1-C6-O6	-6.96	115.73	119.90
52	a	223	U	N1-C2-O2	6.95	127.66	122.80
11	E	245	LEU	CA-CB-CG	6.95	131.27	115.30
31	A	46	C	N3-C2-O2	-6.95	117.04	121.90
31	A	1419	C	N1-C2-O2	6.89	123.03	118.90
31	A	2706	U	N1-C2-O2	6.89	127.62	122.80
52	a	1150	U	N3-C2-O2	-6.89	117.38	122.20
31	A	2116	C	N1-C2-O2	6.86	123.02	118.90
52	a	561	C	N1-C2-O2	6.86	123.02	118.90
31	A	2709	C	C6-N1-C2	-6.86	117.56	120.30
52	a	938	G	N1-C6-O6	6.86	124.02	119.90
31	A	630	C	N1-C2-O2	6.86	123.01	118.90
31	A	900	G	C5-N7-C8	-6.85	100.87	104.30
52	a	55	C	N3-C2-O2	-6.85	117.11	121.90
58	8	283	ILE	CG1-CB-CG2	-6.83	96.37	111.40
31	A	2209	U	N1-C2-O2	6.83	127.58	122.80
31	A	901	C	N1-C2-O2	6.82	122.99	118.90
52	a	491	U	N3-C2-O2	-6.82	117.43	122.20
52	a	55	C	N1-C2-O2	6.82	122.99	118.90
31	A	897	A	C4-C5-N7	6.81	114.11	110.70
31	A	2209	U	C2-N1-C1'	6.81	125.87	117.70
52	a	1150	U	N1-C2-O2	6.80	127.56	122.80
52	a	511	A	C2-N3-C4	6.80	114.00	110.60
31	A	897	A	N1-C6-N6	6.80	122.68	118.60
52	a	301	C	N3-C2-O2	-6.79	117.15	121.90
52	a	1440	G	N7-C8-N9	6.79	116.49	113.10
31	A	31	C	N1-C2-O2	6.79	122.97	118.90
54	d	160	LEU	CA-CB-CG	6.78	130.89	115.30
58	8	316	SER	C-N-CA	6.78	138.64	121.70
31	A	1620	U	N1-C2-O2	6.78	127.54	122.80
52	a	1120	C	N1-C2-O2	6.78	122.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	223	U	C2-N1-C1'	6.77	125.82	117.70
31	A	38	C	N3-C2-O2	-6.76	117.17	121.90
55	v	165	PHE	CB-CG-CD2	-6.75	116.07	120.80
52	a	1092	G	N1-C6-O6	-6.75	115.85	119.90
52	a	1440	G	N1-C2-N3	6.74	127.94	123.90
52	a	1172	G	N3-C4-N9	-6.74	121.96	126.00
31	A	1528	U	N1-C2-O2	6.72	127.51	122.80
31	A	2378	C	N1-C2-O2	6.72	122.93	118.90
52	a	243	C	N1-C2-O2	6.71	122.93	118.90
52	a	784	U	N3-C2-O2	-6.71	117.50	122.20
52	a	890	G	N3-C2-N2	-6.69	115.22	119.90
52	a	150	C	C6-N1-C2	-6.69	117.62	120.30
53	w	133	PRO	CA-N-CD	-6.68	102.15	111.50
52	a	255	C	N3-C4-N4	6.67	122.67	118.00
31	A	2077	C	C6-N1-C1'	-6.66	112.81	120.80
31	A	2706	U	N3-C2-O2	-6.66	117.54	122.20
31	A	1818	U	C5-C6-N1	6.65	126.03	122.70
52	a	558	U	N3-C2-O2	-6.65	117.54	122.20
52	a	1334	G	N1-C6-O6	-6.65	115.91	119.90
52	a	448	G	C5-C6-O6	-6.65	124.61	128.60
52	a	255	C	N3-C2-O2	-6.65	117.25	121.90
52	a	3	U	C5-C6-N1	6.64	126.02	122.70
8	B	61	C	N3-C2-O2	-6.64	117.25	121.90
31	A	1397	C	N1-C2-O2	6.63	122.88	118.90
52	a	1440	G	C5-C6-O6	-6.63	124.62	128.60
52	a	1149	A	C8-N9-C4	6.62	108.45	105.80
31	A	2483	C	N1-C2-O2	6.60	122.86	118.90
31	A	877	C	N1-C2-O2	6.60	122.86	118.90
52	a	1029	A	C6-C5-N7	-6.58	127.69	132.30
52	a	83	C	C6-N1-C2	-6.58	117.67	120.30
52	a	285	C	C6-N1-C2	-6.56	117.68	120.30
52	a	150	C	C2-N1-C1'	6.56	126.01	118.80
31	A	1528	U	N3-C2-O2	-6.55	117.61	122.20
52	a	511	A	N1-C6-N6	-6.55	114.67	118.60
2	2	13	LEU	CA-CB-CG	6.55	130.37	115.30
8	B	61	C	C2-N1-C1'	6.54	126.00	118.80
52	a	90	C	C6-N1-C2	-6.54	117.69	120.30
31	A	928	U	N1-C2-O2	6.53	127.37	122.80
27	W	33	A	P-O3'-C3'	6.53	127.53	119.70
31	A	1459	U	N3-C2-O2	-6.53	117.63	122.20
31	A	2121	C	C2-N1-C1'	6.51	125.96	118.80
31	A	1620	U	N3-C2-O2	-6.51	117.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	1087	G	C5-C6-O6	6.51	132.50	128.60
52	a	976	C	C5-C4-N4	-6.50	115.65	120.20
52	a	958	U	N1-C2-O2	6.49	127.34	122.80
52	a	1254	A	N7-C8-N9	6.48	117.04	113.80
52	a	571	C	N1-C2-O2	6.48	122.79	118.90
52	a	1058	C	N3-C2-O2	-6.48	117.37	121.90
31	A	363	C	N1-C2-O2	6.47	122.78	118.90
34	c	95	LEU	CA-CB-CG	6.46	130.16	115.30
52	a	407	C	C6-N1-C2	-6.46	117.72	120.30
31	A	46	C	C2-N1-C1'	6.45	125.89	118.80
31	A	2447	A	C2-N3-C4	6.44	113.82	110.60
52	a	1487	C	C4-C5-C6	-6.44	114.18	117.40
31	A	168	C	N3-C2-O2	-6.43	117.40	121.90
31	A	901	C	C2-N1-C1'	6.43	125.88	118.80
52	a	1311	C	N3-C2-O2	-6.43	117.40	121.90
52	a	1254	A	C8-N9-C4	-6.43	103.23	105.80
52	a	1029	A	C4-C5-N7	6.43	113.91	110.70
52	a	1077	C	N3-C4-C5	-6.43	119.33	121.90
52	a	1348	C	N1-C2-O2	-6.42	115.05	118.90
52	a	784	U	C2-N1-C1'	6.41	125.40	117.70
52	a	411	U	N1-C2-O2	6.41	127.29	122.80
52	a	1081	C	C5-C6-N1	6.41	124.20	121.00
8	B	69	C	N3-C2-O2	-6.39	117.42	121.90
52	a	59	C	C6-N1-C2	-6.39	117.74	120.30
52	a	828	C	O5'-P-OP1	-6.39	99.95	105.70
31	A	899	A	C8-N9-C4	-6.39	103.25	105.80
52	a	407	C	N1-C2-O2	6.38	122.73	118.90
52	a	1120	C	C6-N1-C2	-6.38	117.75	120.30
52	a	560	C	N1-C2-O2	6.38	122.73	118.90
52	a	890	G	N1-C6-O6	-6.38	116.07	119.90
52	a	682	C	C5-C6-N1	6.38	124.19	121.00
31	A	1013	C	N3-C2-O2	-6.37	117.44	121.90
52	a	371	C	N1-C2-O2	6.37	122.72	118.90
31	A	1528	U	C2-N1-C1'	6.37	125.34	117.70
31	A	2598	G	C4-C5-N7	6.37	113.35	110.80
58	8	329	LYS	CD-CE-NZ	6.36	126.33	111.70
52	a	1078	C	C2-N1-C1'	6.35	125.79	118.80
31	A	783	U	N1-C2-O2	6.35	127.24	122.80
52	a	361	C	N3-C2-O2	-6.34	117.46	121.90
52	a	959	C	N3-C2-O2	-6.34	117.46	121.90
31	A	897	A	N9-C4-C5	-6.33	103.27	105.80
53	w	112	LEU	CB-CG-CD1	-6.33	100.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1335	C	C6-N1-C2	-6.33	117.77	120.30
27	W	32	C	P-O3'-C3'	6.32	127.29	119.70
52	a	1149	A	N9-C4-C5	-6.32	103.27	105.80
31	A	253	C	C2-N1-C1'	6.31	125.75	118.80
52	a	1302	C	C6-N1-C2	-6.30	117.78	120.30
52	a	434	U	N3-C2-O2	-6.30	117.79	122.20
52	a	1374	C	C5-C6-N1	6.30	124.15	121.00
52	a	784	U	N1-C2-O2	6.30	127.21	122.80
38	h	67	ARG	N-CA-CB	-6.30	99.27	110.60
31	A	31	C	C2-N1-C1'	6.29	125.72	118.80
52	a	1353	C	N1-C2-O2	6.29	122.67	118.90
31	A	1250	C	C5-C6-N1	6.27	124.13	121.00
31	A	112	C	N3-C2-O2	-6.27	117.51	121.90
52	a	811	C	N1-C2-O2	6.25	122.65	118.90
52	a	318	G	N1-C6-O6	6.24	123.64	119.90
31	A	448	C	N3-C2-O2	-6.23	117.54	121.90
52	a	794	C	C5-C6-N1	6.23	124.11	121.00
52	a	243	C	N3-C2-O2	-6.22	117.55	121.90
52	a	97	G	N1-C6-O6	-6.22	116.17	119.90
52	a	4	C	N3-C4-N4	6.21	122.35	118.00
31	A	1335	C	C5-C6-N1	6.20	124.10	121.00
31	A	2097	C	N1-C2-O2	6.20	122.62	118.90
52	a	83	C	C2-N3-C4	6.20	123.00	119.90
58	8	69	ASN	N-CA-C	6.20	127.73	111.00
52	a	1360	C	C6-N1-C2	-6.19	117.83	120.30
31	A	38	C	C6-N1-C2	-6.18	117.83	120.30
52	a	755	U	C2-N3-C4	6.18	130.71	127.00
52	a	912	G	N1-C6-O6	-6.17	116.19	119.90
52	a	1077	C	C5-C6-N1	6.17	124.09	121.00
52	a	223	U	N3-C2-O2	-6.17	117.88	122.20
52	a	808	U	N3-C2-O2	-6.17	117.88	122.20
31	A	1108	C	N3-C2-O2	-6.17	117.58	121.90
52	a	1029	A	N1-C6-N6	6.16	122.30	118.60
31	A	2700	C	N1-C2-O2	6.16	122.60	118.90
42	l	7	LEU	CA-CB-CG	6.16	129.47	115.30
52	a	159	C	N3-C2-O2	-6.15	117.59	121.90
52	a	407	C	C5-C6-N1	6.15	124.08	121.00
55	v	142	PHE	CZ-CE2-CD2	6.14	127.47	120.10
31	A	856	U	N3-C2-O2	-6.12	117.91	122.20
52	a	1459	C	N1-C2-O2	6.12	122.57	118.90
52	a	448	G	C6-C5-N7	-6.12	126.73	130.40
52	a	1258	C	N3-C2-O2	-6.12	117.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	2683	C	N3-C2-O2	-6.11	117.62	121.90
58	8	367	ALA	C-N-CA	6.11	136.97	121.70
31	A	2469	C	N1-C2-O2	6.11	122.56	118.90
52	a	434	U	N1-C2-O2	6.11	127.08	122.80
52	a	958	U	N3-C2-O2	-6.11	117.92	122.20
52	a	1158	C	N3-C2-O2	-6.10	117.63	121.90
52	a	1195	G	C6-C5-N7	-6.09	126.75	130.40
52	a	1057	G	C4-N9-C1'	6.09	134.41	126.50
33	b	201	ASP	CA-CB-CG	6.08	126.79	113.40
52	a	698	C	C6-N1-C2	-6.08	117.87	120.30
52	a	1058	C	N1-C2-O2	6.08	122.55	118.90
52	a	1024	C	C5-C6-N1	6.08	124.04	121.00
31	A	1907	C	N1-C2-O2	6.07	122.54	118.90
52	a	411	U	N3-C2-O2	-6.07	117.95	122.20
53	w	126	LEU	CB-CG-CD2	-6.07	100.68	111.00
52	a	1482	C	C6-N1-C2	-6.07	117.87	120.30
31	A	2314	C	C6-N1-C1'	-6.05	113.53	120.80
15	K	239	LEU	CA-CB-CG	6.05	129.21	115.30
42	l	7	LEU	CB-CG-CD2	-6.05	100.72	111.00
31	A	448	C	C2-N1-C1'	6.05	125.45	118.80
52	a	1332	C	N1-C2-O2	6.03	122.52	118.90
52	a	571	C	C6-N1-C2	-6.02	117.89	120.30
52	a	1444	U	C5-C6-N1	6.01	125.71	122.70
31	A	2724	C	N1-C2-O2	6.01	122.51	118.90
31	A	1620	U	C2-N1-C1'	6.01	124.91	117.70
52	a	910	U	N1-C2-N3	6.01	118.50	114.90
52	a	817	C	N1-C2-O2	6.01	122.50	118.90
52	a	1035	U	N3-C2-O2	-6.01	118.00	122.20
47	r	53	ARG	CA-CB-CG	-6.00	100.19	113.40
8	B	69	C	C6-N1-C2	-6.00	117.90	120.30
31	A	253	C	C6-N1-C2	-6.00	117.90	120.30
31	A	38	C	C2-N1-C1'	6.00	125.40	118.80
52	a	591	C	C6-N1-C2	-5.98	117.91	120.30
31	A	186	C	N1-C2-O2	5.98	122.49	118.90
31	A	1013	C	C2-N1-C1'	5.98	125.38	118.80
31	A	173	C	N1-C2-O2	5.98	122.49	118.90
27	W	100	C	N1-C2-O2	5.97	122.48	118.90
52	a	1304	G	N3-C2-N2	5.97	124.08	119.90
52	a	1172	G	C6-C5-N7	5.96	133.97	130.40
52	a	190	C	N1-C2-O2	5.96	122.47	118.90
47	r	21	PRO	N-CA-CB	5.95	110.44	103.30
31	A	1209	U	N1-C2-O2	5.95	126.97	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	921	C	C6-N1-C2	-5.95	117.92	120.30
52	a	1225	C	N3-C2-O2	-5.94	117.74	121.90
31	A	1309	U	N3-C2-O2	-5.93	118.05	122.20
31	A	1142	G	C4-N9-C1'	5.93	134.21	126.50
52	a	1484	C	C4-C5-C6	-5.92	114.44	117.40
31	A	46	C	C5-C6-N1	5.92	123.96	121.00
52	a	282	C	C6-N1-C2	-5.92	117.93	120.30
52	a	313	C	N3-C4-C5	5.92	124.27	121.90
20	P	73	LEU	CA-CB-CG	5.92	128.91	115.30
52	a	571	C	N3-C4-N4	5.92	122.14	118.00
52	a	682	C	C6-N1-C2	-5.92	117.93	120.30
52	a	698	C	C5-C6-N1	5.91	123.96	121.00
52	a	83	C	C2-N1-C1'	5.91	125.30	118.80
31	A	1142	G	N3-C4-C5	-5.91	125.65	128.60
31	A	2789	C	N1-C2-O2	5.91	122.44	118.90
52	a	877	G	C4-C5-N7	5.90	113.16	110.80
31	A	856	U	N1-C2-O2	5.90	126.93	122.80
52	a	564	G	N1-C6-O6	-5.90	116.36	119.90
31	A	2662	C	C6-N1-C1'	-5.89	113.73	120.80
31	A	1770	C	N1-C2-O2	5.89	122.43	118.90
52	a	932	A	C4-N9-C1'	5.89	136.90	126.30
31	A	243	U	N1-C2-O2	5.88	126.92	122.80
52	a	1290	C	N3-C2-O2	-5.88	117.78	121.90
50	u	98	ARG	CA-CB-CG	5.88	126.34	113.40
52	a	484	C	N1-C2-O2	5.88	122.43	118.90
52	a	1296	U	N3-C2-O2	-5.88	118.08	122.20
13	G	206	ASP	CB-CG-OD1	5.88	123.59	118.30
31	A	243	U	N3-C2-O2	-5.88	118.08	122.20
31	A	1748	C	N3-C2-O2	-5.88	117.79	121.90
31	A	2598	G	C5-N7-C8	-5.87	101.36	104.30
55	v	142	PHE	CD1-CE1-CZ	5.86	127.14	120.10
27	W	29	U	P-O3'-C3'	5.86	126.73	119.70
31	A	112	C	C6-N1-C2	-5.86	117.96	120.30
31	A	2654	U	C2-N1-C1'	5.85	124.72	117.70
52	a	107	C	N3-C4-N4	5.85	122.10	118.00
3	3	93	LEU	CA-CB-CG	5.85	128.75	115.30
31	A	9	A	C2-N3-C4	5.84	113.52	110.60
31	A	2706	U	C2-N1-C1'	5.84	124.71	117.70
31	A	1219	U	N3-C2-O2	-5.84	118.11	122.20
31	A	2654	U	N1-C2-O2	5.84	126.89	122.80
33	b	202	ILE	CG1-CB-CG2	-5.84	98.56	111.40
52	a	452	C	C6-N1-C2	-5.84	117.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	178	U	N3-C2-O2	-5.83	118.11	122.20
52	a	450	A	N1-C2-N3	-5.83	126.39	129.30
52	a	848	C	N1-C2-O2	5.83	122.40	118.90
52	a	1172	G	C4-N9-C1'	-5.83	118.92	126.50
31	A	1747	C	C6-N1-C2	-5.82	117.97	120.30
31	A	2491	U	C2-N1-C1'	5.82	124.69	117.70
42	l	24	LEU	CA-CB-CG	5.81	128.66	115.30
31	A	514	A	P-O3'-C3'	5.81	126.67	119.70
52	a	459	C	N1-C2-O2	-5.80	115.42	118.90
52	a	702	C	C2-N1-C1'	5.80	125.18	118.80
31	A	1419	C	N3-C2-O2	-5.79	117.84	121.90
8	B	31	C	N1-C2-O2	5.79	122.37	118.90
31	A	1107	C	C2-N1-C1'	5.79	125.17	118.80
52	a	204	C	C2-N1-C1'	5.79	125.16	118.80
31	A	647	C	C6-N1-C2	-5.78	117.99	120.30
31	A	186	C	N3-C2-O2	-5.78	117.86	121.90
31	A	1784	C	C6-N1-C2	-5.77	117.99	120.30
8	B	7	G	O4'-C1'-N9	5.77	112.82	108.20
52	a	1441	A	N1-C6-N6	-5.77	115.14	118.60
52	a	304	C	N1-C2-O2	5.76	122.36	118.90
52	a	1030	G	C5-C6-O6	-5.76	125.15	128.60
31	A	2653	U	N1-C2-O2	5.75	126.83	122.80
52	a	371	C	C6-N1-C2	-5.75	118.00	120.30
31	A	2121	C	N3-C2-O2	-5.75	117.87	121.90
52	a	293	C	C6-N1-C2	-5.75	118.00	120.30
31	A	1923	C	N1-C2-O2	5.74	122.35	118.90
31	A	2588	U	N1-C2-O2	5.74	126.82	122.80
52	a	137	C	N1-C2-O2	5.74	122.34	118.90
52	a	523	G	N3-C4-N9	-5.74	122.56	126.00
31	A	2007	U	N3-C2-O2	-5.73	118.19	122.20
52	a	374	C	N3-C4-C5	5.73	124.19	121.90
52	a	1172	G	C8-N9-C1'	5.73	134.45	127.00
52	a	1026	G	C6-C5-N7	-5.73	126.96	130.40
52	a	1440	G	N9-C4-C5	5.72	107.69	105.40
31	A	1595	C	C2-N1-C1'	5.72	125.09	118.80
52	a	558	U	N1-C2-O2	5.72	126.81	122.80
52	a	142	G	C5-C6-O6	5.72	132.03	128.60
31	A	210	C	N1-C2-O2	5.71	122.33	118.90
31	A	1334	U	C6-N1-C1'	-5.71	113.21	121.20
31	A	928	U	N3-C2-O2	-5.71	118.20	122.20
31	A	1746	C	N1-C2-O2	5.71	122.32	118.90
31	A	254	U	N3-C2-O2	-5.71	118.21	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	24	C	C5-C6-N1	5.70	123.85	121.00
27	W	74	C	C6-N1-C2	-5.70	118.02	120.30
52	a	797	G	N3-C2-N2	-5.70	115.91	119.90
52	a	71	G	N1-C6-O6	-5.69	116.48	119.90
52	a	1029	A	N9-C4-C5	-5.69	103.53	105.80
31	A	1945	U	N1-C2-O2	5.68	126.78	122.80
52	a	496	G	C6-C5-N7	-5.68	126.99	130.40
31	A	1595	C	N3-C2-O2	-5.68	117.92	121.90
31	A	2111	U	C2-N1-C1'	5.68	124.51	117.70
52	a	1374	C	N1-C2-O2	5.68	122.31	118.90
52	a	411	U	C2-N1-C1'	5.68	124.51	117.70
31	A	2708	C	N1-C2-O2	5.67	122.30	118.90
31	A	1692	C	C6-N1-C2	-5.66	118.03	120.30
52	a	685	U	C5-C6-N1	5.66	125.53	122.70
52	a	1095	C	N3-C2-O2	-5.66	117.94	121.90
55	v	167	PHE	CB-CG-CD2	-5.66	116.83	120.80
58	8	330	LYS	N-CA-CB	5.66	120.79	110.60
31	A	2178	C	N1-C2-O2	5.66	122.29	118.90
31	A	2573	C	N1-C2-O2	5.65	122.29	118.90
31	A	794	A	C2-N3-C4	5.64	113.42	110.60
31	A	367	C	OP1-P-O3'	5.64	117.61	105.20
31	A	1459	U	C2-N1-C1'	5.64	124.47	117.70
31	A	1945	U	C2-N1-C1'	5.64	124.47	117.70
31	A	367	C	P-O3'-C3'	5.63	126.46	119.70
31	A	541	G	C4-N9-C1'	5.63	133.83	126.50
31	A	1923	C	C6-N1-C2	-5.63	118.05	120.30
52	a	410	U	N3-C2-O2	-5.63	118.26	122.20
52	a	1453	G	C5-C6-O6	-5.63	125.22	128.60
31	A	1843	C	C2-N3-C4	-5.63	117.09	119.90
52	a	410	U	N1-C2-O2	5.63	126.74	122.80
52	a	1459	C	C6-N1-C2	-5.63	118.05	120.30
31	A	594	C	C5-C6-N1	5.62	123.81	121.00
52	a	299	C	N1-C2-O2	5.62	122.27	118.90
31	A	210	C	C6-N1-C2	-5.61	118.06	120.30
52	a	765	C	N1-C2-O2	5.61	122.27	118.90
52	a	559	C	N1-C2-O2	5.61	122.27	118.90
31	A	688	C	C6-N1-C2	-5.60	118.06	120.30
31	A	2683	C	C2-N1-C1'	5.60	124.96	118.80
52	a	19	C	C6-N1-C2	-5.59	118.06	120.30
52	a	1446	G	C4-N9-C1'	5.59	133.76	126.50
58	8	280	ILE	CB-CA-C	5.58	122.77	111.60
52	a	976	C	C5-C6-N1	5.58	123.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1142	G	N3-C4-N9	5.58	129.35	126.00
