



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 10:20 PM UTC

PDB ID : 8Y38 / pdb_00008y38
EMDB ID : EMD-38875
Title : Cryo-EM structure of Staphylococcus aureus 70S ribosome (strain 15B196) in complex with MCX-190.
Authors : Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on : 2024-01-28
Resolution : 2.58 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

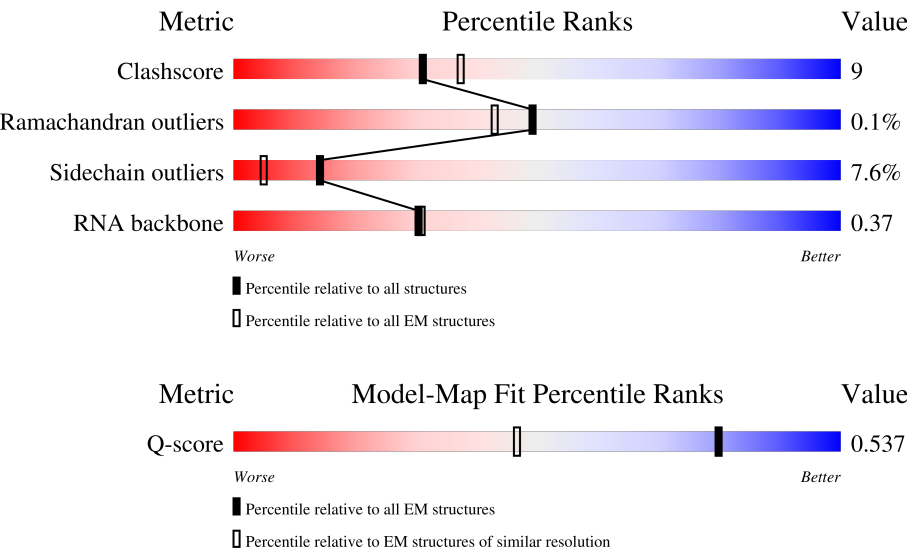
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.58 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7675 (2.08 - 3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	47	70% 26% .
2	2	43	84% 16%
3	3	64	70% 30%

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Mol	Chain	Length	Quality of chain
4	4	37	
5	A	2921	
6	B	115	
7	C	274	
8	D	215	
9	E	206	
10	F	175	
11	G	175	
12	H	145	
13	I	122	
14	J	146	
15	K	137	
16	L	120	
17	M	119	
18	N	114	
19	O	116	
20	P	102	
21	Q	117	
22	R	89	
23	S	103	
24	T	94	
25	U	82	
26	V	58	
27	W	67	
28	X	58	

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Mol	Chain	Length	Quality of chain
29	Y	59	
30	Z	48	
31	a	1548	
32	b	232	
33	c	217	
34	d	200	
35	e	166	
36	f	98	
37	g	156	
38	h	132	
39	i	130	
40	j	102	
41	k	129	
42	l	149	
43	m	121	
44	n	61	
45	o	89	
46	p	91	
47	q	87	
48	r	80	
49	s	108	
50	t	83	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 138224 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 Large ribosomal subunit protein bL33B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2885	Total	C	N	O	P	0	0
			61861	27621	11312	20043	2885		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	274	Total	C	N	O	S	0	0
			2090	1301	415	369	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1317	835	223	253	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	175	Total	C	N	O	S	0	0
			1259	788	239	229	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			891	557	174	159	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O		0	0
			889	563	175	151			

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	112	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	94	Total	C	N	O		0	0
			711	456	127	128			

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	82	Total	C	N	O		0	0
			615	380	121	114			

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	58	Total	C	N	O		0	0
			445	277	96	72			

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	67	Total	C	N	O		0	0
			541	333	102	106			

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 29 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Y	57	Total	C	N	O	0	0
			353	214	65	74		

- Molecule 30 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	48	Total	C	N	O	S	0	0
			361	222	77	59	3		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1479	Total	C	N	O	P	0	0
			31706	14154	5809	10264	1479		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1032	N	C	conflict	GB 1747281577

- Molecule 32 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	224	Total	C	N	O	S	0	0
			1802	1149	314	332	7		

- Molecule 33 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	202	Total	C	N	O	S	0	0
			1596	1005	300	289	2		

- Molecule 34 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	199	Total	C	N	O	S	0	0
			1616	1020	302	292	2		

- Molecule 35 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	156	Total	C	N	O	S	0	0
			1160	731	212	215	2		

- Molecule 36 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	95	Total	C	N	O	S	0	0
			789	498	138	150	3		

- Molecule 37 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	155	Total	C	N	O	S	0	0
			1242	775	239	224	4		

- Molecule 38 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total	C	N	O	S	0	0
			1031	652	183	192	4		

- Molecule 39 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O	S	0	0
			1007	624	201	181	1		

- Molecule 40 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	97	Total	C	N	O	S	0	0
			773	488	141	143	1		

- Molecule 41 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	114	Total	C	N	O	S	0	0
			844	520	160	161	3		

- Molecule 42 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 43 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	116	Total	C	N	O	S	0	0
			922	566	183	172	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 45 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	87	Total	C	N	O	S	0	0
			726	448	149	128	1		

- Molecule 46 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	87	Total	C	N	O	S	0	0
			688	433	127	127	1		

- Molecule 47 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			657	416	117	123	1		

- Molecule 48 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	64	Total	C	N	O	S	0	0
			525	336	98	88	3		

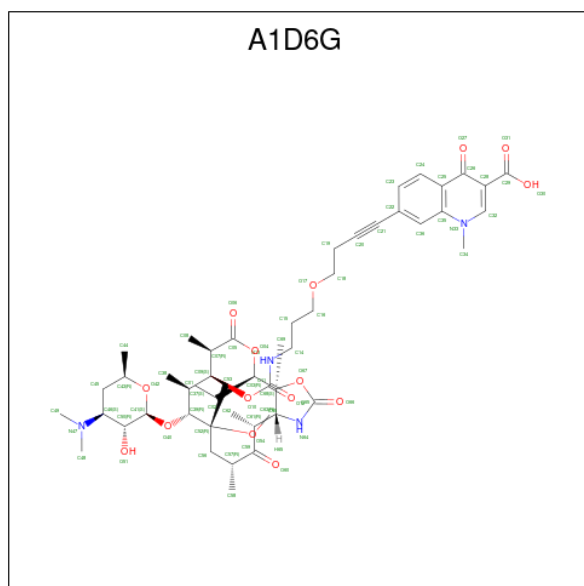
- Molecule 49 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			665	427	121	115	2		

- Molecule 50 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	81	Total	C	N	O	S	0	0
			611	370	120	119	2		

- Molecule 51 is 7-[4-[3-[(1 {S},2 {R},5 {R},6 {S},7 {S},8 {R},9 {R},11 {R},13 {R},14 {R})-8-[(2 {S},3 {R},4 {S},6 {R})-4-(dimethylamino)-6-methyl-3-oxidanyl-oxan-2-yl]oxy-2-ethyl-9-methoxy-1,5,7,9,11,13-hexamethyl-4,12,16-tris(oxidanylidene)-3,17-dioxo-15-azabicyclo[1 2.3.0]heptadecan-6-yl]oxycarbonylamino]propoxy]but-1-ynyl]-1-methyl-4-oxidanylidene-quinoline-3-carboxylic acid (CCD ID: A1D6G) (formula: C₅₀H₇₂N₄O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
51	A	1	Total	C	N	O	0
			69	50	4	15	

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	A	12	Total	Mg	0
			12	12	

- Molecule 53 is water.

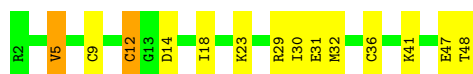
Mol	Chain	Residues	Atoms		AltConf
53	A	4	Total	O	0
			4	4	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Large ribosomal subunit protein bL33B

Chain 1: 



- Molecule 2: Large ribosomal subunit protein bL34

Chain 2: 



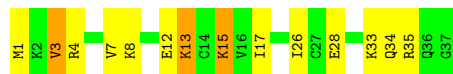
- Molecule 3: Large ribosomal subunit protein bL35

Chain 3: 



- Molecule 4: Large ribosomal subunit protein bL36

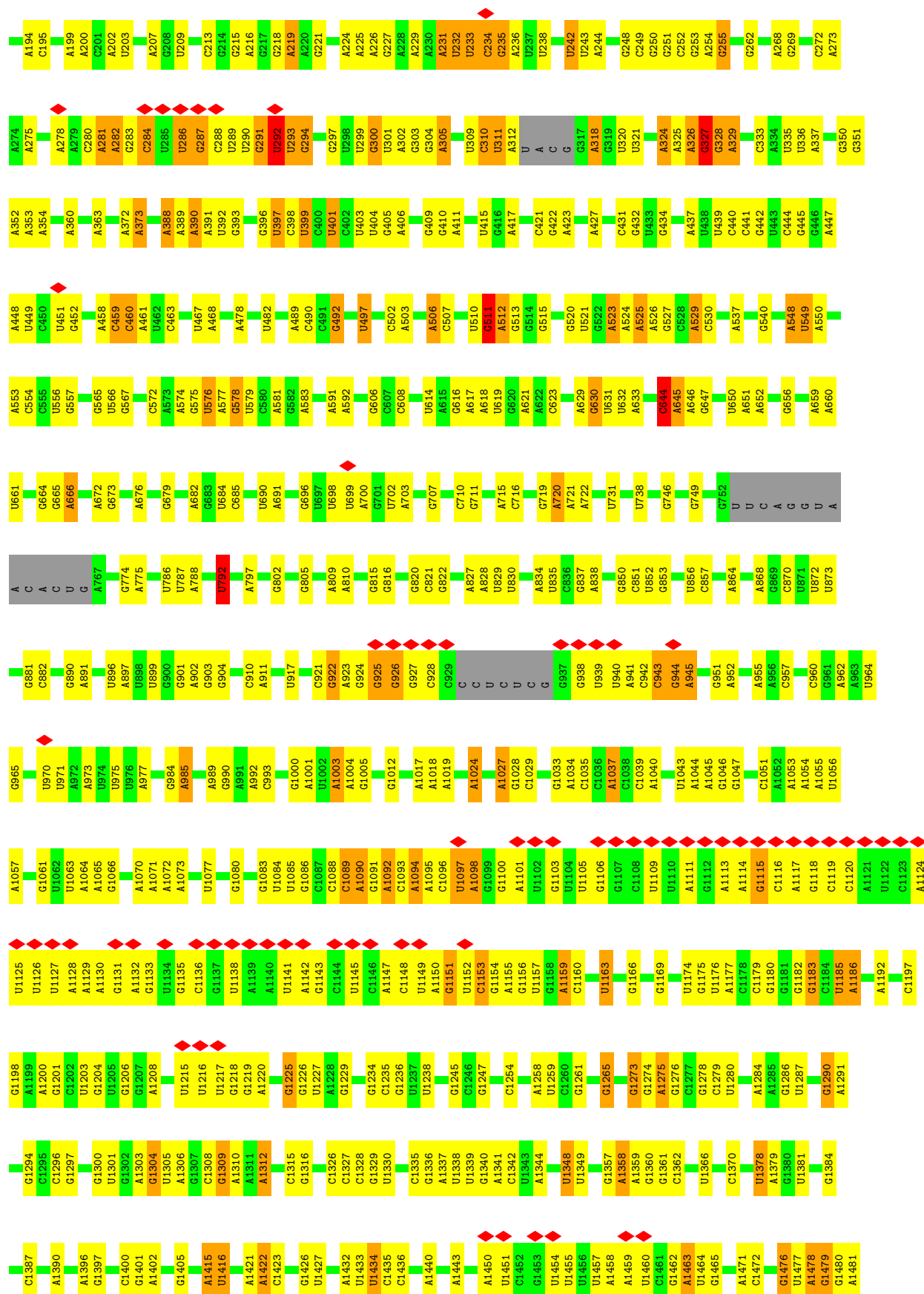
Chain 4: 



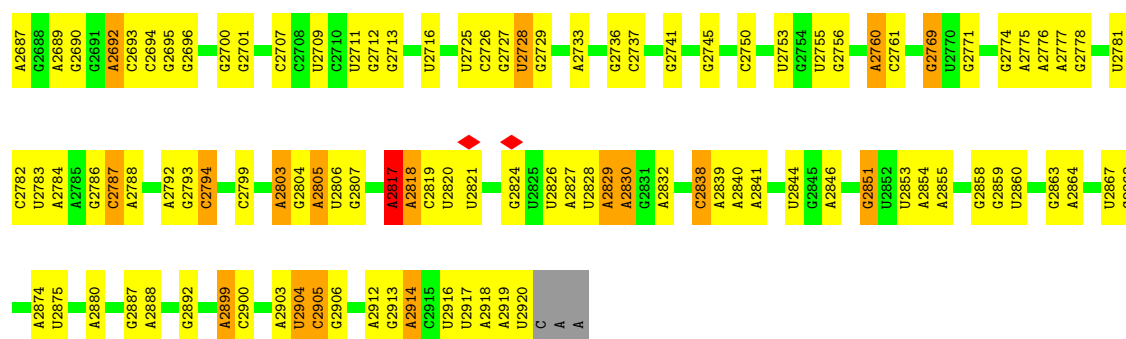
- Molecule 5: 23S ribosomal RNA

Chain A: 

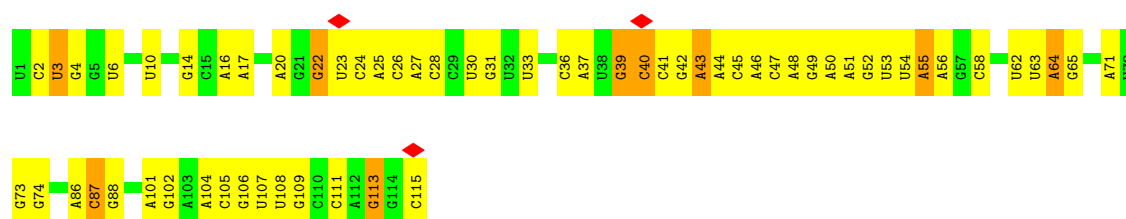




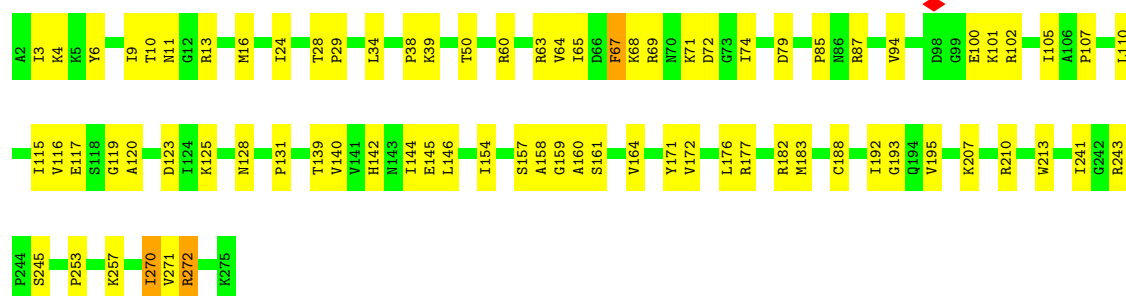
G2609	G2610	G2611	G2612	G2613	G2617	G2618	G2619	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2632	G2633	G2636	G2640	G2641	G2642	G2643	G2644	G2645	G2648	G2649	G2650	G2651	G2652	G2653	A2656	A2661	A2662	A2668	G2669	G2670	G2671	G2672	G2673	C2677	C2678	G2679	G2680	G2681	G2682	G2683	G2684	G2686										
G2521	G2525	G2528	G2529	G2530	G2531	G2532	G2533	G2534	A2540	G2541	G2542	G2543	G2544	G2545	G2547	G2552	G2553	G2554	G2555	G2556	G2557	G2558	G2559	G2562	G2563	G2564	G2565	G2566	G2568	A2569	G2570	U2574	G2575	U2579	G2580	G2581	U2582	U2589	U2590	A2591	A2592	A2593	G2594	U2598	A2599	G2600	G2601	G2605										
C2408	G2409	G2410	A2411	G2412	G2416	G2417	G2418	G2419	C2430	G2431	G2432	G2433	A2434	G2435	G2436	G2437	A2438	G2441	U2450	C2451	A2452	G2453	G2454	G2455	A2457	A2459	A2460	A2461	A2462	G2463	C2464	U2465	C2468	G2472	G2473	G2474	A2475	C2493	C2494	A2495	A2496	G2497	G2498	G2499	A2505	U2506	G2507	G2508										
U2319	C2320	G2326	A2327	A2328	U2329	G2330	G2331	U2332	U2333	G2334	G2335	A2336	A2337	A2338	U2339	C2340	A2341	U2342	A2345	A2346	A2347	G2348	A2349	G2350	U2351	G2352	U2353	A2354	A2355	A2356	G2357	G2358	G2359	A2360	U2361	A2362	A2363	G2364	G2369	U2370	U2371	G2372	A2373	C2374	C2377	A2388	A2396	G2397	G2398	G2399	A2404							
C2223	U2224	A2225	A2226	C2227	C2228	C2229	G2230	G2231	A2232	A2235	U2238	A2239	U2240	C2241	G2244	G2245	G2251	A2252	G2253	A2254	G2257	G2260	G2261	G2265	G2266	U2272	G2273	A2274	G2278	G2279	C2287	A2294	A2295	A2296	G2304	A2305	G2306	G2310	U2311	G2312	A2313	A2314	A2315	G2316	G2317	U2318												
A2162	A2163	C2164	G2165	U2166	G2167	A2168	G2169	C2170	G2171	C2172	U2173	A2174	G2175	C2176	U2177	U2178	A2179	C2180	G2181	U2182	G2183	G2184	A2185	G2186	C2187	C2188	G2189	C2190	U2191	G2192	G2193	U2194	G2195	G2196	G2197	A2198	A2199	A2200	G2201	U2202	A2203	C2204	C2205	C2206	U2207	A2208	G2209	C2210	U2211	G2212	U2213	G2214	U2215	U2216	G2217	G2218	U2221	U2222
G2097	A2098	G2099	C2100	U2101	U2106	G2107	U2108	A2109	G2110	G2114	A2115	U2116	A2117	U2118	U2119	G2120	A2121	A2122	A2123	U2124	U2125	C2126	G2127	G2128	C2129	A2130	C2131	A2132	G2133	C2134	U2135	U2136	G2137	U2138	A2139	A2140	A2141	G2142	G2143	A2144	U2145	A2146	G2147	G2148	U2149	A2150	G2151	G2152	A2153	G2154	C2155	G2156	U2158	U2159	G2160	A2161		
A2008	U2009	U2018	G2019	U2020	C2021	U2022	C2023	A2024	A2025	C2026	G2029	A2032	C2035	G2036	G2037	A2040	A2041	A2042	G2048	U2049	A2050	A2057	A2058	G2059	A2060	U2061	G2062	C2070	C2074	G2075	A2076	C2077	A2078	C2082	G2083	G2084	A2085	A2086	A2087	G2088	A2089	C2090	C2091	C2092	G2093	G2094	U2095	G2096										
G1915	A1916	A1917	A1918	G1919	C1920	A1923	A1928	A1929	C1929	G1932	U1933	G1934	U1938	A1939	A	C	U	A	A1945	A1946	C1947	G1948	U1950	C1951	A1954	A1955	G1956	G1957	U1958	A1964	A1965	U1966	U1967	U1982	G1986	C1989	G1990	C1991	A1993	A1994	G1995	A1996	A1997	U1998	G1999	U2003												
A1814	G1815	A1816	C1817	A1818	G1819	G1820	U1821	G1822	U1823	A1824	U1828	A1830	U1835	A1836	U1843	G1844	U1845	A1856	G1862	U1870	C1870	A1871	C1872	G1873	A1874	A1875	G1876	A1880	A1881	G1882	A1883	A1886	A1893	G1894	U1897	C1898	U1899	G1900	A1903	A1904	G1905	A1908	C1909	A1912														
A1630	G1631	A1632	A1633	A1634	A1635	U1636	G1637	G1638	G1639	U1640	G1641	C1651	A1652	A1653	A1654	G1655	C1656	G1657	A1658	C1659	A1660	C1661	A1662	A1666	C1669	A1670	U1671	C1672	U1675	A1676	A1677	A1678	A1679	U1680	U1681	G1687	A1690	G1691	C1692	G1693	A1699	C1700	U1701	U1707	A1708	A1709	A1712	A1713	C1714	A1616	A1617	A1618	U1623	G1624	U1625	A1626	G1627	U1629
G1565	G1566	C1567	U1568	G1569	G1570	G1571	G1574	A1575	G1576	G1577	A1578	C1579	A1580	U1581	U1582	G1583	U1584	C1585	U1586	C1587	U1588	U1589	C1590	A1591	G1592	G1593	U1594	C1595	G1596	U1597	U1598	G1599	U1602	A1605	A1606	U1613	A1616	A1617	A1618	U1623	G1624	U1625	A1626	G1627	U1629													
U1482	A1483	G1484	G1485	G1486	G1487	A1488	A1489	G1490	U1493	A1494	A1497	U1498	U1499	G1500	U1504	G1505	C1506	A1507	C1508	G1509	U1510	C1511	U1512	A1513	A1517	G1522	G1523	C1524	U1525	G1526	A1527	G1528	U1529	U1530	U1531	U1532	A	C	C	A1537	A1538	A1539	U1540	C1541	C1542	U1548	G1549	U1550	U1551	U1552	A1553	A1554						



• Molecule 6: 5S ribosomal RNA



• Molecule 7: Large ribosomal subunit protein uL2

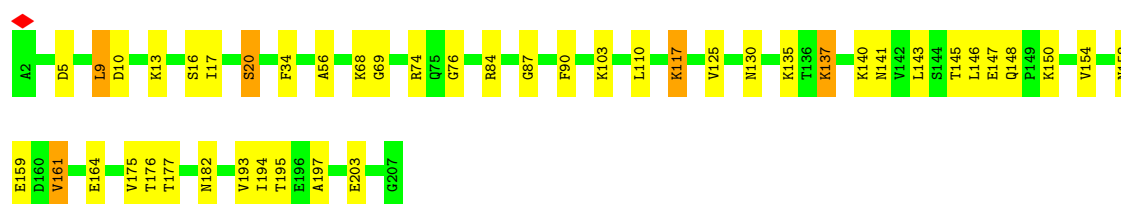


• Molecule 8: Large ribosomal subunit protein uL3



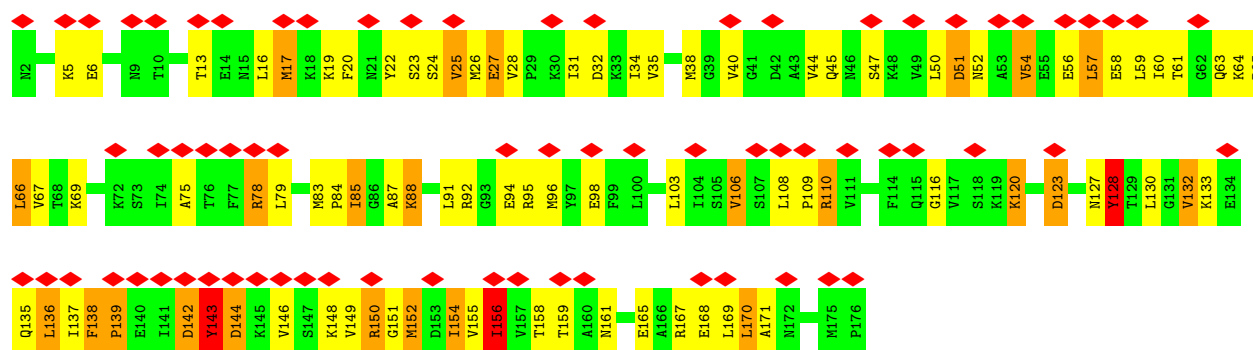
• Molecule 9: Large ribosomal subunit protein uL4

Chain E:  78% 19%



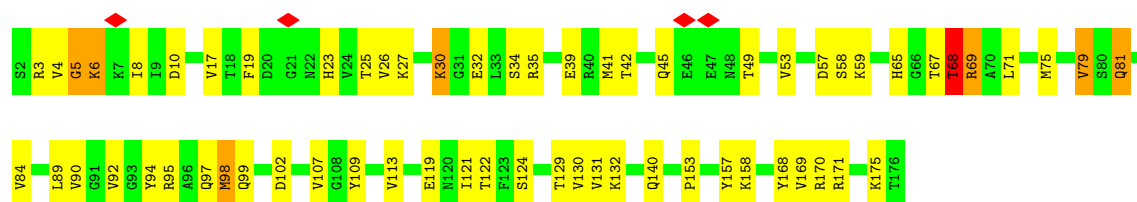
- Molecule 10: Large ribosomal subunit protein uL5

Chain F:  41% 47% 37% 14%



- Molecule 11: Large ribosomal subunit protein uL6

Chain G:  64% 31%



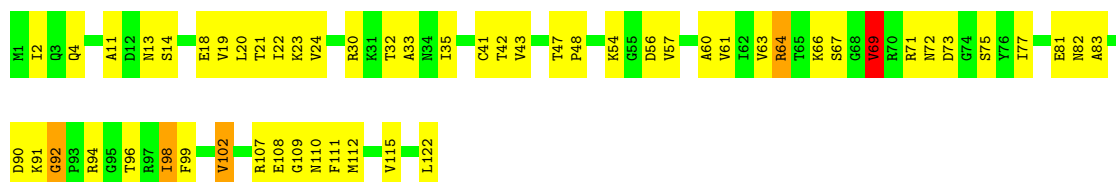
- Molecule 12: Large ribosomal subunit protein uL13

Chain H:  68% 26% 6%

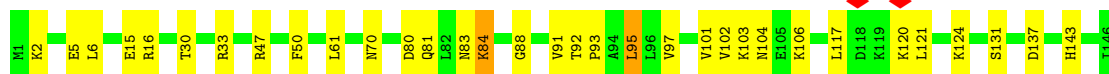
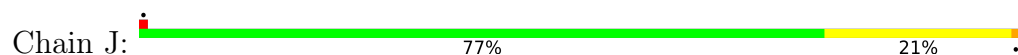


- Molecule 13: Large ribosomal subunit protein uL14

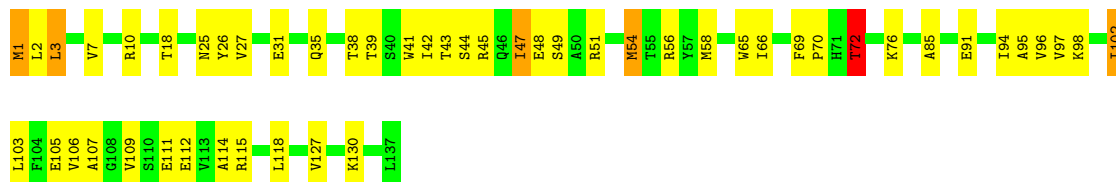
Chain I:  55% 41%



- Molecule 14: Large ribosomal subunit protein uL15



- Molecule 15: Large ribosomal subunit protein uL16



- Molecule 16: Large ribosomal subunit protein bL17



- Molecule 17: Large ribosomal subunit protein uL18



- Molecule 18: Large ribosomal subunit protein bL19





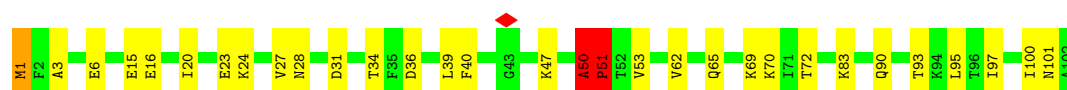
- Molecule 19: Large ribosomal subunit protein bL20

Chain O: 75% 24%



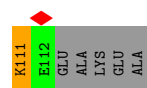
- Molecule 20: Large ribosomal subunit protein bL21

Chain P: 70% 27%



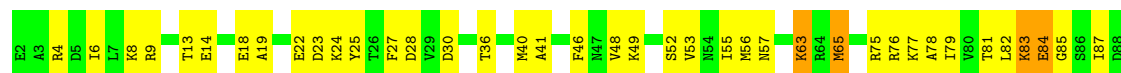
- Molecule 21: Large ribosomal subunit protein uL22

Chain Q: 65% 29%



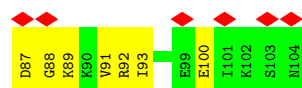
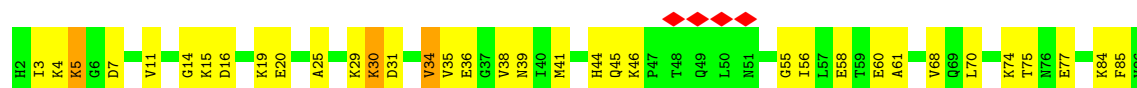
- Molecule 22: Large ribosomal subunit protein uL23

Chain R: 54% 39% 7%

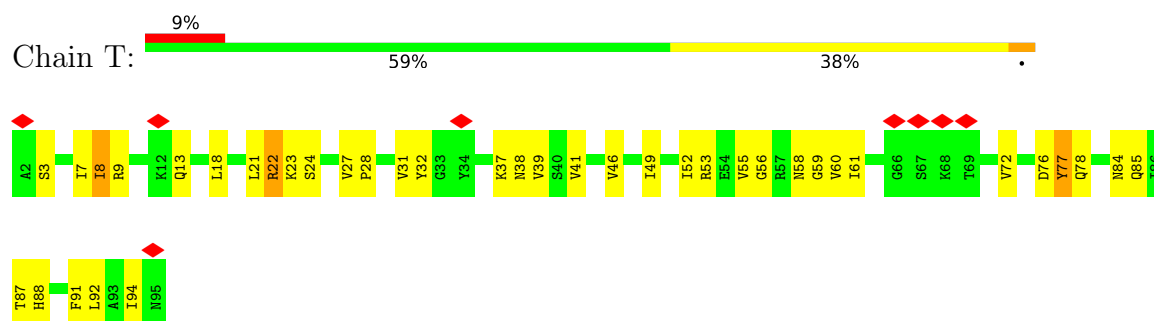


- Molecule 23: Large ribosomal subunit protein uL24

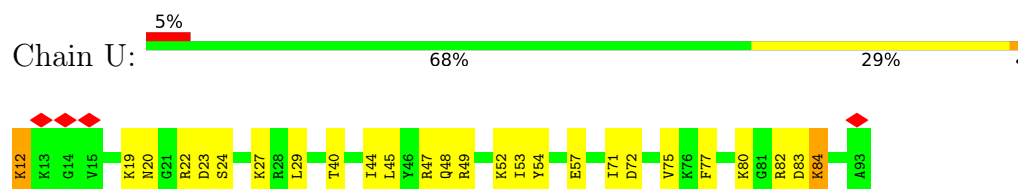
Chain S: 10% 59% 38%



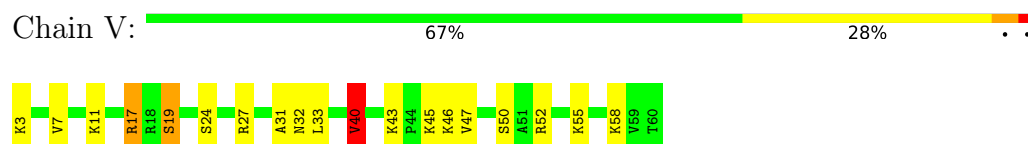
- Molecule 24: Large ribosomal subunit protein bL25



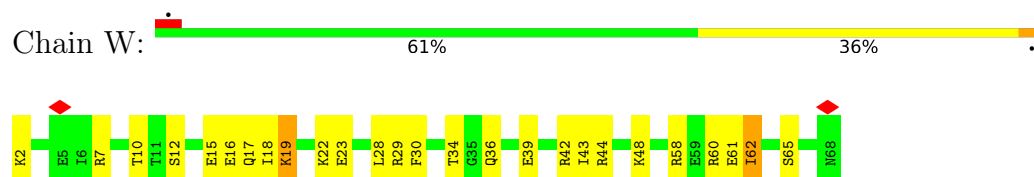
- Molecule 25: Large ribosomal subunit protein bL27



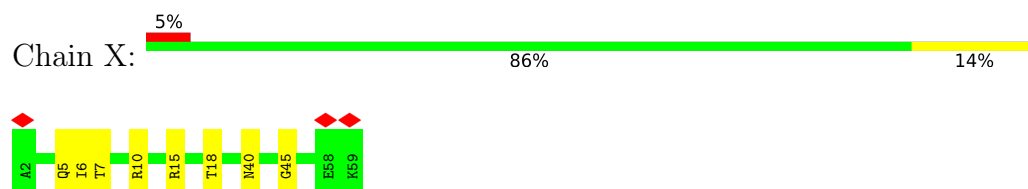
- Molecule 26: Large ribosomal subunit protein bL28



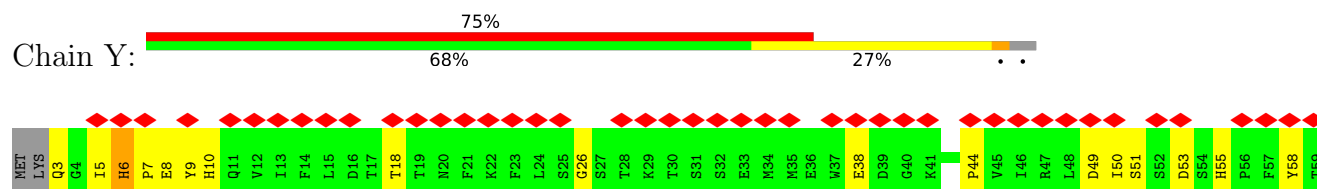
- Molecule 27: Large ribosomal subunit protein uL29



- Molecule 28: Large ribosomal subunit protein uL30



- Molecule 29: Large ribosomal subunit protein bL31B



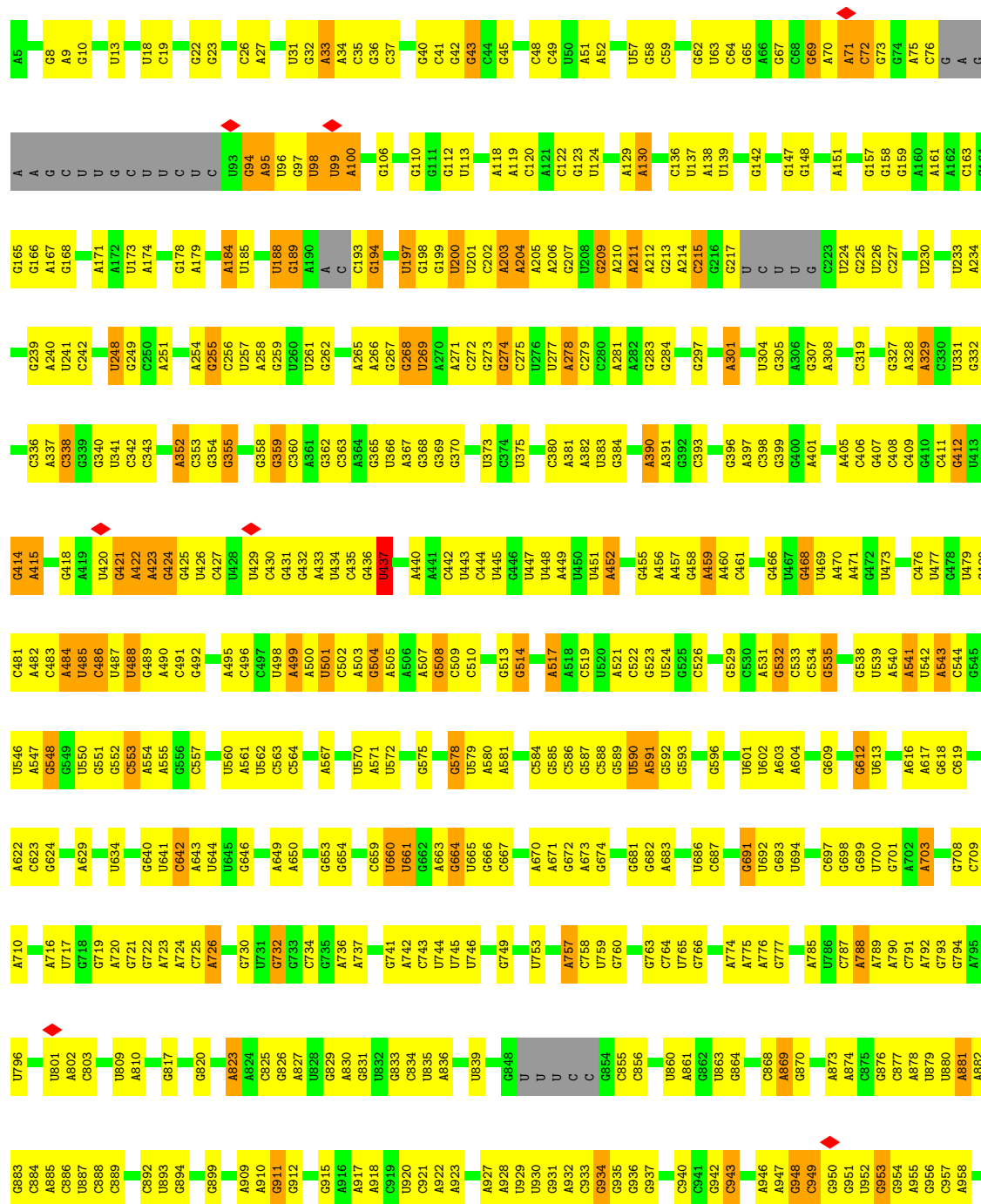
- Molecule 30: Large ribosomal subunit protein bL32

Chain Z:  75% 25%

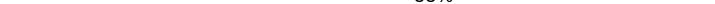


• Molecule 31: 16S ribosomal RNA

Chain a:  39% 45% 11%



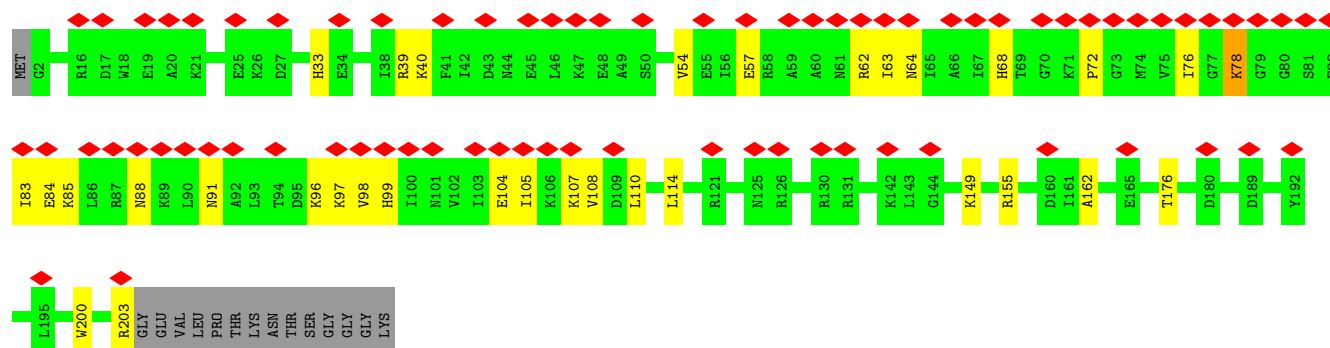
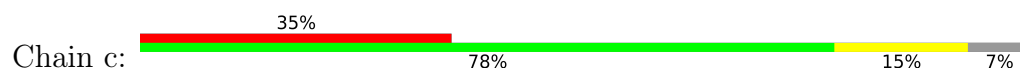


- Chain b:  88% 69% 27% ..

