



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 10, 2017 – 06:32 PM EDT

PDB ID : 5O61
EMDB ID: : EMD-3751
Title : The complete structure of the Mycobacterium smegmatis 70S ribosome
Authors : Hentschel, J.; Burnside, C.; Mignot, I.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on : unknown
Resolution : 3.31 Å(reported)

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

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

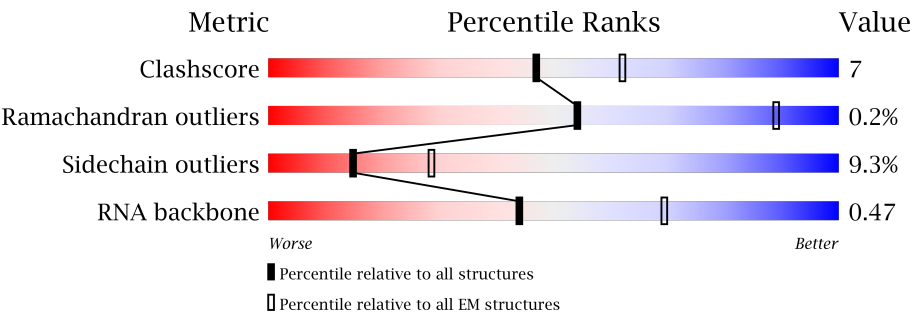
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

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 3.31 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.










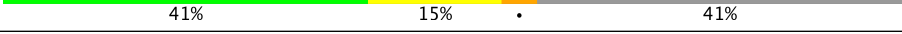


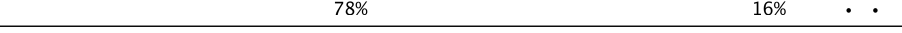
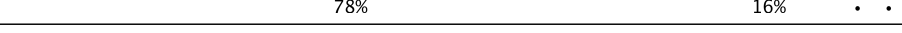
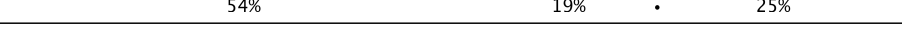


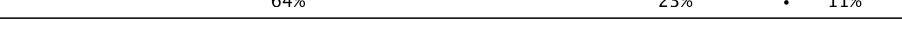









Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	3	24	71% 25% .
2	A	3120	64% 27% 8% .
3	B	118	69% 28% .
4	C	278	64% 31% . .
5	D	217	67% 29% . .
6	E	215	69% 27% . .
7	F	187	65% 27% 5% . .
8	G	179	74% 21% . .














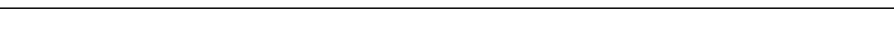










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Mol	Chain	Length	Quality of chain
9	H	151	 79% 19% .
10	I	175	 50% 21% . 28%
11	J	142	 56% 35% . 6%
12	K	147	 80% 18% ..
13	L	122	 74% 23% .
14	M	147	 71% 23% 5% .
15	N	138	 66% 29% . .
16	O	199	 41% 15% . 41%
17	P	127	 80% 18% ..
18	Q	113	 66% 29% .
19	R	129	 78% 16% . .
20	S	103	 78% 16% . .
21	T	153	 54% 19% . 25%
22	U	100	 82% 14% ..
23	V	105	 67% 24% . 8%
24	W	215	 64% 23% . 11%
25	X	88	 72% 18% 10%
26	Y	64	 70% 27% . .
27	Z	77	 65% 17% . 17%
28	a	61	 90% 7% .
29	b	57	 82% 12% 5%
30	c	55	 76% 13% 11%
31	d	47	 89% 9% .
32	e	64	 89% 9% .
33	f	37	 95% 5%

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Mol	Chain	Length	Quality of chain
34	g	75	
35	BA	1528	
36	BB	33	
37	BC	275	
38	BD	201	
39	BE	214	
40	BF	96	
41	BG	156	
42	BH	132	
43	BI	150	
44	BJ	101	
45	BK	138	
46	BL	124	
47	BM	124	
48	BN	61	
49	BO	89	
50	BP	156	
51	BQ	98	
52	BR	84	
53	BS	93	
54	BT	86	
55	BV	277	
56	BW	76	
57	BX	6	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 151463 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 bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3119	Total	C	N	O	P	0	0
			66981	29854	12313	21695	3119		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	126	Total	C	N	O	S	0	0
			956	586	199	171			

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	124	Total	C	N	O	S	0	0
			988	613	203	172			

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	100	Total	C	N	O	S	0	0
			754	478	137	139			

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	W	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 26 is a protein called LSU ribosomal protein L28P.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	a	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 30 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	63	Total	C	N	O	0	0
			502	302	115	85		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 34 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	59	Total	C	N	O	S	0	0
			458	284	84	85	5		

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	1511	Total	C	N	O	P	0	0
			32439	14448	5930	10550	1511		

- Molecule 36 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	32	Total	C	N	O	S	0	0
			280	172	71	36	1		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	208	Total	C	N	O	S	0	0
			1660	1036	322	298	4		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	200	Total	C	N	O	S	0	0
			1641	1028	316	295	2		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	180	Total	C	N	O	S	0	0
			1296	812	245	235	4		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	96	Total	C	N	O	S	0	0
			771	486	138	145	2		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	155	Total	C	N	O	S	0	0
			1232	768	241	221	2		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	131	Total	C	N	O	S	0	0
			1010	633	189	187	1		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BI	122	Total	C	N	O	S	0	0
			994	630	194	170			

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	99	Total	C	N	O	S	0	0
			788	495	146	144	3		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BK	115	Total	C	N	O	S	0	0
			855	528	170	156	1		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BL	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BM	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	60	Total	C	N	O	S	0	0
			477	302	97	73	5		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	BO	88	Total	C	N	O	0	0
			720	449	147	124		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BP	113	Total	C	N	O	0	0
			891	570	162	159		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 52 is a protein called 30S ribosomal protein S18 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BR	65	Total	C	N	O	S	0	0
			513	318	102	90	3		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	82	Total	C	N	O	S	0	0
			662	425	124	112	1		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	BT	85	Total	C	N	O	0	0
			660	402	139	119		

- Molecule 55 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BV	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 56 is a RNA chain called P/P-site Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BW	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 57 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BX	6	Total	C	N	O	P	0	0
			117	54	13	45	5		

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	BA	215	Total	Mg	0
			215	215	
58	BF	1	Total	Mg	0
			1	1	
58	B	9	Total	Mg	0
			9	9	
58	C	4	Total	Mg	0
			4	4	
58	c	1	Total	Mg	0
			1	1	
58	BR	1	Total	Mg	0
			1	1	
58	A	390	Total	Mg	0
			390	390	
58	T	1	Total	Mg	0
			1	1	
58	N	1	Total	Mg	0
			1	1	
58	F	1	Total	Mg	0
			1	1	
58	M	1	Total	Mg	0
			1	1	

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

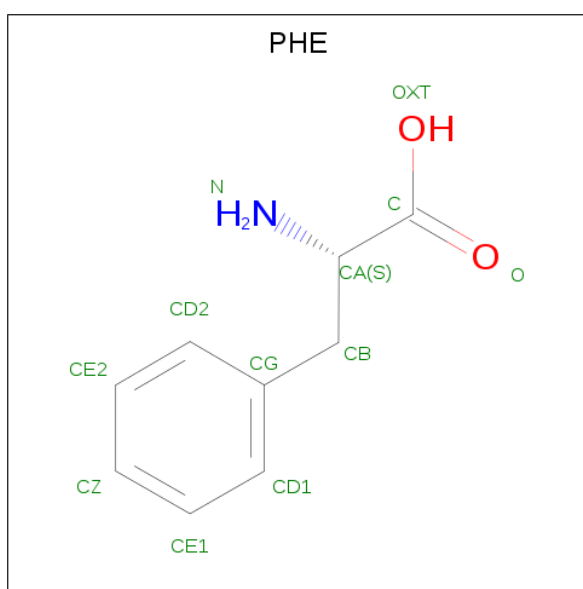
Mol	Chain	Residues	Atoms		AltConf
59	g	1	Total	Zn	0
			1	1	
59	BN	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
59	c	1	Total	Zn	0
			1	1	
59	BR	1	Total	Zn	0
			1	1	
59	Y	1	Total	Zn	0
			1	1	
59	f	1	Total	Zn	0
			1	1	

- Molecule 60 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
60	BW	1	Total	C	N	O	0
			11	9	1	1	

3 Residue-property plots

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

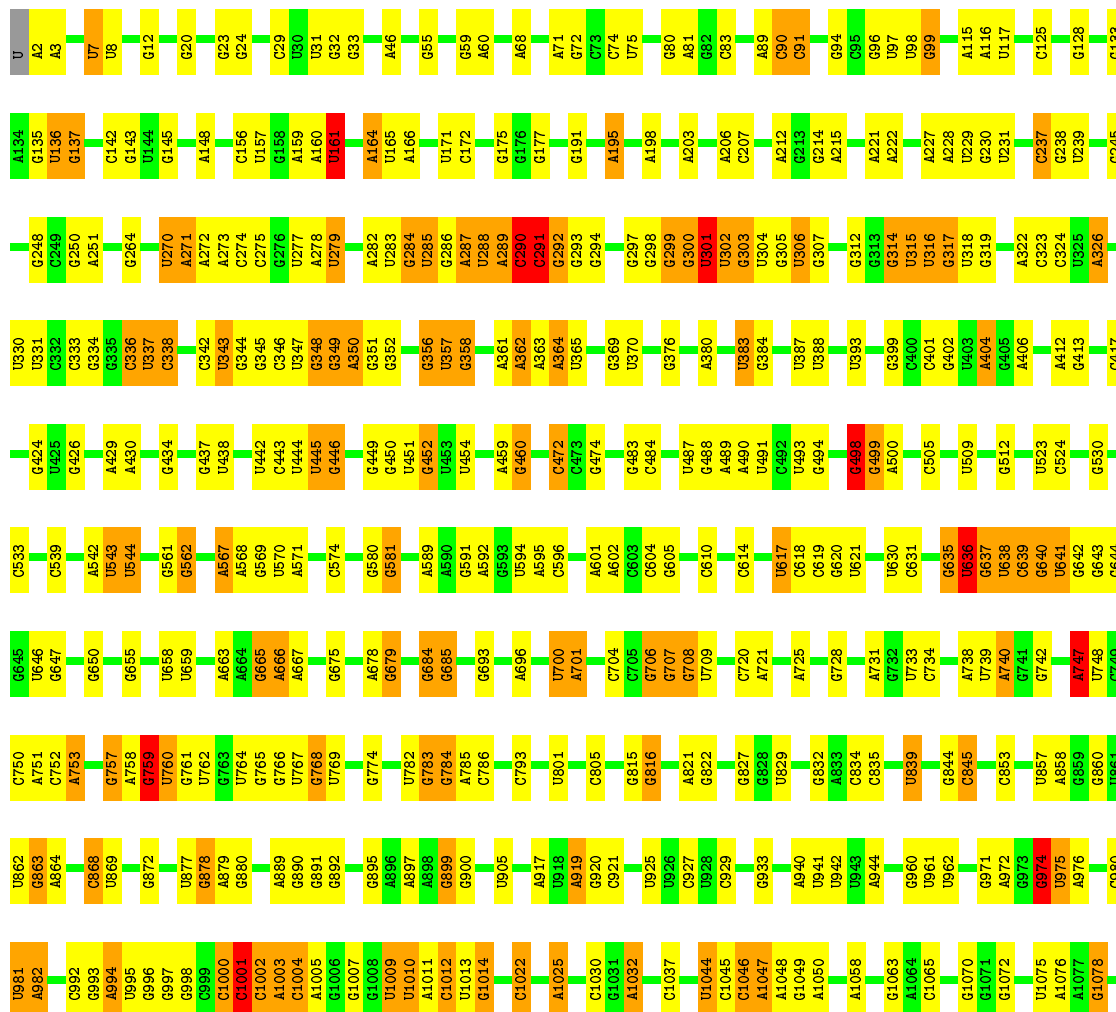
- Molecule 1: 50S ribosomal protein bL37

Chain 3: 

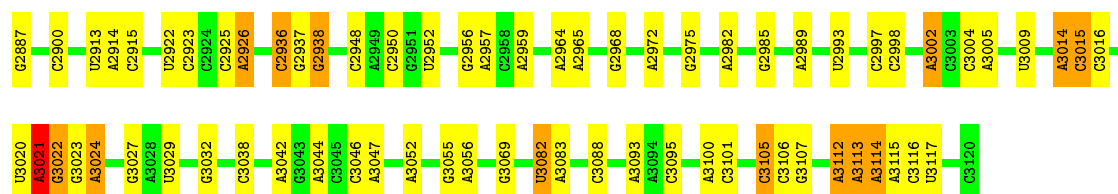


- Molecule 2: 23S rRNA

Chain A: 



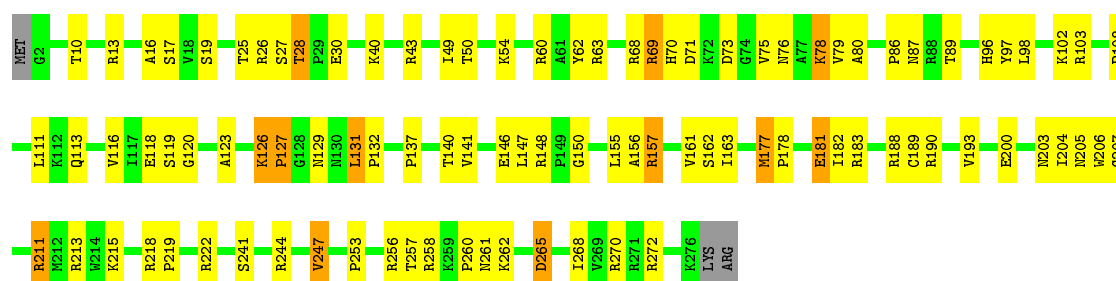
G2750	G2683	G2532	C2423	G2354	U2261	C2129	G2009	A1855	A1731	A1543	C1430	U1294	U1200	C1081
G2753	A2694	U2543	C2424	U2355	C2262	G2130	G2014	C1856	U1732	G1550	U1431	U1295	G1201	U1084
C2757	A2655	U2544	G2427	G2356	G2263	G2131	G2017	U1857	C1733	U1551	C1435	U1303	A1202	G1085
G2759	A2659	G2545	C2431	A2358	C2267	A2137	C2018	G1862	A1737	G1552	C1436	A1304	G1204	A1091
C2760	C2685	U2548	C2434	C2362	C2271	U2138	U2022	G1863	G1738	G1553	C1437	G1312	A1206	G1092
G2761	G2669	U2549	U2435	G2366	C2274	A2140	U2025	U1864	U1745	G1554	C1438	G1207	G1208	A1099
C2762	A2672	U2550	A2436	G2367	A2275	U2147	A2026	A1865	G1746	A1555	C1439	U1324	C1209	C1100
G2772	U2673	A2551	U2437	C2368	G2276	C2148	A2027	G1867	G1747	U1560	C1441	U1325	G1209	A1101
U2778	A2677	G2553	U2442	C2369	G2277	U2149	G2028	A1868	A1748	U1563	G1443	G1332	U1212	G1102
U2779	U2687	A2557	U2443	A2370	A2278	G2153	U2028	G1869	C1753	A1564	C1448	G1335	A1213	G1114
C2780	C2686	C2558	A2444	G2371	C2279	G2154	U2032	G1870	G1754	A1565	C1454	G1339	G1217	C1130
G2781	U2687	U2550	A2445	U2372	G2280	A2159	U2033	A1871	A1755	A1566	U1455	G1339	C1218	G1131
C2782	C2688	A2559	G2373	G2374	A2284	A2160	G2034	U1875	G1756	C1567	U1456	G1343	U1219	G1140
C2689	G2447	U2567	G2448	G2375	G2285	A2162	U2035	A1876	G1757	G1574	C1456	A1344	C1220	
U2786	A2449	U2568	A2449	G2379	A2286	A2163	C2043	U1877	A1759	G1575	C1457	G1345	A1221	
C2691	U2457	G2569	U2457	G2380	C2299	U2164	U2044	U1878	G1760	U1576	C1460	G1353	G1224	G1143
A2692	G2458	U2570	G2458	A2381	C2304	U2179	G2045	A1892	G1761	C1577	C1461	G1353	G1224	A1144
A2693	G2459	C2571	G2382	G2383	A2305	U2184	A2046	C1893	G1762	G1578	C1462	G1359	G1227	A1145
G2694	U2460	U2574	U2383	U2384	A2306	A2184	U2061	C1904	G1763	C1579	G1462	G1381	A1228	A1146
C2698	G2461	G2580	G2385	C2386	U2315	A2190	A2064	G1905	U1767	U1584	C1465	A1362	A1229	A1147
A2700	G2462	U2581	G2386	U2387	G2316	C2191	A2065	C1906	U1774	U1585	C1466	G1363	A1230	G1148
G2800	U2467	U2585	G2388	U2389	C2320	A2194	G2066	U1932	C1785	G1586	C1467	G1365	G1231	U1151
A2702	U2470	U2586	U2390	U2391	A2324	G2196	A2070	U1933	G1786	G1587	C1468	G1365	G1232	U1152
C2703	A2471	U2587	G2391	G2392	U2325	G2197	A2071	A1940	A1787	U1593	C1485	A1368	G1236	U1153
C2803	C2472	U2588	C2472	A2392	U2326	C2198	A2073	A1941	G1788	C1596	C1486	A1369	U1237	U1158
G2806	G2483	U2589	G2483	A2393	G2328	G2199	G2074	U1945	A1789	U1599	C1486	G1371	C1238	G1162
A2826	A2491	G2603	A2491	A2394	G2329	U2215	G2075	U1946	U1792	G1601	C1488	A1380	C1239	A1163
G2827	A2492	U2604	A2492	A2395	U2330	G2216	U2084	U1947	C1795	U1602	C1489	G1381	G1240	A1164
U2833	G2495	G2607	G2495	C2397	U2332	G2217	C2084	U1948	C1796	U1603	G1502	G1386	A1247	G1165
A2837	U2496	U2608	G2496	A2398	G2333	U2217	C2085	C1949	C1797	G1603	G1502	A1387	U1250	G1173
U2839	A2497	U2613	A2497	C2400	U2334	A2221	C2086	G1950	U1798	G1606	G1507	U1388	A1251	G1174
G2718	U2502	U2614	U2502	U2401	U2335	A2227	C2087	C1953	A1799	G1612	A1510	A1390	G1252	A1175
C2843	G2503	C2618	G2503	C2402	U2336	G2234	U2090	C1954	G1801	U1613	A1518	G1400	G1253	G1177
C2853	G2504	U2626	A2405	A2406	U2337	C2235	U2092	G1967	G1802	G1614	C1400	G1257	G1254	U1178
A2856	C2505	C2627	U2406	U2407	U2341	A2244	G2093	C1973	A1803	G1615	C1403	G1258	U1259	G1180
G2729	G2506	U2627	C2408	C2507	A2342	C2245	G2094	A1974	G1805	A1616	C1404	C1260	A1261	A1184
G2732	C2508	U2636	U2409	C2508	G2343	U2246	G2096	A1975	A1806	C1617	C1404	G1260	A1261	A1185
A2862	U2511	G2637	A2410	U2411	U2344	A2247	A2106	U1981	G1813	U1619	C1410	A1261	A1261	A1186
G2864	U2512	U2643	U2412	U2413	G2345	C2248	G2107	C1621	U1717	U1620	G1411	A1275	A1275	A1187
C2869	U2515	U2647	G2413	G2414	U2346	G2251	A2108	G1622	U1820	C1621	C1412	G1276	G1276	A1188
C2741	U2516	C2648	U2418	U2419	G2347	A2252	A2109	G1625	C1825	U1533	C1415	G1282	G1282	C1190
A2742	C2521	U2649	U2421	A2422	U2348	A2253	U2111	G1627	A1826	C1534	A1416	G1282	G1282	A1191
G2885	C2522	U2650	A2421	A2422	G2349	A2254	U2112	U1627	G1840	U1536	A1417	C1290	C1290	G1192
A2886	U2353	U2353	G2352	A2422	G2350	A2255	U2120	U1628	U1728	U1540	U1427	G1291	G1291	C1196
	U2353	U2353	G2352	A2422	G2350	A2255	U2120	U1628	U1728	U1540	U1427	G1291	G1291	U1199



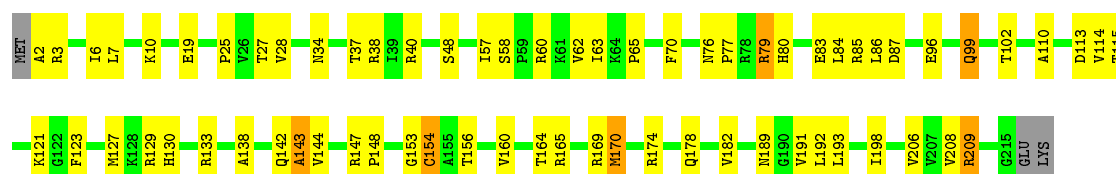
- Molecule 3: 5S rRNA



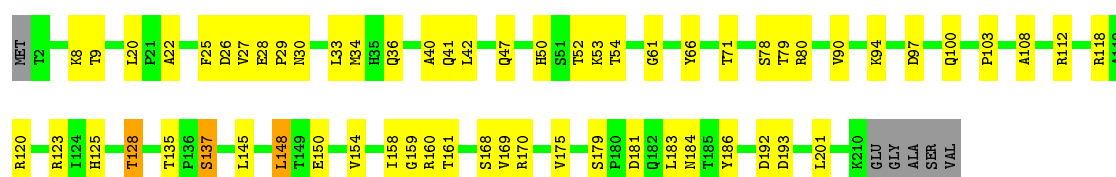
- Molecule 4: 50S ribosomal protein L2



- Molecule 5: 50S ribosomal protein L3

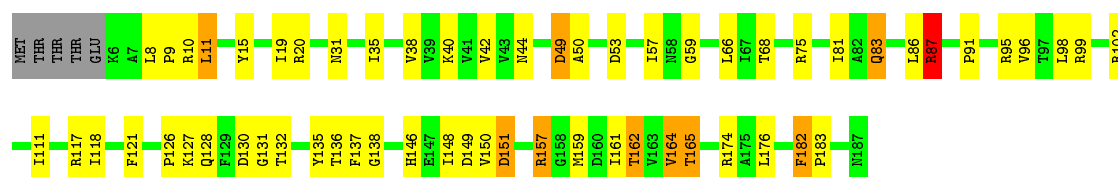


- Molecule 6: 50S ribosomal protein L4

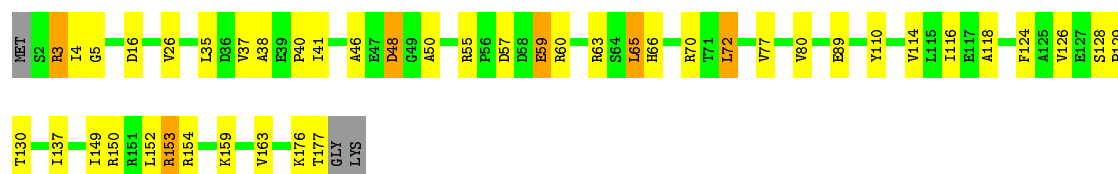


- Molecule 7: 50S ribosomal protein L5

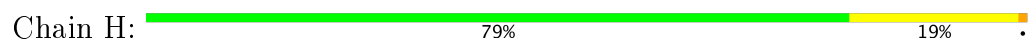




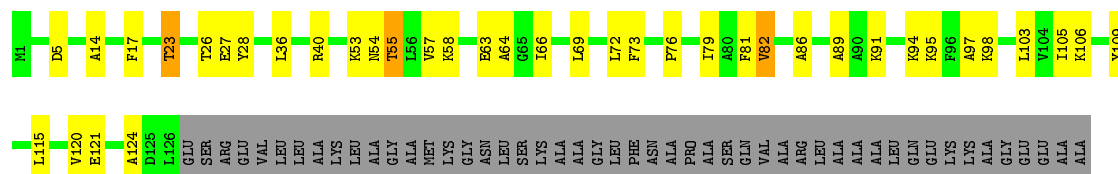
• Molecule 8: 50S ribosomal protein L6



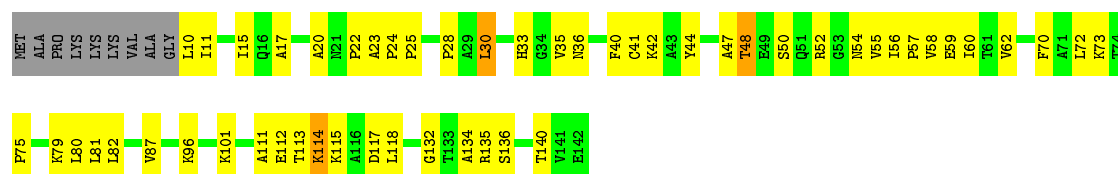
• Molecule 9: 50S ribosomal protein L9



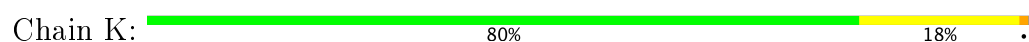
• Molecule 10: 50S ribosomal protein L10



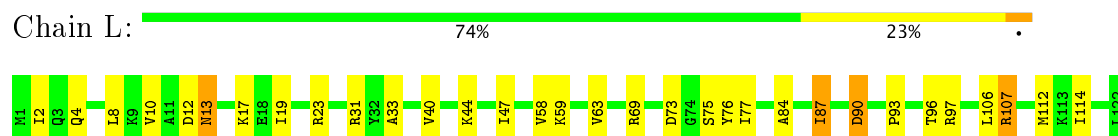
• Molecule 11: 50S ribosomal protein L11



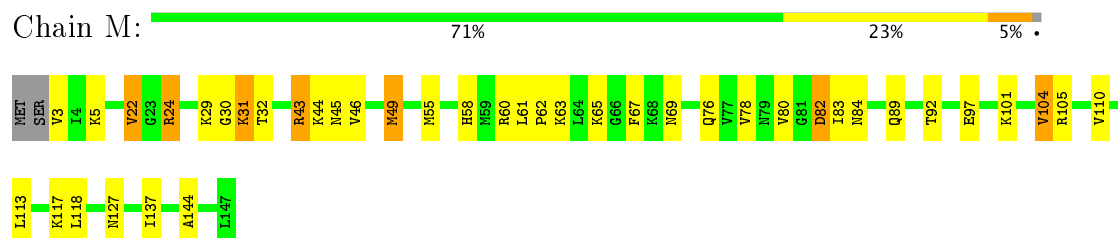
• Molecule 12: 50S ribosomal protein L13



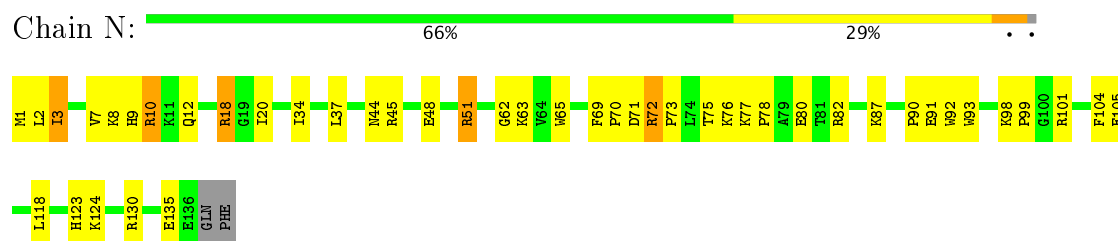
• Molecule 13: 50S ribosomal protein L14



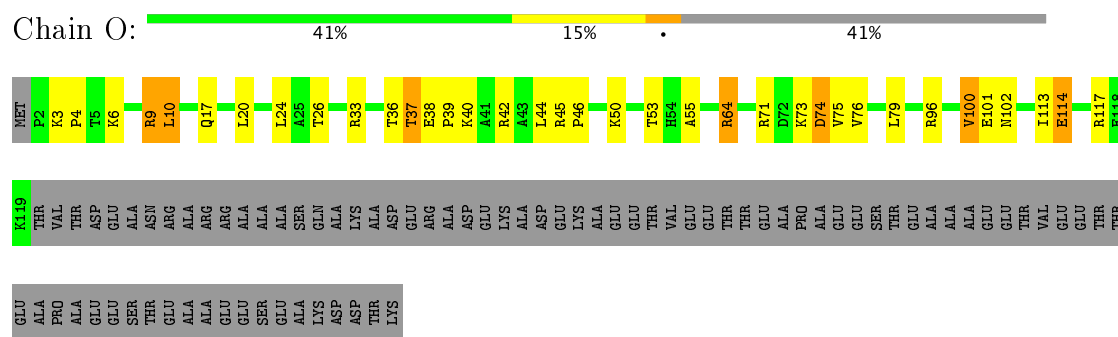
- Molecule 14: 50S ribosomal protein L15



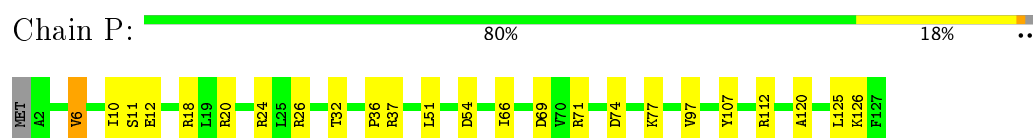
- Molecule 15: 50S ribosomal protein L16



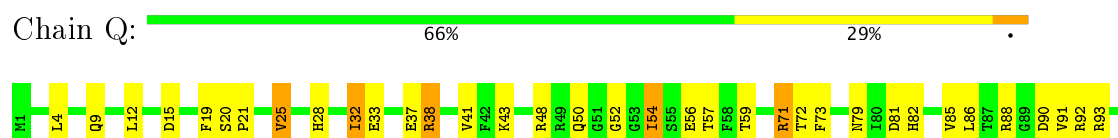
- Molecule 16: 50S ribosomal protein L17



- Molecule 17: 50S ribosomal protein L18



- Molecule 18: 50S ribosomal protein L19





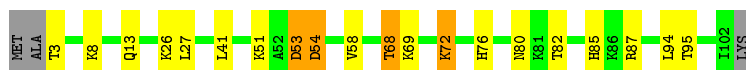
- Molecule 19: 50S ribosomal protein L20

Chain R: 78% 16%



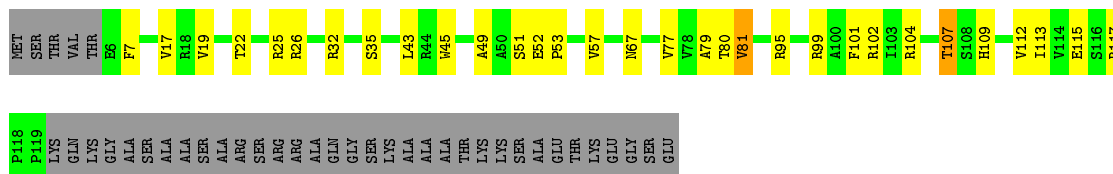
- Molecule 20: 50S ribosomal protein L21

Chain S: 78% 16%



- Molecule 21: 50S ribosomal protein L22

Chain T: 54% 19% 25%



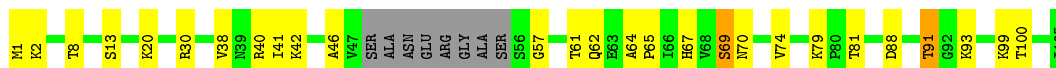
- Molecule 22: 50S ribosomal protein L23

Chain U: 82% 14%



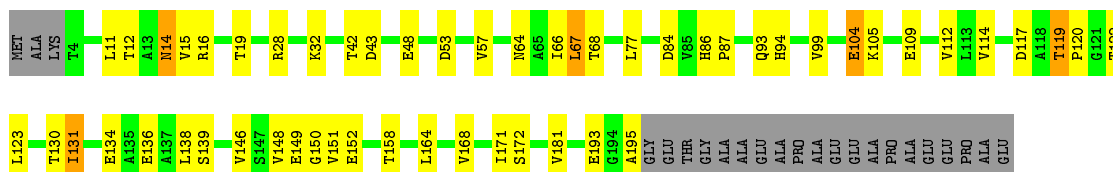
- Molecule 23: 50S ribosomal protein L24

Chain V: 67% 24% 8%

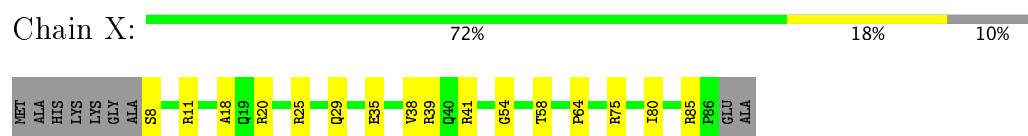


- Molecule 24: 50S ribosomal protein L25

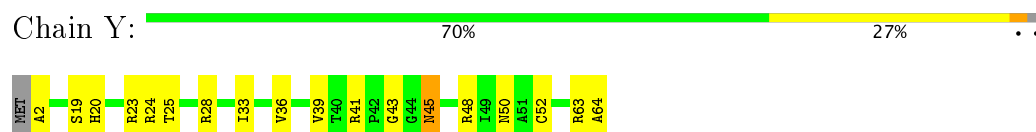
Chain W: 64% 23% 11%



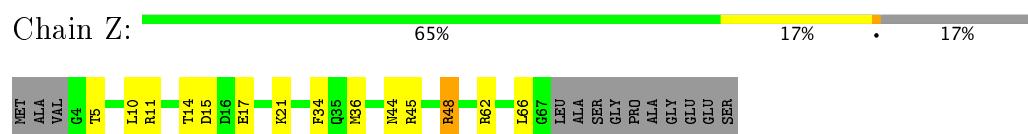
- Molecule 25: 50S ribosomal protein L27