31	A	1981	C	N1-C2-O2	5.58	122.25	118.90
58	8	300	ILE	N-CA-C	-5.58	95.94	111.00
52	a	371	C	N3-C4-N4	5.57	121.90	118.00
52	a	808	U	N1-C2-O2	5.57	126.70	122.80
31	A	2325	G	N3-C4-N9	5.57	129.34	126.00
32	0	87	LEU	CA-CB-CG	5.56	128.09	115.30
52	a	1172	G	N1-C6-O6	-5.56	116.56	119.90
52	a	1374	C	N3-C2-O2	-5.56	118.01	121.90
58	8	73	GLU	CA-CB-CG	5.56	125.63	113.40
8	B	38	C	N1-C2-O2	5.55	122.23	118.90
31	A	683	C	N1-C2-O2	5.55	122.23	118.90
31	A	1317	C	C6-N1-C2	-5.55	118.08	120.30
31	A	594	C	C6-N1-C2	-5.55	118.08	120.30
8	B	69	C	C2-N1-C1'	5.55	124.90	118.80
52	a	131	G	N1-C6-O6	-5.54	116.57	119.90
31	A	448	C	C6-N1-C2	-5.54	118.08	120.30
52	a	1081	C	N3-C4-N4	5.54	121.88	118.00
52	a	1438	G	C8-N9-C4	-5.54	104.18	106.40
52	a	637	C	N1-C2-O2	5.54	122.22	118.90
52	a	1087	G	C2-N3-C4	-5.54	109.13	111.90
31	A	897	A	C5-C6-N1	5.53	120.47	117.70
40	j	135	LEU	CA-CB-CG	5.53	128.02	115.30
52	a	909	U	C2-N1-C1'	5.53	124.33	117.70
31	A	2378	C	N3-C2-O2	-5.53	118.03	121.90
52	a	1358	C	N1-C2-O2	5.52	122.21	118.90
31	A	2421	C	N1-C2-O2	5.52	122.21	118.90
52	a	462	U	C5-C6-N1	5.52	125.46	122.70
31	A	1818	U	N3-C2-O2	-5.52	118.34	122.20
27	W	10	C	N1-C2-O2	5.52	122.21	118.90
27	W	22	A	OP1-P-O3'	5.52	117.34	105.20
31	A	2789	C	N3-C2-O2	-5.52	118.04	121.90
52	a	1058	C	C6-N1-C2	-5.51	118.09	120.30
31	A	2325	G	N3-C4-C5	-5.51	125.85	128.60
31	A	496	C	N1-C2-O2	5.51	122.20	118.90
31	A	1945	U	N3-C2-O2	-5.50	118.35	122.20
52	a	1238	C	C2-N3-C4	-5.50	117.15	119.90
52	a	7	G	N9-C4-C5	5.50	107.60	105.40
31	A	1397	C	N3-C2-O2	-5.50	118.05	121.90
52	a	1005	U	C2-N3-C4	5.49	130.30	127.00
52	a	1330	U	N1-C2-O2	5.49	126.64	122.80
31	A	688	C	N1-C2-O2	5.49	122.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1906	C	N1-C2-O2	5.49	122.19	118.90
52	a	900	G	N3-C2-N2	5.48	123.74	119.90
52	a	1106	C	N1-C2-O2	5.48	122.19	118.90
52	a	484	C	C2-N1-C1'	5.47	124.82	118.80
52	a	1296	U	N1-C2-O2	5.47	126.63	122.80
52	a	285	C	N3-C4-N4	5.47	121.83	118.00
52	a	912	G	C5-C6-O6	5.47	131.88	128.60
31	A	688	C	N3-C2-O2	-5.46	118.08	121.90
31	A	2774	U	C5-C4-O4	5.46	129.18	125.90
52	a	1442	A	N7-C8-N9	5.46	116.53	113.80
31	A	813	C	N1-C2-O2	5.45	122.17	118.90
31	A	2300	U	C2-N1-C1'	5.45	124.24	117.70
52	a	83	C	C5-C6-N1	5.45	123.73	121.00
52	a	910	U	C2-N3-C4	-5.45	123.73	127.00
31	A	1137	C	N1-C2-O2	5.45	122.17	118.90
52	a	152	G	C4-C5-N7	5.44	112.98	110.80
52	a	779	C	C6-N1-C2	-5.44	118.12	120.30
52	a	962	G	N1-C6-O6	-5.44	116.63	119.90
52	a	1290	C	N3-C4-C5	-5.44	119.72	121.90
52	a	454	G	C6-C5-N7	-5.44	127.14	130.40
31	A	2325	G	C4-N9-C1'	5.43	133.56	126.50
52	a	121	C	C2-N1-C1'	5.43	124.77	118.80
53	w	164	THR	CA-CB-CG2	-5.43	104.80	112.40
31	A	178	U	N1-C2-O2	5.43	126.60	122.80
52	a	932	A	C8-N9-C1'	-5.43	117.93	127.70
31	A	2097	C	N3-C2-O2	-5.43	118.10	121.90
52	a	986	C	C6-N1-C2	-5.42	118.13	120.30
52	a	1486	U	C6-N1-C2	-5.42	117.75	121.00
52	a	1352	C	C6-N1-C2	-5.42	118.13	120.30
52	a	147	C	C5-C4-N4	-5.42	116.41	120.20
24	T	67	LEU	CA-CB-CG	5.42	127.76	115.30
52	a	342	G	N3-C2-N2	-5.42	116.11	119.90
31	A	630	C	C2-N1-C1'	5.41	124.75	118.80
31	A	2300	U	C5-C6-N1	5.41	125.41	122.70
31	A	870	U	N1-C2-O2	5.41	126.59	122.80
31	A	1309	U	N1-C2-O2	5.41	126.59	122.80
31	A	856	U	C2-N1-C1'	5.41	124.19	117.70
52	a	1256	U	N3-C4-C5	-5.41	111.36	114.60
52	a	1331	C	N1-C2-O2	5.41	122.14	118.90
31	A	2020	C	N1-C2-O2	5.40	122.14	118.90
35	e	303	MET	CB-CG-SD	5.40	128.59	112.40
55	v	129	LEU	CA-CB-CG	5.40	127.71	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1604	A	N1-C6-N6	5.39	121.84	118.60
31	A	2535	C	N1-C2-O2	5.39	122.14	118.90
52	a	209	G	N1-C6-O6	-5.39	116.66	119.90
52	a	493	C	N3-C4-C5	5.39	124.06	121.90
31	A	186	C	C6-N1-C2	-5.39	118.14	120.30
31	A	2545	U	N1-C2-O2	5.39	126.57	122.80
52	a	1226	U	N1-C2-O2	5.39	126.58	122.80
31	A	1309	U	C2-N1-C1'	5.39	124.17	117.70
52	a	1439	U	C5-C4-O4	-5.39	122.67	125.90
31	A	1283	U	C2-N1-C1'	5.38	124.16	117.70
52	a	566	C	N1-C2-O2	5.38	122.13	118.90
52	a	1087	G	C5-C6-N1	-5.38	108.81	111.50
31	A	2378	C	C6-N1-C2	-5.38	118.15	120.30
31	A	2662	C	C6-N1-C2	-5.38	118.15	120.30
31	A	2699	U	N3-C2-O2	-5.37	118.44	122.20
52	a	784	U	C6-N1-C2	-5.37	117.78	121.00
52	a	850	A	N1-C6-N6	5.37	121.82	118.60
52	a	134	C	C6-N1-C2	-5.37	118.15	120.30
8	B	18	C	N1-C2-O2	5.37	122.12	118.90
31	A	1335	C	N1-C2-O2	5.37	122.12	118.90
52	a	670	A	N3-C4-N9	5.37	131.69	127.40
31	A	703	C	N1-C2-O2	5.36	122.12	118.90
31	A	2007	U	N1-C2-O2	5.36	126.55	122.80
31	A	2653	U	N3-C2-O2	-5.36	118.45	122.20
52	a	1353	C	C6-N1-C2	-5.36	118.16	120.30
31	A	496	C	C5-C6-N1	5.35	123.68	121.00
31	A	2530	U	N3-C2-O2	-5.34	118.46	122.20
52	a	472	G	N3-C2-N2	5.34	123.64	119.90
31	A	2303	A	O4'-C1'-N9	-5.34	103.93	108.20
31	A	2360	U	N1-C2-O2	5.34	126.54	122.80
31	A	907	C	N1-C2-O2	5.34	122.10	118.90
31	A	1175	U	N1-C2-O2	5.33	126.53	122.80
31	A	2737	G	N1-C6-O6	-5.33	116.70	119.90
52	a	1106	C	N3-C2-O2	-5.33	118.17	121.90
31	A	2116	C	N3-C2-O2	-5.33	118.17	121.90
31	A	877	C	N3-C2-O2	-5.33	118.17	121.90
52	a	295	G	N7-C8-N9	5.33	115.77	113.10
52	a	139	G	C5-C6-N1	5.33	114.16	111.50
52	a	784	U	C5-C6-N1	5.33	125.36	122.70
31	A	1209	U	C5-C6-N1	5.33	125.36	122.70
8	B	31	C	C2-N1-C1'	5.32	124.66	118.80
31	A	1397	C	C2-N1-C1'	5.32	124.66	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	1029	A	C5-N7-C8	-5.32	101.24	103.90
52	a	1150	U	C2-N1-C1'	5.32	124.09	117.70
52	a	1238	C	C2-N1-C1'	5.32	124.65	118.80
52	a	1353	C	N3-C2-O2	-5.32	118.18	121.90
52	a	255	C	C5-C4-N4	-5.32	116.48	120.20
31	A	363	C	C2-N1-C1'	5.32	124.65	118.80
52	a	301	C	C6-N1-C2	-5.31	118.17	120.30
31	A	1843	C	N1-C2-N3	5.31	122.92	119.20
52	a	1195	G	N3-C4-N9	5.31	129.19	126.00
52	a	246	G	C4-N9-C1'	5.31	133.40	126.50
31	A	1419	C	C2-N1-C1'	5.31	124.64	118.80
52	a	881	C	C5-C4-N4	-5.31	116.48	120.20
52	a	1106	C	C6-N1-C1'	-5.31	114.43	120.80
52	a	1035	U	N1-C2-O2	5.30	126.51	122.80
31	A	2483	C	N3-C2-O2	-5.30	118.19	121.90
52	a	987	G	C5-C6-O6	5.30	131.78	128.60
21	Q	223	ARG	C-N-CA	5.30	134.94	121.70
31	A	899	A	C5-N7-C8	-5.30	101.25	103.90
53	w	159	LEU	CB-CG-CD1	-5.30	102.00	111.00
31	A	2529	C	C6-N1-C2	-5.29	118.18	120.30
31	A	2708	C	C6-N1-C2	-5.29	118.18	120.30
31	A	1696	C	N1-C2-O2	5.29	122.07	118.90
31	A	2491	U	N1-C2-O2	5.28	126.50	122.80
52	a	1211	C	N1-C2-O2	5.28	122.07	118.90
31	A	1550	U	N1-C2-O2	5.27	126.49	122.80
31	A	2530	U	C2-N1-C1'	5.27	124.02	117.70
53	w	136	ASP	CB-CG-OD2	-5.27	113.56	118.30
52	a	938	G	C5-C6-O6	-5.26	125.44	128.60
58	8	303	VAL	N-CA-C	5.26	125.21	111.00
52	a	229	A	N1-C2-N3	-5.26	126.67	129.30
52	a	90	C	C2-N1-C1'	5.26	124.59	118.80
31	A	630	C	N3-C2-O2	-5.26	118.22	121.90
52	a	800	C	C2-N1-C1'	5.25	124.58	118.80
31	A	972	G	C4-N9-C1'	5.25	133.32	126.50
52	a	139	G	N1-C2-N2	5.25	120.92	116.20
52	a	1295	G	C2-N3-C4	-5.25	109.28	111.90
31	A	563	C	N1-C2-O2	5.24	122.05	118.90
52	a	239	U	N3-C2-O2	-5.24	118.53	122.20
52	a	566	C	C6-N1-C2	-5.24	118.20	120.30
31	A	294	U	C5-C6-N1	5.24	125.32	122.70
31	A	1595	C	C6-N1-C2	-5.24	118.20	120.30
31	A	228	U	N1-C2-O2	5.24	126.47	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	2737	G	C5-C6-O6	5.24	131.74	128.60
52	a	1256	U	N1-C2-N3	-5.24	111.76	114.90
52	a	727	C	N1-C2-O2	5.24	122.04	118.90
52	a	1057	G	C8-N9-C1'	-5.24	120.19	127.00
52	a	204	C	C6-N1-C2	-5.24	118.21	120.30
52	a	336	U	C2-N1-C1'	5.24	123.98	117.70
52	a	912	G	N9-C4-C5	5.24	107.49	105.40
31	A	2683	C	C6-N1-C2	-5.23	118.21	120.30
52	a	444	A	O4'-C1'-N9	5.23	112.38	108.20
52	a	987	G	N1-C2-N2	5.23	120.91	116.20
31	A	541	G	N3-C4-N9	5.23	129.14	126.00
31	A	2654	U	N3-C2-O2	-5.23	118.54	122.20
27	W	29	U	OP2-P-O3'	5.22	116.69	105.20
31	A	2651	C	N1-C2-O2	5.22	122.03	118.90
52	a	523	G	N3-C4-C5	5.22	131.21	128.60
31	A	2300	U	N3-C2-O2	-5.22	118.55	122.20
52	a	361	C	N3-C4-N4	5.22	121.66	118.00
52	a	1290	C	N3-C4-N4	5.22	121.66	118.00
52	a	1446	G	N3-C4-N9	5.22	129.13	126.00
52	a	1099	G	O4'-C1'-N9	5.22	112.38	108.20
31	A	173	C	N3-C2-O2	-5.22	118.25	121.90
52	a	299	C	N3-C2-O2	-5.22	118.25	121.90
52	a	786	C	C5-C4-N4	-5.22	116.55	120.20
31	A	1107	C	N3-C2-O2	-5.22	118.25	121.90
52	a	493	C	C2-N3-C4	-5.22	117.29	119.90
31	A	1901	C	N1-C2-O2	5.21	122.03	118.90
31	A	1907	C	N3-C2-O2	-5.21	118.25	121.90
52	a	88	G	C8-N9-C1'	-5.21	120.22	127.00
52	a	1446	G	C8-N9-C1'	-5.21	120.22	127.00
52	a	909	U	N1-C2-O2	5.21	126.45	122.80
52	a	1334	G	C5-C6-N1	5.21	114.11	111.50
31	A	684	C	C2-N3-C4	-5.21	117.30	119.90
27	W	74	C	C5-C6-N1	5.20	123.60	121.00
31	A	541	G	N3-C4-C5	-5.20	126.00	128.60
52	a	560	C	N3-C2-O2	-5.20	118.26	121.90
52	a	1348	C	C2-N3-C4	-5.20	117.30	119.90
31	A	2699	U	N1-C2-O2	5.20	126.44	122.80
52	a	523	G	N1-C6-O6	5.20	123.02	119.90
52	a	572	C	N3-C4-N4	5.19	121.63	118.00
52	a	933	C	C6-N1-C2	-5.19	118.22	120.30
31	A	2270	G	N3-C4-N9	5.19	129.11	126.00
50	u	103	PHE	CB-CG-CD2	-5.19	117.17	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	372	C	C6-N1-C2	-5.19	118.23	120.30
31	A	404	U	N1-C2-O2	5.18	126.43	122.80
31	A	1092	C	N1-C2-O2	5.18	122.01	118.90
52	a	1234	A	C2-N3-C4	5.18	113.19	110.60
31	A	2447	A	N3-C4-N9	5.18	131.54	127.40
52	a	806	U	N3-C2-O2	-5.18	118.58	122.20
31	A	1604	A	N7-C8-N9	5.17	116.39	113.80
31	A	2593	G	N3-C2-N2	5.17	123.52	119.90
52	a	131	G	C5-C6-N1	5.17	114.09	111.50
52	a	470	C	N1-C2-O2	5.17	122.00	118.90
52	a	568	C	N3-C2-O2	-5.17	118.28	121.90
52	a	702	C	N1-C2-O2	5.17	122.00	118.90
52	a	1453	G	N3-C2-N2	5.16	123.52	119.90
52	a	1017	G	C4-N9-C1'	5.16	133.21	126.50
31	A	1175	U	N3-C2-O2	-5.16	118.59	122.20
52	a	1458	C	C6-N1-C2	-5.16	118.24	120.30
31	A	2121	C	C6-N1-C2	-5.15	118.24	120.30
52	a	1459	C	N3-C4-N4	5.15	121.61	118.00
57	x	85	PRO	C-N-CD	5.15	139.22	128.40
31	A	2367	C	N1-C2-O2	5.15	121.99	118.90
52	a	287	C	N3-C2-O2	-5.15	118.30	121.90
52	a	83	C	N3-C4-C5	-5.14	119.84	121.90
55	v	25	TYR	CB-CG-CD1	5.14	124.09	121.00
31	A	1419	C	C6-N1-C2	-5.14	118.24	120.30
31	A	2360	U	C2-N1-C1'	5.14	123.87	117.70
31	A	703	C	N3-C2-O2	-5.13	118.31	121.90
52	a	190	C	N3-C2-O2	-5.13	118.31	121.90
52	a	1095	C	C2-N1-C1'	5.13	124.44	118.80
52	a	1272	C	N3-C2-O2	-5.13	118.31	121.90
43	m	127	LEU	CA-CB-CG	-5.13	103.50	115.30
52	a	255	C	C6-N1-C2	-5.13	118.25	120.30
52	a	406	U	C5-C6-N1	5.12	125.26	122.70
52	a	1353	C	C5-C6-N1	5.12	123.56	121.00
31	A	1219	U	C6-N1-C2	-5.12	117.93	121.00
52	a	453	G	C4-N9-C1'	5.12	133.16	126.50
31	A	258	C	N3-C2-O2	-5.12	118.31	121.90
52	a	496	G	C4-C5-N7	5.12	112.85	110.80
31	A	845	C	C6-N1-C2	-5.12	118.25	120.30
31	A	275	U	C2-N1-C1'	5.12	123.84	117.70
31	A	112	C	C5-C6-N1	5.12	123.56	121.00
31	A	210	C	N3-C2-O2	-5.11	118.32	121.90
52	a	800	C	C6-N1-C2	-5.11	118.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	797	G	C5-C6-O6	5.11	131.67	128.60
52	a	1244	C	C6-N1-C2	-5.11	118.25	120.30
52	a	83	C	N3-C4-N4	5.11	121.58	118.00
58	8	346	PHE	CB-CG-CD1	-5.11	117.22	120.80
15	K	191	LEU	CA-CB-CG	5.11	127.04	115.30
31	A	258	C	N1-C2-O2	5.11	121.96	118.90
52	a	1163	G	C5-C6-O6	-5.11	125.54	128.60
31	A	543	A	C2-N3-C4	5.10	113.15	110.60
31	A	2432	G	C4-N9-C1'	5.10	133.13	126.50
31	A	1546	C	N1-C2-O2	5.09	121.96	118.90
52	a	295	G	O5'-P-OP2	-5.09	101.12	105.70
52	a	1185	C	C6-N1-C2	-5.09	118.26	120.30
31	A	683	C	C6-N1-C2	-5.08	118.27	120.30
52	a	529	G	C4-C5-N7	5.08	112.83	110.80
52	a	911	C	C6-N1-C2	-5.08	118.27	120.30
31	A	1317	C	N3-C2-O2	-5.08	118.34	121.90
52	a	293	C	C5-C6-N1	5.08	123.54	121.00
52	a	1486	U	C4-C5-C6	-5.08	116.65	119.70
31	A	2243	C	N1-C2-O2	5.08	121.94	118.90
52	a	1332	C	C6-N1-C2	-5.07	118.27	120.30
52	a	35	C	C5-C6-N1	5.07	123.54	121.00
52	a	88	G	N1-C6-O6	5.07	122.94	119.90
52	a	293	C	N3-C2-O2	-5.07	118.35	121.90
52	a	1081	C	N1-C2-N3	5.07	122.75	119.20
31	A	288	C	N1-C2-O2	5.06	121.94	118.90
52	a	1438	G	N1-C6-O6	-5.06	116.86	119.90
31	A	363	C	N3-C2-O2	-5.06	118.36	121.90
31	A	2736	G	N1-C6-O6	-5.06	116.86	119.90
52	a	271	A	N7-C8-N9	5.06	116.33	113.80
52	a	493	C	N3-C4-N4	-5.06	114.46	118.00
52	a	88	G	C6-C5-N7	-5.06	127.36	130.40
52	a	394	G	N3-C4-N9	5.06	129.03	126.00
31	A	502	U	N1-C2-O2	5.05	126.34	122.80
31	A	2518	C	C5-C4-N4	5.05	123.74	120.20
52	a	90	C	C5-C6-N1	5.05	123.53	121.00
31	A	17	C	C6-N1-C2	-5.05	118.28	120.30
31	A	1550	U	N3-C2-O2	-5.05	118.67	122.20
31	A	1770	C	N3-C2-O2	-5.05	118.37	121.90
52	a	1106	C	C6-N1-C2	-5.05	118.28	120.30
42	l	5	LYS	CD-CE-NZ	-5.05	100.09	111.70
31	A	1971	C	N1-C2-O2	5.05	121.93	118.90
29	Y	98	LEU	CA-CB-CG	5.04	126.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	w	136	ASP	N-CA-CB	-5.04	101.52	110.60
31	A	2724	C	C2-N1-C1'	5.04	124.34	118.80
52	a	1318	C	C6-N1-C2	-5.04	118.29	120.30
31	A	97	A	P-O3'-C3'	5.03	125.74	119.70
31	A	827	C	N1-C2-O2	5.03	121.92	118.90
31	A	2300	U	N1-C2-O2	5.03	126.32	122.80
52	a	983	G	C5-C6-N1	5.03	114.02	111.50
31	A	1789	U	C2-N1-C1'	5.03	123.74	117.70
31	A	2063	C	C2-N1-C1'	5.03	124.33	118.80
52	a	806	U	N1-C2-O2	5.03	126.32	122.80
52	a	1092	G	N3-C2-N2	-5.03	116.38	119.90
31	A	253	C	C5-C6-N1	5.03	123.51	121.00
53	w	149	PRO	N-CA-C	5.03	125.17	112.10
52	a	150	C	C5-C6-N1	5.02	123.51	121.00
52	a	1304	G	N3-C4-N9	5.02	129.01	126.00
31	A	1608	C	N1-C2-O2	5.02	121.91	118.90
52	a	881	C	C5-C6-N1	5.02	123.51	121.00
55	v	99	GLU	CA-CB-CG	-5.02	102.36	113.40
31	A	2527	C	N1-C2-O2	5.02	121.91	118.90
52	a	999	G	N1-C6-O6	5.02	122.91	119.90
27	W	100	C	C6-N1-C2	-5.02	118.29	120.30
55	v	37	GLU	CG-CD-OE1	5.02	128.33	118.30
31	A	2469	C	N3-C2-O2	-5.01	118.39	121.90
31	A	1249	C	C6-N1-C2	-5.01	118.30	120.30
31	A	497	C	N1-C2-O2	5.01	121.91	118.90
31	A	1747	C	N1-C2-O2	5.01	121.91	118.90
43	m	118	ARG	NE-CZ-NH1	5.01	122.81	120.30
52	a	423	A	C2-N3-C4	5.01	113.11	110.60
52	a	1189	G	N1-C6-O6	-5.01	116.89	119.90
31	A	496	C	C6-N1-C2	-5.01	118.30	120.30
31	A	1013	C	C6-N1-C2	-5.01	118.30	120.30
52	a	1029	A	C5-C6-N6	-5.00	119.70	123.70