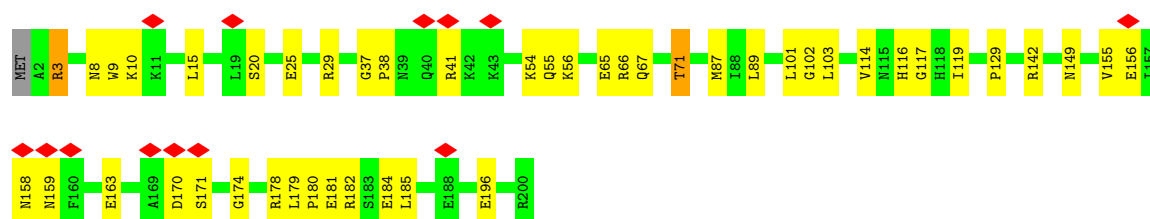
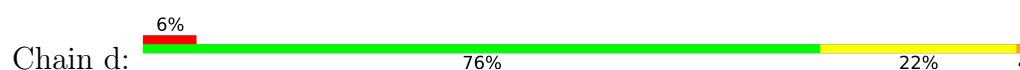




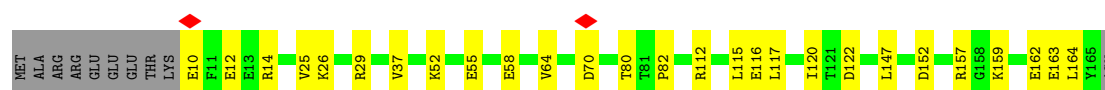
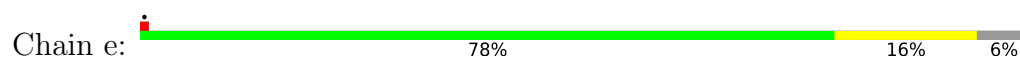
- Molecule 33: Small ribosomal subunit protein uS3



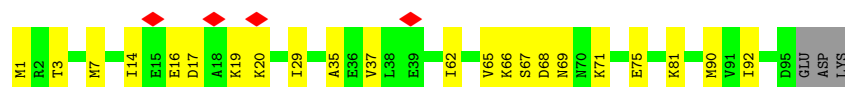
- Molecule 34: Small ribosomal subunit protein uS4



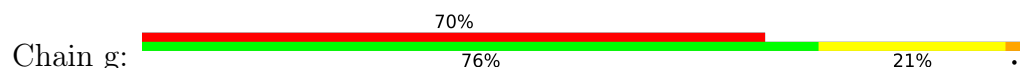
- Molecule 35: Small ribosomal subunit protein uS5

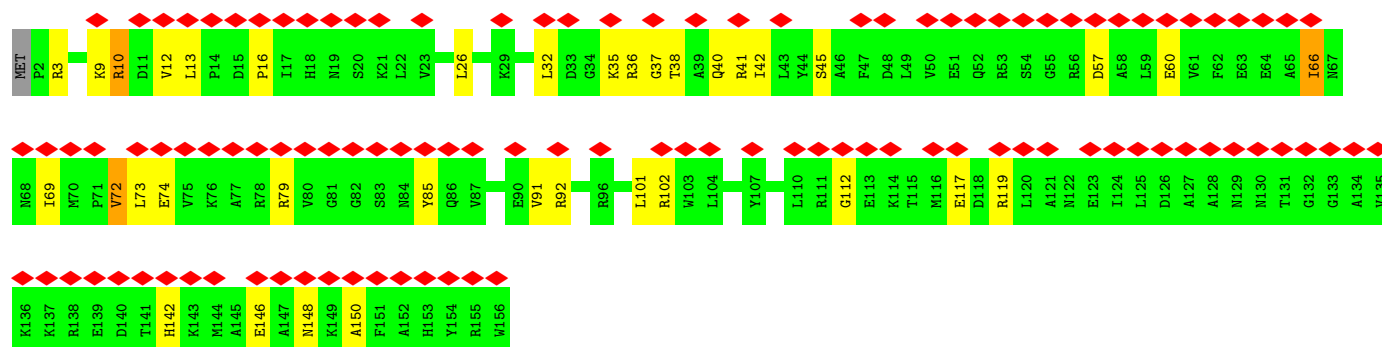


- Molecule 36: Small ribosomal subunit protein bS6

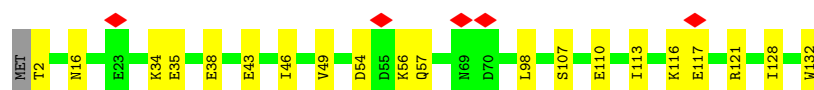
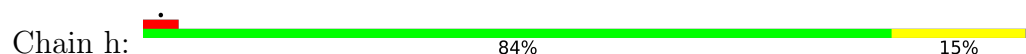


- Molecule 37: Small ribosomal subunit protein uS7

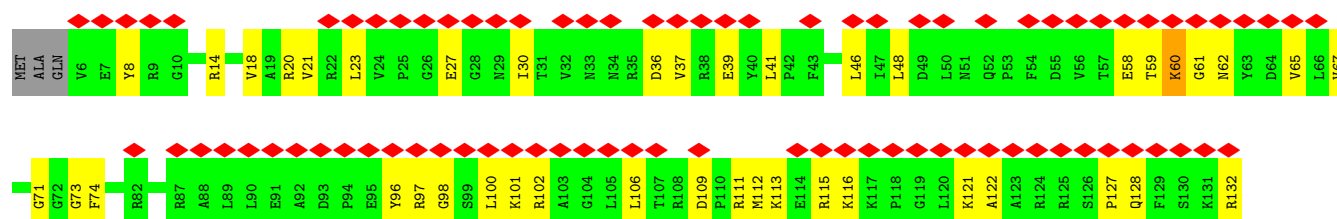




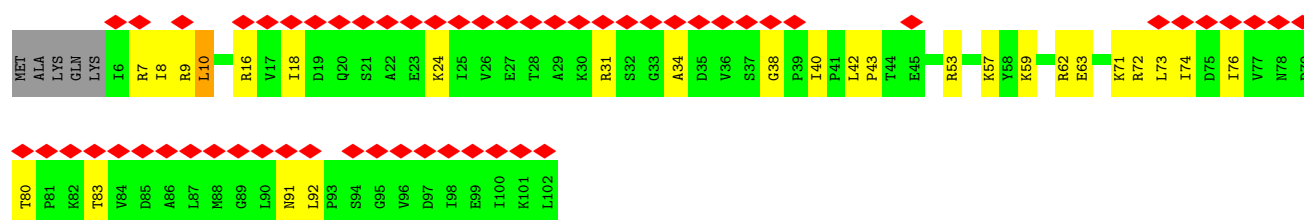
- Molecule 38: Small ribosomal subunit protein uS8



- Molecule 39: Small ribosomal subunit protein uS9

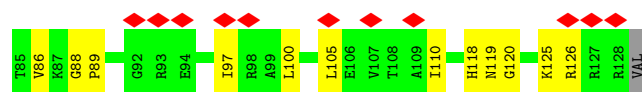


- Molecule 40: Small ribosomal subunit protein uS10

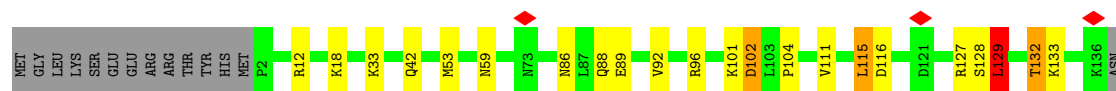
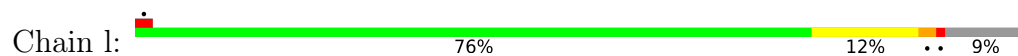


- Molecule 41: Small ribosomal subunit protein uS11

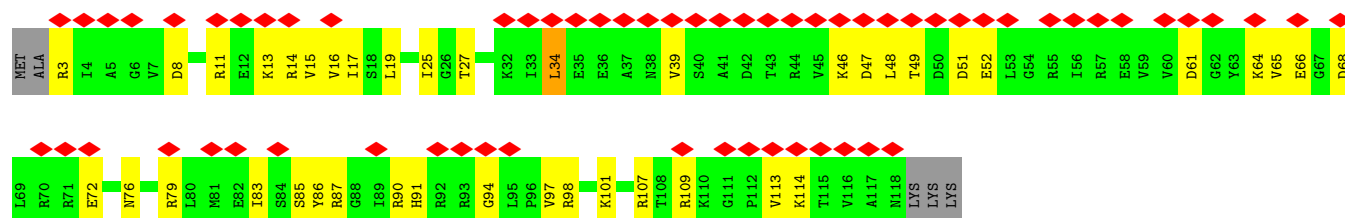




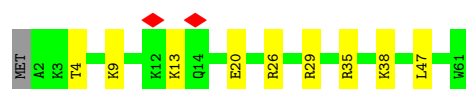
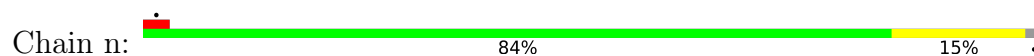
- Molecule 42: Small ribosomal subunit protein uS12



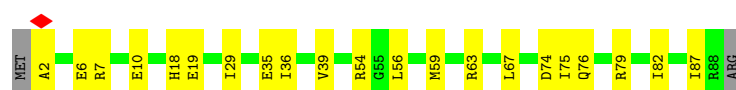
- Molecule 43: Small ribosomal subunit protein uS13



- Molecule 44: Small ribosomal subunit protein uS14B



- Molecule 45: Small ribosomal subunit protein uS15

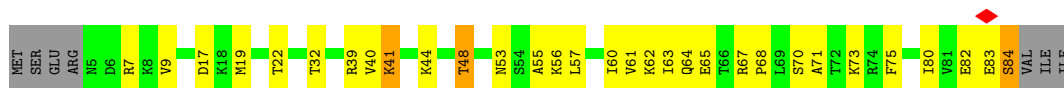


- Molecule 46: Small ribosomal subunit protein bS16



- Molecule 47: Small ribosomal subunit protein uS17

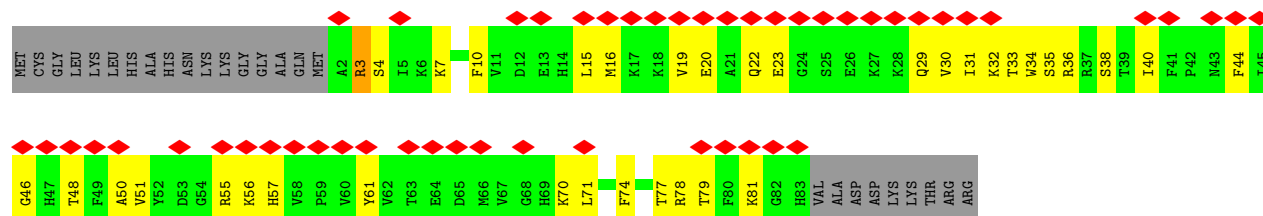
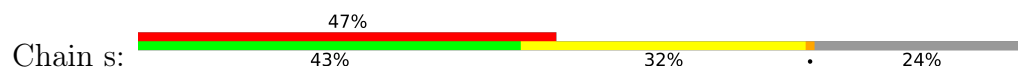




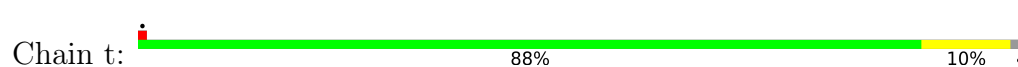
- Molecule 48: Small ribosomal subunit protein bS18



- Molecule 49: Small ribosomal subunit protein uS19



- Molecule 50: Small ribosomal subunit protein bS20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.824, 0.824, 0.824	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1D6G, MA6, 5MU, OMG, 2MA, 2MG, 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 >5	RMSZ	# Z >5
1	1	0.90	0/395	1.23	3/530 (0.6%)
2	2	0.51	0/371	0.75	0/484
3	3	0.89	0/526	1.13	5/690 (0.7%)
4	4	1.12	0/299	1.42	6/393 (1.5%)
5	A	0.44	0/69122	0.68	35/107793 (0.0%)
6	B	0.40	0/2733	0.73	1/4257 (0.0%)
7	C	0.96	0/2125	1.23	10/2853 (0.4%)
8	D	1.08	3/1651 (0.2%)	1.18	10/2215 (0.5%)
9	E	0.98	1/1595 (0.1%)	1.21	11/2154 (0.5%)
10	F	0.67	0/1332	1.29	24/1798 (1.3%)
11	G	0.92	1/1277 (0.1%)	1.31	9/1731 (0.5%)
12	H	0.74	0/1165	0.98	5/1570 (0.3%)
13	I	0.93	0/925	1.10	6/1242 (0.5%)
14	J	0.61	0/1100	0.80	3/1467 (0.2%)
15	K	0.96	1/1095 (0.1%)	1.10	10/1472 (0.7%)
16	L	0.63	0/936	0.64	0/1253
17	M	0.90	0/900	1.23	5/1205 (0.4%)
18	N	0.91	1/901 (0.1%)	0.92	3/1209 (0.2%)
19	O	0.54	0/954	0.61	1/1264 (0.1%)
20	P	0.71	1/800 (0.1%)	0.96	3/1070 (0.3%)
21	Q	0.97	1/861 (0.1%)	1.01	3/1161 (0.3%)
22	R	0.75	0/723	0.96	2/966 (0.2%)
23	S	0.68	0/779	1.02	5/1043 (0.5%)
24	T	0.68	2/719 (0.3%)	0.89	3/969 (0.3%)
25	U	0.72	0/621	0.89	1/825 (0.1%)
26	V	1.05	1/451 (0.2%)	1.25	4/603 (0.7%)
27	W	0.82	0/542	0.86	1/722 (0.1%)
28	X	0.77	0/451	0.73	2/606 (0.3%)
29	Y	0.48	0/361	0.89	2/500 (0.4%)
30	Z	0.84	0/367	0.99	0/490
31	a	0.15	0/35498	0.34	1/55345 (0.0%)
32	b	0.19	0/1829	0.46	0/2455

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.12	0/1618	0.33	0/2173
34	d	0.15	0/1646	0.38	0/2211
35	e	0.25	0/1174	0.47	0/1584
36	f	0.17	0/800	0.45	0/1073
37	g	0.18	0/1262	0.47	1/1698 (0.1%)
38	h	0.22	0/1043	0.41	0/1401
39	i	0.15	0/1023	0.45	0/1374
40	j	0.16	0/785	0.43	0/1060
41	k	0.24	0/859	0.59	0/1161
42	l	0.26	0/1075	0.49	1/1439 (0.1%)
43	m	0.15	0/929	0.40	0/1246
44	n	0.10	0/511	0.33	0/678
45	o	0.12	0/735	0.33	0/982
46	p	0.16	0/699	0.45	0/942
47	q	0.26	0/665	0.48	0/889
48	r	0.25	0/534	0.56	0/715
49	s	0.17	0/683	0.53	1/916 (0.1%)
50	t	0.11	0/611	0.37	0/817
All	All	0.46	12/150056 (0.0%)	0.67	177/224694 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	76	ASP	CA-C	6.56	1.60	1.52
8	D	160	ALA	CA-C	-6.51	1.44	1.52
15	K	97	VAL	C-O	-5.86	1.17	1.24
18	N	59	GLU	CA-C	-5.81	1.45	1.52
8	D	127	PHE	C-O	-5.75	1.17	1.24
11	G	6	LYS	CA-C	-5.23	1.47	1.53
9	E	158	ASN	CA-C	-5.21	1.48	1.53
8	D	13	THR	CA-C	-5.19	1.45	1.52
24	T	77	TYR	N-CA	5.14	1.52	1.45
26	V	19	SER	CA-CB	-5.10	1.45	1.53
21	Q	72	LYS	CA-C	-5.09	1.46	1.52
20	P	3	ALA	CA-C	-5.02	1.46	1.52