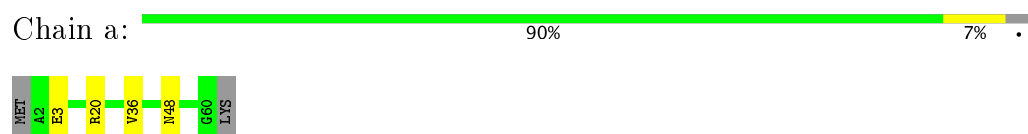
- Molecule 26: LSU ribosomal protein L28P



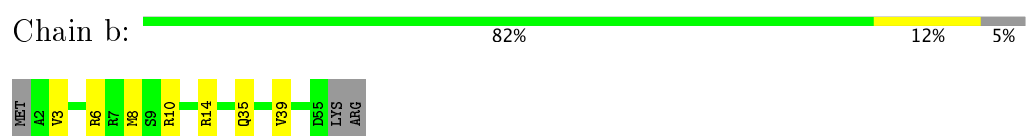
- Molecule 27: 50S ribosomal protein L29



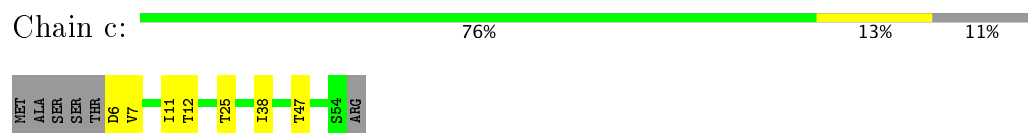
- Molecule 28: 50S ribosomal protein L30



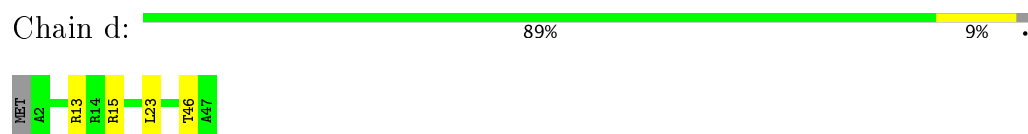
- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33 1



- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35





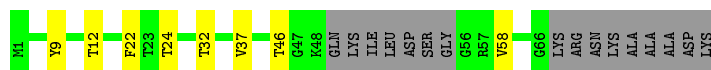
- Molecule 33: 50S ribosomal protein L36

Chain f: 95% 5%



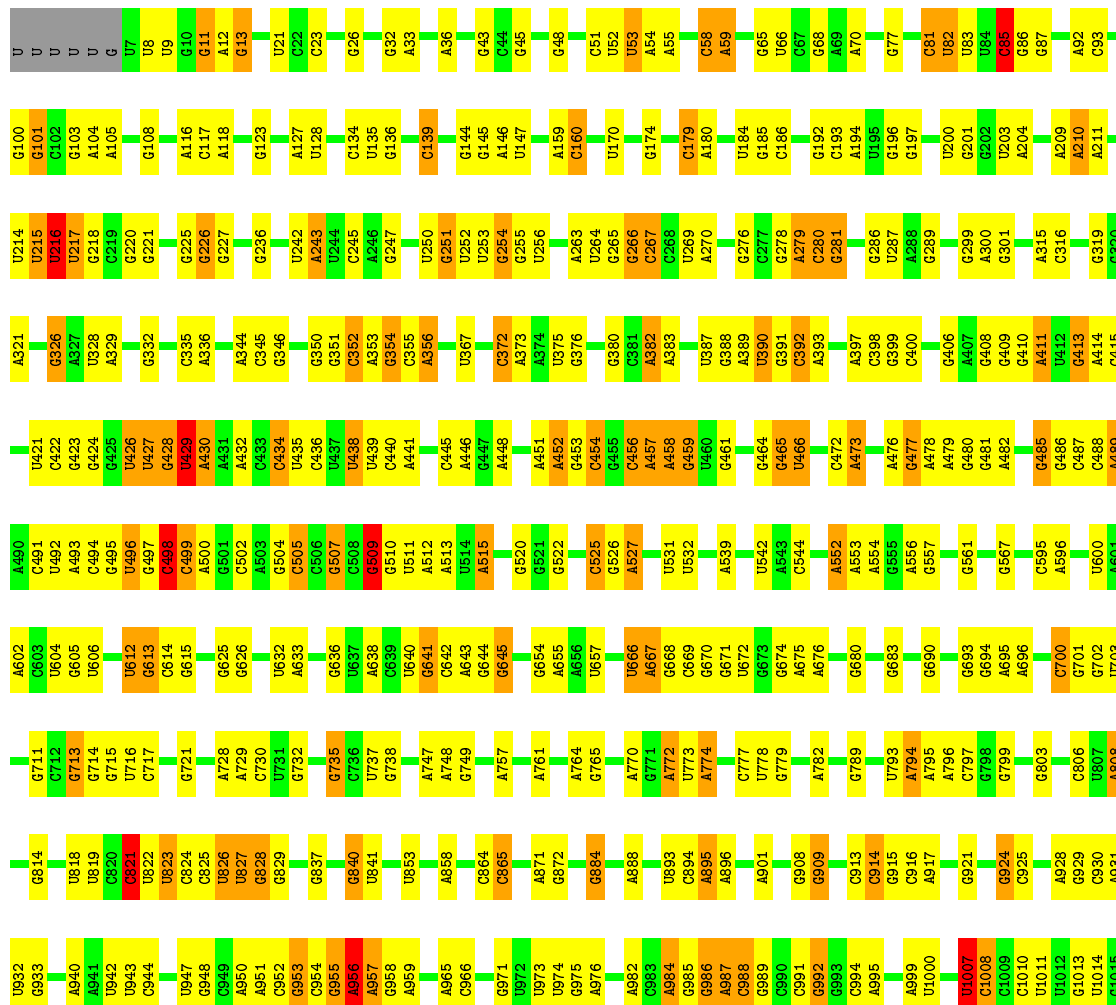
- Molecule 34: 50S ribosomal protein L31

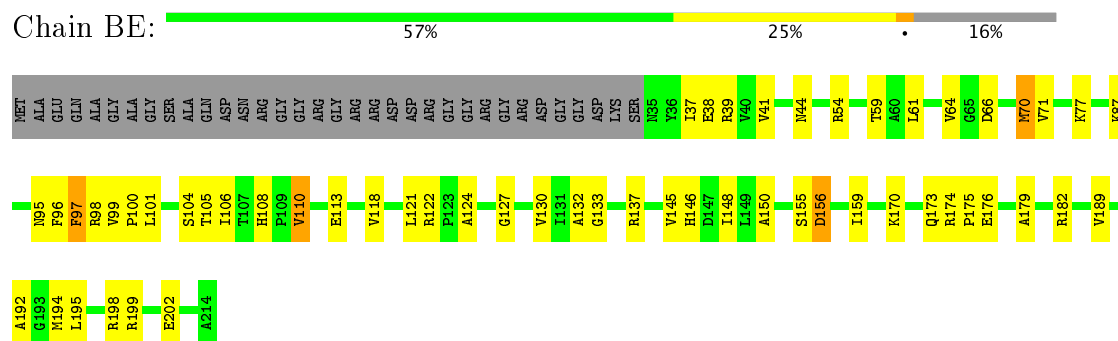
Chain g: 68% 11% 21%



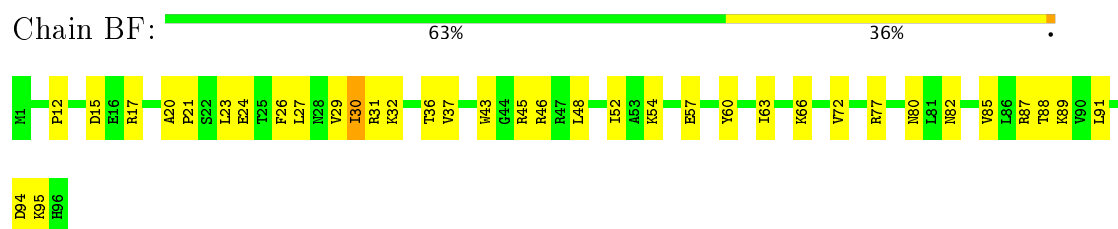
- Molecule 35: 16S rRNA

Chain BA: 57% 32% 10% ..

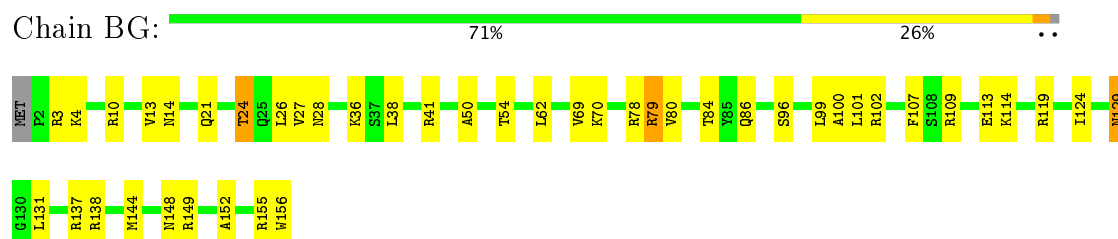




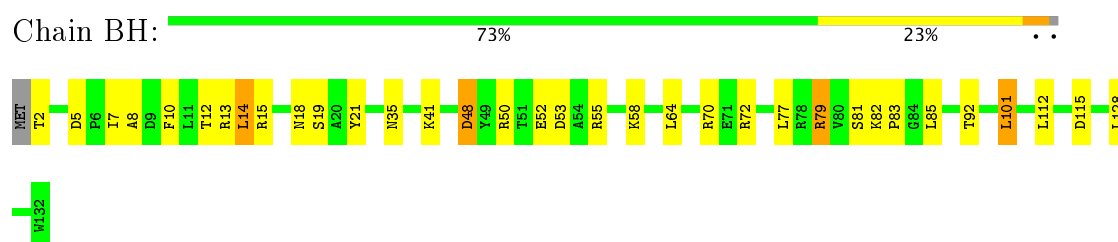
- Molecule 40: 30S ribosomal protein S6



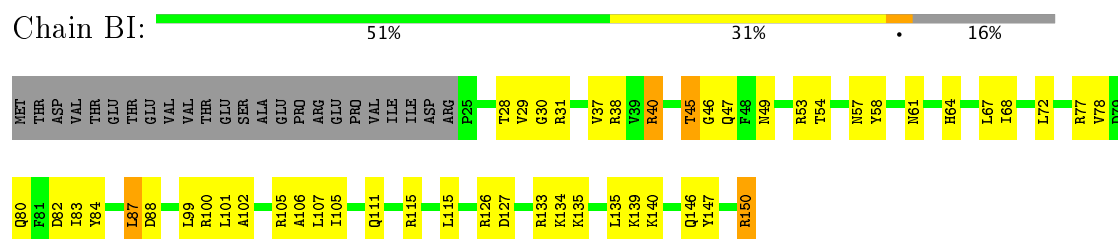
- Molecule 41: 30S ribosomal protein S7



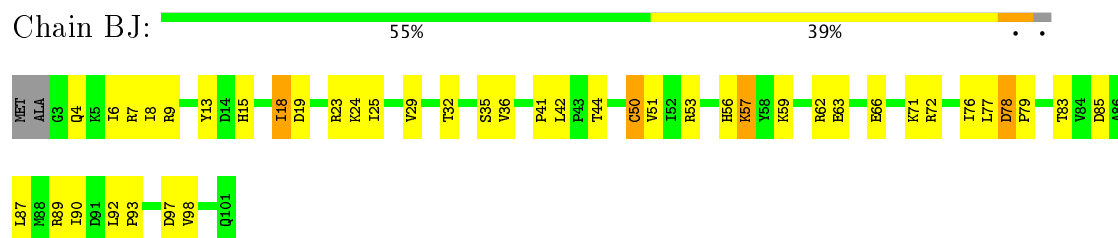
- Molecule 42: 30S ribosomal protein S8



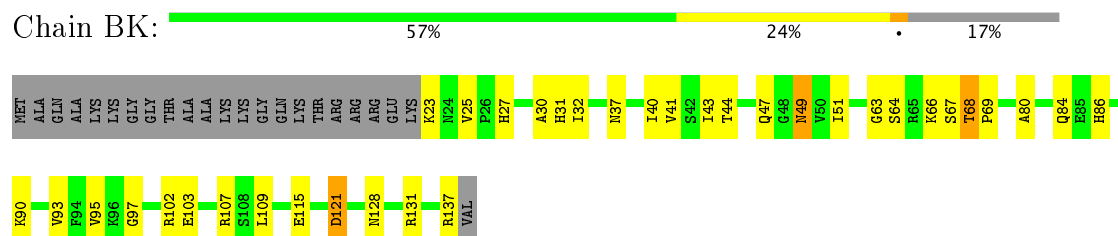
- Molecule 43: 30S ribosomal protein S9



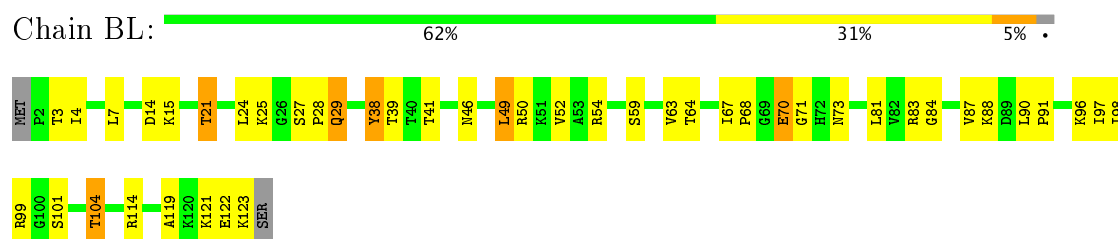
- Molecule 44: 30S ribosomal protein S10



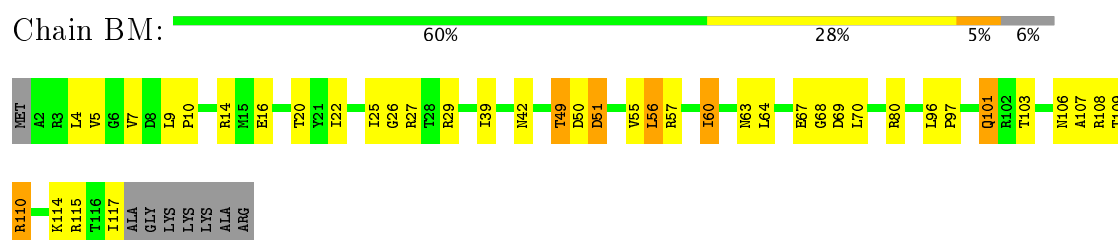
- Molecule 45: 30S ribosomal protein S11



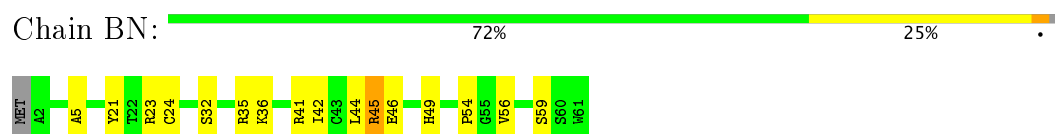
- Molecule 46: 30S ribosomal protein S12



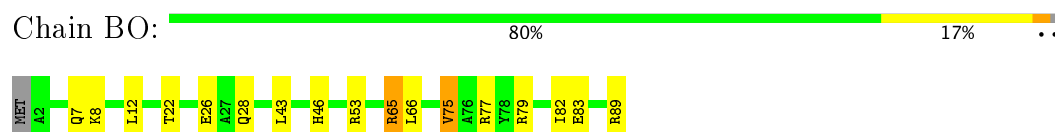
- Molecule 47: 30S ribosomal protein S13



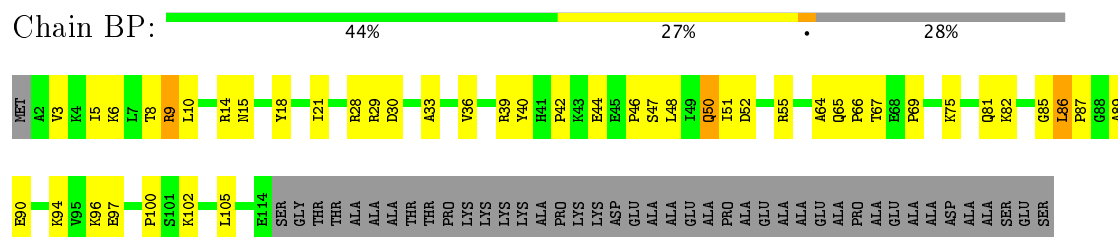
- Molecule 48: 30S ribosomal protein S14 type Z



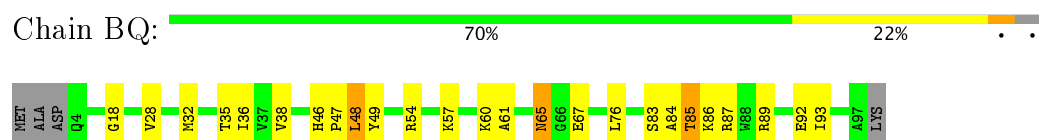
- Molecule 49: 30S ribosomal protein S15



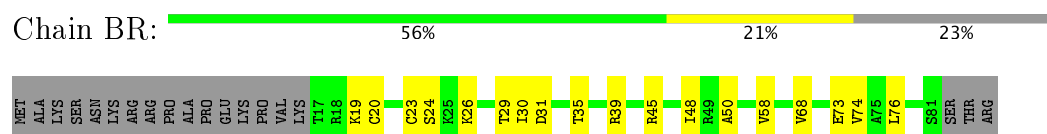
- Molecule 50: 30S ribosomal protein S16



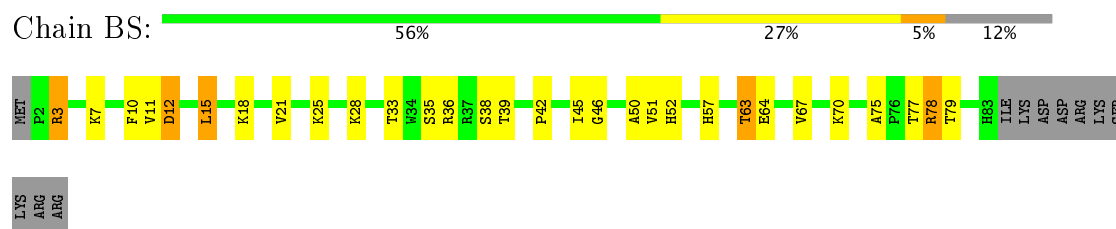
- Molecule 51: 30S ribosomal protein S17



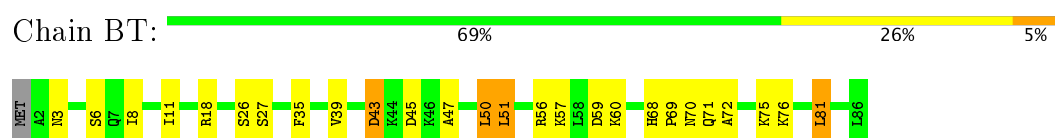
- Molecule 52: 30S ribosomal protein S18 2



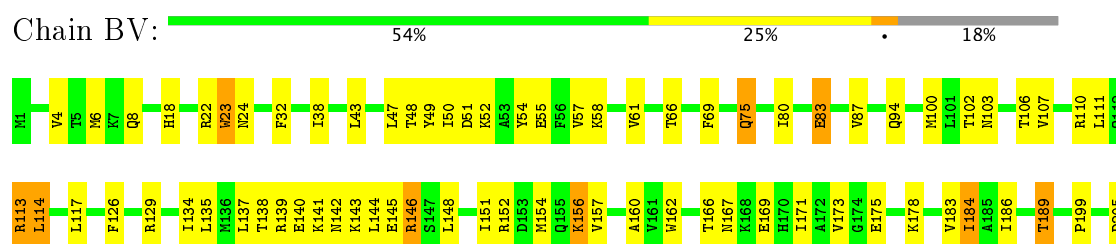
- Molecule 53: 30S ribosomal protein S19

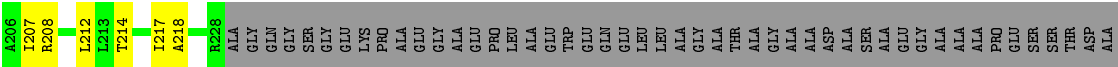


- Molecule 54: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein S2



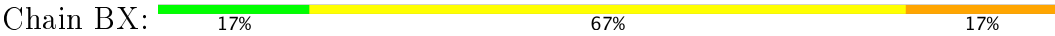


SER

- Molecule 56: P/P-site Phe-tRNA(Phe)



- Molecule 57: mRNA fragment



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224584	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	3	0.46	0/191	0.52	0/247
10	I	0.62	0/925	0.61	0/1246
11	J	0.65	0/1006	0.63	0/1364
12	K	0.46	0/1157	0.56	0/1567
13	L	0.48	0/946	0.58	0/1268
14	M	0.46	0/1091	0.66	0/1457
15	N	0.50	0/1118	0.63	0/1506
16	O	0.46	0/945	0.63	0/1267
17	P	0.36	0/966	0.53	0/1298
18	Q	0.47	0/921	0.64	0/1236
19	R	0.64	1/1000 (0.1%)	0.73	4/1341 (0.3%)
2	A	0.78	4/75001 (0.0%)	1.06	101/117027 (0.1%)
20	S	0.43	0/764	0.61	0/1030
21	T	0.58	0/887	0.63	1/1204 (0.1%)
22	U	0.45	0/766	0.54	0/1030
23	V	0.39	0/738	0.55	0/987
24	W	0.38	0/1443	0.56	0/1970
25	X	0.49	0/595	0.57	0/798
26	Y	0.50	0/478	0.62	0/641
27	Z	0.43	0/534	0.52	0/713
28	a	0.47	0/477	0.59	0/640
29	b	0.46	0/427	0.61	0/572
3	B	0.48	0/2821	0.93	1/4396 (0.0%)
30	c	0.40	0/413	0.56	0/553
31	d	0.49	0/380	0.63	1/500 (0.2%)
32	e	0.44	0/507	0.56	0/672
33	f	0.50	0/303	0.59	0/401
34	g	0.41	0/467	0.53	0/626
35	BA	0.57	1/36309 (0.0%)	1.02	60/56657 (0.1%)
36	BB	0.42	0/280	0.56	0/359
37	BC	0.39	0/1684	0.54	0/2261
38	BD	0.51	1/1672 (0.1%)	0.59	1/2251 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BE	0.40	0/1312	0.54	0/1772
4	C	0.50	0/2153	0.62	0/2895
40	BF	0.40	0/782	0.61	0/1059
41	BG	0.41	0/1252	0.50	0/1690
42	BH	0.35	0/1025	0.58	0/1385
43	BI	0.40	0/1012	0.53	0/1362
44	BJ	0.43	0/802	0.54	0/1086
45	BK	0.39	0/873	0.56	0/1180
46	BL	0.40	0/969	0.58	0/1294
47	BM	0.36	0/942	0.53	0/1260
48	BN	0.34	0/488	0.55	0/650
49	BO	0.37	0/729	0.55	0/977
5	D	0.49	0/1609	0.62	0/2165
50	BP	0.40	0/908	0.64	0/1226
51	BQ	0.39	0/759	0.57	0/1016
52	BR	0.42	0/518	0.53	0/693
53	BS	0.47	0/680	0.58	0/915
54	BT	0.42	0/663	0.54	0/882
55	BV	0.53	0/1822	0.56	0/2457
56	BW	0.68	0/1809	1.08	2/2819 (0.1%)
57	BX	0.57	0/128	0.95	0/196
6	E	0.42	0/1592	0.56	0/2153
7	F	0.38	0/1467	0.60	2/1973 (0.1%)
8	G	0.36	0/1369	0.52	0/1848
9	H	0.44	0/1027	0.53	1/1398 (0.1%)
All	All	0.65	7/163902 (0.0%)	0.95	174/245436 (0.1%)

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
21	T	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	61	TRP	CD2-CE2	8.39	1.51	1.41
38	BD	115	HIS	ND1-CE1	-6.31	1.19	1.34
35	BA	1476	A	N9-C4	5.55	1.41	1.37
2	A	889	A	N3-C4	-5.52	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3021	A	N9-C4	5.24	1.41	1.37
2	A	289	A	N9-C4	5.18	1.41	1.37
2	A	2725	C	N1-C6	-5.13	1.34	1.37

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	61	TRP	CG-CD2-CE3	10.37	143.24	133.90
35	BA	1425	G	C8-N9-C4	-9.91	102.44	106.40
35	BA	1425	G	N7-C8-N9	9.13	117.67	113.10
35	BA	85	C	C2-N1-C1'	8.86	128.55	118.80
35	BA	85	C	N1-C2-O2	8.50	124.00	118.90
7	F	87	ARG	NE-CZ-NH2	8.41	124.51	120.30
35	BA	1149	C	C6-N1-C2	-8.38	116.95	120.30
2	A	445	U	C2-N1-C1'	7.64	126.87	117.70
2	A	2245	C	N1-C2-O2	7.51	123.41	118.90
19	R	61	TRP	CD1-CG-CD2	7.34	112.17	106.30
35	BA	1486	A	N7-C8-N9	7.31	117.46	113.80
2	A	2245	C	C2-N1-C1'	7.11	126.62	118.80
35	BA	415	C	C6-N1-C2	-7.06	117.48	120.30
35	BA	1486	A	C8-N9-C4	-7.03	102.99	105.80
35	BA	1425	G	N3-C2-N2	-7.00	115.00	119.90
35	BA	216	U	N3-C2-O2	-6.99	117.31	122.20
35	BA	85	C	C6-N1-C2	-6.95	117.52	120.30
2	A	2025	C	N3-C2-O2	-6.94	117.04	121.90
35	BA	216	U	N1-C2-O2	6.81	127.57	122.80
2	A	868	C	C6-N1-C2	-6.79	117.58	120.30
35	BA	1482	U	P-O3'-C3'	6.75	127.80	119.70
2	A	291	C	C6-N1-C2	-6.71	117.61	120.30
2	A	1579	C	C5-C6-N1	6.70	124.35	121.00
35	BA	85	C	N3-C2-O2	-6.63	117.26	121.90
2	A	1758	G	C5-C6-O6	-6.62	124.63	128.60
2	A	617	U	C2-N1-C1'	6.56	125.57	117.70
2	A	962	U	C2-N1-C1'	6.56	125.57	117.70
35	BA	1268	C	C5-C6-N1	6.55	124.28	121.00
2	A	1758	G	N1-C6-O6	6.54	123.82	119.90
2	A	1553	C	C6-N1-C2	-6.51	117.69	120.30
35	BA	216	U	C2-N1-C1'	6.50	125.50	117.70
35	BA	1149	C	C2-N1-C1'	6.48	125.92	118.80
2	A	161	U	C2-N1-C1'	6.47	125.47	117.70
2	A	1381	G	C5-C6-N1	6.34	114.67	111.50
35	BA	552	A	C8-N9-C4	6.33	108.33	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1268	C	C2-N1-C1'	6.26	125.69	118.80
35	BA	1425	G	C5-N7-C8	-6.21	101.20	104.30
2	A	1012	C	N1-C2-O2	6.20	122.62	118.90
56	BW	19	G	N7-C8-N9	6.17	116.18	113.10
35	BA	489	A	C8-N9-C4	-6.16	103.34	105.80
2	A	643	G	C4-N9-C1'	6.13	134.47	126.50
35	BA	1149	C	N1-C2-O2	6.12	122.57	118.90
2	A	2245	C	N3-C2-O2	-6.12	117.62	121.90
2	A	445	U	C5-C6-N1	6.11	125.75	122.70
2	A	636	U	C5-C6-N1	6.06	125.73	122.70
2	A	1276	G	C4-N9-C1'	6.05	134.37	126.50
2	A	1403	C	C4-C5-C6	6.04	120.42	117.40
2	A	1621	C	C6-N1-C2	-6.04	117.88	120.30
2	A	445	U	N1-C2-O2	6.00	127.00	122.80
2	A	1276	G	C6-C5-N7	-5.98	126.81	130.40
2	A	2352	C	C5-C6-N1	5.98	123.99	121.00
35	BA	1117	U	O4'-C1'-N1	5.95	112.96	108.20
2	A	445	U	N3-C2-O2	-5.95	118.04	122.20
2	A	2087	C	C5-C6-N1	5.94	123.97	121.00
35	BA	1508	C	C6-N1-C2	-5.93	117.93	120.30
35	BA	1149	C	P-O3'-C3'	5.93	126.81	119.70
2	A	2437	U	C2-N1-C1'	5.91	124.79	117.70
2	A	1534	C	C6-N1-C2	-5.90	117.94	120.30
2	A	2869	C	C6-N1-C2	-5.90	117.94	120.30
2	A	2686	U	N1-C2-O2	5.89	126.93	122.80
2	A	1403	C	N3-C2-O2	-5.89	117.78	121.90
35	BA	415	C	C2-N1-C1'	5.87	125.25	118.80
2	A	1012	C	C2-N1-C1'	5.84	125.23	118.80
35	BA	1149	C	N3-C2-O2	-5.84	117.81	121.90
35	BA	139	C	C6-N1-C2	-5.83	117.97	120.30
35	BA	1117	U	P-O3'-C3'	5.83	126.70	119.70
2	A	1196	C	C6-N1-C2	-5.81	117.98	120.30
2	A	1567	C	C6-N1-C2	-5.79	117.98	120.30
2	A	445	U	P-O3'-C3'	5.78	126.63	119.70
35	BA	413	G	O4'-C1'-N9	5.77	112.81	108.20
2	A	2796	A	O5'-P-OP2	-5.75	100.52	105.70
2	A	2352	C	C6-N1-C2	-5.75	118.00	120.30
2	A	2094	G	P-O3'-C3'	5.75	126.60	119.70
19	R	61	TRP	CE2-CD2-CE3	-5.75	111.81	118.70
2	A	1993	G	C4-N9-C1'	5.73	133.95	126.50
56	BW	17	C	C6-N1-C2	-5.73	118.01	120.30
35	BA	85	C	C6-N1-C1'	-5.72	113.93	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3046	C	N3-C2-O2	-5.72	117.90	121.90
2	A	1631	A	N1-C6-N6	5.71	122.02	118.60
35	BA	489	A	N7-C8-N9	5.71	116.65	113.80
3	B	88	C	C2-N1-C1'	5.70	125.08	118.80
2	A	237	C	C5-C6-N1	5.69	123.84	121.00
35	BA	429	U	P-O3'-C3'	5.68	126.52	119.70
2	A	2521	C	C6-N1-C2	-5.68	118.03	120.30
2	A	617	U	N1-C2-O2	5.67	126.77	122.80
2	A	1567	C	C5-C6-N1	5.67	123.83	121.00
35	BA	1486	A	C5-N7-C8	-5.67	101.07	103.90
35	BA	215	U	N3-C2-O2	-5.66	118.24	122.20
2	A	291	C	C5-C6-N1	5.65	123.83	121.00
35	BA	1149	C	C5-C6-N1	5.65	123.83	121.00
35	BA	821	C	N1-C2-O2	5.63	122.28	118.90
35	BA	1117	U	OP1-P-O3'	5.63	117.58	105.20
2	A	1757	U	C2-N1-C1'	5.60	124.42	117.70
2	A	2245	C	C6-N1-C1'	-5.60	114.08	120.80
35	BA	498	C	P-O3'-C3'	5.58	126.39	119.70
35	BA	354	G	C4-N9-C1'	5.57	133.74	126.50
38	BD	115	HIS	ND1-CG-CD2	-5.57	98.20	106.00
2	A	747	A	O4'-C1'-N9	5.57	112.65	108.20
35	BA	466	U	C2-N1-C1'	5.56	124.38	117.70
2	A	2094	G	OP1-P-O3'	5.55	117.40	105.20
31	d	23	LEU	CA-CB-CG	-5.54	102.55	115.30
2	A	1535	C	C2-N1-C1'	5.53	124.88	118.80
35	BA	956	A	O4'-C1'-N9	5.51	112.61	108.20
2	A	301	U	N1-C2-O2	5.51	126.65	122.80
2	A	2278	A	N1-C2-N3	5.50	132.05	129.30
35	BA	794	A	N1-C6-N6	5.50	121.90	118.60
2	A	533	C	C6-N1-C2	-5.50	118.10	120.30
2	A	1576	C	C6-N1-C2	-5.50	118.10	120.30
2	A	498	G	C4-N9-C1'	5.49	133.64	126.50
2	A	445	U	C6-N1-C2	-5.48	117.71	121.00
2	A	2248	C	C6-N1-C2	-5.48	118.11	120.30
2	A	2843	C	C6-N1-C2	-5.47	118.11	120.30
2	A	362	A	O4'-C1'-N9	5.45	112.56	108.20
2	A	161	U	O4'-C1'-N1	5.45	112.56	108.20
2	A	2085	C	P-O3'-C3'	5.45	126.24	119.70
2	A	974	G	P-O3'-C3'	5.43	126.22	119.70
35	BA	1511	C	C6-N1-C2	-5.42	118.13	120.30
35	BA	509	G	N7-C8-N9	5.42	115.81	113.10
35	BA	730	C	C6-N1-C2	-5.42	118.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	905	U	C2-N1-C1'	5.41	124.19	117.70
2	A	1032	A	N1-C2-N3	5.41	132.00	129.30
2	A	1534	C	N1-C2-O2	5.39	122.14	118.90
2	A	617	U	N3-C2-O2	-5.39	118.43	122.20
2	A	1530	G	N3-C4-N9	-5.38	122.77	126.00
2	A	784	G	C4-N9-C1'	5.37	133.48	126.50
2	A	1621	C	C5-C6-N1	5.35	123.68	121.00
2	A	1276	G	C8-N9-C1'	-5.35	120.04	127.00
35	BA	326	G	N3-C4-C5	-5.34	125.93	128.60
2	A	1993	G	C8-N9-C1'	-5.34	120.06	127.00
2	A	2025	C	N1-C2-O2	5.33	122.09	118.90
2	A	759	G	P-O3'-C3'	5.30	126.06	119.70
35	BA	1206	U	C2-N1-C1'	5.29	124.05	117.70
35	BA	1011	U	C2-N1-C1'	5.29	124.05	117.70
2	A	839	U	C2-N1-C1'	5.28	124.04	117.70
2	A	786	C	C6-N1-C2	-5.27	118.19	120.30
2	A	1767	U	C5-C6-N1	5.27	125.33	122.70
2	A	290	C	C2-N1-C1'	5.26	124.58	118.80
35	BA	454	C	C5-C6-N1	5.22	123.61	121.00
2	A	2271	C	C6-N1-C2	-5.22	118.21	120.30
35	BA	85	C	C5-C6-N1	5.22	123.61	121.00
2	A	191	G	O4'-C1'-N9	5.21	112.37	108.20
35	BA	1007	U	P-O3'-C3'	5.21	125.96	119.70
2	A	1759	A	N1-C6-N6	5.21	121.73	118.60
7	F	87	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
2	A	1004	C	C5-C6-N1	5.19	123.59	121.00
35	BA	1011	U	C5-C6-N1	5.18	125.29	122.70
2	A	635	G	N3-C4-C5	-5.18	126.01	128.60
2	A	3046	C	C6-N1-C2	-5.18	118.23	120.30
2	A	1710	A	C2-N3-C4	5.16	113.18	110.60
2	A	1650	G	C4-N9-C1'	5.14	133.19	126.50
2	A	1602	U	C5-C6-N1	5.14	125.27	122.70
2	A	1631	A	C5-C6-N6	-5.14	119.59	123.70
35	BA	487	C	C6-N1-C2	-5.14	118.25	120.30
2	A	1001	C	C6-N1-C2	-5.13	118.25	120.30
2	A	1758	G	C4-C5-N7	5.12	112.85	110.80
35	BA	1486	A	C6-C5-N7	-5.12	128.71	132.30
35	BA	895	A	P-O3'-C3'	5.11	125.83	119.70
2	A	1276	G	C4-C5-N7	5.10	112.84	110.80
2	A	643	G	C8-N9-C1'	-5.09	120.38	127.00
35	BA	179	C	C2-N1-C1'	5.08	124.39	118.80
9	H	109	GLY	N-CA-C	5.07	125.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	T	109	HIS	ND1-CG-CD2	-5.06	98.92	106.00
2	A	853	C	C6-N1-C2	-5.05	118.28	120.30
2	A	1276	G	N3-C4-N9	5.05	129.03	126.00
19	R	61	TRP	CD2-CE3-CZ3	5.05	125.36	118.80
2	A	2712	U	C2-N3-C4	-5.03	123.98	127.00
2	A	1551	U	C5-C6-N1	5.03	125.21	122.70
2	A	1534	C	C2-N1-C1'	5.02	124.33	118.80
2	A	1412	C	C6-N1-C2	-5.02	118.29	120.30
2	A	2194	A	C8-N9-C4	-5.02	103.79	105.80
35	BA	509	G	C8-N9-C4	-5.01	104.39	106.40
35	BA	179	C	N1-C2-O2	5.01	121.91	118.90
35	BA	823	U	C5-C6-N1	5.01	125.20	122.70
2	A	933	G	C4-N9-C1'	5.00	133.00	126.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	T	117	ARG	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	189	0	205	5	0
2	A	66981	0	33699	491	0
3	B	2522	0	1285	10	0
4	C	2110	0	2165	71	0
5	D	1587	0	1630	41	0
6	E	1569	0	1607	41	0
7	F	1445	0	1476	41	0
8	G	1348	0	1399	32	0
9	H	1018	0	988	19	0
10	I	918	0	959	38	0
11	J	990	0	1021	30	0
12	K	1130	0	1167	22	0
13	L	938	0	1000	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	1078	0	1151	41	0
15	N	1092	0	1128	38	0
16	O	928	0	972	30	0
17	P	956	0	991	11	0
18	Q	907	0	938	27	0
19	R	988	0	1038	22	0
20	S	754	0	802	17	0
21	T	873	0	909	20	0
22	U	756	0	802	12	0
23	V	732	0	782	19	0
24	W	1428	0	1443	29	0
25	X	586	0	601	12	0
26	Y	470	0	480	15	0
27	Z	531	0	541	16	0
28	a	474	0	500	0	0
29	b	423	0	463	0	0
30	c	405	0	407	0	0
31	d	377	0	411	0	0
32	e	502	0	541	0	0
33	f	299	0	321	0	0
34	g	458	0	443	0	0
35	BA	32439	0	16320	340	0
36	BB	280	0	342	9	0
37	BC	1660	0	1707	37	0
38	BD	1641	0	1668	56	0
39	BE	1296	0	1360	37	0
40	BF	771	0	797	23	0
41	BG	1232	0	1282	29	0
42	BH	1010	0	1046	26	0
43	BI	994	0	1050	35	0
44	BJ	788	0	819	33	0
45	BK	855	0	863	19	0
46	BL	958	0	1045	32	0
47	BM	935	0	986	24	0
48	BN	477	0	499	14	0
49	BO	720	0	760	10	0
50	BP	891	0	935	35	0
51	BQ	748	0	795	16	0
52	BR	513	0	537	13	0
53	BS	662	0	677	20	0
54	BT	660	0	712	14	0
55	BV	1793	0	1839	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BW	1619	0	821	22	0
57	BX	117	0	63	3	0
58	A	390	0	0	0	0
58	B	9	0	0	0	0
58	BA	215	0	0	0	0
58	BF	1	0	0	0	0
58	BR	1	0	0	0	0
58	C	4	0	0	0	0
58	F	1	0	0	0	0
58	M	1	0	0	0	0
58	N	1	0	0	0	0
58	T	1	0	0	0	0
58	c	1	0	0	0	0
59	BN	1	0	0	0	0
59	BR	1	0	0	0	0
59	Y	1	0	0	0	0
59	c	1	0	0	0	0
59	f	1	0	0	0	0
59	g	1	0	0	0	0
60	BW	11	0	8	0	0
All	All	151463	0	101196	1781	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 7.