There are no chirality outliers.

All (62) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	0	73	TRP	Peptide
58	8	273	PRO	Peptide
58	8	277	PHE	Peptide
58	8	298	SER	Peptide
58	8	299	ASP	Peptide

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Mol	Chain	Res	Type	Group
58	8	302	THR	Peptide
58	8	303	VAL	Peptide
58	8	304	LEU	Peptide
58	8	315	LEU	Peptide
58	8	329	LYS	Peptide
58	8	346	PHE	Sidechain
58	8	359	ARG	Peptide
58	8	366	MET	Mainchain
58	8	369	ALA	Peptide
58	8	370	ASP	Peptide
58	8	69	ASN	Peptide
58	8	71	PRO	Peptide
58	8	72	MET	Peptide
17	M	143	LEU	Peptide
21	Q	190	VAL	Peptide
23	S	174	THR	Peptide
33	b	168	VAL	Peptide
33	b	201	ASP	Sidechain
34	c	168	ILE	Peptide
34	c	86	GLU	Peptide
34	c	88	ARG	Peptide
54	d	155	SER	Peptide
54	d	23	ASN	Peptide
35	e	147	LYS	Peptide
36	f	102	PRO	Peptide
37	g	8	GLU	Peptide
39	i	78	ARG	Peptide
39	i	96	ILE	Peptide
40	j	135	LEU	Peptide
42	l	24	LEU	Peptide
42	l	27	CYS	Peptide
42	l	8	ILE	Peptide
43	m	137	LYS	Peptide
43	m	34	LYS	Peptide
50	u	103	PHE	Sidechain
55	v	100	LYS	Peptide
55	v	101	PRO	Peptide
55	v	104	GLY	Peptide
55	v	120	SER	Mainchain
55	v	147	LYS	Peptide
55	v	158	GLY	Peptide
55	v	159	THR	Peptide