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	140	GLN	N-CA-C	-10.45	100.27	113.43
10	F	170	LEU	N-CA-C	-10.32	100.68	113.38
10	F	128	TYR	N-CA-C	10.06	122.01	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	58	ILE	N-CA-C	9.41	122.37	112.96
11	G	69	ARG	N-CA-C	-9.06	102.74	113.88
24	T	77	TYR	N-CA-C	8.98	122.80	109.24
11	G	68	THR	CB-CA-C	8.93	124.84	111.17
10	F	45	GLN	N-CA-C	-8.82	102.68	113.97
10	F	19	LYS	N-CA-C	-8.51	102.09	111.36
5	A	1525	U	C4'-C3'-O3'	8.38	121.97	109.40
8	D	23	ILE	CA-C-N	-8.34	110.71	120.13
8	D	23	ILE	C-N-CA	-8.34	110.71	120.13
14	J	84	LYS	N-CA-C	-8.28	102.20	112.88
7	C	146	LEU	N-CA-C	-8.27	103.79	114.04
12	H	3	GLN	N-CA-C	8.27	122.78	111.71
5	A	1918	G	C2'-C3'-O3'	-8.13	101.50	113.70
5	A	1826	G	C3'-C2'-O2'	-8.03	102.56	114.60
13	I	69	VAL	N-CA-C	7.91	120.25	108.46
20	P	50	ALA	CA-C-N	-7.83	110.05	119.84
20	P	50	ALA	C-N-CA	-7.83	110.05	119.84
10	F	52	ASN	N-CA-C	-7.74	102.84	111.28
17	M	19	ARG	N-CA-C	-7.63	103.97	113.20
10	F	171	ALA	N-CA-C	-7.58	104.12	113.15
10	F	142	ASP	N-CA-C	7.53	120.05	110.33
5	A	576	U	C2'-C3'-O3'	7.40	120.61	109.50
10	F	123	ASP	N-CA-C	-7.40	102.20	113.89
5	A	327	G	C2'-C3'-O3'	7.37	120.55	109.50
22	R	18	GLU	N-CA-C	-7.33	103.31	111.82
18	N	28	LEU	N-CA-C	7.29	119.82	108.96
10	F	137	ILE	N-CA-C	7.26	124.45	109.34
26	V	40	VAL	N-CA-C	7.15	118.11	108.11
3	3	18	ALA	N-CA-C	7.14	119.92	111.71
9	E	9	LEU	N-CA-C	-7.09	103.89	112.54
10	F	25	VAL	N-CA-C	-7.06	105.84	112.83
9	E	161	VAL	N-CA-C	6.96	118.56	110.62
4	4	3	VAL	CB-CA-C	6.96	120.03	110.99
29	Y	6	HIS	N-CA-C	6.88	117.51	109.60
5	A	233	U	C4'-C3'-O3'	-6.78	102.83	113.00
5	A	511	G	C4'-C3'-O3'	-6.74	102.89	113.00
7	C	67	PHE	N-CA-C	-6.68	104.95	113.23
4	4	4	ARG	CA-C-N	-6.66	112.76	119.56
4	4	4	ARG	C-N-CA	-6.66	112.76	119.56
8	D	116	ILE	O-C-N	-6.64	115.69	123.00
5	A	1605	A	C2'-C3'-O3'	-6.56	99.66	109.50
21	Q	48	GLU	N-CA-C	-6.55	104.22	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	56	ARG	N-CA-C	-6.55	103.63	111.69
10	F	61	THR	N-CA-C	-6.52	100.33	110.17
5	A	1760	G	C4'-C3'-O3'	6.50	119.16	109.40
9	E	150	LYS	CA-C-N	-6.45	113.90	123.00
9	E	150	LYS	C-N-CA	-6.45	113.90	123.00
23	S	30	LYS	N-CA-C	-6.41	104.16	114.09
10	F	26	MET	N-CA-C	-6.40	105.51	113.38
13	I	72	ASN	N-CA-C	6.40	120.18	112.38
7	C	120	ALA	N-CA-C	-6.38	106.71	114.75
23	S	39	ASN	CA-C-N	-6.37	111.96	120.50
23	S	39	ASN	C-N-CA	-6.37	111.96	120.50
11	G	102	ASP	N-CA-C	-6.32	99.81	109.41
6	B	22	G	C4'-C3'-O3'	6.29	118.83	109.40
37	g	69	ILE	N-CA-C	-6.28	106.84	112.12
10	F	138	PHE	N-CA-C	6.23	122.76	108.93
11	G	30	LYS	N-CA-C	6.22	120.87	113.16
8	D	188	VAL	N-CA-C	-6.21	99.42	108.11
17	M	70	VAL	N-CA-C	-6.18	103.37	111.09
3	3	41	LYS	CA-C-O	-6.16	114.35	120.70
17	M	13	LYS	N-CA-C	-6.11	103.24	112.04
10	F	169	LEU	N-CA-C	-6.11	105.41	112.92
49	s	3	ARG	CB-CA-C	-6.09	109.54	116.54
10	F	143	TYR	N-CA-C	-6.08	105.71	113.01
13	I	61	VAL	N-CA-C	6.05	116.64	108.17
22	R	53	VAL	O-C-N	-6.04	116.36	123.00
3	3	25	SER	O-C-N	-6.03	114.72	122.20
5	A	1526	G	C4'-C3'-O3'	6.02	122.03	113.00
15	K	3	LEU	N-CA-C	5.99	119.34	109.58
5	A	292	U	C4'-C3'-O3'	-5.96	100.47	109.40
18	N	32	VAL	N-CA-C	5.95	117.33	108.46
8	D	170	PRO	N-CA-C	5.95	120.57	111.11
15	K	72	THR	N-CA-C	5.95	118.22	109.42
17	M	95	ASP	CA-CB-CG	-5.95	106.65	112.60
5	A	1556	G	C2'-C3'-O3'	-5.93	104.80	113.70
5	A	207	A	C2'-C3'-O3'	-5.90	100.65	109.50
13	I	92	GLY	CA-C-N	-5.89	114.54	120.31
13	I	92	GLY	C-N-CA	-5.89	114.54	120.31
21	Q	66	THR	N-CA-C	5.87	120.30	113.20
5	A	1024	A	C2'-C3'-O3'	-5.86	104.92	113.70
8	D	161	SER	N-CA-C	-5.84	102.56	110.68
1	1	14	ASP	N-CA-C	5.78	118.73	110.24
5	A	2533	U	C4'-C3'-O3'	5.77	118.05	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	25	VAL	N-CA-C	5.77	118.46	108.95
15	K	96	VAL	N-CA-C	5.77	117.15	109.37
4	4	35	ARG	N-CA-C	5.73	123.01	110.80
11	G	153	PRO	CA-C-N	-5.73	113.88	119.78
11	G	153	PRO	C-N-CA	-5.73	113.88	119.78
9	E	56	ALA	CA-C-N	5.72	130.29	121.71
9	E	56	ALA	C-N-CA	5.72	130.29	121.71
19	O	114	LYS	N-CA-C	-5.68	105.07	112.23
10	F	50	LEU	N-CA-C	-5.68	105.17	111.36
7	C	72	ASP	N-CA-C	5.68	117.99	108.96
5	A	2147	G	C4'-C3'-O3'	-5.67	104.49	113.00
5	A	2817	A	C4'-C3'-O3'	-5.67	100.90	109.40
14	J	95	LEU	N-CA-C	-5.66	105.48	112.90
8	D	130	ALA	N-CA-C	5.63	119.41	112.54
25	U	40	THR	N-CA-C	-5.63	102.43	110.59
26	V	43	LYS	N-CA-C	5.62	117.58	109.48
7	C	177	ARG	N-CA-C	5.62	118.94	111.75
3	3	58	VAL	N-CA-C	5.61	117.83	111.88
26	V	24	SER	N-CA-C	5.60	118.94	109.76
7	C	193	GLY	CA-C-O	-5.59	118.29	122.37
9	E	158	ASN	N-CA-C	-5.59	98.30	108.65
5	A	232	U	C2'-C3'-O3'	-5.57	105.34	113.70
5	A	1555	G	C4'-C3'-O3'	-5.57	101.05	109.40
3	3	26	ARG	N-CA-C	5.56	119.04	110.42
5	A	1348	U	C2'-C3'-O3'	5.55	117.83	109.50
13	I	60	ALA	N-CA-C	5.55	117.53	108.76
10	F	144	ASP	N-CA-C	5.54	118.08	111.71
5	A	1826	G	C1'-C2'-O2'	-5.53	103.50	111.80
12	H	86	LYS	CA-C-N	-5.52	113.93	122.59
12	H	86	LYS	C-N-CA	-5.52	113.93	122.59
20	P	51	PRO	N-CA-C	-5.52	101.11	112.47
1	1	36	CYS	CA-C-N	-5.50	114.02	120.12
1	1	36	CYS	C-N-CA	-5.50	114.02	120.12
26	V	17	ARG	N-CA-C	-5.48	99.80	108.73
8	D	194	VAL	N-CA-C	5.47	115.86	107.77
9	E	87	GLY	N-CA-C	5.46	118.21	111.93
9	E	103	LYS	N-CA-C	5.45	117.92	111.33
12	H	9	GLU	N-CA-C	5.44	119.66	113.19
11	G	5	GLY	N-CA-C	5.44	119.07	112.49
5	A	229	A	C4'-C3'-O3'	-5.43	104.85	113.00
7	C	142	HIS	N-CA-C	-5.43	101.47	109.18
8	D	60	LYS	N-CA-C	-5.43	100.81	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	92	G	C4'-C3'-O3'	-5.41	104.88	113.00
10	F	20	PHE	N-CA-C	-5.41	100.21	109.24
29	Y	44	PRO	N-CA-C	-5.37	101.29	112.36
15	K	31	GLU	N-CA-C	-5.36	106.67	113.43
5	A	2200	A	C2'-C3'-O3'	-5.36	105.66	113.70
7	C	28	THR	CB-CA-C	5.33	117.20	109.20
15	K	85	ALA	N-CA-C	5.33	118.93	111.74
15	K	48	GLU	N-CA-C	-5.32	105.48	111.28
31	a	437	U	C2'-C3'-O3'	-5.30	101.54	109.50
23	S	75	THR	N-CA-C	5.30	118.76	112.72
42	l	129	LEU	N-CA-C	-5.29	102.92	110.59
14	J	137	ASP	N-CA-C	5.26	118.16	111.69
10	F	116	GLY	N-CA-C	-5.25	103.13	110.96
24	T	87	THR	N-CA-C	5.24	119.90	112.93
10	F	57	LEU	N-CA-C	5.23	116.98	111.28
5	A	644	C	O4'-C1'-C2'	-5.23	102.37	107.60
9	E	20	SER	N-CA-C	5.21	117.41	110.53
24	T	28	PRO	CA-C-O	-5.21	115.50	121.86
5	A	1037	A	C2'-C3'-O3'	-5.21	105.89	113.70
4	4	13	LYS	CA-C-N	-5.20	115.85	122.77
4	4	13	LYS	C-N-CA	-5.20	115.85	122.77
5	A	2598	U	C2'-C3'-O3'	-5.18	105.93	113.70
15	K	10	ARG	N-CA-C	5.17	119.58	113.16
5	A	444	C	O3'-P-O5'	-5.17	96.25	104.00
10	F	47	SER	N-CA-C	-5.17	99.79	110.80
5	A	1027	A	C4'-C3'-O3'	-5.17	105.25	113.00
10	F	156	ILE	N-CA-C	5.16	115.49	107.28
21	Q	10	ILE	N-CA-C	-5.16	102.42	109.55
7	C	38	PRO	CB-CA-C	5.16	116.21	111.87
5	A	1555	G	C1'-C2'-O2'	5.16	119.54	111.80
15	K	49	SER	N-CA-C	5.16	116.98	111.36
5	A	1555	G	C2'-C3'-O3'	-5.16	101.77	109.50
9	E	69	GLY	N-CA-C	5.15	119.82	113.79
15	K	41	TRP	N-CA-C	-5.15	101.32	109.76
5	A	2465	U	C4'-C3'-O3'	-5.13	105.31	113.00
5	A	2127	G	C4'-C3'-O3'	-5.12	105.32	113.00
5	A	510	U	C4'-C3'-O3'	-5.09	105.37	113.00
10	F	83	MET	CA-C-N	-5.08	113.98	120.23
10	F	83	MET	C-N-CA	-5.08	113.98	120.23
28	X	15	ARG	CA-C-N	-5.07	114.50	119.92
28	X	15	ARG	C-N-CA	-5.07	114.50	119.92
5	A	492	G	C2'-C3'-O3'	5.04	117.05	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	79	VAL	N-CA-C	-5.03	106.22	113.07
18	N	3	ASN	N-CA-C	-5.02	102.06	109.94
17	M	6	ASP	N-CA-C	-5.01	103.06	110.48
7	C	50	THR	CB-CA-C	5.01	117.95	110.08
23	S	5	LYS	N-CA-C	5.01	118.65	112.54
27	W	18	ILE	N-CA-C	-5.00	105.62	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	390	0	394	3	0
2	2	367	0	415	5	0
3	3	521	0	586	7	0
4	4	296	0	340	7	0
5	A	61861	0	31103	436	0
6	B	2445	0	1240	20	0
7	C	2090	0	2201	47	0
8	D	1627	0	1667	36	0
9	E	1572	0	1619	33	0
10	F	1317	0	1323	62	0
11	G	1259	0	1221	38	0
12	H	1143	0	1134	34	0
13	I	918	0	981	50	0
14	J	1086	0	1125	21	0
15	K	1071	0	1123	26	0
16	L	932	0	983	33	0
17	M	891	0	925	28	0
18	N	889	0	937	22	0
19	O	942	0	1014	37	0
20	P	790	0	830	23	0
21	Q	853	0	905	19	0
22	R	715	0	748	28	0
23	S	770	0	809	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	T	711	0	740	34	0
25	U	615	0	622	18	0
26	V	445	0	466	10	0
27	W	541	0	563	8	0
28	X	449	0	491	2	0
29	Y	353	0	218	13	0
30	Z	361	0	361	11	0
31	a	31706	0	15964	655	0
32	b	1802	0	1866	49	0
33	c	1596	0	1659	24	0
34	d	1616	0	1646	37	0
35	e	1160	0	1223	13	0
36	f	789	0	788	15	0
37	g	1242	0	1276	24	0
38	h	1031	0	1082	14	0
39	i	1007	0	1031	30	0
40	j	773	0	812	19	0
41	k	844	0	851	32	0
42	l	1058	0	1130	16	0
43	m	922	0	970	28	0
44	n	501	0	527	9	0
45	o	726	0	756	15	0
46	p	688	0	713	16	0
47	q	657	0	694	25	0
48	r	525	0	561	11	0
49	s	665	0	668	34	0
50	t	611	0	655	7	0
51	A	69	0	0	0	0
52	A	12	0	0	0	0
53	A	4	0	0	0	0
All	All	138224	0	91956	1998	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1998) 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)
24:T:32:TYR:CE1	24:T:92:LEU:HD21	1.62	1.35
24:T:32:TYR:CD1	24:T:92:LEU:HD23	1.74	1.23
24:T:32:TYR:CD1	24:T:92:LEU:CD2	2.21	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:32:TYR:CE1	24:T:92:LEU:CD2	2.22	1.21
5:A:104:C:H5''	5:A:104:C:H6	1.30	0.96
24:T:32:TYR:HE1	24:T:92:LEU:HD21	1.06	0.93
24:T:32:TYR:CD1	24:T:92:LEU:HD21	1.99	0.92
24:T:32:TYR:HD1	24:T:92:LEU:CD2	1.82	0.91
10:F:79:LEU:HD11	10:F:85:ILE:HG12	1.52	0.90
41:k:18:ASN:H	41:k:81:THR:HB	1.41	0.86
5:A:45:G:H5''	5:A:46:C:H5'	1.57	0.85
5:A:104:C:H5''	5:A:104:C:C6	2.13	0.84
31:a:214:A:H2	31:a:225:G:H1	1.25	0.84
10:F:31:ILE:HG23	10:F:96:MET:SD	2.21	0.80
5:A:162:A:H8	5:A:2244:G:H21	1.28	0.79
4:4:7:VAL:HG22	4:4:34:GLN:HB3	1.64	0.79
5:A:656:G:H21	5:A:660:A:H2	1.31	0.78
7:C:140:VAL:HG13	7:C:161:SER:HB2	1.65	0.78
31:a:672:G:H22	31:a:749:G:H1	1.31	0.78
31:a:950:G:H21	31:a:1353:G:H1	1.32	0.77
32:b:100:LEU:HA	32:b:107:ILE:HG13	1.67	0.77
31:a:214:A:C2	31:a:225:G:N1	2.51	0.76
31:a:481:C:H2'	31:a:482:A:H8	1.50	0.76
31:a:1136:U:H4'	40:j:7:ARG:HH12	1.49	0.76
7:C:79:ASP:C	7:C:79:ASP:OD1	2.28	0.76
10:F:127:ASN:HB3	10:F:155:VAL:HB	1.67	0.76
21:Q:40:ASN:CG	21:Q:40:ASN:O	2.28	0.76
37:g:112:GLY:HA2	37:g:119:ARG:HD3	1.66	0.76
31:a:721:G:H2'	31:a:722:G:C8	2.21	0.76
31:a:75:A:H8	31:a:94:G:H21	1.32	0.75
31:a:725:C:H4'	41:k:119:ASN:HD22	1.50	0.75
31:a:934:G:H1	31:a:1401:U:H3	1.34	0.75
31:a:1484:G:H2'	31:a:1485:G:C8	2.22	0.75
11:G:69:ARG:C	11:G:69:ARG:HD3	2.11	0.75
5:A:2684:A:H1'	5:A:2692:A:N6	2.02	0.74
15:K:25:ASN:C	15:K:26:TYR:HD1	1.94	0.74
31:a:1134:A:H4'	40:j:38:GLY:HA3	1.70	0.74
33:c:88:ASN:HA	33:c:91:ASN:HB2	1.70	0.73
1:1:5:VAL:HG11	1:1:30:ILE:HD11	1.70	0.73
31:a:215:C:H42	31:a:224:U:H3	1.36	0.73
31:a:831:G:HO2'	38:h:2:THR:N	1.86	0.73
17:M:92:ILE:C	17:M:92:ILE:HD12	2.13	0.73
31:a:1082:C:H2'	31:a:1083:G:H8	1.53	0.73
5:A:2575:G:H1'	13:I:23:LYS:NZ	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1478:A:H61	5:A:1605:A:H61	1.35	0.72
15:K:65:TRP:HH2	15:K:107:ALA:HB3	1.54	0.72
13:I:90:ASP:C	13:I:90:ASP:OD1	2.31	0.72
43:m:34:LEU:HD12	43:m:39:VAL:HB	1.72	0.72
5:A:292:U:H1'	5:A:293:U:H5'	1.69	0.72
10:F:65:PRO:HB2	10:F:87:ALA:HB1	1.72	0.72
14:J:84:LYS:HG3	14:J:84:LYS:O	1.87	0.72
5:A:506:A:H2	5:A:515:G:H21	1.35	0.72
5:A:2419:A:H2	5:A:2451:C:H42	1.35	0.72
9:E:154:VAL:HG22	9:E:193:VAL:CG2	2.19	0.71
11:G:119:GLU:OE1	11:G:119:GLU:N	2.23	0.71
32:b:69:PHE:HB3	32:b:80:VAL:HG13	1.72	0.71
16:L:26:ILE:HD12	16:L:71:ILE:HD11	1.72	0.71
5:A:721:A:H8	5:A:2096:G:H21	1.38	0.71
23:S:4:LYS:HE2	23:S:92:ARG:NH1	2.05	0.71
15:K:112:GLU:OE1	15:K:112:GLU:N	2.23	0.71
32:b:114:ILE:HD11	32:b:144:LEU:HB3	1.72	0.71
17:M:63:ILE:O	17:M:72:LEU:HD21	1.91	0.71
31:a:1277:C:N3	31:a:1337:A:O2'	2.23	0.71
5:A:1578:A:H1'	5:A:1588:U:H3	1.56	0.70
6:B:2:C:H41	6:B:113:G:H1	1.37	0.70
16:L:26:ILE:CD1	16:L:71:ILE:HD11	2.21	0.70
14:J:80:ASP:C	14:J:80:ASP:OD1	2.33	0.70
7:C:16:MET:HE1	7:C:207:LYS:HG3	1.72	0.70
31:a:424:G:H2'	31:a:425:G:H8	1.55	0.70
31:a:522:C:H2'	31:a:523:G:H8	1.57	0.70
37:g:72:VAL:H	37:g:142:HIS:HE1	1.40	0.70
13:I:32:THR:CG2	13:I:33:ALA:N	2.55	0.70
23:S:3:ILE:HD12	23:S:4:LYS:N	2.06	0.69
7:C:34:LEU:HD21	7:C:63:ARG:HG3	1.73	0.69
46:p:5:ILE:HG12	46:p:22:VAL:HG22	1.74	0.69
31:a:722:G:H2'	31:a:723:A:C8	2.27	0.69
5:A:1483:A:H62	5:A:1599:G:H8	1.40	0.69
8:D:27:VAL:HG11	18:N:7:ILE:HG13	1.74	0.69
15:K:114:ALA:O	15:K:118:LEU:HG	1.93	0.69
31:a:1248:A:N1	31:a:1309:A:N6	2.40	0.69
17:M:100:LEU:H	17:M:100:LEU:HD12	1.56	0.69
31:a:1544:C:H2'	31:a:1545:A:C8	2.27	0.69
5:A:1881:A:H62	5:A:1915:G:H8	1.40	0.69
7:C:74:ILE:HD12	7:C:74:ILE:H	1.58	0.69
31:a:1407:C:OP2	35:e:29:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2306:G:N7	25:U:22:ARG:NH2	2.37	0.69
39:i:36:ASP:HB3	39:i:39:GLU:HG2	1.75	0.69
5:A:1290:G:N2	19:O:33:LYS:HG2	2.08	0.69
5:A:2859:G:H4'	16:L:45:GLU:OE1	1.92	0.69
31:a:1359:A:H1'	31:a:1384:A:H61	1.58	0.69
39:i:14:ARG:NH1	39:i:109:ASP:OD2	2.26	0.69
30:Z:29:GLU:HG2	30:Z:36:TYR:CE1	2.28	0.69
14:J:83:ASN:ND2	14:J:117:LEU:HA	2.07	0.69
8:D:37:GLN:OE1	8:D:76:HIS:HE1	1.77	0.68
12:H:9:GLU:HG3	12:H:9:GLU:O	1.93	0.68
31:a:22:G:H2'	31:a:23:G:C8	2.29	0.68
31:a:921:C:H2'	31:a:922:A:C8	2.29	0.68
31:a:1002:G:H2'	31:a:1004:C:H41	1.57	0.68
31:a:517:A:H8	31:a:551:G:O2'	1.77	0.68
9:E:193:VAL:O	9:E:193:VAL:HG23	1.93	0.68
7:C:164:VAL:HG13	7:C:172:VAL:HG11	1.74	0.68
15:K:70:PRO:HA	15:K:95:ALA:HB2	1.74	0.68
31:a:459:A:N6	31:a:488:U:O2'	2.27	0.68
31:a:1249:A:H62	31:a:1309:A:H61	1.41	0.68
32:b:61:SER:HB3	32:b:221:ILE:HG13	1.75	0.68
36:f:37:VAL:HG22	36:f:65:VAL:HG12	1.75	0.68
12:H:68:ASN:O	12:H:68:ASN:OD1	2.12	0.68
13:I:32:THR:HG22	13:I:33:ALA:N	2.09	0.68
31:a:791:C:H2'	31:a:792:A:H8	1.59	0.68
5:A:2314:A:H62	5:A:2371:U:H3	1.41	0.67
7:C:145:GLU:HB2	7:C:188:CYS:HB3	1.76	0.67
24:T:32:TYR:CE1	24:T:92:LEU:HD23	2.09	0.67
19:O:105:ALA:HB1	20:P:40:PHE:HZ	1.59	0.67
16:L:92:ARG:HG2	16:L:93:TYR:CE1	2.29	0.67
31:a:224:U:H2'	31:a:225:G:H8	1.59	0.67
31:a:1366:G:H2'	31:a:1367:A:C8	2.30	0.67
7:C:60:ARG:HD3	7:C:85:PRO:HB2	1.76	0.67
9:E:125:VAL:HG13	9:E:194:ILE:HG23	1.77	0.67
31:a:681:G:H2'	31:a:682:G:C8	2.29	0.67
31:a:983:A:OP1	44:n:29:ARG:NH2	2.27	0.67
5:A:1084:U:H3	5:A:1159:A:H61	1.43	0.67
5:A:2037:G:H5''	21:Q:42:ALA:HB2	1.77	0.67
23:S:100:GLU:C	23:S:100:GLU:CD	2.63	0.67
31:a:73:G:H22	31:a:96:U:H3	1.43	0.67
5:A:578:G:N2	19:O:48:ARG:HH22	1.92	0.67
5:A:2341:A:H5'	10:F:35:VAL:HG11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:161:ASN:HB2	10:F:165:GLU:OE1	1.95	0.67
13:I:112:MET:HA	13:I:112:MET:HE3	1.76	0.67
31:a:411:C:H5''	34:d:129:PRO:HD2	1.77	0.67
49:s:79:THR:OG1	49:s:81:LYS:NZ	2.28	0.66
31:a:532:G:H2'	31:a:533:C:C6	2.30	0.66
19:O:104:LYS:H	19:O:104:LYS:CE	2.08	0.66
7:C:74:ILE:HD12	7:C:74:ILE:N	2.10	0.66
31:a:531:A:N6	42:l:102:ASP:OD2	2.28	0.66
31:a:955:A:H2'	31:a:956:G:C8	2.31	0.66
5:A:1556:G:H2'	5:A:1557:C:H5'	1.77	0.66
10:F:69:LYS:HG3	10:F:84:PRO:HA	1.78	0.66
46:p:54:GLU:HG2	46:p:80:ILE:HD11	1.78	0.66
5:A:1304:G:H5''	21:Q:15:ARG:HH22	1.61	0.66
13:I:47:THR:HG23	13:I:48:PRO:HD2	1.78	0.66
48:r:39:SER:OG	48:r:40:GLU:N	2.28	0.66
49:s:50:ALA:HB1	49:s:57:HIS:HB3	1.76	0.66
17:M:33:VAL:HG11	17:M:105:VAL:HG22	1.77	0.65
21:Q:109:ASP:HB3	21:Q:111:LYS:HG2	1.78	0.65
31:a:1026:U:H2'	31:a:1027:A:H8	1.61	0.65
5:A:2575:G:H1'	13:I:23:LYS:HZ2	1.61	0.65
31:a:214:A:H2	31:a:225:G:N1	1.92	0.65
31:a:444:C:H5''	34:d:149:ASN:HD21	1.60	0.65
32:b:129:LEU:HD21	32:b:137:LEU:HD12	1.79	0.65
48:r:17:TYR:O	48:r:17:TYR:HD1	1.80	0.65
31:a:777:G:H4'	31:a:1524:A:H4'	1.77	0.65
31:a:1067:U:H2'	31:a:1068:G:H8	1.62	0.65
10:F:127:ASN:HA	10:F:156:ILE:HG13	1.79	0.65
14:J:83:ASN:HD21	14:J:117:LEU:HA	1.58	0.65
5:A:1290:G:N2	19:O:33:LYS:CG	2.60	0.65
5:A:1478:A:H61	5:A:1605:A:N6	1.94	0.65
10:F:63:GLN:HA	29:Y:7:PRO:HD2	1.78	0.65
17:M:46:ASP:OD1	17:M:48:ASN:N	2.25	0.65
23:S:87:ASP:HB3	23:S:89:LYS:HZ2	1.61	0.65
31:a:106:G:H1	50:t:6:SER:HG	1.43	0.65
31:a:948:G:OP1	37:g:102:ARG:NH1	2.30	0.65
31:a:1003:A:C8	31:a:1226:A:H4'	2.32	0.65
5:A:78:U:H2'	5:A:79:U:C6	2.32	0.64
11:G:8:ILE:C	11:G:69:ARG:HH21	2.05	0.64
21:Q:14:PRO:HA	21:Q:17:VAL:HG22	1.79	0.64
31:a:1422:C:H2'	31:a:1423:A:C8	2.31	0.64
11:G:5:GLY:HA2	11:G:69:ARG:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:130:A:H5'	47:q:67:ARG:HD3	1.80	0.64
31:a:470:A:H2'	31:a:471:A:C8	2.32	0.64
9:E:159:GLU:OE2	9:E:177:THR:HG21	1.98	0.64
25:U:49:ARG:HG2	25:U:49:ARG:HH11	1.62	0.64
31:a:1092:G:N7	35:e:52:LYS:NZ	2.45	0.64
31:a:1533:U:H2'	31:a:1534:G:H8	1.62	0.64
49:s:46:GLY:HA2	49:s:61:TYR:HE1	1.62	0.64
15:K:118:LEU:HD23	15:K:118:LEU:N	2.11	0.64
31:a:1437:C:H2'	31:a:1438:A:H8	1.62	0.64
40:j:40:ILE:HB	40:j:73:LEU:HB2	1.80	0.64
5:A:1575:A:O2'	5:A:1576:A:O5'	2.16	0.64
12:H:70:GLU:OE1	12:H:70:GLU:HA	1.97	0.64
31:a:18:U:H2'	31:a:19:C:C6	2.33	0.64
31:a:507:A:H1'	31:a:508:G:C8	2.32	0.64
31:a:1260:A:H2'	31:a:1261:A:C8	2.32	0.64
7:C:34:LEU:CD2	7:C:63:ARG:HG3	2.27	0.64
12:H:22:GLU:HA	12:H:62:LYS:HB2	1.79	0.64
5:A:162:A:H8	5:A:2244:G:N2	1.95	0.64
10:F:91:LEU:HD12	10:F:95:ARG:HB2	1.80	0.64
23:S:55:GLY:C	23:S:56:ILE:HD12	2.23	0.64
31:a:98:U:O2	31:a:99:U:N3	2.31	0.64
31:a:1387:A:OP1	37:g:92:ARG:NH1	2.25	0.64
31:a:1552:U:O5'	32:b:22:ARG:NH2	2.31	0.64
17:M:55:GLN:OE1	17:M:56:ALA:CA	2.45	0.64
20:P:62:VAL:HG22	20:P:95:LEU:CD2	2.28	0.64
23:S:3:ILE:HD12	23:S:3:ILE:C	2.23	0.64
31:a:485:U:H2'	31:a:486:C:C6	2.33	0.64
31:a:682:G:H2'	31:a:683:A:H8	1.63	0.64
43:m:3:ARG:HA	43:m:8:ASP:HA	1.80	0.64
31:a:546:U:H2'	31:a:547:A:H8	1.63	0.63
5:A:2332:U:H1'	10:F:151:GLY:HA3	1.79	0.63
32:b:6:MET:SD	32:b:6:MET:N	2.69	0.63
22:R:8:LYS:HE3	22:R:30:ASP:HA	1.80	0.63
31:a:382:A:H5'	31:a:459:A:H2	1.63	0.63
31:a:691:G:N2	41:k:39:GLY:O	2.31	0.63
7:C:253:PRO:HB2	7:C:257:LYS:HG3	1.80	0.63
10:F:51:ASP:HA	10:F:54:VAL:HB	1.79	0.63
31:a:214:A:N1	31:a:225:G:O6	2.32	0.63
31:a:699:G:O6	41:k:57:LYS:NZ	2.28	0.63
31:a:147:G:H2'	31:a:148:G:C8	2.34	0.63
31:a:943:C:H42	31:a:948:G:H1	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1383:G:OP2	31:a:1383:G:N2	2.26	0.63
36:f:3:THR:OG1	36:f:66:LYS:NZ	2.32	0.63
50:t:48:GLU:OE1	50:t:48:GLU:N	2.29	0.63
5:A:2859:G:C4'	16:L:45:GLU:OE1	2.46	0.63
31:a:436:G:H5''	34:d:10:LYS:HG3	1.79	0.63
31:a:670:A:H2'	31:a:671:A:C8	2.34	0.63
11:G:69:ARG:HD3	11:G:69:ARG:O	1.98	0.63
15:K:58:MET:HE2	15:K:109:VAL:HG11	1.80	0.63
31:a:1170:G:N2	31:a:1192:G:H22	1.96	0.63
33:c:63:ILE:HB	33:c:97:LYS:HB3	1.80	0.63
33:c:107:LYS:HD2	33:c:110:LEU:HD12	1.79	0.63
9:E:164:GLU:HG3	9:E:175:VAL:HG11	1.80	0.63
31:a:513:G:H2'	31:a:514:G:C8	2.34	0.63
31:a:1276:G:N2	31:a:1279:A:OP2	2.31	0.63
39:i:121:LYS:HG3	39:i:127:PRO:HB3	1.80	0.63
19:O:104:LYS:H	19:O:104:LYS:CD	2.10	0.62
22:R:22:GLU:OE1	22:R:24:LYS:HG3	1.99	0.62
31:a:455:G:H21	31:a:495:A:H2	1.44	0.62
31:a:736:A:H2'	31:a:737:A:C8	2.34	0.62
31:a:1129:A:H1'	31:a:1189:A:C4	2.34	0.62
9:E:193:VAL:CG2	9:E:193:VAL:O	2.47	0.62
17:M:46:ASP:OD1	17:M:46:ASP:C	2.42	0.62
22:R:19:ALA:HB1	22:R:24:LYS:HB2	1.81	0.62
32:b:117:ILE:HA	32:b:120:MET:SD	2.39	0.62
5:A:2432:G:H2'	5:A:2438:A:H61	1.64	0.62
5:A:1216:U:H2'	5:A:1218:G:H8	1.62	0.62
23:S:100:GLU:CD	23:S:100:GLU:O	2.42	0.62
31:a:9:A:N6	34:d:196:GLU:O	2.31	0.62
31:a:560:U:H2'	31:a:561:A:H8	1.64	0.62
31:a:1392:C:H4'	37:g:79:ARG:HH21	1.63	0.62
5:A:2575:G:N3	13:I:23:LYS:NZ	2.47	0.62
11:G:169:VAL:O	11:G:171:ARG:HG2	2.00	0.62
15:K:25:ASN:C	15:K:26:TYR:CD1	2.75	0.62
31:a:517:A:H8	31:a:551:G:HO2'	1.47	0.62
31:a:534:C:OP2	42:l:101:LYS:NZ	2.27	0.62
31:a:1088:G:N2	31:a:1091:A:OP2	2.27	0.62
48:r:42:GLY:O	48:r:68:ARG:NH2	2.31	0.62
19:O:104:LYS:H	19:O:104:LYS:HE2	1.64	0.62
32:b:83:GLU:HG3	32:b:214:THR:HG23	1.80	0.62
41:k:97:ILE:HA	41:k:100:LEU:HD12	1.80	0.62
7:C:9:ILE:HD12	7:C:10:THR:OG1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:20:SER:N	9:E:203:GLU:OE2	2.29	0.62
30:Z:24:VAL:HG13	30:Z:25:PRO:HD2	1.81	0.62
31:a:423:A:HO2'	31:a:424:G:H8	1.48	0.62
5:A:2328:A:H61	5:A:2342:U:H3	1.48	0.61
5:A:1986:G:N3	31:a:1494:A:H2	1.97	0.61
10:F:31:ILE:HD12	10:F:158:THR:CG2	2.29	0.61
13:I:64:ARG:HG3	13:I:83:ALA:HB3	1.81	0.61
16:L:92:ARG:HG2	16:L:93:TYR:CD1	2.35	0.61
13:I:91:LYS:HE3	13:I:111:PHE:CZ	2.35	0.61
15:K:27:VAL:HG13	15:K:105:GLU:HG2	1.82	0.61
49:s:3:ARG:HH11	49:s:10:PHE:HB2	1.66	0.61
9:E:154:VAL:HG22	9:E:193:VAL:HG21	1.82	0.61
33:c:149:LYS:HB3	33:c:200:TRP:HB2	1.82	0.61
5:A:351:G:O2'	23:S:15:LYS:NZ	2.33	0.61
5:A:2499:G:H21	5:A:2505:A:H62	1.48	0.61
11:G:27:LYS:HG2	11:G:32:GLU:CB	2.30	0.61
11:G:41:MET:SD	11:G:65:HIS:HA	2.41	0.61
31:a:469:U:H2'	31:a:470:A:C8	2.35	0.61
36:f:69:ASN:OD1	36:f:71:LYS:NZ	2.22	0.61
5:A:1917:A:C5	5:A:1918:G:H1'	2.35	0.61
5:A:262:G:H21	5:A:666:A:H8	1.49	0.61
31:a:1238:C:H2'	31:a:1239:A:C8	2.36	0.61
31:a:301:A:H5'	31:a:617:A:H61	1.66	0.61
31:a:1170:G:H22	31:a:1192:G:H22	1.49	0.61
31:a:1251:G:H2'	31:a:1252:G:H8	1.66	0.61
31:a:1535:C:H2'	31:a:1536:G:H8	1.65	0.61
31:a:722:G:H2'	31:a:723:A:H8	1.64	0.61
22:R:48:VAL:HG12	22:R:85:GLY:HA3	1.82	0.60
31:a:398:C:H2'	31:a:399:G:H8	1.66	0.60
31:a:918:A:OP1	42:l:18:LYS:NZ	2.31	0.60
41:k:20:VAL:HG12	41:k:83:GLU:HB2	1.83	0.60
10:F:143:TYR:CD1	43:m:3:ARG:NH2	2.68	0.60
31:a:744:U:H2'	31:a:745:U:H6	1.66	0.60
31:a:495:A:H5''	31:a:496:C:H5	1.66	0.60
32:b:15:HIS:HB3	32:b:43:LEU:HD21	1.82	0.60
10:F:108:LEU:HB2	29:Y:51:SER:HA	1.84	0.60
31:a:1527:G:N1	31:a:1530:A:OP2	2.32	0.60
33:c:78:LYS:H	33:c:78:LYS:HD2	1.65	0.60
34:d:9:TRP:CD1	34:d:25:GLU:HG2	2.36	0.60
5:A:221:G:H22	5:A:238:U:H4'	1.66	0.60
10:F:38:MET:HE2	10:F:150:ARG:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:205:A:H2'	31:a:206:A:C8	2.37	0.60
34:d:163:GLU:OE1	34:d:178:ARG:NH1	2.34	0.60
8:D:38:LYS:HE2	8:D:101:VAL:HG23	1.82	0.60
10:F:106:VAL:HG21	10:F:139:PRO:HG3	1.83	0.60
14:J:84:LYS:O	14:J:84:LYS:CG	2.50	0.60
20:P:62:VAL:HG22	20:P:95:LEU:HD21	1.83	0.60
31:a:1336:U:H2'	31:a:1337:A:H8	1.65	0.60
5:A:2863:G:HO2'	18:N:2:THR:N	1.99	0.60
13:I:90:ASP:OD1	13:I:90:ASP:O	2.19	0.60
31:a:483:C:H2'	31:a:484:A:C8	2.37	0.60
31:a:590:U:H2'	31:a:591:A:H8	1.67	0.60
2:2:22:ARG:HD2	2:2:31:VAL:HG21	1.84	0.60
9:E:154:VAL:HA	9:E:193:VAL:HG22	1.84	0.59
31:a:498:U:H2'	31:a:499:A:H8	1.67	0.59
31:a:1261:A:N3	31:a:1379:C:O2'	2.34	0.59
34:d:158:ASN:OD1	34:d:159:ASN:N	2.34	0.59
5:A:1378:U:C6	22:R:79:ILE:HD13	2.37	0.59
31:a:469:U:H2'	31:a:470:A:H8	1.67	0.59
34:d:102:GLY:HA3	34:d:158:ASN:HD22	1.67	0.59
47:q:60:ILE:HD13	47:q:82:GLU:HG3	1.84	0.59
5:A:1218:G:H2'	5:A:1219:G:C8	2.37	0.59
7:C:164:VAL:HG13	7:C:172:VAL:CG1	2.32	0.59
22:R:6:ILE:HD11	22:R:41:ALA:HB2	1.83	0.59
31:a:726:A:H5'	41:k:119:ASN:HD21	1.66	0.59
31:a:1002:G:O2'	31:a:1003:A:N7	2.35	0.59
31:a:1187:G:H3'	31:a:1188:G:H8	1.67	0.59
31:a:1238:C:H2'	31:a:1239:A:H8	1.68	0.59
31:a:535:G:O2'	31:a:543:A:N1	2.33	0.59
31:a:765:U:OP1	31:a:830:A:O2'	2.20	0.59
5:A:1254:C:OP1	19:O:11:ARG:HD2	2.03	0.59
31:a:384:G:H5''	46:p:6:ARG:HB2	1.84	0.59
34:d:117:GLY:O	34:d:142:ARG:NH1	2.36	0.59
47:q:56:LYS:HZ2	47:q:84:SER:HB2	1.67	0.59
47:q:60:ILE:HB	47:q:82:GLU:HG2	1.83	0.59
31:a:563:C:H2'	31:a:564:C:C6	2.38	0.59
39:i:100:LEU:HD13	39:i:106:LEU:HD21	1.84	0.59
9:E:154:VAL:HG22	9:E:193:VAL:HG22	1.84	0.59
10:F:95:ARG:HH22	29:Y:9:TYR:HB3	1.68	0.59
15:K:39:THR:HB	15:K:98:LYS:HA	1.85	0.59
17:M:72:LEU:O	17:M:76:VAL:HG23	2.03	0.59
31:a:981:C:OP2	40:j:59:LYS:NZ	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:17:THR:OG1	3:3:21:GLN:HB2	2.01	0.58
5:A:1934:G:H1	5:A:1950:U:H3	1.51	0.58
10:F:31:ILE:HD12	10:F:158:THR:HG23	1.85	0.58
19:O:36:LYS:O	19:O:40:MET:HG3	2.02	0.58
31:a:513:G:H2'	31:a:514:G:H8	1.67	0.58
31:a:1201:A:H2'	31:a:1202:C:C6	2.38	0.58
13:I:73:ASP:OD1	13:I:75:SER:HB3	2.03	0.58
31:a:1297:A:H2'	31:a:1298:A:C8	2.39	0.58
5:A:1039:C:C5	12:H:1:MET:HA	2.39	0.58
8:D:191:GLU:OE1	8:D:191:GLU:N	2.30	0.58
31:a:723:A:H2'	31:a:724:A:C8	2.37	0.58
5:A:437:A:H4'	5:A:459:C:OP1	2.03	0.58
8:D:56:LYS:HE3	8:D:66:ASN:O	2.04	0.58
10:F:75:ALA:HA	10:F:78:ARG:HH12	1.67	0.58
31:a:1329:A:OP1	49:s:70:LYS:NZ	2.36	0.58
31:a:1338:C:C2	31:a:1339:A:C8	2.91	0.58
2:2:22:ARG:HD2	2:2:31:VAL:CG2	2.34	0.58
10:F:58:GLU:HB2	29:Y:7:PRO:HG2	1.86	0.58
30:Z:8:THR:HG23	30:Z:12:ARG:HB3	1.86	0.58
31:a:744:U:H2'	31:a:745:U:C6	2.39	0.58
31:a:1160:U:H4'	40:j:43:PRO:HG3	1.85	0.58
31:a:1365:A:H2'	31:a:1366:G:H8	1.68	0.58
48:r:74:PRO:HG3	48:r:77:LYS:HD3	1.84	0.58
5:A:227:G:H1	5:A:233:U:H3	1.51	0.58
25:U:27:LYS:O	25:U:29:LEU:HG	2.04	0.58
31:a:1084:U:O2	32:b:103:ASN:ND2	2.37	0.58
5:A:1401:G:OP1	26:V:3:LYS:HE3	2.04	0.58
7:C:13:ARG:O	7:C:13:ARG:HG3	2.04	0.58
7:C:160:ALA:H	7:C:195:VAL:HG22	1.68	0.58
23:S:56:ILE:HD12	23:S:56:ILE:N	2.18	0.58
31:a:547:A:H2'	31:a:548:G:C8	2.38	0.58
5:A:1051:C:OP1	12:H:38:ARG:NH1	2.37	0.57
7:C:140:VAL:CG1	7:C:161:SER:HB2	2.33	0.57
10:F:32:ASP:C	10:F:32:ASP:OD1	2.46	0.57
23:S:87:ASP:HB3	23:S:89:LYS:NZ	2.18	0.57
31:a:721:G:H2'	31:a:722:G:H8	1.66	0.57
5:A:630:G:N7	14:J:33:ARG:NH1	2.51	0.57
5:A:1115:G:N1	5:A:1136:C:OP2	2.36	0.57
20:P:23:GLU:OE1	20:P:23:GLU:HA	2.03	0.57
25:U:49:ARG:HG2	25:U:49:ARG:NH1	2.18	0.57
31:a:765:U:H2'	31:a:766:G:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:949:C:H3'	31:a:950:G:H8	1.68	0.57
31:a:1133:U:O4	31:a:1134:A:N6	2.37	0.57
31:a:1260:A:H2'	31:a:1261:A:H8	1.69	0.57
31:a:1434:U:H2'	31:a:1435:A:C8	2.39	0.57
33:c:96:LYS:HG2	33:c:98:VAL:HG13	1.86	0.57
5:A:925:G:H3'	5:A:926:G:C8	2.39	0.57
31:a:328:A:HO2'	31:a:1445:G:HO2'	1.53	0.57
31:a:682:G:H2'	31:a:683:A:C8	2.39	0.57
40:j:24:LYS:HD2	40:j:91:ASN:HB2	1.85	0.57
12:H:117:GLU:O	12:H:121:LYS:HG3	2.03	0.57
15:K:65:TRP:HZ3	15:K:106:VAL:C	2.12	0.57
31:a:1366:G:H2'	31:a:1367:A:H8	1.68	0.57
34:d:178:ARG:NH2	34:d:184:GLU:OE2	2.37	0.57
20:P:72:THR:HG23	20:P:72:THR:O	2.04	0.57
24:T:31:VAL:HG12	24:T:91:PHE:HB2	1.86	0.57
29:Y:38:GLU:OE1	29:Y:38:GLU:N	2.37	0.57
31:a:22:G:H2'	31:a:23:G:H8	1.70	0.57
3:3:4:MET:HE1	3:3:60:GLN:NE2	2.20	0.57
31:a:1330:C:H2'	31:a:1331:U:C6	2.40	0.57
31:a:570:U:H1'	42:l:12:ARG:HD2	1.86	0.57
5:A:650:U:H3	5:A:666:A:H2	1.51	0.57
21:Q:34:ALA:HB3	30:Z:27:MET:HE1	1.84	0.57
31:a:398:C:H2'	31:a:399:G:C8	2.39	0.57
31:a:563:C:H2'	31:a:564:C:H6	1.70	0.57
31:a:996:A:H61	31:a:1228:U:H3	1.53	0.57
5:A:1065:A:H62	5:A:1185:U:H3	1.52	0.57
7:C:154:ILE:HG21	7:C:176:LEU:HD22	1.87	0.57
10:F:94:GLU:O	10:F:98:GLU:OE1	2.23	0.57
31:a:206:A:H2'	31:a:207:G:C8	2.40	0.57
31:a:1357:G:N7	39:i:14:ARG:NH2	2.52	0.57
48:r:38:ILE:HD12	48:r:42:GLY:HA2	1.86	0.57
5:A:2049:U:OP2	30:Z:12:ARG:NH2	2.37	0.57
23:S:7:ASP:OD1	23:S:7:ASP:N	2.36	0.57
31:a:994:C:H2'	31:a:995:A:H8	1.68	0.57
31:a:588:C:H2'	31:a:589:G:O4'	2.04	0.56
31:a:1170:G:H22	31:a:1192:G:H1	1.51	0.56
38:h:113:ILE:HB	38:h:117:GLU:OE2	2.05	0.56
1:l:5:VAL:HG13	1:l:47:GLU:HG3	1.86	0.56
5:A:1183:G:OP2	12:H:73:LYS:NZ	2.36	0.56
17:M:55:GLN:OE1	17:M:56:ALA:N	2.38	0.56
20:P:50:ALA:HB3	20:P:51:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:422:A:H3'	31:a:423:A:H8	1.70	0.56
31:a:653:G:C2	31:a:654:G:C8	2.93	0.56
31:a:1329:A:C8	31:a:1333:G:C5	2.93	0.56
3:3:21:GLN:HB3	3:3:49:LEU:HD22	1.87	0.56
5:A:320:U:H5	5:A:326:A:N7	2.04	0.56
5:A:1044:A:H2'	5:A:1045:A:C8	2.40	0.56
5:A:2361:U:H5'	17:M:17:ARG:HG2	1.87	0.56
8:D:44:ASP:OD1	8:D:44:ASP:O	2.23	0.56
12:H:21:ALA:HB3	12:H:60:ALA:H	1.71	0.56
15:K:38:THR:OG1	15:K:127:VAL:HG23	2.04	0.56
31:a:547:A:H2'	31:a:548:G:H8	1.70	0.56
31:a:736:A:H2'	31:a:737:A:H8	1.70	0.56
31:a:1323:U:H2'	31:a:1324:C:H6	1.70	0.56
31:a:1531:G:H2'	31:a:1532:G:C8	2.40	0.56
34:d:178:ARG:NH2	34:d:181:GLU:OE1	2.37	0.56
46:p:40:TYR:HD1	46:p:50:ILE:HG22	1.69	0.56
33:c:62:ARG:HD2	33:c:98:VAL:HG22	1.86	0.56
10:F:130:LEU:HB2	10:F:154:ILE:CD1	2.35	0.56
22:R:27:PHE:HZ	22:R:87:ILE:HG21	1.70	0.56
31:a:1082:C:H2'	31:a:1083:G:C8	2.39	0.56
31:a:1261:A:H2'	31:a:1262:A:C8	2.41	0.56
5:A:2222:U:H2'	5:A:2223:C:C6	2.41	0.56
31:a:1071:U:H2'	31:a:1072:G:H8	1.71	0.56
5:A:1259:U:OP1	20:P:69:LYS:NZ	2.38	0.56
5:A:1479:G:H2'	5:A:1480:G:C8	2.41	0.56
31:a:1074:C:OP2	31:a:1075:G:O2'	2.23	0.56
38:h:107:SER:HB2	38:h:128:ILE:HD11	1.88	0.56
46:p:83:LYS:HA	46:p:86:GLU:HG2	1.88	0.56
31:a:508:G:H2'	31:a:509:C:C6	2.41	0.56
31:a:546:U:H2'	31:a:547:A:C8	2.41	0.56
31:a:331:U:H2'	31:a:332:G:O4'	2.06	0.56
31:a:495:A:H5''	31:a:496:C:C5	2.41	0.56
31:a:787:C:H2'	31:a:788:A:O4'	2.06	0.56
31:a:1304:U:H2'	31:a:1305:U:C6	2.41	0.56
37:g:26:LEU:HD13	37:g:101:LEU:HD22	1.87	0.56
43:m:64:LYS:HD2	43:m:68:ASP:HB2	1.88	0.56
47:q:9:VAL:HG22	47:q:64:GLN:HG3	1.87	0.56
5:A:2618:C:N4	5:A:2619:G:O6	2.39	0.56
31:a:1541:G:H2'	31:a:1542:A:C2	2.40	0.56
7:C:29:PRO:HB2	7:C:34:LEU:HD11	1.87	0.55
8:D:186:VAL:HG22	8:D:196:LEU:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:84:ASN:O	24:T:85:GLN:HG3	2.06	0.55
25:U:19:LYS:NZ	25:U:19:LYS:HB3	2.20	0.55
5:A:926:G:H21	5:A:941:A:H62	1.54	0.55
31:a:193:C:HO2'	31:a:194:G:P	2.29	0.55
43:m:11:ARG:O	43:m:13:LYS:HG2	2.06	0.55
31:a:106:G:N1	50:t:6:SER:OG	2.32	0.55
47:q:17:ASP:OD2	47:q:57:LEU:N	2.38	0.55
5:A:1574:G:H1	5:A:1590:C:H5	1.54	0.55
17:M:28:LYS:HG2	17:M:93:VAL:HG22	1.88	0.55
22:R:25:TYR:CE2	22:R:82:LEU:HD21	2.40	0.55
31:a:352:A:H5''	31:a:353:C:H5	1.71	0.55
31:a:1437:C:H2'	31:a:1438:A:C8	2.41	0.55
11:G:6:LYS:N	11:G:65:HIS:HE1	2.04	0.55
17:M:55:GLN:CD	17:M:55:GLN:C	2.75	0.55
31:a:397:A:H3'	31:a:398:C:H6	1.71	0.55
31:a:1141:A:O2'	31:a:1142:U:O5'	2.25	0.55
5:A:2048:G:OP1	30:Z:9:SER:OG	2.24	0.55
13:I:71:ARG:HH11	18:N:74:ARG:CZ	2.19	0.55
16:L:106:GLN:NE2	16:L:118:ILE:HD12	2.22	0.55
31:a:590:U:H2'	31:a:591:A:C8	2.41	0.55
31:a:720:A:H2'	31:a:721:G:C8	2.41	0.55
37:g:45:SER:HB3	37:g:117:GLU:HG2	1.88	0.55
31:a:42:G:H2'	31:a:43:G:C8	2.41	0.55
31:a:35:C:H2'	31:a:36:G:H8	1.72	0.55
31:a:448:U:C2	31:a:449:A:C8	2.94	0.55
31:a:1324:C:H2'	31:a:1325:U:O2	2.07	0.55
34:d:65:GLU:C	34:d:67:GLN:H	2.15	0.55
5:A:901:G:H2'	5:A:902:A:C8	2.42	0.55
6:B:40:C:C6	10:F:66:LEU:HD13	2.42	0.55
12:H:70:GLU:OE1	12:H:70:GLU:CA	2.53	0.55
27:W:44:ARG:HD2	27:W:48:LYS:NZ	2.22	0.55
36:f:20:LYS:H	36:f:20:LYS:HD2	1.72	0.55
49:s:31:ILE:H	49:s:31:ILE:HD12	1.70	0.55
31:a:509:C:H2'	31:a:510:C:C6	2.43	0.54
32:b:219:ASP:HA	32:b:222:LEU:HD12	1.89	0.54
35:e:159:LYS:HE3	35:e:163:GLU:HB3	1.88	0.54
5:A:1003:A:H2'	5:A:1004:A:C8	2.42	0.54
18:N:60:THR:CG2	18:N:60:THR:O	2.55	0.54
5:A:1378:U:C6	22:R:79:ILE:CD1	2.91	0.54
31:a:661:U:C2	38:h:56:LYS:HD2	2.42	0.54
31:a:1026:U:H2'	31:a:1027:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1167:A:N6	31:a:1187:G:N7	2.55	0.54
37:g:85:TYR:HH	41:k:55:SER:HG	1.53	0.54
5:A:2098:A:H2'	5:A:2099:G:C8	2.42	0.54
22:R:9:ARG:HG2	22:R:28:ASP:HB3	1.90	0.54
31:a:458:G:OP2	31:a:459:A:O2'	2.26	0.54
33:c:155:ARG:H	33:c:162:ALA:HA	1.72	0.54
36:f:35:ALA:HA	36:f:67:SER:HB3	1.88	0.54
5:A:1478:A:N6	5:A:1605:A:H61	2.06	0.54
5:A:2838:C:OP2	16:L:38:LYS:NZ	2.40	0.54
11:G:69:ARG:C	11:G:69:ARG:CD	2.81	0.54
16:L:95:GLU:O	16:L:97:GLN:NE2	2.40	0.54
26:V:17:ARG:HB2	26:V:27:ARG:HG3	1.89	0.54
31:a:433:A:H2'	31:a:434:U:C6	2.43	0.54
37:g:57:ASP:HB3	37:g:60:GLU:HB2	1.89	0.54
46:p:42:PRO:HA	46:p:48:PRO:HB3	1.89	0.54
23:S:41:MET:O	23:S:58:GLU:HA	2.07	0.54
23:S:89:LYS:N	23:S:89:LYS:HD2	2.22	0.54
31:a:723:A:H2'	31:a:724:A:H8	1.73	0.54
31:a:1398:U:H2'	31:a:1399:C:C6	2.42	0.54
35:e:80:THR:HG22	35:e:122:ASP:HB2	1.88	0.54
22:R:55:ILE:HD12	22:R:78:ALA:HB2	1.89	0.54
24:T:94:ILE:HD12	24:T:94:ILE:N	2.23	0.54
31:a:521:A:H2'	31:a:522:C:C6	2.42	0.54
31:a:873:A:H2'	31:a:874:A:C8	2.43	0.54
38:h:110:GLU:OE1	38:h:110:GLU:N	2.40	0.54
31:a:508:G:H2'	31:a:509:C:H6	1.73	0.54
31:a:753:U:OP1	31:a:860:U:O2'	2.26	0.54
41:k:52:PHE:HD1	41:k:56:LYS:HB3	1.73	0.54
13:I:91:LYS:HD2	13:I:111:PHE:CE1	2.43	0.54
17:M:18:VAL:C	17:M:20:THR:H	2.16	0.54
22:R:49:LYS:HB3	22:R:84:GLU:HB3	1.90	0.54
31:a:33:A:H2'	31:a:34:A:C8	2.43	0.54
31:a:57:U:H2'	31:a:58:G:H8	1.72	0.54
31:a:876:G:O2'	31:a:882:A:N1	2.40	0.54
31:a:1235:A:H1'	49:s:78:ARG:HD3	1.89	0.54
41:k:45:SER:HB3	41:k:70:ALA:HB2	1.87	0.54
5:A:1089:C:H4'	5:A:1090:A:H5''	1.90	0.54
13:I:71:ARG:HD2	18:N:74:ARG:HH21	1.73	0.54
31:a:277:U:H2'	31:a:278:A:H8	1.73	0.54
43:m:90:ARG:HB2	43:m:97:VAL:HG12	1.90	0.54
46:p:79:GLY:O	46:p:83:LYS:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1290:G:H21	19:O:33:LYS:HG2	1.71	0.53
9:E:34:PHE:CE1	14:J:6:LEU:HD13	2.43	0.53
24:T:49:ILE:HG22	24:T:53:ARG:NH1	2.23	0.53
31:a:1365:A:H2'	31:a:1366:G:C8	2.42	0.53
40:j:53:ARG:HG2	40:j:63:GLU:HB2	1.90	0.53
5:A:1290:G:H21	19:O:33:LYS:CG	2.20	0.53
12:H:24:GLN:HG2	12:H:29:LEU:HD12	1.88	0.53
13:I:32:THR:CG2	13:I:33:ALA:H	2.20	0.53
13:I:71:ARG:HH11	18:N:74:ARG:NH2	2.06	0.53
31:a:34:A:N3	42:l:42:GLN:NE2	2.55	0.53
31:a:445:U:O2'	34:d:116:HIS:ND1	2.35	0.53
31:a:1167:A:N6	31:a:1188:G:H1'	2.23	0.53
31:a:214:A:N1	31:a:225:G:C6	2.77	0.53
5:A:293:U:H2'	5:A:294:G:O4'	2.08	0.53
22:R:49:LYS:HG2	22:R:83:LYS:HE2	1.90	0.53
31:a:423:A:O2'	31:a:424:G:H8	1.92	0.53
31:a:424:G:H2'	31:a:425:G:C8	2.39	0.53
31:a:1402:G:O2'	31:a:1513:A:O5'	2.26	0.53
32:b:54:TYR:HE2	32:b:216:LYS:HG3	1.73	0.53
37:g:85:TYR:OH	41:k:55:SER:OG	2.25	0.53
3:3:12:LYS:NZ	5:A:252:C:O2	2.40	0.53
19:O:104:LYS:H	19:O:104:LYS:HD3	1.72	0.53
31:a:1131:C:C2	31:a:1132:U:C5	2.96	0.53
42:l:59:ASN:ND2	42:l:102:ASP:OD1	2.42	0.53
46:p:53:ASP:OD1	46:p:54:GLU:N	2.42	0.53
5:A:665:G:H4'	5:A:666:A:H5''	1.91	0.53
9:E:141:ASN:O	9:E:145:THR:HG23	2.09	0.53
12:H:37:LEU:HD11	12:H:110:LEU:HD11	1.91	0.53
27:W:58:ARG:NH1	27:W:61:GLU:OE2	2.39	0.53
12:H:54:TYR:CE1	12:H:122:LYS:HD2	2.43	0.53
31:a:63:U:OP1	31:a:393:C:O2'	2.26	0.53
31:a:205:A:H2'	31:a:206:A:H8	1.72	0.53
31:a:860:U:H2'	31:a:861:A:H8	1.74	0.53
31:a:1543:U:H2'	31:a:1544:C:O4'	2.09	0.53
32:b:127:GLU:OE1	32:b:127:GLU:N	2.42	0.53
33:c:84:GLU:O	33:c:88:ASN:ND2	2.41	0.53
39:i:8:TYR:HB2	39:i:23:LEU:HB2	1.91	0.53
5:A:1484:G:H3'	5:A:1485:G:H8	1.73	0.53
16:L:6:LEU:HD13	16:L:16:MET:HE1	1.89	0.53
19:O:116:ALA:O	19:O:117:LEU:C	2.49	0.53
31:a:272:C:H2'	31:a:273:G:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1075:G:H1'	31:a:1200:G:H21	1.74	0.53
37:g:72:VAL:H	37:g:142:HIS:CE1	2.21	0.53
5:A:512:A:H5''	5:A:512:A:H8	1.72	0.53
6:B:73:G:H21	24:T:88:HIS:HD2	1.56	0.53
34:d:9:TRP:CG	34:d:25:GLU:HG2	2.44	0.53
5:A:458:A:C5	5:A:459:C:H1'	2.44	0.53
5:A:2122:A:H2'	5:A:2123:A:O4'	2.08	0.53
5:A:2372:G:H4'	5:A:2373:A:H5''	1.91	0.53
19:O:107:ALA:O	19:O:111:THR:HG23	2.08	0.53
21:Q:4:LYS:HD2	21:Q:106:VAL:HG22	1.90	0.53
22:R:56:MET:HE1	22:R:79:ILE:HD11	1.90	0.53
5:A:1080:G:H1	5:A:1163:U:H3	1.57	0.52
5:A:2452:A:H4'	5:A:2453:A:H5''	1.90	0.52
5:A:2774:G:O2'	11:G:67:THR:HG23	2.09	0.52
7:C:210:ARG:HA	7:C:213:TRP:CE3	2.44	0.52
31:a:500:A:H2'	31:a:501:U:C6	2.44	0.52
31:a:823:A:N7	31:a:1520:C:O2'	2.30	0.52
5:A:684:U:H2'	5:A:685:C:C6	2.43	0.52
5:A:1463:A:H2	5:A:1625:U:H3	1.57	0.52
12:H:36:ILE:HD11	12:H:141:TYR:CE1	2.43	0.52
31:a:1153:G:H2'	31:a:1154:G:C8	2.44	0.52
31:a:1289:A:O2'	31:a:1291:U:OP2	2.20	0.52
31:a:1542:A:H2'	31:a:1543:U:C6	2.44	0.52
36:f:1:MET:SD	36:f:68:ASP:HB3	2.49	0.52
5:A:2146:A:H62	5:A:2195:G:H22	1.58	0.52
19:O:102:ASP:OD1	19:O:104:LYS:HE2	2.08	0.52
31:a:213:G:H2'	31:a:214:A:C8	2.45	0.52
31:a:950:G:N2	31:a:1353:G:H1	2.04	0.52
41:k:17:GLU:OE1	41:k:17:GLU:N	2.42	0.52
5:A:1150:A:H3'	5:A:1151:G:H8	1.74	0.52
7:C:29:PRO:CB	7:C:34:LEU:HD11	2.39	0.52
16:L:102:ARG:HH22	16:L:122:VAL:HG23	1.74	0.52
20:P:6:GLU:HB2	20:P:39:LEU:HD11	1.90	0.52
24:T:8:ILE:HG13	24:T:41:VAL:HG12	1.91	0.52
31:a:42:G:H2'	31:a:43:G:H8	1.75	0.52
31:a:366:U:C2	31:a:367:A:C8	2.97	0.52
31:a:381:A:C2	31:a:382:A:C8	2.98	0.52
5:A:84:A:H1'	5:A:85:G:O4'	2.10	0.52
5:A:548:A:H4'	5:A:549:U:H5'	1.92	0.52
5:A:792:5MU:H4'	21:Q:92:ARG:HH12	1.74	0.52
5:A:1699:A:H4'	8:D:128:GLN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:191:GLU:HG2	8:D:192:ASN:N	2.24	0.52
9:E:164:GLU:HA	9:E:175:VAL:HG21	1.92	0.52
10:F:132:VAL:O	10:F:151:GLY:HA2	2.10	0.52
31:a:934:G:H1'	31:a:1513:A:C4	2.45	0.52
31:a:1167:A:N7	31:a:1190:A:N6	2.57	0.52
36:f:29:ILE:HD12	36:f:29:ILE:H	1.73	0.52
37:g:16:PRO:HA	39:i:48:LEU:HD22	1.91	0.52
5:A:896:U:H2'	5:A:897:A:C8	2.44	0.52
24:T:52:ILE:O	24:T:56:GLY:N	2.38	0.52
5:A:352:A:H4'	23:S:14:GLY:HA2	1.92	0.52
5:A:1669:C:H2'	5:A:1670:A:O4'	2.10	0.52
5:A:1758:A:H61	5:A:1771:A:H62	1.57	0.52
5:A:2136:U:H3'	5:A:2147:G:OP1	2.09	0.52
31:a:523:G:H2'	31:a:524:U:H6	1.75	0.52
31:a:541:A:O2'	31:a:543:A:OP1	2.28	0.52
31:a:1062:G:H2'	31:a:1063:U:C6	2.45	0.52
31:a:1141:A:C2'	31:a:1142:U:O5'	2.58	0.52
31:a:1286:G:N3	31:a:1292:C:O2'	2.40	0.52
40:j:8:ILE:HB	40:j:74:ILE:HG13	1.90	0.52
5:A:1485:G:O2'	5:A:1672:G:OP1	2.24	0.52
5:A:2316:G:O6	5:A:2370:U:H5	1.93	0.52
5:A:2854:A:H2'	5:A:2899:A:H61	1.75	0.52
7:C:94:VAL:HG22	7:C:102:ARG:O	2.10	0.52
10:F:130:LEU:HB2	10:F:154:ILE:HD12	1.91	0.52
20:P:27:VAL:CG2	20:P:31:ASP:HB2	2.40	0.52
31:a:612:G:H2'	31:a:613:U:C6	2.45	0.52
5:A:2540:A:H2'	5:A:2541:U:C6	2.45	0.52
5:A:2581:U:H2'	5:A:2582:U:C6	2.45	0.52
5:A:2760:A:C5	8:D:216:LYS:HE2	2.45	0.52
7:C:67:PHE:HE1	7:C:105:ILE:HD11	1.75	0.52
8:D:47:ASN:OD1	8:D:47:ASN:O	2.28	0.52
24:T:37:LYS:HG3	24:T:38:ASN:N	2.23	0.52
31:a:257:U:H2'	31:a:258:A:C8	2.45	0.52
31:a:368:G:H2'	31:a:369:G:C8	2.45	0.52
31:a:407:G:H2'	31:a:408:C:C6	2.45	0.52
31:a:420:U:H1'	34:d:29:ARG:CZ	2.40	0.52
31:a:724:A:H1'	41:k:120:GLY:HA2	1.92	0.52
31:a:1260:A:C8	31:a:1297:A:C2	2.98	0.52
36:f:16:GLU:HG3	36:f:20:LYS:NZ	2.25	0.52
43:m:49:THR:HB	43:m:52:GLU:HG3	1.92	0.52
5:A:2711:U:OP1	18:N:60:THR:HG21	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:22:ILE:HD11	13:I:42:THR:HG23	1.91	0.51
24:T:39:VAL:HG12	24:T:41:VAL:HG13	1.93	0.51
31:a:1394:C:H2'	31:a:1395:G:H8	1.75	0.51
2:2:31:VAL:HG12	2:2:34:ARG:NH2	2.25	0.51
31:a:521:A:H2'	31:a:522:C:H6	1.75	0.51
31:a:617:A:C2	31:a:618:G:H1'	2.45	0.51
32:b:89:GLN:HE21	32:b:221:ILE:HG12	1.75	0.51
38:h:54:ASP:OD1	38:h:56:LYS:N	2.43	0.51
49:s:22:GLN:HE22	49:s:31:ILE:HD11	1.75	0.51
5:A:388:A:H2'	5:A:389:A:H2	1.74	0.51
5:A:1315:C:H2'	5:A:1316:G:H8	1.75	0.51
13:I:112:MET:HE3	13:I:112:MET:CA	2.37	0.51
31:a:776:A:H4'	31:a:1534:G:H21	1.75	0.51
31:a:1333:G:H2'	31:a:1334:A:C8	2.46	0.51
33:c:39:ARG:NH1	33:c:54:VAL:O	2.43	0.51
5:A:2435:U:H2'	5:A:2436:G:C8	2.46	0.51
10:F:120:LYS:HD3	10:F:167:ARG:HH21	1.76	0.51
17:M:83:LYS:O	17:M:87:LYS:HG2	2.11	0.51
31:a:18:U:H2'	31:a:19:C:H6	1.71	0.51
31:a:384:G:OP1	46:p:68:THR:HG21	2.11	0.51
31:a:1169:U:O4'	31:a:1192:G:N2	2.44	0.51
31:a:1532:G:H2'	31:a:1533:U:C2	2.46	0.51
5:A:921:C:H2'	5:A:922:G:C8	2.45	0.51
5:A:1055:A:OP1	19:O:75:SER:OG	2.28	0.51
5:A:2760:A:C6	8:D:216:LYS:HG2	2.45	0.51
12:H:29:LEU:HA	12:H:143:LEU:HD11	1.93	0.51
13:I:2:ILE:HD11	13:I:82:ASN:OD1	2.10	0.51
17:M:30:ARG:HH21	17:M:45:ILE:HG12	1.74	0.51
32:b:67:VAL:HG22	32:b:160:ALA:HB3	1.91	0.51
5:A:297:G:H4'	5:A:304:G:O3'	2.11	0.51
5:A:738:U:O2'	5:A:1390:A:N3	2.44	0.51
5:A:2144:A:C8	5:A:2176:C:H5'	2.46	0.51
8:D:118:VAL:HG12	8:D:183:LEU:HD12	1.93	0.51
23:S:87:ASP:O	23:S:89:LYS:HD2	2.11	0.51
24:T:60:VAL:C	24:T:61:ILE:HD13	2.35	0.51
31:a:370:G:N2	31:a:373:U:OP2	2.42	0.51
5:A:702:U:H2'	5:A:703:A:C8	2.46	0.51
5:A:2599:A:OP1	5:A:2601:G:H4'	2.10	0.51
18:N:29:ARG:HD3	18:N:89:LYS:HD3	1.92	0.51
23:S:11:VAL:HG12	23:S:68:VAL:HG12	1.92	0.51
24:T:61:ILE:HD13	24:T:61:ILE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:709:C:H5'	31:a:710:A:H3'	1.93	0.51
32:b:94:GLN:HG3	32:b:146:LYS:HG2	1.91	0.51
41:k:68:GLU:O	41:k:72:LYS:HG2	2.10	0.51
45:o:29:ILE:HD13	45:o:67:LEU:HG	1.92	0.51
5:A:2163:A:H62	5:A:2183:G:H21	1.57	0.51
10:F:143:TYR:O	10:F:146:VAL:HG22	2.11	0.51
11:G:23:HIS:NE2	11:G:34:SER:HB3	2.26	0.51
31:a:1535:C:H2'	31:a:1536:G:C8	2.46	0.51
32:b:80:VAL:HG12	32:b:91:TYR:HB2	1.93	0.51
5:A:943:C:H2'	5:A:944:G:C8	2.46	0.51
5:A:1261:G:N7	20:P:70:LYS:NZ	2.56	0.51
5:A:2085:MA6:H92	5:A:2086:A:N6	2.26	0.51
11:G:90:VAL:O	11:G:94:TYR:HD2	1.93	0.51
13:I:111:PHE:O	13:I:115:VAL:HG23	2.10	0.51
31:a:199:G:H2'	31:a:200:U:C6	2.46	0.51
31:a:870:G:HO2'	31:a:883:G:HO2'	1.59	0.51
31:a:987:A:C2	31:a:1329:A:C4	2.98	0.51
31:a:1232:G:OP1	31:a:1331:U:O2'	2.22	0.51
34:d:66:ARG:O	34:d:66:ARG:HG2	2.10	0.51
47:q:55:ALA:HB2	47:q:80:ILE:HD11	1.93	0.51
10:F:31:ILE:HA	10:F:158:THR:HG22	1.93	0.51
17:M:18:VAL:C	17:M:20:THR:N	2.69	0.51
19:O:104:LYS:CD	19:O:104:LYS:N	2.74	0.51
31:a:96:U:H2'	31:a:97:G:H8	1.75	0.51
31:a:911:G:H2'	31:a:912:G:H8	1.75	0.51
31:a:955:A:H2'	31:a:956:G:H8	1.74	0.51
31:a:1106:U:H2'	31:a:1107:C:C6	2.46	0.51
5:A:396:G:H2'	5:A:397:U:O4'	2.11	0.50
5:A:631:U:H1'	9:E:90:PHE:HB3	1.93	0.50
5:A:2036:G:C2	5:A:2037:G:C8	3.00	0.50
8:D:67:LYS:HA	8:D:86:ARG:HH22	1.76	0.50
5:A:644:C:O2'	5:A:645:A:H8	1.94	0.50
19:O:104:LYS:HD3	19:O:104:LYS:N	2.26	0.50
31:a:834:C:O2	38:h:16:ASN:ND2	2.44	0.50
4:4:17:ILE:HD13	4:4:26:ILE:HG12	1.93	0.50
5:A:162:A:H2	5:A:166:A:H61	1.59	0.50
5:A:1992:C:H2'	5:A:1993:A:C8	2.46	0.50
5:A:2328:A:N6	5:A:2342:U:H3	2.09	0.50
5:A:2622:G:N2	5:A:2625:A:OP2	2.38	0.50
9:E:195:THR:HG22	9:E:197:ALA:H	1.76	0.50
22:R:89:LEU:O	22:R:90:PHE:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:468:G:O6	31:a:482:A:N6	2.44	0.50
31:a:504:G:H21	31:a:505:A:H3'	1.75	0.50
8:D:5:ILE:HG21	8:D:195:ILE:CD1	2.41	0.50
17:M:55:GLN:OE1	17:M:56:ALA:HA	2.10	0.50
40:j:18:ILE:HG13	40:j:72:ARG:HG2	1.92	0.50
5:A:283:G:H3'	5:A:284:C:C6	2.47	0.50
5:A:1400:C:O2'	5:A:1836:A:N3	2.37	0.50
5:A:1741:G:OP2	5:A:1742:A:O2'	2.23	0.50
7:C:11:ASN:C	7:C:13:ARG:H	2.19	0.50
7:C:79:ASP:OD1	7:C:79:ASP:O	2.29	0.50
10:F:32:ASP:OD2	17:M:2:ILE:HD11	2.10	0.50
12:H:74:VAL:CG2	12:H:87:SER:HB2	2.42	0.50
18:N:60:THR:O	18:N:60:THR:HG23	2.11	0.50
23:S:100:GLU:C	23:S:100:GLU:OE1	2.54	0.50
31:a:948:G:H2'	31:a:949:C:C6	2.47	0.50
31:a:966:U:H4'	49:s:79:THR:HG23	1.94	0.50
5:A:1265:G:N7	19:O:16:LYS:NZ	2.59	0.50
31:a:592:G:H2'	31:a:593:G:H8	1.76	0.50
31:a:791:C:H2'	31:a:792:A:C8	2.44	0.50
49:s:30:VAL:O	49:s:30:VAL:HG12	2.11	0.50
5:A:94:A:H2'	5:A:95:A:C8	2.46	0.50
5:A:1707:U:O2'	5:A:2713:G:H4'	2.12	0.50
5:A:1806:U:H5	5:A:1811:A:N7	2.10	0.50
5:A:2123:A:C2	5:A:2124:U:C5	3.00	0.50
6:B:44:A:H5''	17:M:7:LYS:HE3	1.94	0.50
9:E:159:GLU:OE2	9:E:177:THR:CG2	2.59	0.50
11:G:89:LEU:HD22	11:G:95:ARG:O	2.11	0.50
13:I:32:THR:HG23	13:I:33:ALA:H	1.77	0.50
16:L:91:GLU:OE1	16:L:91:GLU:N	2.44	0.50
31:a:123:G:H2'	31:a:124:U:C6	2.47	0.50
31:a:366:U:H2'	31:a:367:A:H8	1.76	0.50
31:a:1142:U:H6	31:a:1142:U:H5''	1.77	0.50
31:a:1323:U:H2'	31:a:1324:C:C6	2.46	0.50
31:a:1441:C:H2'	31:a:1442:G:O4'	2.12	0.50
39:i:30:ILE:HG13	39:i:65:VAL:CG2	2.42	0.50
5:A:1401:G:OP1	26:V:3:LYS:CE	2.59	0.50
5:A:2024:A:H5''	8:D:131:ILE:HD11	1.94	0.50
31:a:1524:A:H2'	31:a:1525:U:C6	2.47	0.50
33:c:68:HIS:HB3	33:c:105:ILE:HD11	1.93	0.50
39:i:116:LYS:HG3	39:i:122:ALA:HA	1.93	0.50
5:A:194:A:H2'	5:A:195:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:324:A:H2'	5:A:325:A:O4'	2.11	0.50
14:J:2:LYS:HB2	14:J:5:GLU:HG3	1.94	0.50
31:a:41:C:H2'	31:a:42:G:H8	1.77	0.50
31:a:383:U:OP1	46:p:70:THR:HG21	2.12	0.50
31:a:483:C:O2'	31:a:484:A:H5'	2.12	0.50
31:a:726:A:H5'	41:k:119:ASN:ND2	2.25	0.50
7:C:157:SER:O	7:C:195:VAL:HG21	2.11	0.49
13:I:42:THR:HG22	13:I:57:VAL:HG22	1.93	0.49
31:a:699:G:H22	31:a:703:A:H5''	1.77	0.49
31:a:920:U:H2'	31:a:921:C:C6	2.47	0.49
31:a:1376:C:O2'	40:j:62:ARG:NH2	2.44	0.49
31:a:1398:U:H2'	31:a:1399:C:H6	1.77	0.49
31:a:1477:C:H2'	31:a:1478:G:O4'	2.12	0.49
5:A:1182:G:N3	12:H:109:MET:HE2	2.26	0.49
16:L:24:LEU:HD23	16:L:44:VAL:HG21	1.94	0.49
17:M:6:ASP:OD1	17:M:7:LYS:N	2.45	0.49
31:a:860:U:H2'	31:a:861:A:C8	2.48	0.49
31:a:1001:U:N3	31:a:1054:G:O2'	2.42	0.49
31:a:1353:G:H2'	31:a:1354:C:C6	2.46	0.49
31:a:1394:C:C2	31:a:1395:G:C8	3.00	0.49
33:c:57:GLU:HB2	33:c:64:ASN:HB3	1.93	0.49
38:h:46:ILE:HD11	38:h:49:VAL:HG22	1.94	0.49
5:A:327:G:H1	5:A:399:U:H3	1.59	0.49
5:A:2142:G:N2	5:A:2188:C:OP1	2.45	0.49
5:A:2775:A:H5''	11:G:4:VAL:HG21	1.94	0.49
9:E:164:GLU:HG3	9:E:175:VAL:CG1	2.42	0.49
11:G:23:HIS:C	11:G:23:HIS:ND1	2.70	0.49
15:K:72:THR:HB	15:K:94:ILE:HG12	1.95	0.49
27:W:2:LYS:O	27:W:2:LYS:HD2	2.12	0.49
31:a:509:C:OP1	42:l:127:ARG:NH2	2.46	0.49
34:d:41:ARG:NE	34:d:41:ARG:HA	2.27	0.49
37:g:142:HIS:O	37:g:146:GLU:HG2	2.13	0.49
5:A:2858:G:C4	5:A:2859:G:C8	3.01	0.49
29:Y:9:TYR:CE1	29:Y:26:GLY:HA2	2.47	0.49
29:Y:55:HIS:ND1	29:Y:58:TYR:O	2.43	0.49
31:a:1438:A:H2'	31:a:1439:C:H6	1.77	0.49
38:h:117:GLU:O	38:h:121:ARG:HG2	2.13	0.49
39:i:59:THR:HG22	39:i:62:ASN:HB2	1.93	0.49
5:A:787:U:H2'	5:A:788:A:C8	2.47	0.49
7:C:119:GLY:O	7:C:131:PRO:HD3	2.12	0.49
19:O:78:ARG:CD	19:O:78:ARG:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:202:C:H2'	31:a:203:A:C8	2.48	0.49
31:a:499:A:C2	31:a:500:A:C5	3.00	0.49
31:a:1172:C:C2	31:a:1173:G:C8	3.00	0.49
41:k:74:ALA:HB1	41:k:79:LEU:HG	1.94	0.49
5:A:1097:U:H4'	5:A:1098:A:OP2	2.12	0.49
18:N:19:LEU:H	18:N:19:LEU:CD2	2.26	0.49
19:O:76:TYR:CZ	19:O:80:MET:HG3	2.48	0.49
31:a:917:A:H2'	31:a:918:A:H8	1.77	0.49
31:a:954:G:C2	31:a:955:A:C8	3.01	0.49
31:a:1106:U:H2'	31:a:1107:C:H6	1.78	0.49
5:A:579:U:H5'	19:O:42:SER:OG	2.13	0.49
5:A:897:A:H5'	28:X:45:GLY:HA3	1.94	0.49
5:A:1530:A:H2'	5:A:1531:U:C6	2.47	0.49
5:A:2338:A:O2'	10:F:79:LEU:HD22	2.12	0.49
5:A:2786:G:H1'	5:A:2787:C:H5'	1.95	0.49
16:L:100:TYR:O	16:L:101:THR:HG23	2.13	0.49
20:P:1:MET:O	20:P:15:GLU:HB3	2.13	0.49
31:a:975:G:H4'	39:i:132:ARG:HB3	1.94	0.49
42:l:88:GLN:N	42:l:88:GLN:OE1	2.45	0.49
5:A:2154:G:H2'	5:A:2155:C:C6	2.47	0.49
15:K:111:GLU:OE2	15:K:115:ARG:NH2	2.45	0.49
31:a:36:G:N2	42:l:128:SER:OG	2.46	0.49
31:a:161:A:N6	31:a:355:G:O2'	2.46	0.49
31:a:266:A:H2'	31:a:267:G:H8	1.78	0.49
31:a:953:G:N1	31:a:1348:G:OP2	2.27	0.49
31:a:1006:U:H2'	31:a:1007:C:C6	2.48	0.49
32:b:87:ALA:HB1	32:b:221:ILE:HG21	1.93	0.49
5:A:90:A:H4'	5:A:91:A:H5'	1.94	0.49
5:A:104:C:C6	5:A:104:C:C5'	2.92	0.49
5:A:707:G:H5''	14:J:16:ARG:HB3	1.94	0.49
5:A:1699:A:N6	5:A:2032:A:O2'	2.46	0.49
5:A:2867:U:H2'	5:A:2868:G:O4'	2.13	0.49
15:K:35:GLN:HA	15:K:102:ILE:HA	1.95	0.49
31:a:274:G:H3'	47:q:71:ALA:HB2	1.94	0.49
31:a:341:U:C2	31:a:342:C:C5	3.00	0.49
31:a:502:C:O2'	31:a:504:G:H1'	2.13	0.49
31:a:774:A:C2	31:a:775:A:H1'	2.47	0.49
31:a:946:A:H2'	31:a:947:A:C8	2.47	0.49
31:a:1260:A:H4'	39:i:71:GLY:HA2	1.94	0.49
31:a:1513:A:H2	31:a:1516:G:H22	1.59	0.49
34:d:114:VAL:HG22	34:d:119:ILE:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1754:C:H2'	5:A:1755:U:C6	2.48	0.49
12:H:103:GLU:HB2	12:H:125:VAL:HG11	1.95	0.49
31:a:209:G:H2'	31:a:210:A:C8	2.48	0.49
31:a:963:G:H2'	31:a:964:U:C6	2.48	0.49
31:a:1340:U:H2'	31:a:1341:G:O4'	2.13	0.49
47:q:56:LYS:NZ	47:q:84:SER:HB2	2.28	0.49
47:q:63:ILE:HG23	47:q:75:PHE:HB3	1.95	0.49
5:A:281:A:H2'	5:A:282:A:C8	2.48	0.48
5:A:578:G:H21	19:O:48:ARG:HH22	1.58	0.48
9:E:5:ASP:HA	9:E:13:LYS:NZ	2.28	0.48
11:G:168:TYR:CE2	11:G:170:ARG:HG2	2.48	0.48
16:L:55:ASP:C	16:L:55:ASP:OD1	2.55	0.48
16:L:73:ASN:HB2	16:L:77:THR:OG1	2.13	0.48
31:a:63:U:H2'	31:a:64:C:C6	2.48	0.48
34:d:87:MET:HE1	34:d:182:ARG:CZ	2.43	0.48
35:e:157:ARG:HH21	38:h:43:GLU:HB3	1.78	0.48
5:A:427:A:N1	5:A:439:U:H5	2.10	0.48
5:A:852:U:C2	5:A:853:G:C8	3.01	0.48
5:A:1753:U:H1'	5:A:2880:A:H1'	1.94	0.48
5:A:2338:A:O2'	10:F:79:LEU:CD2	2.62	0.48
16:L:70:GLU:OE1	16:L:80:THR:HG22	2.13	0.48
31:a:994:C:H2'	31:a:995:A:C8	2.47	0.48
5:A:1701:U:OP1	8:D:149:ARG:N	2.47	0.48
20:P:27:VAL:HG22	20:P:28:ASN:N	2.26	0.48
31:a:618:G:C2	31:a:619:C:C6	3.02	0.48
31:a:1129:A:C2	31:a:1130:G:C8	3.01	0.48
31:a:1538:C:H2'	31:a:1539:U:C6	2.49	0.48
49:s:35:SER:OG	49:s:38:SER:OG	2.30	0.48
5:A:1821:U:H2'	5:A:1822:C:C6	2.48	0.48
22:R:22:GLU:OE1	22:R:23:ASP:N	2.47	0.48
31:a:592:G:H2'	31:a:593:G:C8	2.48	0.48
46:p:11:GLY:HA3	46:p:16:PRO:HA	1.95	0.48
49:s:15:LEU:HD11	49:s:33:THR:HG23	1.94	0.48
5:A:1072:A:N6	5:A:1169:G:H2'	2.27	0.48
12:H:17:TYR:HA	12:H:139:GLU:O	2.13	0.48
19:O:111:THR:O	19:O:115:ASP:OD2	2.31	0.48
31:a:1136:U:H1'	31:a:1137:U:H2'	1.95	0.48
31:a:1518:A:H2'	31:a:1519:G:C8	2.49	0.48
32:b:76:ALA:HB2	32:b:164:VAL:HG11	1.96	0.48
39:i:21:VAL:HA	39:i:67:VAL:HG12	1.94	0.48
5:A:78:U:H2'	5:A:79:U:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2022:U:O2'	5:A:2023:C:OP1	2.29	0.48
13:I:63:VAL:HB	13:I:102:VAL:HG22	1.94	0.48
31:a:899:G:O2'	31:a:915:G:O6	2.30	0.48
31:a:1135:G:O2'	31:a:1155:C:N3	2.46	0.48
31:a:1473:C:O2'	31:a:1474:C:H5'	2.14	0.48
45:o:36:ILE:HG23	45:o:56:LEU:HD11	1.96	0.48
49:s:32:LYS:HA	49:s:50:ALA:HB3	1.96	0.48
5:A:529:A:C8	23:S:44:HIS:HD2	2.31	0.48
5:A:1290:G:N2	19:O:33:LYS:HG3	2.28	0.48
17:M:77:GLY:O	17:M:80:ILE:HG22	2.13	0.48
25:U:71:ILE:HD12	25:U:72:ASP:O	2.13	0.48
33:c:33:HIS:HE1	44:n:38:LYS:HB3	1.79	0.48
47:q:70:SER:OG	47:q:73:LYS:HG3	2.13	0.48
5:A:1279:C:C2	5:A:1280:U:C5	3.02	0.48
5:A:2632:U:H2'	5:A:2633:C:C6	2.48	0.48
5:A:2903:A:H5'	5:A:2904:U:H5''	1.96	0.48
8:D:205:LYS:HB2	8:D:205:LYS:HE2	1.65	0.48
12:H:15:LYS:HD2	12:H:17:TYR:OH	2.14	0.48
13:I:19:VAL:HG22	13:I:20:LEU:N	2.28	0.48
19:O:76:TYR:O	19:O:80:MET:HG2	2.13	0.48
25:U:48:GLN:OE1	25:U:52:LYS:N	2.46	0.48
31:a:271:A:H2'	31:a:272:C:C6	2.49	0.48
31:a:1326:G:N2	31:a:1328:A:H3'	2.28	0.48
31:a:1473:C:C2'	31:a:1474:C:H5'	2.44	0.48
40:j:9:ARG:HB3	40:j:73:LEU:HD23	1.96	0.48
41:k:53:LYS:HD3	41:k:54:GLY:O	2.14	0.48
21:Q:5:ALA:HB3	21:Q:54:ALA:HB2	1.96	0.48
29:Y:18:THR:HG21	29:Y:49:ASP:O	2.14	0.48
31:a:1470:U:H2'	31:a:1471:A:H8	1.78	0.48
32:b:121:GLU:HG3	32:b:126:PHE:CD2	2.49	0.48
42:l:92:VAL:O	42:l:116:ASP:HB3	2.13	0.48
49:s:35:SER:HG	49:s:38:SER:HG	1.59	0.48
5:A:1315:C:H5'	16:L:20:LEU:CD2	2.43	0.48
5:A:1805:U:H3'	5:A:1811:A:N6	2.29	0.48
23:S:87:ASP:O	23:S:89:LYS:CE	2.62	0.48
31:a:855:C:H2'	31:a:856:C:H6	1.79	0.48
31:a:1191:G:H1'	31:a:1192:G:C8	2.49	0.48
43:m:14:ARG:HH21	43:m:17:ILE:HD11	1.79	0.48
5:A:38:A:H2'	5:A:39:C:O4'	2.14	0.47
10:F:152:MET:HB2	10:F:152:MET:HE2	1.62	0.47
11:G:8:ILE:CB	11:G:69:ARG:NH2	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:94:THR:HG23	16:L:95:GLU:HG3	1.95	0.47
31:a:59:C:O2	31:a:59:C:H2'	2.14	0.47
31:a:498:U:H2'	31:a:499:A:C8	2.47	0.47