All (1781) 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)
35:BA:531:U:O2'	46:BL:83:ARG:NH1	1.92	1.01
2:A:1786:G:OP1	4:C:211:ARG:NH1	1.97	0.98
2:A:2772:G:H1'	13:L:23:ARG:HH12	1.29	0.96
2:A:142:C:H5''	22:U:41:GLN:HE21	1.32	0.94
37:BC:169:ARG:HH11	37:BC:169:ARG:HB2	1.31	0.94
2:A:2245:C:OP1	19:R:25:ARG:NH1	2.02	0.92
6:E:112:ARG:HH11	6:E:112:ARG:HG2	1.33	0.92
6:E:192:ASP:OD1	14:M:5:LYS:NZ	2.05	0.90
35:BA:1350:U:H5'	44:BJ:62:ARG:HH11	1.37	0.90
44:BJ:66:GLU:HB2	48:BN:59:SER:HB2	1.56	0.88
39:BE:132:ALA:O	39:BE:137:ARG:NH1	2.08	0.87
2:A:2343:G:O6	2:A:2399:A:N6	2.07	0.87
2:A:1612:U:H1'	40:BF:17:ARG:HH12	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:U:H5'	2:A:302:U:H5''	1.55	0.86
1:3:8:LYS:NZ	2:A:2253:A:OP2	2.08	0.85
40:BF:24:GLU:OE2	40:BF:31:ARG:NH1	2.09	0.84
35:BA:1350:U:H5'	44:BJ:62:ARG:NH1	1.94	0.83
2:A:1730:U:H5''	2:A:1731:A:H8	1.43	0.83
35:BA:1301:A:OP1	53:BS:70:LYS:NZ	2.11	0.83
2:A:2357:A:H1'	2:A:2382:G:H21	1.41	0.83
2:A:1730:U:H5''	2:A:1731:A:C8	2.14	0.82
2:A:1552:A:H1'	2:A:1618:C:H42	1.45	0.81
2:A:2358:A:N6	2:A:2379:G:O2'	2.12	0.81
10:I:40:ARG:HH11	10:I:40:ARG:HG3	1.46	0.81
2:A:1578:G:H22	2:A:1593:U:H3	1.24	0.81
35:BA:427:U:OP2	38:BD:29:ARG:NH1	2.15	0.80
2:A:2363:A:H61	2:A:2374:U:H3	1.27	0.80
2:A:2234:G:H5''	21:T:49:ALA:HB2	1.61	0.80
45:BK:90:LYS:HG3	45:BK:115:GLU:HB2	1.63	0.80
2:A:1365:G:OP2	14:M:24:ARG:NH1	2.16	0.79
47:BM:20:THR:HG23	47:BM:26:GLY:HA2	1.65	0.79
35:BA:986:G:N1	35:BA:1016:G:O6	2.16	0.78
35:BA:644:G:H22	35:BA:721:G:H1	1.30	0.78
40:BF:12:PRO:O	40:BF:45:ARG:NH1	2.17	0.78
44:BJ:63:GLU:OE1	48:BN:45:ARG:NH1	2.15	0.78
35:BA:393:A:OP1	50:BP:14:ARG:NH2	2.16	0.77
2:A:160:A:H3'	2:A:161:U:H5''	1.66	0.77
2:A:2032:A:OP2	4:C:54:LYS:NZ	2.18	0.77
49:BO:26:GLU:OE2	49:BO:77:ARG:NH1	2.17	0.77
41:BG:10:ARG:HG3	41:BG:10:ARG:HH11	1.50	0.77
2:A:1541:G:OP2	2:A:1629:G:N2	2.17	0.77
19:R:114:ARG:HH11	19:R:114:ARG:HG3	1.50	0.77
13:L:17:LYS:HE3	13:L:47:ILE:HG22	1.67	0.76
2:A:1825:C:N4	2:A:1840:G:OP2	2.18	0.76
2:A:2386:U:OP1	2:A:2393:A:O2'	2.03	0.76
1:3:21:ARG:HG2	1:3:22:PRO:HD2	1.67	0.76
54:BT:35:PHE:HA	54:BT:50:LEU:HD21	1.67	0.76
23:V:88:ASP:HB2	23:V:93:LYS:HB2	1.67	0.76
35:BA:392:C:OP1	50:BP:9:ARG:NH2	2.18	0.76
19:R:28:ARG:NH1	19:R:38:GLN:OE1	2.18	0.75
2:A:290:C:H42	2:A:298:G:H22	1.35	0.75
35:BA:1177:A:O2'	35:BA:1178:A:OP1	2.02	0.75
2:A:1530:G:H22	2:A:1805:G:H1	1.35	0.75
2:A:543:U:H3'	2:A:544:U:H5''	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2044:U:OP2	4:C:222:ARG:NH1	2.19	0.74
4:C:80:ALA:O	4:C:113:GLN:NE2	2.20	0.74
8:G:55:ARG:HH12	8:G:63:ARG:HG3	1.49	0.74
26:Y:36:VAL:HG12	26:Y:63:ARG:HH21	1.50	0.74
14:M:43:ARG:HG3	14:M:43:ARG:HH11	1.53	0.74
19:R:73:ASP:O	19:R:114:ARG:NH2	2.20	0.74
41:BG:69:VAL:HG23	41:BG:100:ALA:HB1	1.70	0.73
15:N:18:ARG:O	15:N:98:LYS:NZ	2.18	0.73
56:BW:49:C:H42	56:BW:65:G:H1	1.35	0.73
7:F:75:ARG:HH21	7:F:95:ARG:NH1	1.86	0.73
53:BS:3:ARG:NH1	53:BS:10:PHE:HB2	2.04	0.73
20:S:76:HIS:HE1	20:S:85:HIS:HB3	1.54	0.73
35:BA:413:G:N7	38:BD:28:LYS:NZ	2.31	0.73
2:A:679:G:OP2	14:M:24:ARG:NH2	2.21	0.72
43:BI:126:ARG:NH1	43:BI:127:ASP:O	2.22	0.72
39:BE:70:MET:HE3	39:BE:98:ARG:NH1	2.05	0.72
2:A:1612:U:H2'	2:A:1613:G:C8	2.24	0.72
26:Y:41:ARG:HG2	26:Y:43:GLY:H	1.55	0.72
2:A:2332:U:H1'	2:A:2404:G:H21	1.52	0.72
47:BM:5:VAL:HG21	47:BM:60:ILE:HD11	1.70	0.72
55:BV:18:HIS:HB3	55:BV:22:ARG:HD2	1.71	0.72
14:M:84:ASN:HD21	14:M:118:LEU:HA	1.52	0.72
2:A:383:U:O4	23:V:79:LYS:NZ	2.22	0.72
35:BA:1332:A:OP2	43:BI:140:LYS:NZ	2.16	0.71
2:A:1551:U:H3	2:A:1619:U:H3	1.39	0.71
2:A:2975:G:H4'	8:G:4:ILE:HD11	1.73	0.71
2:A:1257:G:H5''	12:K:72:LYS:NZ	2.06	0.70
6:E:112:ARG:HH11	6:E:112:ARG:CG	2.05	0.70
4:C:247:VAL:HG12	4:C:253:PRO:HA	1.73	0.70
35:BA:531:U:HO2'	46:BL:83:ARG:NH1	1.89	0.70
43:BI:135:LYS:HB2	43:BI:135:LEU:HD12	1.73	0.70
19:R:89:GLU:OE1	20:S:8:LYS:NZ	2.22	0.70
35:BA:819:U:H3	35:BA:829:G:H1	1.39	0.70
2:A:2914:A:OP1	16:O:9:ARG:NH1	2.24	0.70
21:T:81:VAL:HG13	21:T:112:VAL:HG22	1.74	0.70
38:BD:10:ARG:HD2	38:BD:33:PRO:HG3	1.72	0.70
4:C:126:LYS:HD3	4:C:127:PRO:HD2	1.72	0.70
10:I:17:PHE:CE2	10:I:64:ALA:HB3	2.27	0.70
2:A:2348:G:O2'	2:A:2396:A:N6	2.22	0.69
10:I:94:LYS:NZ	10:I:121:GLU:HA	2.07	0.69
20:S:87:ARG:HG3	20:S:87:ARG:HH11	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:5:THR:HG21	27:Z:21:LYS:HZ2	1.56	0.69
2:A:753:A:H61	2:A:762:U:H3	1.40	0.69
2:A:2529:A:H5''	7:F:138:GLY:HA3	1.72	0.69
50:BP:44:GLU:HB3	50:BP:47:SER:HA	1.72	0.69
50:BP:48:LEU:HB2	50:BP:96:LYS:HE3	1.73	0.69
50:BP:46:PRO:HG3	50:BP:96:LYS:HA	1.73	0.69
35:BA:772:A:O2'	35:BA:774:A:N7	2.25	0.69
2:A:1187:A:H5''	2:A:1188:A:C8	2.27	0.69
2:A:2862:G:O2'	2:A:3002:A:N6	2.26	0.69
2:A:2343:G:N2	2:A:2401:U:O2	2.23	0.69
39:BE:61:LEU:HD22	39:BE:159:ILE:HD13	1.75	0.69
35:BA:1375:G:H21	35:BA:1486:A:H8	1.41	0.69
37:BC:58:ARG:HG2	37:BC:63:VAL:HG22	1.74	0.69
2:A:2276:G:H4'	5:D:153:GLY:O	1.93	0.68
55:BV:6:MET:HG2	55:BV:47:LEU:HD11	1.76	0.68
10:I:23:THR:HG23	10:I:109:TYR:HB3	1.75	0.68
41:BG:129:ASN:HB2	41:BG:131:LEU:HG	1.73	0.68
55:BV:114:LEU:HD13	55:BV:152:ARG:HH11	1.56	0.68
2:A:1187:A:H5''	2:A:1188:A:H8	1.59	0.68
35:BA:700:C:H5'	52:BR:50:ALA:HA	1.74	0.68
35:BA:1300:A:OP1	53:BS:3:ARG:NH2	2.27	0.68
7:F:136:THR:HG23	7:F:162:THR:HB	1.74	0.68
2:A:290:C:N4	2:A:298:G:H22	1.90	0.68
35:BA:184:U:H5''	54:BT:81:LEU:HD13	1.76	0.68
46:BL:54:ARG:HH11	46:BL:64:THR:HG23	1.56	0.68
2:A:639:C:HO2'	2:A:640:G:H8	1.39	0.68
35:BA:1287:G:HO2'	35:BA:1288:A:H8	1.42	0.68
14:M:137:ILE:HG21	14:M:144:ALA:HB2	1.76	0.67
35:BA:953:G:O2'	35:BA:1348:G:O2'	2.06	0.67
2:A:1673:A:O2'	2:A:2926:A:OP2	2.12	0.67
35:BA:1304:C:OP1	53:BS:78:ARG:NH2	2.28	0.67
11:J:40:PHE:HE1	11:J:58:VAL:HG21	1.59	0.67
2:A:2350:G:O2'	2:A:2351:A:O4'	2.13	0.67
35:BA:821:C:H42	35:BA:826:U:H3	1.42	0.67
15:N:51:ARG:NH2	24:W:193:GLU:O	2.27	0.67
35:BA:1486:A:H2	35:BA:1489:G:H1	1.42	0.67
4:C:132:PRO:HD3	4:C:190:ARG:HH11	1.60	0.67
27:Z:10:LEU:HD21	27:Z:21:LYS:NZ	2.10	0.67
2:A:997:G:H1	2:A:1010:U:H3	1.43	0.67
39:BE:113:GLU:HG2	39:BE:118:VAL:HG22	1.77	0.67
40:BF:29:VAL:HA	40:BF:32:LYS:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2618:C:H5"	14:M:63:LYS:HD2	1.77	0.67
2:A:1456:G:OP1	2:A:1820:U:O2'	2.13	0.66
2:A:706:G:O2'	6:E:160:ARG:NH2	2.28	0.66
42:BH:79:ARG:NE	42:BH:81:SER:O	2.28	0.66
2:A:994:A:N6	2:A:1014:G:O2'	2.26	0.66
2:A:2882:C:H5"	8:G:159:LYS:HD2	1.78	0.66
2:A:2862:G:OP1	5:D:85:ARG:NH1	2.28	0.66
44:BJ:59:LYS:HE2	44:BJ:62:ARG:NH2	2.11	0.66
11:J:96:LYS:HE2	24:W:120:PRO:HB2	1.78	0.66
2:A:2626:U:H4'	2:A:2627:C:OP2	1.96	0.66
3:B:76:G:H5"	24:W:19:THR:HG21	1.77	0.66
35:BA:1289:U:H5"	47:BM:101:GLN:HE22	1.60	0.66
35:BA:1160:A:OP2	43:BI:115:ARG:NH2	2.29	0.66
2:A:75:U:H5'	27:Z:11:ARG:HH22	1.60	0.66
35:BA:984:A:H61	35:BA:1018:C:H42	1.43	0.66
35:BA:1018:C:H2'	35:BA:1019:U:C6	2.30	0.65
37:BC:76:ILE:HG22	37:BC:83:ALA:HB2	1.77	0.65
35:BA:507:G:O6	46:BL:46:ASN:ND2	2.28	0.65
56:BW:35:A:H61	57:BX:5:C:H42	1.44	0.65
2:A:164:A:O2'	26:Y:41:ARG:NH1	2.29	0.65
2:A:164:A:H4'	26:Y:41:ARG:HH12	1.62	0.65
38:BD:55:LYS:HB2	38:BD:190:LEU:HD11	1.78	0.65
40:BF:26:PHE:HZ	40:BF:82:ASN:HD22	1.43	0.65
41:BG:26:LEU:HD13	41:BG:101:LEU:HD22	1.77	0.65
4:C:19:SER:HB2	4:C:204:ILE:HD11	1.77	0.65
2:A:2735:U:O2'	5:D:148:PRO:O	2.14	0.65
3:B:81:U:OP1	15:N:18:ARG:NH2	2.26	0.65
2:A:1551:U:H3'	2:A:1552:A:H8	1.62	0.65
35:BA:1117:U:H1'	35:BA:1118:A:H5"	1.77	0.65
35:BA:11:G:H1	39:BE:122:ARG:HH11	1.45	0.65
35:BA:315:A:N7	35:BA:328:U:H5	1.95	0.65
39:BE:179:ALA:HA	39:BE:189:VAL:HG21	1.79	0.65
56:BW:51:U:H3	56:BW:63:G:H1	1.44	0.65
2:A:333:C:H2'	2:A:334:G:H8	1.61	0.65
39:BE:101:LEU:HD21	39:BE:145:VAL:HG22	1.77	0.65
2:A:659:U:OP2	14:M:31:LYS:NZ	2.28	0.65
35:BA:1434:U:O2'	35:BA:1435:U:H5"	1.95	0.65
10:I:36:LEU:O	10:I:40:ARG:HG2	1.97	0.65
2:A:1072:G:OP1	15:N:87:LYS:NZ	2.25	0.65
37:BC:90:LEU:HD13	37:BC:98:VAL:HG11	1.79	0.65
47:BM:14:ARG:NH2	47:BM:16:GLU:OE2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1084:U:O2'	2:A:1085:G:OP1	2.14	0.65
6:E:118:ARG:HH12	14:M:3:VAL:HG13	1.62	0.65
2:A:3113:A:H4'	2:A:3114:A:OP2	1.98	0.64
18:Q:32:ILE:HG22	18:Q:37:GLU:HG2	1.79	0.64
2:A:2708:G:OP1	15:N:45:ARG:NH1	2.29	0.64
37:BC:72:PRO:HD3	37:BC:104:GLU:HB3	1.79	0.64
38:BD:112:LEU:HB3	38:BD:118:PHE:HE1	1.62	0.64
2:A:1875:U:H4'	5:D:143:ALA:HB1	1.79	0.64
2:A:1002:C:H2'	2:A:1003:A:H5''	1.79	0.64
35:BA:525:C:OP2	38:BD:54:GLN:NE2	2.25	0.64
2:A:2795:C:O2'	5:D:156:THR:O	2.16	0.64
35:BA:481:G:H2'	35:BA:482:A:C8	2.32	0.64
7:F:130:ASP:O	7:F:132:THR:N	2.26	0.64
12:K:76:ARG:HB3	12:K:85:ARG:NH1	2.12	0.64
2:A:1457:A:O2'	2:A:1459:U:OP2	2.15	0.64
43:BI:150:ARG:NH1	56:BW:35:A:OP2	2.31	0.64
8:G:35:LEU:HD11	8:G:72:LEU:HB3	1.79	0.64
35:BA:436:C:H5''	38:BD:148:LEU:HD12	1.79	0.64
35:BA:858:A:H1'	42:BH:12:THR:HG21	1.80	0.64
2:A:2424:C:OP1	26:Y:48:ARG:NH2	2.31	0.64
8:G:37:VAL:HG22	47:BM:57:ARG:HH12	143.72	0.64
2:A:1260:C:H6	12:K:27:ARG:HH12	1.46	0.64
14:M:43:ARG:HH11	14:M:43:ARG:CG	2.10	0.64
27:Z:10:LEU:HD21	27:Z:21:LYS:HZ3	1.62	0.64
35:BA:1400:A:H5'	36:BB:31:LEU:HD21	1.79	0.63
38:BD:47:ARG:HG2	38:BD:47:ARG:HH11	1.63	0.63
2:A:2404:G:H2'	2:A:2405:A:C8	2.34	0.63
2:A:2412:U:H2'	2:A:2413:G:C8	2.32	0.63
35:BA:1130:C:OP1	43:BI:31:ARG:NH1	2.30	0.63
35:BA:1471:G:OP1	36:BB:23:ARG:NH2	2.32	0.63
35:BA:438:U:P	38:BD:117:HIS:HE2	2.21	0.63
55:BV:117:LEU:HB3	55:BV:141:LYS:HE3	1.80	0.63
55:BV:162:TRP:HH2	55:BV:214:THR:HG22	1.62	0.63
2:A:3014:A:O2'	2:A:3015:C:H5''	1.98	0.63
35:BA:390:U:O3'	50:BP:29:ARG:NH2	2.32	0.63
2:A:1403:C:H5	2:A:1441:C:N3	1.96	0.63
2:A:2374:U:H2'	2:A:2375:G:C8	2.34	0.63
35:BA:1220:A:H62	35:BA:1281:A:H62	1.46	0.63
13:L:10:VAL:HG12	13:L:12:ASP:H	1.64	0.63
2:A:543:U:H3'	2:A:544:U:C5'	2.29	0.63
39:BE:145:VAL:HG11	39:BE:148:ILE:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:40:ALA:HA	6:E:100:GLN:HE21	1.63	0.63
20:S:87:ARG:HG3	20:S:87:ARG:NH1	2.12	0.63
2:A:2557:A:OP1	25:X:75:ARG:NH2	2.32	0.62
2:A:2772:G:H1'	13:L:23:ARG:NH1	2.08	0.62
39:BE:38:GLU:HG2	39:BE:64:VAL:HG22	1.80	0.62
9:H:127:VAL:HG21	9:H:150:ALA:HB2	1.81	0.62
2:A:1554:U:H3	2:A:1617:C:H42	1.46	0.62
2:A:292:G:N2	2:A:343:U:O2	2.31	0.62
35:BA:448:A:OP2	35:BA:465:G:N2	2.31	0.62
41:BG:107:PHE:HZ	41:BG:137:ARG:NH1	1.96	0.62
2:A:567:A:H4'	2:A:568:A:H5'	1.80	0.62
42:BH:85:LEU:HB2	46:BL:4:ILE:HD12	1.81	0.62
55:BV:4:VAL:HG13	55:BV:8:GLN:HB3	1.81	0.62
2:A:1201:G:N2	2:A:1203:A:H3'	2.14	0.62
2:A:2221:A:H5''	5:D:127:MET:HE1	1.82	0.62
2:A:2369:C:H5''	2:A:2370:A:C8	2.35	0.62
42:BH:50:ARG:NH1	42:BH:52:GLU:OE2	2.33	0.62
53:BS:33:THR:HG22	53:BS:35:SER:H	1.64	0.62
14:M:110:VAL:H	14:M:127:ASN:HD22	1.45	0.62
2:A:1675:U:O2	16:O:64:ARG:NH1	2.32	0.62
9:H:112:LEU:HD13	9:H:134:VAL:HG11	1.82	0.62
18:Q:90:ASP:HB2	18:Q:110:LYS:HB2	1.81	0.62
19:R:114:ARG:HG3	19:R:114:ARG:NH1	2.15	0.62
2:A:899:G:H5'	2:A:899:G:H8	1.64	0.62
35:BA:438:U:OP1	38:BD:117:HIS:NE2	2.29	0.62
35:BA:254:G:H4'	51:BQ:35:THR:HG21	1.82	0.62
2:A:2404:G:H2'	2:A:2405:A:H8	1.65	0.62
44:BJ:6:ILE:HB	44:BJ:76:ILE:HG23	1.82	0.62
47:BM:4:LEU:HG	47:BM:5:VAL:HG23	1.82	0.62
2:A:1869:G:OP1	16:O:40:LYS:NZ	2.33	0.62
2:A:2089:C:O2	2:A:2094:G:N2	2.33	0.62
2:A:2340:A:H61	2:A:2389:U:H3	1.48	0.62
35:BA:612:U:H5'	35:BA:613:G:C8	2.34	0.62
35:BA:1265:U:H5''	35:BA:1266:U:H4'	1.82	0.61
37:BC:169:ARG:NH1	37:BC:169:ARG:HB2	2.09	0.61
38:BD:51:GLN:HB3	38:BD:55:LYS:HE3	1.82	0.61
10:I:94:LYS:HD3	10:I:121:GLU:HG2	1.80	0.61
35:BA:1382:C:H4'	35:BA:1383:C:H5''	1.81	0.61
35:BA:987:A:H8	35:BA:1007:U:H1'	1.63	0.61
25:X:18:ALA:HB3	25:X:20:ARG:NH1	2.15	0.61
35:BA:1515:A:H2'	35:BA:1516:U:O4'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BV:114:LEU:HD21	55:BV:145:GLU:HG3	1.82	0.61
11:J:20:ALA:HB1	11:J:41:CYS:HB3	1.82	0.61
35:BA:1220:A:H62	35:BA:1281:A:N6	1.98	0.61
35:BA:193:C:N4	51:BQ:18:GLY:O	2.33	0.61
43:BI:53:ARG:HB3	43:BI:57:ASN:HD22	1.66	0.61
45:BK:30:ALA:HB3	45:BK:93:VAL:HG12	1.81	0.61
15:N:37:LEU:O	15:N:99:PRO:HB3	2.01	0.61
22:U:46:ILE:HD12	22:U:84:VAL:HG21	1.83	0.61
55:BV:111:LEU:HD13	55:BV:148:LEU:HD23	1.82	0.61
2:A:333:C:H2'	2:A:334:G:C8	2.35	0.61
2:A:752:C:H2'	2:A:753:A:C8	2.35	0.61
35:BA:561:G:OP1	49:BO:65:ARG:NH2	2.33	0.61
4:C:108:PRO:HG2	4:C:111:LEU:HB2	1.82	0.61
2:A:604:C:O2'	21:T:25:ARG:NH2	2.34	0.61
2:A:2351:A:N3	2:A:2396:A:O2'	2.34	0.61
35:BA:956:A:OP2	48:BN:41:ARG:NH1	2.33	0.61
4:C:96:HIS:CD2	4:C:102:LYS:HG2	2.35	0.61
24:W:16:ARG:HG2	24:W:48:GLU:HG3	1.81	0.61
2:A:1551:U:H3'	2:A:1552:A:C8	2.34	0.61
51:BQ:65:ASN:N	51:BQ:65:ASN:OD1	2.34	0.61
10:I:69:LEU:HD22	10:I:72:LEU:HD12	1.82	0.61
38:BD:96:VAL:HG13	38:BD:166:LEU:HD21	1.81	0.61
26:Y:19:SER:OG	26:Y:20:HIS:N	2.34	0.61
2:A:142:C:H5''	22:U:41:GLN:NE2	2.11	0.60
35:BA:1170:U:H5''	37:BC:5:ILE:HD13	1.82	0.60
3:B:31:C:H5'	17:P:11:SER:HB3	1.83	0.60
38:BD:15:LEU:HD22	38:BD:55:LYS:HG3	1.83	0.60
2:A:1153:U:H4'	8:G:60:ARG:CZ	2.32	0.60
2:A:1722:C:OP1	4:C:78:LYS:NZ	2.20	0.60
2:A:292:G:H1	2:A:343:U:H3	1.47	0.60
35:BA:11:G:H1	39:BE:122:ARG:NH1	1.99	0.60
35:BA:808:A:H62	35:BA:840:G:H21	1.49	0.60
47:BM:97:PRO:HB2	47:BM:101:GLN:HG3	1.84	0.60
35:BA:216:U:O2'	35:BA:217:U:H5'	2.02	0.60
55:BV:162:TRP:CH2	55:BV:214:THR:HG22	2.36	0.60
56:BW:17:C:H3'	56:BW:18:G:H5''	1.84	0.60
8:G:116:ILE:HD13	8:G:149:ILE:HG12	1.82	0.60
16:O:33:ARG:HB3	16:O:114:GLU:HG3	1.84	0.60
50:BP:40:TYR:CE2	50:BP:42:PRO:HG3	2.37	0.60
5:D:130:HIS:CD2	5:D:165:ARG:HB3	2.37	0.60
2:A:1455:U:OP2	22:U:62:ARG:NH1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BI:61:ASN:HD22	43:BI:64:HIS:CD2	2.19	0.60
9:H:124:ILE:HG22	9:H:125:LYS:H	1.67	0.60
13:L:90:ASP:N	13:L:90:ASP:OD1	2.33	0.60
2:A:1621:C:H2'	2:A:1622:G:C8	2.37	0.60
2:A:733:U:H2'	2:A:734:C:H6	1.66	0.60
13:L:76:TYR:HB2	18:Q:72:THR:HB	1.84	0.60
18:Q:19:PHE:HA	18:Q:88:ARG:HH12	1.67	0.60
20:S:54:ASP:OD1	20:S:54:ASP:N	2.35	0.60
2:A:1174:G:O2'	2:A:1221:A:N6	2.34	0.59
41:BG:107:PHE:HZ	41:BG:137:ARG:HH11	1.50	0.59
2:A:1158:U:H3	2:A:1233:A:H61	1.49	0.59
35:BA:382:A:H2'	35:BA:383:A:H8	1.66	0.59
38:BD:21:GLY:HA3	38:BD:160:ARG:HH22	1.67	0.59
7:F:128:GLN:HB2	7:F:135:TYR:CE1	2.37	0.59
2:A:1530:G:N2	2:A:1805:G:H1	2.01	0.59
35:BA:481:G:H2'	35:BA:482:A:H8	1.66	0.59
41:BG:79:ARG:HA	41:BG:84:THR:HA	1.84	0.59
2:A:380:A:P	23:V:99:LYS:HZ3	2.25	0.59
2:A:1146:A:N3	2:A:2710:G:O2'	2.33	0.59
2:A:2381:A:H4'	2:A:2382:G:O5'	2.00	0.59
2:A:2580:G:H2'	2:A:2581:G:O4'	2.02	0.59
2:A:759:G:H1	25:X:64:PRO:HB3	1.66	0.59
22:U:34:HIS:ND1	22:U:36:ASP:OD1	2.36	0.59
48:BN:21:TYR:HE1	48:BN:23:ARG:HE	1.50	0.59
40:BF:89:LYS:NZ	52:BR:73:GLU:OE1	2.36	0.59
2:A:1164:A:H4'	10:I:55:THR:HB	1.84	0.59
2:A:451:U:H2'	2:A:452:G:C8	2.38	0.59
44:BJ:25:ILE:HD11	44:BJ:92:LEU:HD11	1.84	0.59
12:K:77:HIS:CD2	12:K:79:GLY:H	2.20	0.59
24:W:43:ASP:N	24:W:43:ASP:OD1	2.34	0.59
2:A:858:A:O2'	2:A:1877:U:OP1	2.19	0.59
40:BF:27:LEU:O	40:BF:30:ILE:HG13	2.03	0.59
2:A:1410:C:H5''	16:O:71:ARG:HH11	1.67	0.59
46:BL:121:LYS:HG3	46:BL:122:GLU:N	2.18	0.58
52:BR:20:CYS:HB3	52:BR:23:CYS:HB2	1.86	0.58
6:E:52:THR:O	6:E:94:LYS:NZ	2.36	0.58
10:I:72:LEU:HD22	10:I:106:LYS:HB3	1.84	0.58
35:BA:1199:C:H2'	35:BA:1200:A:C8	2.39	0.58
35:BA:600:U:H1'	38:BD:127:ILE:HG21	1.85	0.58
43:BI:40:ARG:HG2	43:BI:84:TYR:HB2	1.85	0.58
10:I:14:ALA:HB1	10:I:63:GLU:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:1261:A:P	44:BJ:9:ARG:HH22	2.26	0.58
38:BD:188:VAL:HG22	38:BD:189:PRO:HD2	1.86	0.58
42:BH:12:THR:HG22	42:BH:15:ARG:HH12	1.68	0.58
44:BJ:24:LYS:HD2	44:BJ:92:LEU:HD23	1.85	0.58
35:BA:502:C:H41	46:BL:50:ARG:HH12	1.51	0.58
2:A:2137:A:N6	35:BA:1392:C:O2	2.36	0.58
35:BA:1267:U:H3'	35:BA:1268:C:H5'	1.86	0.58
10:I:94:LYS:HZ3	10:I:121:GLU:HA	1.67	0.58
37:BC:41:LEU:HD13	37:BC:89:ASP:HB3	1.85	0.58
24:W:105:LYS:NZ	24:W:136:GLU:OE2	2.27	0.58
40:BF:80:ASN:HD21	40:BF:88:THR:HG22	1.68	0.58
39:BE:100:PRO:HB3	39:BE:174:ARG:HG2	1.85	0.58
9:H:32:PRO:HB3	26:Y:64:ALA:HA	1.85	0.58
11:J:79:LYS:HD3	11:J:82:LEU:HD12	1.86	0.58
2:A:860:G:HO2'	2:A:863:G:HO2'	1.36	0.58
46:BL:83:ARG:HH21	46:BL:96:LYS:HD2	1.68	0.58
2:A:2009:G:H5'	4:C:205:ASN:ND2	2.19	0.58
5:D:6:ILE:HG22	5:D:208:VAL:HG22	1.85	0.58
25:X:8:SER:N	56:BW:2:C:H4'	2.18	0.58
2:A:752:C:H2'	2:A:753:A:H8	1.68	0.57
54:BT:39:VAL:HG22	54:BT:47:ALA:HB1	1.85	0.57
10:I:27:GLU:HG3	10:I:76:PRO:HG2	1.86	0.57
2:A:2304:C:H4'	26:Y:25:THR:HG21	1.86	0.57
2:A:1427:U:H4'	2:A:1428:U:O5'	2.04	0.57
35:BA:500:A:H62	35:BA:509:G:H8	1.53	0.57
46:BL:121:LYS:HG3	46:BL:122:GLU:H	1.67	0.57
15:N:91:GLU:HB3	15:N:92:TRP:CE3	2.39	0.57
18:Q:43:LYS:HZ2	18:Q:86:LEU:HD12	1.68	0.57
2:A:2936:C:OP1	2:A:2938:G:H4'	2.04	0.57
37:BC:46:LEU:HD13	37:BC:75:VAL:HG13	1.86	0.57
40:BF:30:ILE:HG22	40:BF:36:THR:HG21	1.85	0.57
15:N:63:LYS:HD3	15:N:65:TRP:CZ2	2.40	0.57
2:A:3023:G:H2'	2:A:3024:A:O4'	2.03	0.57
2:A:273:A:H61	2:A:314:G:H1'	1.69	0.57
35:BA:452:A:H62	50:BP:94:LYS:H	1.52	0.57
35:BA:1077:C:H5''	55:BV:143:LYS:NZ	2.20	0.57
49:BO:43:LEU:HD13	49:BO:53:ARG:HG2	1.85	0.57
51:BQ:32:MET:HB2	51:BQ:35:THR:OG1	2.05	0.57
2:A:1640:A:H3'	2:A:1641:U:H5''	1.87	0.57
38:BD:3:ARG:HD2	38:BD:110:ARG:HH11	1.70	0.57
55:BV:18:HIS:NE2	55:BV:205:ASP:OD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:28:HIS:ND1	18:Q:41:VAL:HG12	2.19	0.57
2:A:571:A:H5''	23:V:46:ALA:HB2	1.86	0.57
35:BA:1145:G:H1	35:BA:1153:U:H3	1.52	0.57
25:X:41:ARG:NE	25:X:41:ARG:HA	2.19	0.57
38:BD:86:LEU:HD13	38:BD:186:ILE:HG21	1.87	0.57
40:BF:23:LEU:HD13	40:BF:63:ILE:HD11	1.86	0.57
4:C:132:PRO:HA	4:C:190:ARG:HA	1.87	0.57
24:W:11:LEU:HD12	24:W:67:LEU:HD13	1.87	0.57
2:A:356:G:H21	2:A:362:A:H62	1.53	0.57
43:BI:77:ARG:HH22	43:BI:111:GLN:HG2	1.70	0.57
5:D:114:VAL:HG12	5:D:208:VAL:HG12	1.87	0.57
56:BW:14:A:N1	56:BW:22:G:H1'	2.19	0.56
47:BM:97:PRO:HG2	47:BM:103:THR:HG22	1.87	0.56
11:J:101:LYS:HG3	11:J:140:THR:HB	1.86	0.56
14:M:30:GLY:O	14:M:32:THR:N	2.31	0.56
2:A:1410:C:H5''	16:O:71:ARG:NH1	2.20	0.56
35:BA:243:A:N1	35:BA:281:G:O2'	2.37	0.56
4:C:141:VAL:HG13	4:C:162:SER:HB2	1.87	0.56
11:J:56:ILE:HD11	11:J:72:LEU:HB3	1.86	0.56
24:W:14:ASN:N	24:W:14:ASN:OD1	2.38	0.56
35:BA:958:G:H22	35:BA:1345:A:H5'	1.69	0.56
35:BA:526:G:OP1	38:BD:65:LYS:HG2	2.05	0.56
41:BG:50:ALA:O	41:BG:54:THR:HG22	2.04	0.56
35:BA:1106:U:P	44:BJ:7:ARG:HH22	2.27	0.56
12:K:102:GLU:HG3	12:K:124:VAL:HG11	1.86	0.56
14:M:84:ASN:ND2	14:M:117:LYS:O	2.39	0.56
35:BA:956:A:P	48:BN:41:ARG:HH12	2.28	0.56
42:BH:7:ILE:HB	42:BH:79:ARG:NH1	2.21	0.56
43:BI:54:THR:HG23	43:BI:57:ASN:H	1.69	0.56
2:A:1875:U:H5''	5:D:143:ALA:O	2.06	0.56
2:A:2900:C:OP1	13:L:31:ARG:NH2	2.37	0.56
2:A:3032:G:H5''	5:D:63:ILE:HD12	1.87	0.56
2:A:314:G:H5'	2:A:315:U:OP2	2.05	0.56
2:A:2491:A:H5''	2:A:2492:A:H5'	1.86	0.56
35:BA:931:A:O2'	35:BA:1346:A:OP2	2.23	0.56
35:BA:925:C:H1'	43:BI:146:GLN:HE22	1.70	0.56
4:C:258:ARG:HH12	4:C:268:ILE:CD1	2.18	0.56
7:F:20:ARG:HD3	7:F:35:ILE:HG21	1.87	0.56
8:G:55:ARG:NH1	8:G:63:ARG:HG3	2.20	0.56
35:BA:372:C:N4	35:BA:388:G:OP2	2.39	0.56
47:BM:39:ILE:HD12	47:BM:56:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BQ:83:SER:OG	51:BQ:84:ALA:O	2.22	0.56
5:D:115:THR:HG21	5:D:174:ARG:HE	1.70	0.56
21:T:32:ARG:HH11	21:T:32:ARG:HG3	1.71	0.56
2:A:380:A:P	23:V:99:LYS:NZ	2.79	0.56
44:BJ:50:CYS:SG	44:BJ:62:ARG:HD3	2.46	0.56
44:BJ:51:VAL:HG11	48:BN:44:LEU:HD23	1.88	0.56
4:C:262:LYS:O	4:C:265:ASP:HB2	2.05	0.56
14:M:110:VAL:H	14:M:127:ASN:ND2	2.04	0.56
17:P:26:ARG:NH1	17:P:54:ASP:OD2	2.34	0.56
24:W:66:ILE:HD11	24:W:77:LEU:HD21	1.88	0.56
44:BJ:29:VAL:HG11	44:BJ:36:VAL:HB	1.87	0.56
4:C:206:TRP:CH2	4:C:215:LYS:HE3	2.39	0.56
45:BK:27:HIS:HD2	45:BK:90:LYS:HB3	1.70	0.56
5:D:37:THR:HG21	5:D:70:PHE:HE1	1.70	0.56
6:E:118:ARG:NH1	14:M:3:VAL:HG13	2.20	0.56
2:A:733:U:H2'	2:A:734:C:C6	2.41	0.55
35:BA:1458:G:H2'	35:BA:1459:G:O4'	2.06	0.55
55:BV:111:LEU:HD11	55:BV:152:ARG:HA	1.87	0.55
19:R:90:VAL:HG21	20:S:41:LEU:HD22	1.87	0.55
2:A:2571:C:OP1	4:C:40:LYS:NZ	94.17	0.55
37:BC:12:LEU:HA	37:BC:16:THR:HG23	1.88	0.55
35:BA:1202:G:O3'	53:BS:77:THR:HG21	2.05	0.55
18:Q:52:GLY:H	18:Q:56:GLU:HB2	1.71	0.55
2:A:2018:G:H22	2:A:2028:G:P	2.29	0.55
2:A:2862:G:HO2'	2:A:3002:A:N6	2.04	0.55
35:BA:382:A:H2'	35:BA:383:A:C8	2.42	0.55
48:BN:32:SER:O	48:BN:32:SER:OG	2.20	0.55
51:BQ:65:ASN:HB2	51:BQ:67:GLU:HG3	1.88	0.55
35:BA:439:U:O2'	38:BD:126:ASP:OD2	2.24	0.55
43:BI:101:LEU:HG	43:BI:105:ARG:HD2	1.88	0.55
2:A:3014:A:N6	2:A:3112:A:H2'	2.21	0.55
2:A:639:C:O2'	2:A:640:G:H8	1.89	0.55
35:BA:21:U:OP1	39:BE:44:ASN:ND2	2.34	0.55
4:C:155:LEU:HD13	4:C:177:MET:HE1	1.88	0.55
4:C:26:ARG:HG2	4:C:28:THR:H	1.70	0.55
14:M:67:PHE:HD2	14:M:69:ASN:H	1.55	0.55
24:W:119:THR:HG23	24:W:150:GLY:HA2	1.87	0.55
2:A:1552:A:H2	2:A:1617:C:H5	1.53	0.55
2:A:363:A:H2'	2:A:364:A:O4'	2.06	0.55
35:BA:458:A:OP1	35:BA:459:G:H1'	2.07	0.55
46:BL:14:ASP:OD1	46:BL:15:LYS:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BS:36:ARG:NH2	53:BS:77:THR:OG1	2.39	0.55
4:C:147:LEU:HD21	4:C:155:LEU:HD11	1.88	0.55
2:A:1756:G:N3	2:A:1756:G:H2'	2.22	0.55
15:N:10:ARG:HH12	56:BW:64:A:H4'	1.72	0.55
10:I:94:LYS:NZ	10:I:120:VAL:O	2.39	0.55
27:Z:62:ARG:HH21	27:Z:66:LEU:HD21	1.71	0.55
2:A:1722:C:H2'	2:A:1723:U:O4'	2.07	0.55
2:A:3021:A:H4'	2:A:3022:G:C8	2.42	0.55
35:BA:452:A:N6	50:BP:94:LYS:H	2.05	0.55
53:BS:15:LEU:HD23	53:BS:33:THR:HG21	1.89	0.55
55:BV:114:LEU:HD13	55:BV:152:ARG:NH1	2.22	0.55
11:J:11:ILE:HG21	11:J:33:HIS:CD2	2.42	0.55
2:A:998:G:H22	2:A:1009:U:H3	1.55	0.55
2:A:1564:A:H2'	2:A:1565:A:C8	2.42	0.55
2:A:316:U:O2'	2:A:317:G:OP1	2.20	0.55
38:BD:99:ARG:HH22	38:BD:188:VAL:HG23	1.71	0.55
47:BM:96:LEU:O	47:BM:110:ARG:NH1	2.39	0.55
6:E:192:ASP:HA	14:M:5:LYS:HZ3	1.71	0.55
2:A:857:U:H2'	2:A:858:A:C8	2.42	0.54
35:BA:987:A:C8	35:BA:1007:U:H1'	2.42	0.54
53:BS:3:ARG:HH11	53:BS:10:PHE:HB2	1.72	0.54
15:N:72:ARG:HB3	15:N:72:ARG:NH1	2.22	0.54
37:BC:22:TRP:CE2	48:BN:54:PRO:HG3	2.42	0.54
39:BE:130:VAL:O	39:BE:137:ARG:NH2	2.41	0.54
4:C:26:ARG:HG2	4:C:27:SER:N	2.22	0.54
15:N:62:GLY:HA2	24:W:123:LEU:HD11	1.89	0.54
35:BA:1110:A:H4'	43:BI:40:ARG:NH1	2.22	0.54
9:H:82:VAL:HG11	9:H:91:LEU:HD13	1.89	0.54
15:N:65:TRP:HB2	15:N:105:GLU:HB2	1.88	0.54
2:A:2707:C:N3	15:N:124:LYS:NZ	2.53	0.54
35:BA:108:G:OP2	50:BP:28:ARG:NH2	2.40	0.54
35:BA:1298:G:N7	53:BS:7:LYS:NZ	2.55	0.54
55:BV:110:ARG:HD3	55:BV:144:LEU:HD11	1.89	0.54
55:BV:75:GLN:HG3	55:BV:207:ILE:HB	1.89	0.54
10:I:82:VAL:HG13	10:I:89:ALA:HB2	1.90	0.54
35:BA:924:G:H21	43:BI:146:GLN:NE2	2.05	0.54
37:BC:186:LEU:HD13	37:BC:199:LYS:HG2	1.90	0.54
38:BD:77:GLN:NE2	38:BD:88:ILE:HD11	2.22	0.54
45:BK:23:LYS:HE3	45:BK:86:HIS:CD2	2.42	0.54
11:J:114:LYS:O	11:J:118:LEU:N	2.41	0.54
16:O:26:THR:HG23	16:O:75:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:41:ILE:O	23:V:61:THR:HA	2.06	0.54
2:A:2761:U:H2'	2:A:2762:C:C6	2.43	0.54
3:B:15:U:OP2	3:B:71:C:O2'	2.26	0.54
35:BA:1237:C:H3'	37:BC:26:LYS:HZ2	1.73	0.54
37:BC:46:LEU:HD12	37:BC:51:ILE:HD11	1.88	0.54
38:BD:165:TRP:CE3	38:BD:181:PRO:HB3	2.43	0.54
40:BF:37:VAL:HB	40:BF:66:LYS:HB2	1.90	0.54
47:BM:56:LEU:O	47:BM:60:ILE:HG23	2.06	0.54
35:BA:1201:G:H1'	53:BS:52:HIS:HD2	1.73	0.54
2:A:539:C:H4'	6:E:53:LYS:NZ	2.23	0.54
7:F:57:ILE:HD13	7:F:91:PRO:HB2	1.89	0.54
16:O:33:ARG:NH2	16:O:114:GLU:OE2	2.40	0.54
18:Q:71:ARG:HG2	18:Q:73:PHE:CZ	2.42	0.54
2:A:1627:U:H2'	2:A:1628:A:H8	1.73	0.54
2:A:1640:A:H3'	2:A:1641:U:C5'	2.37	0.54
35:BA:1470:G:H2'	35:BA:1471:G:O4'	2.08	0.54
35:BA:299:G:H2'	35:BA:300:A:C8	2.43	0.54
54:BT:68:HIS:ND1	54:BT:69:PRO:HD2	2.22	0.54
2:A:1162:G:O2'	2:A:1229:A:N6	2.41	0.54
2:A:2422:A:O2'	26:Y:63:ARG:NH1	2.41	0.54
10:I:40:ARG:HG3	10:I:40:ARG:NH1	2.17	0.54
39:BE:110:VAL:HG12	39:BE:121:LEU:HB2	1.90	0.54
13:L:13:ASN:N	13:L:13:ASN:OD1	2.41	0.54
14:M:49:MET:HE3	14:M:49:MET:H	1.73	0.54
23:V:67:HIS:HD2	23:V:69:SER:H	1.56	0.54
2:A:2343:G:H2'	2:A:2344:G:C8	2.43	0.54
2:A:288:U:H4'	2:A:289:A:O5'	2.07	0.54
2:A:336:C:N4	2:A:337:U:O4	2.41	0.54
45:BK:103:GLU:HB3	45:BK:107:ARG:NH2	2.22	0.54
9:H:4:ILE:HG13	9:H:39:ALA:HB2	1.89	0.54
2:A:1679:A:H4'	2:A:1679:A:OP1	2.08	0.53
2:A:2147:U:H2'	2:A:2148:C:C6	2.43	0.53
35:BA:1232:A:H2'	35:BA:1233:A:O4'	2.08	0.53
9:H:124:ILE:O	9:H:125:LYS:HB2	2.08	0.53
10:I:94:LYS:HZ1	10:I:124:ALA:HB2	1.73	0.53
18:Q:28:HIS:CD2	18:Q:82:HIS:HB2	2.42	0.53
2:A:1533:U:H3'	2:A:1534:C:H5''	1.91	0.53
39:BE:105:THR:HG21	39:BE:124:ALA:H	1.74	0.53
2:A:2864:G:H5'	12:K:99:ARG:HH22	1.73	0.53
35:BA:793:U:H5''	35:BA:796:A:N6	2.22	0.53
35:BA:954:C:O3'	44:BJ:59:LYS:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BM:7:VAL:HG21	47:BM:22:ILE:HG12	1.90	0.53
56:BW:28:G:H1	56:BW:42:C:H42	1.56	0.53
4:C:68:ARG:NH1	4:C:150:GLY:O	2.41	0.53
17:P:77:LYS:HB3	17:P:112:ARG:HD3	1.90	0.53
2:A:574:C:O2'	21:T:67:ASN:ND2	2.40	0.53
35:BA:269:U:H2'	35:BA:270:A:C8	2.43	0.53
43:BI:58:TYR:HE2	43:BI:87:LEU:HD12	1.72	0.53
10:I:54:ASN:ND2	10:I:73:PHE:O	2.42	0.53
13:L:2:ILE:HG13	13:L:8:LEU:HD21	1.90	0.53
2:A:442:U:H2'	2:A:443:C:C6	2.44	0.53
4:C:108:PRO:HD2	4:C:111:LEU:HD22	1.90	0.53
2:A:1260:C:H6	12:K:27:ARG:NH1	2.04	0.53
18:Q:19:PHE:HA	18:Q:88:ARG:NH1	2.23	0.53
25:X:41:ARG:HE	25:X:41:ARG:HA	1.74	0.53
2:A:2387:U:H3'	2:A:2388:G:H8	1.74	0.53
35:BA:1513:G:N7	36:BB:7:LYS:HE3	2.23	0.53
11:J:132:GLY:HA2	11:J:135:ARG:HD2	1.91	0.53
2:A:1206:A:H62	11:J:136:SER:HB3	1.74	0.53
12:K:116:ARG:HH11	12:K:116:ARG:HG3	1.73	0.53
55:BV:151:ILE:HA	55:BV:154:MET:HB2	1.90	0.53
5:D:154:CYS:C	5:D:156:THR:H	2.11	0.53
6:E:112:ARG:NH1	6:E:112:ARG:CG	2.66	0.53
24:W:28:ARG:HH21	24:W:93:GLN:HB3	1.74	0.53
2:A:2334:U:H4'	2:A:2341:U:O2'	2.08	0.53
2:A:302:U:H1'	2:A:303:G:C8	2.44	0.53
55:BV:23:TRP:HA	55:BV:189:THR:HG23	1.91	0.53
8:G:116:ILE:HD11	8:G:152:LEU:HD11	1.91	0.53
2:A:1756:G:H1'	2:A:1758:G:N1	2.23	0.53
35:BA:645:G:H1'	35:BA:713:G:H1'	1.91	0.53
16:O:36:THR:OG1	16:O:37:THR:N	2.42	0.53
17:P:26:ARG:HD3	17:P:37:ARG:NH1	2.24	0.53
2:A:3052:A:O2'	2:A:3105:C:OP1	2.23	0.53
35:BA:252:U:H2'	35:BA:253:U:C6	2.44	0.53
40:BF:20:ALA:HB3	40:BF:21:PRO:HD3	1.91	0.53
35:BA:482:A:OP1	46:BL:114:ARG:N	2.42	0.53
54:BT:8:ILE:HA	54:BT:11:ILE:HD12	1.91	0.53
13:L:13:ASN:HD21	13:L:97:ARG:N	2.06	0.53
2:A:306:U:H5''	9:H:41:ARG:HG2	1.90	0.52
5:D:79:ARG:HG2	5:D:80:HIS:CE1	2.44	0.52
6:E:154:VAL:HG12	6:E:175:VAL:HG22	1.91	0.52
9:H:77:ASP:HB3	9:H:147:ASN:HD21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:114:LYS:HB3	11:J:118:LEU:HG	1.91	0.52
2:A:337:U:H5'	2:A:338:C:O5'	2.09	0.52
46:BL:21:THR:HG22	46:BL:24:LEU:HG	1.91	0.52
46:BL:71:GLY:O	46:BL:99:ARG:NH2	2.35	0.52
52:BR:35:THR:O	52:BR:39:ARG:HG2	2.09	0.52
53:BS:50:ALA:HB1	53:BS:57:HIS:HB3	1.91	0.52
15:N:1:MET:SD	15:N:45:ARG:HG2	2.49	0.52
35:BA:488:C:H1'	35:BA:489:A:H2	1.74	0.52
8:G:38:ALA:HB1	8:G:40:PRO:HD2	1.92	0.52
9:H:100:VAL:HG22	9:H:146:LEU:HD21	1.90	0.52
10:I:94:LYS:HZ1	10:I:124:ALA:CB	2.22	0.52
11:J:111:ALA:O	11:J:115:LYS:HB2	2.10	0.52
2:A:2356:G:H2'	2:A:2380:G:H22	1.74	0.52
2:A:7:U:H5	2:A:2853:C:N3	2.06	0.52
56:BW:49:C:N4	56:BW:65:G:H1	2.05	0.52
5:D:110:ALA:O	5:D:182:VAL:HG12	2.09	0.52
13:L:63:VAL:HG12	13:L:106:LEU:HD11	1.91	0.52
17:P:66:ILE:HG23	17:P:71:ARG:HH21	1.74	0.52
2:A:1312:G:O2'	19:R:12:LYS:NZ	2.42	0.52
35:BA:928:A:H2'	35:BA:929:G:C8	2.45	0.52
10:I:17:PHE:CZ	10:I:64:ALA:HB3	2.45	0.52
35:BA:23:C:OP1	39:BE:155:SER:OG	2.28	0.52
35:BA:411:A:C4	35:BA:413:G:H1'	2.45	0.52
35:BA:909:G:O2'	35:BA:1487:A:N7	2.40	0.52
35:BA:994:C:H2'	35:BA:995:A:C8	2.45	0.52
38:BD:134:GLN:HG2	38:BD:179:GLN:HA	1.92	0.52
38:BD:29:ARG:HD3	38:BD:31:TYR:OH	2.10	0.52
11:J:114:LYS:HE3	11:J:117:ASP:HB3	1.92	0.52
2:A:2:A:H2'	2:A:3:A:C8	2.45	0.52
35:BA:1477:A:H4'	35:BA:1478:G:OP1	2.09	0.52
50:BP:100:PRO:HB2	50:BP:105:LEU:HD21	1.91	0.52
10:I:26:THR:HG22	10:I:105:ILE:HA	1.91	0.52
27:Z:14:THR:HG23	27:Z:17:GLU:H	1.75	0.52
35:BA:1267:U:H3'	35:BA:1268:C:C5'	2.39	0.52
45:BK:32:ILE:HG12	45:BK:41:VAL:HG12	1.92	0.52
4:C:26:ARG:HD3	4:C:28:THR:O	2.10	0.52
11:J:40:PHE:CD1	11:J:60:ILE:HD11	2.44	0.52
17:P:18:ARG:HD2	17:P:107:TYR:CZ	2.45	0.52
23:V:40:ARG:HA	23:V:62:GLN:O	2.10	0.52
27:Z:5:THR:HG21	27:Z:21:LYS:NZ	2.24	0.52
2:A:2704:C:H5'	2:A:2705:G:OP2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:444:U:H5'	2:A:446:G:H4'	1.91	0.52
2:A:523:U:H2'	2:A:524:C:H5'	1.92	0.52
35:BA:821:C:N4	35:BA:826:U:H3	2.08	0.52
50:BP:21:ILE:HD13	50:BP:33:ALA:HB2	1.91	0.52
35:BA:1502:A:H5'	36:BB:19:LYS:NZ	2.25	0.51
35:BA:440:C:H2'	35:BA:441:A:H8	1.75	0.51
37:BC:28:TYR:HE2	44:BJ:13:TYR:HH	1.57	0.51
45:BK:97:GLY:O	45:BK:102:ARG:NH2	2.43	0.51
4:C:200:GLU:OE1	4:C:200:GLU:N	2.40	0.51
7:F:117:ARG:HD2	7:F:146:HIS:CE1	2.45	0.51
21:T:32:ARG:HG3	21:T:32:ARG:NH1	2.26	0.51
2:A:2495:G:OP1	25:X:18:ALA:HB1	2.10	0.51
2:A:287:A:C6	2:A:300:G:C6	2.98	0.51
35:BA:638:A:H1'	49:BO:22:THR:HG21	1.91	0.51
35:BA:695:A:H2'	35:BA:696:A:C8	2.45	0.51
39:BE:66:ASP:OD1	39:BE:70:MET:HB2	2.10	0.51
45:BK:64:SER:O	45:BK:67:SER:OG	2.28	0.51
7:F:20:ARG:HH11	7:F:20:ARG:HG3	1.75	0.51
35:BA:440:C:H2'	35:BA:441:A:C8	2.45	0.51
43:BI:68:ILE:HD13	43:BI:99:LEU:HD23	1.91	0.51
35:BA:376:G:H5''	50:BP:6:LYS:HB3	1.92	0.51
7:F:42:VAL:HB	7:F:162:THR:HG23	1.90	0.51
26:Y:2:ALA:HA	26:Y:33:ILE:HD11	1.91	0.51
2:A:1455:U:OP1	22:U:19:LYS:NZ	2.40	0.51
2:A:1619:U:H2'	2:A:1620:U:O4'	2.10	0.51
2:A:164:A:H2'	2:A:165:U:C6	2.46	0.51
2:A:1755:A:H2	2:A:1759:A:N6	2.09	0.51
2:A:635:G:H1'	2:A:636:U:H5'	1.91	0.51
35:BA:492:U:H2'	35:BA:493:A:C8	2.45	0.51
10:I:14:ALA:CB	10:I:63:GLU:HG3	2.40	0.51
23:V:91:THR:HB	23:V:93:LYS:HG3	1.91	0.51
2:A:1000:C:H3'	2:A:1001:C:H5''	1.92	0.51
2:A:2306:A:H61	2:A:2460:U:H3	1.59	0.51
2:A:2552:A:H2'	2:A:2553:G:C8	2.45	0.51
2:A:2636:A:H2'	2:A:2637:G:O4'	2.09	0.51
2:A:80:G:N2	2:A:99:G:H1'	2.26	0.51
35:BA:495:G:H2'	35:BA:496:U:C6	2.44	0.51
35:BA:1273:C:OP1	41:BG:41:ARG:NH1	2.44	0.51
12:K:76:ARG:HB3	12:K:85:ARG:HH12	1.74	0.51
22:U:7:PRO:HG3	22:U:48:LYS:HD3	1.93	0.51
2:A:1044:U:H5'	2:A:1045:C:OP2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1224:G:O2'	10:I:28:TYR:OH	2.12	0.51
2:A:334:G:N2	2:A:347:U:O2	2.44	0.51
35:BA:1237:C:H2'	37:BC:26:LYS:NZ	2.26	0.51
56:BW:14:A:C2	56:BW:22:G:H1'	2.46	0.51
4:C:146:GLU:HB2	4:C:189:CYS:HB2	1.93	0.51
2:A:380:A:OP1	23:V:99:LYS:NZ	2.36	0.51
38:BD:64:GLU:OE2	38:BD:199:TYR:OH	2.27	0.51
39:BE:156:ASP:OD1	39:BE:156:ASP:N	2.42	0.51
40:BF:94:ASP:OD1	40:BF:95:LYS:N	2.35	0.51
50:BP:15:ASN:N	50:BP:15:ASN:OD1	2.43	0.51
56:BW:2:C:H2'	56:BW:3:C:C6	2.46	0.51
15:N:75:THR:HG22	15:N:90:PRO:HA	1.91	0.51
1:3:4:ARG:NH2	1:3:8:LYS:HZ1	2.09	0.51
55:BV:113:ARG:NH1	55:BV:117:LEU:HD21	2.26	0.51
5:D:142:GLN:O	5:D:143:ALA:HB3	2.10	0.51
5:D:7:LEU:H	5:D:34:ASN:ND2	2.09	0.51
27:Z:45:ARG:NH1	27:Z:48:ARG:HE	2.08	0.51
2:A:357:U:H4'	2:A:358:G:O5'	2.11	0.51
35:BA:251:G:HO2'	35:BA:266:G:H8	1.59	0.51
44:BJ:35:SER:HB2	44:BJ:77:LEU:HB2	1.92	0.51
43:BI:37:VAL:HG21	43:BI:99:LEU:HA	1.92	0.51
56:BW:51:U:O2	56:BW:63:G:N2	2.43	0.51
4:C:68:ARG:HH12	4:C:150:GLY:CA	2.24	0.51
5:D:28:VAL:HG22	5:D:193:LEU:HD22	1.92	0.51
8:G:5:GLY:HA3	8:G:66:HIS:CD2	2.46	0.51
2:A:1250:U:H3'	2:A:1251:A:H5''	1.93	0.50
2:A:1552:A:H2	2:A:1617:C:C5	2.29	0.50
35:BA:399:G:H2'	35:BA:400:C:C6	2.47	0.50
38:BD:47:ARG:HG2	38:BD:47:ARG:NH1	2.25	0.50
35:BA:956:A:P	48:BN:41:ARG:NH1	2.84	0.50
5:D:57:ILE:HG21	5:D:62:VAL:HG13	1.93	0.50
2:A:925:U:C4	14:M:31:LYS:O	2.64	0.50
35:BA:409:G:OP1	38:BD:104:ARG:NH2	2.43	0.50
38:BD:70:TYR:HE1	38:BD:131:ARG:HE	1.58	0.50
8:G:37:VAL:HG22	47:BM:57:ARG:NH1	144.12	0.50
50:BP:86:LEU:HB2	50:BP:87:PRO:CD	2.41	0.50
55:BV:69:PHE:HB3	55:BV:80:ILE:HG23	1.93	0.50
56:BW:17:C:O2'	56:BW:18:G:H3'	2.11	0.50
2:A:404:A:OP1	6:E:170:ARG:HD2	2.10	0.50
15:N:72:ARG:HH11	15:N:72:ARG:HB3	1.76	0.50
2:A:1178:U:C2	2:A:1180:G:H5'	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1542:A:N6	2:A:1628:A:O2'	2.44	0.50
2:A:2338:G:H4'	2:A:2388:G:H22	1.76	0.50
35:BA:642:C:H2'	35:BA:643:A:C8	2.46	0.50
35:BA:955:G:OP1	44:BJ:59:LYS:HE3	2.11	0.50
55:BV:129:ARG:CZ	55:BV:137:LEU:HD11	2.42	0.50
11:J:23:ALA:HB3	11:J:24:PRO:HD3	1.92	0.50
2:A:2463:G:OP1	4:C:244:ARG:NH2	2.29	0.50
35:BA:872:G:O2'	35:BA:888:A:N6	2.44	0.50
35:BA:893:U:H2'	35:BA:894:C:H6	1.75	0.50
53:BS:42:PRO:HA	53:BS:45:ILE:HG13	1.92	0.50
55:BV:50:ILE:O	55:BV:54:TYR:HB2	2.10	0.50
8:G:55:ARG:HH11	8:G:63:ARG:HA	1.76	0.50
35:BA:427:U:P	38:BD:13:ARG:HH22	2.34	0.50
2:A:725:A:OP1	14:M:65:LYS:HE3	2.12	0.50
2:A:1187:A:H4'	2:A:1188:A:H5''	1.93	0.50
35:BA:826:U:H2'	35:BA:828:G:H5'	1.94	0.50
55:BV:162:TRP:CD1	55:BV:217:ILE:HD13	2.45	0.50
56:BW:68:C:H2'	56:BW:69:G:O4'	2.12	0.50
2:A:2515:U:H2'	2:A:2516:U:C6	2.47	0.50
2:A:561:G:H2'	2:A:562:G:H5'	1.93	0.50
35:BA:1076:C:O2'	35:BA:1151:A:O2'	2.28	0.50
35:BA:498:C:H5	35:BA:509:G:H3'	1.77	0.50
35:BA:837:G:OP2	35:BA:853:U:N3	2.40	0.50
4:C:76:ASN:ND2	4:C:118:GLU:HB3	2.27	0.50
11:J:75:PRO:HG2	11:J:80:LEU:HD21	1.94	0.50
2:A:1612:U:H1'	40:BF:17:ARG:NH1	2.17	0.50
2:A:1729:A:H2'	2:A:1731:A:C8	2.47	0.50
35:BA:1375:G:N2	35:BA:1486:A:H8	2.09	0.50
2:A:1037:C:O2'	25:X:29:GLN:NE2	2.45	0.50
2:A:2350:G:H21	2:A:2396:A:H1'	1.76	0.50
2:A:289:A:C5	2:A:290:C:H5	2.30	0.50
42:BH:14:LEU:HD21	42:BH:64:LEU:HD21	1.93	0.50
44:BJ:41:PRO:HB3	44:BJ:72:ARG:NH1	2.27	0.50
47:BM:51:ASP:O	47:BM:55:VAL:HG23	2.12	0.50
14:M:78:VAL:HG23	14:M:104:VAL:HG13	1.93	0.50
16:O:44:LEU:HD23	16:O:113:ILE:HD13	1.94	0.50
2:A:1001:C:H4'	2:A:1001:C:OP1	2.12	0.49
35:BA:958:G:N2	35:BA:1345:A:H5'	2.26	0.49
38:BD:112:LEU:HB3	38:BD:118:PHE:CE1	2.43	0.49
4:C:43:ARG:NH2	4:C:49:ILE:HD11	2.27	0.49
16:O:37:THR:HG23	16:O:40:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:45:ARG:HB2	16:O:46:PRO:HD3	1.95	0.49
2:A:1754:G:C6	2:A:1755:A:C2	2.99	0.49
2:A:1940:A:H2'	2:A:1941:A:O4'	2.12	0.49
2:A:2022:U:O2	4:C:50:THR:HB	2.12	0.49
2:A:919:A:H8	2:A:919:A:H5''	1.76	0.49
35:BA:1122:U:H2'	35:BA:1123:G:H8	1.77	0.49
41:BG:28:ASN:HD21	41:BG:36:LYS:NZ	2.10	0.49
42:BH:35:ASN:HB2	42:BH:112:LEU:HD12	1.94	0.49
55:BV:54:TYR:HE1	55:BV:58:LYS:HE3	1.77	0.49
6:E:137:SER:O	6:E:168:SER:OG	2.26	0.49
56:BW:29:G:H1	56:BW:41:C:H42	1.59	0.49
4:C:76:ASN:O	4:C:98:LEU:HG	2.13	0.49
7:F:87:ARG:NH1	56:BW:19:G:N1	2.60	0.49
11:J:60:ILE:HD13	11:J:70:PHE:HB3	1.94	0.49
21:T:17:VAL:O	21:T:107:THR:OG1	2.24	0.49
2:A:1805:G:H2'	2:A:1806:A:H8	1.76	0.49
2:A:992:C:H2'	2:A:993:G:O4'	2.12	0.49
49:BO:8:LYS:O	49:BO:12:LEU:HB2	2.12	0.49
54:BT:56:ARG:O	54:BT:60:LYS:HG2	2.12	0.49
4:C:68:ARG:HH12	4:C:150:GLY:HA2	1.77	0.49
7:F:49:ASP:N	7:F:49:ASP:OD1	2.45	0.49
10:I:53:LYS:O	10:I:57:VAL:HG23	2.12	0.49
20:S:76:HIS:CE1	20:S:85:HIS:HB3	2.41	0.49
2:A:1678:U:H5'	2:A:1679:A:OP2	2.13	0.49
2:A:760:U:H2'	2:A:761:G:C8	2.48	0.49
35:BA:632:U:O4	35:BA:732:G:O2'	2.23	0.49
35:BA:749:G:H4'	35:BA:1497:A:H4'	1.94	0.49
11:J:30:LEU:HA	11:J:33:HIS:HD2	1.76	0.49
2:A:287:A:N6	2:A:299:G:O2'	2.46	0.49
35:BA:770:A:OP1	56:BW:38:A:O2'	2.30	0.49
38:BD:154:ARG:HG2	38:BD:155:GLU:HG3	1.94	0.49
2:A:658:U:H5'	14:M:31:LYS:NZ	2.28	0.49
39:BE:104:SER:HA	39:BE:146:HIS:HD2	1.78	0.49
43:BI:72:LEU:HD23	43:BI:107:LEU:HD11	1.95	0.49
50:BP:102:LYS:HA	50:BP:105:LEU:HD12	1.94	0.49
6:E:118:ARG:HH12	14:M:3:VAL:CG1	2.25	0.49
14:M:84:ASN:ND2	14:M:118:LEU:HA	2.25	0.49
2:A:1702:A:H61	2:A:1732:U:H3	1.60	0.49
2:A:2342:A:C2	2:A:2392:A:H2'	2.48	0.49
35:BA:335:C:H2'	35:BA:336:A:C8	2.48	0.49
35:BA:636:G:O2'	49:BO:28:GLN:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BD:110:ARG:HE	38:BD:128:PRO:HB2	1.77	0.49
41:BG:10:ARG:CG	41:BG:10:ARG:HH11	2.22	0.49
55:BV:166:THR:HG23	55:BV:173:VAL:HG21	1.94	0.49
14:M:104:VAL:HG11	14:M:110:VAL:HG22	1.95	0.49
16:O:20:LEU:HD21	16:O:40:LYS:HE3	1.95	0.49
21:T:43:LEU:O	21:T:51:SER:OG	2.30	0.49
2:A:574:C:H4'	21:T:67:ASN:ND2	2.27	0.49
2:A:270:U:H2'	2:A:271:A:H5'	1.93	0.49
2:A:639:C:O2'	2:A:640:G:O5'	2.31	0.49
35:BA:1186:U:H5''	37:BC:195:ARG:HH21	1.78	0.49
56:BW:5:G:H1'	56:BW:69:G:N2	2.27	0.49
5:D:121:LYS:HG3	5:D:170:MET:HE3	1.95	0.49
11:J:48:THR:HG21	11:J:56:ILE:HG21	1.94	0.49
17:P:36:PRO:HG2	17:P:97:VAL:HG11	1.94	0.49
2:A:1639:G:H5'	2:A:1640:A:OP1	2.13	0.49
2:A:349:G:H2'	2:A:350:A:H8	1.77	0.49
35:BA:146:A:H2'	35:BA:147:U:C6	2.48	0.49
4:C:79:VAL:HG21	4:C:111:LEU:HD21	1.94	0.49
5:D:40:ARG:O	5:D:48:SER:HA	2.13	0.49
14:M:78:VAL:HG11	14:M:83:ILE:HD11	1.95	0.49
2:A:1550:G:O2'	2:A:1551:U:OP2	2.29	0.48
2:A:610:C:O2	2:A:646:U:O2'	2.31	0.48
42:BH:8:ALA:O	42:BH:12:THR:HG23	2.12	0.48
54:BT:43:ASP:OD1	54:BT:43:ASP:N	2.45	0.48
4:C:182:ILE:HB	4:C:270:ARG:NH1	2.28	0.48
4:C:96:HIS:HD2	4:C:102:LYS:HG2	1.78	0.48
6:E:9:THR:HG22	6:E:128:THR:HG21	1.95	0.48
8:G:118:ALA:HB2	8:G:124:PHE:CE2	2.46	0.48
20:S:80:ASN:C	20:S:82:THR:H	2.15	0.48
21:T:80:THR:OG1	21:T:113:ILE:HB	2.13	0.48
2:A:365:U:H3	2:A:437:G:H1	1.61	0.48
2:A:90:C:H2'	2:A:91:C:O4'	2.13	0.48
41:BG:10:ARG:HG3	41:BG:10:ARG:NH1	2.26	0.48
2:A:284:G:H5''	2:A:285:U:OP2	2.14	0.48
2:A:273:A:N6	2:A:314:G:H1'	2.27	0.48
35:BA:1417:A:H2'	35:BA:1418:G:O4'	2.14	0.48
7:F:81:ILE:HG22	7:F:86:LEU:HD23	1.94	0.48
19:R:51:ARG:HG3	19:R:51:ARG:HH11	1.77	0.48
19:R:94:ASN:HD21	20:S:13:GLN:HB2	1.78	0.48
35:BA:1476:A:H2'	35:BA:1477:A:H2'	1.95	0.48
39:BE:132:ALA:HB2	39:BE:150:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BG:152:ALA:HB1	41:BG:155:ARG:NH2	2.28	0.48
35:BA:1357:A:OP1	41:BG:36:LYS:NZ	2.46	0.48
42:BH:41:LYS:NZ	42:BH:48:ASP:OD1	2.44	0.48
43:BI:77:ARG:O	43:BI:80:GLN:HG2	2.13	0.48
2:A:2975:G:C4	8:G:3:ARG:HD3	2.48	0.48
16:O:101:GLU:HG3	16:O:102:ASN:N	2.27	0.48
2:A:621:U:H5'	19:R:42:SER:OG	2.13	0.48
2:A:760:U:H2'	2:A:761:G:H8	1.78	0.48
2:A:80:G:H22	2:A:99:G:H1'	1.77	0.48
38:BD:55:LYS:CB	38:BD:190:LEU:HD11	2.42	0.48
39:BE:192:ALA:HA	39:BE:195:LEU:HD12	1.95	0.48
40:BF:30:ILE:HB	40:BF:36:THR:OG1	2.13	0.48
5:D:147:ARG:HB2	5:D:148:PRO:HD2	1.94	0.48
2:A:2043:C:O2'	2:A:2195:U:OP2	2.32	0.48
35:BA:612:U:H5'	35:BA:613:G:H8	1.77	0.48
38:BD:80:LYS:HB2	39:BE:127:GLY:HA3	1.95	0.48
2:A:1260:C:O2'	12:K:27:ARG:NH2	2.47	0.48
2:A:2199:G:H4'	36:BB:30:LYS:HG2	1.94	0.48
35:BA:737:U:H2'	35:BA:738:G:O4'	2.13	0.48
38:BD:126:ASP:N	38:BD:126:ASP:OD1	2.47	0.48
41:BG:70:LYS:HD2	41:BG:96:SER:HB3	1.96	0.48
46:BL:122:GLU:HG2	46:BL:123:LYS:H	1.78	0.48
35:BA:1284:U:O4	47:BM:14:ARG:HD3	2.14	0.48
5:D:27:THR:HG21	5:D:198:ILE:HG12	1.95	0.48
13:L:59:LYS:HB3	13:L:87:ILE:HG22	1.95	0.48
15:N:63:LYS:HD3	15:N:65:TRP:CH2	2.48	0.48
18:Q:48:ARG:HD2	18:Q:50:GLN:HE21	1.78	0.48
2:A:1753:C:N4	2:A:1754:G:O6	2.47	0.48
2:A:1760:G:H2'	2:A:1761:G:C8	2.49	0.48
2:A:7:U:H3'	2:A:8:U:H6	1.79	0.48
35:BA:988:C:H4'	35:BA:1018:C:H1'	1.95	0.48
35:BA:210:A:HO2'	35:BA:221:G:HO2'	1.58	0.48
35:BA:372:C:H41	35:BA:387:U:H2'	1.79	0.48
35:BA:476:A:H5'	35:BA:477:G:OP2	2.13	0.48
37:BC:61:ASP:HB2	37:BC:96:LYS:HD3	1.96	0.48
35:BA:1280:C:H2'	41:BG:114:LYS:NZ	2.29	0.48
55:BV:162:TRP:HD1	55:BV:184:ILE:HB	1.79	0.48
10:I:94:LYS:NZ	10:I:124:ALA:HB3	2.28	0.48
15:N:34:ILE:HD12	15:N:104:PHE:HB2	1.95	0.48
16:O:55:ALA:HB2	16:O:79:LEU:HD22	1.96	0.48
19:R:51:ARG:NH1	19:R:51:ARG:HG3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:159:A:C6	2:A:160:A:C6	3.02	0.48
2:A:2356:G:H2'	2:A:2380:G:H1	1.78	0.48
39:BE:70:MET:HE3	39:BE:98:ARG:CZ	2.43	0.48
44:BJ:83:THR:O	44:BJ:87:LEU:HG	2.14	0.48
6:E:27:VAL:O	6:E:120:ARG:NH2	2.47	0.48
14:M:44:LYS:HG3	14:M:45:ASN:H	1.77	0.48
15:N:69:PHE:HA	15:N:70:PRO:HD3	1.72	0.48
23:V:1:MET:O	23:V:2:LYS:HB2	2.14	0.48
2:A:1704:U:H2'	2:A:1705:C:C6	2.49	0.48
2:A:2569:G:H4'	2:A:2570:A:H5''	1.96	0.48
35:BA:1488:G:OP1	35:BA:1491:A:H4'	2.14	0.48
38:BD:99:ARG:HB3	38:BD:166:LEU:HD11	1.96	0.48
7:F:117:ARG:HH11	7:F:146:HIS:CE1	2.31	0.48
11:J:54:ASN:HB3	11:J:75:PRO:HB3	1.96	0.48
2:A:1282:G:OP1	20:S:26:LYS:NZ	2.46	0.47
2:A:1560:U:O2	40:BF:17:ARG:HD3	2.14	0.47
2:A:356:G:H4'	2:A:358:G:N1	2.30	0.47
35:BA:1109:C:H1'	35:BA:1127:A:H61	1.78	0.47
36:BB:22:ARG:HH11	36:BB:22:ARG:HG2	1.79	0.47
42:BH:77:LEU:HD12	42:BH:77:LEU:HA	1.67	0.47
55:BV:48:THR:O	55:BV:51:ASP:HB3	2.14	0.47
7:F:149:ASP:HB3	7:F:151:ASP:OD1	2.14	0.47
10:I:97:ALA:HB2	10:I:103:LEU:HD22	1.94	0.47
11:J:44:TYR:HD2	11:J:72:LEU:HD21	1.79	0.47
2:A:1258:C:P	12:K:68:LYS:HZ2	2.38	0.47
25:X:25:ARG:NH2	25:X:35:GLU:OE2	2.47	0.47
2:A:2780:C:H2'	2:A:2781:G:O4'	2.13	0.47
2:A:3055:G:H2'	2:A:3100:A:H61	1.79	0.47
35:BA:100:G:H2'	35:BA:101:G:H5''	1.96	0.47
35:BA:1132:U:H5''	44:BJ:44:THR:HG23	1.96	0.47
35:BA:1342:A:OP2	48:BN:35:ARG:NH2	2.47	0.47
35:BA:456:C:H6	35:BA:456:C:H2'	1.45	0.47
54:BT:68:HIS:CG	54:BT:69:PRO:HD2	2.48	0.47
4:C:258:ARG:HH12	4:C:268:ILE:HD12	1.79	0.47
14:M:110:VAL:N	14:M:127:ASN:HD22	2.10	0.47
18:Q:38:ARG:NH2	35:BA:346:G:OP1	2.47	0.47
2:A:1400:G:H21	2:A:1443:G:H5''	1.79	0.47
2:A:2997:C:H2'	2:A:2998:C:H6	1.80	0.47
35:BA:263:A:H2'	35:BA:264:U:C6	2.49	0.47
42:BH:18:ASN:O	42:BH:72:ARG:NH1	2.47	0.47
50:BP:9:ARG:O	50:BP:10:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BW:2:C:H2'	56:BW:3:C:H6	1.79	0.47
2:A:2445:A:H4'	4:C:188:ARG:HH12	1.79	0.47
24:W:14:ASN:HD21	24:W:32:LYS:NZ	2.13	0.47