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Mol	Chain	Res	Type	Group
55	v	165	PHE	Sidechain
55	v	168	VAL	Peptide
55	v	184	ASN	Peptide
55	v	185	ASN	Peptide
55	v	187	VAL	Peptide
55	v	188	LEU	Peptide
55	v	194	ARG	Sidechain
55	v	33	LEU	Peptide
53	w	108	LYS	Peptide
53	w	110	ILE	Peptide
53	w	126	LEU	Peptide
53	w	130	TYR	Peptide
53	w	148	LYS	Peptide
53	w	176	ASN	Peptide
53	w	98	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	378	0	415	7	0
2	2	415	0	434	7	0
3	3	445	0	501	12	0
4	4	563	0	623	9	0
5	5	304	0	345	7	0
6	6	422	0	508	8	0
7	7	368	0	386	7	0
8	B	2500	0	1263	15	0
9	C	1904	0	1985	42	0
10	D	1620	0	1699	34	0
11	E	1655	0	1725	41	0
12	F	1351	0	1407	29	0
13	G	1353	0	1416	18	0
14	H	423	0	490	8	0
15	K	1568	0	1595	24	0
16	L	942	0	995	17	0
17	M	1342	0	1417	24	0
18	N	1067	0	1122	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	O	944	0	1004	28	0
20	P	947	0	966	29	0
21	Q	953	0	1042	37	0
22	R	996	0	1062	35	0
23	S	1171	0	1216	23	0
24	T	1149	0	1220	22	0
25	U	740	0	795	14	0
26	V	993	0	1055	25	0
27	W	2187	0	1102	18	0
28	X	810	0	847	13	0
29	Y	605	0	652	17	0
30	Z	754	0	808	13	0
31	A	60324	0	30373	516	0
32	0	521	0	498	14	0
33	b	1787	0	1828	0	0
34	c	1719	0	1807	0	0
35	e	1292	0	1355	0	0
36	f	886	0	888	0	0
37	g	1161	0	1237	0	0
38	h	1088	0	1149	0	0
39	i	1020	0	1072	0	0
40	j	796	0	841	0	0
41	k	887	0	933	0	0
42	l	967	0	1046	0	0
43	m	898	0	949	0	0
44	o	525	0	572	0	0
45	p	664	0	703	0	0
46	q	635	0	667	0	0
47	r	518	0	544	0	0
48	s	627	0	653	0	0
49	t	832	0	883	0	0
50	u	393	0	406	0	0
51	y	845	0	892	0	0
52	a	31777	0	16003	0	0
53	w	689	0	706	0	0
54	d	1633	0	1727	0	0
55	v	1464	0	1456	0	0
56	n	819	0	858	0	0
57	x	289	0	301	0	0
58	8	1201	0	1220	46	0
All	All	147126	0	101662	970	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 (970) 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)
31:A:1466:G:C8	31:A:1934:C:OP1	108.10	1.24
21:Q:160:ARG:HH12	31:A:317:G:H1'	136.27	1.14
21:Q:160:ARG:HH22	31:A:317:G:C1'	136.78	1.10
21:Q:160:ARG:NH1	31:A:317:G:H1'	136.21	1.10
17:M:122:GLY:O	31:A:897:A:O2'	108.58	1.07
21:Q:160:ARG:NH2	31:A:317:G:C8	135.55	1.02
31:A:63:A:H61	31:A:89:A:N6	1.59	1.01
31:A:293:G:H21	31:A:365:A:N6	1.62	0.98
31:A:293:G:N2	31:A:365:A:H62	1.61	0.98
31:A:1505:C:H42	31:A:1515:G:H1	1.09	0.98
31:A:2118:U:H3	31:A:2199:G:H1	1.08	0.97
31:A:313:A:H2	31:A:323:G:H1	1.02	0.97
31:A:63:A:H61	31:A:89:A:H61	0.98	0.96
58:8:317:HIS:HA	58:8:324:VAL:HA	1.47	0.94
21:Q:160:ARG:NH2	31:A:317:G:N9	135.96	0.94
31:A:1084:G:H21	31:A:1131:A:N6	1.65	0.93
31:A:1121:G:H21	31:A:1126:A:H62	1.09	0.93
31:A:63:A:N6	31:A:89:A:H61	1.66	0.92
31:A:1084:G:N2	31:A:1131:A:H62	1.67	0.92
12:F:106:ALA:O	12:F:110:LEU:HB3	1.72	0.90
21:Q:160:ARG:NH2	31:A:317:G:C1'	136.71	0.89
20:P:73:LEU:HA	20:P:85:GLN:O	1.73	0.88
31:A:1235:A:H62	31:A:1256:G:H21	1.24	0.86
31:A:1084:G:H21	31:A:1131:A:H62	0.88	0.86
31:A:1196:A:H61	31:A:1201:A:H61	1.25	0.85
13:G:57:ALA:HB3	13:G:64:LYS:O	1.77	0.84
31:A:313:A:C2	31:A:323:G:N1	2.45	0.83
17:M:122:GLY:O	31:A:897:A:C2'	109.34	0.83
58:8:291:GLN:HB3	58:8:327:SER:HA	1.60	0.83
58:8:342:PRO:HA	58:8:345:VAL:HB	1.61	0.83
31:A:313:A:H2	31:A:323:G:N1	1.77	0.82
32:0:49:ALA:HB3	32:0:61:THR:O	1.79	0.82
12:F:105:ALA:O	12:F:109:GLU:HB2	1.80	0.81
31:A:1505:C:N4	31:A:1515:G:H1	1.78	0.80
13:G:101:ALA:O	13:G:105:HIS:HB2	1.82	0.79
31:A:892:C:O2'	31:A:893:C:H5'	1.82	0.79
58:8:63:ALA:O	58:8:66:ARG:C	2.22	0.78
31:A:2764:U:O4	31:A:2774:U:C4	2.38	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:162:GLN:O	13:G:174:SER:HB2	1.85	0.77
18:N:37:LEU:HB2	18:N:41:TRP:CZ2	18.41	0.76
31:A:293:G:H21	31:A:365:A:H62	0.83	0.75
31:A:721:U:H3	31:A:732:A:H61	1.33	0.74
58:8:365:ALA:O	58:8:366:MET:O	2.03	0.74
31:A:1121:G:N2	31:A:1126:A:H62	1.86	0.74
31:A:2107:G:H1	31:A:2210:C:H42	1.34	0.74
21:Q:160:ARG:CZ	31:A:317:G:H1'	136.19	0.73
11:E:251:THR:O	11:E:255:LEU:HB2	1.88	0.73
58:8:354:GLN:OE1	58:8:357:ARG:NH1	2.18	0.73
22:R:81:PHE:O	22:R:85:LEU:HB2	1.86	0.73
31:A:901:C:H2'	31:A:902:G:H5''	1.70	0.73
31:A:722:G:H1	31:A:731:U:H3	1.37	0.73
58:8:64:TYR:HA	58:8:67:CYS:HB2	1.72	0.72
10:D:260:LYS:HD2	31:A:2790:C:H5''	1.72	0.71
31:A:1260:G:C5'	32:0:100:LYS:HD3	177.95	0.71
31:A:1462:G:H1	31:A:1584:C:H42	1.38	0.71
31:A:2112:U:H3	31:A:2205:G:H1	1.39	0.70
31:A:2764:U:O4	31:A:2774:U:C5	2.45	0.70
10:D:127:LYS:O	10:D:135:ASN:HA	1.92	0.69
31:A:1260:G:H5'	32:0:100:LYS:HB3	180.04	0.69
31:A:55:G:H1	31:A:112:C:H42	1.42	0.69
14:H:51:ILE:HA	14:H:85:GLU:O	1.93	0.68
58:8:318:ASP:HB3	58:8:323:ARG:HB2	1.74	0.68
16:L:22:ILE:HB	16:L:40:VAL:O	1.94	0.68
17:M:122:GLY:CA	31:A:897:A:H2'	109.78	0.68
58:8:359:ARG:HG3	58:8:360:ILE:HG13	1.75	0.68
14:H:57:ILE:HG22	14:H:59:ASP:H	1.58	0.68
31:A:2707:A:H62	31:A:2737:G:N2	1.92	0.68
9:C:167:SER:HA	9:C:180:ILE:O	1.93	0.67
58:8:257:GLN:HE22	58:8:283:ILE:HA	1.60	0.67
31:A:2492:C:H42	31:A:2546:G:H22	1.41	0.67
26:V:75:VAL:HA	26:V:135:MET:O	1.95	0.67
31:A:2464:G:H1	31:A:2467:A:H62	1.40	0.67
28:X:121:GLY:HA3	28:X:138:TYR:O	1.94	0.67
31:A:1060:A:H2	31:A:1150:G:H1	1.43	0.66
18:N:65:TRP:HB2	18:N:105:GLU:HB2	1.77	0.66
10:D:98:GLY:H	10:D:286:PRO:HB3	1.59	0.66
31:A:2134:G:H22	31:A:2192:U:H3	1.42	0.66
31:A:2764:U:C4	31:A:2774:U:O4	2.49	0.66
18:N:30:GLY:HA2	18:N:107:SER:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:148:ILE:HG12	21:Q:168:ILE:HG12	1.77	0.66
21:Q:160:ARG:CZ	31:A:317:G:C8	135.49	0.66
10:D:275:VAL:HG21	21:Q:122:ILE:HG21	1.78	0.66
18:N:35:GLN:HE21	18:N:100:GLY:HA2	1.60	0.66
27:W:53:G:H8	27:W:70:G:H21	1.44	0.66
31:A:1385:G:H4'	31:A:1818:U:H3	1.61	0.66
10:D:125:GLN:O	10:D:138:GLN:HB3	1.96	0.65
12:F:91:CYS:O	12:F:139:GLY:HA2	1.96	0.65
17:M:122:GLY:O	31:A:897:A:H2'	109.89	0.65
5:5:14:CYS:HA	5:5:26:ILE:O	1.97	0.65
31:A:2764:U:O4	31:A:2774:U:O4	2.14	0.65
31:A:1196:A:N6	31:A:1201:A:H61	1.93	0.65
21:Q:216:LYS:HG3	21:Q:218:ARG:H	1.61	0.65
31:A:1235:A:H62	31:A:1256:G:N2	1.93	0.65
16:L:2:ILE:HB	16:L:33:ALA:HB3	1.78	0.64
15:K:56:LYS:O	15:K:60:GLU:HB2	1.97	0.64
13:G:91:ARG:HA	13:G:109:ARG:HH22	1.62	0.64
9:C:37:LYS:HE3	9:C:50:ARG:HE	1.61	0.64
12:F:89:VAL:HA	12:F:206:ASP:O	1.97	0.64
23:S:198:PHE:HA	23:S:208:ARG:O	1.97	0.64
19:O:108:ILE:O	19:O:122:TYR:HB3	1.98	0.64
22:R:97:LEU:O	22:R:101:ALA:HB2	1.99	0.63
3:3:146:ARG:HH22	25:U:140:VAL:HG21	1.64	0.63
31:A:1505:C:N3	31:A:1515:G:N2	2.43	0.63
23:S:211:GLY:H	31:A:1245:U:H4'	1.64	0.62
17:M:203:GLU:HB3	31:A:649:A:H5''	1.82	0.62
9:C:29:ILE:HG22	9:C:57:LEU:HD22	1.81	0.62
9:C:146:ARG:NH2	31:A:1811:A:OP2	2.33	0.62
31:A:670:A:H61	31:A:681:A:H61	28.23	0.62
21:Q:123:MET:O	21:Q:127:ASN:HB2	1.99	0.62
31:A:540:A:H62	31:A:2055:U:H3	1.48	0.62
14:H:57:ILE:HB	14:H:61:GLY:H	1.65	0.62
23:S:214:GLN:HE22	31:A:1189:G:H21	1.47	0.62
26:V:76:LYS:O	26:V:134:VAL:HA	1.99	0.62
9:C:139:ASN:O	9:C:186:ALA:HA	2.00	0.62
31:A:1438:G:H2'	31:A:1439:U:C6	2.70	0.62
13:G:104:MET:HA	13:G:107:LEU:HB3	1.81	0.62
24:T:139:ILE:HG12	24:T:160:LEU:HD22	14.75	0.61
18:N:14:ARG:NH1	31:A:984:G:N7	2.48	0.61
22:R:6:ARG:NH2	31:A:29:A:OP2	2.33	0.61
4:4:110:ILE:H	4:4:143:TYR:HE1	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:198:LYS:HG3	13:G:200:LYS:HB3	1.82	0.61
31:A:890:G:O2'	31:A:891:G:H5'	2.00	0.61
31:A:1238:G:H1	31:A:1252:C:H42	1.47	0.61
12:F:155:ARG:O	12:F:159:LEU:HB2	2.01	0.61
31:A:1196:A:H61	31:A:1201:A:N6	1.97	0.61
11:E:97:ARG:NH1	31:A:38:C:O2	2.33	0.61
8:B:58:A:H5'	12:F:77:ASN:HD22	1.65	0.61
15:K:84:MET:HG2	15:K:96:TRP:HE1	1.66	0.61
28:X:123:VAL:HG12	28:X:137:VAL:HG22	1.83	0.61
31:A:2492:C:H42	31:A:2546:G:N2	1.99	0.60
31:A:1121:G:H21	31:A:1126:A:N6	1.92	0.60
21:Q:160:ARG:NH2	31:A:317:G:H1'	136.26	0.60
26:V:152:LEU:HD12	26:V:154:ASP:H	1.67	0.60
31:A:721:U:H3	31:A:732:A:N6	1.99	0.60
31:A:903:G:O2'	31:A:904:U:H5'	2.02	0.60
9:C:137:ILE:HG21	9:C:186:ALA:HB1	1.84	0.60
15:K:123:ILE:HG12	15:K:246:ILE:HG23	1.84	0.60
58:8:304:LEU:HD13	58:8:306:PRO:HD3	1.82	0.60
12:F:92:GLY:HA3	31:A:2323:C:H42	1.67	0.60
31:A:904:U:O5'	31:A:904:U:H6	1.83	0.60
28:X:142:ILE:HG22	28:X:143:GLN:HG3	1.84	0.60
31:A:899:A:H2'	31:A:900:G:C8	2.37	0.60
31:A:1133:U:H2'	31:A:1134:G:H8	1.67	0.59
58:8:268:VAL:HG21	58:8:305:GLN:HB3	1.84	0.59
3:3:127:ARG:NH2	31:A:478:A:OP1	2.35	0.59
19:O:17:ILE:HD12	31:A:2707:A:H4'	1.84	0.59
21:Q:151:ILE:HB	21:Q:165:TYR:HB2	1.84	0.59
31:A:890:G:C2'	31:A:891:G:H5'	2.32	0.59
10:D:200:SER:HA	10:D:259:THR:O	2.02	0.59
19:O:60:LYS:O	19:O:64:LEU:HB2	2.03	0.59
11:E:86:ARG:NH2	31:A:670:A:N3	2.45	0.59
10:D:227:LYS:HB3	31:A:2596:C:H4'	1.84	0.59
22:R:92:LEU:O	23:S:133:GLN:NE2	2.36	0.59
31:A:1443:G:H2'	31:A:1926:A:O2'	105.81	0.59
31:A:313:A:N1	31:A:323:G:O6	2.36	0.59
29:Y:87:ARG:NH1	31:A:2095:U:OP1	2.36	0.59
31:A:525:A:N3	31:A:591:C:O2'	2.35	0.58
31:A:984:G:H2'	31:A:985:A:H2'	1.85	0.58
12:F:116:GLN:HE21	12:F:148:LEU:HD21	1.68	0.58
24:T:47:ARG:HA	24:T:50:ILE:HG22	1.86	0.58
22:R:16:LYS:NZ	31:A:1248:G:N7	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:33:ARG:O	31:A:1273:G:N2	2.36	0.58
31:A:1789:U:OP2	31:A:1794:A:N6	2.36	0.58
31:A:17:C:O2'	31:A:564:U:OP1	2.21	0.58
9:C:142:ILE:HA	9:C:180:ILE:HD11	1.85	0.58
3:3:140:ASN:ND2	31:A:125:A:OP2	2.36	0.58
18:N:39:PRO:HB3	18:N:99:PRO:HD3	1.85	0.58
31:A:1260:G:OP2	32:0:96:LYS:HG3	174.98	0.58
3:3:125:LYS:HE2	31:A:164:A:H5''	1.86	0.58
31:A:2456:A:N6	31:A:2602:U:OP1	2.37	0.58
17:M:138:ARG:NH2	31:A:235:G:O2'	2.37	0.58
17:M:122:GLY:HA3	31:A:897:A:C8	110.93	0.58
11:E:126:ARG:HH21	31:A:1278:U:H5''	1.68	0.58
4:4:150:LEU:HD22	4:4:153:LEU:HG	1.86	0.58
31:A:1296:A:OP2	31:A:1682:C:N4	2.37	0.58
12:F:68:LEU:O	12:F:72:GLU:HB2	2.03	0.58
14:H:43:LYS:HG2	14:H:44:LYS:HG2	1.85	0.58
16:L:23:ARG:NH1	31:A:2579:U:O2'	2.37	0.58
31:A:1291:C:H5''	31:A:1292:G:H5'	1.86	0.57
10:D:240:THR:HG23	31:A:2046:G:H21	1.69	0.57
31:A:1260:G:H5''	32:0:100:LYS:HD3	176.98	0.57
31:A:2707:A:H62	31:A:2737:G:H21	1.51	0.57
19:O:21:SER:N	31:A:698:C:HO2'	46.51	0.57
2:2:34:ILE:HG12	31:A:2303:A:H61	1.68	0.57
21:Q:160:ARG:HH12	31:A:317:G:C1'	136.74	0.57
25:U:162:VAL:HG12	25:U:176:ILE:HG22	1.86	0.57
58:8:316:SER:HB3	58:8:325:SER:HB2	1.86	0.57
26:V:85:LYS:HD3	26:V:104:LEU:HD13	1.87	0.57
4:4:114:ARG:HE	4:4:132:LEU:HD23	1.69	0.57
29:Y:102:ASN:HB3	31:A:2247:C:H1'	1.85	0.57
30:Z:110:LYS:NZ	31:A:75:C:OP1	2.38	0.57
12:F:107:ILE:O	12:F:111:ALA:CB	2.53	0.57
14:H:55:GLU:OE1	14:H:83:LYS:NZ	2.37	0.57
26:V:107:LYS:HB2	26:V:125:ILE:O	2.05	0.57
31:A:1260:G:H5'	32:0:100:LYS:HD3	178.27	0.57
3:3:127:ARG:NH1	3:3:134:ILE:O	2.37	0.57
6:6:106:MET:O	6:6:110:LYS:HB2	2.04	0.57
31:A:1130:C:H2'	31:A:1131:A:H8	1.68	0.57
31:A:2705:G:OP1	31:A:2731:C:N4	2.38	0.57
31:A:318:A:N3	31:A:338:G:O2'	2.36	0.57
9:C:206:SER:HA	9:C:209:TRP:HD1	1.69	0.57
21:Q:143:ILE:HD11	21:Q:206:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:52:G:N2	27:W:71:C:O2'	2.37	0.57
31:A:1103:C:C4	31:A:1104:C:N4	2.73	0.57
6:6:123:ARG:NH2	31:A:1405:A:OP2	2.37	0.57
22:R:11:ARG:O	22:R:15:LYS:HB2	2.05	0.57
11:E:99:THR:OG1	31:A:454:G:N3	2.38	0.56
20:P:152:VAL:HA	20:P:155:LEU:HB3	1.85	0.56
21:Q:124:GLY:O	21:Q:128:LYS:HB2	2.05	0.56
23:S:197:VAL:HG23	23:S:210:ILE:HG13	1.85	0.56
31:A:1111:G:N2	31:A:1114:A:OP2	2.38	0.56
11:E:204:LYS:HA	11:E:225:THR:HB	1.87	0.56
20:P:64:VAL:HG11	20:P:142:ASP:HB3	1.87	0.56
58:8:262:SER:OG	58:8:281:GLY:O	2.22	0.56
11:E:253:GLN:O	11:E:257:GLN:HB2	2.05	0.56
31:A:1020:C:H2'	31:A:1021:A:H8	1.70	0.56
31:A:1573:C:H2'	31:A:1574:G:H8	1.71	0.56
11:E:222:ASN:ND2	31:A:329:C:O2'	2.36	0.56
19:O:27:ARG:NH1	31:A:2707:A:OP2	2.38	0.56
58:8:366:MET:SD	58:8:366:MET:N	2.78	0.56
10:D:235:ILE:O	10:D:248:LYS:NZ	2.37	0.56
12:F:89:VAL:HG22	12:F:207:VAL:HG22	1.88	0.56
58:8:320:GLU:OE1	58:8:323:ARG:NH2	2.35	0.56
31:A:2599:G:OP2	31:A:2600:G:N2	2.38	0.56
31:A:2707:A:N6	31:A:2737:G:H21	2.03	0.56
10:D:275:VAL:HG11	21:Q:126:LEU:HD11	1.86	0.56
16:L:97:ARG:HH12	31:A:309:A:H5''	159.24	0.56
22:R:49:ASP:OD1	22:R:52:ARG:NH1	2.38	0.56
11:E:79:LYS:NZ	31:A:609:G:OP1	2.39	0.55
23:S:204:LYS:HG2	31:A:1001:A:H5'	1.88	0.55
12:F:208:CYS:SG	31:A:2320:G:N2	2.80	0.55
1:1:34:LEU:HD23	24:T:67:LEU:HD21	1.88	0.55
31:A:1486:U:H2'	31:A:1487:C:C6	3.26	0.55
11:E:105:ARG:NH2	31:A:685:G:OP1	2.38	0.55
19:O:51:ALA:HA	19:O:123:ILE:HD11	1.89	0.55
31:A:1096:G:N2	31:A:1123:A:O2'	2.39	0.55
10:D:210:GLY:HA2	10:D:251:PRO:HB3	1.88	0.55
23:S:128:VAL:HG22	23:S:133:GLN:HG2	1.89	0.55
31:A:1041:G:H1	31:A:1176:C:H42	1.55	0.55
6:6:123:ARG:HH22	31:A:1404:C:H3'	1.72	0.55
31:A:423:G:OP2	31:A:2423:A:O2'	2.24	0.55
16:L:61:VAL:O	16:L:84:ALA:HA	2.06	0.55
23:S:146:ARG:NH1	31:A:1189:G:OP1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1343:A:N1	31:A:1354:C:O2'	2.38	0.55
31:A:641:C:O2	31:A:651:U:O2'	2.25	0.55
31:A:962:G:N7	31:A:966:G:N1	15.27	0.55
11:E:168:ALA:HB1	11:E:245:LEU:HD11	1.89	0.55
26:V:76:LYS:HB2	26:V:137:ILE:HD11	1.89	0.55
28:X:123:VAL:HA	28:X:136:SER:O	2.06	0.55
19:O:37:GLN:HE22	31:A:1298:A:H2	1.55	0.55
31:A:1801:A:N6	31:A:1838:G:O2'	2.36	0.55
31:A:1393:U:O2'	31:A:2230:A:N3	2.37	0.55
31:A:542:C:OP1	31:A:571:G:N1	2.39	0.55
22:R:25:ARG:HH22	31:A:2035:A:H5'	1.71	0.55
22:R:3:ARG:N	31:A:1269:G:N7	2.55	0.55
31:A:1466:G:N9	31:A:1934:C:OP1	108.94	0.55
20:P:100:THR:O	20:P:104:ALA:HB2	2.06	0.55
29:Y:107:ARG:HG2	29:Y:116:PHE:HB3	1.89	0.55
3:3:127:ARG:HE	3:3:132:ARG:HG3	1.72	0.55
31:A:1155:A:N7	31:A:2505:A:O2'	2.39	0.55
31:A:2300:U:O2	31:A:2342:G:O6	2.24	0.55
16:L:6:THR:OG1	16:L:21:CYS:SG	2.65	0.55
31:A:709:C:O2'	31:A:745:A:N6	2.38	0.54
31:A:902:G:H2'	31:A:903:G:H5'	1.88	0.54
31:A:1793:A:H1'	31:A:2624:G:H21	1.72	0.54
31:A:2612:G:N2	31:A:2615:A:OP2	2.36	0.54
17:M:122:GLY:C	31:A:897:A:H2'	109.52	0.54
16:L:34:ARG:NH1	31:A:2690:G:OP1	2.41	0.54
23:S:214:GLN:HE21	31:A:1021:A:H1'	1.72	0.54
16:L:31:ARG:HH11	31:A:2009:U:H1'	1.70	0.54
31:A:2464:G:N2	31:A:2467:A:N7	2.53	0.54
21:Q:174:ASN:HA	21:Q:179:THR:HA	1.89	0.54
26:V:105:ASN:OD1	26:V:107:LYS:NZ	2.39	0.54
28:X:70:ARG:NH1	31:A:2274:A:O2'	2.41	0.54
5:5:6:SER:HB3	31:A:2483:C:H5"	1.89	0.54
31:A:833:U:H4'	31:A:834:G:H5"	5.59	0.54
9:C:256:ARG:HE	9:C:260:LYS:HD3	1.72	0.54
23:S:139:GLY:H	23:S:221:ILE:HB	1.72	0.54
58:8:280:ILE:HG23	58:8:283:ILE:HG12	1.90	0.54
7:7:74:ARG:NH1	31:A:1177:U:O4	2.40	0.54
18:N:124:LYS:NZ	31:A:2500:C:N3	2.48	0.54
20:P:61:ARG:NH2	20:P:89:ASP:OD1	2.41	0.54
15:K:219:ASN:O	15:K:222:LYS:NZ	2.41	0.54
16:L:24:ILE:HG22	16:L:39:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1260:G:H5'	32:O:100:LYS:CB	180.70	0.54
16:L:24:ILE:HG21	16:L:33:ALA:HB2	1.89	0.53
20:P:75:VAL:HA	20:P:83:TYR:O	2.08	0.53
11:E:207:PHE:HB2	11:E:246:VAL:HG22	1.91	0.53
15:K:58:THR:O	15:K:62:ARG:HB2	2.07	0.53
19:O:19:ARG:NH1	31:A:1689:C:O2'	2.41	0.53
24:T:57:SER:HA	24:T:99:ILE:HA	1.90	0.53
26:V:114:LYS:HD3	26:V:118:GLU:HB2	1.89	0.53
31:A:579:U:O2'	31:A:1011:A:N1	2.40	0.53
22:R:77:ASN:ND2	31:A:1040:U:OP1	2.41	0.53
31:A:1379:C:N4	31:A:1393:U:OP2	2.41	0.53
31:A:2300:U:O2	31:A:2342:G:C6	2.61	0.53
10:D:142:GLU:OE1	10:D:166:ARG:NH2	2.38	0.53
31:A:992:U:O2'	31:A:2290:A:N3	2.37	0.53
18:N:46:GLN:NE2	31:A:2502:G:OP1	2.41	0.53
31:A:259:C:H42	31:A:268:G:H1	1.56	0.53
12:F:87:ILE:HA	12:F:208:CYS:O	2.08	0.53
8:B:10:G:O5'	20:P:61:ARG:NH1	2.41	0.53
19:O:73:ARG:HH21	31:A:1475:U:H4'	1.73	0.53
31:A:309:A:N3	31:A:328:C:O2'	2.40	0.53
14:H:47:LYS:NZ	31:A:412:G:OP2	2.37	0.53
26:V:89:ILE:HG22	26:V:101:ILE:HG22	1.91	0.53
3:3:133:LYS:HE3	31:A:471:U:H5''	1.91	0.53
31:A:1234:A:H2'	31:A:1235:A:H4'	4.06	0.53
9:C:152:ARG:HG2	31:A:1828:U:H2'	1.91	0.53
2:2:24:ASN:HB2	2:2:27:SER:HB3	1.91	0.53
31:A:1533:A:N3	31:A:1611:G:O2'	2.42	0.53
9:C:181:SER:OG	9:C:184:CYS:SG	2.67	0.53
12:F:87:ILE:HG22	12:F:209:ILE:HA	1.90	0.53
19:O:44:ILE:HG22	19:O:123:ILE:HB	1.91	0.53
21:Q:122:ILE:HA	21:Q:125:ILE:HG22	1.91	0.53