31:a:886:C:C2	31:a:887:U:C5	3.02	0.47
31:a:1083:G:H2'	31:a:1084:U:C6	2.49	0.47
31:a:1255:A:N6	31:a:1303:G:O6	2.47	0.47
34:d:101:LEU:HD11	34:d:174:GLY:HA3	1.95	0.47
50:t:72:ASP:OD1	50:t:72:ASP:N	2.47	0.47
5:A:881:G:C6	5:A:882:C:C5	3.02	0.47
5:A:1300:G:C6	5:A:1301:U:C4	3.02	0.47
6:B:55:A:H4'	10:F:27:GLU:HG2	1.95	0.47
23:S:3:ILE:HD12	23:S:4:LYS:O	2.14	0.47
31:a:434:U:OP1	34:d:29:ARG:HD2	2.14	0.47
31:a:1438:A:H2'	31:a:1439:C:C6	2.49	0.47
31:a:1544:C:H2'	31:a:1545:A:H8	1.74	0.47
5:A:1206:G:N2	20:P:90:GLN:OE1	2.47	0.47
5:A:2272:U:H5''	5:A:2273:G:H5'	1.96	0.47
11:G:45:GLN:O	11:G:45:GLN:HG2	2.13	0.47
31:a:509:C:H2'	31:a:510:C:H6	1.77	0.47
31:a:586:C:O2'	31:a:736:A:N3	2.41	0.47
31:a:1326:G:N1	31:a:1329:A:OP2	2.42	0.47
31:a:1392:C:H2'	31:a:1393:C:H6	1.78	0.47
32:b:99:GLY:O	32:b:103:ASN:HB3	2.13	0.47
40:j:42:LEU:HB3	40:j:71:LYS:HB2	1.96	0.47
5:A:388:A:H8	5:A:389:A:C2	2.33	0.47
5:A:1512:U:H2'	5:A:1567:A:N6	2.29	0.47
5:A:1575:A:HO2'	5:A:1576:A:P	2.38	0.47
5:A:2727:G:H2'	5:A:2728:U:C6	2.49	0.47
10:F:13:THR:O	10:F:17:MET:HB2	2.13	0.47
10:F:78:ARG:HD3	10:F:78:ARG:HA	1.57	0.47
31:a:1197:G:H4'	39:i:115:ARG:NH1	2.29	0.47
31:a:1217:C:C2'	31:a:1218:C:H5'	2.44	0.47
33:c:72:PRO:HG3	33:c:104:GLU:HG3	1.96	0.47
39:i:58:GLU:OE1	39:i:58:GLU:N	2.47	0.47
5:A:2224:U:H2'	5:A:2251:G:H1	1.80	0.47
13:I:81:GLU:OE1	13:I:82:ASN:O	2.32	0.47
31:a:1325:U:H2'	31:a:1326:G:O4'	2.14	0.47
33:c:96:LYS:HB2	33:c:96:LYS:HE3	1.66	0.47
5:A:944:G:H2'	5:A:945:A:O4'	2.15	0.47
5:A:1315:C:H5'	16:L:20:LEU:HD21	1.96	0.47
5:A:2318:U:H2'	5:A:2319:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2432:G:H2'	5:A:2438:A:N6	2.28	0.47
6:B:47:C:H2'	6:B:48:A:C8	2.49	0.47
23:S:85:PHE:HD1	23:S:88:GLY:C	2.23	0.47
31:a:34:A:H2'	31:a:35:C:C6	2.50	0.47
31:a:266:A:H2'	31:a:267:G:C8	2.50	0.47
31:a:553:C:OP1	34:d:54:LYS:NZ	2.47	0.47
41:k:54:GLY:C	41:k:56:LYS:H	2.22	0.47
43:m:72:GLU:OE2	43:m:76:ASN:ND2	2.47	0.47
5:A:1494:G:H5''	5:A:1574:G:O3'	2.14	0.47
5:A:1633:A:H1'	5:A:1634:A:H5'	1.96	0.47
5:A:1929:C:H5''	7:C:241:ILE:HB	1.96	0.47
5:A:2662:U:O2'	8:D:90:GLU:OE1	2.32	0.47
5:A:2839:A:O2'	5:A:2841:A:N7	2.47	0.47
8:D:54:GLU:O	8:D:85:LYS:HD3	2.15	0.47
13:I:73:ASP:OD1	13:I:75:SER:CB	2.62	0.47
20:P:62:VAL:HG22	20:P:95:LEU:HD23	1.96	0.47
31:a:643:A:H2'	31:a:644:U:C6	2.50	0.47
31:a:698:G:H2'	31:a:699:G:C8	2.50	0.47
31:a:745:U:H2'	31:a:746:U:H6	1.78	0.47
31:a:749:G:OP1	45:o:2:ALA:HB2	2.15	0.47
31:a:884:C:C4	31:a:885:A:N7	2.83	0.47
31:a:920:U:C2	31:a:921:C:C5	3.02	0.47
31:a:1541:G:H2'	31:a:1542:A:N3	2.29	0.47
32:b:12:ALA:HA	32:b:208:ARG:HG3	1.95	0.47
45:o:6:GLU:OE1	45:o:6:GLU:N	2.40	0.47
7:C:100:GLU:OE2	7:C:102:ARG:HD3	2.15	0.47
7:C:157:SER:O	7:C:195:VAL:CG2	2.63	0.47
10:F:69:LYS:HE2	10:F:69:LYS:HB2	1.70	0.47
14:J:6:LEU:C	14:J:6:LEU:HD12	2.40	0.47
18:N:19:LEU:H	18:N:19:LEU:HD23	1.80	0.47
31:a:612:G:H2'	31:a:613:U:H6	1.80	0.47
41:k:17:GLU:HG2	41:k:18:ASN:OD1	2.14	0.47
5:A:1084:U:H2'	5:A:1085:U:O4'	2.15	0.47
5:A:1726:A:OP2	5:A:1743:G:N2	2.47	0.47
13:I:42:THR:HA	13:I:56:ASP:O	2.15	0.47
14:J:70:ASN:OD1	14:J:70:ASN:O	2.33	0.47
26:V:40:VAL:HG23	26:V:45:LYS:HB3	1.96	0.47
31:a:932:A:H2'	31:a:933:C:C6	2.50	0.47
32:b:83:GLU:OE1	32:b:86:ARG:NH1	2.46	0.47
34:d:149:ASN:N	34:d:149:ASN:OD1	2.46	0.47
41:k:84:VAL:HB	41:k:110:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:25:HIS:ND1	48:r:25:HIS:C	2.73	0.47
49:s:71:LEU:HD23	49:s:71:LEU:H	1.79	0.47
5:A:1072:A:H2'	5:A:1073:A:C8	2.50	0.47
6:B:40:C:O4'	10:F:66:LEU:HD22	2.15	0.47
22:R:4:ARG:HD2	27:W:23:GLU:HA	1.97	0.47
23:S:25:ALA:HB3	23:S:34:VAL:CG1	2.45	0.47
24:T:32:TYR:HE1	24:T:92:LEU:CD2	1.86	0.47
26:V:46:LYS:C	26:V:47:VAL:HG13	2.40	0.47
31:a:1007:C:H2'	31:a:1008:C:O4'	2.14	0.47
31:a:1333:G:H2'	31:a:1334:A:H8	1.80	0.47
35:e:112:ARG:NH1	35:e:116:GLU:OE2	2.43	0.47
5:A:901:G:H2'	5:A:902:A:H8	1.80	0.46
5:A:962:A:H5''	5:A:2295:A:H61	1.80	0.46
5:A:1290:G:C2	19:O:33:LYS:HG3	2.51	0.46
5:A:1876:G:H1	5:A:1920:C:H42	1.63	0.46
9:E:5:ASP:HB2	9:E:13:LYS:HE2	1.96	0.46
24:T:78:GLN:HB2	24:T:88:HIS:H	1.80	0.46
31:a:468:G:C6	31:a:482:A:C6	3.03	0.46
31:a:776:A:H4'	31:a:1534:G:N2	2.29	0.46
31:a:1090:G:H2'	31:a:1091:A:C8	2.50	0.46
31:a:1339:A:C5	31:a:1340:U:C5	3.03	0.46
32:b:9:LEU:HB3	32:b:14:VAL:HB	1.97	0.46
32:b:86:ARG:NE	32:b:222:LEU:HD11	2.29	0.46
32:b:166:PRO:HG2	32:b:187:VAL:HG12	1.97	0.46
43:m:46:LYS:HG3	43:m:47:ASP:OD1	2.15	0.46
5:A:896:U:H2'	5:A:897:A:H8	1.80	0.46
6:B:86:A:H8	6:B:87:C:H5''	1.80	0.46
31:a:305:G:N2	31:a:308:A:OP2	2.37	0.46
31:a:1142:U:H6	31:a:1142:U:C5'	2.28	0.46
31:a:1170:G:C5	31:a:1171:C:C6	3.04	0.46
31:a:1464:A:H2'	31:a:1465:G:C8	2.51	0.46
36:f:1:MET:SD	36:f:1:MET:N	2.76	0.46
36:f:29:ILE:HG21	36:f:75:GLU:HB3	1.97	0.46
39:i:58:GLU:HB3	39:i:60:LYS:HZ3	1.80	0.46
5:A:2359:C:OP1	25:U:54:TYR:OH	2.29	0.46
9:E:137:LYS:HB3	9:E:137:LYS:HE2	1.42	0.46
10:F:17:MET:HE3	10:F:17:MET:HB3	1.71	0.46
20:P:16:GLU:HA	20:P:97:ILE:HB	1.96	0.46
31:a:1229:U:H2'	31:a:1230:G:C8	2.50	0.46
35:e:25:VAL:HG22	35:e:26:LYS:H	1.80	0.46
47:q:61:VAL:HG12	47:q:80:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:350:G:H8	5:A:373:A:N6	2.14	0.46
5:A:363:A:OP1	9:E:135:LYS:NZ	2.48	0.46
5:A:441:C:H2'	5:A:442:G:C8	2.51	0.46
5:A:1829:A:H2'	5:A:1830:A:C8	2.50	0.46
6:B:71:A:C2	24:T:38:ASN:ND2	2.84	0.46
10:F:92:ARG:O	10:F:96:MET:CE	2.64	0.46
25:U:80:LYS:HE3	25:U:80:LYS:HB3	1.77	0.46
31:a:328:A:O2'	31:a:1445:G:O2'	2.24	0.46
31:a:561:A:H2'	31:a:562:U:C6	2.50	0.46
31:a:732:G:OP2	31:a:863:U:O2'	2.23	0.46
31:a:1388:C:O4'	37:g:92:ARG:NH1	2.48	0.46
31:a:1445:G:H2'	31:a:1446:C:C6	2.51	0.46
49:s:40:ILE:HD11	49:s:71:LEU:HB3	1.98	0.46
5:A:1578:A:H1'	5:A:1588:U:N3	2.28	0.46
5:A:1693:G:C6	5:A:2036:G:O6	2.68	0.46
5:A:1823:U:H2'	5:A:1824:C:C6	2.50	0.46
5:A:2146:A:N6	5:A:2195:G:H22	2.13	0.46
5:A:2645:G:H21	8:D:163:VAL:HG21	1.81	0.46
25:U:23:ASP:OD1	25:U:24:SER:N	2.43	0.46
31:a:203:A:O2'	31:a:204:A:O5'	2.30	0.46
31:a:390:A:H2'	31:a:391:A:C8	2.50	0.46
31:a:425:G:H2'	31:a:426:U:C6	2.51	0.46
31:a:716:A:H2'	31:a:717:U:C6	2.50	0.46
31:a:745:U:C2	31:a:746:U:C5	3.03	0.46
31:a:1197:G:H2'	31:a:1198:A:C8	2.50	0.46
34:d:3:ARG:HD2	34:d:3:ARG:HA	1.47	0.46
4:4:1:MET:HE2	4:4:1:MET:HB2	1.80	0.46
5:A:720:A:OP1	9:E:76:GLY:HA3	2.16	0.46
5:A:924:G:H2'	5:A:925:G:C8	2.51	0.46
5:A:1198:G:OP2	19:O:58:ARG:NH2	2.40	0.46
5:A:1737:U:H5''	5:A:1738:C:H5	1.80	0.46
5:A:2144:A:H1'	5:A:2175:G:H4'	1.97	0.46
5:A:2459:A:H2'	5:A:2460:A:C8	2.50	0.46
5:A:2817:A:H1'	5:A:2818:A:H5'	1.96	0.46
16:L:106:GLN:NE2	16:L:118:ILE:CD1	2.79	0.46
31:a:1278:G:H2'	31:a:1279:A:C8	2.51	0.46
34:d:67:GLN:O	34:d:71:THR:OG1	2.32	0.46
35:e:115:LEU:HD22	35:e:120:ILE:HG21	1.98	0.46
41:k:74:ALA:O	41:k:79:LEU:HD23	2.16	0.46
5:A:1422:A:H1'	5:A:1423:C:C6	2.51	0.46
5:A:1899:U:H1'	5:A:1900:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2124:U:C4	5:A:2125:U:C4	3.04	0.46
5:A:2854:A:H2'	5:A:2899:A:N6	2.31	0.46
7:C:139:THR:HG21	7:C:192:ILE:HD12	1.97	0.46
31:a:41:C:H2'	31:a:42:G:C8	2.51	0.46
31:a:552:G:OP1	34:d:55:GLN:NE2	2.46	0.46
31:a:887:U:H2'	31:a:888:C:H6	1.81	0.46
32:b:154:MET:HE3	32:b:155:LYS:H	1.81	0.46
4:4:15:LYS:HB3	4:4:15:LYS:HE3	1.66	0.46
5:A:2575:G:H1'	13:I:23:LYS:HZ1	1.76	0.46
13:I:71:ARG:HH11	18:N:74:ARG:NE	2.14	0.46
31:a:1154:G:N2	31:a:1156:A:H62	2.14	0.46
33:c:57:GLU:O	33:c:64:ASN:N	2.36	0.46
47:q:53:ASN:O	47:q:53:ASN:ND2	2.49	0.46
8:D:33:ASN:HB2	8:D:105:VAL:HB	1.98	0.46
15:K:65:TRP:CH2	15:K:107:ALA:HB3	2.42	0.46
18:N:91:ARG:HG3	18:N:92:GLY:H	1.81	0.46
31:a:137:U:OP1	46:p:66:LYS:NZ	2.48	0.46
31:a:470:A:H2'	31:a:471:A:H8	1.79	0.46
31:a:501:U:H2'	31:a:502:C:C2	2.51	0.46
31:a:692:U:H2'	31:a:693:G:O4'	2.15	0.46
31:a:927:A:H2'	31:a:928:A:C8	2.51	0.46
31:a:1185:G:C2	31:a:1186:A:C8	3.04	0.46
46:p:20:ILE:HG22	46:p:37:ILE:HB	1.98	0.46
2:2:17:HIS:CE1	5:A:511:G:H4'	2.51	0.46
5:A:64:A:H1'	22:R:65:MET:HB2	1.98	0.46
12:H:68:ASN:O	12:H:68:ASN:CG	2.58	0.46
12:H:93:LEU:HA	12:H:93:LEU:HD23	1.77	0.46
19:O:45:TYR:CD1	19:O:48:ARG:NH2	2.84	0.46
19:O:78:ARG:N	19:O:78:ARG:HD3	2.31	0.46
23:S:36:GLU:HA	23:S:60:GLU:OE2	2.16	0.46
25:U:57:GLU:CD	25:U:57:GLU:N	2.73	0.46
27:W:7:ARG:O	27:W:60:ARG:NH2	2.49	0.46
29:Y:9:TYR:CZ	29:Y:26:GLY:HA2	2.51	0.46
31:a:272:C:O2'	47:q:68:PRO:O	2.29	0.46
31:a:435:C:H5''	34:d:10:LYS:HD3	1.98	0.46
43:m:65:VAL:HG13	43:m:66:GLU:H	1.80	0.46
5:A:84:A:H1'	5:A:85:G:C1'	2.46	0.45
5:A:632:U:H2'	5:A:633:A:H8	1.81	0.45
5:A:2431:C:H2'	5:A:2432:G:O4'	2.15	0.45
24:T:55:VAL:HG21	24:T:59:GLY:HA3	1.98	0.45
31:a:1278:G:N2	31:a:1337:A:H1'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1435:A:H2'	31:a:1436:A:O4'	2.16	0.45
5:A:2153:A:C4'	5:A:2190:C:H42	2.29	0.45
8:D:128:GLN:HG3	8:D:173:MET:HE3	1.98	0.45
11:G:92:VAL:O	11:G:92:VAL:HG23	2.16	0.45
31:a:36:G:H2'	31:a:37:C:C6	2.51	0.45
31:a:412:G:O6	31:a:507:A:N1	2.49	0.45
31:a:562:U:C2	31:a:563:C:C5	3.03	0.45
31:a:622:A:H2'	31:a:623:C:C6	2.52	0.45
31:a:1097:U:H2'	31:a:1098:G:H8	1.80	0.45
31:a:1417:C:C2	31:a:1418:A:C8	3.04	0.45
34:d:8:ASN:OD1	34:d:20:SER:OG	2.29	0.45
39:i:98:GLY:O	39:i:102:ARG:NH2	2.49	0.45
50:t:33:LYS:HE3	50:t:33:LYS:HB3	1.78	0.45
5:A:1880:A:H2'	5:A:1881:A:C8	2.51	0.45
13:I:18:GLU:OE2	13:I:19:VAL:N	2.49	0.45
13:I:35:ILE:HD13	13:I:69:VAL:HG22	1.98	0.45
20:P:100:ILE:HG22	20:P:101:ASN:N	2.32	0.45
21:Q:11:ARG:C	21:Q:11:ARG:HH11	2.23	0.45
27:W:62:ILE:HA	27:W:62:ILE:HD12	1.68	0.45
31:a:1243:G:H2'	31:a:1244:C:C6	2.51	0.45
31:a:1505:G:C2	31:a:1506:U:C5	3.04	0.45
37:g:10:ARG:H	37:g:10:ARG:HG2	1.49	0.45
41:k:36:ASP:OD1	41:k:40:ASN:N	2.48	0.45
45:o:75:ILE:H	45:o:75:ILE:HD12	1.81	0.45
5:A:631:U:H2'	5:A:632:U:C6	2.52	0.45
5:A:1278:G:C8	5:A:1279:C:C6	3.05	0.45
10:F:120:LYS:HD3	10:F:120:LYS:HA	1.66	0.45
12:H:73:LYS:O	12:H:73:LYS:HG3	2.17	0.45
14:J:15:GLU:OE2	14:J:16:ARG:O	2.34	0.45
31:a:197:U:C2	31:a:198:G:C8	3.04	0.45
31:a:775:A:C4	31:a:776:A:C8	3.04	0.45
31:a:954:G:H1	31:a:1246:A:H61	1.65	0.45
31:a:1310:G:P	31:a:1345:C:H42	2.38	0.45
31:a:1336:U:H2'	31:a:1337:A:C8	2.48	0.45
31:a:1390:U:C4	37:g:3:ARG:HG2	2.52	0.45
39:i:27:GLU:HA	39:i:61:GLY:O	2.17	0.45
49:s:33:THR:HB	49:s:51:VAL:HA	1.98	0.45
1:l:9:CYS:SG	1:l:12:CYS:N	2.88	0.45
5:A:273:A:N1	5:A:415:U:H4'	2.32	0.45
5:A:651:A:H2'	5:A:652:A:C8	2.50	0.45
5:A:1128:A:C8	5:A:1129:A:C8	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1308:C:H5''	5:A:1309:G:C5'	2.47	0.45
9:E:5:ASP:HA	9:E:13:LYS:HZ1	1.81	0.45
22:R:57:ASN:OD1	22:R:76:ARG:NH1	2.48	0.45
23:S:16:ASP:OD1	23:S:19:LYS:NZ	2.46	0.45
31:a:659:C:H2'	31:a:660:U:C6	2.51	0.45
42:l:86:ASN:OD1	42:l:86:ASN:N	2.48	0.45
5:A:719:G:H5''	9:E:76:GLY:N	2.32	0.45
5:A:2253:C:C2	5:A:2254:A:C8	3.05	0.45
8:D:118:VAL:HG23	8:D:209:VAL:HB	1.99	0.45
13:I:91:LYS:HE3	13:I:111:PHE:CE1	2.51	0.45
31:a:1001:U:H4'	31:a:1002:G:O5'	2.15	0.45
34:d:179:LEU:HD12	34:d:180:PRO:HD2	1.98	0.45
48:r:44:ILE:HD13	48:r:61:THR:HG23	1.99	0.45
5:A:523:A:H2'	5:A:524:A:C8	2.52	0.45
5:A:925:G:H3'	5:A:926:G:H8	1.82	0.45
5:A:1225:G:H3'	5:A:1226:G:H8	1.81	0.45
5:A:2122:A:C4	5:A:2123:A:C8	3.04	0.45
5:A:2294:A:H5''	5:A:2295:A:H5'	1.97	0.45
9:E:146:LEU:O	9:E:148:GLN:OE1	2.34	0.45
10:F:110:ARG:HD3	10:F:136:LEU:HA	1.99	0.45
15:K:51:ARG:HA	15:K:54:MET:HE2	1.97	0.45
20:P:27:VAL:CG2	20:P:28:ASN:N	2.79	0.45
21:Q:40:ASN:O	21:Q:40:ASN:ND2	2.50	0.45
22:R:9:ARG:HG2	22:R:28:ASP:CB	2.46	0.45
31:a:409:C:O2'	31:a:629:A:N3	2.49	0.45
31:a:967:A:H2'	31:a:968:A:C8	2.52	0.45
31:a:1394:C:H2'	31:a:1395:G:C8	2.52	0.45
32:b:113:ARG:O	32:b:117:ILE:HG13	2.17	0.45
43:m:51:ASP:OD1	43:m:52:GLU:N	2.49	0.45
5:A:1000:G:N2	5:A:1003:A:H3'	2.32	0.45
5:A:1801:C:O2	5:A:1801:C:H2'	2.16	0.45
5:A:1818:A:C2'	5:A:1819:G:H5'	2.47	0.45
11:G:98:MET:HE3	11:G:98:MET:HB3	1.81	0.45
16:L:55:ASP:OD1	16:L:55:ASP:O	2.35	0.45
31:a:382:A:C6	31:a:383:U:C4	3.04	0.45
31:a:444:C:H2'	31:a:445:U:C6	2.52	0.45
31:a:451:U:O2'	31:a:452:A:O5'	2.35	0.45
31:a:839:U:O2'	31:a:1550:C:OP1	2.31	0.45
31:a:1132:U:C2	31:a:1133:U:C5	3.04	0.45
31:a:1187:G:H3'	31:a:1188:G:C8	2.49	0.45
31:a:1259:C:O2'	39:i:73:GLY:O	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:36:ARG:HG3	37:g:40:GLN:HG3	1.99	0.45
40:j:10:LEU:HB2	40:j:18:ILE:HD11	1.98	0.45
5:A:90:A:H1'	5:A:91:A:C8	2.52	0.45
5:A:249:C:O2'	5:A:431:C:H4'	2.16	0.45
5:A:1315:C:H2'	5:A:1316:G:C8	2.52	0.45
5:A:1758:A:H5''	5:A:1759:G:H21	1.80	0.45
5:A:1932:C:H4'	5:A:1956:G:H8	1.82	0.45
5:A:2279:G:C8	25:U:12:LYS:HD2	2.51	0.45
8:D:29:GLU:OE2	8:D:31:LYS:HD3	2.16	0.45
9:E:146:LEU:C	9:E:147:GLU:HG3	2.41	0.45
20:P:27:VAL:CG2	20:P:31:ASP:CB	2.94	0.45
26:V:40:VAL:CG2	26:V:45:LYS:HB3	2.47	0.45
31:a:205:A:C2	31:a:206:A:C5	3.04	0.45
31:a:561:A:H2'	31:a:562:U:H6	1.81	0.45
31:a:987:A:C8	31:a:988:C:H5	2.34	0.45
31:a:1516:G:H5''	31:a:1517:U:H2'	1.99	0.45
32:b:17:GLY:HA2	32:b:188:ASP:OD1	2.16	0.45
44:n:20:GLU:OE1	44:n:20:GLU:N	2.45	0.45
3:3:24:ARG:HD2	14:J:61:LEU:HD21	1.98	0.45
5:A:1680:U:H2'	5:A:1681:U:C6	2.51	0.45
13:I:71:ARG:NH1	18:N:74:ARG:CZ	2.80	0.45
31:a:328:A:H2'	31:a:329:A:C8	2.52	0.45
31:a:341:U:H2'	31:a:342:C:H6	1.82	0.45
31:a:452:A:N6	31:a:499:A:N6	2.64	0.45
31:a:674:G:H5'	31:a:734:C:H1'	1.99	0.45
31:a:920:U:H2'	31:a:921:C:H6	1.82	0.45
31:a:1197:G:H2'	31:a:1198:A:H8	1.81	0.45
32:b:18:HIS:HB2	32:b:189:THR:HB	1.98	0.45
33:c:76:ILE:HA	33:c:83:ILE:HB	1.99	0.45
45:o:56:LEU:HA	45:o:59:MET:HE3	1.99	0.45
49:s:32:LYS:HG3	49:s:34:TRP:HZ3	1.81	0.45
5:A:1115:G:N2	5:A:1136:C:OP2	2.50	0.44
5:A:2564:U:H2'	5:A:2565:C:C6	2.53	0.44
31:a:34:A:H2'	31:a:35:C:H6	1.82	0.44
31:a:271:A:H2'	31:a:272:C:C5	2.52	0.44
31:a:1118:C:C4	31:a:1119:G:C8	3.05	0.44
33:c:33:HIS:CE1	44:n:38:LYS:HB3	2.51	0.44
40:j:34:ALA:HB1	40:j:76:ILE:HD11	1.99	0.44
41:k:53:LYS:HD3	41:k:54:GLY:N	2.32	0.44
47:q:19:MET:HE3	47:q:22:THR:HG22	1.99	0.44
5:A:1712:A:O2'	5:A:1718:G:N7	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2260:A:H2'	5:A:2261:G:C8	2.51	0.44
5:A:2369:C:H3'	5:A:2370:U:O2	2.17	0.44
5:A:2917:U:H2'	5:A:2918:A:C8	2.52	0.44
11:G:23:HIS:CE1	11:G:34:SER:HB3	2.52	0.44
18:N:35:ILE:H	18:N:35:ILE:HG12	1.50	0.44
19:O:33:LYS:HB2	19:O:33:LYS:HE3	1.75	0.44
20:P:20:ILE:HG13	20:P:95:LEU:HB2	1.98	0.44
22:R:46:PHE:CE2	22:R:87:ILE:HG23	2.52	0.44
31:a:110:G:H1	31:a:338:C:H41	1.65	0.44
31:a:550:U:H2'	31:a:551:G:C8	2.52	0.44
31:a:666:G:C6	31:a:667:C:C4	3.05	0.44
31:a:1094:U:O2'	31:a:1113:A:OP2	2.35	0.44
31:a:1395:G:C4	31:a:1396:G:C8	3.06	0.44
32:b:120:MET:HA	32:b:123:ASP:CG	2.42	0.44
33:c:85:LYS:HA	33:c:88:ASN:HD21	1.82	0.44
37:g:150:ALA:HB3	41:k:56:LYS:NZ	2.32	0.44
3:3:7:HIS:ND1	3:3:10:ALA:N	2.66	0.44
5:A:1379:A:HO2'	5:A:1381:U:P	2.38	0.44
5:A:2670:G:H2'	5:A:2671:A:C8	2.52	0.44
15:K:43:THR:O	15:K:47:ILE:HG13	2.17	0.44
31:a:929:U:H2'	31:a:930:U:C6	2.52	0.44
31:a:1396:G:N3	31:a:1397:G:C8	2.86	0.44
32:b:28:LYS:HE3	32:b:28:LYS:HB3	1.72	0.44
33:c:110:LEU:HD13	33:c:203:ARG:HD3	1.98	0.44
48:r:31:THR:O	48:r:35:LYS:HG3	2.17	0.44
5:A:1312:A:N7	16:L:12:GLN:HG2	2.33	0.44
5:A:2022:U:H3'	5:A:2023:C:H2'	1.98	0.44
5:A:2212:G:H2'	5:A:2213:U:C6	2.52	0.44
6:B:28:C:H1'	6:B:55:A:H61	1.82	0.44
13:I:107:ARG:HD3	13:I:115:VAL:HG11	1.98	0.44
21:Q:46:VAL:O	21:Q:50:VAL:HG23	2.17	0.44
30:Z:29:GLU:OE1	30:Z:34:GLY:O	2.34	0.44
31:a:423:A:O2'	31:a:424:G:O5'	2.36	0.44
31:a:683:A:H1'	41:k:118:HIS:CG	2.53	0.44
31:a:911:G:C2	31:a:912:G:C8	3.06	0.44
31:a:1102:U:C2	31:a:1106:U:C4	3.06	0.44
31:a:1228:U:OP1	44:n:9:LYS:HE3	2.17	0.44
31:a:1297:A:H8	31:a:1363:G:O2'	2.00	0.44
31:a:1552:U:H3'	32:b:22:ARG:HH12	1.83	0.44
4:4:13:LYS:HD2	4:4:28:GLU:CD	2.42	0.44
5:A:529:A:H5'	23:S:44:HIS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:923:A:H2'	5:A:924:G:C8	2.53	0.44
6:B:64:A:N6	6:B:104:A:H2'	2.33	0.44
31:a:63:U:H2'	31:a:64:C:H6	1.82	0.44
31:a:277:U:H2'	31:a:278:A:C8	2.51	0.44
31:a:490:A:H2'	31:a:491:C:O4'	2.18	0.44
31:a:1325:U:H2'	31:a:1326:G:C8	2.53	0.44
39:i:46:LEU:HD11	39:i:74:PHE:HD1	1.81	0.44
43:m:107:ARG:NH2	43:m:113:VAL:HG22	2.33	0.44
5:A:1617:A:H2'	5:A:1618:A:C8	2.53	0.44
5:A:1806:U:H5'	5:A:1807:A:O5'	2.18	0.44
5:A:2035:C:H2'	5:A:2036:G:H8	1.82	0.44
5:A:2591:A:O2'	5:A:2592:A:O5'	2.26	0.44
5:A:2874:A:H2'	5:A:2875:U:C6	2.53	0.44
7:C:74:ILE:N	7:C:74:ILE:CD1	2.80	0.44
11:G:17:VAL:HG13	11:G:26:VAL:HG22	1.99	0.44
31:a:189:G:N2	31:a:202:C:H1'	2.32	0.44
31:a:616:A:H2'	31:a:617:A:O4'	2.17	0.44
31:a:660:U:C5	31:a:760:G:C4	3.06	0.44
31:a:951:G:C2	31:a:1352:C:C2	3.06	0.44
31:a:957:C:OP2	43:m:107:ARG:HG2	2.18	0.44
31:a:1107:C:H2'	31:a:1108:C:H6	1.82	0.44
31:a:1330:C:H42	49:s:36:ARG:HB2	1.82	0.44
31:a:1359:A:H1'	31:a:1384:A:N6	2.28	0.44
31:a:1550:C:OP2	31:a:1550:C:H6	2.01	0.44
34:d:182:ARG:HA	34:d:185:LEU:HD12	1.99	0.44
45:o:29:ILE:HG23	45:o:63:ARG:HG3	1.99	0.44
10:F:34:ILE:HG13	10:F:91:LEU:HB2	1.99	0.44
10:F:35:VAL:HG12	10:F:155:VAL:HG22	1.99	0.44
16:L:69:VAL:HG12	16:L:70:GLU:N	2.32	0.44
31:a:479:U:H2'	31:a:480:G:H8	1.82	0.44
31:a:485:U:O2'	31:a:486:C:H5'	2.17	0.44
40:j:16:ARG:HD3	40:j:16:ARG:HA	1.64	0.44
5:A:1054:A:OP1	19:O:66:ASN:ND2	2.43	0.44
10:F:103:LEU:HD12	10:F:103:LEU:HA	1.89	0.44
16:L:92:ARG:HD2	16:L:93:TYR:CZ	2.52	0.44
24:T:72:VAL:HG21	24:T:91:PHE:HB3	2.00	0.44
26:V:31:ALA:HB3	26:V:33:LEU:HG	1.99	0.44
31:a:421:G:H5''	31:a:436:G:N2	2.32	0.44
31:a:434:U:H2'	31:a:435:C:C6	2.53	0.44
31:a:563:C:C2	31:a:564:C:C5	3.06	0.44
31:a:855:C:C2	31:a:856:C:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1541:G:C2	31:a:1542:A:C6	3.06	0.44
4:4:33:LYS:HB2	4:4:33:LYS:HE2	1.86	0.44
5:A:1328:C:C2	5:A:1329:G:C8	3.05	0.44
5:A:1712:A:N3	5:A:1714:C:N4	2.65	0.44
5:A:1745:A:H2	31:a:1485:G:O2'	2.01	0.44
5:A:2786:G:HO2'	5:A:2787:C:H6	1.66	0.44
5:A:2793:G:C2	5:A:2794:C:C6	3.06	0.44
11:G:90:VAL:O	11:G:94:TYR:CD2	2.71	0.44
17:M:41:TYR:CD2	17:M:57:SER:OG	2.65	0.44
23:S:45:GLN:OE1	23:S:46:LYS:N	2.51	0.44
23:S:91:VAL:HG22	23:S:92:ARG:N	2.31	0.44
24:T:84:ASN:C	24:T:85:GLN:HG3	2.42	0.44
31:a:262:G:O6	31:a:281:A:N6	2.50	0.44
31:a:697:C:OP1	41:k:46:SER:OG	2.30	0.44
31:a:758:C:C2	31:a:759:U:C5	3.06	0.44
31:a:909:A:H2'	31:a:910:A:C8	2.53	0.44
31:a:1005:A:C5	31:a:1006:U:C4	3.05	0.44
31:a:1131:C:H2'	31:a:1132:U:H6	1.83	0.44
31:a:1182:C:H2'	31:a:1183:C:H6	1.83	0.44
31:a:1287:C:H1'	31:a:1292:C:O2	2.18	0.44
47:q:32:THR:HG22	47:q:39:ARG:HG2	2.00	0.44
49:s:15:LEU:HD12	49:s:15:LEU:HA	1.75	0.44
5:A:1103:G:O6	5:A:1124:A:N6	2.51	0.43
5:A:2278:OMG:HM23	5:A:2278:OMG:H1'	1.48	0.43
5:A:2611:U:H2'	5:A:2612:U:H2'	2.00	0.43
5:A:2725:U:H2'	5:A:2726:C:C6	2.53	0.43
13:I:77:ILE:O	13:I:77:ILE:HG23	2.18	0.43
18:N:17:THR:C	18:N:19:LEU:H	2.26	0.43
25:U:54:TYR:HE2	25:U:84:LYS:HG2	1.83	0.43
31:a:618:G:C6	31:a:619:C:C5	3.05	0.43
31:a:764:C:H2'	31:a:765:U:C6	2.53	0.43
31:a:932:A:H2'	31:a:933:C:H6	1.82	0.43
31:a:987:A:N7	31:a:1328:A:N6	2.65	0.43
32:b:6:MET:O	32:b:10:LEU:HD23	2.18	0.43
34:d:89:LEU:HD23	34:d:89:LEU:HA	1.90	0.43
35:e:162:GLU:OE1	35:e:162:GLU:N	2.49	0.43
36:f:90:MET:HG2	36:f:92:ILE:HD13	1.99	0.43
45:o:75:ILE:HD12	45:o:75:ILE:N	2.33	0.43
47:q:19:MET:HG3	47:q:22:THR:HB	2.00	0.43
49:s:19:VAL:HG21	49:s:44:PHE:CE1	2.53	0.43
49:s:71:LEU:HA	49:s:74:PHE:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2123:A:C4	5:A:2124:U:C5	3.06	0.43
23:S:7:ASP:HB2	23:S:70:LEU:HD21	2.00	0.43
23:S:84:LYS:CE	23:S:93:ILE:HD12	2.48	0.43
31:a:1171:C:C2	31:a:1172:C:C5	3.06	0.43
36:f:90:MET:HE1	48:r:66:ARG:HB3	1.99	0.43
37:g:150:ALA:HB3	41:k:56:LYS:HZ2	1.83	0.43
39:i:112:MET:SD	39:i:113:LYS:N	2.91	0.43
43:m:19:LEU:HD22	43:m:25:ILE:HG21	1.99	0.43
43:m:114:LYS:O	43:m:114:LYS:HG2	2.18	0.43
47:q:62:LYS:HE2	47:q:62:LYS:HB2	1.75	0.43
5:A:300:G:N1	5:A:467:U:O2'	2.50	0.43
7:C:74:ILE:H	7:C:74:ILE:CD1	2.28	0.43
12:H:36:ILE:HG22	12:H:37:LEU:N	2.32	0.43
22:R:52:SER:OG	22:R:81:THR:CG2	2.66	0.43
23:S:3:ILE:CD1	23:S:4:LYS:O	2.66	0.43
31:a:342:C:C2	31:a:343:C:C5	3.07	0.43
31:a:365:G:C2	31:a:366:U:C5	3.06	0.43
32:b:81:LYS:HG3	32:b:91:TYR:CZ	2.53	0.43
4:4:1:MET:HE3	5:A:2769:G:H5''	2.01	0.43
5:A:305:A:H62	5:A:410:G:H21	1.67	0.43
5:A:409:G:H3'	5:A:410:G:C8	2.54	0.43
5:A:2273:G:H2'	5:A:2274:A:H8	1.83	0.43
5:A:2793:G:H2'	5:A:2793:G:N3	2.34	0.43
5:A:2829:A:H3'	5:A:2830:A:H8	1.84	0.43
6:B:73:G:H21	24:T:88:HIS:CD2	2.35	0.43
12:H:19:ILE:HG13	12:H:55:VAL:HG13	2.00	0.43
12:H:37:LEU:C	12:H:37:LEU:HD12	2.42	0.43
13:I:43:VAL:HG23	13:I:54:LYS:HA	2.01	0.43
31:a:383:U:C2	31:a:384:G:C8	3.07	0.43
31:a:1137:U:C4	40:j:73:LEU:HD11	2.53	0.43
31:a:1229:U:H2'	31:a:1230:G:H8	1.83	0.43
47:q:41:LYS:HB2	47:q:41:LYS:HE2	1.71	0.43
50:t:3:ASN:HB3	50:t:8:ILE:HD11	1.99	0.43
5:A:1185:U:H4'	5:A:1186:A:O5'	2.18	0.43
5:A:1804:U:O2	5:A:1804:U:O4'	2.37	0.43
8:D:123:LYS:HE3	8:D:204:PRO:HA	2.00	0.43
13:I:91:LYS:CE	13:I:109:GLY:O	2.66	0.43
14:J:143:HIS:ND1	14:J:143:HIS:O	2.51	0.43
31:a:13:U:H4'	31:a:534:C:H4'	2.01	0.43
31:a:57:U:H2'	31:a:58:G:C8	2.54	0.43
31:a:304:U:O2'	31:a:564:C:O2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:358:G:H2'	31:a:359:G:C8	2.54	0.43
31:a:522:C:H2'	31:a:523:G:C8	2.46	0.43
31:a:725:C:H4'	41:k:119:ASN:ND2	2.27	0.43
31:a:742:A:H2'	31:a:743:C:H6	1.83	0.43
31:a:1216:G:C4	31:a:1217:C:C6	3.06	0.43
31:a:1455:U:O2'	31:a:1456:A:OP1	2.29	0.43
37:g:66:ILE:HA	37:g:66:ILE:HD13	1.69	0.43
49:s:23:GLU:OE1	49:s:23:GLU:N	2.51	0.43
49:s:29:GLN:HA	49:s:29:GLN:OE1	2.17	0.43
5:A:786:U:H2'	5:A:787:U:O4'	2.18	0.43
5:A:2799:C:H5'	8:D:181:GLN:NE2	2.34	0.43
9:E:146:LEU:O	9:E:147:GLU:CD	2.61	0.43
15:K:111:GLU:HG2	15:K:112:GLU:OE1	2.19	0.43
17:M:11:ARG:HE	17:M:11:ARG:HB3	1.63	0.43
17:M:95:ASP:OD1	17:M:95:ASP:C	2.60	0.43
24:T:94:ILE:HD12	24:T:94:ILE:H	1.82	0.43
31:a:184:A:C8	31:a:207:G:N2	2.85	0.43
31:a:204:A:C2	31:a:205:A:C5	3.06	0.43
31:a:956:G:H2'	31:a:957:C:C6	2.54	0.43
31:a:1201:A:H2'	31:a:1202:C:H6	1.81	0.43
31:a:1302:U:H2'	31:a:1303:G:C8	2.53	0.43
42:l:129:LEU:H	42:l:129:LEU:HG	1.49	0.43
8:D:168:LYS:HB2	8:D:168:LYS:HE3	1.36	0.43
10:F:69:LYS:HG3	10:F:84:PRO:CA	2.47	0.43
11:G:23:HIS:C	11:G:23:HIS:HD1	2.26	0.43
18:N:98:LYS:C	18:N:99:LEU:HD22	2.43	0.43
19:O:76:TYR:CE1	19:O:80:MET:HG3	2.53	0.43
31:a:122:C:OP1	31:a:319:C:O2'	2.35	0.43
31:a:414:G:C2	31:a:415:A:C8	3.07	0.43
31:a:877:C:H2'	31:a:878:A:O4'	2.18	0.43
31:a:921:C:H2'	31:a:922:A:H8	1.82	0.43
31:a:1170:G:C6	31:a:1171:C:C5	3.07	0.43
39:i:30:ILE:HG22	39:i:37:VAL:HB	2.01	0.43
42:l:96:ARG:HG2	42:l:111:VAL:HG22	2.01	0.43
5:A:1152:U:C5	5:A:1153:C:C2	3.07	0.43
5:A:2656:A:C6	5:A:2914:A:C4	3.07	0.43
5:A:2701:G:H4'	13:I:30:ARG:HD3	2.00	0.43
7:C:67:PHE:CE1	7:C:105:ILE:HD11	2.54	0.43
13:I:24:VAL:HG23	13:I:24:VAL:O	2.18	0.43
17:M:55:GLN:CD	17:M:56:ALA:N	2.77	0.43
22:R:23:ASP:OD2	22:R:82:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:71:A:H3'	31:a:72:C:C5'	2.49	0.43
31:a:340:G:C2	31:a:341:U:C6	3.06	0.43
31:a:422:A:C8	31:a:423:A:C8	3.07	0.43
31:a:479:U:H2'	31:a:480:G:C8	2.54	0.43
31:a:742:A:H2'	31:a:743:C:C6	2.54	0.43
31:a:835:U:H5	31:a:881:A:N1	2.17	0.43
31:a:956:G:H5''	43:m:107:ARG:HB2	2.00	0.43
31:a:1161:A:O2'	31:a:1162:A:H5''	2.19	0.43
31:a:1182:C:H2'	31:a:1183:C:C6	2.54	0.43
31:a:1536:G:H2'	31:a:1537:G:H8	1.83	0.43
32:b:57:LEU:HD23	32:b:57:LEU:HA	1.82	0.43
32:b:90:PHE:HE1	32:b:153:ASP:HB2	1.84	0.43
34:d:15:LEU:HD13	34:d:56:LYS:HA	2.00	0.43
34:d:155:VAL:HG13	34:d:156:GLU:HG3	2.01	0.43
5:A:441:C:H2'	5:A:442:G:H8	1.83	0.43
5:A:1141:U:H2'	5:A:1142:A:C4	2.53	0.43
5:A:1435:C:H2'	5:A:1436:C:C6	2.53	0.43
5:A:2106:U:H2'	5:A:2107:G:O4'	2.19	0.43
5:A:2332:U:H1'	10:F:151:GLY:CA	2.48	0.43
13:I:35:ILE:H	13:I:35:ILE:HD12	1.84	0.43
14:J:80:ASP:OD1	14:J:81:GLN:N	2.52	0.43
14:J:88:GLY:N	14:J:120:LYS:O	2.50	0.43
21:Q:11:ARG:HH21	21:Q:98:LYS:HB3	1.83	0.43
31:a:888:C:H2'	31:a:889:C:H6	1.83	0.43
31:a:1126:U:H2'	31:a:1127:U:C6	2.54	0.43
31:a:1242:U:P	39:i:128:GLN:HE21	2.42	0.43
39:i:41:LEU:HD13	39:i:46:LEU:HB3	2.01	0.43
43:m:85:SER:OG	43:m:87:ARG:O	2.37	0.43
43:m:91:HIS:ND1	43:m:97:VAL:HG11	2.34	0.43
5:A:556:U:H4'	5:A:1273:G:H4'	2.01	0.43
5:A:1197:C:H2'	5:A:1198:G:O4'	2.19	0.43
5:A:1583:G:H4'	5:A:1584:U:O4'	2.19	0.43
5:A:2859:G:C4	5:A:2860:U:C5	3.07	0.43
11:G:92:VAL:O	11:G:92:VAL:CG2	2.67	0.43
16:L:16:MET:HE2	16:L:16:MET:HB3	1.84	0.43
20:P:65:GLN:HG2	20:P:93:THR:HG22	2.00	0.43
31:a:165:G:C2	31:a:166:G:C8	3.07	0.43
31:a:484:A:C4	31:a:485:U:C5	3.06	0.43
31:a:952:U:O2'	39:i:128:GLN:OE1	2.29	0.43
31:a:1176:G:H3'	31:a:1177:A:C5'	2.48	0.43
31:a:1228:U:H2'	31:a:1229:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1271:A:N6	31:a:1284:A:O2'	2.52	0.43
5:A:1094:A:C6	5:A:2778:G:C2	3.07	0.42
5:A:2707:C:H5'	8:D:202:PRO:HA	2.01	0.42
22:R:65:MET:HE2	22:R:65:MET:HB3	1.91	0.42
27:W:28:LEU:HD21	27:W:42:ARG:NH1	2.34	0.42
28:X:40:ASN:OD1	28:X:40:ASN:C	2.62	0.42
31:a:203:A:C2	31:a:204:A:C5	3.07	0.42
31:a:483:C:H2'	31:a:484:A:H8	1.81	0.42
31:a:560:U:N3	31:a:561:A:N7	2.67	0.42
31:a:617:A:C5	31:a:618:G:C8	3.07	0.42
31:a:946:A:H2'	31:a:947:A:H8	1.84	0.42
31:a:1171:C:C2'	31:a:1172:C:H5'	2.49	0.42
32:b:117:ILE:HG23	32:b:120:MET:HE1	2.01	0.42
5:A:1000:G:H2'	5:A:1001:A:H2'	2.01	0.42
5:A:1630:A:H1'	5:A:1631:G:C8	2.54	0.42
5:A:2135:U:H4'	5:A:2177:U:H1'	2.00	0.42
5:A:2355:A:H2'	5:A:2356:A:C8	2.53	0.42
15:K:69:PHE:HA	15:K:70:PRO:HD3	1.85	0.42
15:K:130:LYS:HE2	15:K:130:LYS:HB3	1.94	0.42
19:O:102:ASP:OD1	19:O:104:LYS:CE	2.67	0.42
20:P:34:THR:HG23	20:P:34:THR:O	2.18	0.42
20:P:36:ASP:OD1	20:P:36:ASP:N	2.44	0.42
24:T:31:VAL:HG12	24:T:91:PHE:CB	2.47	0.42
31:a:123:G:H2'	31:a:124:U:H6	1.84	0.42
31:a:267:G:O2'	31:a:268:G:H5'	2.20	0.42
31:a:432:G:H2'	31:a:433:A:C8	2.54	0.42
31:a:612:G:C6	31:a:643:A:C6	3.07	0.42
31:a:1085:G:O2'	31:a:1112:A:N1	2.48	0.42
31:a:1133:U:H2'	31:a:1134:A:C8	2.54	0.42
32:b:114:ILE:CD1	32:b:144:LEU:HB3	2.44	0.42
37:g:37:GLY:O	37:g:41:ARG:HD2	2.19	0.42
45:o:76:GLN:OE1	45:o:76:GLN:HA	2.19	0.42
49:s:30:VAL:HG22	49:s:48:THR:HG21	2.01	0.42
5:A:1844:G:H2'	5:A:1845:U:H5'	2.01	0.42
5:A:2304:G:OP2	25:U:20:ASN:OD1	2.37	0.42
12:H:15:LYS:HD2	12:H:17:TYR:CZ	2.54	0.42
15:K:76:LYS:HB3	15:K:91:GLU:OE1	2.19	0.42
23:S:45:GLN:OE1	23:S:45:GLN:CA	2.67	0.42
31:a:261:U:H2'	31:a:262:G:H8	1.84	0.42
38:h:116:LYS:HE2	38:h:116:LYS:HB2	1.83	0.42
41:k:88:GLY:HA2	41:k:89:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:o:7:ARG:HA	45:o:10:GLU:OE1	2.20	0.42
5:A:283:G:H3'	5:A:284:C:H6	1.83	0.42
5:A:300:G:H1	5:A:467:U:HO2'	1.65	0.42
5:A:460:C:N4	5:A:2435:U:O4	2.52	0.42
5:A:1726:A:H2'	5:A:1727:C:C6	2.55	0.42
7:C:117:GLU:O	7:C:128:ASN:HB2	2.19	0.42
10:F:22:TYR:HB3	10:F:27:GLU:HB3	2.01	0.42
13:I:4:GLN:HA	13:I:21:THR:HG23	2.00	0.42
17:M:40:ILE:HG23	17:M:76:VAL:HG21	2.01	0.42
31:a:211:A:H1'	31:a:212:A:O4'	2.20	0.42
31:a:973:A:H4'	40:j:57:LYS:HE3	2.00	0.42
31:a:1271:A:C5	31:a:1272:A:C8	3.07	0.42
35:e:55:GLU:HB2	35:e:58:GLU:OE1	2.19	0.42
5:A:37:C:H4'	5:A:497:U:OP1	2.20	0.42
5:A:231:A:H3'	5:A:231:A:N3	2.35	0.42
5:A:1917:A:H3'	5:A:1918:G:O4'	2.20	0.42
6:B:43:A:H2'	6:B:44:A:O4'	2.19	0.42
7:C:69:ARG:HE	7:C:69:ARG:HB3	1.56	0.42
7:C:100:GLU:OE2	7:C:102:ARG:CD	2.68	0.42
12:H:15:LYS:CD	12:H:17:TYR:CZ	3.02	0.42
13:I:20:LEU:O	13:I:41:CYS:HB2	2.19	0.42
16:L:22:THR:O	16:L:26:ILE:HG12	2.20	0.42
25:U:54:TYR:HD2	25:U:80:LYS:HD3	1.85	0.42
31:a:468:G:H2'	31:a:469:U:C6	2.54	0.42
31:a:571:A:H2'	31:a:575:G:C8	2.54	0.42
31:a:617:A:C6	31:a:618:G:C8	3.07	0.42
31:a:699:G:H2'	31:a:700:U:C6	2.55	0.42
31:a:745:U:H2'	31:a:746:U:C6	2.54	0.42
31:a:992:A:H5'	31:a:993:C:OP2	2.19	0.42
31:a:1167:A:C2	31:a:1191:G:C5	3.07	0.42
31:a:1327:C:H2'	31:a:1328:A:O4'	2.20	0.42
37:g:74:GLU:HB2	37:g:91:VAL:HG22	2.01	0.42
37:g:148:ASN:HD22	37:g:148:ASN:N	2.16	0.42
43:m:86:TYR:CZ	43:m:90:ARG:HD2	2.54	0.42
44:n:26:ARG:HD2	44:n:47:LEU:HD11	2.00	0.42
5:A:27:G:N2	5:A:557:G:H1'	2.34	0.42
5:A:1873:G:H2'	5:A:1874:A:C8	2.54	0.42
5:A:2142:G:O2'	5:A:2192:G:N1	2.45	0.42
5:A:2346:U:OP2	5:A:2346:U:C6	2.73	0.42
7:C:171:TYR:HB3	7:C:183:MET:HB3	2.02	0.42
23:S:20:GLU:OE1	23:S:20:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:44:ILE:HG21	25:U:47:ARG:HG2	2.01	0.42
31:a:500:A:O2'	31:a:501:U:H5'	2.20	0.42
31:a:911:G:N3	31:a:912:G:C8	2.87	0.42
38:h:98:LEU:HD22	38:h:132:TRP:HB2	2.00	0.42
41:k:105:LEU:HD23	41:k:105:LEU:HA	1.91	0.42
43:m:16:VAL:HG13	43:m:17:ILE:HG12	2.01	0.42
5:A:286:U:H4'	5:A:287:G:C8	2.54	0.42
5:A:1238:U:O4'	19:O:4:VAL:HG23	2.20	0.42
5:A:1296:C:O2'	5:A:1297:G:H5'	2.19	0.42
5:A:1378:U:H3'	5:A:1434:U:O2	2.20	0.42
5:A:2273:G:H2'	5:A:2274:A:C8	2.55	0.42
8:D:6:LEU:HD23	8:D:6:LEU:HA	1.89	0.42
13:I:20:LEU:HD12	13:I:21:THR:N	2.35	0.42
13:I:90:ASP:OD1	13:I:92:GLY:N	2.53	0.42
23:S:41:MET:CE	23:S:61:ALA:HB2	2.50	0.42
25:U:77:PHE:CD1	25:U:77:PHE:N	2.88	0.42
31:a:248:U:H2'	31:a:249:G:C8	2.55	0.42
31:a:265:A:H2'	31:a:266:A:C8	2.55	0.42
31:a:421:G:H3'	31:a:436:G:H22	1.83	0.42
31:a:661:U:H5	38:h:57:GLN:OE1	2.02	0.42
31:a:1370:A:OP2	44:n:35:ARG:NH2	2.53	0.42
32:b:121:GLU:HG3	32:b:126:PHE:HD2	1.83	0.42
34:d:103:LEU:HD13	34:d:103:LEU:HA	1.93	0.42
36:f:14:ILE:HG21	36:f:19:LYS:HG3	2.02	0.42
42:l:33:LYS:HD3	42:l:33:LYS:HA	1.77	0.42
46:p:20:ILE:HD13	46:p:52:VAL:HG22	2.02	0.42
47:q:7:ARG:HB3	47:q:65:GLU:HG3	2.01	0.42
47:q:56:LYS:HE3	47:q:56:LYS:HB3	1.70	0.42
5:A:328:G:H1'	5:A:329:A:H5'	2.00	0.42
11:G:68:THR:HA	11:G:71:LEU:HB2	2.01	0.42
13:I:108:GLU:C	13:I:110:ASN:H	2.27	0.42
14:J:121:LEU:C	14:J:121:LEU:HD12	2.44	0.42
16:L:37:ALA:HA	16:L:40:VAL:HG12	2.00	0.42
31:a:432:G:H2'	31:a:433:A:H8	1.85	0.42
31:a:609:G:C6	31:a:646:G:C6	3.08	0.42
31:a:1058:G:H5''	44:n:4:THR:HG21	2.01	0.42
31:a:1434:U:H2'	31:a:1435:A:H8	1.82	0.42
31:a:1533:U:H2'	31:a:1534:G:C8	2.50	0.42
32:b:54:TYR:CE2	32:b:216:LYS:HG3	2.53	0.42
35:e:82:PRO:HG2	35:e:147:LEU:HD22	2.02	0.42
49:s:55:ARG:HG2	49:s:56:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1306:A:H1'	5:A:2040:A:N6	2.35	0.42
5:A:2161:A:H61	5:A:2184:G:C2'	2.33	0.42
5:A:2228:C:H2'	5:A:2229:C:C6	2.55	0.42
11:G:35:ARG:HB2	11:G:75:MET:HE1	2.01	0.42
11:G:89:LEU:H	11:G:129:THR:HG23	1.84	0.42
16:L:105:LYS:HA	16:L:117:VAL:HG12	2.02	0.42
22:R:56:MET:CE	22:R:79:ILE:HD11	2.49	0.42
31:a:51:A:O2'	31:a:368:G:N2	2.53	0.42
31:a:69:G:H22	31:a:100:A:H2	1.67	0.42
31:a:94:G:H5'	31:a:95:A:OP1	2.20	0.42
31:a:562:U:H2'	31:a:563:C:H6	1.84	0.42
31:a:892:C:H2'	31:a:893:U:C6	2.54	0.42
31:a:910:A:C5	31:a:911:G:H1'	2.55	0.42
31:a:1310:G:H1'	31:a:1313:C:N4	2.35	0.42
33:c:40:LYS:NZ	33:c:40:LYS:HB3	2.35	0.42
34:d:37:GLY:N	34:d:38:PRO:HD2	2.35	0.42
35:e:37:VAL:HG11	35:e:64:VAL:HG22	2.02	0.42
41:k:53:LYS:O	41:k:56:LYS:HB2	2.19	0.42
43:m:90:ARG:HD3	43:m:97:VAL:HA	2.01	0.42
5:A:318:A:H62	5:A:401:U:H3	1.66	0.42
5:A:870:C:H4'	5:A:2455:G:C5	2.55	0.42
5:A:1203:U:C2	5:A:1204:G:C8	3.08	0.42
5:A:1751:G:H1'	5:A:1783:G:C4	2.55	0.42
5:A:1816:A:H2'	5:A:1817:C:O4'	2.20	0.42
5:A:2253:C:H2'	5:A:2254:A:O4'	2.19	0.42
7:C:157:SER:O	7:C:158:ALA:C	2.63	0.42
12:H:60:ALA:HB3	12:H:127:GLY:HA2	2.02	0.42
13:I:63:VAL:HG23	13:I:64:ARG:HG2	2.02	0.42
31:a:26:C:H2'	31:a:27:A:H8	1.85	0.42
31:a:112:G:H2'	31:a:113:U:C6	2.55	0.42
31:a:262:G:OP1	47:q:70:SER:OG	2.28	0.42
31:a:470:A:C6	31:a:480:G:C6	3.08	0.42
31:a:1267:A:O2'	31:a:1268:G:N7	2.53	0.42
31:a:1357:G:H8	39:i:111:ARG:O	2.02	0.42
37:g:38:THR:O	37:g:42:ILE:HG12	2.20	0.42
41:k:23:ILE:HB	41:k:86:VAL:HG12	2.02	0.42
42:l:53:MET:HE1	42:l:104:PRO:HD2	2.01	0.42
43:m:94:GLY:HA2	43:m:109:ARG:HH21	1.85	0.42
46:p:52:VAL:HG12	46:p:53:ASP:O	2.19	0.42
49:s:32:LYS:HG3	49:s:34:TRP:CZ3	2.55	0.42
5:A:351:G:H2'	5:A:352:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:390:A:H2'	5:A:391:A:C8	2.55	0.41
5:A:1235:C:C2	5:A:1236:G:C8	3.08	0.41
5:A:1303:A:O4'	5:A:1305:U:C6	2.73	0.41
5:A:1476:G:H5''	5:A:1476:G:H8	1.85	0.41
5:A:1692:C:H5	5:A:2036:G:H1	1.68	0.41
5:A:1862:G:H1	5:A:1932:C:H5	1.68	0.41
6:B:108:U:H2'	6:B:109:G:C8	2.55	0.41
14:J:47:ARG:NH2	14:J:50:PHE:HD1	2.18	0.41
21:Q:22:ASP:OD1	21:Q:25:ARG:NH1	2.47	0.41
22:R:63:LYS:HB3	22:R:63:LYS:HE2	1.81	0.41
24:T:84:ASN:O	24:T:85:GLN:CG	2.68	0.41
25:U:19:LYS:HB3	25:U:19:LYS:HZ3	1.84	0.41
31:a:203:A:N3	31:a:204:A:C8	2.88	0.41
31:a:248:U:H2'	31:a:249:G:H8	1.84	0.41
31:a:956:G:H2'	31:a:957:C:H6	1.84	0.41
31:a:1248:A:H8	31:a:1251:G:O2'	2.04	0.41
31:a:1489:A:H2'	31:a:1490:A:H8	1.83	0.41
46:p:46:ASN:HB3	46:p:47:ALA:H	1.65	0.41
5:A:234:C:H3'	5:A:235:G:H4'	2.01	0.41
5:A:291:G:H2'	5:A:292:U:C2	2.55	0.41
5:A:458:A:H61	5:A:2438:A:H1'	1.85	0.41
5:A:525:A:H1'	5:A:526:A:H5''	2.01	0.41
5:A:1335:C:H2'	5:A:1336:G:O4'	2.20	0.41
5:A:1800:A:C8	5:A:1856:A:C8	3.08	0.41
5:A:2101:U:O2'	5:A:2624:G:H1'	2.20	0.41
5:A:2345:A:H5'	5:A:2346:U:OP2	2.20	0.41
5:A:2541:U:H2'	5:A:2542:C:C6	2.55	0.41
5:A:2803:A:C2	5:A:2805:A:C2	3.08	0.41
11:G:3:ARG:O	11:G:4:VAL:C	2.62	0.41
29:Y:18:THR:HG22	29:Y:53:ASP:OD2	2.20	0.41
31:a:26:C:H2'	31:a:27:A:C8	2.54	0.41
31:a:188:U:H5'	31:a:189:G:OP2	2.19	0.41
31:a:342:C:H2'	31:a:343:C:H6	1.85	0.41
31:a:744:U:C2	31:a:745:U:C5	3.08	0.41
31:a:1099:G:O2'	31:a:1178:C:N4	2.48	0.41
31:a:1347:G:H5''	31:a:1348:G:OP1	2.20	0.41
35:e:14:ARG:HB2	35:e:117:LEU:HD11	2.02	0.41
49:s:16:MET:O	49:s:20:GLU:HG2	2.20	0.41
5:A:242:U:H2'	5:A:243:U:O4'	2.20	0.41
5:A:1692:C:O2	5:A:1692:C:O4'	2.38	0.41
5:A:1751:G:H1'	5:A:1783:G:N3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1804:U:H5	5:A:1814:A:N1	2.18	0.41
5:A:2859:G:O4'	16:L:45:GLU:OE1	2.38	0.41
8:D:49:ILE:HD12	8:D:51:VAL:HG23	2.03	0.41
9:E:68:LYS:HB3	9:E:68:LYS:HE3	1.75	0.41
10:F:128:TYR:HB2	10:F:156:ILE:HG12	2.02	0.41
11:G:131:VAL:HG12	11:G:132:LYS:N	2.34	0.41
15:K:1:MET:HG2	15:K:66:ILE:HG21	2.01	0.41
15:K:38:THR:OG1	15:K:127:VAL:CG2	2.69	0.41
20:P:24:LYS:NZ	20:P:24:LYS:HB3	2.35	0.41
21:Q:34:ALA:HB3	30:Z:27:MET:CE	2.50	0.41
31:a:224:U:H2'	31:a:225:G:C8	2.48	0.41
31:a:254:A:H1'	31:a:255:G:H4'	2.03	0.41
31:a:307:G:H2'	31:a:308:A:C8	2.54	0.41
31:a:561:A:C4	31:a:562:U:C5	3.08	0.41
31:a:1338:C:N3	31:a:1339:A:N7	2.68	0.41
31:a:1343:A:H2'	31:a:1344:G:O4'	2.20	0.41
32:b:120:MET:HA	32:b:123:ASP:OD1	2.20	0.41
39:i:23:LEU:HD23	39:i:65:VAL:HG12	2.02	0.41
43:m:61:ASP:OD1	43:m:61:ASP:N	2.49	0.41
45:o:18:HIS:ND1	45:o:19:GLU:O	2.53	0.41
49:s:3:ARG:HB3	49:s:4:SER:H	1.61	0.41
49:s:33:THR:HG21	49:s:71:LEU:HD11	2.02	0.41
5:A:710:C:H2'	5:A:711:G:H8	1.86	0.41
5:A:2332:U:O4	10:F:40:VAL:HG12	2.19	0.41
5:A:2338:A:H1'	10:F:79:LEU:HD22	2.02	0.41
5:A:2863:G:C2	5:A:2864:A:C8	3.08	0.41
7:C:107:PRO:HD2	7:C:110:LEU:HD22	2.01	0.41
11:G:158:LYS:HA	11:G:171:ARG:NH2	2.35	0.41
31:a:98:U:H4'	31:a:99:U:H5'	2.02	0.41
31:a:241:U:H2'	31:a:242:C:C6	2.55	0.41
31:a:507:A:H62	31:a:554:A:H2'	1.85	0.41
31:a:509:C:H1'	31:a:557:C:H1'	2.03	0.41
31:a:686:U:H2'	31:a:687:C:H6	1.86	0.41
31:a:757:A:C2	31:a:758:C:C5	3.09	0.41
31:a:931:G:H2'	31:a:932:A:C8	2.55	0.41
31:a:957:C:H2'	31:a:958:A:H8	1.85	0.41
31:a:1057:A:N6	31:a:1221:U:O2'	2.52	0.41
31:a:1376:C:H2'	31:a:1377:U:C6	2.56	0.41
34:d:170:ASP:O	34:d:171:SER:OG	2.33	0.41
40:j:18:ILE:HD12	40:j:18:ILE:HA	1.82	0.41
5:A:127:C:H2'	5:A:128:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:253:G:H2'	5:A:254:A:C8	2.55	0.41
5:A:864:A:N7	5:A:1227:U:C5	2.88	0.41
5:A:1053:A:C8	5:A:1197:C:O2'	2.72	0.41
5:A:2109:A:H3'	5:A:2110:G:H8	1.86	0.41
5:A:2680:U:H2'	5:A:2681:A:C2	2.55	0.41
6:B:3:U:H2'	6:B:4:G:C8	2.56	0.41
9:E:110:LEU:HD23	9:E:110:LEU:HA	1.95	0.41
10:F:57:LEU:HD23	10:F:57:LEU:HA	1.82	0.41
18:N:93:LYS:O	18:N:93:LYS:HG2	2.20	0.41
19:O:104:LYS:HE2	19:O:104:LYS:N	2.33	0.41
21:Q:111:LYS:HB3	21:Q:111:LYS:HE3	1.66	0.41
31:a:138:A:H2'	31:a:139:U:C6	2.55	0.41
31:a:352:A:O2'	31:a:354:G:N1	2.48	0.41
31:a:1176:G:H3'	31:a:1177:A:H5''	2.01	0.41
32:b:129:LEU:HD12	32:b:129:LEU:HA	1.90	0.41
38:h:34:LYS:O	38:h:38:GLU:HG3	2.19	0.41
39:i:102:ARG:CZ	39:i:102:ARG:HB2	2.50	0.41
47:q:56:LYS:NZ	47:q:83:GLU:O	2.46	0.41
3:3:48:ARG:HG2	3:3:48:ARG:HH11	1.85	0.41
5:A:219:A:C8	5:A:478:A:N6	2.88	0.41
5:A:1415:A:H1'	5:A:1416:U:C5	2.55	0.41
5:A:2330:G:H4'	10:F:123:ASP:HA	2.02	0.41
5:A:2553:G:C2	5:A:2554:C:H1'	2.56	0.41
6:B:47:C:H2'	6:B:48:A:H8	1.85	0.41
8:D:197:VAL:O	8:D:197:VAL:HG23	2.21	0.41
12:H:38:ARG:HH11	12:H:38:ARG:HG3	1.85	0.41
12:H:69:LYS:HE2	12:H:69:LYS:HB3	1.83	0.41
15:K:26:TYR:CD1	15:K:26:TYR:N	2.87	0.41
18:N:19:LEU:HD23	18:N:19:LEU:O	2.20	0.41
31:a:1086:U:H5''	32:b:178:LYS:HE3	2.02	0.41
31:a:1179:A:H2'	31:a:1180:A:C8	2.56	0.41
31:a:1497:G:H2'	31:a:1498:G:C8	2.55	0.41
34:d:41:ARG:HA	34:d:41:ARG:HE	1.85	0.41
39:i:97:ARG:HG3	39:i:101:LYS:HG3	2.03	0.41
43:m:15:VAL:HG22	43:m:48:LEU:HD11	2.02	0.41
2:2:4:ARG:O	2:2:7:GLN:OE1	2.39	0.41
5:A:250:G:C2	5:A:255:G:C6	3.08	0.41
5:A:902:A:O2'	5:A:903:G:H5'	2.20	0.41
5:A:1229:G:OP1	14:J:30:THR:OG1	2.39	0.41
5:A:1928:A:H2'	5:A:1929:C:C6	2.55	0.41
10:F:95:ARG:HH22	29:Y:9:TYR:CB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:130:LEU:HB2	10:F:154:ILE:HD11	2.01	0.41
11:G:5:GLY:HA2	11:G:69:ARG:CG	2.46	0.41
31:a:69:G:C2	31:a:70:A:H1'	2.56	0.41
31:a:75:A:N6	31:a:94:G:O2'	2.34	0.41
31:a:261:U:H2'	31:a:262:G:C8	2.55	0.41
31:a:736:A:N7	45:o:54:ARG:HD2	2.36	0.41
31:a:855:C:H2'	31:a:856:C:C6	2.54	0.41
31:a:887:U:H2'	31:a:888:C:C6	2.55	0.41
31:a:1183:C:H2'	31:a:1184:G:C8	2.56	0.41
31:a:1270:G:OP1	31:a:1294:C:H4'	2.21	0.41
31:a:1337:A:C4	31:a:1338:C:C5	3.09	0.41
31:a:1422:C:H2'	31:a:1423:A:H8	1.79	0.41
31:a:1489:A:H2'	31:a:1490:A:C8	2.56	0.41
32:b:30:TYR:HE2	32:b:199:VAL:HG11	1.84	0.41
33:c:64:ASN:HA	33:c:99:HIS:HB2	2.01	0.41
45:o:82:ILE:HG12	45:o:87:ILE:O	2.20	0.41
5:A:409:G:H3'	5:A:410:G:H8	1.85	0.41
5:A:1712:A:N3	5:A:1714:C:C4	2.89	0.41
5:A:1989:C:H4'	5:A:1990:C:C5	2.56	0.41
5:A:2107:G:H5'	26:V:19:SER:CB	2.51	0.41
5:A:2905:C:N4	30:Z:39:SER:OG	2.47	0.41
6:B:64:A:H61	6:B:104:A:H2'	1.86	0.41
7:C:272:ARG:H	7:C:272:ARG:HG2	1.79	0.41
13:I:11:ALA:HB1	13:I:99:PHE:O	2.21	0.41
17:M:92:ILE:HD12	17:M:93:VAL:N	2.36	0.41
24:T:22:ARG:HE	24:T:22:ARG:HB2	1.67	0.41
31:a:476:C:H2'	31:a:477:U:H6	1.86	0.41
31:a:602:U:H2'	31:a:603:A:C8	2.55	0.41
31:a:612:G:O6	31:a:643:A:N6	2.54	0.41
31:a:987:A:C4	31:a:1329:A:C2	3.08	0.41
31:a:1319:G:OP2	43:m:98:ARG:NH2	2.54	0.41
31:a:1340:U:C4	31:a:1341:G:C6	3.09	0.41
45:o:35:GLU:O	45:o:39:VAL:HG23	2.20	0.41
5:A:310:C:O2'	5:A:311:U:H2'	2.21	0.41
5:A:398:C:H2'	5:A:399:U:O4'	2.20	0.41
5:A:422:G:H2'	5:A:423:A:H8	1.86	0.41
5:A:445:G:OP2	26:V:55:LYS:NZ	2.51	0.41
5:A:579:U:O2'	19:O:49:ASP:OD2	2.30	0.41
5:A:774:G:O4'	7:C:207:LYS:NZ	2.53	0.41
5:A:1326:C:H2'	5:A:1327:C:H6	1.86	0.41
5:A:1329:G:H2'	5:A:1330:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1708:A:N3	5:A:1709:A:C8	2.88	0.41
5:A:1747:G:O2'	31:a:1439:C:H4'	2.21	0.41
5:A:2115:A:H2'	5:A:2116:U:O4'	2.21	0.41
5:A:2319:U:O2'	5:A:2320:C:H5'	2.21	0.41
5:A:2617:A:H2'	5:A:2618:C:C6	2.56	0.41
5:A:2851:G:H1'	5:A:2903:A:H2'	2.02	0.41
6:B:39:G:H8	6:B:40:C:H3'	1.86	0.41
7:C:6:TYR:CD2	7:C:16:MET:HG2	2.56	0.41
7:C:100:GLU:HG3	7:C:101:LYS:N	2.35	0.41
8:D:15:VAL:HG23	8:D:23:ILE:HB	2.03	0.41
8:D:37:GLN:OE1	8:D:76:HIS:CE1	2.66	0.41
8:D:40:THR:OG1	8:D:43:VAL:HB	2.21	0.41
10:F:31:ILE:CG2	10:F:96:MET:SD	3.03	0.41
11:G:10:ASP:OD1	11:G:69:ARG:CZ	2.68	0.41
11:G:130:VAL:O	11:G:130:VAL:HG12	2.20	0.41
11:G:157:TYR:O	11:G:171:ARG:NH2	2.53	0.41
24:T:13:GLN:HB3	24:T:18:LEU:CD2	2.50	0.41
31:a:178:G:C2	31:a:179:A:C8	3.08	0.41
31:a:418:G:H2'	31:a:437:U:C4	2.56	0.41
31:a:484:A:O2'	31:a:485:U:H6	2.04	0.41
31:a:663:A:H2'	31:a:664:G:O4'	2.21	0.41
31:a:665:U:C2	31:a:666:G:C8	3.09	0.41
31:a:833:G:O6	31:a:885:A:N6	2.54	0.41
31:a:1081:U:H2'	31:a:1082:C:H6	1.85	0.41
31:a:1122:A:N1	33:c:176:THR:HG22	2.36	0.41
31:a:1235:A:OP1	43:m:101:LYS:HA	2.21	0.41
31:a:1547:C:H6	31:a:1547:C:H2'	1.66	0.41
47:q:48:THR:HG21	47:q:63:ILE:HG13	2.03	0.41
49:s:3:ARG:HH21	49:s:7:LYS:HD2	1.86	0.41
49:s:4:SER:HB2	49:s:7:LYS:HE3	2.03	0.41
5:A:1358:A:H3'	5:A:1359:A:H8	1.86	0.41
5:A:2026:C:H5''	5:A:2750:C:O2'	2.20	0.41
5:A:2544:C:C2	5:A:2569:A:N6	2.89	0.41
5:A:2677:C:H2'	5:A:2678:C:C6	2.56	0.41
5:A:2727:G:H2'	5:A:2728:U:H6	1.86	0.41
6:B:46:A:H2'	6:B:47:C:O4'	2.20	0.41
7:C:39:LYS:HB2	7:C:39:LYS:HE2	1.67	0.41
7:C:159:GLY:H	7:C:195:VAL:HG23	1.86	0.41
8:D:133:ARG:HG3	8:D:173:MET:HG3	2.03	0.41
10:F:63:GLN:HG3	29:Y:6:HIS:HB2	2.03	0.41
11:G:19:PHE:CD1	11:G:45:GLN:NE2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:71:ARG:NH1	18:N:74:ARG:NE	2.69	0.41
18:N:31:HIS:CD2	18:N:85:LYS:HG2	2.56	0.41
23:S:5:LYS:O	23:S:5:LYS:HG3	2.15	0.41
24:T:49:ILE:O	24:T:53:ARG:HG2	2.21	0.41
31:a:432:G:C2	31:a:433:A:C5	3.09	0.41
31:a:642:C:H2'	31:a:643:A:C8	2.56	0.41
31:a:642:C:H2'	31:a:643:A:H8	1.86	0.41
31:a:1084:U:C2	31:a:1085:G:C8	3.09	0.41
31:a:1185:G:N3	31:a:1186:A:C8	2.89	0.41
31:a:1216:G:C5	31:a:1217:C:C5	3.09	0.41
31:a:1384:A:H2'	31:a:1384:A:N3	2.36	0.41
31:a:1527:G:C6	31:a:1531:G:C6	3.08	0.41
36:f:7:MET:HG2	48:r:70:MET:HE2	2.01	0.41
5:A:4:U:H2'	5:A:5:A:C8	2.56	0.40
5:A:851:C:C2	5:A:852:U:C5	3.09	0.40
5:A:1539:A:H2'	5:A:1541:C:C5	2.56	0.40
5:A:2074:C:H2'	5:A:2075:G:H8	1.86	0.40
5:A:2590:U:C2	5:A:2592:A:OP2	2.74	0.40
5:A:2652:G:H2'	5:A:2653:C:O4'	2.20	0.40
10:F:88:LYS:HB2	10:F:88:LYS:HE3	1.75	0.40
11:G:30:LYS:HE3	11:G:81:GLN:C	2.46	0.40
12:H:95:ARG:CG	12:H:96:THR:HG23	2.51	0.40
13:I:13:ASN:HD21	13:I:96:THR:H	1.69	0.40
16:L:102:ARG:NH2	16:L:122:VAL:HG23	2.35	0.40
21:Q:9:THR:HG23	21:Q:80:PRO:HD2	2.03	0.40
21:Q:39:THR:OG1	30:Z:25:PRO:HG3	2.21	0.40
31:a:203:A:C4	31:a:204:A:C8	3.08	0.40
31:a:623:C:H2'	31:a:624:G:H8	1.86	0.40
31:a:869:A:H3'	31:a:870:G:H8	1.86	0.40
31:a:992:A:H2	31:a:993:C:C6	2.40	0.40
31:a:1067:U:H2'	31:a:1068:G:C8	2.50	0.40
32:b:176:ALA:HB3	32:b:183:ILE:HD11	2.02	0.40
36:f:62:ILE:HG12	48:r:29:LYS:NZ	2.36	0.40
43:m:79:ARG:O	43:m:83:ILE:HG13	2.20	0.40
5:A:27:G:H22	5:A:557:G:H1'	1.84	0.40
5:A:512:A:H5''	5:A:512:A:C8	2.55	0.40
5:A:660:A:H8	9:E:182:ASN:HB3	1.85	0.40
5:A:1088:C:H5'	5:A:1092:A:H1'	2.02	0.40
5:A:1247:G:O2'	5:A:1275:A:N1	2.40	0.40
5:A:2041:A:H2'	5:A:2042:A:C8	2.57	0.40
5:A:2564:U:H2'	5:A:2565:C:H6	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2725:U:C2	5:A:2726:C:C5	3.09	0.40
6:B:74:G:H5'	24:T:18:LEU:HD11	2.03	0.40
9:E:34:PHE:CD1	14:J:6:LEU:HD13	2.56	0.40
9:E:146:LEU:O	9:E:147:GLU:HG3	2.21	0.40
12:H:107:LYS:NZ	12:H:120:GLY:O	2.55	0.40
14:J:93:PRO:HD3	14:J:124:LYS:O	2.22	0.40
16:L:99:GLY:O	16:L:100:TYR:HB2	2.21	0.40
22:R:6:ILE:HD11	22:R:41:ALA:CB	2.51	0.40
31:a:283:G:C2	31:a:284:G:C8	3.09	0.40
31:a:451:U:HO2'	31:a:452:A:H8	1.68	0.40
31:a:457:A:H2'	31:a:458:G:O4'	2.22	0.40
31:a:885:A:H2'	31:a:886:C:C6	2.56	0.40
31:a:1131:C:H2'	31:a:1132:U:C6	2.57	0.40
31:a:1535:C:C2	31:a:1536:G:N7	2.89	0.40
32:b:54:TYR:CE1	32:b:220:ALA:HA	2.56	0.40
32:b:116:GLU:O	32:b:119:LYS:HB3	2.21	0.40
44:n:13:LYS:HD2	44:n:13:LYS:HA	1.87	0.40
45:o:75:ILE:HG22	45:o:79:ARG:HE	1.85	0.40
49:s:3:ARG:NH1	49:s:10:PHE:HB2	2.34	0.40
5:A:2091:C:H2'	5:A:2092:C:C6	2.56	0.40
5:A:2136:U:H5'	5:A:2169:G:H21	1.87	0.40
10:F:142:ASP:HB3	10:F:144:ASP:H	1.86	0.40
17:M:72:LEU:HD23	17:M:75:LYS:HG3	2.03	0.40
21:Q:14:PRO:HG3	21:Q:78:GLU:HG3	2.03	0.40
24:T:3:SER:O	24:T:3:SER:OG	2.31	0.40
31:a:369:G:H2'	31:a:370:G:O4'	2.20	0.40
31:a:1384:A:O2'	31:a:1385:A:H5'	2.22	0.40
5:A:421:C:H2'	5:A:422:G:H8	1.86	0.40
5:A:650:U:H5	5:A:664:G:C5	2.39	0.40
5:A:2257:G:H1'	26:V:32:ASN:HA	2.04	0.40
5:A:2689:A:C4	5:A:2690:G:H1'	2.57	0.40
5:A:2736:G:C6	5:A:2737:C:C4	3.09	0.40
12:H:92:GLU:OE2	12:H:95:ARG:NH1	2.54	0.40
15:K:54:MET:HE2	15:K:54:MET:HB2	1.82	0.40
27:W:19:LYS:HB3	27:W:19:LYS:HE3	1.24	0.40
31:a:240:A:H2'	31:a:241:U:C6	2.57	0.40
31:a:578:G:H2'	31:a:579:U:C6	2.57	0.40
31:a:776:A:C4	31:a:777:G:C8	3.09	0.40
31:a:809:U:H2'	31:a:810:A:C8	2.56	0.40
31:a:1004:C:N3	31:a:1005:A:C2	2.90	0.40
31:a:1185:G:H2'	31:a:1186:A:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1283:C:H2'	31:a:1284:A:O4'	2.21	0.40
31:a:1535:C:C2	31:a:1536:G:C8	3.09	0.40
33:c:108:VAL:HG13	33:c:114:LEU:HD13	2.04	0.40
40:j:80:THR:O	40:j:83:THR:OG1	2.35	0.40
5:A:984:G:H2'	5:A:985:A:O4'	2.21	0.40
5:A:1426:G:H2'	5:A:1427:U:O4'	2.20	0.40
5:A:1708:A:C4	5:A:1709:A:N7	2.89	0.40
5:A:2434:A:N3	5:A:2434:A:H2'	2.37	0.40
7:C:16:MET:HE3	7:C:16:MET:HB2	1.81	0.40
7:C:182:ARG:HG3	7:C:270:ILE:HG22	2.03	0.40
9:E:117:LYS:HD3	9:E:117:LYS:HA	1.55	0.40
10:F:109:PRO:HA	29:Y:50:ILE:HG12	2.02	0.40
10:F:159:THR:O	10:F:159:THR:HG22	2.21	0.40
16:L:100:TYR:C	16:L:122:VAL:HG12	2.47	0.40
18:N:82:LYS:HE3	18:N:82:LYS:HB3	1.52	0.40
22:R:52:SER:OG	22:R:81:THR:HG21	2.22	0.40
30:Z:48:SER:O	30:Z:49:TYR:C	2.64	0.40
31:a:269:U:H2'	31:a:271:A:OP2	2.21	0.40
31:a:601:U:H2'	31:a:602:U:C6	2.57	0.40
31:a:623:C:H2'	31:a:624:G:C8	2.57	0.40
31:a:719:G:H2'	31:a:720:A:H8	1.87	0.40
31:a:1141:A:H2'	31:a:1142:U:C6	2.56	0.40
39:i:20:ARG:O	39:i:67:VAL:HA	2.22	0.40
42:l:92:VAL:HG12	42:l:115:LEU:HD13	2.04	0.40
47:q:19:MET:H	47:q:19:MET:HG2	1.72	0.40
49:s:3:ARG:HH21	49:s:7:LYS:CD	2.34	0.40
50:t:60:ALA:HB1	50:t:65:LEU:HB2	2.03	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	1	45/47 (96%)	41 (91%)	4 (9%)	0	100	100
2	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
3	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
4	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
7	C	272/274 (99%)	245 (90%)	26 (10%)	1 (0%)	30	49
8	D	213/215 (99%)	200 (94%)	13 (6%)	0	100	100
9	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
10	F	173/175 (99%)	144 (83%)	28 (16%)	1 (1%)	21	39
11	G	173/175 (99%)	157 (91%)	16 (9%)	0	100	100
12	H	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
13	I	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	32
14	J	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
15	K	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	L	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
17	M	117/119 (98%)	107 (92%)	10 (8%)	0	100	100
18	N	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
19	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
20	P	100/102 (98%)	93 (93%)	5 (5%)	2 (2%)	6	11
21	Q	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
22	R	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
23	S	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
24	T	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
25	U	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
26	V	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
27	W	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
28	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
29	Y	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
30	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
32	b	222/232 (96%)	212 (96%)	10 (4%)	0	100	100
33	c	200/217 (92%)	190 (95%)	10 (5%)	0	100	100
34	d	197/200 (98%)	187 (95%)	10 (5%)	0	100	100
35	e	154/166 (93%)	149 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	f	93/98 (95%)	87 (94%)	6 (6%)	0	100	100
37	g	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	h	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
39	i	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
40	j	95/102 (93%)	89 (94%)	6 (6%)	0	100	100
41	k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
42	l	133/149 (89%)	122 (92%)	10 (8%)	1 (1%)	16	32
43	m	114/121 (94%)	105 (92%)	9 (8%)	0	100	100
44	n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
45	o	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
46	p	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
47	q	78/87 (90%)	74 (95%)	4 (5%)	0	100	100
48	r	62/80 (78%)	60 (97%)	2 (3%)	0	100	100
49	s	80/108 (74%)	73 (91%)	7 (9%)	0	100	100
50	t	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
All	All	5323/5563 (96%)	4979 (94%)	338 (6%)	6 (0%)	49	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	P	51	PRO
13	I	98	ILE
10	F	139	PRO
20	P	50	ALA
42	l	132	THR
7	C	271	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	44/45 (98%)	35 (80%)	9 (20%)	1	2
2	2	39/39 (100%)	38 (97%)	1 (3%)	40	66
3	3	55/55 (100%)	51 (93%)	4 (7%)	13	27
4	4	35/35 (100%)	31 (89%)	4 (11%)	5	11
7	C	220/221 (100%)	203 (92%)	17 (8%)	12	25
8	D	173/173 (100%)	155 (90%)	18 (10%)	7	13
9	E	168/168 (100%)	155 (92%)	13 (8%)	12	25
10	F	139/154 (90%)	100 (72%)	39 (28%)	0	1
11	G	123/153 (80%)	101 (82%)	22 (18%)	2	3
12	H	122/123 (99%)	110 (90%)	12 (10%)	7	16
13	I	100/100 (100%)	91 (91%)	9 (9%)	9	19
14	J	109/112 (97%)	99 (91%)	10 (9%)	8	18
15	K	108/114 (95%)	95 (88%)	13 (12%)	5	9
16	L	96/101 (95%)	96 (100%)	0	100	100
17	M	86/95 (90%)	75 (87%)	11 (13%)	4	8
18	N	93/100 (93%)	74 (80%)	19 (20%)	1	2
19	O	96/96 (100%)	91 (95%)	5 (5%)	21	42
20	P	84/86 (98%)	80 (95%)	4 (5%)	23	45
21	Q	89/94 (95%)	78 (88%)	11 (12%)	4	8
22	R	78/80 (98%)	66 (85%)	12 (15%)	2	4
23	S	81/88 (92%)	73 (90%)	8 (10%)	7	15
24	T	75/82 (92%)	64 (85%)	11 (15%)	3	5
25	U	60/64 (94%)	53 (88%)	7 (12%)	5	10
26	V	44/49 (90%)	38 (86%)	6 (14%)	3	7
27	W	58/60 (97%)	43 (74%)	15 (26%)	0	1
28	X	52/52 (100%)	47 (90%)	5 (10%)	8	16
29	Y	21/56 (38%)	17 (81%)	4 (19%)	1	2
30	Z	36/44 (82%)	36 (100%)	0	100	100
32	b	194/201 (96%)	192 (99%)	2 (1%)	68	84
33	c	164/175 (94%)	163 (99%)	1 (1%)	78	89
34	d	174/175 (99%)	172 (99%)	2 (1%)	65	83
35	e	122/131 (93%)	117 (96%)	5 (4%)	27	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	83/86 (96%)	81 (98%)	2 (2%)	43	68
37	g	131/132 (99%)	122 (93%)	9 (7%)	14	30
38	h	112/113 (99%)	111 (99%)	1 (1%)	70	85
39	i	105/107 (98%)	102 (97%)	3 (3%)	37	63
40	j	87/91 (96%)	84 (97%)	3 (3%)	32	58
41	k	90/104 (86%)	88 (98%)	2 (2%)	45	70
42	l	117/130 (90%)	111 (95%)	6 (5%)	21	43
43	m	100/104 (96%)	98 (98%)	2 (2%)	48	72
44	n	52/53 (98%)	52 (100%)	0	100	100
45	o	79/81 (98%)	78 (99%)	1 (1%)	61	81
46	p	74/77 (96%)	72 (97%)	2 (3%)	39	65
47	q	75/82 (92%)	70 (93%)	5 (7%)	15	31
48	r	57/68 (84%)	55 (96%)	2 (4%)	32	57
49	s	71/91 (78%)	70 (99%)	1 (1%)	59	79
50	t	67/69 (97%)	67 (100%)	0	100	100
All	All	4438/4709 (94%)	4100 (92%)	338 (8%)	14	26