2:A:929:C:H1'	2:A:1339:G:H21	1.79	0.47
2:A:1535:C:H2'	2:A:1536:A:O4'	2.14	0.47
2:A:1762:C:H2'	2:A:1763:G:O4'	2.14	0.47
2:A:750:C:H2'	2:A:751:A:C8	2.49	0.47
44:BJ:56:HIS:C	44:BJ:57:LYS:HG3	2.35	0.47
50:BP:86:LEU:HB2	50:BP:87:PRO:HD3	1.96	0.47
2:A:1542:A:H2'	2:A:1543:A:C8	2.48	0.47
2:A:543:U:H5	2:A:561:G:H5'	1.80	0.47
2:A:805:C:O2'	2:A:895:G:OP1	2.31	0.47
35:BA:279:A:H4'	35:BA:280:C:H5'	1.96	0.47
35:BA:413:G:O2'	35:BA:428:G:N2	2.48	0.47
35:BA:428:G:OP2	38:BD:10:ARG:NH1	2.35	0.47
37:BC:94:THR:C	37:BC:96:LYS:H	2.17	0.47
6:E:108:ALA:O	6:E:112:ARG:HG3	2.14	0.47
24:W:11:LEU:HD21	24:W:57:VAL:HG21	1.95	0.47
35:BA:436:C:O2'	38:BD:149:PRO:HG3	2.15	0.47
37:BC:87:ARG:O	37:BC:91:GLU:HG2	2.14	0.47
11:J:23:ALA:O	11:J:28:PRO:HD2	2.15	0.47
2:A:1875:U:H2'	2:A:1876:A:H8	1.79	0.47
2:A:2394:A:O2'	2:A:2396:A:OP1	2.32	0.47
35:BA:1465:C:C2'	35:BA:1466:G:H5'	2.44	0.47
51:BQ:46:HIS:HD2	51:BQ:49:TYR:H	1.62	0.47
6:E:22:ALA:O	6:E:26:ASP:HB2	2.15	0.47
18:Q:43:LYS:NZ	18:Q:86:LEU:HD12	2.30	0.47
2:A:1250:U:H2'	2:A:1251:A:C8	2.50	0.47
2:A:1555:A:H2'	2:A:1556:A:O4'	2.15	0.47
2:A:707:G:H2'	2:A:707:G:N3	2.29	0.47
35:BA:1120:G:H4'	35:BA:1121:G:H5'	1.97	0.47
35:BA:409:G:H2'	35:BA:410:G:O4'	2.14	0.47
5:D:63:ILE:CG2	5:D:65:PRO:HD2	2.44	0.47
18:Q:25:VAL:HG23	18:Q:85:VAL:HA	1.97	0.47
20:S:26:LYS:HE2	20:S:26:LYS:HB3	1.71	0.47
21:T:79:ALA:HB2	21:T:115:GLU:HG2	1.97	0.47
2:A:2543:U:H4'	2:A:2544:U:H5'	1.97	0.47
35:BA:928:A:O2'	35:BA:1315:A:N3	2.39	0.47
35:BA:255:G:H2'	35:BA:256:U:C6	2.50	0.47
38:BD:192:GLU:O	38:BD:196:VAL:HG23	2.15	0.47
42:BH:115:ASP:N	42:BH:115:ASP:OD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:502:C:H41	46:BL:50:ARG:NH1	2.13	0.47
53:BS:63:THR:HG22	53:BS:64:GLU:H	1.79	0.47
2:A:1552:A:H1'	2:A:1618:C:N4	2.22	0.47
2:A:1554:U:H3	2:A:1617:C:N4	2.13	0.47
2:A:2588:C:H2'	2:A:2589:G:O4'	2.14	0.47
2:A:270:U:C2'	2:A:271:A:H5'	2.45	0.47
2:A:380:A:N1	2:A:404:A:O2'	2.40	0.47
3:B:110:G:H2'	3:B:111:C:C6	2.50	0.47
35:BA:1266:U:H2'	35:BA:1267:U:H5''	1.97	0.47
35:BA:495:G:H2'	35:BA:496:U:H6	1.79	0.47
42:BH:21:TYR:CE2	42:BH:70:ARG:HG3	2.50	0.47
55:BV:140:GLU:O	55:BV:144:LEU:HB2	2.15	0.47
57:BX:3:U:HO2'	57:BX:4:U:H5	1.62	0.47
8:G:128:SER:HB3	8:G:129:PRO:HD2	1.97	0.47
19:R:11:GLN:HB3	19:R:15:ARG:NH2	2.30	0.47
2:A:1660:A:H2'	2:A:1661:G:O4'	2.15	0.47
2:A:739:U:O3'	2:A:740:A:H2'	2.15	0.47
40:BF:48:LEU:HD13	40:BF:52:ILE:HD12	1.96	0.47
4:C:126:LYS:HB2	4:C:126:LYS:HE3	1.58	0.47
4:C:260:PRO:O	4:C:261:ASN:HB2	2.15	0.47
6:E:61:GLY:HA3	6:E:80:ARG:HG2	1.96	0.47
2:A:1003:A:OP1	2:A:1003:A:H2'	2.15	0.46
2:A:1904:C:H2'	2:A:1905:G:O4'	2.14	0.46
2:A:2801:A:H5''	2:A:2802:G:H5'	1.97	0.46
2:A:665:G:O2'	2:A:666:A:H3'	2.14	0.46
35:BA:1159:G:N2	35:BA:1162:G:OP2	2.30	0.46
35:BA:675:A:H2'	35:BA:676:A:C8	2.50	0.46
35:BA:827:U:OP1	52:BR:19:LYS:HB2	2.15	0.46
39:BE:159:ILE:HG12	39:BE:159:ILE:H	1.61	0.46
46:BL:49:LEU:HD12	46:BL:49:LEU:HA	1.72	0.46
4:C:182:ILE:HD12	4:C:270:ARG:NH1	2.30	0.46
7:F:20:ARG:NH1	7:F:20:ARG:HG3	2.29	0.46
10:I:69:LEU:HD21	10:I:109:TYR:HB2	1.97	0.46
12:K:114:LEU:HA	12:K:114:LEU:HD12	1.73	0.46
2:A:1201:G:H4'	10:I:40:ARG:NH1	2.30	0.46
2:A:137:G:H8	2:A:137:G:OP1	1.98	0.46
2:A:2362:C:H2'	2:A:2363:A:C8	2.50	0.46
2:A:238:G:H2'	2:A:239:U:O4'	2.16	0.46
35:BA:429:U:O4'	35:BA:430:A:H8	1.98	0.46
35:BA:614:C:H2'	35:BA:615:G:C8	2.50	0.46
37:BC:21:ARG:HG2	37:BC:57:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BD:55:LYS:HD3	38:BD:190:LEU:HD21	1.97	0.46
4:C:137:PRO:O	4:C:140:THR:HG23	2.15	0.46
7:F:40:LYS:HD3	7:F:99:ARG:NH2	2.30	0.46
16:O:10:LEU:HB2	16:O:17:GLN:HE21	1.80	0.46
2:A:571:A:O2'	23:V:57:GLY:HA3	2.16	0.46
26:Y:33:ILE:HD12	26:Y:50:ASN:HB3	1.95	0.46
2:A:1343:G:HO2'	2:A:1345:G:H8	1.60	0.46
2:A:195:A:N3	2:A:195:A:H2'	2.29	0.46
2:A:277:U:H2'	2:A:278:A:C8	2.50	0.46
35:BA:1163:G:H4'	35:BA:1164:U:H5'	1.98	0.46
37:BC:134:ARG:HD2	37:BC:134:ARG:HA	1.73	0.46
37:BC:156:ARG:NH1	37:BC:193:PHE:HB3	2.31	0.46
37:BC:60:ARG:HD3	37:BC:60:ARG:HA	1.84	0.46
43:BI:134:LYS:HE3	43:BI:139:LYS:O	2.15	0.46
35:BA:606:U:H4'	50:BP:39:ARG:CZ	2.45	0.46
55:BV:135:LEU:O	55:BV:139:ARG:HG2	2.14	0.46
10:I:58:LYS:HE3	10:I:73:PHE:HB2	1.97	0.46
15:N:1:MET:HG2	15:N:48:GLU:HG3	1.96	0.46
15:N:51:ARG:NH1	24:W:195:ALA:HB2	2.30	0.46
2:A:650:G:H5''	12:K:112:ASN:ND2	2.30	0.46
3:B:17:G:N2	3:B:70:G:H1'	2.30	0.46
35:BA:522:G:OP1	38:BD:10:ARG:NH2	2.48	0.46
38:BD:15:LEU:HD13	38:BD:55:LYS:HA	1.97	0.46
42:BH:70:ARG:HD2	42:BH:70:ARG:HA	1.60	0.46
7:F:40:LYS:HG3	7:F:164:VAL:HG13	1.96	0.46
2:A:637:G:HO2'	2:A:638:U:H6	1.64	0.46
2:A:747:A:H2'	2:A:748:U:O4'	2.15	0.46
35:BA:1075:U:H2'	35:BA:1076:C:O4'	2.15	0.46
35:BA:464:G:H4'	35:BA:465:G:H4'	1.98	0.46
35:BA:640:U:H2'	35:BA:641:G:O4'	2.16	0.46
40:BF:21:PRO:O	40:BF:24:GLU:HB3	2.15	0.46
41:BG:113:GLU:HG3	41:BG:119:ARG:HA	1.96	0.46
43:BI:45:THR:HG22	43:BI:46:GLY:H	1.80	0.46
43:BI:37:VAL:HB	43:BI:87:LEU:HD22	1.97	0.46
2:A:976:A:C2	2:A:1032:A:C4	3.03	0.46
35:BA:1237:C:H2'	37:BC:26:LYS:HZ1	1.79	0.46
35:BA:472:C:H2'	35:BA:473:A:C8	2.51	0.46
35:BA:85:C:H4'	35:BA:86:G:C8	2.50	0.46
35:BA:236:G:H5''	51:BQ:57:LYS:NZ	2.30	0.46
51:BQ:85:THR:H	51:BQ:87:ARG:NH1	2.14	0.46
4:C:218:ARG:HB3	4:C:219:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:8:LEU:HD23	7:F:9:PRO:HD2	1.98	0.46
2:A:2567:U:H2'	2:A:2568:U:C6	2.51	0.46
2:A:2672:A:H4'	2:A:2673:U:OP2	2.15	0.46
2:A:2778:U:H2'	2:A:2779:U:C6	2.51	0.46
2:A:74:C:O2'	27:Z:11:ARG:NH2	2.48	0.46
35:BA:1123:G:C2	35:BA:1124:G:H1'	2.51	0.46
39:BE:97:PHE:CZ	39:BE:170:LYS:HG2	2.51	0.46
35:BA:1099:C:OP2	43:BI:31:ARG:NH2	2.49	0.46
55:BV:57:VAL:HG21	55:BV:217:ILE:HD11	1.98	0.46
7:F:15:TYR:HA	7:F:19:ILE:HD12	1.98	0.46
14:M:43:ARG:NH1	14:M:43:ARG:CG	2.70	0.46
17:P:126:LYS:HD3	17:P:126:LYS:HA	1.76	0.46
35:BA:1287:G:O2'	35:BA:1288:A:H8	1.98	0.46
35:BA:278:G:H5'	35:BA:279:A:OP1	2.16	0.46
43:BI:49:ASN:HD22	43:BI:84:TYR:HD1	1.64	0.46
45:BK:80:ALA:O	45:BK:84:GLN:HG2	2.15	0.46
50:BP:9:ARG:HB2	50:BP:29:ARG:NH1	2.30	0.46
5:D:198:ILE:HD12	5:D:206:VAL:HG11	1.98	0.46
5:D:84:LEU:HB3	5:D:209:ARG:CZ	2.46	0.46
7:F:118:ILE:HB	7:F:121:PHE:HB2	1.98	0.46
18:Q:9:GLN:HA	18:Q:12:LEU:HD12	1.98	0.46
2:A:1022:C:O2'	15:N:101:ARG:NH2	2.47	0.46
2:A:1081:C:O2'	2:A:2497:A:N3	2.43	0.46
2:A:284:G:H1'	2:A:303:G:C6	2.51	0.46
2:A:3116:C:H2'	2:A:3117:U:H6	1.81	0.46
2:A:81:A:N1	2:A:96:G:O2'	2.36	0.46
35:BA:352:C:O2	35:BA:355:C:N4	2.49	0.46
35:BA:957:A:N3	35:BA:957:A:H5'	2.30	0.46
35:BA:914:C:H5'	41:BG:4:LYS:HE2	1.98	0.46
35:BA:1197:U:H5''	48:BN:5:ALA:HB2	1.97	0.46
4:C:118:GLU:H	4:C:129:ASN:ND2	2.14	0.46
19:R:11:GLN:HB3	19:R:15:ARG:HH21	1.80	0.46
1:3:21:ARG:NH2	2:A:1100:C:N3	2.64	0.46
2:A:1454:G:OP2	22:U:62:ARG:NH2	2.49	0.46
2:A:1530:G:N2	2:A:1805:G:H22	2.14	0.46
2:A:356:G:H5''	2:A:357:U:OP1	2.16	0.46
35:BA:225:G:H2'	35:BA:226:G:O4'	2.16	0.46
35:BA:375:U:OP1	50:BP:69:PRO:HB3	2.16	0.46
35:BA:814:G:H5''	52:BR:58:VAL:HG21	1.98	0.46
54:BT:72:ALA:O	54:BT:76:LYS:HG3	2.16	0.46
8:G:129:PRO:HG2	8:G:130:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:82:VAL:HG11	9:H:91:LEU:HD22	1.97	0.46
27:Z:14:THR:HG22	27:Z:17:GLU:HB2	1.98	0.46
35:BA:1494:C:OP1	36:BB:11:ARG:HB2	2.16	0.45
35:BA:265:G:H2'	35:BA:267:C:H5	1.81	0.45
35:BA:694:G:H2'	35:BA:695:A:C8	2.50	0.45
39:BE:175:PRO:HB3	39:BE:194:MET:HE3	1.97	0.45
14:M:55:MET:O	14:M:60:ARG:NH1	2.48	0.45
2:A:2558:C:H5''	17:P:20:ARG:HH21	1.80	0.45
2:A:1065:C:H1'	2:A:1102:G:C8	2.51	0.45
2:A:2959:A:H61	2:A:2993:U:H3	1.64	0.45
35:BA:1084:G:O5'	55:BV:110:ARG:HD2	2.16	0.45
7:F:127:LYS:HA	7:F:127:LYS:HD3	1.78	0.45
12:K:89:ILE:O	12:K:93:LEU:HB2	2.17	0.45
21:T:35:SER:HA	21:T:77:VAL:HA	1.99	0.45
2:A:1001:C:C5	2:A:1002:C:H1'	2.52	0.45
35:BA:58:C:O2'	35:BA:59:A:H5''	2.16	0.45
46:BL:81:LEU:HB3	46:BL:98:ILE:HG22	1.99	0.45
2:A:708:G:N2	6:E:184:ASN:HD21	2.15	0.45
7:F:81:ILE:HG22	7:F:86:LEU:HB3	1.98	0.45
2:A:2394:A:O2'	2:A:2395:U:H3'	2.15	0.45
2:A:2937:G:H3'	2:A:2938:G:H5''	1.99	0.45
2:A:530:G:O4'	6:E:47:GLN:NE2	2.50	0.45
2:A:571:A:H4'	23:V:46:ALA:HB2	1.99	0.45
35:BA:1338:G:H2'	35:BA:1339:A:C8	2.52	0.45
37:BC:34:GLU:HB3	37:BC:58:ARG:HH22	1.81	0.45
35:BA:567:G:OP1	42:BH:83:PRO:HB3	2.16	0.45
44:BJ:19:ASP:O	44:BJ:23:ARG:HG2	2.16	0.45
47:BM:27:ARG:HB2	47:BM:27:ARG:NH1	2.31	0.45
56:BW:28:G:H1	56:BW:42:C:N4	2.14	0.45
4:C:156:ALA:HB2	4:C:163:ILE:HG13	1.99	0.45
12:K:35:LEU:HA	12:K:35:LEU:HD23	1.74	0.45
12:K:36:LEU:O	12:K:51:GLY:HA3	2.16	0.45
14:M:82:ASP:N	14:M:82:ASP:OD1	2.49	0.45
2:A:1755:A:C2	2:A:1758:G:O6	2.70	0.45
2:A:2922:U:H2'	2:A:2923:C:C6	2.52	0.45
35:BA:1076:C:H2'	35:BA:1077:C:C6	2.51	0.45
35:BA:1444:A:H2'	35:BA:1445:G:O4'	2.17	0.45
35:BA:480:G:H2'	35:BA:481:G:C8	2.51	0.45
35:BA:944:C:H1'	35:BA:1182:A:N6	2.32	0.45
44:BJ:4:GLN:O	44:BJ:79:PRO:HD3	2.17	0.45
4:C:177:MET:HG3	4:C:181:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2014:G:O2'	4:C:257:THR:OG1	2.20	0.45
5:D:121:LYS:HG3	5:D:170:MET:CE	2.47	0.45
26:Y:45:ASN:HA	26:Y:45:ASN:HD22	1.52	0.45
2:A:1236:G:H2'	2:A:1237:U:O4'	2.16	0.45
2:A:1875:U:H2'	2:A:1876:A:C8	2.52	0.45
2:A:2457:U:H2'	2:A:2458:G:C8	2.52	0.45
2:A:498:G:H5'	2:A:499:G:O5'	2.17	0.45
2:A:899:G:C8	2:A:899:G:H5'	2.49	0.45
35:BA:146:A:H2'	35:BA:147:U:H6	1.82	0.45
35:BA:666:U:H2'	35:BA:667:A:C8	2.52	0.45
5:D:142:GLN:O	5:D:143:ALA:CB	2.64	0.45
10:I:91:LYS:HG2	10:I:95:LYS:HE3	1.99	0.45
27:Z:62:ARG:NH2	27:Z:66:LEU:HD21	2.30	0.45
2:A:1799:A:H2'	2:A:1800:G:O4'	2.16	0.45
2:A:2137:A:H2	35:BA:1478:G:C8	2.35	0.45
2:A:877:U:H4'	2:A:878:G:O5'	2.16	0.45
35:BA:1266:U:O2'	35:BA:1267:U:OP1	2.30	0.45
35:BA:196:G:C2	35:BA:197:G:C5	3.05	0.45
35:BA:505:C:H5'	46:BL:88:LYS:HE3	1.99	0.45
50:BP:9:ARG:HG2	50:BP:18:TYR:CE1	2.51	0.45
7:F:130:ASP:C	7:F:132:THR:H	2.17	0.45
8:G:55:ARG:NH1	8:G:63:ARG:HA	2.32	0.45
13:L:19:ILE:HD11	13:L:84:ALA:HB3	1.99	0.45
16:O:101:GLU:OE1	21:T:45:TRP:HZ3	1.99	0.45
22:U:14:PRO:HD3	27:Z:34:PHE:CD1	2.51	0.45
2:A:1202:A:O2'	2:A:1203:A:O4'	2.22	0.45
2:A:1566:A:H2'	2:A:1567:C:C5	2.51	0.45
2:A:2061:U:H5''	4:C:256:ARG:HG2	1.99	0.45
2:A:23:G:C6	2:A:24:G:N1	2.84	0.45
37:BC:69:THR:HG21	37:BC:75:VAL:HG21	1.98	0.45
39:BE:77:LYS:O	39:BE:87:LYS:NZ	2.32	0.45
51:BQ:46:HIS:CD2	51:BQ:48:LEU:H	2.34	0.45
20:S:53:ASP:N	20:S:53:ASP:OD1	2.49	0.45
26:Y:33:ILE:HA	26:Y:52:CYS:HA	1.99	0.45
2:A:2106:A:H3'	2:A:2107:G:H5''	1.97	0.45
2:A:974:G:O2'	2:A:975:U:P	2.75	0.45
35:BA:976:A:C8	35:BA:1197:U:H4'	2.52	0.45
39:BE:97:PHE:CE1	39:BE:170:LYS:HG2	2.52	0.45
48:BN:42:ILE:O	48:BN:46:GLU:HG2	2.17	0.45
50:BP:29:ARG:HD2	50:BP:30:ASP:OD1	2.16	0.45
4:C:270:ARG:HH11	4:C:270:ARG:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:95:LYS:HD2	12:K:95:LYS:HA	1.63	0.45
2:A:2421:A:C2	9:H:29:TYR:HB2	2.52	0.45
2:A:2800:G:O2'	2:A:2803:C:OP2	2.31	0.45
2:A:636:U:H5''	2:A:637:G:C4	2.52	0.45
3:B:81:U:H2'	3:B:82:A:C8	2.52	0.45
35:BA:625:G:H2'	35:BA:626:G:H8	1.82	0.45
4:C:147:LEU:HD23	4:C:147:LEU:HA	1.84	0.45
10:I:17:PHE:HB2	10:I:81:PHE:CE1	2.52	0.45
16:O:74:ASP:OD1	16:O:74:ASP:N	2.47	0.45
21:T:43:LEU:HA	21:T:43:LEU:HD23	1.59	0.45
2:A:2315:U:P	26:Y:63:ARG:HH12	2.40	0.45
2:A:1733:C:H2'	2:A:1734:C:C6	2.52	0.44
2:A:2251:G:N2	2:A:2261:U:C2	2.85	0.44
2:A:347:U:H2'	2:A:348:G:C8	2.52	0.44
35:BA:1170:U:OP1	44:BJ:53:ARG:NH2	2.46	0.44
41:BG:101:LEU:HA	41:BG:101:LEU:HD23	1.72	0.44
42:BH:5:ASP:OD1	42:BH:79:ARG:NH1	2.50	0.44
35:BA:1110:A:H4'	43:BI:40:ARG:HH12	1.82	0.44
44:BJ:85:ASP:O	44:BJ:89:ARG:HG3	2.17	0.44
55:BV:126:PHE:HD1	55:BV:134:ILE:HG23	1.81	0.44
6:E:42:LEU:HD21	6:E:186:TYR:CE1	2.52	0.44
7:F:83:GLN:H	7:F:83:GLN:HG2	1.32	0.44
2:A:1174:G:H5'	2:A:1175:A:O4'	2.16	0.44
2:A:863:G:OP1	21:T:95:ARG:NH1	2.49	0.44
35:BA:1408:A:H2'	35:BA:1409:A:O4'	2.17	0.44
35:BA:492:U:H2'	35:BA:493:A:H8	1.81	0.44
35:BA:991:C:H2'	35:BA:992:G:O4'	2.18	0.44
38:BD:15:LEU:HB3	38:BD:55:LYS:HG2	1.98	0.44
50:BP:51:ILE:HG22	50:BP:52:ASP:O	2.17	0.44
51:BQ:85:THR:N	51:BQ:87:ARG:NH1	2.65	0.44
7:F:111:ILE:HD11	7:F:182:PHE:CD2	2.52	0.44
16:O:100:VAL:HB	16:O:101:GLU:H	1.67	0.44
2:A:2521:C:H42	2:A:2545:G:H1	1.66	0.44
2:A:245:G:O2'	2:A:472:C:O2	2.23	0.44
35:BA:1324:C:H2'	35:BA:1325:G:C8	2.53	0.44
35:BA:456:C:H4'	35:BA:457:A:OP1	2.18	0.44
35:BA:714:G:N2	52:BR:73:GLU:OE2	2.50	0.44
38:BD:167:GLN:HB2	38:BD:178:HIS:HE1	1.82	0.44
54:BT:27:SER:HB3	54:BT:57:LYS:NZ	2.31	0.44
55:BV:94:GLN:HG3	55:BV:146:ARG:O	2.16	0.44
4:C:97:TYR:HE2	4:C:103:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:120:ALA:O	17:P:125:LEU:HB2	2.17	0.44
22:U:34:HIS:HA	22:U:35:PRO:HD3	1.86	0.44
2:A:1430:C:H2'	2:A:1431:U:C6	2.52	0.44
2:A:206:A:H2'	2:A:207:C:O4'	2.17	0.44
2:A:2367:G:H1'	2:A:2371:G:H22	1.83	0.44
2:A:291:C:H1'	2:A:338:C:OP2	2.17	0.44
2:A:700:U:H2'	2:A:701:A:H5'	1.99	0.44
2:A:782:U:H2'	2:A:783:G:O4'	2.17	0.44
2:A:821:A:H2'	2:A:822:G:O4'	2.18	0.44
2:A:869:U:P	5:D:2:ALA:HB2	79.40	0.44
2:A:998:G:H1	2:A:1009:U:H3	1.65	0.44
35:BA:445:C:H2'	35:BA:446:A:H8	1.82	0.44
35:BA:532:U:H4'	46:BL:84:GLY:O	2.18	0.44
35:BA:747:A:H2'	35:BA:748:A:O4'	2.17	0.44
35:BA:893:U:H2'	35:BA:894:C:C6	2.52	0.44
53:BS:36:ARG:NH1	53:BS:75:ALA:O	2.39	0.44
55:BV:111:LEU:HD12	55:BV:111:LEU:HA	1.79	0.44
13:L:93:PRO:HG3	13:L:114:ILE:HG12	1.99	0.44
15:N:2:LEU:HB3	15:N:69:PHE:CE1	2.52	0.44
24:W:53:ASP:O	24:W:57:VAL:HG23	2.17	0.44
2:A:1584:U:H2'	2:A:1586:C:H5	1.82	0.44
2:A:2740:G:C6	2:A:2741:C:N4	2.85	0.44
2:A:291:C:HO2'	2:A:337:U:HO2'	1.64	0.44
35:BA:1019:U:H2'	35:BA:1020:G:O4'	2.18	0.44
35:BA:1135:G:H2'	35:BA:1136:A:H8	1.83	0.44
39:BE:182:ARG:NH2	39:BE:189:VAL:HA	2.33	0.44
41:BG:62:LEU:HD13	41:BG:124:ILE:HD13	1.97	0.44
42:BH:7:ILE:O	42:BH:10:PHE:HB3	2.17	0.44
35:BA:1168:G:O2'	43:BI:133:ARG:NH1	2.51	0.44
51:BQ:38:VAL:HG21	51:BQ:76:LEU:HD11	1.99	0.44
55:BV:171:ILE:O	55:BV:175:GLU:HG3	2.18	0.44
4:C:118:GLU:HG3	4:C:129:ASN:ND2	2.33	0.44
2:A:3055:G:H2'	2:A:3100:A:N6	2.31	0.44
2:A:580:G:H2'	2:A:581:G:O4'	2.18	0.44
35:BA:493:A:H2'	35:BA:494:C:C6	2.52	0.44
37:BC:120:ALA:HB1	37:BC:189:ALA:HB2	1.99	0.44
38:BD:140:VAL:HG21	38:BD:150:PHE:CZ	2.53	0.44
4:C:69:ARG:H	4:C:69:ARG:HG3	1.61	0.44
8:G:55:ARG:HD2	8:G:57:ASP:O	2.18	0.44
18:Q:111:GLU:N	18:Q:111:GLU:OE1	2.51	0.44
20:S:51:LYS:HB2	20:S:54:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:104:GLU:O	24:W:136:GLU:HA	2.18	0.44
24:W:134:GLU:HB2	24:W:171:ILE:HD11	1.99	0.44
2:A:1953:C:H2'	2:A:1954:C:O4'	2.18	0.44
2:A:2085:C:O2'	2:A:2086:U:P	2.76	0.44
2:A:2094:G:O2'	2:A:2095:G:H8	2.00	0.44
2:A:3044:A:OP1	5:D:123:PHE:HB2	2.17	0.44
35:BA:81:C:H3'	35:BA:82:U:H5''	2.00	0.44
35:BA:13:G:H5'	39:BE:133:GLY:HA3	2.00	0.44
46:BL:114:ARG:HG2	46:BL:119:ALA:HB3	1.99	0.44
49:BO:75:VAL:HB	49:BO:79:ARG:NH2	2.33	0.44
7:F:59:GLY:HA3	7:F:157:ARG:HH12	1.82	0.44
18:Q:48:ARG:HD2	18:Q:50:GLN:NE2	2.33	0.44
18:Q:54:ILE:O	18:Q:54:ILE:HD13	2.18	0.44
2:A:1131:G:H21	19:R:122:ASN:ND2	2.16	0.44
2:A:1158:U:H3	2:A:1233:A:N6	2.13	0.44
2:A:2027:A:H2'	2:A:2028:G:O4'	2.17	0.44
35:BA:1098:U:H1'	35:BA:1160:A:C4	2.53	0.44
35:BA:1281:A:N3	35:BA:1281:A:H2'	2.32	0.44
35:BA:427:U:OP1	38:BD:13:ARG:NH2	2.51	0.44
35:BA:452:A:H2	50:BP:47:SER:HB2	1.83	0.44
35:BA:504:G:H2'	35:BA:505:C:C6	2.53	0.44
35:BA:806:C:H5'	42:BH:13:ARG:HH21	1.83	0.44
37:BC:123:LEU:HB3	37:BC:196:ILE:HD11	1.99	0.44
43:BI:30:GLY:N	43:BI:102:ALA:HB2	2.33	0.44
55:BV:57:VAL:O	55:BV:61:VAL:HG23	2.18	0.44
4:C:163:ILE:HG12	4:C:178:PRO:HD3	1.99	0.44
10:I:66:ILE:HG22	10:I:109:TYR:CG	2.53	0.44
18:Q:4:LEU:HA	18:Q:4:LEU:HD23	1.62	0.44
2:A:159:A:H2'	2:A:160:A:C8	2.53	0.44
2:A:1665:U:H2'	2:A:1666:A:H8	1.82	0.44
2:A:747:A:N6	2:A:768:G:O2'	2.51	0.44
35:BA:103:G:H2'	35:BA:104:A:O4'	2.17	0.44
35:BA:1406:G:H2'	35:BA:1407:U:O4'	2.18	0.44
35:BA:426:U:OP1	38:BD:31:TYR:OH	2.36	0.44
45:BK:37:ASN:HA	45:BK:67:SER:HB3	2.00	0.44
54:BT:81:LEU:HA	54:BT:81:LEU:HD12	1.84	0.44
5:D:96:GLU:O	5:D:99:GLN:HB3	2.17	0.44
8:G:152:LEU:HA	8:G:152:LEU:HD23	1.83	0.44
13:L:4:GLN:HE21	13:L:23:ARG:NH1	2.16	0.44
16:O:117:ARG:HA	16:O:117:ARG:HD3	1.78	0.44
21:T:7:PHE:HB2	21:T:115:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1530:G:H2'	2:A:1531:C:O4'	2.18	0.43
35:BA:1152:C:H2'	35:BA:1153:U:C6	2.53	0.43
35:BA:1465:C:H2'	35:BA:1466:G:H5'	2.00	0.43
35:BA:498:C:H4'	35:BA:499:C:O5'	2.17	0.43
41:BG:10:ARG:CG	41:BG:10:ARG:NH1	2.81	0.43
55:BV:4:VAL:HG11	55:BV:212:LEU:HD21	1.99	0.43
55:BV:87:VAL:HG21	55:BV:218:ALA:HB1	2.00	0.43
4:C:120:GLY:O	4:C:131:LEU:HB3	2.18	0.43
5:D:113:ASP:OD1	5:D:178:GLN:HA	2.18	0.43
6:E:145:LEU:HD23	6:E:145:LEU:HA	1.76	0.43
10:I:94:LYS:HB2	10:I:94:LYS:HE3	1.56	0.43
11:J:57:PRO:HG2	11:J:73:LYS:HB2	2.00	0.43
16:O:9:ARG:HD3	16:O:9:ARG:HA	1.82	0.43
24:W:122:THR:HG23	24:W:181:VAL:HG13	2.00	0.43
2:A:1294:U:H2'	2:A:1295:U:C6	2.53	0.43
2:A:561:G:C2'	2:A:562:G:H5'	2.47	0.43
2:A:768:G:H2'	2:A:769:U:C6	2.53	0.43
35:BA:427:U:H5''	35:BA:428:G:O5'	2.18	0.43
47:BM:106:ASN:O	47:BM:107:ALA:HB3	2.18	0.43
50:BP:55:ARG:HD3	50:BP:55:ARG:HA	1.61	0.43
56:BW:34:G:H1	57:BX:6:U:H3	1.65	0.43
9:H:10:GLU:HB3	9:H:11:HIS:CD2	2.53	0.43
14:M:31:LYS:HE3	14:M:32:THR:HG23	1.99	0.43
15:N:2:LEU:O	15:N:3:ILE:HG23	2.17	0.43
23:V:8:THR:O	23:V:74:VAL:HG12	2.17	0.43
2:A:1260:C:C6	12:K:27:ARG:NH1	2.85	0.43
2:A:1637:G:O2'	2:A:1805:G:O2'	2.36	0.43
35:BA:1185:A:H2'	35:BA:1186:U:O4'	2.18	0.43
37:BC:19:LYS:O	37:BC:55:GLU:HA	2.18	0.43
35:BA:527:A:OP2	38:BD:2:ALA:N	2.51	0.43
41:BG:24:THR:O	41:BG:27:VAL:HG22	2.18	0.43
45:BK:63:GLY:O	45:BK:66:LYS:HG2	2.18	0.43
46:BL:25:LYS:HD3	46:BL:59:SER:HB3	2.00	0.43
4:C:25:THR:HG21	4:C:113:GLN:HE22	1.83	0.43
8:G:150:ARG:HG2	8:G:150:ARG:HH11	1.82	0.43
15:N:51:ARG:HH12	24:W:195:ALA:HB2	1.82	0.43
25:X:18:ALA:HB3	25:X:20:ARG:HH12	1.82	0.43
2:A:2366:C:H2'	2:A:2367:G:O4'	2.19	0.43
35:BA:185:G:H2'	35:BA:186:C:C6	2.53	0.43
35:BA:203:U:H2'	35:BA:204:A:H8	1.83	0.43
41:BG:28:ASN:HD21	41:BG:36:LYS:HZ1	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BI:53:ARG:NH1	43:BI:58:TYR:HD1	2.17	0.43
37:BC:6:ASN:HD22	48:BN:49:HIS:HB3	1.84	0.43
5:D:189:ASN:O	5:D:191:VAL:HG23	2.18	0.43
14:M:61:LEU:HA	14:M:62:PRO:HD3	1.84	0.43
2:A:2074:G:C6	2:A:2075:G:N1	2.86	0.43
2:A:2442:U:H2'	2:A:2443:U:O4'	2.19	0.43
2:A:356:G:H4'	2:A:358:G:C2	2.53	0.43
35:BA:1187:G:H2'	35:BA:1188:C:O4'	2.18	0.43
39:BE:137:ARG:NH1	39:BE:137:ARG:HB2	2.34	0.43
44:BJ:92:LEU:HD12	44:BJ:98:VAL:HG21	1.99	0.43
44:BJ:24:LYS:NZ	44:BJ:93:PRO:HD3	2.34	0.43
46:BL:38:TYR:N	46:BL:38:TYR:CD1	2.86	0.43
47:BM:67:GLU:HB3	47:BM:68:GLY:H	1.60	0.43
52:BR:48:ILE:HG12	52:BR:68:VAL:HG11	2.00	0.43
53:BS:18:LYS:HA	53:BS:18:LYS:HD3	1.88	0.43
54:BT:35:PHE:CE1	54:BT:51:LEU:HB2	2.53	0.43
8:G:46:ALA:HB3	8:G:50:ALA:HB3	2.00	0.43
2:A:1530:G:N2	2:A:1806:A:C6	2.86	0.43
2:A:2613:G:O5'	2:A:2614:U:H5'	2.19	0.43
2:A:460:G:O2'	2:A:488:G:O6	2.28	0.43
35:BA:1384:G:C6	35:BA:1385:C:C2	3.06	0.43
35:BA:144:G:H2'	35:BA:145:G:C8	2.54	0.43
40:BF:15:ASP:OD1	40:BF:15:ASP:N	2.50	0.43
42:BH:53:ASP:OD1	42:BH:58:LYS:HG2	2.19	0.43
47:BM:49:THR:HG22	47:BM:50:ASP:H	1.83	0.43
51:BQ:35:THR:HG22	51:BQ:86:LYS:NZ	2.33	0.43
53:BS:12:ASP:OD1	53:BS:38:SER:HB3	2.18	0.43
55:BV:160:ALA:HB1	55:BV:184:ILE:HD11	2.01	0.43
4:C:16:ALA:HB2	4:C:207:GLY:HA3	2.01	0.43
4:C:68:ARG:O	4:C:68:ARG:HG3	2.18	0.43
7:F:50:ALA:HB1	7:F:57:ILE:HD11	2.00	0.43
2:A:1048:A:C6	2:A:1050:A:C8	3.06	0.43
2:A:156:C:H2'	2:A:157:U:H6	1.83	0.43
2:A:2757:C:H2'	2:A:2758:A:O4'	2.19	0.43
39:BE:182:ARG:HH21	39:BE:189:VAL:HA	1.84	0.43
35:BA:803:G:HO2'	42:BH:2:THR:N	2.16	0.43
44:BJ:78:ASP:N	44:BJ:78:ASP:OD1	2.52	0.43
52:BR:24:SER:HB3	52:BR:26:LYS:HG2	2.00	0.43
6:E:20:LEU:HB3	6:E:25:PHE:CD1	2.54	0.43
14:M:49:MET:HB2	14:M:58:HIS:HE1	1.83	0.43
24:W:105:LYS:HA	24:W:105:LYS:HD3	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:117:ASP:H	24:W:149:GLU:HG3	1.83	0.43
2:A:1339:G:OP1	20:S:72:LYS:NZ	2.49	0.43
2:A:1640:A:C3'	2:A:1641:U:H5''	2.47	0.43
35:BA:53:U:H6	35:BA:53:U:H5''	1.84	0.43
35:BA:65:G:H2'	35:BA:66:U:O4'	2.19	0.43
35:BA:994:C:H2'	35:BA:995:A:H8	1.83	0.43
46:BL:54:ARG:NH1	46:BL:64:THR:HG23	2.30	0.43
50:BP:65:GLN:HA	50:BP:66:PRO:HD2	1.78	0.43
5:D:83:GLU:O	5:D:84:LEU:HD23	2.19	0.43
7:F:66:LEU:HD23	7:F:66:LEU:HA	1.77	0.43
8:G:41:ILE:HD11	8:G:65:LEU:HB3	2.01	0.43
10:I:40:ARG:CG	10:I:40:ARG:NH1	2.81	0.43
16:O:73:LYS:HA	16:O:76:VAL:HG22	1.99	0.43
26:Y:39:VAL:HG21	26:Y:64:ALA:HB3	2.00	0.43
2:A:1400:G:N2	2:A:1443:G:H5''	2.34	0.43
2:A:1565:A:N6	2:A:1606:G:H1	2.17	0.43
2:A:159:A:N3	2:A:2431:C:O2'	2.52	0.43
2:A:1755:A:C2	2:A:1759:A:N6	2.87	0.43
2:A:2008:A:N6	2:A:2045:G:O2'	2.48	0.43
35:BA:196:G:H2'	35:BA:197:G:C8	2.54	0.43
35:BA:390:U:H2'	35:BA:391:G:H8	1.84	0.43
35:BA:614:C:H2'	35:BA:615:G:H8	1.83	0.43
35:BA:864:C:O2'	35:BA:865:C:H5'	2.19	0.43
42:BH:19:SER:HA	42:BH:72:ARG:NH1	2.33	0.43
46:BL:39:THR:HA	46:BL:50:ARG:O	2.19	0.43
46:BL:70:GLU:H	46:BL:70:GLU:CD	2.21	0.43
50:BP:40:TYR:CZ	50:BP:42:PRO:HG3	2.54	0.43
6:E:29:PRO:HD3	6:E:120:ARG:NH1	2.34	0.43
7:F:50:ALA:HA	7:F:53:ASP:O	2.19	0.43
25:X:54:GLY:N	25:X:58:THR:O	2.47	0.43
2:A:1855:A:H2'	2:A:1856:C:C6	2.54	0.43
2:A:2585:U:H2'	2:A:2586:G:H5'	2.01	0.43
2:A:3082:U:H2'	2:A:3083:A:H8	1.83	0.43
2:A:601:A:H2'	2:A:602:A:O4'	2.19	0.43
35:BA:595:C:H2'	35:BA:596:A:H8	1.84	0.43
45:BK:109:LEU:HD23	45:BK:109:LEU:HA	1.81	0.43
6:E:94:LYS:HD3	6:E:94:LYS:HA	1.59	0.43
7:F:75:ARG:HA	7:F:75:ARG:HD3	1.86	0.43
8:G:110:TYR:CE1	8:G:153:ARG:NH1	2.87	0.43
9:H:98:ALA:HB2	9:H:114:LYS:HD2	2.01	0.43
10:I:82:VAL:HG21	10:I:86:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:24:ARG:HD3	14:M:24:ARG:HA	1.42	0.43
2:A:250:G:H2'	2:A:251:A:C8	2.54	0.42
35:BA:203:U:H2'	35:BA:204:A:C8	2.54	0.42
39:BE:99:VAL:HG12	39:BE:101:LEU:HG	2.01	0.42
47:BM:9:LEU:HA	47:BM:10:PRO:HD3	1.91	0.42
50:BP:48:LEU:HD11	50:BP:50:GLN:HG2	2.01	0.42
55:BV:52:LYS:O	55:BV:55:GLU:HG2	2.19	0.42
4:C:26:ARG:NH1	4:C:30:GLU:OE1	2.49	0.42
6:E:28:GLU:HA	6:E:120:ARG:HH22	1.81	0.42
22:U:44:ILE:HA	22:U:47:GLU:OE2	2.18	0.42
24:W:77:LEU:HA	24:W:77:LEU:HD12	1.87	0.42
2:A:2548:U:H5'	2:A:2549:G:H5'	2.01	0.42
35:BA:1271:A:H2'	35:BA:1272:G:H5'	2.01	0.42
35:BA:32:G:H2'	35:BA:33:A:O4'	2.19	0.42
35:BA:380:G:N2	35:BA:383:A:OP2	2.47	0.42
35:BA:728:A:OP2	35:BA:728:A:H8	2.01	0.42
36:BB:3:SER:OG	36:BB:5:ILE:HG13	2.19	0.42
44:BJ:90:ILE:HG22	44:BJ:92:LEU:HG	2.01	0.42
35:BA:735:G:OP2	49:BO:65:ARG:HD3	2.19	0.42
50:BP:82:LYS:HB2	50:BP:89:ALA:HB2	2.01	0.42
4:C:70:HIS:CG	4:C:71:ASP:N	2.87	0.42
4:C:62:TYR:HA	4:C:87:ASN:HD21	1.84	0.42
11:J:10:LEU:N	11:J:62:VAL:HG22	2.33	0.42
16:O:38:GLU:N	16:O:39:PRO:HD2	2.33	0.42
21:T:52:GLU:HB2	21:T:53:PRO:HD3	2.02	0.42
1:3:8:LYS:O	1:3:11:ARG:HG2	2.19	0.42
2:A:306:U:H2'	2:A:307:G:H8	1.84	0.42
2:A:684:G:H3'	2:A:685:G:C5'	2.49	0.42
35:BA:1209:C:OP1	47:BM:108:ARG:NH1	2.43	0.42
35:BA:434:C:H2'	35:BA:435:U:C6	2.55	0.42
35:BA:642:C:H2'	35:BA:643:A:H8	1.83	0.42
35:BA:654:G:H2'	35:BA:655:A:C8	2.54	0.42
35:BA:669:C:H2'	35:BA:670:G:O4'	2.19	0.42
35:BA:672:U:O2'	35:BA:674:G:N7	2.45	0.42
35:BA:965:A:H5'	35:BA:966:C:OP2	2.19	0.42
35:BA:884:G:H5'	36:BB:18:ARG:NH1	2.34	0.42
41:BG:155:ARG:HD3	41:BG:155:ARG:HA	1.67	0.42
52:BR:45:ARG:HD3	52:BR:45:ARG:HA	1.88	0.42
12:K:7:LYS:HA	12:K:7:LYS:HD3	1.67	0.42
14:M:80:VAL:HG23	14:M:113:LEU:O	2.18	0.42
22:U:44:ILE:O	22:U:47:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1202:A:H62	10:I:36:LEU:HD11	1.84	0.42
2:A:1229:A:C8	2:A:1230:G:H1'	2.54	0.42
2:A:1795:C:H2'	2:A:1796:U:O4'	2.20	0.42
2:A:289:A:N7	2:A:290:C:H5	2.17	0.42
2:A:326:A:H61	2:A:449:G:H1	1.67	0.42
35:BA:390:U:H2'	35:BA:391:G:C8	2.55	0.42
35:BA:480:G:C6	35:BA:526:G:N2	2.86	0.42
35:BA:657:U:H3	35:BA:693:G:H22	1.67	0.42
38:BD:145:LEU:HG	38:BD:154:ARG:HH12	1.84	0.42
55:BV:100:MET:HA	55:BV:107:VAL:HG21	2.01	0.42
8:G:26:VAL:HG12	8:G:80:VAL:HG21	2.02	0.42
21:T:53:PRO:O	21:T:57:VAL:HG23	2.19	0.42
27:Z:45:ARG:HA	27:Z:45:ARG:HD3	1.76	0.42
2:A:1805:G:H2'	2:A:1806:A:C8	2.54	0.42
2:A:2581:G:OP2	2:A:2581:G:H8	2.02	0.42
3:B:76:G:O2'	24:W:94:HIS:HE1	2.03	0.42
35:BA:1461:U:H2'	35:BA:1462:C:C6	2.54	0.42
35:BA:70:A:H4'	35:BA:170:U:C5	2.54	0.42
38:BD:182:GLU:O	38:BD:186:ILE:HG13	2.19	0.42
46:BL:90:LEU:HA	46:BL:91:PRO:HD3	1.81	0.42
50:BP:28:ARG:HG2	50:BP:28:ARG:HH11	1.84	0.42
55:BV:156:LYS:O	55:BV:157:VAL:HG22	2.20	0.42
6:E:123:ARG:O	6:E:125:HIS:HD2	2.02	0.42
7:F:68:THR:HG21	7:F:96:VAL:HG11	2.01	0.42
9:H:77:ASP:HB3	9:H:147:ASN:ND2	2.35	0.42
18:Q:48:ARG:HG2	18:Q:59:THR:HB	2.01	0.42
27:Z:45:ARG:NH1	27:Z:48:ARG:NE	2.67	0.42
2:A:300:G:N2	2:A:303:G:H5''	2.35	0.42
35:BA:1110:A:H4'	43:BI:40:ARG:CZ	2.49	0.42
35:BA:1374:U:H2'	35:BA:1375:G:C8	2.55	0.42
38:BD:132:VAL:HG13	38:BD:136:ASP:OD2	2.20	0.42
39:BE:108:HIS:HE1	39:BE:173:GLN:H	1.66	0.42
41:BG:13:VAL:HG22	41:BG:14:ASN:H	1.83	0.42
45:BK:43:ILE:O	45:BK:51:ILE:HG13	2.20	0.42
55:BV:173:VAL:HG13	55:BV:183:VAL:HG11	2.01	0.42
7:F:98:LEU:HD23	7:F:98:LEU:HA	1.81	0.42
15:N:76:LYS:HB3	15:N:91:GLU:HG3	2.01	0.42
23:V:64:ALA:HA	23:V:65:PRO:HD3	1.92	0.42
2:A:2035:U:OP2	4:C:157:ARG:NH1	2.53	0.42
2:A:2348:G:H21	2:A:2397:C:H42	1.68	0.42
35:BA:159:A:C5	35:BA:160:C:H1'	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:457:A:O2'	35:BA:458:A:O5'	2.27	0.42
35:BA:613:G:H2'	35:BA:614:C:C6	2.55	0.42
35:BA:693:G:H2'	35:BA:694:G:C8	2.55	0.42
46:BL:28:PRO:C	46:BL:29:GLN:HE21	2.22	0.42
13:L:2:ILE:HB	13:L:33:ALA:HB3	2.02	0.42
21:T:95:ARG:HG3	21:T:101:PHE:CD2	2.55	0.42
24:W:109:GLU:HA	24:W:131:ILE:O	2.19	0.42
2:A:1257:G:OP2	12:K:72:LYS:NZ	2.37	0.42
2:A:1756:G:H1'	2:A:1758:G:C2	2.55	0.42
2:A:3038:C:OP1	16:O:42:ARG:NH2	2.52	0.42
2:A:326:A:H2'	2:A:326:A:N3	2.34	0.42
2:A:443:C:H2'	2:A:444:U:O4'	2.18	0.42
2:A:834:C:O2'	2:A:835:C:H5'	2.19	0.42
35:BA:690:G:H5"	40:BF:54:LYS:HZ1	1.84	0.42
37:BC:126:ARG:HA	37:BC:126:ARG:HD3	1.76	0.42
37:BC:175:LEU:HD23	37:BC:182:ILE:HD12	2.02	0.42
53:BS:28:LYS:NZ	53:BS:46:GLY:HA3	2.34	0.42
10:I:98:LYS:HE2	10:I:98:LYS:HB2	1.77	0.42
15:N:77:LYS:HB2	15:N:78:PRO:HD2	2.01	0.42
2:A:2925:C:O2'	16:O:73:LYS:HE3	2.20	0.42
23:V:81:THR:HG23	23:V:100:THR:HG23	2.01	0.42
23:V:81:THR:HG21	23:V:100:THR:H	1.85	0.42
2:A:2350:G:H22	2:A:2384:C:H2'	1.85	0.42
2:A:2925:C:H3'	2:A:2926:A:C5'	2.50	0.42
2:A:2964:A:H2'	2:A:2965:A:C8	2.55	0.42
2:A:720:C:H42	14:M:76:GLN:NE2	2.18	0.42
2:A:929:C:H1'	2:A:1339:G:N2	2.35	0.42
35:BA:1183:U:H2'	35:BA:1184:C:O4'	2.20	0.42
35:BA:1208:A:C2	47:BM:117:ILE:HG21	2.54	0.42
35:BA:1258:C:H2'	35:BA:1260:A:H8	1.85	0.42
35:BA:1353:G:C2	35:BA:1354:G:C8	3.07	0.42
35:BA:253:U:H2'	35:BA:254:G:H8	1.84	0.42
35:BA:493:A:H2'	35:BA:494:C:H6	1.85	0.42
35:BA:510:G:H2'	35:BA:510:G:N3	2.35	0.42
35:BA:485:G:C8	35:BA:515:A:C4	3.08	0.42
37:BC:190:LYS:HD3	37:BC:195:ARG:CZ	2.49	0.42
38:BD:41:ILE:HG21	38:BD:47:ARG:CZ	2.50	0.42
39:BE:106:ILE:HD13	39:BE:148:ILE:HD11	2.01	0.42
41:BG:21:GLN:HA	41:BG:24:THR:HG22	2.00	0.42
45:BK:121:ASP:N	45:BK:121:ASP:OD1	2.53	0.42
4:C:73:ASP:C	4:C:75:VAL:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:79:ARG:HG2	5:D:80:HIS:NE2	2.35	0.42
8:G:55:ARG:HG2	8:G:66:HIS:CE1	2.54	0.42
16:O:3:LYS:HA	16:O:4:PRO:HD3	1.81	0.42
2:A:1485:C:H2'	2:A:1486:G:O4'	2.20	0.42
2:A:1642:G:C2	2:A:1643:G:C8	3.08	0.42
2:A:483:G:H2'	2:A:484:C:C6	2.55	0.42
35:BA:1310:C:H2'	35:BA:1311:G:O4'	2.19	0.42
42:BH:128:LEU:HD23	42:BH:128:LEU:HA	1.77	0.42
51:BQ:36:ILE:HG13	51:BQ:61:ALA:HB3	2.02	0.42
55:BV:49:TYR:HB3	55:BV:199:PRO:O	2.20	0.42
9:H:85:ALA:HB2	9:H:92:PHE:CE1	2.55	0.42
13:L:44:LYS:HA	13:L:44:LYS:HD3	1.82	0.42
2:A:1046:C:H4'	2:A:1047:A:OP2	2.20	0.41
2:A:1131:G:H21	19:R:122:ASN:HD22	1.68	0.41
35:BA:1261:A:O2'	35:BA:1262:U:H5'	2.20	0.41
35:BA:1315:A:H2'	35:BA:1316:G:O4'	2.20	0.41
35:BA:408:G:OP1	38:BD:107:ARG:HB2	2.20	0.41
43:BI:150:ARG:HD3	43:BI:150:ARG:HA	1.79	0.41
50:BP:5:ILE:HG13	50:BP:64:ALA:HB1	2.02	0.41
55:BV:83:GLU:OE2	55:BV:214:THR:HB	2.20	0.41
9:H:5:LEU:HD12	9:H:17:ASP:HB2	2.01	0.41
11:J:81:LEU:HD13	11:J:134:ALA:HB2	2.01	0.41
12:K:109:LEU:HD23	12:K:109:LEU:HA	1.85	0.41
2:A:2718:G:H4'	15:N:80:GLU:HG2	2.01	0.41
2:A:334:G:H1	2:A:347:U:H3	1.66	0.41
2:A:940:A:H2'	2:A:941:U:O4'	2.20	0.41
35:BA:715:G:H1'	52:BR:73:GLU:OE2	2.20	0.41
35:BA:777:C:H2'	35:BA:778:U:C6	2.55	0.41
42:BH:50:ARG:HG3	42:BH:52:GLU:OE2	2.20	0.41
43:BI:61:ASN:HD22	43:BI:64:HIS:HD2	1.62	0.41
46:BL:38:TYR:CE1	46:BL:52:VAL:HG12	2.55	0.41
49:BO:66:LEU:HD23	49:BO:66:LEU:HA	1.78	0.41
5:D:10:LYS:HB2	5:D:198:ILE:HD11	2.02	0.41
6:E:8:LYS:HD2	6:E:148:LEU:HD13	2.01	0.41
6:E:158:ILE:O	6:E:179:SER:HA	2.19	0.41
7:F:38:VAL:HA	7:F:165:THR:HG23	2.01	0.41
7:F:75:ARG:NH2	7:F:95:ARG:NH1	2.62	0.41
14:M:97:GLU:O	14:M:101:LYS:HG2	2.19	0.41
2:A:2084:A:H2'	2:A:2085:C:O4'	2.20	0.41
2:A:278:A:C2	2:A:279:U:H1'	2.55	0.41
2:A:2952:U:O2'	5:D:25:PRO:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:543:U:C5	2:A:561:G:H5'	2.55	0.41
38:BD:13:ARG:HD2	38:BD:31:TYR:O	2.19	0.41
47:BM:108:ARG:NH2	47:BM:114:LYS:HA	2.36	0.41
55:BV:103:ASN:ND2	55:BV:106:THR:OG1	2.52	0.41
4:C:25:THR:HG21	4:C:113:GLN:NE2	2.36	0.41
7:F:126:PRO:O	7:F:174:ARG:NH1	2.53	0.41
11:J:40:PHE:CE1	11:J:58:VAL:HG21	2.45	0.41
15:N:37:LEU:HD21	15:N:130:ARG:HD3	2.02	0.41
24:W:119:THR:HG21	24:W:152:GLU:HG2	2.01	0.41
2:A:2074:G:O6	2:A:2075:G:N1	2.54	0.41
2:A:2691:C:H4'	15:N:123:HIS:CD2	2.55	0.41
35:BA:210:A:H8	35:BA:210:A:OP2	2.02	0.41
35:BA:276:G:H4'	51:BQ:60:LYS:NZ	2.35	0.41
35:BA:988:C:H2'	35:BA:989:G:O4'	2.20	0.41
41:BG:78:ARG:HB2	41:BG:156:TRP:CZ3	2.56	0.41
46:BL:7:LEU:HA	46:BL:7:LEU:HD23	1.89	0.41
46:BL:67:ILE:HG12	46:BL:97:ILE:HD12	2.02	0.41
35:BA:1081:A:N7	55:BV:171:ILE:HG23	2.35	0.41
4:C:17:SER:O	4:C:211:ARG:NH2	2.53	0.41
6:E:183:LEU:HD12	6:E:183:LEU:HA	1.80	0.41
7:F:11:LEU:HD23	7:F:11:LEU:HA	1.87	0.41
9:H:121:LYS:HA	9:H:121:LYS:HD3	1.91	0.41
10:I:17:PHE:CZ	10:I:66:ILE:HG12	2.55	0.41
11:J:59:GLU:O	11:J:70:PHE:HA	2.19	0.41
15:N:8:LYS:HB3	15:N:9:HIS:ND1	2.36	0.41
18:Q:32:ILE:O	18:Q:32:ILE:HG13	2.19	0.41
13:L:75:SER:CB	18:Q:71:ARG:HH21	2.33	0.41
19:R:109:LEU:HA	19:R:109:LEU:HD23	1.86	0.41
2:A:1185:A:H2'	2:A:1186:G:C8	2.54	0.41
2:A:1201:G:H21	2:A:1203:A:H3'	1.82	0.41
2:A:2532:G:H2'	2:A:2532:G:N3	2.36	0.41
35:BA:134:C:H2'	35:BA:135:U:O4'	2.21	0.41
35:BA:286:G:H2'	35:BA:287:U:O4'	2.20	0.41
35:BA:716:U:H2'	35:BA:717:C:C6	2.56	0.41
35:BA:772:A:O2'	35:BA:774:A:C8	2.68	0.41
42:BH:101:LEU:HD23	42:BH:101:LEU:HA	1.80	0.41
43:BI:28:THR:HG21	43:BI:106:ALA:HB2	2.03	0.41
44:BJ:8:ILE:HD11	44:BJ:87:LEU:HD13	2.02	0.41
49:BO:7:GLN:H	49:BO:7:GLN:HG3	1.73	0.41
50:BP:81:GLN:O	50:BP:85:GLY:N	2.40	0.41
55:BV:138:THR:O	55:BV:142:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BV:83:GLU:O	55:BV:87:VAL:HG23	2.21	0.41
4:C:123:ALA:HB3	4:C:131:LEU:HD22	2.02	0.41
7:F:137:PHE:CE1	7:F:161:ILE:HB	2.56	0.41
8:G:149:ILE:HG22	8:G:163:VAL:HG11	2.01	0.41
15:N:72:ARG:H	15:N:72:ARG:HG2	1.32	0.41
16:O:24:LEU:HD23	16:O:24:LEU:HA	1.83	0.41
18:Q:20:SER:OG	18:Q:21:PRO:HD2	2.21	0.41
20:S:68:THR:HG22	20:S:94:LEU:HB2	2.03	0.41
35:BA:1125:G:H21	35:BA:1127:A:H62	1.67	0.41
35:BA:1177:A:HO2'	35:BA:1178:A:P	2.37	0.41
35:BA:1221:U:O4	41:BG:109:ARG:NH2	2.51	0.41
35:BA:410:G:H21	35:BA:432:A:H62	1.67	0.41
43:BI:47:GLN:HB2	43:BI:82:ASP:OD1	2.21	0.41
46:BL:101:SER:O	46:BL:104:THR:HG23	2.20	0.41
47:BM:25:ILE:HG23	47:BM:29:ARG:HB2	2.03	0.41
2:A:2017:C:P	4:C:183:ARG:HH12	2.43	0.41
2:A:693:G:OP1	6:E:30:ASN:ND2	2.54	0.41
20:S:69:LYS:HE3	20:S:69:LYS:HB2	1.78	0.41
2:A:1078:G:N2	2:A:2254:A:OP1	2.47	0.41
2:A:2505:C:O2'	2:A:2506:G:H5'	2.20	0.41
2:A:487:U:H2'	2:A:488:G:O4'	2.20	0.41
2:A:844:G:H5'	2:A:845:C:H5''	2.02	0.41
3:B:12:C:H4'	3:B:13:C:OP2	2.20	0.41
35:BA:1410:C:H2'	35:BA:1411:A:C8	2.56	0.41
37:BC:107:ASN:HA	37:BC:108:PRO:HD3	1.91	0.41
38:BD:191:THR:HG22	38:BD:193:GLN:HG2	2.03	0.41
41:BG:86:GLN:HB2	41:BG:148:ASN:ND2	2.36	0.41
42:BH:14:LEU:HA	42:BH:14:LEU:HD23	1.86	0.41
44:BJ:42:LEU:HB2	44:BJ:71:LYS:HB2	2.01	0.41
50:BP:75:LYS:HA	50:BP:81:GLN:HE21	1.85	0.41
6:E:158:ILE:HG22	6:E:159:GLY:O	2.21	0.41
7:F:165:THR:HG21	7:F:176:LEU:HD23	2.03	0.41
11:J:47:ALA:O	11:J:50:SER:HB2	2.21	0.41
23:V:13:SER:HB2	23:V:70:ASN:ND2	2.36	0.41
2:A:1199:U:H2'	2:A:1200:U:C6	2.56	0.41
2:A:1787:A:H2'	4:C:86:PRO:HG3	2.02	0.41
2:A:2070:A:H2'	2:A:2071:A:C8	2.55	0.41
2:A:944:A:C8	2:A:2472:C:H5'	2.56	0.41
2:A:3082:U:H2'	2:A:3083:A:C8	2.55	0.41
2:A:757:G:H2'	25:X:85:ARG:HD2	2.02	0.41
35:BA:1110:A:H61	35:BA:1125:G:H1'	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:605:G:H2'	35:BA:606:U:H6	1.86	0.41
35:BA:933:G:HO2'	35:BA:952:C:HO2'	1.69	0.41
43:BI:53:ARG:HD3	43:BI:57:ASN:ND2	2.36	0.41
52:BR:29:THR:HG22	52:BR:30:ILE:H	1.85	0.41
53:BS:21:VAL:HG13	53:BS:25:LYS:HE3	2.02	0.41
55:BV:111:LEU:HD21	55:BV:152:ARG:HA	2.03	0.41
7:F:182:PHE:HA	7:F:183:PRO:HD3	1.69	0.41
15:N:71:ASP:N	15:N:71:ASP:OD1	2.37	0.41
2:A:3069:G:H3'	18:Q:92:ARG:O	2.21	0.41
2:A:2781:G:H2'	2:A:2782:C:C6	2.56	0.41
2:A:2926:A:OP1	16:O:73:LYS:NZ	2.48	0.41
2:A:641:U:H2'	2:A:641:U:H6	1.69	0.41
2:A:981:U:O2'	2:A:982:A:O5'	2.38	0.41
35:BA:376:G:C4	35:BA:389:A:C2	3.09	0.41
40:BF:29:VAL:O	40:BF:32:LYS:HG2	2.21	0.41
40:BF:46:ARG:HB3	40:BF:60:TYR:CE2	2.56	0.41
45:BK:103:GLU:HB3	45:BK:107:ARG:HH21	1.83	0.41
46:BL:67:ILE:HA	46:BL:68:PRO:HD3	1.77	0.41
48:BN:36:LYS:HE2	48:BN:36:LYS:HB3	1.77	0.41
55:BV:137:LEU:HB3	55:BV:141:LYS:NZ	2.36	0.41
4:C:182:ILE:HB	4:C:270:ARG:HH12	1.86	0.41
14:M:22:VAL:HG23	14:M:29:LYS:HD2	2.02	0.41
19:R:38:GLN:O	19:R:42:SER:HB2	2.21	0.41
19:R:58:ARG:HA	19:R:61:TRP:CE3	2.55	0.41
12:K:145:VAL:HG12	19:R:73:ASP:OD1	2.21	0.41
2:A:1439:G:C2	2:A:1443:G:C6	3.08	0.41
2:A:1615:G:H2'	2:A:1616:A:O4'	2.21	0.41
2:A:1732:U:H2'	2:A:1733:C:C6	2.56	0.41
2:A:2367:G:H1'	2:A:2371:G:N2	2.36	0.41
35:BA:604:U:H2'	35:BA:605:G:H8	1.86	0.41
45:BK:31:HIS:CE1	45:BK:44:THR:HG21	2.55	0.41
13:L:107:ARG:NH1	18:Q:33:GLU:OE2	2.54	0.41
14:M:137:ILE:HD13	14:M:137:ILE:HA	1.94	0.41
15:N:34:ILE:HD11	15:N:118:LEU:HD22	2.03	0.41
15:N:73:PRO:HB3	15:N:93:TRP:CZ3	2.56	0.41
24:W:86:HIS:HA	24:W:87:PRO:HD3	1.86	0.41
27:Z:14:THR:OG1	27:Z:15:ASP:N	2.54	0.41
2:A:1303:U:O2'	2:A:1304:A:H5'	2.21	0.41
2:A:1533:U:OP2	2:A:1535:C:N4	2.53	0.41
2:A:1602:U:H2'	2:A:1603:G:C8	2.56	0.41
2:A:1715:A:H2'	2:A:1716:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:429:A:H2'	2:A:430:A:C8	2.56	0.41
2:A:844:G:H4'	2:A:878:G:H5'	2.03	0.41
35:BA:1077:C:H5''	55:BV:143:LYS:HZ1	1.85	0.41
35:BA:127:A:H1'	35:BA:263:A:O2'	2.21	0.41
39:BE:199:ARG:HA	39:BE:202:GLU:OE1	2.21	0.41
39:BE:54:ARG:HG2	39:BE:54:ARG:HH11	1.86	0.41
44:BJ:57:LYS:HE3	44:BJ:57:LYS:HB2	1.75	0.41
55:BV:43:LEU:O	55:BV:47:LEU:HG	2.20	0.41
5:D:38:ARG:HD3	5:D:40:ARG:NH1	2.36	0.41
6:E:118:ARG:HA	6:E:118:ARG:HD3	1.93	0.41
6:E:150:GLU:H	6:E:150:GLU:HG2	1.68	0.41
8:G:176:LYS:HG3	8:G:177:THR:H	1.86	0.41
18:Q:88:ARG:HB2	18:Q:112:LYS:HB2	2.03	0.41
19:R:83:LEU:HA	19:R:83:LEU:HD23	1.63	0.41
2:A:1078:G:H22	2:A:2254:A:P	2.45	0.40
2:A:1760:G:H2'	2:A:1761:G:H8	1.85	0.40
2:A:700:U:OP1	6:E:103:PRO:HA	2.21	0.40
35:BA:1107:G:H1'	35:BA:1261:A:C6	2.56	0.40
35:BA:105:A:C6	35:BA:326:G:C6	3.09	0.40
35:BA:498:C:C5	35:BA:509:G:H3'	2.55	0.40
52:BR:74:VAL:HG23	52:BR:76:LEU:HG	2.03	0.40
54:BT:68:HIS:HD2	54:BT:70:ASN:HB2	1.86	0.40
54:BT:71:GLN:HE21	54:BT:75:LYS:NZ	2.19	0.40
2:A:2217:U:H4'	5:D:138:ALA:HB3	2.03	0.40
6:E:54:THR:HG23	6:E:94:LYS:HZ1	1.85	0.40
14:M:31:LYS:HG3	14:M:32:THR:N	2.35	0.40
2:A:1204:A:H5''	2:A:1205:G:OP1	2.20	0.40
2:A:1688:G:N2	2:A:1748:A:H1'	2.36	0.40
35:BA:1486:A:H2'	35:BA:1488:G:C8	2.56	0.40
35:BA:355:C:H2'	35:BA:356:A:O4'	2.21	0.40
35:BA:595:C:H2'	35:BA:596:A:C8	2.56	0.40
44:BJ:18:ILE:HD12	44:BJ:18:ILE:HA	1.73	0.40
45:BK:68:THR:OG1	45:BK:69:PRO:HD2	2.21	0.40
51:BQ:46:HIS:CG	51:BQ:47:PRO:HD2	2.56	0.40
6:E:29:PRO:CD	6:E:120:ARG:HH12	2.34	0.40
8:G:4:ILE:CG2	8:G:70:ARG:HD2	2.51	0.40
19:R:72:ASN:N	19:R:72:ASN:HD22	2.19	0.40
21:T:95:ARG:HG3	21:T:101:PHE:CE2	2.57	0.40
24:W:84:ASP:OD2	24:W:94:HIS:HB3	2.20	0.40
2:A:1541:G:N2	2:A:1631:A:H61	2.20	0.40
2:A:1640:A:H2'	2:A:1642:G:N7	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1655:A:H2'	2:A:1656:A:O4'	2.21	0.40
2:A:159:A:C5	2:A:166:A:C2	3.10	0.40
2:A:2470:A:H2'	2:A:2471:A:C8	2.56	0.40
2:A:322:A:OP2	2:A:322:A:H8	2.05	0.40
3:B:50:C:H2'	3:B:51:G:H8	1.86	0.40
35:BA:1007:U:H4'	35:BA:1008:C:H5'	2.04	0.40
35:BA:671:G:O6	45:BK:66:LYS:HE2	2.22	0.40
37:BC:46:LEU:HD21	37:BC:86:ILE:HD11	2.04	0.40
45:BK:47:GLN:HB2	45:BK:49:ASN:ND2	2.36	0.40
4:C:127:PRO:HA	4:C:193:VAL:O	2.20	0.40
11:J:112:GLU:O	11:J:115:LYS:HB3	2.22	0.40
15:N:2:LEU:O	15:N:44:ASN:ND2	2.55	0.40
16:O:10:LEU:HB2	16:O:17:GLN:NE2	2.37	0.40
18:Q:43:LYS:NZ	18:Q:86:LEU:CD1	2.85	0.40
24:W:164:LEU:HD13	24:W:168:VAL:HG12	2.02	0.40
2:A:135:G:H3'	2:A:136:U:H5''	2.04	0.40
2:A:1431:U:H1'	2:A:1507:G:H21	1.86	0.40
35:BA:1193:U:O2'	35:BA:1194:A:O4'	2.34	0.40
2:A:1612:U:O2	40:BF:17:ARG:NH1	2.54	0.40
6:E:41:GLN:HE22	6:E:184:ASN:HB2	1.86	0.40
2:A:2750:G:P	8:G:154:ARG:HH22	2.43	0.40
8:G:59:GLU:HG3	8:G:59:GLU:H	1.49	0.40
9:H:82:VAL:HG21	9:H:148:VAL:HG13	2.04	0.40
11:J:22:PRO:HB2	11:J:25:PRO:HD2	2.02	0.40
15:N:3:ILE:HG22	15:N:93:TRP:CD1	2.56	0.40
16:O:50:LYS:O	16:O:53:THR:HB	2.21	0.40
20:S:26:LYS:HA	20:S:95:THR:OG1	2.21	0.40
2:A:1025:A:H62	15:N:12:GLN:HA	1.86	0.40
2:A:1553:C:C4	2:A:1618:C:H1'	2.57	0.40
2:A:2603:G:H2'	2:A:2604:U:C6	2.56	0.40
2:A:303:G:H2'	2:A:304:U:C6	2.56	0.40
2:A:401:C:H2'	2:A:402:G:O4'	2.21	0.40
2:A:815:G:H2'	2:A:816:G:O4'	2.21	0.40
35:BA:250:U:H4'	35:BA:251:G:O5'	2.21	0.40
35:BA:604:U:C2	35:BA:605:G:C8	3.08	0.40
35:BA:864:C:C2'	35:BA:865:C:H5'	2.52	0.40
37:BC:90:LEU:HB3	37:BC:98:VAL:HG21	2.03	0.40
50:BP:8:THR:O	50:BP:18:TYR:HA	2.22	0.40
53:BS:10:PHE:O	53:BS:39:THR:HG22	2.21	0.40
5:D:76:ASN:HA	5:D:77:PRO:HD3	1.81	0.40
6:E:154:VAL:HG23	6:E:193:ASP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:48:ASP:N	8:G:48:ASP:OD1	2.52	0.40
10:I:115:LEU:HB2	10:I:120:VAL:HG23	2.04	0.40
7:F:132:THR:OG1	17:P:6:VAL:HG21	2.22	0.40
23:V:20:LYS:NZ	23:V:74:VAL:HG21	2.36	0.40
27:Z:62:ARG:HD2	27:Z:62:ARG:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	21/24 (88%)	21 (100%)	0	0	100	100
4	C	273/278 (98%)	261 (96%)	12 (4%)	0	100	100
5	D	212/217 (98%)	199 (94%)	12 (6%)	1 (0%)	32	67
6	E	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	32	67
7	F	180/187 (96%)	167 (93%)	12 (7%)	1 (1%)	28	63
8	G	174/179 (97%)	167 (96%)	7 (4%)	0	100	100
9	H	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	25	61
10	I	124/175 (71%)	115 (93%)	9 (7%)	0	100	100
11	J	131/142 (92%)	124 (95%)	6 (5%)	1 (1%)	22	58
12	K	144/147 (98%)	136 (94%)	8 (6%)	0	100	100
13	L	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
14	M	143/147 (97%)	135 (94%)	7 (5%)	1 (1%)	25	61
15	N	134/138 (97%)	123 (92%)	11 (8%)	0	100	100
16	O	116/199 (58%)	111 (96%)	5 (4%)	0	100	100
17	P	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
18	Q	111/113 (98%)	105 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	R	122/129 (95%)	117 (96%)	5 (4%)	0	100	100
20	S	98/103 (95%)	96 (98%)	2 (2%)	0	100	100
21	T	112/153 (73%)	109 (97%)	3 (3%)	0	100	100
22	U	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
23	V	93/105 (89%)	89 (96%)	4 (4%)	0	100	100
24	W	190/215 (88%)	185 (97%)	5 (3%)	0	100	100
25	X	77/88 (88%)	73 (95%)	4 (5%)	0	100	100
26	Y	61/64 (95%)	61 (100%)	0	0	100	100
27	Z	62/77 (80%)	60 (97%)	2 (3%)	0	100	100
28	a	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
29	b	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
30	c	47/55 (86%)	45 (96%)	1 (2%)	1 (2%)	8	38
31	d	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
32	e	61/64 (95%)	61 (100%)	0	0	100	100
33	f	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
34	g	55/75 (73%)	54 (98%)	1 (2%)	0	100	100
36	BB	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
37	BC	206/275 (75%)	190 (92%)	14 (7%)	2 (1%)	18	54
38	BD	198/201 (98%)	186 (94%)	12 (6%)	0	100	100
39	BE	178/214 (83%)	170 (96%)	8 (4%)	0	100	100
40	BF	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
41	BG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
42	BH	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
43	BI	124/150 (83%)	119 (96%)	5 (4%)	0	100	100
44	BJ	97/101 (96%)	90 (93%)	7 (7%)	0	100	100
45	BK	113/138 (82%)	106 (94%)	7 (6%)	0	100	100
46	BL	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
47	BM	114/124 (92%)	106 (93%)	8 (7%)	0	100	100
48	BN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
49	BO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
50	BP	111/156 (71%)	106 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BQ	92/98 (94%)	88 (96%)	4 (4%)	0	100	100
52	BR	63/84 (75%)	62 (98%)	1 (2%)	0	100	100
53	BS	80/93 (86%)	76 (95%)	4 (5%)	0	100	100
54	BT	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
55	BV	226/277 (82%)	207 (92%)	18 (8%)	1 (0%)	38	72
All	All	5979/6679 (90%)	5688 (95%)	281 (5%)	10 (0%)	54	81