22:R:10:ALA:O	22:R:14:ARG:HB2	2.09	0.53
23:S:148:LYS:HB2	31:A:1189:G:H5'	1.89	0.53
31:A:763:A:OP2	31:A:1791:C:N4	2.42	0.53
1:1:16:ARG:NH2	31:A:2633:C:OP1	2.42	0.53
31:A:724:G:H21	31:A:729:A:H62	1.56	0.53
24:T:90:ASN:ND2	31:A:506:G:O2'	2.42	0.53
9:C:103:PRO:HA	9:C:191:VAL:HA	1.90	0.53
11:E:69:PHE:O	11:E:256:ASN:ND2	2.39	0.53
16:L:104:ARG:NH1	16:L:121:LEU:O	2.42	0.53
29:Y:115:ARG:HH12	29:Y:145:LEU:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1836:C:O2'	31:A:1985:A:OP2	2.27	0.52
13:G:63:LEU:HB2	13:G:76:TYR:HE1	1.73	0.52
31:A:1117:G:N2	31:A:1118:U:O4	2.42	0.52
31:A:845:C:H2'	31:A:846:A:H8	1.74	0.52
31:A:88:A:H3'	31:A:89:A:H2'	1.91	0.52
28:X:97:ARG:HH22	31:A:2279:U:H5''	1.72	0.52
31:A:1615:G:H2'	31:A:1616:A:H8	1.73	0.52
9:C:141:GLU:HB2	9:C:184:CYS:HB3	1.92	0.52
6:6:140:LYS:HE2	31:A:1461:G:H5'	1.90	0.52
31:A:656:A:H61	31:A:2366:G:H21	1.55	0.52
10:D:99:MET:HG2	10:D:113:THR:HG22	1.92	0.52
21:Q:170:ILE:HG23	21:Q:219:LEU:HB2	1.92	0.52
25:U:144:LYS:NZ	25:U:162:VAL:O	2.43	0.52
2:2:35:THR:O	31:A:2303:A:N6	2.41	0.52
31:A:2133:A:N6	31:A:2181:U:O2'	2.40	0.52
31:A:2761:U:OP2	31:A:2773:C:N4	2.38	0.52
31:A:890:G:H2'	31:A:891:G:H8	1.75	0.52
10:D:204:ILE:HG23	10:D:284:GLY:HA2	1.91	0.52
11:E:120:LYS:HA	31:A:2073:A:H4'	1.92	0.52
15:K:99:THR:HA	22:R:99:GLN:HE22	1.73	0.52
24:T:57:SER:OG	24:T:60:GLU:OE1	2.25	0.52
32:0:71:GLU:HG3	32:0:72:VAL:HG13	1.92	0.52
2:2:15:CYS:O	2:2:31:SER:HA	2.10	0.52
31:A:182:A:N6	31:A:2447:A:O2'	2.43	0.52
31:A:902:G:C2'	31:A:903:G:H5'	2.40	0.52
15:K:58:THR:O	15:K:62:ARG:CB	2.58	0.52
18:N:37:LEU:HB2	18:N:41:TRP:HZ2	18.72	0.52
18:N:71:ASP:OD2	31:A:916:G:N2	2.42	0.52
31:A:1886:A:H2'	31:A:1887:G:H8	1.75	0.52
31:A:901:C:C2'	31:A:902:G:H5''	2.39	0.52
16:L:22:ILE:O	16:L:40:VAL:HB	2.09	0.52
24:T:79:LEU:HD22	24:T:134:ILE:HD12	1.92	0.52
21:Q:144:ARG:HH12	27:W:53:G:H22	1.57	0.52
6:6:115:ARG:HH12	31:A:1490:G:H5''	1.74	0.52
58:8:363:ALA:O	58:8:364:GLU:HB3	2.09	0.52
31:A:1876:A:H62	31:A:1889:G:H21	1.57	0.52
9:C:178:ARG:NH1	31:A:1810:C:OP2	2.43	0.52
1:1:47:PHE:HZ	19:O:45:LYS:HE2	1.75	0.52
25:U:112:TYR:HB2	30:Z:84:LYS:HE2	1.91	0.52
58:8:285:GLY:HA2	58:8:324:VAL:O	2.09	0.52
31:A:2495:A:O2'	31:A:2553:G:N2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:208:A:O2'	31:A:432:G:N3	2.42	0.52
15:K:172:LEU:HB2	15:K:174:ARG:HH11	1.75	0.52
20:P:72:ARG:NH1	20:P:142:ASP:OD2	2.41	0.52
8:B:38:C:O2	20:P:149:HIS:NE2	2.42	0.52
31:A:622:G:H2'	31:A:623:A:H8	5.69	0.52
24:T:99:ILE:HD11	24:T:137:ARG:HD3	1.92	0.52
26:V:76:LYS:HE2	26:V:137:ILE:HD11	1.93	0.52
30:Z:135:LYS:O	30:Z:139:ALA:HB2	2.10	0.52
7:7:48:SER:OG	7:7:49:SER:N	2.43	0.51
31:A:1443:G:C2'	31:A:1926:A:O2'	105.98	0.51
31:A:1462:G:H1	31:A:1584:C:N4	2.05	0.51
31:A:2107:G:H1	31:A:2210:C:N4	2.04	0.51
31:A:232:G:OP2	31:A:234:C:N4	2.43	0.51
22:R:40:ILE:HG23	23:S:198:PHE:HE2	1.74	0.51
25:U:167:ARG:NH1	25:U:171:THR:OG1	2.42	0.51
27:W:61:G:N2	27:W:64:A:OP2	2.44	0.51
12:F:180:ASN:HB3	31:A:2332:G:H4'	1.92	0.51
9:C:64:ARG:NH2	9:C:145:GLY:O	2.43	0.51
11:E:78:GLU:O	17:M:88:GLN:NE2	2.43	0.51
31:A:1949:G:N2	31:A:1976:C:O2'	2.43	0.51
10:D:199:ILE:O	10:D:260:LYS:HA	2.11	0.51
20:P:87:ILE:HG22	20:P:94:THR:HG22	1.91	0.51
24:T:121:ARG:O	31:A:1650:A:N6	2.44	0.51
26:V:109:LYS:HD3	26:V:125:ILE:HD12	1.91	0.51
27:W:30:A:O2'	27:W:38:G:O2'	2.28	0.51
31:A:1391:C:O2'	31:A:1821:G:O2'	2.28	0.51
31:A:545:U:H2'	31:A:546:G:H8	1.76	0.51
21:Q:138:ARG:HH12	21:Q:201:PRO:HA	1.75	0.51
31:A:704:A:O2'	31:A:1374:A:N3	2.41	0.51
31:A:2492:C:N4	31:A:2546:G:H22	2.06	0.51
8:B:81:U:O2'	31:A:927:A:N3	2.42	0.51
19:O:43:ARG:HA	19:O:123:ILE:O	2.10	0.51
19:O:77:LEU:HD11	19:O:83:LYS:HD2	1.91	0.51
20:P:128:ALA:HB2	20:P:159:ALA:HA	1.93	0.51
58:8:342:PRO:O	58:8:346:PHE:N	2.40	0.51
2:2:45:ARG:NH2	31:A:2361:U:OP1	2.44	0.51
31:A:817:C:O2	31:A:2461:A:O2'	2.28	0.51
26:V:167:ILE:HG22	26:V:169:ASP:H	1.75	0.51
31:A:290:A:H2'	31:A:291:G:H8	1.76	0.51
9:C:56:ARG:HG3	9:C:81:PRO:HB2	1.92	0.51
26:V:138:LEU:HG	26:V:140:GLU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:8:257:GLN:NE2	58:8:283:ILE:HA	2.25	0.51
31:A:1332:G:OP2	31:A:1332:G:N2	2.44	0.51
8:B:9:U:OP1	20:P:53:ARG:NH2	2.39	0.51
17:M:122:GLY:C	31:A:897:A:C2'	108.97	0.51
1:1:45:SER:HA	19:O:108:ILE:HG23	1.93	0.51
58:8:317:HIS:HB3	58:8:324:VAL:HG12	1.93	0.51
31:A:1457:G:O2'	31:A:1496:A:N1	2.43	0.51
12:F:116:GLN:OE1	32:O:42:HIS:ND1	2.43	0.51
12:F:70:LYS:HD2	12:F:75:TYR:HB2	1.91	0.51
31:A:1874:U:OP1	31:A:2427:G:O2'	2.28	0.50
13:G:119:VAL:HG12	13:G:176:ARG:HD2	1.93	0.50
15:K:169:THR:HG23	15:K:170:GLN:HG2	1.93	0.50
19:O:101:ASN:O	27:W:43:G:N2	2.43	0.50
58:8:291:GLN:CD	58:8:327:SER:HB2	2.31	0.50
6:6:127:LYS:NZ	31:A:1402:G:OP2	2.45	0.50
31:A:804:A:OP2	31:A:2085:A:O2'	2.29	0.50
25:U:127:ASN:ND2	25:U:131:GLU:OE1	2.43	0.50
26:V:52:GLU:HG3	26:V:53:ARG:HG3	1.92	0.50
22:R:52:ARG:O	22:R:56:ASP:HB2	2.11	0.50
15:K:56:LYS:O	24:T:147:LYS:NZ	2.45	0.50
26:V:67:ARG:HH12	26:V:92:ILE:HD11	1.77	0.50
31:A:892:C:O5'	31:A:892:C:H6	1.95	0.50
18:N:41:TRP:N	18:N:41:TRP:CD1	3.26	0.50
30:Z:65:LEU:HB3	30:Z:68:LEU:HD13	1.93	0.50
27:W:19:A:N3	31:A:2020:C:O2'	2.45	0.50
9:C:140:ILE:HD11	9:C:150:LEU:HD12	1.93	0.50
13:G:55:ALA:HB3	13:G:66:LYS:HB2	1.93	0.50
18:N:115:ARG:O	18:N:119:ALA:HB3	2.12	0.50
6:6:113:ARG:NH1	31:A:1548:A:OP1	2.45	0.50
11:E:250:GLY:O	11:E:254:TYR:CB	2.60	0.50
17:M:143:LEU:O	17:M:147:ALA:N	2.44	0.50
19:O:106:ARG:HE	19:O:124:GLU:HG3	1.76	0.50
20:P:103:LYS:HE3	20:P:122:LYS:HB3	1.93	0.50
21:Q:147:ASP:OD1	21:Q:211:HIS:ND1	2.40	0.50
30:Z:129:GLY:H	30:Z:132:LEU:HD12	1.76	0.50
58:8:365:ALA:C	58:8:366:MET:O	2.50	0.50
31:A:1454:G:H2'	31:A:1455:A:H8	1.76	0.50
4:4:118:GLN:NE2	31:A:2436:U:O4	2.45	0.50
22:R:11:ARG:NH2	31:A:524:A:O2'	2.45	0.50
9:C:51:GLY:HA3	31:A:702:C:H5"	1.94	0.50
19:O:43:ARG:NE	19:O:124:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:111:LEU:HB2	24:T:127:ARG:HB3	1.93	0.50
26:V:75:VAL:HB	26:V:134:VAL:HB	1.93	0.50
9:C:194:VAL:HG13	31:A:1830:U:H3	1.77	0.49
10:D:237:ALA:HB3	10:D:241:PRO:HG3	1.93	0.49
19:O:21:SER:N	31:A:699:U:O4'	49.59	0.49
9:C:27:ASN:ND2	31:A:1445:G:OP2	2.45	0.49
31:A:376:U:O2'	31:A:378:A:N1	2.38	0.49
31:A:894:G:C5	31:A:895:C:N4	2.80	0.49
3:3:142:SER:O	31:A:1636:U:O2'	2.28	0.49
31:A:1052:G:H5''	31:A:1053:A:H5''	1.93	0.49
10:D:200:SER:HB2	10:D:291:ARG:HB2	1.94	0.49
12:F:150:TYR:O	12:F:154:ASP:HB2	2.13	0.49
17:M:135:PRO:HD2	17:M:138:ARG:HD2	1.95	0.49
27:W:54:A:OP2	27:W:70:G:N2	2.35	0.49
20:P:70:ARG:HH12	31:A:2395:A:H5''	1.78	0.49
3:3:96:THR:O	31:A:697:U:O2'	2.30	0.49
11:E:249:GLU:HA	11:E:252:ILE:HG22	1.95	0.49
11:E:60:PHE:O	11:E:196:ARG:NH1	2.45	0.49
58:8:63:ALA:HA	58:8:66:ARG:HB2	1.94	0.49
15:K:194:ARG:NH1	31:A:2657:G:OP2	2.41	0.49
5:5:20:ARG:NH1	31:A:2758:A:OP1	2.46	0.49
31:A:864:U:H2'	31:A:865:A:H8	1.77	0.49
15:K:155:VAL:HB	15:K:223:VAL:HG22	1.94	0.49
4:4:149:ALA:HB2	17:M:127:ARG:HG3	1.94	0.49
19:O:101:ASN:OD1	27:W:44:U:O2'	2.30	0.49
23:S:124:PHE:HE1	23:S:135:ILE:HG23	1.77	0.49
29:Y:87:ARG:HD2	29:Y:97:ARG:HD3	1.93	0.49
31:A:2422:G:O2'	31:A:2428:A:N6	2.44	0.49
15:K:85:PHE:HB3	15:K:96:TRP:HZ2	1.78	0.49
18:N:101:ARG:NH1	31:A:916:G:O2'	2.39	0.49
11:E:250:GLY:O	11:E:254:TYR:HB2	2.13	0.49
31:A:2108:G:H1	31:A:2209:U:H3	1.59	0.49
31:A:2308:U:O2'	31:A:2391:C:O2	2.30	0.49
31:A:883:C:H2'	31:A:884:G:H8	1.77	0.49
31:A:894:G:C6	31:A:895:C:N4	2.81	0.49
25:U:106:ARG:NH2	25:U:143:ASP:OD1	2.43	0.49
58:8:315:LEU:O	58:8:317:HIS:N	2.45	0.49
31:A:699:U:H2'	31:A:700:A:H8	1.78	0.49
12:F:118:PRO:HB2	12:F:140:ILE:HG22	1.94	0.49
22:R:114:GLU:HG3	23:S:172:ILE:HD13	1.94	0.49
22:R:17:ILE:HG22	22:R:35:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:79:LEU:O	24:T:83:ALA:HB2	2.13	0.49
31:A:693:G:O6	31:A:805:A:N6	2.46	0.48
10:D:117:PHE:O	10:D:274:ARG:NH2	2.46	0.48
19:O:26:GLN:NE2	31:A:1296:A:O4'	2.46	0.48
31:A:1935:G:H2'	31:A:1936:G:C8	2.48	0.48
20:P:125:GLU:OE2	20:P:162:HIS:NE2	2.42	0.48
11:E:150:ILE:HG23	31:A:671:C:H5''	1.95	0.48
31:A:68:C:H2'	31:A:69:G:H8	2.84	0.48
15:K:176:HIS:NE2	15:K:179:ARG:O	2.45	0.48
22:R:78:TYR:CZ	22:R:82:ILE:HD11	2.49	0.48
31:A:1103:C:N4	31:A:1104:C:N4	2.61	0.48
31:A:133:A:O2'	31:A:134:A:N7	2.45	0.48
9:C:174:SER:OG	31:A:1809:G:O6	2.30	0.48
31:A:309:A:N1	31:A:331:A:O2'	2.37	0.48
31:A:596:A:H62	31:A:1272:A:H2	1.61	0.48
10:D:219:ARG:HH12	31:A:2006:G:H21	1.61	0.48
11:E:208:PHE:HB3	11:E:229:LEU:HB2	1.96	0.48
19:O:31:LEU:HD23	19:O:54:MET:HE1	1.95	0.48
2:2:18:CYS:O	2:2:49:ARG:NH2	2.47	0.48
58:8:288:HIS:O	58:8:292:ILE:HG13	2.12	0.48
18:N:128:ARG:NH1	31:A:1057:A:OP1	2.40	0.48
31:A:1401:G:H21	31:A:1604:A:H2	1.61	0.48
21:Q:215:ARG:HD3	31:A:1763:G:H5''	1.95	0.48
31:A:2118:U:N3	31:A:2199:G:N1	2.51	0.48
31:A:68:C:H2'	31:A:69:G:C8	3.22	0.48
31:A:895:C:H6	31:A:895:C:H3'	1.79	0.48
9:C:46:THR:OG1	31:A:1815:U:O2	2.31	0.48
15:K:84:MET:HB2	15:K:84:MET:HE2	1.58	0.48
18:N:51:ARG:HG3	18:N:64:ILE:HD11	1.94	0.48
23:S:165:GLY:HA2	23:S:170:THR:HA	1.96	0.48
26:V:74:THR:OG1	26:V:137:ILE:O	2.31	0.48
30:Z:86:GLU:HA	30:Z:89:MET:HE2	1.94	0.48
1:1:21:LYS:HG2	24:T:48:ARG:HB3	1.96	0.48
31:A:1757:G:H2'	31:A:1758:G:C8	2.48	0.48
18:N:115:ARG:O	18:N:119:ALA:CB	2.62	0.48
22:R:52:ARG:HG2	22:R:55:ARG:HE	1.79	0.48
21:Q:138:ARG:NH1	21:Q:200:SER:O	2.47	0.48
24:T:50:ILE:HD13	24:T:76:ILE:HD12	1.94	0.48
1:1:13:LYS:HD3	31:A:1284:U:H5''	1.95	0.48
11:E:125:ARG:HE	31:A:685:G:H1'	1.78	0.48
11:E:81:ARG:O	11:E:85:HIS:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1367:A:H2	31:A:1962:G:N3	84.64	0.48
15:K:161:VAL:HG21	15:K:200:ILE:HD11	1.95	0.48
31:A:2114:G:H1	31:A:2203:U:H3	1.61	0.48
31:A:615:G:H21	31:A:669:C:H5'	1.79	0.48
31:A:932:A:H2'	31:A:933:G:H8	1.79	0.48
31:A:976:C:H2'	31:A:977:G:H8	1.78	0.48
9:C:71:TYR:HA	9:C:113:VAL:HB	1.95	0.48
8:B:45:G:H3'	12:F:145:ARG:HH12	1.79	0.48
31:A:2692:A:H61	31:A:2750:G:H1	1.61	0.47
9:C:254:ARG:NH2	31:A:1854:C:O3'	2.47	0.47
21:Q:116:ARG:HH22	27:W:35:U:H5''	1.79	0.47
23:S:145:GLN:HE21	31:A:1189:G:H1'	1.78	0.47
31:A:827:C:OP1	31:A:1206:C:O2'	2.29	0.47
31:A:903:G:C2'	31:A:904:U:H5'	2.44	0.47
11:E:89:ILE:O	11:E:93:GLN:HB2	2.14	0.47
15:K:123:ILE:HD11	15:K:126:ARG:HD2	1.97	0.47
15:K:131:ILE:HG23	15:K:153:VAL:HG21	1.96	0.47
21:Q:124:GLY:O	21:Q:128:LYS:CB	2.62	0.47
29:Y:87:ARG:HB3	29:Y:97:ARG:HE	1.79	0.47
31:A:2118:U:O2	31:A:2199:G:N2	2.37	0.47
31:A:1466:G:N7	31:A:1934:C:OP1	107.69	0.47
31:A:182:A:H2	31:A:2451:A:H62	1.61	0.47
31:A:898:G:H3'	31:A:899:A:H5'	1.96	0.47
22:R:90:LEU:HD23	22:R:93:ASN:HD21	1.79	0.47
17:M:111:GLY:HA2	31:A:1211:G:H5''	1.96	0.47
31:A:1513:C:H2'	31:A:1514:A:H8	1.79	0.47
31:A:2563:U:H5''	31:A:2564:U:H5'	1.96	0.47
10:D:204:ILE:HG21	10:D:285:LYS:HG2	1.96	0.47
15:K:57:CYS:O	15:K:61:TRP:HB2	2.14	0.47
11:E:242:ALA:HB3	17:M:81:ARG:HD3	1.97	0.47
29:Y:120:ARG:NH1	31:A:1385:G:OP2	2.48	0.47
58:8:63:ALA:O	58:8:66:ARG:O	2.33	0.47
31:A:1466:G:O6	31:A:1485:U:O2	2.33	0.47
20:P:160:ARG:NH1	31:A:2393:A:O2'	2.31	0.47
10:D:239:THR:OG1	31:A:2589:A:N7	2.35	0.47
58:8:61:GLU:O	58:8:65:GLU:HG3	2.15	0.47
10:D:239:THR:N	31:A:2589:A:OP2	2.45	0.47
31:A:8:G:O2'	31:A:2646:U:O4	2.28	0.47
31:A:2013:A:O3'	31:A:2740:G:N2	2.47	0.47
17:M:131:GLY:O	31:A:842:G:N2	2.47	0.47
15:K:175:ARG:HH21	15:K:184:LYS:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:77:VAL:HG11	26:V:82:GLU:HG2	1.96	0.47
31:A:1260:G:C5'	32:O:100:LYS:CD	178.60	0.47
25:U:106:ARG:NH1	31:A:128:U:OP2	2.48	0.47
31:A:1859:G:H2'	31:A:1860:G:H8	1.80	0.47
29:Y:118:LYS:NZ	31:A:2234:G:OP1	2.38	0.47
31:A:599:C:H2'	31:A:600:A:H8	1.79	0.47
31:A:2345:A:H2'	31:A:2346:A:C8	2.50	0.47
31:A:2594:A:H5'	31:A:2595:G:H5'	1.97	0.47
30:Z:107:ARG:HA	30:Z:110:LYS:HB3	1.97	0.47
9:C:255:SER:OG	31:A:1813:A:O2'	2.32	0.47
12:F:107:ILE:O	12:F:111:ALA:HB3	2.14	0.47
29:Y:74:ILE:HG22	29:Y:81:LYS:HG2	1.97	0.47
31:A:1407:C:H2'	31:A:1408:A:H8	1.80	0.47
31:A:737:G:O5'	31:A:1453:G:O2'	2.31	0.47
22:R:97:LEU:HA	22:R:100:ILE:HG12	1.96	0.47
58:8:257:GLN:NE2	58:8:282:GLY:O	2.48	0.47
31:A:1235:A:N6	31:A:1256:G:H21	2.01	0.47
31:A:1487:C:H42	31:A:1557:G:N2	2.13	0.47
31:A:2490:U:OP1	31:A:2546:G:N2	2.44	0.47
9:C:208:ARG:HD3	9:C:214:PRO:HD3	1.97	0.47
10:D:125:GLN:O	10:D:138:GLN:CB	2.63	0.47
23:S:194:LYS:HG2	23:S:213:ARG:HD3	1.97	0.47
30:Z:135:LYS:O	30:Z:139:ALA:CB	2.63	0.47
31:A:744:G:N2	31:A:745:A:N7	2.63	0.46
9:C:104:ARG:HB3	9:C:190:GLN:HG3	1.95	0.46
3:3:146:ARG:HH12	25:U:140:VAL:HG11	1.80	0.46
28:X:152:ALA:O	28:X:156:GLU:HB2	2.16	0.46
29:Y:108:VAL:HG21	29:Y:129:ILE:HD13	1.97	0.46
31:A:1725:A:H2'	31:A:1726:A:H8	1.80	0.46
16:L:38:VAL:HG12	16:L:61:VAL:HG22	1.97	0.46
20:P:138:LYS:HA	20:P:165:VAL:HB	1.98	0.46
5:5:16:LEU:HD21	31:A:1060:A:H4'	1.97	0.46
31:A:1260:G:H5'	32:O:100:LYS:CD	178.92	0.46
31:A:670:A:N6	31:A:681:A:H61	27.82	0.46
9:C:34:ARG:NH2	9:C:40:ASN:O	2.49	0.46
13:G:128:GLN:HA	13:G:170:LYS:HA	1.98	0.46
21:Q:217:ALA:HB2	27:W:52:G:C8	2.50	0.46
24:T:138:ASP:OD1	24:T:139:ILE:N	2.49	0.46
10:D:223:THR:HG21	31:A:1712:A:H1'	1.97	0.46
31:A:1871:U:H2'	31:A:1872:G:H8	1.81	0.46
31:A:1844:U:O4	31:A:1914:A:N6	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:890:G:H2'	31:A:891:G:H5'	1.98	0.46
17:M:215:ARG:HG3	17:M:216:ALA:H	1.81	0.46
22:R:10:ALA:O	22:R:14:ARG:CB	2.63	0.46
6:6:123:ARG:NH1	31:A:1404:C:OP2	2.49	0.46
31:A:652:C:N4	31:A:657:U:O4	2.49	0.46
22:R:82:ILE:HA	22:R:85:LEU:HB3	1.97	0.46
31:A:1640:C:O2'	31:A:1646:A:N1	2.38	0.46
9:C:269:ARG:HH22	31:A:1808:C:H5	1.63	0.46
31:A:2116:C:N3	31:A:2201:G:O6	2.49	0.46
31:A:2296:G:HO2'	31:A:2344:A:HO2'	1.62	0.46
26:V:67:ARG:HD3	26:V:97:SER:HA	1.98	0.46
58:8:343:LYS:HA	58:8:346:PHE:CE2	2.50	0.46
31:A:471:U:H2'	31:A:472:A:H8	1.81	0.46
17:M:115:ARG:NH1	31:A:578:U:OP1	2.49	0.46
31:A:1271:G:O2'	31:A:1310:C:O2'	66.29	0.46
18:N:39:PRO:HD3	18:N:99:PRO:HG3	1.98	0.46
22:R:52:ARG:HD2	22:R:55:ARG:HH11	1.81	0.46
31:A:2270:G:H5''	31:A:2271:C:H5	1.80	0.46
31:A:670:A:H61	31:A:681:A:N6	28.25	0.46
58:8:318:ASP:OD2	58:8:323:ARG:NH2	2.45	0.45
31:A:1081:C:N3	31:A:1087:G:O6	25.80	0.45
31:A:902:G:O2'	31:A:903:G:H5'	2.16	0.45
9:C:37:LYS:HD3	9:C:56:ARG:HH22	1.81	0.45
22:R:81:PHE:O	22:R:85:LEU:CB	2.60	0.45
31:A:2085:A:H2'	31:A:2086:G:H8	1.80	0.45
31:A:2417:G:H1	31:A:2433:C:H42	1.63	0.45
18:N:56:ARG:NE	31:A:2486:A:O2'	2.49	0.45
31:A:376:U:OP1	31:A:377:G:O2'	11.61	0.45
22:R:33:ARG:NH2	31:A:588:A:O2'	2.49	0.45
28:X:76:ARG:HD2	31:A:2373:C:H4'	1.98	0.45
58:8:356:PHE:O	58:8:359:ARG:HG2	2.16	0.45
31:A:2009:U:H3'	31:A:2010:C:H2'	1.99	0.45
9:C:256:ARG:NH1	31:A:1809:G:OP1	2.50	0.45
10:D:115:ILE:O	10:D:275:VAL:HA	2.16	0.45
11:E:148:TRP:CD1	11:E:150:ILE:HG12	2.51	0.45
11:E:82:ALA:HB2	17:M:88:GLN:HG3	1.99	0.45
19:O:77:LEU:HA	19:O:86:VAL:HG21	1.98	0.45
25:U:116:GLN:HB2	25:U:137:THR:O	2.16	0.45
9:C:37:LYS:NZ	31:A:1825:A:OP2	2.47	0.45
31:A:1157:A:O2'	31:A:2532:C:O2	2.31	0.45
31:A:705:U:OP1	31:A:770:G:O2'	33.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:163:VAL:HG12	13:G:173:VAL:HA	1.98	0.45
18:N:38:GLU:HB3	18:N:127:ILE:HB	1.97	0.45
28:X:88:LYS:HB2	28:X:91:ALA:HB2	1.98	0.45
31:A:1732:G:N2	31:A:1991:A:O2'	2.50	0.45
31:A:1844:U:H5''	31:A:1845:G:H5'	1.98	0.45
10:D:222:MET:HB3	31:A:2007:U:H5'	1.99	0.45
31:A:1873:G:H4'	31:A:2428:A:H4'	1.98	0.45
8:B:41:U:H1'	8:B:46:A:H61	1.80	0.45
11:E:202:ALA:HA	11:E:225:THR:HG21	1.98	0.45
12:F:160:ALA:O	12:F:164:THR:OG1	2.29	0.45
24:T:113:LYS:HE2	31:A:1344:G:H5''	1.97	0.45
26:V:110:HIS:HB3	31:A:495:A:H5'	1.99	0.45
26:V:136:LEU:HD13	26:V:168:VAL:HG11	1.99	0.45
4:4:119:HIS:CE1	4:4:120:LEU:HD13	2.52	0.45
58:8:264:VAL:HG22	58:8:281:GLY:H	1.81	0.45
31:A:1077:C:H2'	31:A:1078:A:H8	1.82	0.45
31:A:925:G:N2	31:A:1311:C:OP2	117.54	0.45
31:A:1433:U:H2'	31:A:1434:G:C8	2.52	0.45
31:A:144:A:N3	31:A:2223:A:O2'	2.48	0.45
31:A:1423:U:O2'	31:A:1555:G:O2'	2.33	0.45