All (338) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	5	VAL
1	1	12	CYS
1	1	18	ILE
1	1	23	LYS
1	1	29	ARG
1	1	31	GLU
1	1	32	MET
1	1	41	LYS
1	1	48	THR
2	2	2	VAL
3	3	52	LYS
3	3	53	SER
3	3	56	LYS
3	3	62	LEU
4	4	3	VAL
4	4	8	LYS
4	4	12	GLU

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Mol	Chain	Res	Type
4	4	15	LYS
7	C	3	ILE
7	C	4	LYS
7	C	24	ILE
7	C	64	VAL
7	C	65	ILE
7	C	68	LYS
7	C	71	LYS
7	C	87	ARG
7	C	115	ILE
7	C	116	VAL
7	C	123	ASP
7	C	125	LYS
7	C	144	ILE
7	C	243	ARG
7	C	245	SER
7	C	270	ILE
7	C	272	ARG
8	D	13	THR
8	D	18	GLU
8	D	21	GLU
8	D	22	LEU
8	D	27	VAL
8	D	54	GLU
8	D	74	GLU
8	D	100	GLU
8	D	106	SER
8	D	107	VAL
8	D	108	ASP
8	D	131	ILE
8	D	137	SER
8	D	158	SER
8	D	168	LYS
8	D	193	LYS
8	D	200	ASN
8	D	205	LYS
9	E	9	LEU
9	E	10	ASP
9	E	16	SER
9	E	17	ILE
9	E	74	ARG
9	E	84	ARG