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	c	7	VAL
37	BC	125	ASN
5	D	143	ALA
14	M	31	LYS
6	E	90	VAL
11	J	17	ALA
37	BC	162	MET
55	BV	156	LYS
9	H	124	ILE
7	F	131	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	3	18/19 (95%)	17 (94%)	1 (6%)	25	61
4	C	215/218 (99%)	190 (88%)	25 (12%)	6	27
5	D	160/163 (98%)	141 (88%)	19 (12%)	6	26
6	E	169/173 (98%)	152 (90%)	17 (10%)	9	33
7	F	151/156 (97%)	134 (89%)	17 (11%)	7	28
8	G	148/150 (99%)	136 (92%)	12 (8%)	14	44
9	H	90/116 (78%)	86 (96%)	4 (4%)	33	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	89/120 (74%)	84 (94%)	5 (6%)	25	61
11	J	102/108 (94%)	91 (89%)	11 (11%)	7	30
12	K	119/120 (99%)	111 (93%)	8 (7%)	19	54
13	L	100/100 (100%)	89 (89%)	11 (11%)	7	30
14	M	112/114 (98%)	102 (91%)	10 (9%)	11	40
15	N	114/116 (98%)	105 (92%)	9 (8%)	14	46
16	O	97/158 (61%)	88 (91%)	9 (9%)	10	37
17	P	93/94 (99%)	85 (91%)	8 (9%)	12	42
18	Q	100/100 (100%)	89 (89%)	11 (11%)	7	30
19	R	97/99 (98%)	92 (95%)	5 (5%)	27	63
20	S	81/83 (98%)	74 (91%)	7 (9%)	12	42
21	T	90/117 (77%)	82 (91%)	8 (9%)	11	40
22	U	83/85 (98%)	80 (96%)	3 (4%)	40	72
23	V	81/86 (94%)	76 (94%)	5 (6%)	21	56
24	W	155/168 (92%)	134 (86%)	21 (14%)	4	20
25	X	58/63 (92%)	54 (93%)	4 (7%)	18	53
26	Y	50/51 (98%)	46 (92%)	4 (8%)	14	45
27	Z	58/66 (88%)	55 (95%)	3 (5%)	27	63
28	a	52/54 (96%)	48 (92%)	4 (8%)	15	47
29	b	43/46 (94%)	36 (84%)	7 (16%)	3	13
30	c	47/52 (90%)	41 (87%)	6 (13%)	5	22
31	d	35/36 (97%)	32 (91%)	3 (9%)	12	42
32	e	53/54 (98%)	47 (89%)	6 (11%)	7	28
33	f	35/35 (100%)	33 (94%)	2 (6%)	24	60
34	g	51/63 (81%)	43 (84%)	8 (16%)	3	15
36	BB	30/31 (97%)	26 (87%)	4 (13%)	4	21
37	BC	170/212 (80%)	156 (92%)	14 (8%)	13	44
38	BD	175/176 (99%)	162 (93%)	13 (7%)	16	49
39	BE	127/147 (86%)	114 (90%)	13 (10%)	8	33
40	BF	85/85 (100%)	77 (91%)	8 (9%)	10	36
41	BG	131/132 (99%)	120 (92%)	11 (8%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BH	107/108 (99%)	100 (94%)	7 (6%)	20	55
43	BI	102/125 (82%)	90 (88%)	12 (12%)	6	26
44	BJ	89/90 (99%)	82 (92%)	7 (8%)	14	46
45	BK	89/105 (85%)	80 (90%)	9 (10%)	9	33
46	BL	103/105 (98%)	91 (88%)	12 (12%)	6	27
47	BM	99/104 (95%)	85 (86%)	14 (14%)	4	19
48	BN	49/50 (98%)	46 (94%)	3 (6%)	22	57
49	BO	76/77 (99%)	70 (92%)	6 (8%)	14	46
50	BP	92/118 (78%)	84 (91%)	8 (9%)	12	41
51	BQ	80/83 (96%)	72 (90%)	8 (10%)	9	33
52	BR	55/72 (76%)	54 (98%)	1 (2%)	64	83
53	BS	73/84 (87%)	64 (88%)	9 (12%)	5	24
54	BT	69/70 (99%)	59 (86%)	10 (14%)	4	18
55	BV	191/218 (88%)	173 (91%)	18 (9%)	10	36
All	All	4938/5375 (92%)	4478 (91%)	460 (9%)	15	37