21:Q:218:ARG:HG2	31:A:2736:G:H4'	1.99	0.45
31:A:313:A:N1	31:A:323:G:C6	2.85	0.45
11:E:162:SER:O	11:E:166:ALA:HB2	2.17	0.45
20:P:100:THR:O	20:P:104:ALA:CB	2.64	0.45
24:T:111:LEU:O	24:T:126:LYS:HA	2.17	0.45
31:A:2051:G:H2'	31:A:2052:G:C8	2.51	0.45
31:A:2557:C:O2'	31:A:2758:A:N3	2.41	0.45
31:A:686:A:N3	31:A:2460:U:O2'	2.49	0.45
9:C:65:ARG:HH12	9:C:124:ASN:HA	1.81	0.45
18:N:28:CYS:HB2	18:N:67:ARG:HH12	1.81	0.45
7:7:60:MET:SD	31:A:977:G:O2'	2.66	0.45
31:A:1238:G:H1	31:A:1252:C:N4	2.15	0.45
31:A:170:U:H2'	31:A:171:G:H8	1.82	0.45
31:A:22:G:H2'	31:A:23:G:C8	2.81	0.45
31:A:621:G:H2'	31:A:622:G:C8	3.56	0.45
10:D:145:ARG:HE	10:D:147:ARG:HD2	1.82	0.45
11:E:81:ARG:O	11:E:85:HIS:HB2	2.17	0.45
16:L:15:GLY:HA3	16:L:50:THR:HG21	1.99	0.45
5:5:7:VAL:HG12	5:5:36:GLN:HE22	1.82	0.45
58:8:329:LYS:HE2	58:8:332:GLU:OE2	2.16	0.45
31:A:1604:A:H2'	31:A:1605:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:241:A:H2'	31:A:242:A:H8	1.81	0.45
31:A:605:C:H2'	31:A:606:A:H8	1.82	0.45
31:A:892:C:C2'	31:A:893:C:H5'	2.47	0.45
13:G:165:VAL:HG22	13:G:171:VAL:HG22	1.99	0.45
19:O:106:ARG:HB3	19:O:124:GLU:HB2	1.97	0.45
28:X:122:LEU:O	28:X:137:VAL:HA	2.17	0.45
1:1:18:ASN:ND2	31:A:14:A:O3'	2.48	0.45
9:C:57:LEU:O	9:C:59:ARG:NH2	2.47	0.45
12:F:178:HIS:HB2	12:F:181:TYR:HA	1.98	0.45
21:Q:149:VAL:HG12	21:Q:208:VAL:HA	1.98	0.45
58:8:317:HIS:CA	58:8:324:VAL:HA	2.33	0.44
58:8:329:LYS:HB3	58:8:332:GLU:OE2	2.17	0.44
31:A:1260:G:H5''	32:0:100:LYS:CD	177.63	0.44
31:A:1384:C:O2'	31:A:1819:A:N3	2.46	0.44
31:A:199:G:N2	31:A:201:A:N3	2.64	0.44
29:Y:100:PHE:CE2	31:A:2247:C:H5''	2.52	0.44
26:V:157:LYS:NZ	31:A:306:G:O3'	2.50	0.44
31:A:885:G:H1	31:A:911:U:H3	1.63	0.44
25:U:121:THR:HG23	25:U:124:ALA:H	1.82	0.44
31:A:1529:A:H2'	31:A:1530:G:C8	2.52	0.44
31:A:1739:G:H2'	31:A:1740:G:H8	1.82	0.44
4:4:107:LYS:HB2	31:A:663:A:H5'	1.99	0.44
31:A:892:C:C6	31:A:892:C:O5'	2.70	0.44
11:E:59:ASN:HB3	11:E:178:PHE:HE1	1.82	0.44
31:A:55:G:H1	31:A:112:C:N4	2.11	0.44
19:O:38:LEU:HD22	19:O:58:VAL:HG21	1.97	0.44
29:Y:77:PHE:HA	29:Y:141:ALA:HB2	1.99	0.44
58:8:69:ASN:HB3	58:8:73:GLU:HG2	1.99	0.44
31:A:1354:C:H2'	31:A:1355:G:H8	1.82	0.44
31:A:1454:G:H2'	31:A:1455:A:C8	2.52	0.44
31:A:1605:A:H2'	31:A:1606:A:C8	2.52	0.44
8:B:8:G:O6	8:B:115:C:N4	2.50	0.44
18:N:33:ALA:O	18:N:131:PHE:HA	2.17	0.44
26:V:90:SER:HB2	26:V:102:LYS:HD3	1.99	0.44
30:Z:120:ARG:NE	30:Z:123:GLU:OE1	2.50	0.44
31:A:1408:A:H5'	31:A:1488:A:H1'	1.99	0.44
31:A:2627:C:H4'	31:A:2628:C:H5'	2.00	0.44
18:N:36:ALA:HA	18:N:129:THR:HG22	2.00	0.44
20:P:128:ALA:HB1	20:P:162:HIS:HB2	1.99	0.44
31:A:1385:G:N2	31:A:1388:A:OP2	2.45	0.44
31:A:1665:U:O4	31:A:1666:A:N6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:149:HIS:HB2	31:A:307:C:H5''	2.00	0.44
17:M:203:GLU:HG2	31:A:649:A:H8	1.83	0.44
8:B:92:U:OP1	18:N:17:MET:N	2.50	0.44
20:P:126:MET:HA	20:P:129:LYS:HG2	2.00	0.44
3:3:102:ARG:NH2	3:3:138:LYS:O	2.44	0.44
58:8:354:GLN:HA	58:8:357:ARG:NH1	2.33	0.44
31:A:1487:C:H42	31:A:1557:G:H22	1.66	0.44
11:E:106:ALA:HB2	31:A:812:G:H8	1.83	0.44
9:C:116:THR:OG1	9:C:117:GLU:OE1	2.31	0.44
15:K:115:TYR:HB2	15:K:153:VAL:HG12	1.99	0.44
18:N:37:LEU:O	18:N:41:TRP:CH2	17.34	0.44
24:T:58:TYR:O	24:T:62:LEU:HB2	2.17	0.44
31:A:2599:G:C2	31:A:2600:G:H1'	2.53	0.44
31:A:283:C:H2'	31:A:284:A:C8	4.23	0.44
31:A:545:U:H2'	31:A:546:G:C8	2.53	0.44
27:W:12:C:O2'	27:W:87:A:O2'	2.31	0.44
58:8:364:GLU:HA	58:8:364:GLU:OE1	2.18	0.44
31:A:1994:G:O2'	31:A:1996:U:OP2	2.32	0.44
31:A:631:G:OP2	31:A:632:G:N2	2.51	0.44
22:R:3:ARG:NH2	31:A:1220:U:O2	2.36	0.43
31:A:1407:C:H2'	31:A:1408:A:C8	2.53	0.43
31:A:818:U:O2'	31:A:2074:A:N1	2.51	0.43
31:A:570:C:H2'	31:A:571:G:C8	2.53	0.43
25:U:157:VAL:HG21	25:U:178:LEU:HD13	1.99	0.43
58:8:367:ALA:HB3	58:8:368:ARG:HG2	2.00	0.43
31:A:1968:G:H5'	31:A:2567:G:H21	1.82	0.43
13:G:129:LEU:HG	13:G:202:VAL:HG22	2.00	0.43
15:K:116:VAL:HG22	15:K:154:ILE:HB	2.00	0.43
27:W:13:G:N2	27:W:40:U:O2'	2.43	0.43
22:R:5:LYS:NZ	31:A:1219:U:O2	2.37	0.43
17:M:161:ASN:HD21	31:A:639:A:H62	1.65	0.43
19:O:38:LEU:HD11	19:O:123:ILE:HG21	1.99	0.43
19:O:80:ILE:HD12	19:O:86:VAL:HG22	2.00	0.43
26:V:120:GLY:O	31:A:495:A:O2'	2.24	0.43
31:A:1704:A:N3	31:A:1706:C:N4	2.66	0.43
9:C:152:ARG:NE	31:A:1828:U:OP2	2.50	0.43
31:A:2022:C:H2'	31:A:2023:G:H8	1.82	0.43
31:A:663:A:H2'	31:A:664:A:C8	3.41	0.43
31:A:794:A:H2'	31:A:795:U:H4'	2.01	0.43
4:4:112:ARG:NH1	31:A:2377:C:OP1	2.51	0.43
31:A:146:U:O2	31:A:148:C:N4	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:68:LEU:HA	12:F:71:GLU:HG2	2.00	0.43
23:S:145:GLN:NE2	23:S:214:GLN:OE1	2.51	0.43
58:8:369:ALA:O	58:8:371:MET:HG2	2.18	0.43
31:A:1874:U:O3'	31:A:2426:G:N2	2.50	0.43
31:A:2601:U:H5'	31:A:2602:U:H5'	2.01	0.43
8:B:92:U:H5'	18:N:17:MET:HB2	2.00	0.43
21:Q:217:ALA:HB2	27:W:52:G:H8	1.83	0.43
31:A:330:U:O2'	31:A:349:A:N3	2.52	0.43
31:A:426:C:H2'	31:A:427:A:C8	2.54	0.43
31:A:591:C:H2'	31:A:592:G:C8	2.54	0.43
30:Z:107:ARG:O	30:Z:111:ARG:HB2	2.19	0.43
31:A:1704:A:O2'	31:A:1710:G:N7	2.49	0.43
15:K:214:GLY:HA2	15:K:217:LEU:HG	2.01	0.43
18:N:53:ALA:O	18:N:57:ASN:HB2	2.19	0.43
20:P:123:ILE:HA	20:P:123:ILE:HD12	1.87	0.43
20:P:73:LEU:HD23	20:P:139:VAL:HG21	2.00	0.43
2:2:46:LEU:HB2	2:2:57:LYS:HD2	2.00	0.43
31:A:1986:G:H2'	31:A:1987:G:C8	2.54	0.43
31:A:2464:G:C8	31:A:2518:C:H5''	2.54	0.43
31:A:715:G:O2'	31:A:737:G:N2	2.43	0.43
18:N:12:GLN:HA	31:A:919:A:H62	1.84	0.43
23:S:188:GLU:OE2	23:S:218:ARG:NH1	2.52	0.43
29:Y:107:ARG:HA	29:Y:117:VAL:O	2.19	0.43
31:A:2204:A:H3'	31:A:2205:G:H8	1.84	0.43
31:A:2316:G:H2'	31:A:2317:G:C8	2.54	0.43
31:A:468:U:O2	31:A:471:U:O2'	2.35	0.43
15:K:147:VAL:HG23	15:K:149:MET:HG2	2.00	0.43
16:L:11:ALA:O	16:L:99:PHE:N	2.46	0.43
20:P:73:LEU:HB3	20:P:86:VAL:HG22	2.01	0.43
31:A:1125:U:H3'	31:A:1126:A:H8	1.84	0.42
31:A:2539:U:C2	31:A:2783:A:N7	2.87	0.42
31:A:383:A:H61	31:A:413:A:H3'	1.84	0.42
31:A:592:G:H2'	31:A:593:G:H8	1.84	0.42
10:D:135:ASN:HD22	10:D:175:SER:HA	1.83	0.42
8:B:91:G:N2	18:N:38:GLU:OE2	2.46	0.42
4:4:140:ARG:HA	4:4:143:TYR:HB3	2.02	0.42
13:G:43:ILE:HG12	31:A:2769:G:H4'	2.01	0.42
11:E:251:THR:O	11:E:255:LEU:CB	2.62	0.42
13:G:166:GLU:OE2	13:G:170:LYS:NZ	2.52	0.42
30:Z:72:THR:OG1	30:Z:75:GLN:OE1	2.37	0.42
7:7:88:GLU:HG3	7:7:89:TRP:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1443:G:O2'	31:A:1926:A:O2'	105.70	0.42
31:A:226:A:H61	31:A:240:A:H5''	1.84	0.42
28:X:122:LEU:HG	28:X:140:ARG:HG3	2.02	0.42
30:Z:88:PHE:HA	30:Z:91:ARG:HE	1.85	0.42
21:Q:160:ARG:NH2	31:A:317:G:O4'	136.73	0.42
11:E:158:ARG:NH1	31:A:630:C:OP2	2.51	0.42
31:A:74:G:H22	31:A:109:A:H2	1.67	0.42
31:A:756:G:O2'	31:A:759:G:O2'	2.31	0.42
31:A:92:U:H2'	31:A:93:A:C8	2.54	0.42
7:7:80:PRO:HA	7:7:81:PRO:HD3	1.93	0.42
31:A:1154:A:H4'	31:A:1155:A:H5''	2.00	0.42
19:O:116:ASP:OD2	31:A:1685:G:O2'	2.34	0.42
20:P:125:GLU:HG3	20:P:129:LYS:HE3	2.01	0.42
31:A:1118:U:H2'	31:A:1119:G:C8	2.54	0.42
31:A:825:C:O2'	31:A:1245:U:O2	2.29	0.42
31:A:1406:A:O2'	31:A:1417:U:O2	2.30	0.42
31:A:2316:G:H2'	31:A:2317:G:H8	1.85	0.42
31:A:596:A:N1	31:A:820:G:O2'	2.40	0.42
31:A:843:C:H2'	31:A:844:G:C8	2.54	0.42
9:C:68:LYS:HB3	9:C:115:GLY:HA2	2.01	0.42
12:F:107:ILE:O	12:F:111:ALA:HB2	2.18	0.42
21:Q:127:ASN:HD21	21:Q:177:ILE:N	2.18	0.42
28:X:101:PHE:HB3	28:X:135:VAL:HG23	2.02	0.42
29:Y:95:THR:HG21	31:A:2095:U:H4'	2.01	0.42
31:A:2047:A:O2'	31:A:2049:G:OP2	2.31	0.42
18:N:124:LYS:NZ	31:A:2484:C:O2	2.46	0.42
17:M:134:MET:HA	17:M:135:PRO:HD3	1.82	0.42
31:A:1450:G:H2'	31:A:1451:G:C8	2.55	0.42
31:A:1468:C:O2'	31:A:1578:A:N3	2.39	0.42
12:F:88:VAL:HG11	31:A:2331:G:H5'	2.01	0.42
31:A:919:A:H2'	31:A:920:A:C8	2.54	0.42
10:D:269:ILE:HG22	10:D:276:VAL:HG13	2.01	0.42
13:G:43:ILE:HG13	31:A:2766:A:H5'	2.02	0.42
17:M:223:GLU:O	17:M:227:ALA:HB2	2.20	0.42
20:P:124:GLY:HA2	20:P:127:ILE:HG22	2.02	0.42
31:A:2767:A:H3'	31:A:2768:A:H5''	2.02	0.42
10:D:141:TYR:CD2	10:D:142:GLU:HG3	2.55	0.42
11:E:96:ARG:HD2	31:A:455:A:C6	2.55	0.42
22:R:27:ALA:O	22:R:34:THR:OG1	2.36	0.42
31:A:1060:A:N1	31:A:1150:G:O6	2.53	0.42
31:A:25:G:H4'	31:A:1281:G:H4'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:932:A:H2'	31:A:933:G:C8	2.55	0.42
9:C:228:HIS:CE1	9:C:237:ILE:HG13	2.55	0.42
10:D:149:LEU:HD21	10:D:157:LEU:HD12	2.02	0.42
31:A:1843:C:H42	31:A:1986:G:H1	1.68	0.41
31:A:2308:U:H2'	31:A:2309:U:C6	2.55	0.41
31:A:818:U:H2'	31:A:819:G:C8	2.55	0.41
8:B:78:U:O2	8:B:101:A:N7	2.53	0.41
10:D:95:THR:HG21	10:D:118:LYS:HE3	2.02	0.41
16:L:21:CYS:HA	16:L:41:ALA:HA	2.01	0.41
58:8:271:LEU:CD1	58:8:304:LEU:HA	2.50	0.41
31:A:1063:U:H2'	31:A:1064:A:C8	2.55	0.41
20:P:143:ARG:HH11	31:A:2310:U:H5''	1.85	0.41
31:A:587:G:O2'	31:A:1275:A:OP1	2.38	0.41
31:A:682:C:H2'	31:A:683:C:H6	1.85	0.41
31:A:865:A:H2'	31:A:866:G:H8	1.85	0.41
21:Q:141:PRO:HD2	21:Q:206:ILE:HD11	2.02	0.41
22:R:31:LEU:HD12	22:R:31:LEU:HA	1.84	0.41
23:S:146:ARG:O	23:S:217:THR:OG1	2.30	0.41
24:T:33:THR:HG22	24:T:135:VAL:HG22	2.02	0.41
31:A:10:G:H2'	31:A:11:G:C8	2.55	0.41
31:A:2283:A:N6	31:A:2290:A:OP2	2.52	0.41
13:G:160:GLU:OE1	13:G:176:ARG:NH2	2.49	0.41
18:N:13:HIS:CD2	31:A:982:G:H5''	2.55	0.41
23:S:202:LYS:HG3	23:S:203:LYS:H	1.86	0.41
58:8:280:ILE:HD13	58:8:280:ILE:HG21	1.69	0.41
31:A:867:G:N2	31:A:2286:A:O4'	2.51	0.41
20:P:70:ARG:NH2	20:P:139:VAL:O	2.40	0.41
24:T:47:ARG:HH22	31:A:529:G:P	2.43	0.41
31:A:1260:G:P	32:0:96:LYS:HE3	175.05	0.41
31:A:577:G:H21	31:A:581:A:H8	1.68	0.41
12:F:126:SER:HA	12:F:132:VAL:HG12	2.02	0.41
13:G:134:TYR:HA	13:G:146:SER:O	2.21	0.41
19:O:12:LYS:HB2	31:A:1689:C:H3'	2.03	0.41
27:W:51:U:O2	31:A:2709:C:O2'	2.39	0.41
31:A:1015:C:O2'	31:A:1028:A:N3	2.43	0.41
3:3:119:SER:OG	31:A:693:G:O3'	2.37	0.41
9:C:88:CYS:O	9:C:99:TYR:HA	2.21	0.41
21:Q:174:ASN:HB3	21:Q:179:THR:HG23	2.02	0.41
22:R:49:ASP:OD1	31:A:569:G:N2	2.53	0.41
25:U:105:PRO:O	31:A:131:C:N4	2.54	0.41
23:S:182:VAL:HG22	23:S:224:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:103:ALA:HA	24:T:134:ILE:HA	2.02	0.41
7:7:69:ARG:HG3	7:7:73:LYS:NZ	2.36	0.41
58:8:268:VAL:HG11	58:8:305:GLN:HB3	2.03	0.41
31:A:1762:C:H42	31:A:1766:G:H1	1.69	0.41
11:E:102:THR:HG21	11:E:142:GLY:HA3	2.02	0.41
11:E:133:LEU:O	31:A:1277:G:N2	2.53	0.41
12:F:175:PHE:HA	31:A:2320:G:H4'	2.02	0.41
27:W:59:C:H2'	27:W:60:A:H8	1.86	0.41
27:W:26:G:H8	27:W:87:A:H2	1.67	0.41
11:E:254:TYR:OH	11:E:258:ARG:NH1	2.39	0.41
20:P:126:MET:O	20:P:130:SER:HB3	2.21	0.41
22:R:28:HIS:HB3	22:R:38:GLN:HG3	2.02	0.41
31:A:872:A:O2'	31:A:1348:C:OP2	103.71	0.41
31:A:1488:A:H2'	31:A:1489:A:C8	2.56	0.41
31:A:1592:A:H4'	31:A:1593:U:H3'	2.02	0.41
31:A:2356:G:H2'	31:A:2357:A:H8	1.86	0.41
8:B:32:A:H61	8:B:54:G:H21	1.69	0.41
10:D:167:HIS:CD2	10:D:289:LEU:HD22	2.56	0.41
17:M:210:LEU:H	17:M:230:CYS:HB2	1.85	0.41
29:Y:99:GLN:HG3	31:A:2248:U:H5''	2.02	0.41
30:Z:104:ASP:O	30:Z:108:MET:HB2	2.21	0.41
7:7:54:LYS:O	7:7:58:HIS:N	2.50	0.41
58:8:315:LEU:HD23	58:8:327:SER:H	1.85	0.41
22:R:33:ARG:HG2	31:A:1273:G:H21	1.86	0.41
31:A:1487:C:N4	31:A:1557:G:H22	2.18	0.41
5:5:10:ILE:HG21	31:A:2494:C:H42	1.85	0.41
31:A:895:C:C6	31:A:895:C:C3'	3.03	0.41
28:X:154:LYS:NZ	31:A:960:A:N1	2.69	0.41
32:0:95:GLU:HA	32:0:98:ARG:HG2	2.03	0.41
5:5:6:SER:O	5:5:6:SER:OG	2.26	0.41
9:C:94:ASP:HA	31:A:1530:G:H21	1.86	0.41
31:A:1330:G:H21	31:A:1647:C:H5'	1.85	0.41
31:A:530:U:H2'	31:A:531:A:H8	1.86	0.41
31:A:838:U:O2'	31:A:2082:U:N3	2.53	0.41
9:C:90:ILE:HD11	9:C:98:ARG:HB2	2.03	0.41
11:E:201:PRO:O	11:E:225:THR:OG1	2.36	0.41
14:H:77:PHE:HE2	14:H:79:LEU:HD12	11.41	0.41
14:H:74:LEU:HA	14:H:78:LEU:HB2	2.01	0.41
31:A:1444:A:H2'	31:A:1445:G:H8	1.86	0.41
31:A:2045:A:O2'	31:A:2471:G:N2	2.51	0.41
29:Y:92:ASN:OD1	29:Y:94:LYS:NZ	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1424:A:O2'	31:A:1490:G:O2'	2.31	0.40
31:A:645:A:O2'	31:A:2421:C:OP1	2.31	0.40
8:B:10:G:OP1	20:P:57:HIS:NE2	2.52	0.40
12:F:132:VAL:HG22	12:F:138:LEU:HD21	2.03	0.40
22:R:36:ALA:O	22:R:40:ILE:HG12	2.22	0.40
24:T:102:LYS:HG2	24:T:135:VAL:HB	2.02	0.40
31:A:1050:G:H4'	31:A:1051:U:H5'	2.02	0.40
18:N:6:ARG:HB3	31:A:880:U:H5"	2.01	0.40
21:Q:170:ILE:N	21:Q:182:ARG:O	2.42	0.40
27:W:67:U:H2'	27:W:68:A:C8	2.56	0.40
29:Y:103:LEU:HA	29:Y:122:SER:HA	2.03	0.40
31:A:568:C:H2'	31:A:569:G:C8	2.57	0.40
31:A:1941:A:H2'	31:A:1942:A:C8	2.56	0.40
31:A:385:U:H2'	31:A:386:A:H8	1.86	0.40
31:A:426:C:H2'	31:A:427:A:H8	1.85	0.40
11:E:233:SER:OG	31:A:623:A:N6	2.53	0.40
31:A:828:C:O2'	31:A:850:G:OP1	2.33	0.40
8:B:24:G:H2'	8:B:25:G:C5	2.57	0.40
10:D:157:LEU:HD13	10:D:165:MET:H	1.87	0.40
11:E:90:THR:O	11:E:94:ASN:HB2	2.22	0.40
16:L:102:ILE:HD12	16:L:106:LEU:HD11	2.03	0.40
23:S:192:ASP:HB3	23:S:216:ILE:HD13	2.04	0.40
31:A:1227:U:H2'	31:A:1228:A:H8	1.86	0.40
31:A:2653:U:H3	31:A:2800:G:H1	1.69	0.40
31:A:2118:U:O4	31:A:2199:G:O6	2.40	0.40
31:A:2464:G:N7	31:A:2518:C:H2'	2.36	0.40
31:A:2013:A:H1'	31:A:2704:U:H1'	2.04	0.40
31:A:530:U:OP2	31:A:706:G:N1	72.68	0.40
9:C:25:ARG:NH2	31:A:1603:A:OP1	2.54	0.40
25:U:140:VAL:HA	25:U:172:LYS:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	44/56 (79%)	40 (91%)	4 (9%)	0	100	100
2	2	49/65 (75%)	39 (80%)	10 (20%)	0	100	100
3	3	55/61 (90%)	49 (89%)	6 (11%)	0	100	100
4	4	67/73 (92%)	59 (88%)	8 (12%)	0	100	100
5	5	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
6	6	47/142 (33%)	46 (98%)	1 (2%)	0	100	100
7	7	44/116 (38%)	41 (93%)	3 (7%)	0	100	100
9	C	245/271 (90%)	213 (87%)	32 (13%)	0	100	100
10	D	210/221 (95%)	188 (90%)	22 (10%)	0	100	100
11	E	208/243 (86%)	180 (86%)	28 (14%)	0	100	100
12	F	173/220 (79%)	161 (93%)	12 (7%)	0	100	100
13	G	171/182 (94%)	161 (94%)	10 (6%)	0	100	100
14	H	51/155 (33%)	47 (92%)	4 (8%)	0	100	100
15	K	191/197 (97%)	178 (93%)	13 (7%)	0	100	100
16	L	119/121 (98%)	104 (87%)	15 (13%)	0	100	100
17	M	175/192 (91%)	163 (93%)	11 (6%)	1 (1%)	28	68
18	N	132/135 (98%)	111 (84%)	21 (16%)	0	100	100
19	O	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
20	P	118/123 (96%)	116 (98%)	2 (2%)	0	100	100
21	Q	116/156 (74%)	100 (86%)	16 (14%)	0	100	100
22	R	113/127 (89%)	105 (93%)	8 (7%)	0	100	100
23	S	145/201 (72%)	118 (81%)	27 (19%)	0	100	100
24	T	142/199 (71%)	125 (88%)	17 (12%)	0	100	100
25	U	90/122 (74%)	86 (96%)	4 (4%)	0	100	100
26	V	122/145 (84%)	109 (89%)	13 (11%)	0	100	100
28	X	98/137 (72%)	87 (89%)	11 (11%)	0	100	100
29	Y	72/77 (94%)	66 (92%)	6 (8%)	0	100	100
30	Z	88/109 (81%)	87 (99%)	1 (1%)	0	100	100
32	0	62/94 (66%)	54 (87%)	6 (10%)	2 (3%)	5	34
33	b	225/236 (95%)	195 (87%)	29 (13%)	1 (0%)	38	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	c	211/218 (97%)	181 (86%)	28 (13%)	2 (1%)	20	61
35	e	169/253 (67%)	150 (89%)	17 (10%)	2 (1%)	15	54
36	f	109/146 (75%)	85 (78%)	24 (22%)	0	100	100
37	g	147/155 (95%)	130 (88%)	16 (11%)	1 (1%)	25	65
38	h	132/134 (98%)	116 (88%)	16 (12%)	0	100	100
39	i	131/157 (83%)	107 (82%)	23 (18%)	1 (1%)	22	62
40	j	96/122 (79%)	83 (86%)	13 (14%)	0	100	100
41	k	116/138 (84%)	104 (90%)	12 (10%)	0	100	100
42	l	121/123 (98%)	100 (83%)	21 (17%)	0	100	100
43	m	108/126 (86%)	90 (83%)	18 (17%)	0	100	100
44	o	60/90 (67%)	59 (98%)	1 (2%)	0	100	100
45	p	78/88 (89%)	61 (78%)	17 (22%)	0	100	100
46	q	76/108 (70%)	64 (84%)	12 (16%)	0	100	100
47	r	62/101 (61%)	58 (94%)	4 (6%)	0	100	100
48	s	76/92 (83%)	61 (80%)	15 (20%)	0	100	100
49	t	103/108 (95%)	93 (90%)	10 (10%)	0	100	100
50	u	42/137 (31%)	39 (93%)	3 (7%)	0	100	100
51	y	106/236 (45%)	96 (91%)	10 (9%)	0	100	100
53	w	82/121 (68%)	79 (96%)	0	3 (4%)	4	30
54	d	197/201 (98%)	173 (88%)	22 (11%)	2 (1%)	18	59
55	v	188/198 (95%)	171 (91%)	14 (7%)	3 (2%)	11	48
56	n	97/100 (97%)	90 (93%)	7 (7%)	0	100	100
57	x	35/47 (74%)	30 (86%)	4 (11%)	1 (3%)	5	36
58	8	150/370 (40%)	116 (77%)	18 (12%)	16 (11%)	0	6
All	All	6213/7898 (79%)	5499 (88%)	679 (11%)	35 (1%)	33	68