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Mol	Chain	Res	Type
9	E	117	LYS
9	E	130	ASN
9	E	137	LYS
9	E	140	LYS
9	E	143	LEU
9	E	161	VAL
9	E	176	THR
10	F	5	LYS
10	F	6	GLU
10	F	16	LEU
10	F	17	MET
10	F	23	SER
10	F	24	SER
10	F	25	VAL
10	F	27	GLU
10	F	28	VAL
10	F	44	VAL
10	F	51	ASP
10	F	54	VAL
10	F	56	GLU
10	F	59	LEU
10	F	60	ILE
10	F	64	LYS
10	F	66	LEU
10	F	67	VAL
10	F	78	ARG
10	F	85	ILE
10	F	88	LYS
10	F	106	VAL
10	F	110	ARG
10	F	120	LYS
10	F	128	TYR
10	F	132	VAL
10	F	133	LYS
10	F	135	GLN
10	F	136	LEU
10	F	138	PHE
10	F	143	TYR
10	F	148	LYS
10	F	149	VAL
10	F	150	ARG
10	F	152	MET

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Mol	Chain	Res	Type
10	F	154	ILE
10	F	156	ILE
10	F	168	GLU
10	F	170	LEU
11	G	25	THR
11	G	39	GLU
11	G	42	THR
11	G	49	THR
11	G	53	VAL
11	G	57	ASP
11	G	58	SER
11	G	59	LYS
11	G	68	THR
11	G	79	VAL
11	G	81	GLN
11	G	84	VAL
11	G	97	GLN
11	G	98	MET
11	G	99	GLN
11	G	107	VAL
11	G	109	TYR
11	G	113	VAL
11	G	121	ILE
11	G	122	THR
11	G	124	SER
11	G	175	LYS
12	H	3	GLN
12	H	18	VAL
12	H	19	ILE
12	H	20	ASP
12	H	24	GLN
12	H	25	THR
12	H	58	ILE
12	H	63	ILE
12	H	86	LYS
12	H	125	VAL
12	H	139	GLU
12	H	143	LEU
13	I	14	SER
13	I	64	ARG
13	I	66	LYS
13	I	67	SER

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Mol	Chain	Res	Type
13	I	69	VAL
13	I	94	ARG
13	I	98	ILE
13	I	102	VAL
13	I	122	LEU
14	J	91	VAL
14	J	92	THR
14	J	95	LEU
14	J	97	VAL
14	J	101	VAL
14	J	102	VAL
14	J	103	LYS
14	J	104	ASN
14	J	106	LYS
14	J	131	SER
15	K	1	MET
15	K	2	LEU
15	K	3	LEU
15	K	7	VAL
15	K	18	THR
15	K	42	ILE
15	K	44	SER
15	K	45	ARG
15	K	47	ILE
15	K	54	MET
15	K	72	THR
15	K	102	ILE
15	K	103	LEU
17	M	9	LYS
17	M	11	ARG
17	M	13	LYS
17	M	33	VAL
17	M	45	ILE
17	M	58	SER
17	M	66	THR
17	M	74	THR
17	M	93	VAL
17	M	113	ARG
17	M	114	GLU
18	N	5	LYS
18	N	7	ILE
18	N	10	VAL