All (460) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	7	LYS
4	C	10	THR
4	C	13	ARG
4	C	28	THR
4	C	60	ARG
4	C	63	ARG
4	C	69	ARG
4	C	78	LYS
4	C	89	THR
4	C	116	VAL
4	C	119	SER
4	C	126	LYS
4	C	127	PRO
4	C	131	LEU
4	C	148	ARG
4	C	157	ARG
4	C	161	VAL
4	C	177	MET

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Mol	Chain	Res	Type
4	C	181	GLU
4	C	203	ASN
4	C	211	ARG
4	C	213	ARG
4	C	241	SER
4	C	247	VAL
4	C	265	ASP
4	C	272	ARG
5	D	3	ARG
5	D	19	GLU
5	D	58	SER
5	D	60	ARG
5	D	79	ARG
5	D	86	LEU
5	D	87	ASP
5	D	99	GLN
5	D	102	THR
5	D	129	ARG
5	D	133	ARG
5	D	144	VAL
5	D	154	CYS
5	D	160	VAL
5	D	164	THR
5	D	169	ARG
5	D	170	MET
5	D	192	LEU
5	D	209	ARG
6	E	33	LEU
6	E	34	MET
6	E	36	GLN
6	E	50	HIS
6	E	66	TYR
6	E	71	THR
6	E	78	SER
6	E	79	THR
6	E	97	ASP
6	E	128	THR
6	E	135	THR
6	E	137	SER
6	E	148	LEU
6	E	161	THR
6	E	169	VAL