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	0	72	VAL
35	e	148	ILE
53	w	149	PRO
55	v	105	MET
58	8	72	MET

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Mol	Chain	Res	Type
58	8	73	GLU
58	8	299	ASP
58	8	300	ILE
58	8	303	VAL
58	8	316	SER
58	8	330	LYS
58	8	366	MET
58	8	367	ALA
58	8	370	ASP
58	8	371	MET
34	c	89	PRO
54	d	5	ARG
55	v	121	PRO
58	8	360	ILE
58	8	368	ARG
17	M	197	PRO
33	b	169	ASP
39	i	159	ALA
53	w	150	TRP
34	c	88	ARG
35	e	302	PRO
57	x	90	ILE
58	8	306	PRO
58	8	364	GLU
37	g	9	GLU
32	0	73	TRP
54	d	168	PRO
55	v	120	SER
53	w	119	PRO
58	8	307	GLY

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	1	39/49 (80%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	48/59 (81%)	46 (96%)	2 (4%)	34	70
3	3	47/50 (94%)	47 (100%)	0	100	100
4	4	59/62 (95%)	58 (98%)	1 (2%)	66	86
5	5	34/34 (100%)	34 (100%)	0	100	100
6	6	46/124 (37%)	46 (100%)	0	100	100
7	7	40/96 (42%)	40 (100%)	0	100	100
9	C	195/216 (90%)	194 (100%)	1 (0%)	91	96
10	D	174/182 (96%)	174 (100%)	0	100	100
11	E	176/205 (86%)	173 (98%)	3 (2%)	66	86
12	F	148/183 (81%)	148 (100%)	0	100	100
13	G	147/154 (96%)	147 (100%)	0	100	100
14	H	47/134 (35%)	47 (100%)	0	100	100
15	K	167/171 (98%)	165 (99%)	2 (1%)	75	89
16	L	101/101 (100%)	101 (100%)	0	100	100
17	M	135/144 (94%)	133 (98%)	2 (2%)	70	87
18	N	107/108 (99%)	107 (100%)	0	100	100
19	O	96/96 (100%)	96 (100%)	0	100	100
20	P	99/100 (99%)	99 (100%)	0	100	100
21	Q	104/135 (77%)	103 (99%)	1 (1%)	80	91
22	R	102/114 (90%)	102 (100%)	0	100	100
23	S	129/174 (74%)	129 (100%)	0	100	100
24	T	126/176 (72%)	126 (100%)	0	100	100
25	U	81/103 (79%)	80 (99%)	1 (1%)	75	89
26	V	112/129 (87%)	111 (99%)	1 (1%)	82	92
28	X	85/111 (77%)	84 (99%)	1 (1%)	75	89
29	Y	64/67 (96%)	63 (98%)	1 (2%)	68	86
30	Z	83/97 (86%)	82 (99%)	1 (1%)	75	89
32	0	56/83 (68%)	55 (98%)	1 (2%)	64	85
33	b	192/201 (96%)	188 (98%)	4 (2%)	59	83
34	c	185/188 (98%)	185 (100%)	0	100	100
35	e	132/203 (65%)	128 (97%)	4 (3%)	46	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	98/125 (78%)	98 (100%)	0	100	100
37	g	120/126 (95%)	120 (100%)	0	100	100
38	h	117/117 (100%)	115 (98%)	2 (2%)	66	86
39	i	103/123 (84%)	102 (99%)	1 (1%)	80	91
40	j	90/110 (82%)	90 (100%)	0	100	100
41	k	92/109 (84%)	92 (100%)	0	100	100
42	l	106/106 (100%)	106 (100%)	0	100	100
43	m	97/109 (89%)	97 (100%)	0	100	100
44	o	58/85 (68%)	58 (100%)	0	100	100
45	p	71/79 (90%)	70 (99%)	1 (1%)	71	88
46	q	70/95 (74%)	70 (100%)	0	100	100
47	r	56/96 (58%)	56 (100%)	0	100	100
48	s	67/81 (83%)	67 (100%)	0	100	100
49	t	86/89 (97%)	84 (98%)	2 (2%)	56	82
50	u	40/118 (34%)	40 (100%)	0	100	100
51	y	97/213 (46%)	94 (97%)	3 (3%)	45	77
53	w	75/109 (69%)	74 (99%)	1 (1%)	73	89
54	d	178/180 (99%)	175 (98%)	3 (2%)	66	86
55	v	160/168 (95%)	158 (99%)	2 (1%)	73	89
56	n	89/90 (99%)	89 (100%)	0	100	100
57	x	28/37 (76%)	28 (100%)	0	100	100
58	8	129/310 (42%)	125 (97%)	4 (3%)	45	77
All	All	5383/6724 (80%)	5338 (99%)	45 (1%)	86	93

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	13	LEU
2	2	48	LEU
4	4	153	LEU
9	C	39	ARG
11	E	71	ASN
11	E	81	ARG
11	E	245	LEU

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Mol	Chain	Res	Type
15	K	62	ARG
15	K	174	ARG
17	M	196	LEU
17	M	252	ARG
21	Q	127	ASN
25	U	106	ARG
26	V	64	LEU
28	X	73	LYS
29	Y	103	LEU
30	Z	107	ARG
32	0	76	ASN
33	b	30	ARG
33	b	40	LYS
33	b	94	HIS
33	b	201	ASP
35	e	144	LYS
35	e	266	LEU
35	e	303	MET
35	e	305	GLU
38	h	67	ARG
38	h	79	LEU
39	i	176	ARG
45	p	46	THR
49	t	103	ARG
49	t	162	ARG
51	y	91	ARG
51	y	119	ARG
51	y	159	LEU
53	w	103	PHE
54	d	27	ARG
54	d	40	LYS
54	d	160	LEU
55	v	24	LEU
55	v	37	GLU
58	8	283	ILE
58	8	304	LEU
58	8	314	ILE
58	8	368	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	58	HIS
4	4	95	HIS
4	4	118	GLN
4	4	145	ASN
9	C	54	HIS
9	C	84	ASN
10	D	167	HIS
10	D	209	GLN
11	E	71	ASN
11	E	118	GLN
11	E	153	ASN
11	E	222	ASN
12	F	60	ASN
12	F	77	ASN
12	F	116	GLN
13	G	103	GLN
15	K	97	ASN
15	K	139	ASN
16	L	3	GLN
16	L	73	ASN
16	L	82	ASN
17	M	161	ASN
18	N	13	HIS
19	O	37	GLN
20	P	81	HIS
21	Q	127	ASN
22	R	28	HIS
22	R	77	ASN
22	R	99	GLN
23	S	145	GLN
23	S	212	HIS
23	S	214	GLN
24	T	52	GLN
24	T	106	ASN
26	V	130	HIS
32	0	76	ASN
34	c	18	HIS
34	c	34	GLN
34	c	187	GLN
35	e	225	HIS
35	e	264	ASN
38	h	19	ASN
38	h	51	HIS

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Mol	Chain	Res	Type
38	h	68	ASN
39	i	127	ASN
39	i	161	HIS
40	j	126	ASN
40	j	149	HIS
40	j	151	HIS
41	k	127	HIS
41	k	128	ASN
42	l	77	HIS
43	m	56	ASN
43	m	65	GLN
43	m	83	ASN
43	m	125	HIS
47	r	59	GLN
47	r	83	GLN
48	s	23	ASN
50	u	124	ASN
51	y	165	GLN
53	w	155	GLN
53	w	162	GLN
53	w	172	GLN
54	d	57	HIS
54	d	112	ASN
54	d	115	HIS
54	d	142	GLN
55	v	45	HIS
55	v	96	ASN
55	v	163	ASN
55	v	196	ASN
58	8	58	GLN
58	8	269	GLN
58	8	294	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	W	101/106 (95%)	30 (29%)	4 (3%)
31	A	2808/2810 (99%)	596 (21%)	4 (0%)
52	a	1477/1491 (99%)	310 (20%)	0
8	B	116/121 (95%)	21 (18%)	1 (0%)
All	All	4502/4528 (99%)	957 (21%)	9 (0%)