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Mol	Chain	Res	Type
18	N	12	LYS
18	N	14	GLN
18	N	17	THR
18	N	27	THR
18	N	28	LEU
18	N	32	VAL
18	N	34	ILE
18	N	35	ILE
18	N	41	ARG
18	N	57	VAL
18	N	63	VAL
18	N	65	LYS
18	N	78	LEU
18	N	82	LYS
18	N	85	LYS
18	N	87	GLU
19	O	8	THR
19	O	9	VAL
19	O	89	ASP
19	O	90	ILE
19	O	117	LEU
20	P	1	MET
20	P	47	LYS
20	P	53	VAL
20	P	83	LYS
21	Q	1	MET
21	Q	9	THR
21	Q	38	LEU
21	Q	43	SER
21	Q	51	LEU
21	Q	52	MET
21	Q	65	ASN
21	Q	67	ASP
21	Q	70	VAL
21	Q	81	THR
21	Q	111	LYS
22	R	13	THR
22	R	14	GLU
22	R	36	THR
22	R	40	MET
22	R	63	LYS
22	R	65	MET

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Mol	Chain	Res	Type
22	R	75	ARG
22	R	77	LYS
22	R	83	LYS
22	R	84	GLU
22	R	89	LEU
22	R	90	PHE
23	S	29	LYS
23	S	30	LYS
23	S	31	ASP
23	S	34	VAL
23	S	35	VAL
23	S	38	VAL
23	S	74	LYS
23	S	77	GLU
24	T	7	ILE
24	T	8	ILE
24	T	9	ARG
24	T	21	LEU
24	T	22	ARG
24	T	23	LYS
24	T	24	SER
24	T	27	VAL
24	T	46	VAL
24	T	58	ASN
24	T	77	TYR
25	U	12	LYS
25	U	45	LEU
25	U	53	ILE
25	U	75	VAL
25	U	82	ARG
25	U	83	ASP
25	U	84	LYS
26	V	7	VAL
26	V	11	LYS
26	V	40	VAL
26	V	50	SER
26	V	52	ARG
26	V	58	LYS
27	W	10	THR
27	W	12	SER
27	W	15	GLU
27	W	16	GLU

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Mol	Chain	Res	Type
27	W	17	GLN
27	W	19	LYS
27	W	22	LYS
27	W	29	ARG
27	W	30	PHE
27	W	34	THR
27	W	36	GLN
27	W	39	GLU
27	W	43	ILE
27	W	62	ILE
27	W	65	SER
28	X	5	GLN
28	X	6	ILE
28	X	7	THR
28	X	10	ARG
28	X	18	THR
29	Y	3	GLN
29	Y	5	ILE
29	Y	8	GLU
29	Y	10	HIS
32	b	6	MET
32	b	43	LEU
33	c	78	LYS
34	d	3	ARG
34	d	71	THR
35	e	10	GLU
35	e	12	GLU
35	e	70	ASP
35	e	152	ASP
35	e	164	LEU
36	f	17	ASP
36	f	81	LYS
37	g	9	LYS
37	g	10	ARG
37	g	12	VAL
37	g	13	LEU
37	g	32	LEU
37	g	35	LYS
37	g	66	ILE
37	g	72	VAL
37	g	73	LEU
38	h	35	GLU

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Mol	Chain	Res	Type
39	i	18	VAL
39	i	60	LYS
39	i	96	TYR
40	j	10	LEU
40	j	31	ARG
40	j	92	LEU
41	k	125	LYS
41	k	126	ARG
42	l	89	GLU
42	l	102	ASP
42	l	115	LEU
42	l	129	LEU
42	l	132	THR
42	l	133	LYS
43	m	27	THR
43	m	34	LEU
45	o	74	ASP
46	p	43	THR
46	p	81	MET
47	q	40	VAL
47	q	41	LYS
47	q	44	LYS
47	q	48	THR
47	q	84	SER
48	r	17	TYR
48	r	25	HIS
49	s	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	26	ASN
2	2	7	GLN
3	3	60	GLN
4	4	34	GLN
7	C	15	ASN
7	C	75	ASN
7	C	86	ASN
7	C	134	ASN
7	C	143	ASN
8	D	134	HIS
8	D	148	HIS

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Mol	Chain	Res	Type
8	D	182	ASN
9	E	29	ASN
10	F	161	ASN
10	F	172	ASN
12	H	68	ASN
12	H	81	HIS
12	H	131	HIS
14	J	81	GLN
14	J	83	ASN
14	J	126	HIS
16	L	12	GLN
16	L	106	GLN
17	M	8	ASN
17	M	39	HIS
17	M	48	ASN
18	N	113	GLN
20	P	18	GLN
21	Q	40	ASN
22	R	37	GLN
22	R	54	ASN
23	S	44	HIS
24	T	20	GLN
24	T	38	ASN
24	T	88	HIS
32	b	15	HIS
32	b	77	GLN
33	c	88	ASN
33	c	185	HIS
34	d	85	ASN
34	d	146	GLN
37	g	122	ASN
37	g	130	ASN
37	g	148	ASN
39	i	77	GLN
41	k	119	ASN
42	l	39	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1470/1548 (94%)	382 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	2879/2921 (98%)	951 (33%)	78 (2%)
6	B	114/115 (99%)	47 (41%)	4 (3%)
All	All	4463/4584 (97%)	1380 (30%)	82 (1%)

All (1380) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	5	A
5	A	13	A
5	A	18	C
5	A	19	G
5	A	23	G
5	A	24	G
5	A	28	A
5	A	29	U
5	A	34	U
5	A	36	G
5	A	39	C
5	A	43	A
5	A	46	C
5	A	47	C
5	A	50	U
5	A	51	G
5	A	54	G
5	A	55	G
5	A	58	G
5	A	62	C
5	A	63	U
5	A	64	A
5	A	66	C
5	A	70	G
5	A	71	A
5	A	74	U
5	A	75	G
5	A	80	G
5	A	83	G
5	A	84	A
5	A	88	G
5	A	90	A
5	A	91	A
5	A	92	G
5	A	93	U

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Mol	Chain	Res	Type
5	A	94	A
5	A	96	G
5	A	100	U
5	A	101	G
5	A	102	A
5	A	103	U
5	A	104	C
5	A	105	C
5	A	106	A
5	A	117	A
5	A	118	A
5	A	119	U
5	A	122	G
5	A	124	A
5	A	125	A
5	A	135	G
5	A	140	A
5	A	153	G
5	A	158	G
5	A	162	A
5	A	163	U
5	A	164	A
5	A	165	C
5	A	166	A
5	A	167	U
5	A	169	G
5	A	170	C
5	A	171	A
5	A	173	A
5	A	176	A
5	A	177	G
5	A	179	A
5	A	180	G
5	A	183	A
5	A	184	C
5	A	185	A
5	A	199	A
5	A	200	A
5	A	202	A
5	A	203	U
5	A	209	U
5	A	213	C

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Mol	Chain	Res	Type
5	A	215	G
5	A	216	A
5	A	218	G
5	A	219	A
5	A	224	A
5	A	225	A
5	A	226	A
5	A	231	A
5	A	232	U
5	A	234	C
5	A	235	G
5	A	236	A
5	A	242	U
5	A	244	A
5	A	248	G
5	A	251	G
5	A	255	G
5	A	268	A
5	A	269	G
5	A	272	C
5	A	275	A
5	A	278	A
5	A	280	C
5	A	281	A
5	A	282	A
5	A	284	C
5	A	286	U
5	A	287	G
5	A	288	C
5	A	289	U
5	A	290	U
5	A	292	U
5	A	293	U
5	A	294	G
5	A	299	U
5	A	300	G
5	A	301	U
5	A	302	A
5	A	303	G
5	A	305	A
5	A	309	U
5	A	310	C

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Mol	Chain	Res	Type
5	A	311	U
5	A	312	A
5	A	318	A
5	A	321	U
5	A	324	A
5	A	326	A
5	A	327	G
5	A	328	G
5	A	329	A
5	A	333	C
5	A	335	U
5	A	336	U
5	A	353	A
5	A	354	A
5	A	360	A
5	A	372	A
5	A	388	A
5	A	390	A
5	A	392	U
5	A	393	G
5	A	397	U
5	A	399	U
5	A	401	U
5	A	403	U
5	A	404	U
5	A	405	G
5	A	406	A
5	A	411	A
5	A	417	A
5	A	432	G
5	A	434	G
5	A	440	C
5	A	447	A
5	A	448	A
5	A	449	U
5	A	451	U
5	A	452	G
5	A	459	C
5	A	460	C
5	A	461	A
5	A	463	C
5	A	468	A

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Mol	Chain	Res	Type
5	A	482	U
5	A	489	A
5	A	490	C
5	A	492	G
5	A	497	U
5	A	502	C
5	A	503	A
5	A	506	A
5	A	507	C
5	A	511	G
5	A	512	A
5	A	513	G
5	A	520	G
5	A	521	U
5	A	523	A
5	A	525	A
5	A	527	G
5	A	529	A
5	A	530	C
5	A	537	A
5	A	540	G
5	A	548	A
5	A	549	U
5	A	550	A
5	A	553	A
5	A	554	C
5	A	565	G
5	A	566	U
5	A	567	G
5	A	572	C
5	A	574	A
5	A	575	G
5	A	576	U
5	A	577	A
5	A	578	G
5	A	581	A
5	A	583	A
5	A	591	A
5	A	592	A
5	A	606	G
5	A	608	C
5	A	616	G

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Mol	Chain	Res	Type
5	A	617	A
5	A	618	A
5	A	619	U
5	A	621	A
5	A	623	C
5	A	629	A
5	A	630	G
5	A	644	C
5	A	645	A
5	A	646	A
5	A	647	G
5	A	659	A
5	A	661	U
5	A	666	A
5	A	672	A
5	A	673	G
5	A	676	A
5	A	679	G
5	A	682	A
5	A	690	U
5	A	691	A
5	A	696	G
5	A	698	U
5	A	699	U
5	A	700	A
5	A	715	A
5	A	716	C
5	A	720	A
5	A	722	A
5	A	731	U
5	A	746	G
5	A	749	G
5	A	775	A
5	A	792	5MU
5	A	797	A
5	A	802	G
5	A	805	G
5	A	809	A
5	A	810	A
5	A	815	G
5	A	816	G
5	A	820	G

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Mol	Chain	Res	Type
5	A	821	C
5	A	822	G
5	A	827	A
5	A	828	A
5	A	829	U
5	A	830	U
5	A	834	A
5	A	835	U
5	A	837	G
5	A	838	A
5	A	850	G
5	A	856	U
5	A	857	C
5	A	868	A
5	A	872	U
5	A	873	U
5	A	890	G
5	A	891	A
5	A	899	U
5	A	904	G
5	A	911	A
5	A	917	U
5	A	922	G
5	A	925	G
5	A	926	G
5	A	927	G
5	A	928	C
5	A	938	G
5	A	939	U
5	A	940	U
5	A	942	C
5	A	943	C
5	A	944	G
5	A	945	A
5	A	951	G
5	A	952	A
5	A	955	A
5	A	957	C
5	A	960	C
5	A	964	U
5	A	965	G
5	A	970	U

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Mol	Chain	Res	Type
5	A	971	U
5	A	973	A
5	A	975	U
5	A	977	A
5	A	985	A
5	A	989	A
5	A	990	G
5	A	992	A
5	A	993	C
5	A	1003	A
5	A	1005	G
5	A	1012	G
5	A	1017	A
5	A	1018	A
5	A	1019	A
5	A	1024	A
5	A	1027	A
5	A	1028	G
5	A	1029	C
5	A	1033	G
5	A	1034	A
5	A	1035	C
5	A	1037	A
5	A	1040	A
5	A	1043	U
5	A	1046	G
5	A	1047	G
5	A	1056	U
5	A	1057	A
5	A	1061	G
5	A	1063	U
5	A	1064	A
5	A	1066	G
5	A	1070	A
5	A	1071	A
5	A	1077	U
5	A	1083	G
5	A	1086	G
5	A	1089	C
5	A	1090	A
5	A	1091	G
5	A	1092	A

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Mol	Chain	Res	Type
5	A	1093	C
5	A	1094	A
5	A	1095	A
5	A	1096	C
5	A	1097	U
5	A	1098	A
5	A	1100	G
5	A	1101	A
5	A	1105	U
5	A	1106	G
5	A	1109	U
5	A	1111	A
5	A	1113	A
5	A	1114	A
5	A	1115	G
5	A	1116	C
5	A	1117	A
5	A	1118	G
5	A	1119	C
5	A	1120	C
5	A	1125	U
5	A	1126	U
5	A	1127	U
5	A	1130	A
5	A	1131	G
5	A	1132	A
5	A	1133	G
5	A	1135	G
5	A	1138	U
5	A	1143	G
5	A	1145	U
5	A	1147	A
5	A	1148	C
5	A	1149	U
5	A	1151	G
5	A	1153	C
5	A	1154	G
5	A	1155	A
5	A	1156	G
5	A	1157	U
5	A	1159	A
5	A	1160	C

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Mol	Chain	Res	Type
5	A	1163	U
5	A	1166	G
5	A	1174	U
5	A	1175	G
5	A	1176	U
5	A	1177	A
5	A	1179	C
5	A	1180	G
5	A	1183	G
5	A	1185	U
5	A	1186	A
5	A	1192	A
5	A	1200	A
5	A	1201	G
5	A	1208	A
5	A	1215	U
5	A	1217	U
5	A	1220	A
5	A	1225	G
5	A	1234	G
5	A	1245	G
5	A	1258	A
5	A	1265	G
5	A	1273	G
5	A	1274	G
5	A	1275	A
5	A	1276	G
5	A	1284	A
5	A	1286	G
5	A	1287	U
5	A	1290	G
5	A	1291	A
5	A	1294	G
5	A	1304	G
5	A	1309	G
5	A	1310	A
5	A	1312	A
5	A	1337	A
5	A	1338	U
5	A	1339	U
5	A	1340	G
5	A	1341	A

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Mol	Chain	Res	Type
5	A	1342	C
5	A	1344	A
5	A	1348	U
5	A	1349	U
5	A	1357	G
5	A	1358	A
5	A	1360	G
5	A	1361	G
5	A	1362	C
5	A	1366	U
5	A	1370	C
5	A	1378	U
5	A	1384	G
5	A	1387	C
5	A	1396	A
5	A	1397	G
5	A	1402	A
5	A	1405	G
5	A	1415	A
5	A	1416	U
5	A	1421	A
5	A	1422	A
5	A	1432	A
5	A	1433	U
5	A	1434	U
5	A	1440	A
5	A	1443	A
5	A	1450	A
5	A	1451	U
5	A	1454	U
5	A	1455	U
5	A	1457	U
5	A	1458	A
5	A	1459	A
5	A	1460	U
5	A	1462	G
5	A	1463	A
5	A	1464	U
5	A	1465	G
5	A	1471	A
5	A	1472	C
5	A	1476	G

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Mol	Chain	Res	Type
5	A	1477	U
5	A	1478	A
5	A	1479	G
5	A	1481	A
5	A	1482	U
5	A	1484	G
5	A	1487	G
5	A	1488	A
5	A	1489	A
5	A	1490	G
5	A	1493	U
5	A	1494	G
5	A	1497	A
5	A	1498	U
5	A	1499	U
5	A	1500	G
5	A	1504	U
5	A	1505	G
5	A	1506	C
5	A	1507	A
5	A	1508	C
5	A	1509	G
5	A	1511	C
5	A	1512	U
5	A	1513	A
5	A	1517	A
5	A	1522	G
5	A	1523	G
5	A	1524	C
5	A	1525	U
5	A	1526	G
5	A	1528	G
5	A	1532	U
5	A	1538	A
5	A	1539	A
5	A	1540	U
5	A	1542	C
5	A	1550	G
5	A	1551	U
5	A	1552	U
5	A	1553	A
5	A	1554	A

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Mol	Chain	Res	Type
5	A	1555	G
5	A	1556	G
5	A	1557	C
5	A	1558	U
5	A	1560	A
5	A	1562	C
5	A	1568	U
5	A	1569	G
5	A	1571	G
5	A	1575	A
5	A	1576	A
5	A	1577	G
5	A	1578	A
5	A	1579	C
5	A	1580	A
5	A	1581	U
5	A	1582	U
5	A	1583	G
5	A	1584	U
5	A	1585	G
5	A	1586	U
5	A	1587	C
5	A	1588	U
5	A	1589	U
5	A	1590	C
5	A	1591	G
5	A	1592	A
5	A	1593	G
5	A	1594	U
5	A	1596	G
5	A	1598	U
5	A	1599	G
5	A	1602	U
5	A	1605	A
5	A	1606	C
5	A	1613	G
5	A	1616	A
5	A	1623	U
5	A	1624	C
5	A	1625	U
5	A	1627	G
5	A	1628	A

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Mol	Chain	Res	Type
5	A	1629	U
5	A	1630	A
5	A	1631	G
5	A	1632	A
5	A	1633	A
5	A	1634	A
5	A	1635	A
5	A	1636	U
5	A	1637	A
5	A	1639	G
5	A	1641	G
5	A	1651	C
5	A	1652	A
5	A	1653	A
5	A	1654	A
5	A	1656	C
5	A	1657	G
5	A	1658	A
5	A	1660	A
5	A	1661	C
5	A	1662	A
5	A	1666	A
5	A	1678	A
5	A	1679	A
5	A	1687	G
5	A	1690	A
5	A	1691	G
5	A	1692	C
5	A	1707	U
5	A	1717	G
5	A	1718	G
5	A	1719	C
5	A	1737	U
5	A	1740	G
5	A	1757	U
5	A	1758	A
5	A	1759	G
5	A	1760	G
5	A	1761	G
5	A	1762	U
5	A	1763	U
5	A	1764	A

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Mol	Chain	Res	Type
5	A	1766	C
5	A	1769	C
5	A	1770	C
5	A	1771	A
5	A	1790	G
5	A	1791	G
5	A	1796	A
5	A	1797	G
5	A	1800	A
5	A	1803	G
5	A	1805	U
5	A	1806	U
5	A	1808	U
5	A	1809	C
5	A	1811	A
5	A	1813	A
5	A	1827	C
5	A	1828	U
5	A	1829	A
5	A	1835	U
5	A	1843	U
5	A	1844	G
5	A	1856	A
5	A	1870	C
5	A	1871	U
5	A	1874	A
5	A	1876	G
5	A	1883	A
5	A	1886	A
5	A	1893	A
5	A	1894	G
5	A	1897	U
5	A	1898	C
5	A	1899	U
5	A	1903	A
5	A	1904	A
5	A	1905	G
5	A	1908	A
5	A	1909	C
5	A	1912	A
5	A	1919	C
5	A	1923	A

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Mol	Chain	Res	Type
5	A	1933	G
5	A	1934	G
5	A	1938	U
5	A	1939	A
5	A	1945	A
5	A	1946	A
5	A	1948	G
5	A	1950	U
5	A	1951	C
5	A	1954	A
5	A	1956	G
5	A	1957	G
5	A	1958	U
5	A	1964	A
5	A	1965	A
5	A	1966	5MU
5	A	1967	U
5	A	1982	U
5	A	1992	C
5	A	1994	C
5	A	1996	A
5	A	1997	A
5	A	1998	A
5	A	1999	G
5	A	2003	U
5	A	2008	A
5	A	2009	U
5	A	2018	U
5	A	2019	G
5	A	2020	U
5	A	2023	C
5	A	2024	A
5	A	2029	G
5	A	2048	G
5	A	2050	A
5	A	2057	A
5	A	2058	A
5	A	2059	G
5	A	2060	A
5	A	2061	U
5	A	2062	G
5	A	2070	C

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Mol	Chain	Res	Type
5	A	2075	G
5	A	2076	A
5	A	2078	A
5	A	2082	C
5	A	2083	G
5	A	2087	A
5	A	2088	G
5	A	2089	A
5	A	2090	C
5	A	2095	U
5	A	2096	G
5	A	2107	G
5	A	2109	A
5	A	2114	G
5	A	2117	A
5	A	2119	U
5	A	2120	G
5	A	2127	G
5	A	2128	G
5	A	2129	C
5	A	2130	A
5	A	2132	A
5	A	2133	G
5	A	2134	C
5	A	2135	U
5	A	2136	U
5	A	2137	G
5	A	2138	U
5	A	2139	A
5	A	2140	C
5	A	2143	G
5	A	2144	A
5	A	2145	U
5	A	2146	A
5	A	2147	G
5	A	2148	G
5	A	2149	U
5	A	2153	A
5	A	2155	C
5	A	2156	C
5	A	2158	U
5	A	2159	U

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Mol	Chain	Res	Type
5	A	2161	A
5	A	2163	A
5	A	2164	C
5	A	2169	G
5	A	2170	C
5	A	2172	C
5	A	2173	U
5	A	2175	G
5	A	2177	U
5	A	2185	A
5	A	2186	G
5	A	2188	C
5	A	2190	C
5	A	2193	G
5	A	2194	U
5	A	2195	G
5	A	2196	G
5	A	2198	A
5	A	2200	A
5	A	2204	C
5	A	2205	C
5	A	2206	C
5	A	2208	A
5	A	2209	G
5	A	2210	C
5	A	2211	U
5	A	2212	G
5	A	2214	G
5	A	2215	U
5	A	2217	G
5	A	2221	U
5	A	2224	U
5	A	2225	A
5	A	2226	A
5	A	2230	G
5	A	2231	C
5	A	2232	A
5	A	2235	A
5	A	2238	U
5	A	2239	A
5	A	2240	U
5	A	2241	C

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Mol	Chain	Res	Type
5	A	2245	G
5	A	2252	A
5	A	2265	G
5	A	2266	G
5	A	2287	C
5	A	2296	A
5	A	2306	G
5	A	2310	C
5	A	2311	U
5	A	2312	C
5	A	2313	A
5	A	2314	A
5	A	2315	A
5	A	2326	G
5	A	2328	A
5	A	2329	U
5	A	2330	G
5	A	2331	G
5	A	2332	U
5	A	2333	U
5	A	2334	G
5	A	2335	G
5	A	2336	A
5	A	2337	A
5	A	2338	A
5	A	2339	U
5	A	2342	U
5	A	2345	A
5	A	2346	U
5	A	2347	A
5	A	2348	G
5	A	2349	A
5	A	2350	G
5	A	2352	G
5	A	2353	U
5	A	2354	A
5	A	2358	G
5	A	2360	A
5	A	2362	A
5	A	2364	G
5	A	2370	U
5	A	2371	U

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Mol	Chain	Res	Type
5	A	2372	G
5	A	2374	C
5	A	2377	C
5	A	2388	A
5	A	2396	A
5	A	2397	G
5	A	2398	G
5	A	2399	G
5	A	2404	A
5	A	2408	C
5	A	2410	G
5	A	2411	A
5	A	2412	C
5	A	2416	G
5	A	2417	U
5	A	2418	G
5	A	2430	C
5	A	2433	C
5	A	2434	A
5	A	2437	G
5	A	2441	G
5	A	2450	U
5	A	2451	C
5	A	2452	A
5	A	2453	A
5	A	2455	G
5	A	2456	G
5	A	2457	A
5	A	2461	A
5	A	2463	G
5	A	2468	C
5	A	2474	G
5	A	2475	A
5	A	2493	C
5	A	2497	G
5	A	2505	A
5	A	2506	U
5	A	2508	G
5	A	2521	G
5	A	2525	C
5	A	2528	C
5	A	2529	G

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Mol	Chain	Res	Type
5	A	2530	2MA
5	A	2531	U
5	A	2532	G
5	A	2533	U
5	A	2534	C
5	A	2543	G
5	A	2545	A
5	A	2547	C
5	A	2552	G
5	A	2554	C
5	A	2556	G
5	A	2558	A
5	A	2559	G
5	A	2562	G
5	A	2568	A
5	A	2569	A
5	A	2570	G
5	A	2574	U
5	A	2579	U
5	A	2580	G
5	A	2589	U
5	A	2592	A
5	A	2593	A
5	A	2594	G
5	A	2599	A
5	A	2600	C
5	A	2601	G
5	A	2605	G
5	A	2609	G
5	A	2612	U
5	A	2613	C
5	A	2626	G
5	A	2629	A
5	A	2636	U
5	A	2640	U
5	A	2642	U
5	A	2648	G
5	A	2649	U
5	A	2650	G
5	A	2656	A
5	A	2661	A
5	A	2668	A

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Mol	Chain	Res	Type
5	A	2672	G
5	A	2673	C
5	A	2681	A
5	A	2682	G
5	A	2683	U
5	A	2684	A
5	A	2685	C
5	A	2687	A
5	A	2692	A
5	A	2693	C
5	A	2694	C
5	A	2695	G
5	A	2696	G
5	A	2700	G
5	A	2709	U
5	A	2712	G
5	A	2716	U
5	A	2728	U
5	A	2729	G
5	A	2733	A
5	A	2741	G
5	A	2745	G
5	A	2753	U
5	A	2755	U
5	A	2756	G
5	A	2760	A
5	A	2761	C
5	A	2769	G
5	A	2771	G
5	A	2776	A
5	A	2777	A
5	A	2781	U
5	A	2782	C
5	A	2783	U
5	A	2784	A
5	A	2787	C
5	A	2788	A
5	A	2792	A
5	A	2794	C
5	A	2803	A
5	A	2804	G
5	A	2805	A

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Mol	Chain	Res	Type
5	A	2806	U
5	A	2807	G
5	A	2817	A
5	A	2818	A
5	A	2819	C
5	A	2820	U
5	A	2821	U
5	A	2824	G
5	A	2826	U
5	A	2827	A
5	A	2828	U
5	A	2829	A
5	A	2830	A
5	A	2832	A
5	A	2838	C
5	A	2840	A
5	A	2844	U
5	A	2846	A
5	A	2851	G
5	A	2853	U
5	A	2855	A
5	A	2887	G
5	A	2888	A
5	A	2892	G
5	A	2899	A
5	A	2900	C
5	A	2904	U
5	A	2905	C
5	A	2906	G
5	A	2913	G
5	A	2914	A
5	A	2916	U
5	A	2919	A
5	A	2920	U
6	B	3	U
6	B	6	U
6	B	10	U
6	B	14	G
6	B	16	A
6	B	17	A
6	B	20	A
6	B	22	G

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Mol	Chain	Res	Type
6	B	23	U
6	B	24	C
6	B	25	A
6	B	26	C
6	B	27	A
6	B	30	U
6	B	31	G
6	B	33	U
6	B	36	C
6	B	37	A
6	B	39	G
6	B	40	C
6	B	41	C
6	B	42	G
6	B	43	A
6	B	45	C
6	B	49	G
6	B	50	A
6	B	51	A
6	B	52	G
6	B	53	U
6	B	54	U
6	B	55	A
6	B	56	A
6	B	58	C
6	B	62	U
6	B	63	U
6	B	64	A
6	B	65	G
6	B	87	C
6	B	88	G
6	B	101	A
6	B	102	G
6	B	105	C
6	B	106	G
6	B	107	U
6	B	111	C
6	B	113	G
6	B	115	C
31	a	8	G
31	a	10	G
31	a	31	U

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Mol	Chain	Res	Type
31	a	32	G
31	a	33	A
31	a	40	G
31	a	43	G
31	a	45	G
31	a	48	C
31	a	49	C
31	a	52	A
31	a	62	G
31	a	65	G
31	a	67	G
31	a	69	G
31	a	71	A
31	a	72	C
31	a	76	C
31	a	94	G
31	a	95	A
31	a	98	U
31	a	99	U
31	a	100	A
31	a	118	A
31	a	119	A
31	a	120	C
31	a	129	A
31	a	130	A
31	a	136	C
31	a	142	G
31	a	151	A
31	a	157	G
31	a	158	G
31	a	159	G
31	a	163	C
31	a	167	A
31	a	168	G
31	a	171	A
31	a	173	U
31	a	174	A
31	a	184	A
31	a	185	U
31	a	188	U
31	a	189	G
31	a	194	G

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Mol	Chain	Res	Type
31	a	197	U
31	a	200	U
31	a	201	U
31	a	203	A
31	a	204	A
31	a	209	G
31	a	211	A
31	a	215	C
31	a	217	G
31	a	226	U
31	a	227	C
31	a	230	U
31	a	233	U
31	a	234	A
31	a	239	G
31	a	248	U
31	a	251	A
31	a	255	G
31	a	256	C
31	a	259	G
31	a	268	G
31	a	269	U
31	a	274	G
31	a	275	C
31	a	278	A
31	a	279	C
31	a	297	G
31	a	301	A
31	a	327	G
31	a	329	A
31	a	336	C
31	a	337	A
31	a	338	C
31	a	352	A
31	a	355	G
31	a	359	G
31	a	360	C
31	a	362	G
31	a	363	C
31	a	375	U
31	a	380	C
31	a	390	A

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Mol	Chain	Res	Type
31	a	396	G
31	a	401	A
31	a	405	A
31	a	406	C
31	a	412	G
31	a	414	G
31	a	415	A
31	a	421	G
31	a	422	A
31	a	423	A
31	a	424	G
31	a	427	C
31	a	429	U
31	a	430	C
31	a	431	G
31	a	437	U
31	a	440	A
31	a	442	C
31	a	443	U
31	a	447	U
31	a	452	A
31	a	456	A
31	a	459	A
31	a	460	A
31	a	461	C
31	a	466	G
31	a	468	G
31	a	473	U
31	a	484	A
31	a	485	U
31	a	486	C
31	a	487	U
31	a	488	U
31	a	489	G
31	a	492	G
31	a	499	A
31	a	501	U
31	a	503	A
31	a	504	G
31	a	508	G
31	a	514	G
31	a	517	A

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Mol	Chain	Res	Type
31	a	519	C
31	a	526	C
31	a	529	G
31	a	532	G
31	a	535	G
31	a	538	G
31	a	539	U
31	a	540	A
31	a	541	A
31	a	542	U
31	a	543	A
31	a	544	C
31	a	548	G
31	a	553	C
31	a	555	A
31	a	567	A
31	a	572	U
31	a	578	G
31	a	580	A
31	a	581	A
31	a	584	C
31	a	585	G
31	a	587	G
31	a	590	U
31	a	591	A
31	a	596	G
31	a	604	A
31	a	612	G
31	a	634	U
31	a	640	G
31	a	641	U
31	a	642	C
31	a	649	A
31	a	650	A
31	a	660	U
31	a	661	U
31	a	664	G
31	a	673	A
31	a	691	G
31	a	694	U
31	a	701	G
31	a	703	A

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Mol	Chain	Res	Type
31	a	708	G
31	a	726	A
31	a	730	G
31	a	732	G
31	a	741	G
31	a	757	A
31	a	763	G
31	a	785	A
31	a	788	A
31	a	789	A
31	a	790	A
31	a	793	G
31	a	794	G
31	a	796	U
31	a	801	U
31	a	802	A
31	a	803	C
31	a	817	G
31	a	820	G
31	a	823	A
31	a	825	C
31	a	826	G
31	a	827	A
31	a	829	G
31	a	836	A
31	a	864	G
31	a	868	C
31	a	869	A
31	a	879	U
31	a	880	U
31	a	881	A
31	a	894	G
31	a	911	G
31	a	923	A
31	a	934	G
31	a	935	G
31	a	936	G
31	a	937	G
31	a	940	C
31	a	942	G
31	a	943	C
31	a	948	G

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Mol	Chain	Res	Type
31	a	949	C
31	a	953	G
31	a	969	U
31	a	970	U
31	a	973	A
31	a	978	A
31	a	980	G
31	a	983	A
31	a	984	A
31	a	986	A
31	a	987	A
31	a	991	U
31	a	993	C
31	a	998	U
31	a	1000	U
31	a	1001	U
31	a	1002	G
31	a	1005	A
31	a	1007	C
31	a	1008	C
31	a	1029	A
31	a	1055	A
31	a	1060	U
31	a	1064	G
31	a	1067	U
31	a	1075	G
31	a	1076	U
31	a	1092	G
31	a	1097	U
31	a	1105	G
31	a	1110	G
31	a	1112	A
31	a	1113	A
31	a	1119	G
31	a	1120	C
31	a	1122	A
31	a	1124	C
31	a	1128	A
31	a	1132	U
31	a	1135	G
31	a	1137	U
31	a	1139	C

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Mol	Chain	Res	Type
31	a	1140	C
31	a	1141	A
31	a	1143	C
31	a	1144	A
31	a	1152	G
31	a	1155	C
31	a	1156	A
31	a	1167	A
31	a	1168	C
31	a	1169	U
31	a	1172	C
31	a	1174	G
31	a	1175	U
31	a	1177	A
31	a	1178	C
31	a	1179	A
31	a	1182	C
31	a	1187	G
31	a	1189	A
31	a	1194	G
31	a	1203	G
31	a	1205	C
31	a	1206	A
31	a	1207	A
31	a	1218	C
31	a	1222	U
31	a	1223	A
31	a	1225	G
31	a	1235	A
31	a	1236	C
31	a	1237	A
31	a	1239	A
31	a	1246	A
31	a	1248	A
31	a	1250	U
31	a	1254	C
31	a	1255	A
31	a	1256	A
31	a	1264	G
31	a	1266	C
31	a	1268	G
31	a	1269	C

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Mol	Chain	Res	Type
31	a	1270	G
31	a	1271	A
31	a	1278	G
31	a	1279	A
31	a	1280	G
31	a	1283	C
31	a	1289	A
31	a	1290	A
31	a	1292	C
31	a	1296	U
31	a	1297	A
31	a	1298	A
31	a	1303	G
31	a	1307	U
31	a	1308	C
31	a	1310	G
31	a	1312	U
31	a	1313	C
31	a	1315	G
31	a	1326	G
31	a	1329	A
31	a	1330	C
31	a	1331	U
31	a	1332	C
31	a	1333	G
31	a	1334	A
31	a	1335	C
31	a	1338	C
31	a	1341	G
31	a	1346	U
31	a	1347	G
31	a	1356	A
31	a	1357	G
31	a	1358	U
31	a	1363	G
31	a	1374	U
31	a	1380	G
31	a	1384	A
31	a	1385	A
31	a	1387	A
31	a	1388	C
31	a	1389	G

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Mol	Chain	Res	Type
31	a	1390	U
31	a	1391	U
31	a	1393	C
31	a	1397	G
31	a	1401	U
31	a	1404	A
31	a	1407	C
31	a	1408	A
31	a	1409	C
31	a	1410	C
31	a	1415	G
31	a	1420	A
31	a	1429	G
31	a	1445	G
31	a	1451	G
31	a	1452	G
31	a	1456	A
31	a	1457	A
31	a	1460	U
31	a	1474	C
31	a	1475	G
31	a	1476	U
31	a	1490	A
31	a	1498	G
31	a	1500	G
31	a	1504	A
31	a	1505	G
31	a	1508	G
31	a	1510	A
31	a	1514	A
31	a	1515	G
31	a	1517	U
31	a	1518	A
31	a	1528	G
31	a	1529	A
31	a	1530	A
31	a	1532	G
31	a	1540	G
31	a	1541	G
31	a	1547	C
31	a	1548	U
31	a	1549	C

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Mol	Chain	Res	Type
31	a	1550	C

All (82) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	63	U
5	A	82	G
5	A	90	A
5	A	98	U
5	A	104	C
5	A	199	A
5	A	202	A
5	A	291	G
5	A	299	U
5	A	327	G
5	A	328	G
5	A	337	A
5	A	373	A
5	A	403	U
5	A	502	C
5	A	513	G
5	A	520	G
5	A	548	A
5	A	576	U
5	A	577	A
5	A	614	U
5	A	672	A
5	A	690	U
5	A	715	A
5	A	809	A
5	A	890	G
5	A	910	C
5	A	1017	A
5	A	1028	G
5	A	1077	U
5	A	1096	C
5	A	1097	U
5	A	1130	A
5	A	1153	C
5	A	1312	A
5	A	1357	G
5	A	1361	G

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Mol	Chain	Res	Type
5	A	1433	U
5	A	1434	U
5	A	1455	U
5	A	1458	A
5	A	1525	U
5	A	1552	U
5	A	1554	A
5	A	1555	G
5	A	1577	G
5	A	1581	U
5	A	1591	G
5	A	1593	G
5	A	1605	A
5	A	1628	A
5	A	1629	U
5	A	1634	A
5	A	1652	A
5	A	1757	U
5	A	1760	G
5	A	1789	A
5	A	1826	G
5	A	2089	A
5	A	2094	G
5	A	2137	G
5	A	2224	U
5	A	2225	A
5	A	2238	U
5	A	2329	U
5	A	2347	A
5	A	2353	U
5	A	2409	G
5	A	2457	A
5	A	2495	A
5	A	2505	A
5	A	2533	U
5	A	2599	A
5	A	2628	C
5	A	2672	G
5	A	2829	A
5	A	2887	G
5	A	2912	A
6	B	22	G

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Mol	Chain	Res	Type
6	B	37	A
6	B	50	A
6	B	105	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	5MU	A	1966	5	19,22,23	1.66	5 (26%)	27,32,35	2.35	8 (29%)
5	MA6	A	2085	5	23,26,27	1.53	5 (21%)	33,38,41	2.36	13 (39%)
5	2MA	A	2530	5,52	22,25,26	1.46	5 (22%)	32,37,40	2.45	9 (28%)
5	2MG	A	2472	5	23,26,27	1.37	3 (13%)	33,38,41	2.75	12 (36%)
5	OMG	A	2278	5	23,26,27	1.27	4 (17%)	32,38,41	2.07	7 (21%)
5	5MU	A	792	5	19,22,23	1.48	5 (26%)	27,32,35	2.29	8 (29%)