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Mol	Chain	Res	Type
6	E	181	ASP
6	E	201	LEU
7	F	10	ARG
7	F	11	LEU
7	F	31	ASN
7	F	44	ASN
7	F	49	ASP
7	F	83	GLN
7	F	87	ARG
7	F	102	ARG
7	F	148	ILE
7	F	150	VAL
7	F	151	ASP
7	F	157	ARG
7	F	159	MET
7	F	162	THR
7	F	164	VAL
7	F	165	THR
7	F	182	PHE
8	G	3	ARG
8	G	16	ASP
8	G	48	ASP
8	G	59	GLU
8	G	65	LEU
8	G	72	LEU
8	G	77	VAL
8	G	89	GLU
8	G	114	VAL
8	G	126	VAL
8	G	137	ILE
8	G	153	ARG
9	H	4	ILE
9	H	25	TYR
9	H	88	THR
9	H	137	HIS
10	I	5	ASP
10	I	23	THR
10	I	55	THR
10	I	79	ILE
10	I	82	VAL
11	J	15	ILE
11	J	30	LEU

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Mol	Chain	Res	Type
11	J	35	VAL
11	J	36	ASN
11	J	42	LYS
11	J	48	THR
11	J	52	ARG
11	J	55	VAL
11	J	87	VAL
11	J	113	THR
11	J	114	LYS
12	K	10	ASP
12	K	17	VAL
12	K	70	THR
12	K	93	LEU
12	K	96	HIS
12	K	118	ILE
12	K	129	ASP
12	K	145	VAL
13	L	13	ASN
13	L	40	VAL
13	L	58	VAL
13	L	69	ARG
13	L	73	ASP
13	L	77	ILE
13	L	87	ILE
13	L	90	ASP
13	L	96	THR
13	L	107	ARG
13	L	112	MET
14	M	22	VAL
14	M	24	ARG
14	M	43	ARG
14	M	46	VAL
14	M	49	MET
14	M	82	ASP
14	M	89	GLN
14	M	92	THR
14	M	104	VAL
14	M	105	ARG
15	N	3	ILE
15	N	7	VAL
15	N	10	ARG
15	N	18	ARG

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Mol	Chain	Res	Type
15	N	20	ILE
15	N	51	ARG
15	N	72	ARG
15	N	82	ARG
15	N	135	GLU
16	O	6	LYS
16	O	9	ARG
16	O	10	LEU
16	O	37	THR
16	O	64	ARG
16	O	74	ASP
16	O	96	ARG
16	O	100	VAL
16	O	114	GLU
17	P	6	VAL
17	P	10	ILE
17	P	12	GLU
17	P	24	ARG
17	P	32	THR
17	P	51	LEU
17	P	69	ASP
17	P	74	ASP
18	Q	15	ASP
18	Q	25	VAL
18	Q	32	ILE
18	Q	38	ARG
18	Q	54	ILE
18	Q	57	THR
18	Q	71	ARG
18	Q	79	ASN
18	Q	81	ASP
18	Q	91	VAL
18	Q	93	ARG
19	R	6	ARG
19	R	28	ARG
19	R	29	SER
19	R	33	ARG
19	R	44	THR
20	S	3	THR
20	S	27	LEU
20	S	53	ASP
20	S	54	ASP

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Mol	Chain	Res	Type
20	S	58	VAL
20	S	68	THR
20	S	72	LYS
21	T	19	VAL
21	T	22	THR
21	T	26	ARG
21	T	81	VAL
21	T	99	ARG
21	T	102	ARG
21	T	104	ARG
21	T	107	THR
22	U	20	SER
22	U	62	ARG
22	U	81	ARG
23	V	30	ARG
23	V	38	VAL
23	V	42	LYS
23	V	69	SER
23	V	91	THR
24	W	12	THR
24	W	14	ASN
24	W	15	VAL
24	W	42	THR
24	W	64	ASN
24	W	67	LEU
24	W	68	THR
24	W	99	VAL
24	W	104	GLU
24	W	112	VAL
24	W	114	VAL
24	W	119	THR
24	W	130	THR
24	W	131	ILE
24	W	138	LEU
24	W	139	SER
24	W	146	VAL
24	W	148	VAL
24	W	151	VAL
24	W	158	THR
24	W	172	SER
25	X	11	ARG
25	X	38	VAL

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Mol	Chain	Res	Type
25	X	39	ARG
25	X	80	ILE
26	Y	23	ARG
26	Y	24	ARG
26	Y	28	ARG
26	Y	45	ASN
27	Z	36	MET
27	Z	44	ASN
27	Z	48	ARG
28	a	3	GLU
28	a	20	ARG
28	a	36	VAL
28	a	48	ASN
29	b	3	VAL
29	b	6	ARG
29	b	8	MET
29	b	10	ARG
29	b	14	ARG
29	b	35	GLN
29	b	39	VAL
30	c	6	ASP
30	c	11	ILE
30	c	12	THR
30	c	25	THR
30	c	38	ILE
30	c	47	THR
31	d	13	ARG
31	d	15	ARG
31	d	46	THR
32	e	11	SER
32	e	13	ARG
32	e	19	THR
32	e	47	ARG
32	e	56	SER
32	e	59	ASN
33	f	2	LYS
33	f	7	VAL
34	g	9	TYR
34	g	12	THR
34	g	22	PHE
34	g	24	THR
34	g	32	THR

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Mol	Chain	Res	Type
34	g	37	VAL
34	g	46	THR
34	g	58	VAL
36	BB	4	VAL
36	BB	6	LYS
36	BB	10	LYS
36	BB	24	THR
37	BC	21	ARG
37	BC	23	TYR
37	BC	35	ASP
37	BC	46	LEU
37	BC	62	ARG
37	BC	71	ARG
37	BC	82	GLU
37	BC	103	LEU
37	BC	153	CYS
37	BC	167	PHE
37	BC	169	ARG
37	BC	182	ILE
37	BC	193	PHE
37	BC	204	LYS
38	BD	10	ARG
38	BD	20	VAL
38	BD	23	ASP
38	BD	86	LEU
38	BD	102	LEU
38	BD	110	ARG
38	BD	119	LEU
38	BD	123	VAL
38	BD	131	ARG
38	BD	145	LEU
38	BD	156	THR
38	BD	177	VAL
38	BD	188	VAL
39	BE	37	ILE
39	BE	39	ARG
39	BE	41	VAL
39	BE	59	THR
39	BE	70	MET
39	BE	71	VAL
39	BE	95	ASN
39	BE	96	PHE