All (957) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	B	4	U
8	B	10	G
8	B	14	U
8	B	15	A
8	B	16	G
8	B	25	G
8	B	31	C
8	B	36	A
8	B	42	C
8	B	53	U
8	B	54	G
8	B	58	A
8	B	61	C
8	B	67	U
8	B	74	A
8	B	89	A
8	B	92	U
8	B	101	A
8	B	111	G
8	B	117	A
8	B	119	G
27	W	16	G
27	W	17	A
27	W	22	A
27	W	23	G
27	W	28	U
27	W	29	U
27	W	30	A
27	W	31	U
27	W	32	C
27	W	33	A
27	W	34	U
27	W	35	U
27	W	36	A
27	W	37	C
27	W	38	G
27	W	39	A
27	W	48	A
27	W	53	G
27	W	64	A
27	W	65	U
27	W	71	C

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Mol	Chain	Res	Type
27	W	76	G
27	W	77	A
27	W	83	C
27	W	84	C
27	W	88	C
27	W	90	G
27	W	95	A
27	W	97	A
27	W	98	G
31	A	9	A
31	A	10	G
31	A	11	G
31	A	12	A
31	A	13	A
31	A	14	A
31	A	15	G
31	A	26	G
31	A	33	A
31	A	45	A
31	A	46	C
31	A	54	G
31	A	70	A
31	A	72	A
31	A	73	U
31	A	74	G
31	A	82	G
31	A	84	G
31	A	85	U
31	A	98	G
31	A	99	A
31	A	100	G
31	A	112	C
31	A	116	A
31	A	117	A
31	A	118	U
31	A	123	C
31	A	130	U
31	A	131	C
31	A	143	G
31	A	144	A
31	A	147	C
31	A	149	A

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Mol	Chain	Res	Type
31	A	158	C
31	A	159	A
31	A	173	C
31	A	181	A
31	A	184	A
31	A	189	A
31	A	201	A
31	A	207	A
31	A	226	A
31	A	233	G
31	A	250	A
31	A	251	G
31	A	252	C
31	A	262	G
31	A	264	A
31	A	266	A
31	A	275	U
31	A	276	G
31	A	284	A
31	A	287	A
31	A	294	U
31	A	295	C
31	A	297	U
31	A	298	G
31	A	304	A
31	A	316	G
31	A	320	U
31	A	330	U
31	A	331	A
31	A	332	G
31	A	333	A
31	A	338	G
31	A	340	A
31	A	347	G
31	A	352	C
31	A	361	C
31	A	365	A
31	A	368	U
31	A	370	A
31	A	377	G
31	A	378	A
31	A	379	C

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Mol	Chain	Res	Type
31	A	383	A
31	A	384	G
31	A	392	G
31	A	398	G
31	A	399	U
31	A	415	U
31	A	416	C
31	A	417	A
31	A	418	G
31	A	423	G
31	A	424	A
31	A	436	G
31	A	447	C
31	A	448	C
31	A	466	A
31	A	467	G
31	A	468	U
31	A	469	A
31	A	479	G
31	A	489	A
31	A	491	A
31	A	493	G
31	A	504	G
31	A	507	G
31	A	512	A
31	A	515	U
31	A	516	A
31	A	519	A
31	A	524	A
31	A	529	G
31	A	541	G
31	A	542	C
31	A	543	A
31	A	544	G
31	A	545	U
31	A	554	G
31	A	555	A
31	A	557	C
31	A	558	A
31	A	559	G
31	A	560	A
31	A	573	G

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Mol	Chain	Res	Type
31	A	583	G
31	A	585	A
31	A	608	U
31	A	609	G
31	A	610	G
31	A	611	C
31	A	613	U
31	A	614	G
31	A	623	A
31	A	624	A
31	A	630	C
31	A	632	G
31	A	633	A
31	A	638	U
31	A	639	A
31	A	643	A
31	A	646	G
31	A	649	A
31	A	657	U
31	A	665	U
31	A	667	G
31	A	680	G
31	A	686	A
31	A	688	C
31	A	696	A
31	A	697	U
31	A	722	G
31	A	724	G
31	A	728	A
31	A	731	U
31	A	734	G
31	A	737	G
31	A	740	G
31	A	741	U
31	A	745	A
31	A	757	U
31	A	758	U
31	A	768	G
31	A	773	U
31	A	775	A
31	A	776	G
31	A	782	G

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Mol	Chain	Res	Type
31	A	786	G
31	A	787	G
31	A	788	G
31	A	793	A
31	A	795	U
31	A	802	C
31	A	803	G
31	A	811	A
31	A	816	G
31	A	823	C
31	A	838	U
31	A	841	G
31	A	856	U
31	A	857	G
31	A	859	A
31	A	861	A
31	A	866	G
31	A	869	G
31	A	879	G
31	A	887	G
31	A	889	G
31	A	890	G
31	A	891	G
31	A	892	C
31	A	893	C
31	A	895	C
31	A	897	A
31	A	900	G
31	A	901	C
31	A	902	G
31	A	903	G
31	A	905	A
31	A	906	C
31	A	907	C
31	A	908	A
31	A	915	G
31	A	916	G
31	A	919	A
31	A	924	U
31	A	937	U
31	A	938	G
31	A	946	A

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Mol	Chain	Res	Type
31	A	947	A
31	A	970	G
31	A	974	G
31	A	981	G
31	A	987	A
31	A	989	G
31	A	993	C
31	A	1001	A
31	A	1002	G
31	A	1008	A
31	A	1011	A
31	A	1013	C
31	A	1017	G
31	A	1018	A
31	A	1024	A
31	A	1037	A
31	A	1040	U
31	A	1041	G
31	A	1045	G
31	A	1050	G
31	A	1051	U
31	A	1054	U
31	A	1055	A
31	A	1061	G
31	A	1062	G
31	A	1065	G
31	A	1072	A
31	A	1075	G
31	A	1098	A
31	A	1099	G
31	A	1101	A
31	A	1105	A
31	A	1106	C
31	A	1112	A
31	A	1116	A
31	A	1118	U
31	A	1125	U
31	A	1139	A
31	A	1140	G
31	A	1143	C
31	A	1147	U
31	A	1148	G

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Mol	Chain	Res	Type
31	A	1150	G
31	A	1155	A
31	A	1158	U
31	A	1160	A
31	A	1162	C
31	A	1163	G
31	A	1169	A
31	A	1170	A
31	A	1175	U
31	A	1183	A
31	A	1196	A
31	A	1197	A
31	A	1198	A
31	A	1225	G
31	A	1227	U
31	A	1240	G
31	A	1241	U
31	A	1245	U
31	A	1254	U
31	A	1258	A
31	A	1259	C
31	A	1261	A
31	A	1271	G
31	A	1272	A
31	A	1274	A
31	A	1277	G
31	A	1286	A
31	A	1293	C
31	A	1294	A
31	A	1296	A
31	A	1305	A
31	A	1308	A
31	A	1310	C
31	A	1315	G
31	A	1321	A
31	A	1322	A
31	A	1333	U
31	A	1342	A
31	A	1346	U
31	A	1366	C
31	A	1371	C
31	A	1373	U

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Mol	Chain	Res	Type
31	A	1379	C
31	A	1386	A
31	A	1399	A
31	A	1400	U
31	A	1405	A
31	A	1413	A
31	A	1416	A
31	A	1423	U
31	A	1424	A
31	A	1427	A
31	A	1431	C
31	A	1432	U
31	A	1433	U
31	A	1436	U
31	A	1437	G
31	A	1448	A
31	A	1449	C
31	A	1458	C
31	A	1461	G
31	A	1472	A
31	A	1476	G
31	A	1480	A
31	A	1481	U
31	A	1484	G
31	A	1486	U
31	A	1493	C
31	A	1494	G
31	A	1497	A
31	A	1501	G
31	A	1502	A
31	A	1511	U
31	A	1512	U
31	A	1513	C
31	A	1519	A
31	A	1520	A
31	A	1521	G
31	A	1522	A
31	A	1524	G
31	A	1525	G
31	A	1528	U
31	A	1529	A
31	A	1531	A

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Mol	Chain	Res	Type
31	A	1532	G
31	A	1544	A
31	A	1557	G
31	A	1558	U
31	A	1559	A
31	A	1568	U
31	A	1569	A
31	A	1570	C
31	A	1571	G
31	A	1592	A
31	A	1593	U
31	A	1594	A
31	A	1600	A
31	A	1603	A
31	A	1612	A
31	A	1620	U
31	A	1621	C
31	A	1622	A
31	A	1628	A
31	A	1635	C
31	A	1643	G
31	A	1644	A
31	A	1662	A
31	A	1682	C
31	A	1683	G
31	A	1684	C
31	A	1708	C
31	A	1710	G
31	A	1711	C
31	A	1734	A
31	A	1750	C
31	A	1751	A
31	A	1752	C
31	A	1753	A
31	A	1755	A
31	A	1756	G
31	A	1762	C
31	A	1766	G
31	A	1774	G
31	A	1778	G
31	A	1783	A
31	A	1796	A

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Mol	Chain	Res	Type
31	A	1801	A
31	A	1810	C
31	A	1812	A
31	A	1818	U
31	A	1819	A
31	A	1821	G
31	A	1826	U
31	A	1829	A
31	A	1839	A
31	A	1882	U
31	A	1884	A
31	A	1885	C
31	A	1915	A
31	A	1920	G
31	A	1923	C
31	A	1926	A
31	A	1927	A
31	A	1928	C
31	A	1930	A
31	A	1931	U
31	A	1943	G
31	A	1944	G
31	A	1945	U
31	A	1950	A
31	A	1951	A
31	A	1957	U
31	A	1969	U
31	A	1974	A
31	A	1981	C
31	A	1984	A
31	A	1985	A
31	A	1986	G
31	A	1996	U
31	A	2005	U
31	A	2006	G
31	A	2007	U
31	A	2011	G
31	A	2034	C
31	A	2035	A
31	A	2037	G
31	A	2045	A
31	A	2046	G

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Mol	Chain	Res	Type
31	A	2047	A
31	A	2048	U
31	A	2069	C
31	A	2070	A
31	A	2073	A
31	A	2074	A
31	A	2075	G
31	A	2076	A
31	A	2077	C
31	A	2082	U
31	A	2083	G
31	A	2091	A
31	A	2094	G
31	A	2101	G
31	A	2103	G
31	A	2106	U
31	A	2107	G
31	A	2118	U
31	A	2122	C
31	A	2123	U
31	A	2124	G
31	A	2125	C
31	A	2126	G
31	A	2128	A
31	A	2129	G
31	A	2130	C
31	A	2132	U
31	A	2133	A
31	A	2134	G
31	A	2137	G
31	A	2139	A
31	A	2140	A
31	A	2142	G
31	A	2144	G
31	A	2145	A
31	A	2146	A
31	A	2147	G
31	A	2148	A
31	A	2151	G
31	A	2159	C
31	A	2160	C
31	A	2162	G

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Mol	Chain	Res	Type
31	A	2163	G
31	A	2173	G
31	A	2174	C
31	A	2175	C
31	A	2176	A
31	A	2178	C
31	A	2179	A
31	A	2181	U
31	A	2183	A
31	A	2184	G
31	A	2185	A
31	A	2186	U
31	A	2187	A
31	A	2189	C
31	A	2191	C
31	A	2192	U
31	A	2195	G
31	A	2198	A
31	A	2199	G
31	A	2201	G
31	A	2204	A
31	A	2209	U
31	A	2212	A
31	A	2220	G
31	A	2229	U
31	A	2230	A
31	A	2240	G
31	A	2242	A
31	A	2254	A
31	A	2255	G
31	A	2256	A
31	A	2266	U
31	A	2268	G
31	A	2269	G
31	A	2271	C
31	A	2272	G
31	A	2283	A
31	A	2286	A
31	A	2295	A
31	A	2297	G
31	A	2300	U
31	A	2304	A

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Mol	Chain	Res	Type
31	A	2317	G
31	A	2322	A
31	A	2323	C
31	A	2325	G
31	A	2342	G
31	A	2343	C
31	A	2344	A
31	A	2348	G
31	A	2352	A
31	A	2353	A
31	A	2361	U
31	A	2362	G
31	A	2364	C
31	A	2367	C
31	A	2374	C
31	A	2378	C
31	A	2394	A
31	A	2396	G
31	A	2400	G
31	A	2402	C
31	A	2405	A
31	A	2406	G
31	A	2408	G
31	A	2419	G
31	A	2423	A
31	A	2432	G
31	A	2436	U
31	A	2442	A
31	A	2443	A
31	A	2444	C
31	A	2445	G
31	A	2446	G
31	A	2452	A
31	A	2458	U
31	A	2464	G
31	A	2465	A
31	A	2466	U
31	A	2487	G
31	A	2493	A
31	A	2508	U
31	A	2509	U
31	A	2511	G

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Mol	Chain	Res	Type
31	A	2515	C
31	A	2518	C
31	A	2519	G
31	A	2520	A
31	A	2521	U
31	A	2522	G
31	A	2524	C
31	A	2535	C
31	A	2537	C
31	A	2549	G
31	A	2552	U
31	A	2579	U
31	A	2583	A
31	A	2584	G
31	A	2589	A
31	A	2590	C
31	A	2591	G
31	A	2593	G
31	A	2594	A
31	A	2597	U
31	A	2598	G
31	A	2599	G
31	A	2601	U
31	A	2602	U
31	A	2603	C
31	A	2619	A
31	A	2626	U
31	A	2627	C
31	A	2630	U
31	A	2632	U
31	A	2646	U
31	A	2647	A
31	A	2653	U
31	A	2671	A
31	A	2672	G
31	A	2674	A
31	A	2680	G
31	A	2690	G
31	A	2702	G
31	A	2706	U
31	A	2708	C
31	A	2719	G

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Mol	Chain	Res	Type
31	A	2729	A
31	A	2731	C
31	A	2732	G
31	A	2736	G
31	A	2744	A
31	A	2751	A
31	A	2753	C
31	A	2762	G
31	A	2764	U
31	A	2766	A
31	A	2768	A
31	A	2770	C
31	A	2771	A
31	A	2780	G
31	A	2783	A
31	A	2784	G
31	A	2796	A
52	a	5	A
52	a	6	U
52	a	7	G
52	a	10	G
52	a	31	U
52	a	32	G
52	a	33	A
52	a	40	G
52	a	45	A
52	a	48	C
52	a	49	U
52	a	50	U
52	a	52	A
52	a	55	C
52	a	62	G
52	a	72	A
52	a	75	U
52	a	82	U
52	a	83	C
52	a	85	A
52	a	90	C
52	a	92	G
52	a	100	A
52	a	104	A
52	a	105	C

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Mol	Chain	Res	Type
52	a	106	G
52	a	114	A
52	a	115	C
52	a	121	C
52	a	127	A
52	a	130	G
52	a	143	G
52	a	147	C
52	a	148	G
52	a	150	C
52	a	152	G
52	a	166	G
52	a	167	G
52	a	174	A
52	a	180	A
52	a	191	G
52	a	202	G
52	a	216	U
52	a	218	G
52	a	221	A
52	a	222	G
52	a	230	G
52	a	237	G
52	a	238	C
52	a	252	G
52	a	260	G
52	a	269	A
52	a	277	A
52	a	287	C
52	a	296	A
52	a	299	C
52	a	300	A
52	a	303	G
52	a	315	A
52	a	317	G
52	a	322	G
52	a	323	C
52	a	324	A
52	a	325	G
52	a	338	U
52	a	343	C
52	a	344	A

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Mol	Chain	Res	Type
52	a	349	G
52	a	353	A
52	a	355	G
52	a	358	U
52	a	360	A
52	a	369	U
52	a	377	G
52	a	382	C
52	a	383	A
52	a	384	G
52	a	392	A
52	a	393	C
52	a	395	G
52	a	399	G
52	a	400	U
52	a	410	U
52	a	411	U
52	a	416	G
52	a	423	A
52	a	424	G
52	a	426	A
52	a	429	G
52	a	432	G
52	a	433	G
52	a	434	U
52	a	443	A
52	a	444	A
52	a	447	A
52	a	453	G
52	a	456	U
52	a	459	C
52	a	466	C
52	a	469	G
52	a	472	G
52	a	475	G
52	a	478	G
52	a	479	U
52	a	481	A
52	a	495	A
52	a	507	A
52	a	510	G
52	a	511	A

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Mol	Chain	Res	Type
52	a	512	U
52	a	514	G
52	a	520	A
52	a	521	A
52	a	524	C
52	a	525	G
52	a	536	G
52	a	543	A
52	a	544	A
52	a	566	C
52	a	577	A
52	a	578	C
52	a	579	A
52	a	580	G
52	a	600	U
52	a	601	G
52	a	602	G
52	a	613	G
52	a	630	G
52	a	650	A
52	a	651	G
52	a	659	A
52	a	660	A
52	a	669	A
52	a	670	A
52	a	671	C
52	a	672	G
52	a	695	A
52	a	696	C
52	a	697	A
52	a	703	A
52	a	725	A
52	a	741	U
52	a	742	A
52	a	757	G
52	a	762	A
52	a	763	A
52	a	765	C
52	a	766	G
52	a	768	U
52	a	769	G
52	a	775	U

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Mol	Chain	Res	Type
52	a	776	A
52	a	780	G
52	a	784	U
52	a	790	U
52	a	791	C
52	a	794	C
52	a	795	C
52	a	796	C
52	a	797	G
52	a	798	U
52	a	799	G
52	a	821	A
52	a	822	A
52	a	825	A
52	a	834	G
52	a	838	A
52	a	849	A
52	a	851	G
52	a	863	A
52	a	875	G
52	a	876	G
52	a	883	C
52	a	884	A
52	a	909	U
52	a	915	G
52	a	918	A
52	a	920	G
52	a	924	A
52	a	925	G
52	a	926	A
52	a	938	G
52	a	941	U
52	a	942	G
52	a	945	A
52	a	946	U
52	a	948	C
52	a	953	A
52	a	954	A
52	a	958	U
52	a	961	U
52	a	963	A
52	a	964	A

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Mol	Chain	Res	Type
52	a	969	A
52	a	973	G
52	a	974	U
52	a	975	G
52	a	978	U
52	a	980	C
52	a	981	G
52	a	982	G
52	a	985	A
52	a	986	C
52	a	992	C
52	a	994	C
52	a	995	A
52	a	1003	C
52	a	1005	U
52	a	1014	U
52	a	1027	U
52	a	1034	U
52	a	1038	G
52	a	1041	A
52	a	1043	G
52	a	1044	U
52	a	1047	C
52	a	1050	A
52	a	1057	G
52	a	1066	G
52	a	1073	G
52	a	1074	U
52	a	1075	U
52	a	1079	A
52	a	1080	A
52	a	1082	G
52	a	1088	U
52	a	1089	U
52	a	1091	G
52	a	1095	C
52	a	1099	G
52	a	1100	A
52	a	1105	A
52	a	1107	U
52	a	1114	G
52	a	1115	A

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Mol	Chain	Res	Type
52	a	1116	U
52	a	1119	G
52	a	1130	G
52	a	1131	U
52	a	1132	G
52	a	1144	A
52	a	1149	A
52	a	1150	U
52	a	1160	U
52	a	1161	A
52	a	1162	U
52	a	1163	G
52	a	1174	C
52	a	1175	A
52	a	1184	A
52	a	1186	A
52	a	1187	A
52	a	1188	U
52	a	1189	G
52	a	1195	G
52	a	1198	A
52	a	1204	U
52	a	1205	C
52	a	1206	G
52	a	1208	G
52	a	1222	G
52	a	1223	A
52	a	1227	A
52	a	1229	C
52	a	1233	A
52	a	1234	A
52	a	1235	A
52	a	1243	C
52	a	1246	C
52	a	1247	A
52	a	1248	G
52	a	1250	U
52	a	1253	G
52	a	1265	C
52	a	1266	A
52	a	1267	A
52	a	1271	G

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Mol	Chain	Res	Type
52	a	1280	A
52	a	1288	A
52	a	1294	A
52	a	1295	G
52	a	1311	C
52	a	1312	A
52	a	1317	G
52	a	1319	G
52	a	1327	C
52	a	1328	G
52	a	1346	C
52	a	1347	A
52	a	1351	C
52	a	1368	G
52	a	1371	G
52	a	1390	A
52	a	1395	A
52	a	1397	C
52	a	1400	C
52	a	1401	A
52	a	1402	A
52	a	1403	G
52	a	1405	A
52	a	1418	A
52	a	1441	A
52	a	1443	G
52	a	1452	A
52	a	1454	G
52	a	1455	U
52	a	1466	G
52	a	1478	G
52	a	1479	G
52	a	1480	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	B	57	U
27	W	29	U
27	W	32	C
27	W	33	A
27	W	97	A

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Mol	Chain	Res	Type
31	A	5	A
31	A	97	A
31	A	514	A
31	A	556	C

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.