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Mol	Chain	Res	Type
39	BE	97	PHE
39	BE	110	VAL
39	BE	156	ASP
39	BE	176	GLU
39	BE	198	ARG
40	BF	30	ILE
40	BF	43	TRP
40	BF	57	GLU
40	BF	72	VAL
40	BF	77	ARG
40	BF	85	VAL
40	BF	87	ARG
40	BF	91	LEU
41	BG	3	ARG
41	BG	24	THR
41	BG	38	LEU
41	BG	79	ARG
41	BG	80	VAL
41	BG	99	LEU
41	BG	102	ARG
41	BG	129	ASN
41	BG	138	ARG
41	BG	144	MET
41	BG	149	ARG
42	BH	14	LEU
42	BH	48	ASP
42	BH	55	ARG
42	BH	79	ARG
42	BH	82	LYS
42	BH	92	THR
42	BH	101	LEU
43	BI	29	VAL
43	BI	38	ARG
43	BI	40	ARG
43	BI	45	THR
43	BI	67	LEU
43	BI	78	VAL
43	BI	83	ILE
43	BI	87	LEU
43	BI	88	ASP
43	BI	100	ARG
43	BI	147	TYR

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Mol	Chain	Res	Type
43	BI	150	ARG
44	BJ	15	HIS
44	BJ	18	ILE
44	BJ	32	THR
44	BJ	50	CYS
44	BJ	57	LYS
44	BJ	78	ASP
44	BJ	97	ASP
45	BK	25	VAL
45	BK	40	ILE
45	BK	49	ASN
45	BK	68	THR
45	BK	95	VAL
45	BK	121	ASP
45	BK	128	ASN
45	BK	131	ARG
45	BK	137	ARG
46	BL	3	THR
46	BL	21	THR
46	BL	27	SER
46	BL	29	GLN
46	BL	38	TYR
46	BL	41	THR
46	BL	49	LEU
46	BL	63	VAL
46	BL	70	GLU
46	BL	73	ASN
46	BL	87	VAL
46	BL	104	THR
47	BM	42	ASN
47	BM	49	THR
47	BM	51	ASP
47	BM	56	LEU
47	BM	60	ILE
47	BM	63	ASN
47	BM	64	LEU
47	BM	69	ASP
47	BM	70	LEU
47	BM	80	ARG
47	BM	101	GLN
47	BM	109	THR
47	BM	110	ARG

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Mol	Chain	Res	Type
47	BM	115	ARG
48	BN	24	CYS
48	BN	45	ARG
48	BN	56	VAL
49	BO	46	HIS
49	BO	65	ARG
49	BO	75	VAL
49	BO	82	ILE
49	BO	83	GLU
49	BO	89	ARG
50	BP	3	VAL
50	BP	9	ARG
50	BP	36	VAL
50	BP	50	GLN
50	BP	67	THR
50	BP	86	LEU
50	BP	90	GLU
50	BP	97	GLU
51	BQ	28	VAL
51	BQ	48	LEU
51	BQ	54	ARG
51	BQ	65	ASN
51	BQ	85	THR
51	BQ	89	ARG
51	BQ	92	GLU
51	BQ	93	ILE
52	BR	31	ASP
53	BS	3	ARG
53	BS	11	VAL
53	BS	12	ASP
53	BS	15	LEU
53	BS	51	VAL
53	BS	63	THR
53	BS	67	VAL
53	BS	78	ARG
53	BS	79	THR
54	BT	3	ASN
54	BT	6	SER
54	BT	18	ARG
54	BT	26	SER
54	BT	43	ASP
54	BT	45	ASP

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Mol	Chain	Res	Type
54	BT	50	LEU
54	BT	51	LEU
54	BT	59	ASP
54	BT	81	LEU
55	BV	23	TRP
55	BV	24	ASN
55	BV	32	PHE
55	BV	38	ILE
55	BV	66	THR
55	BV	75	GLN
55	BV	83	GLU
55	BV	102	THR
55	BV	113	ARG
55	BV	114	LEU
55	BV	146	ARG
55	BV	167	ASN
55	BV	169	GLU
55	BV	178	LYS
55	BV	184	ILE
55	BV	186	ILE
55	BV	189	THR
55	BV	208	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	17	ASN
1	3	18	HIS
4	C	76	ASN
4	C	91	ASN
4	C	129	ASN
4	C	130	ASN
4	C	143	HIS
4	C	205	ASN
5	D	34	ASN
5	D	130	HIS
5	D	179	ASN
6	E	100	GLN
6	E	125	HIS
6	E	151	ASN
6	E	202	ASN
7	F	146	HIS

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Mol	Chain	Res	Type
8	G	66	HIS
8	G	86	GLN
9	H	11	HIS
9	H	147	ASN
10	I	100	ASN
11	J	32	GLN
11	J	33	HIS
12	K	77	HIS
12	K	103	ASN
12	K	132	HIS
13	L	3	GLN
14	M	54	GLN
14	M	58	HIS
14	M	76	GLN
14	M	127	ASN
15	N	123	HIS
16	O	17	GLN
17	P	22	HIS
18	Q	26	ASN
18	Q	79	ASN
19	R	11	GLN
19	R	41	HIS
19	R	72	ASN
19	R	94	ASN
19	R	122	ASN
20	S	67	HIS
20	S	76	HIS
20	S	85	HIS
21	T	67	ASN
22	U	41	GLN
22	U	61	ASN
23	V	31	ASN
23	V	67	HIS
23	V	101	ASN
24	W	46	HIS
24	W	93	GLN
24	W	94	HIS
25	X	29	GLN
25	X	44	HIS
26	Y	22	HIS
26	Y	45	ASN
29	b	36	GLN

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Mol	Chain	Res	Type
30	c	22	ASN
30	c	48	HIS
32	e	25	GLN
32	e	31	HIS
37	BC	8	HIS
38	BD	51	GLN
38	BD	77	GLN
38	BD	84	ASN
38	BD	115	HIS
39	BE	146	HIS
39	BE	157	ASN
39	BE	160	ASN
39	BE	163	HIS
40	BF	80	ASN
41	BG	28	ASN
41	BG	106	ASN
43	BI	57	ASN
43	BI	64	HIS
43	BI	146	GLN
45	BK	27	HIS
45	BK	49	ASN
45	BK	128	ASN
46	BL	29	GLN
46	BL	73	ASN
47	BM	101	GLN
48	BN	11	ASN
49	BO	28	GLN
50	BP	41	HIS
50	BP	81	GLN
51	BQ	46	HIS
51	BQ	62	HIS
53	BS	52	HIS
53	BS	57	HIS
54	BT	52	HIS
54	BT	68	HIS
54	BT	70	ASN
54	BT	71	GLN
55	BV	24	ASN
55	BV	103	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3118/3120 (99%)	740 (23%)	29 (0%)
3	B	117/118 (99%)	23 (19%)	1 (0%)
35	BA	1510/1528 (98%)	362 (23%)	13 (0%)
56	BW	75/76 (98%)	20 (26%)	0
57	BX	5/6 (83%)	2 (40%)	0
All	All	4825/4848 (99%)	1147 (23%)	43 (0%)

All (1147) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	7	U
2	A	12	G
2	A	20	G
2	A	29	C
2	A	31	U
2	A	32	G
2	A	33	G
2	A	46	A
2	A	55	G
2	A	59	G
2	A	60	A
2	A	68	A
2	A	71	A
2	A	72	G
2	A	83	C
2	A	89	A
2	A	90	C
2	A	91	C
2	A	94	G
2	A	98	U
2	A	99	G
2	A	115	A
2	A	116	A
2	A	117	U
2	A	125	C
2	A	128	G
2	A	133	G
2	A	136	U
2	A	137	G
2	A	143	G
2	A	145	G
2	A	148	A
2	A	161	U

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Mol	Chain	Res	Type
2	A	164	A
2	A	171	U
2	A	172	C
2	A	175	G
2	A	177	G
2	A	195	A
2	A	198	A
2	A	203	A
2	A	212	A
2	A	214	G
2	A	215	A
2	A	221	A
2	A	222	A
2	A	227	A
2	A	228	A
2	A	229	U
2	A	230	G
2	A	231	U
2	A	237	C
2	A	248	G
2	A	264	G
2	A	270	U
2	A	271	A
2	A	272	A
2	A	274	C
2	A	275	C
2	A	279	U
2	A	282	A
2	A	283	U
2	A	285	U
2	A	286	G
2	A	287	A
2	A	288	U
2	A	290	C
2	A	291	C
2	A	292	G
2	A	293	G
2	A	294	G
2	A	297	G
2	A	299	G
2	A	300	G
2	A	301	U

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Mol	Chain	Res	Type
2	A	302	U
2	A	303	G
2	A	305	G
2	A	306	U
2	A	312	G
2	A	314	G
2	A	315	U
2	A	316	U
2	A	317	G
2	A	318	U
2	A	319	G
2	A	323	C
2	A	324	C
2	A	326	A
2	A	330	U
2	A	331	U
2	A	336	C
2	A	337	U
2	A	338	C
2	A	342	C
2	A	343	U
2	A	344	G
2	A	345	G
2	A	346	C
2	A	348	G
2	A	349	G
2	A	350	A
2	A	351	G
2	A	352	G
2	A	356	G
2	A	357	U
2	A	358	G
2	A	361	A
2	A	364	A
2	A	369	G
2	A	370	U
2	A	376	G
2	A	383	U
2	A	384	G
2	A	387	U
2	A	388	U
2	A	393	U

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Mol	Chain	Res	Type
2	A	399	G
2	A	404	A
2	A	406	A
2	A	412	A
2	A	413	G
2	A	417	C
2	A	424	G
2	A	426	G
2	A	434	G
2	A	438	U
2	A	445	U
2	A	446	G
2	A	450	G
2	A	452	G
2	A	454	U
2	A	459	A
2	A	460	G
2	A	472	C
2	A	474	G
2	A	489	A
2	A	490	A
2	A	491	U
2	A	493	U
2	A	494	G
2	A	498	G
2	A	499	G
2	A	500	A
2	A	505	C
2	A	509	U
2	A	512	G
2	A	542	A
2	A	543	U
2	A	544	U
2	A	562	G
2	A	567	A
2	A	569	G
2	A	570	U
2	A	581	G
2	A	589	A
2	A	591	G
2	A	592	A
2	A	594	U

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Mol	Chain	Res	Type
2	A	595	A
2	A	596	C
2	A	605	G
2	A	614	C
2	A	617	U
2	A	618	C
2	A	619	C
2	A	620	G
2	A	630	U
2	A	631	C
2	A	636	U
2	A	637	G
2	A	638	U
2	A	639	C
2	A	640	G
2	A	641	U
2	A	642	G
2	A	644	G
2	A	647	G
2	A	655	G
2	A	663	A
2	A	665	G
2	A	666	A
2	A	667	A
2	A	675	G
2	A	678	A
2	A	679	G
2	A	684	G
2	A	685	G
2	A	696	A
2	A	700	U
2	A	701	A
2	A	704	C
2	A	706	G
2	A	707	G
2	A	708	G
2	A	709	U
2	A	721	A
2	A	728	G
2	A	731	A
2	A	738	A
2	A	740	A

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Mol	Chain	Res	Type
2	A	742	G
2	A	747	A
2	A	753	A
2	A	757	G
2	A	758	A
2	A	759	G
2	A	760	U
2	A	764	U
2	A	765	G
2	A	766	G
2	A	767	U
2	A	768	G
2	A	774	G
2	A	783	G
2	A	784	G
2	A	785	A
2	A	793	C
2	A	801	U
2	A	816	G
2	A	827	G
2	A	829	U
2	A	832	G
2	A	839	U
2	A	845	C
2	A	862	U
2	A	863	G
2	A	864	A
2	A	868	C
2	A	872	G
2	A	878	G
2	A	879	A
2	A	880	G
2	A	890	G
2	A	891	G
2	A	892	G
2	A	897	A
2	A	899	G
2	A	900	G
2	A	917	A
2	A	919	A
2	A	920	G
2	A	921	C

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Mol	Chain	Res	Type
2	A	927	C
2	A	942	U
2	A	960	G
2	A	961	U
2	A	971	G
2	A	972	A
2	A	974	G
2	A	975	U
2	A	981	U
2	A	982	A
2	A	994	A
2	A	995	U
2	A	996	G
2	A	1000	C
2	A	1001	C
2	A	1002	C
2	A	1003	A
2	A	1005	A
2	A	1007	G
2	A	1009	U
2	A	1010	U
2	A	1011	A
2	A	1012	C
2	A	1013	U
2	A	1014	G
2	A	1022	C
2	A	1025	A
2	A	1030	C
2	A	1044	U
2	A	1046	C
2	A	1047	A
2	A	1049	G
2	A	1058	A
2	A	1063	G
2	A	1070	G
2	A	1075	U
2	A	1076	A
2	A	1078	G
2	A	1084	U
2	A	1085	G
2	A	1091	A
2	A	1092	G

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Mol	Chain	Res	Type
2	A	1099	A
2	A	1101	A
2	A	1114	G
2	A	1130	C
2	A	1131	G
2	A	1140	G
2	A	1143	G
2	A	1144	A
2	A	1148	G
2	A	1151	U
2	A	1163	A
2	A	1164	A
2	A	1165	G
2	A	1173	G
2	A	1174	G
2	A	1175	A
2	A	1176	G
2	A	1178	U
2	A	1184	U
2	A	1185	A
2	A	1186	G
2	A	1187	A
2	A	1188	A
2	A	1189	G
2	A	1190	C
2	A	1191	A
2	A	1192	G
2	A	1201	G
2	A	1202	A
2	A	1203	A
2	A	1204	A
2	A	1205	G
2	A	1206	A
2	A	1207	G
2	A	1208	U
2	A	1209	G
2	A	1212	U
2	A	1213	A
2	A	1214	A
2	A	1217	G
2	A	1219	U
2	A	1227	C

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Mol	Chain	Res	Type
2	A	1229	A
2	A	1230	G
2	A	1232	G
2	A	1233	A
2	A	1237	U
2	A	1238	G
2	A	1239	C
2	A	1240	G
2	A	1247	A
2	A	1250	U
2	A	1251	A
2	A	1253	C
2	A	1254	G
2	A	1260	C
2	A	1261	A
2	A	1275	A
2	A	1290	C
2	A	1292	U
2	A	1293	G
2	A	1294	U
2	A	1324	G
2	A	1325	U
2	A	1332	G
2	A	1335	G
2	A	1339	G
2	A	1344	A
2	A	1345	G
2	A	1353	G
2	A	1359	G
2	A	1362	A
2	A	1363	G
2	A	1368	A
2	A	1369	A
2	A	1371	G
2	A	1380	A
2	A	1386	G
2	A	1387	A
2	A	1389	U
2	A	1390	A
2	A	1404	C
2	A	1415	A
2	A	1416	A

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Mol	Chain	Res	Type
2	A	1417	A
2	A	1435	C
2	A	1437	A
2	A	1440	C
2	A	1448	C
2	A	1456	G
2	A	1457	A
2	A	1461	G
2	A	1462	G
2	A	1465	C
2	A	1467	U
2	A	1480	A
2	A	1494	U
2	A	1499	A
2	A	1502	G
2	A	1507	G
2	A	1510	A
2	A	1518	A
2	A	1521	C
2	A	1522	G
2	A	1531	C
2	A	1532	G
2	A	1533	U
2	A	1534	C
2	A	1540	U
2	A	1541	G
2	A	1543	A
2	A	1550	G
2	A	1551	U
2	A	1552	A
2	A	1553	C
2	A	1554	U
2	A	1563	A
2	A	1564	A
2	A	1565	A
2	A	1566	A
2	A	1574	G
2	A	1578	G
2	A	1579	C
2	A	1587	G
2	A	1596	C
2	A	1599	U

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Mol	Chain	Res	Type
2	A	1600	G
2	A	1625	G
2	A	1627	U
2	A	1628	A
2	A	1629	G
2	A	1631	A
2	A	1632	G
2	A	1633	U
2	A	1637	G
2	A	1638	C
2	A	1639	G
2	A	1640	A
2	A	1641	U
2	A	1648	A
2	A	1649	C
2	A	1659	U
2	A	1670	G
2	A	1673	A
2	A	1674	G
2	A	1679	A
2	A	1680	A
2	A	1681	U
2	A	1688	G
2	A	1703	G
2	A	1710	A
2	A	1711	G
2	A	1714	A
2	A	1715	A
2	A	1717	U
2	A	1723	U
2	A	1724	G
2	A	1728	U
2	A	1729	A
2	A	1730	U
2	A	1731	A
2	A	1737	A
2	A	1738	G
2	A	1745	U
2	A	1746	G
2	A	1754	G
2	A	1755	A
2	A	1756	G

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Mol	Chain	Res	Type
2	A	1757	U
2	A	1761	G
2	A	1767	U
2	A	1774	U
2	A	1785	C
2	A	1786	G
2	A	1789	A
2	A	1792	A
2	A	1796	U
2	A	1798	U
2	A	1802	G
2	A	1803	A
2	A	1806	A
2	A	1813	C
2	A	1826	A
2	A	1845	G
2	A	1857	U
2	A	1862	C
2	A	1864	U
2	A	1866	C
2	A	1867	G
2	A	1869	G
2	A	1870	U
2	A	1871	G
2	A	1872	A
2	A	1892	G
2	A	1893	C
2	A	1916	A
2	A	1932	U
2	A	1933	G
2	A	1945	U
2	A	1946	U
2	A	1947	U
2	A	1948	A
2	A	1950	G
2	A	1967	G
2	A	1973	C
2	A	1974	A
2	A	1975	A
2	A	1981	U
2	A	1990	A
2	A	1999	U

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Mol	Chain	Res	Type
2	A	2008	A
2	A	2017	C
2	A	2018	G
2	A	2026	A
2	A	2033	U
2	A	2046	A
2	A	2064	A
2	A	2065	A
2	A	2066	G
2	A	2073	A
2	A	2075	G
2	A	2084	A
2	A	2085	C
2	A	2086	U
2	A	2087	C
2	A	2088	C
2	A	2089	C
2	A	2091	U
2	A	2092	U
2	A	2093	G
2	A	2094	G
2	A	2095	G
2	A	2096	G
2	A	2106	A
2	A	2107	G
2	A	2108	A
2	A	2111	U
2	A	2112	U
2	A	2120	A
2	A	2129	C
2	A	2130	G
2	A	2131	G
2	A	2137	A
2	A	2138	C
2	A	2140	A
2	A	2141	U
2	A	2153	G
2	A	2154	G
2	A	2160	A
2	A	2162	A
2	A	2163	U
2	A	2164	U

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Mol	Chain	Res	Type
2	A	2179	U
2	A	2184	A
2	A	2190	A
2	A	2191	C
2	A	2194	A
2	A	2195	U
2	A	2196	G
2	A	2197	G
2	A	2215	U
2	A	2217	U
2	A	2221	A
2	A	2227	A
2	A	2235	C
2	A	2244	A
2	A	2247	A
2	A	2251	G
2	A	2254	A
2	A	2255	A
2	A	2256	G
2	A	2257	A
2	A	2263	G
2	A	2267	C
2	A	2274	C
2	A	2276	G
2	A	2279	C
2	A	2280	G
2	A	2284	A
2	A	2285	G
2	A	2286	A
2	A	2299	C
2	A	2316	G
2	A	2320	C
2	A	2324	A
2	A	2325	U
2	A	2328	G
2	A	2329	G
2	A	2333	G
2	A	2334	U
2	A	2335	G
2	A	2336	U
2	A	2338	G
2	A	2339	G

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Mol	Chain	Res	Type
2	A	2340	A
2	A	2341	U
2	A	2342	A
2	A	2343	G
2	A	2346	G
2	A	2349	A
2	A	2351	A
2	A	2354	G
2	A	2355	U
2	A	2356	G
2	A	2357	A
2	A	2362	C
2	A	2368	C
2	A	2371	G
2	A	2372	U
2	A	2380	G
2	A	2382	G
2	A	2383	U
2	A	2384	C
2	A	2386	U
2	A	2387	U
2	A	2388	G
2	A	2389	U
2	A	2390	U
2	A	2391	G
2	A	2392	A
2	A	2393	A
2	A	2394	A
2	A	2395	U
2	A	2396	A
2	A	2400	C
2	A	2401	U
2	A	2402	C
2	A	2407	C
2	A	2408	G
2	A	2409	U
2	A	2410	A
2	A	2413	G
2	A	2418	U
2	A	2421	A
2	A	2422	A
2	A	2427	G

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Mol	Chain	Res	Type
2	A	2434	A
2	A	2436	A
2	A	2447	G
2	A	2449	A
2	A	2462	G
2	A	2463	G
2	A	2467	U
2	A	2483	G
2	A	2502	A
2	A	2503	G
2	A	2504	G
2	A	2507	C
2	A	2508	C
2	A	2511	A
2	A	2529	A
2	A	2532	G
2	A	2545	G
2	A	2549	G
2	A	2551	A
2	A	2558	C
2	A	2559	A
2	A	2567	U
2	A	2571	C
2	A	2574	C
2	A	2585	U
2	A	2607	G
2	A	2609	A
2	A	2613	G
2	A	2626	U
2	A	2627	C
2	A	2643	U
2	A	2647	U
2	A	2649	A
2	A	2650	A
2	A	2653	G
2	A	2654	A
2	A	2655	U
2	A	2659	A
2	A	2665	C
2	A	2669	G
2	A	2672	A
2	A	2673	U

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Mol	Chain	Res	Type
2	A	2677	A
2	A	2688	C
2	A	2689	C
2	A	2693	A
2	A	2694	G
2	A	2698	C
2	A	2700	A
2	A	2702	A
2	A	2705	G
2	A	2715	U
2	A	2726	G
2	A	2729	G
2	A	2732	G
2	A	2742	A
2	A	2744	C
2	A	2753	G
2	A	2759	G
2	A	2778	U
2	A	2786	U
2	A	2790	A
2	A	2791	G
2	A	2796	A
2	A	2797	C
2	A	2802	G
2	A	2806	G
2	A	2826	A
2	A	2827	G
2	A	2833	U
2	A	2837	U
2	A	2839	U
2	A	2853	C
2	A	2856	A
2	A	2862	G
2	A	2885	G
2	A	2887	G
2	A	2913	U
2	A	2915	C
2	A	2926	A
2	A	2936	C
2	A	2938	G
2	A	2948	C
2	A	2950	C

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Mol	Chain	Res	Type
2	A	2956	G
2	A	2957	A
2	A	2968	G
2	A	2972	A
2	A	2982	A
2	A	2985	G
2	A	2989	A
2	A	3002	A
2	A	3004	C
2	A	3005	A
2	A	3009	U
2	A	3014	A
2	A	3015	C
2	A	3016	C
2	A	3020	U
2	A	3021	A
2	A	3022	G
2	A	3024	A
2	A	3027	G
2	A	3029	U
2	A	3042	A
2	A	3047	A
2	A	3056	A
2	A	3082	U
2	A	3088	C
2	A	3093	A
2	A	3095	C
2	A	3101	C
2	A	3105	C
2	A	3106	C
2	A	3107	G
2	A	3112	A
2	A	3113	A
2	A	3114	A
2	A	3115	A
3	B	4	A
3	B	7	G
3	B	11	U
3	B	12	C
3	B	13	C
3	B	14	A
3	B	22	A

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Mol	Chain	Res	Type
3	B	23	G
3	B	25	G
3	B	30	G
3	B	31	C
3	B	35	G
3	B	42	C
3	B	57	U
3	B	58	A
3	B	85	C
3	B	87	U
3	B	89	C
3	B	90	G
3	B	103	G
3	B	107	A
3	B	112	C
3	B	115	A
35	BA	8	U
35	BA	9	U
35	BA	11	G
35	BA	12	A
35	BA	13	G
35	BA	26	G
35	BA	36	A
35	BA	43	G
35	BA	45	G
35	BA	48	G
35	BA	51	C
35	BA	52	U
35	BA	53	U
35	BA	54	A
35	BA	55	A
35	BA	58	C
35	BA	59	A
35	BA	68	G
35	BA	77	G
35	BA	81	C
35	BA	82	U
35	BA	83	U
35	BA	85	C
35	BA	87	G
35	BA	92	A
35	BA	93	C

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Mol	Chain	Res	Type
35	BA	101	G
35	BA	116	A
35	BA	117	C
35	BA	118	A
35	BA	123	G
35	BA	128	U
35	BA	136	G
35	BA	139	C
35	BA	160	C
35	BA	174	G
35	BA	179	C
35	BA	180	A
35	BA	192	G
35	BA	194	A
35	BA	200	U
35	BA	201	G
35	BA	209	A
35	BA	210	A
35	BA	211	A
35	BA	214	U
35	BA	215	U
35	BA	216	U
35	BA	217	U
35	BA	218	G
35	BA	220	G
35	BA	226	G
35	BA	227	G
35	BA	242	U
35	BA	243	A
35	BA	245	C
35	BA	247	G
35	BA	251	G
35	BA	254	G
35	BA	266	G
35	BA	267	C
35	BA	279	A
35	BA	280	C
35	BA	281	G
35	BA	289	G
35	BA	301	G
35	BA	316	C
35	BA	319	G

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Mol	Chain	Res	Type
35	BA	321	A
35	BA	329	A
35	BA	332	G
35	BA	344	A
35	BA	345	C
35	BA	350	G
35	BA	351	G
35	BA	352	C
35	BA	353	A
35	BA	354	G
35	BA	356	A
35	BA	367	U
35	BA	372	C
35	BA	373	A
35	BA	382	A
35	BA	390	U
35	BA	392	C
35	BA	397	A
35	BA	398	C
35	BA	406	G
35	BA	411	A
35	BA	414	A
35	BA	421	U
35	BA	422	C
35	BA	423	G
35	BA	424	G
35	BA	426	U
35	BA	427	U
35	BA	428	G
35	BA	429	U
35	BA	430	A
35	BA	434	C
35	BA	438	U
35	BA	451	A
35	BA	452	A
35	BA	453	G
35	BA	454	C
35	BA	456	C
35	BA	457	A
35	BA	458	A
35	BA	459	G
35	BA	461	G

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Mol	Chain	Res	Type
35	BA	465	G
35	BA	466	U
35	BA	473	A
35	BA	477	G
35	BA	478	A
35	BA	479	A
35	BA	485	G
35	BA	486	G
35	BA	491	C
35	BA	496	U
35	BA	497	G
35	BA	498	C
35	BA	499	C
35	BA	505	C
35	BA	507	G
35	BA	509	G
35	BA	511	U
35	BA	512	A
35	BA	513	A
35	BA	515	A
35	BA	520	G
35	BA	525	C
35	BA	527	A
35	BA	539	A
35	BA	542	U
35	BA	544	C
35	BA	552	A
35	BA	553	A
35	BA	554	A
35	BA	556	A
35	BA	557	G
35	BA	602	A
35	BA	612	U
35	BA	613	G
35	BA	633	A
35	BA	641	G
35	BA	645	G
35	BA	666	U
35	BA	667	A
35	BA	668	G
35	BA	680	G
35	BA	683	G

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Mol	Chain	Res	Type
35	BA	700	C
35	BA	701	G
35	BA	702	G
35	BA	703	U
35	BA	711	G
35	BA	713	G
35	BA	729	A
35	BA	735	G
35	BA	757	A
35	BA	761	A
35	BA	764	A
35	BA	765	G
35	BA	772	A
35	BA	773	U
35	BA	774	A
35	BA	779	G
35	BA	782	A
35	BA	789	G
35	BA	794	A
35	BA	795	A
35	BA	797	C
35	BA	799	G
35	BA	808	A
35	BA	818	U
35	BA	821	C
35	BA	822	U
35	BA	823	U
35	BA	824	C
35	BA	825	C
35	BA	826	U
35	BA	827	U
35	BA	828	G
35	BA	840	G
35	BA	841	U
35	BA	865	C
35	BA	871	A
35	BA	884	G
35	BA	896	A
35	BA	901	A
35	BA	908	G
35	BA	909	G
35	BA	913	C

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Mol	Chain	Res	Type
35	BA	914	C
35	BA	915	G
35	BA	916	C
35	BA	917	A
35	BA	921	G
35	BA	924	G
35	BA	930	C
35	BA	932	U
35	BA	940	A
35	BA	942	U
35	BA	943	U
35	BA	947	U
35	BA	948	G
35	BA	950	A
35	BA	951	A
35	BA	953	G
35	BA	955	G
35	BA	956	A
35	BA	957	A
35	BA	959	A
35	BA	971	G
35	BA	973	U
35	BA	974	U
35	BA	975	G
35	BA	982	A
35	BA	984	A
35	BA	985	G
35	BA	986	G
35	BA	987	A
35	BA	988	C
35	BA	992	G
35	BA	999	A
35	BA	1000	U
35	BA	1007	U
35	BA	1008	C
35	BA	1010	C
35	BA	1013	G
35	BA	1014	U
35	BA	1020	G
35	BA	1021	U
35	BA	1024	G
35	BA	1025	C

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Mol	Chain	Res	Type
35	BA	1028	G
35	BA	1030	G
35	BA	1033	G
35	BA	1034	C
35	BA	1045	U
35	BA	1048	G
35	BA	1054	G
35	BA	1074	G
35	BA	1075	U
35	BA	1079	G
35	BA	1081	A
35	BA	1088	G
35	BA	1104	G
35	BA	1108	C
35	BA	1112	C
35	BA	1115	G
35	BA	1116	U
35	BA	1117	U
35	BA	1118	A
35	BA	1120	G
35	BA	1123	G
35	BA	1128	C
35	BA	1129	U
35	BA	1132	U
35	BA	1138	A
35	BA	1139	C
35	BA	1140	U
35	BA	1141	G
35	BA	1147	G
35	BA	1149	C
35	BA	1150	A
35	BA	1152	C
35	BA	1162	G
35	BA	1164	U
35	BA	1165	G
35	BA	1176	C
35	BA	1177	A
35	BA	1178	A
35	BA	1181	C
35	BA	1182	A
35	BA	1183	U
35	BA	1193	U

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Mol	Chain	Res	Type
35	BA	1194	A
35	BA	1206	U
35	BA	1207	C
35	BA	1217	A
35	BA	1219	A
35	BA	1231	A
35	BA	1233	A
35	BA	1238	U
35	BA	1239	G
35	BA	1241	G
35	BA	1248	U
35	BA	1251	G
35	BA	1260	A
35	BA	1261	A
35	BA	1266	U
35	BA	1267	U
35	BA	1268	C
35	BA	1269	A
35	BA	1271	A
35	BA	1272	G
35	BA	1281	A
35	BA	1282	G
35	BA	1283	U
35	BA	1284	U
35	BA	1285	C
35	BA	1287	G
35	BA	1299	C
35	BA	1301	A
35	BA	1302	C
35	BA	1304	C
35	BA	1305	G
35	BA	1313	G
35	BA	1320	G
35	BA	1322	G
35	BA	1327	U
35	BA	1328	A
35	BA	1329	G
35	BA	1335	G
35	BA	1343	G
35	BA	1344	C
35	BA	1345	A
35	BA	1346	A

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Mol	Chain	Res	Type
35	BA	1347	C
35	BA	1351	G
35	BA	1353	G
35	BA	1357	A
35	BA	1363	U
35	BA	1364	U
35	BA	1381	A
35	BA	1382	C
35	BA	1383	C
35	BA	1385	C
35	BA	1389	U
35	BA	1402	G
35	BA	1405	G
35	BA	1407	U
35	BA	1409	A
35	BA	1424	G
35	BA	1425	G
35	BA	1426	C
35	BA	1429	A
35	BA	1430	A
35	BA	1433	C
35	BA	1434	U
35	BA	1435	U
35	BA	1436	G
35	BA	1438	G
35	BA	1459	G
35	BA	1466	G
35	BA	1471	G
35	BA	1478	G
35	BA	1481	G
35	BA	1483	A
35	BA	1486	A
35	BA	1487	A
35	BA	1488	G
35	BA	1490	U
35	BA	1501	G
35	BA	1502	A
35	BA	1503	A
35	BA	1504	G
35	BA	1513	G
35	BA	1514	G
35	BA	1516	U

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Mol	Chain	Res	Type
56	BW	2	C
56	BW	6	G
56	BW	8	U
56	BW	16	U
56	BW	17	C
56	BW	18	G
56	BW	19	G
56	BW	20	U
56	BW	21	A
56	BW	22	G
56	BW	23	A
56	BW	32	U
56	BW	37	A
56	BW	42	C
56	BW	46	G
56	BW	47	U
56	BW	48	C
56	BW	52	G
56	BW	69	G
56	BW	76	A
57	BX	2	U
57	BX	3	U

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	89	A
2	A	97	U
2	A	284	G
2	A	287	A
2	A	316	U
2	A	357	U
2	A	445	U
2	A	759	G
2	A	919	A
2	A	974	G
2	A	980	C
2	A	981	U
2	A	1004	C
2	A	1010	U
2	A	1046	C
2	A	1084	U

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Mol	Chain	Res	Type
2	A	1186	G
2	A	1231	U
2	A	1368	A
2	A	1713	U
2	A	1730	U
2	A	1947	U
2	A	2085	C
2	A	2088	C
2	A	2094	G
2	A	2350	G
2	A	2381	A
2	A	2626	U
2	A	3113	A
3	B	10	G
35	BA	422	C
35	BA	429	U
35	BA	456	C
35	BA	485	G
35	BA	498	C
35	BA	895	A
35	BA	1007	U
35	BA	1116	U
35	BA	1117	U
35	BA	1149	C
35	BA	1266	U
35	BA	1477	A
35	BA	1482	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 632 ligands modelled in this entry, 631 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	PHE	BW	101	-	11,11,12	1.06	1 (9%)	12,13,15	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PHE	BW	101	-	-	0/4/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BW	101	PHE	CA-C	2.36	1.53	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.