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
5	5MU	A	1966	5	-	0/7/25/26	0/2/2/2
5	MA6	A	2085	5	-	2/11/29/30	0/3/3/3
5	2MA	A	2530	5,52	-	0/7/25/26	0/3/3/3
5	2MG	A	2472	5	-	0/9/27/28	0/3/3/3
5	OMG	A	2278	5	-	1/9/27/28	0/3/3/3
5	5MU	A	792	5	-	0/7/25/26	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2085	MA6	C5-C4	4.25	1.46	1.39
5	A	2530	2MA	C5-C4	4.00	1.46	1.39
5	A	2472	2MG	C6-N1	-3.42	1.32	1.38
5	A	1966	5MU	C4-N3	-3.25	1.32	1.38
5	A	792	5MU	C4-N3	-3.24	1.32	1.38
5	A	1966	5MU	C6-C5	3.16	1.39	1.34
5	A	1966	5MU	C2-N3	-3.08	1.32	1.38
5	A	2278	OMG	C6-N1	-2.99	1.33	1.38
5	A	2472	2MG	C5-N7	-2.88	1.33	1.39
5	A	2085	MA6	C5-C6	2.87	1.48	1.41
5	A	2530	2MA	C5-N7	-2.76	1.34	1.39
5	A	792	5MU	C6-N1	-2.72	1.33	1.38
5	A	792	5MU	C2-N3	-2.72	1.33	1.38
5	A	2472	2MG	C4-N9	-2.69	1.31	1.38
5	A	1966	5MU	C2-N1	2.61	1.42	1.38
5	A	2278	OMG	C5-C4	2.60	1.45	1.38
5	A	2085	MA6	C4-N9	-2.50	1.32	1.37
5	A	2278	OMG	C5-N7	-2.46	1.34	1.39
5	A	2530	2MA	C5-C6	2.35	1.47	1.41
5	A	1966	5MU	C4-C5	2.30	1.48	1.44
5	A	2085	MA6	C5-N7	-2.29	1.34	1.39
5	A	2085	MA6	C8-N9	-2.21	1.33	1.37
5	A	792	5MU	C2-N1	2.19	1.41	1.38
5	A	792	5MU	C6-C5	2.16	1.38	1.34
5	A	2530	2MA	C4-N9	-2.14	1.33	1.37
5	A	2278	OMG	C4-N9	-2.08	1.32	1.38
5	A	2530	2MA	C8-N9	-2.01	1.34	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2472	2MG	C2-N3-C4	8.92	123.16	112.00
5	A	2530	2MA	C5-C4-N3	-8.23	118.51	127.18
5	A	2472	2MG	N1-C2-N2	7.06	123.76	116.56
5	A	2530	2MA	N3-C4-N9	6.92	135.77	126.99
5	A	2278	OMG	C5-C4-N3	-6.16	118.58	128.39
5	A	1966	5MU	N3-C2-N1	5.99	122.69	114.89
5	A	2472	2MG	C5-C4-N3	-5.59	119.49	128.39
5	A	792	5MU	N3-C2-N1	5.44	121.97	114.89
5	A	1966	5MU	C5-C4-N3	5.29	119.92	115.32
5	A	2278	OMG	C2-N3-C4	5.27	121.37	112.30
5	A	1966	5MU	C4-N3-C2	-5.06	120.71	127.34
5	A	792	5MU	C4-N3-C2	-5.03	120.75	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2085	MA6	C5-C4-N3	-4.96	119.89	126.72
5	A	2085	MA6	C10-N6-C6	-4.66	108.66	120.52
5	A	2085	MA6	C2-N1-C6	4.57	122.98	111.83
5	A	2278	OMG	N9-C4-N3	4.51	134.98	125.95
5	A	2085	MA6	C4-C5-N7	-4.32	105.64	110.58
5	A	2472	2MG	C6-C5-N7	4.28	138.09	130.29
5	A	792	5MU	O4-C4-C5	-4.05	120.29	124.92
5	A	792	5MU	C5-C4-N3	3.95	118.75	115.32
5	A	2085	MA6	N3-C4-N9	3.78	133.60	127.17
5	A	2085	MA6	N1-C2-N3	-3.71	122.96	128.58
5	A	2085	MA6	C2-N3-C4	3.63	120.70	111.83
5	A	2472	2MG	N9-C4-N3	3.54	133.03	125.95
5	A	1966	5MU	O4-C4-C5	-3.36	121.07	124.92
5	A	2278	OMG	C6-C5-N7	3.35	136.38	130.29
5	A	792	5MU	C5-C6-N1	-3.30	119.73	123.31
5	A	1966	5MU	O2-C2-N3	-3.26	115.48	121.49
5	A	2530	2MA	C4-C5-N7	-3.19	106.93	110.58
5	A	2530	2MA	C4-N9-C8	3.16	109.05	105.74
5	A	2085	MA6	C4-N9-C8	3.14	109.04	105.74
5	A	2530	2MA	N6-C6-N1	3.13	121.25	117.03
5	A	2472	2MG	N2-C2-N3	-3.09	116.57	120.51
5	A	792	5MU	C3'-C2'-C1'	2.99	107.12	101.46
5	A	2085	MA6	C5-N7-C8	2.99	108.15	103.45
5	A	2085	MA6	C6-C5-N7	2.91	138.07	133.43
5	A	1966	5MU	O4'-C1'-N1	2.87	114.87	108.36
5	A	2472	2MG	C4-C5-N7	-2.75	106.31	110.67
5	A	2530	2MA	C2-N1-C6	2.65	122.17	118.10
5	A	1966	5MU	C6-N1-C2	-2.63	118.68	121.30
5	A	2530	2MA	C5-N7-C8	2.63	107.59	103.45
5	A	792	5MU	C1'-N1-C2	2.59	122.24	117.59
5	A	792	5MU	O2-C2-N3	-2.52	116.84	121.49
5	A	1966	5MU	C5-C6-N1	-2.45	120.65	123.31
5	A	2278	OMG	O6-C6-C5	-2.45	120.06	126.53
5	A	2472	2MG	N1-C2-N3	-2.39	119.65	123.68
5	A	2278	OMG	C4-C5-N7	-2.34	106.96	110.67
5	A	2085	MA6	N9-C8-N7	-2.32	110.65	113.94
5	A	2530	2MA	N9-C8-N7	-2.28	110.70	113.94
5	A	2278	OMG	C5-C6-N1	2.25	118.98	113.25
5	A	2472	2MG	C5-C6-N1	2.25	118.97	113.25
5	A	2085	MA6	C10-N6-C9	-2.21	109.09	116.18
5	A	2085	MA6	C2'-C1'-N9	-2.16	107.94	113.30
5	A	2472	2MG	C6-C5-C4	-2.15	115.59	118.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2530	2MA	C6-C5-N7	2.12	136.17	132.09
5	A	2472	2MG	O6-C6-C5	-2.11	120.96	126.53
5	A	2472	2MG	C8-N7-C5	2.02	107.86	104.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2085	MA6	C5-C6-N6-C10
5	A	2278	OMG	C1'-C2'-O2'-CM2
5	A	2085	MA6	N1-C6-N6-C10

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2085	MA6	1	0
5	A	2278	OMG	1	0
5	A	792	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 12 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
51	A1D6G	A	3000	52	72,73,73	2.44	26 (36%)	97,107,107	1.84	30 (30%)

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
51	A1D6G	A	3000	52	-	11/82/113/113	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	3000	A1D6G	C65-N64	8.77	1.45	1.33
51	A	3000	A1D6G	C11-N13	7.43	1.50	1.34
51	A	3000	A1D6G	O67-C65	4.92	1.43	1.36
51	A	3000	A1D6G	O10-C11	4.88	1.43	1.35
51	A	3000	A1D6G	C22-C21	4.59	1.55	1.44
51	A	3000	A1D6G	O67-C68	-4.43	1.41	1.47
51	A	3000	A1D6G	O04-C03	-4.32	1.39	1.46
51	A	3000	A1D6G	C19-C20	3.81	1.56	1.47
51	A	3000	A1D6G	C25-C26	-3.81	1.40	1.48
51	A	3000	A1D6G	O04-C05	3.55	1.42	1.34
51	A	3000	A1D6G	C50-C46	-3.18	1.47	1.53
51	A	3000	A1D6G	C28-C29	3.15	1.53	1.48
51	A	3000	A1D6G	C35-N33	-3.13	1.33	1.39
51	A	3000	A1D6G	O42-C41	3.04	1.49	1.41
51	A	3000	A1D6G	C32-N33	-3.04	1.32	1.35
51	A	3000	A1D6G	C63-N64	-2.96	1.40	1.45
51	A	3000	A1D6G	C25-C35	-2.76	1.36	1.41
51	A	3000	A1D6G	O10-C09	-2.57	1.41	1.44
51	A	3000	A1D6G	O54-C52	-2.38	1.39	1.44
51	A	3000	A1D6G	C45-C46	-2.37	1.48	1.53
51	A	3000	A1D6G	O27-C26	-2.30	1.18	1.23
51	A	3000	A1D6G	O60-C59	-2.21	1.18	1.21
51	A	3000	A1D6G	O42-C43	2.13	1.48	1.44
51	A	3000	A1D6G	C28-C26	-2.09	1.39	1.44
51	A	3000	A1D6G	C21-C20	2.06	1.22	1.19
51	A	3000	A1D6G	C56-C52	2.04	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	A	3000	A1D6G	C63-N64-C65	-4.32	106.75	112.39
51	A	3000	A1D6G	O10-C11-N13	4.31	118.03	111.01
51	A	3000	A1D6G	O42-C43-C45	4.27	115.45	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	A	3000	A1D6G	C52-C39-C37	-4.12	107.24	113.54
51	A	3000	A1D6G	C02-C03-C68	-3.95	109.79	115.23
51	A	3000	A1D6G	C44-C43-C45	-3.89	107.38	113.27
51	A	3000	A1D6G	C41-O42-C43	3.79	118.75	112.91
51	A	3000	A1D6G	O04-C05-C07	3.30	118.57	111.53
51	A	3000	A1D6G	C35-N33-C32	3.16	123.13	120.03
51	A	3000	A1D6G	O30-C29-C28	3.05	122.84	115.69
51	A	3000	A1D6G	O66-C65-N64	-3.04	125.59	129.19
51	A	3000	A1D6G	O67-C68-C69	3.02	112.13	106.80
51	A	3000	A1D6G	O67-C65-O66	2.99	125.53	121.64
51	A	3000	A1D6G	C03-O04-C05	-2.96	113.04	118.20
51	A	3000	A1D6G	O10-C11-O12	-2.86	120.35	124.55
51	A	3000	A1D6G	C28-C32-N33	-2.64	119.57	123.31
51	A	3000	A1D6G	C14-N13-C11	-2.63	117.53	121.98
51	A	3000	A1D6G	C38-C37-C09	-2.59	106.83	111.40
51	A	3000	A1D6G	C56-C52-C39	-2.33	107.38	110.18
51	A	3000	A1D6G	C45-C46-N47	-2.31	109.11	115.59
51	A	3000	A1D6G	C53-C52-C39	2.23	113.07	109.79
51	A	3000	A1D6G	O12-C11-N13	-2.20	121.62	124.93
51	A	3000	A1D6G	C69-C68-C03	-2.17	108.49	112.36
51	A	3000	A1D6G	O30-C29-O31	-2.17	118.74	123.90
51	A	3000	A1D6G	C57-C59-C61	2.12	122.71	119.13
51	A	3000	A1D6G	O42-C41-C50	2.08	114.65	110.37
51	A	3000	A1D6G	O31-C29-C28	-2.06	118.42	122.67
51	A	3000	A1D6G	O40-C39-C52	2.05	111.20	106.44
51	A	3000	A1D6G	C56-C57-C59	-2.05	109.89	113.32
51	A	3000	A1D6G	C15-C14-N13	-2.02	106.54	112.20

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	A	3000	A1D6G	C18-C19-C20-C21
51	A	3000	A1D6G	O10-C11-N13-C14
51	A	3000	A1D6G	O12-C11-N13-C14
51	A	3000	A1D6G	C19-C20-C21-C22
51	A	3000	A1D6G	N13-C11-O10-C09
51	A	3000	A1D6G	O42-C41-O40-C39
51	A	3000	A1D6G	C01-C02-C03-O04
51	A	3000	A1D6G	O12-C11-O10-C09
51	A	3000	A1D6G	C19-C18-O17-C16
51	A	3000	A1D6G	C50-C41-O40-C39

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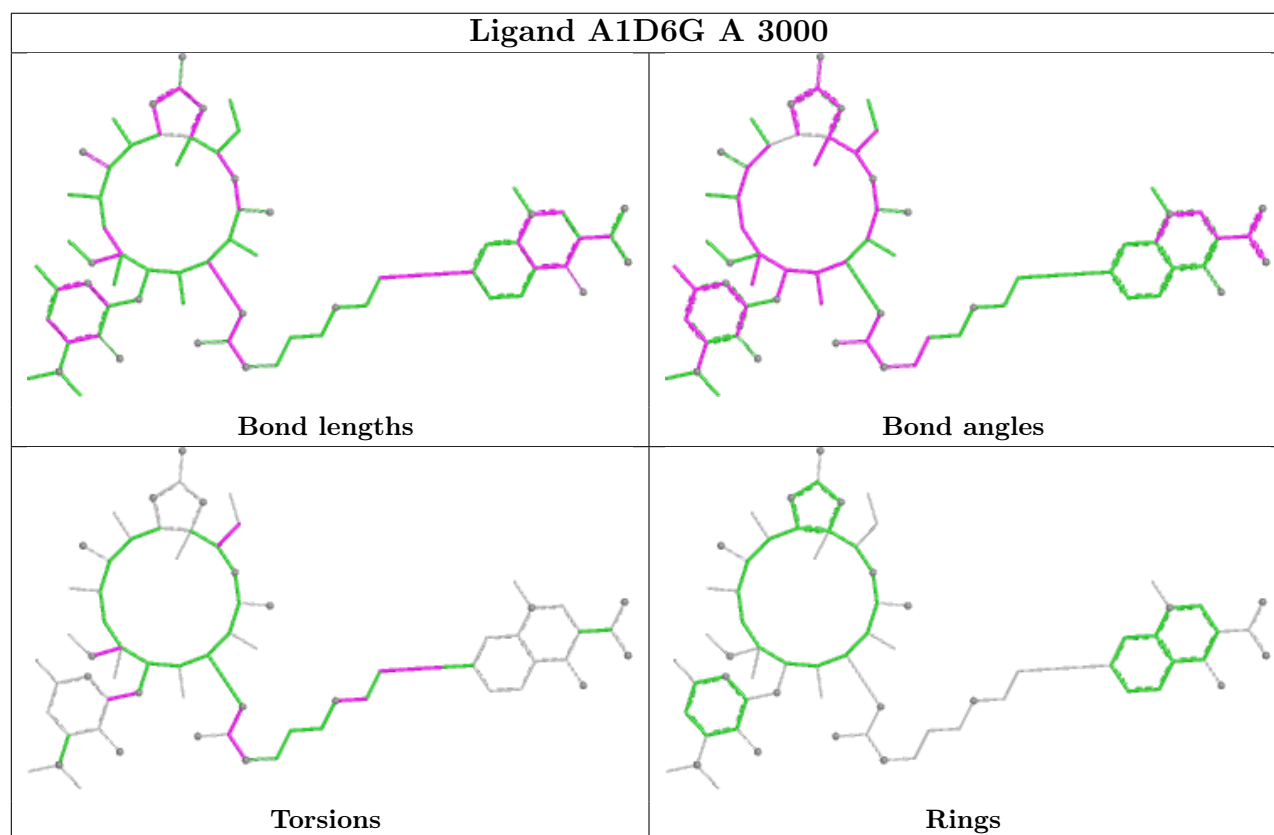
Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	A	3000	A1D6G	C56-C52-O54-C55

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

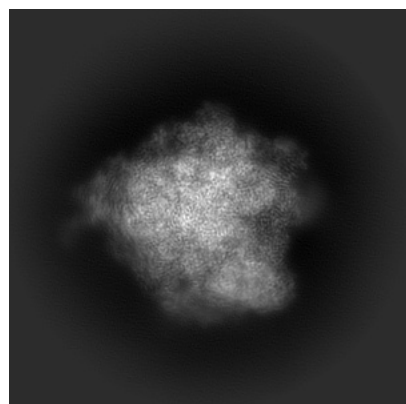
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38875. These allow visual inspection of the internal detail of the map and identification of artifacts.

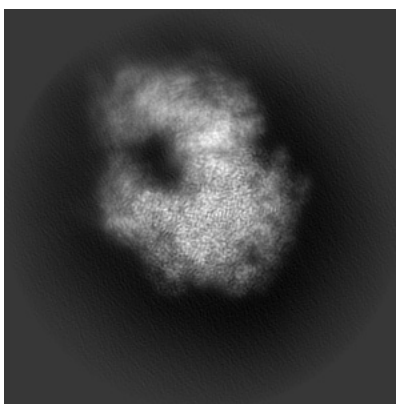
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

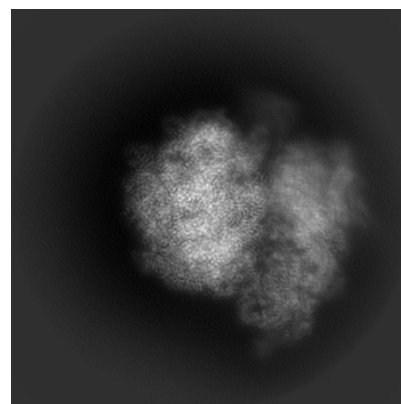
6.1.1 Primary map



X

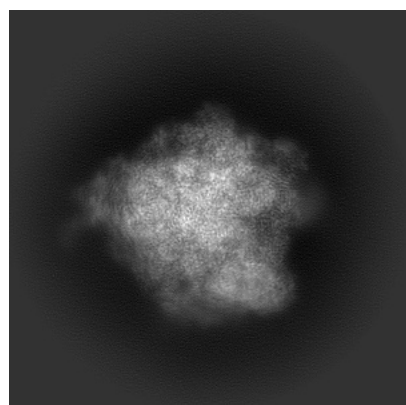


Y

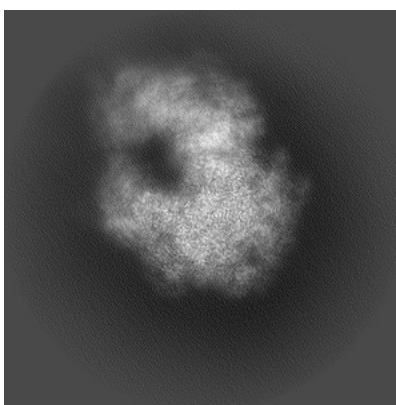


Z

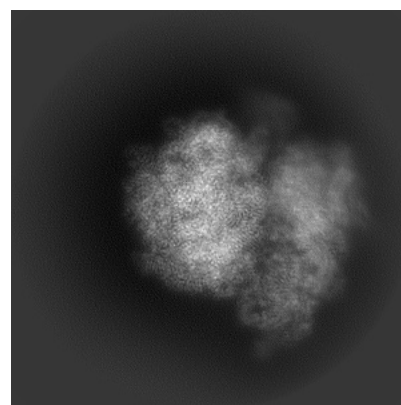
6.1.2 Raw map



X



Y

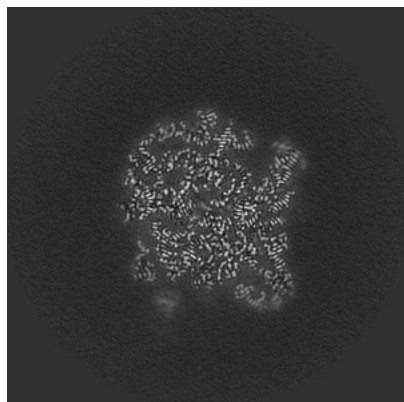


Z

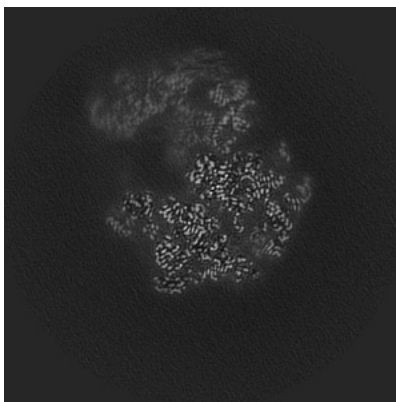
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

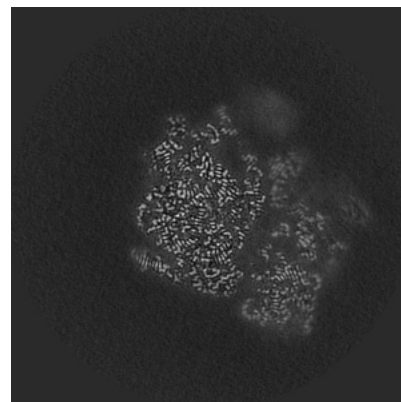
6.2.1 Primary map



X Index: 240

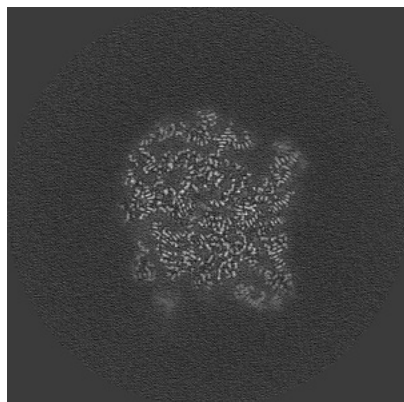


Y Index: 240

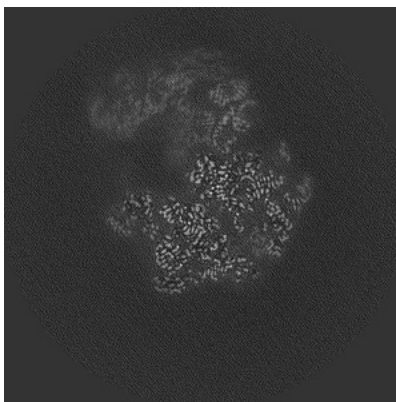


Z Index: 240

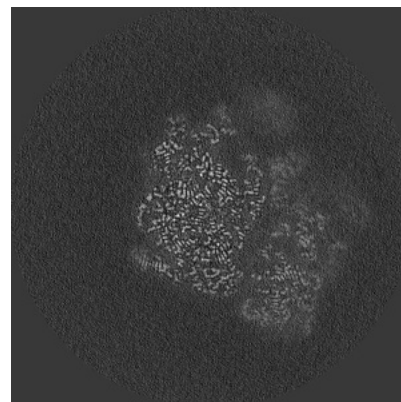
6.2.2 Raw map



X Index: 240



Y Index: 240

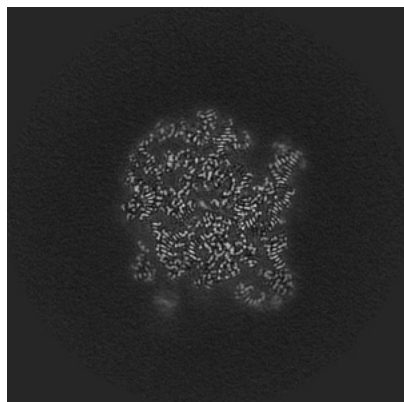


Z Index: 240

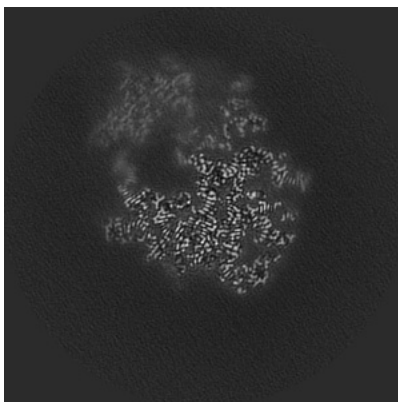
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

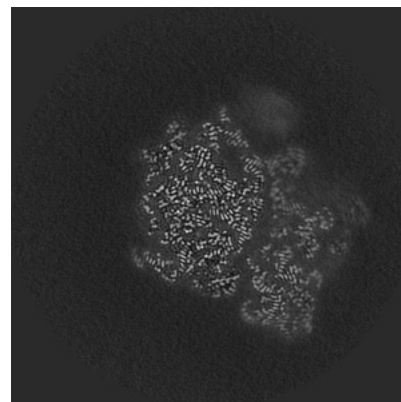
6.3.1 Primary map



X Index: 239

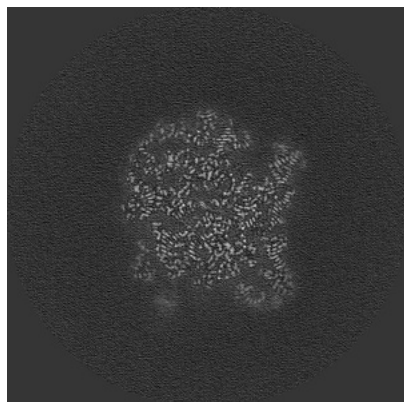


Y Index: 257

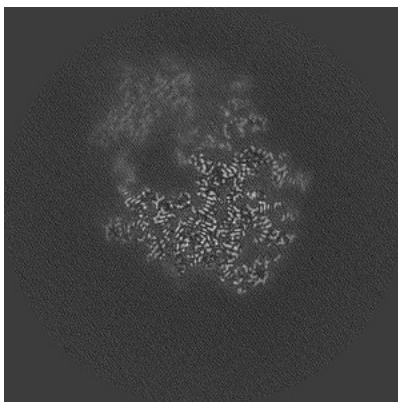


Z Index: 244

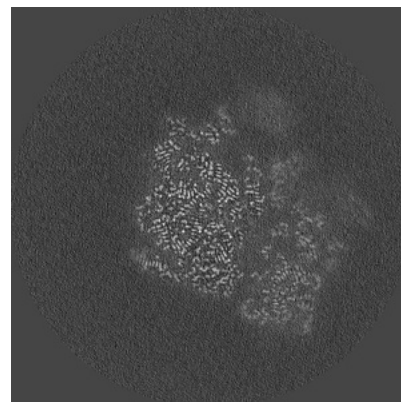
6.3.2 Raw map



X Index: 239



Y Index: 257

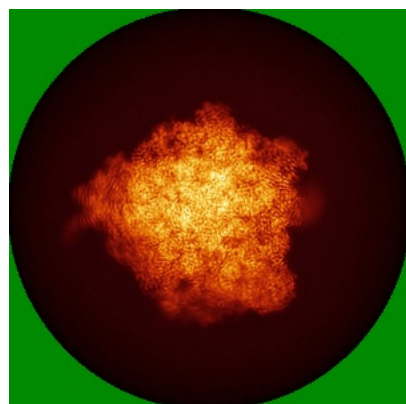


Z Index: 239

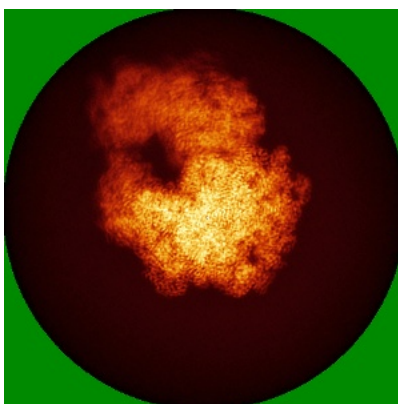
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

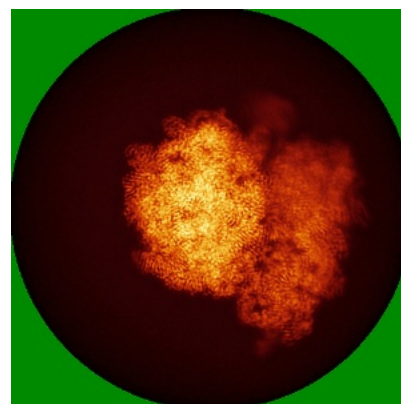
6.4.1 Primary map



X

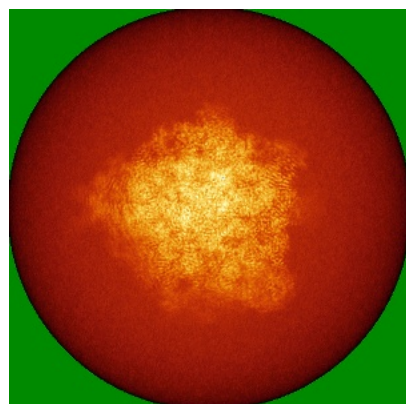


Y

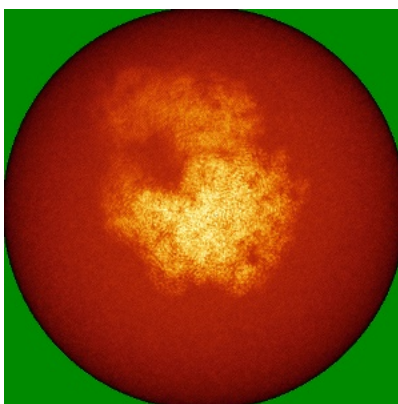


Z

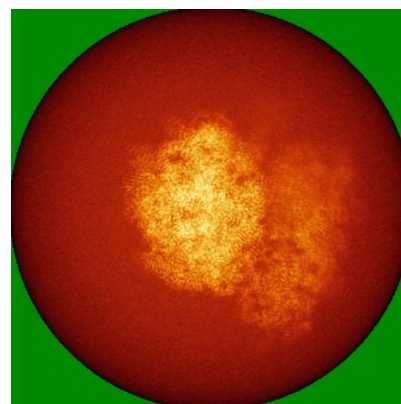
6.4.2 Raw map



X



Y

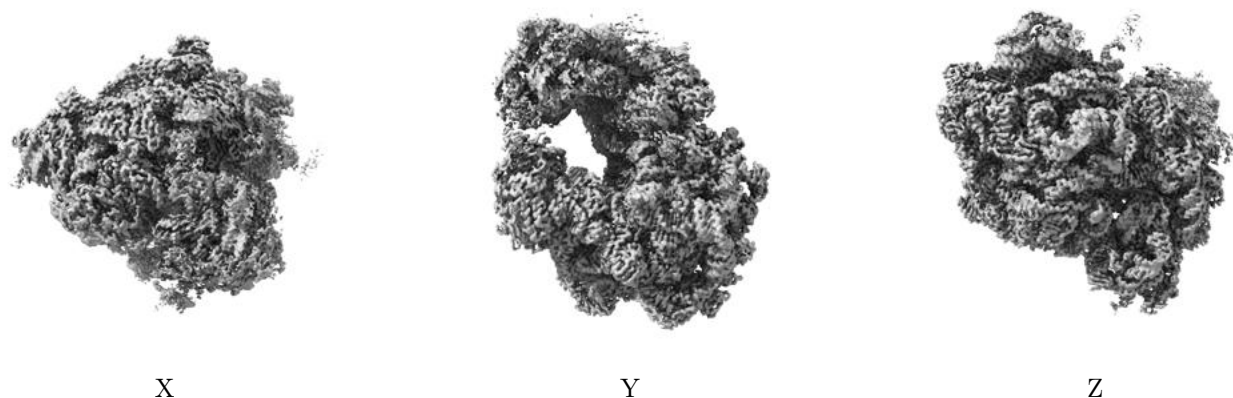


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

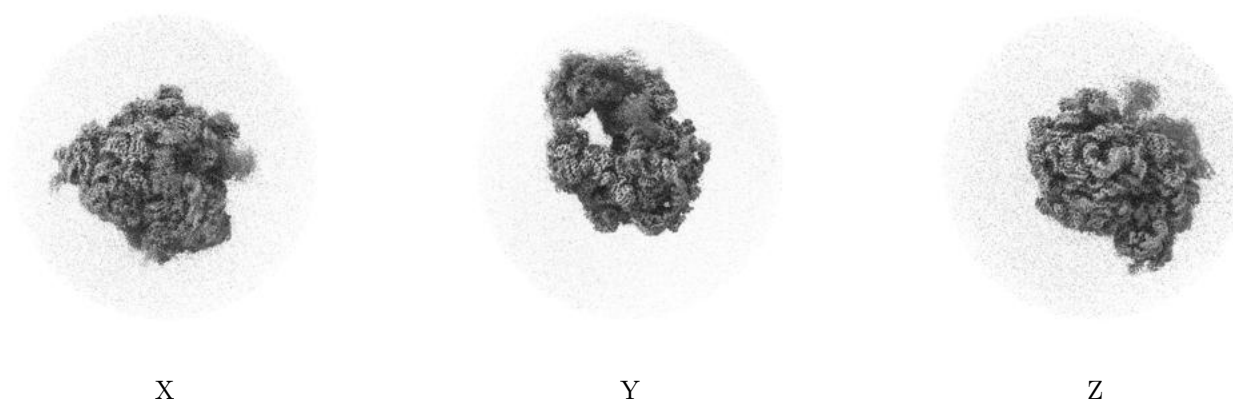
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

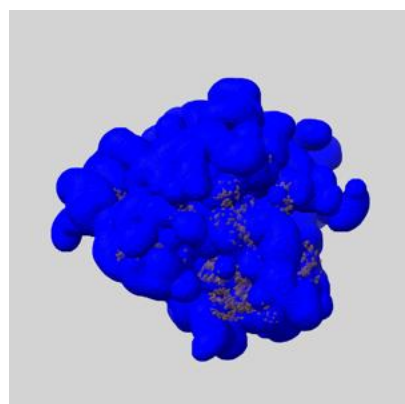
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

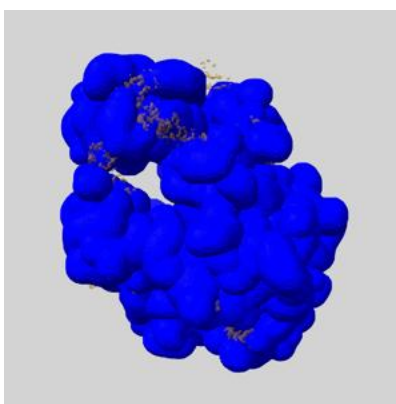
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

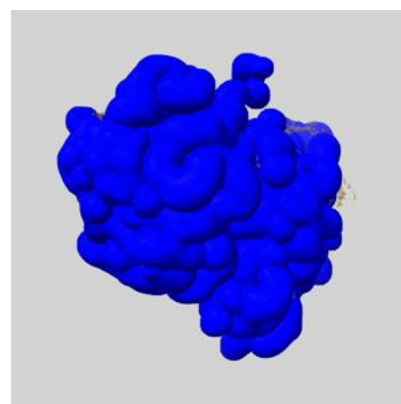
6.6.1 emd_38875_msk_1.map [i](#)



X



Y

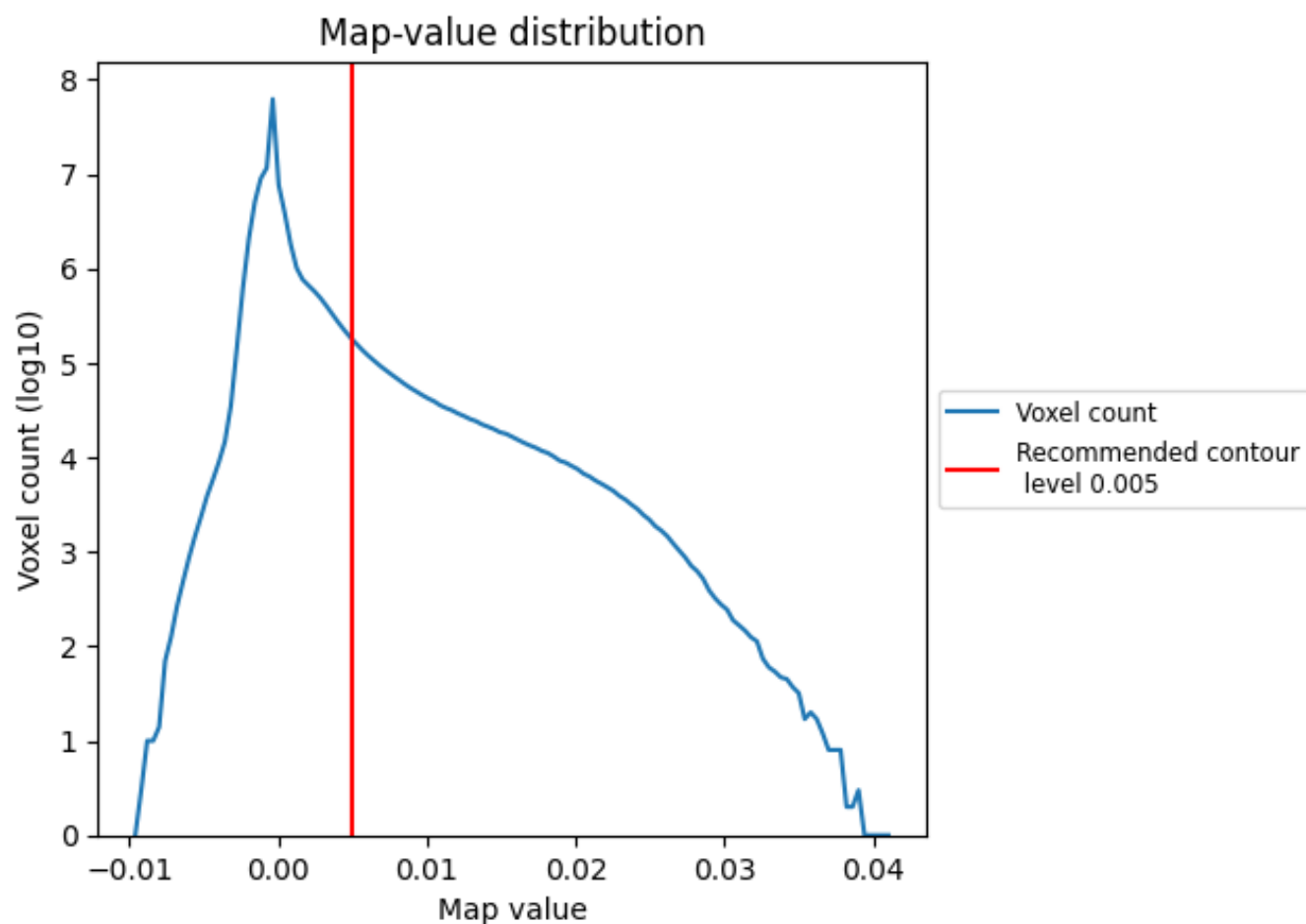


Z

7 Map analysis [i](#)

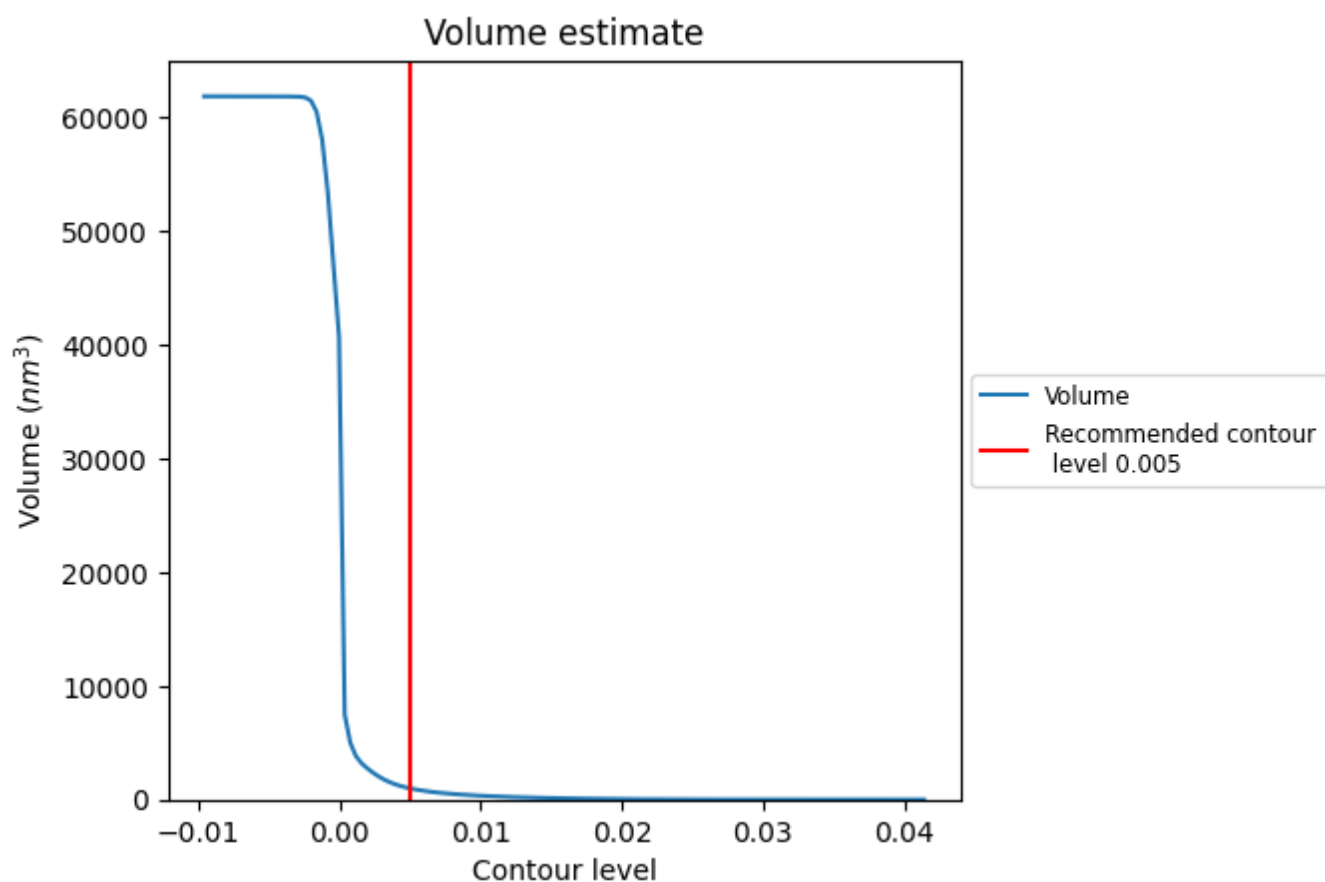
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

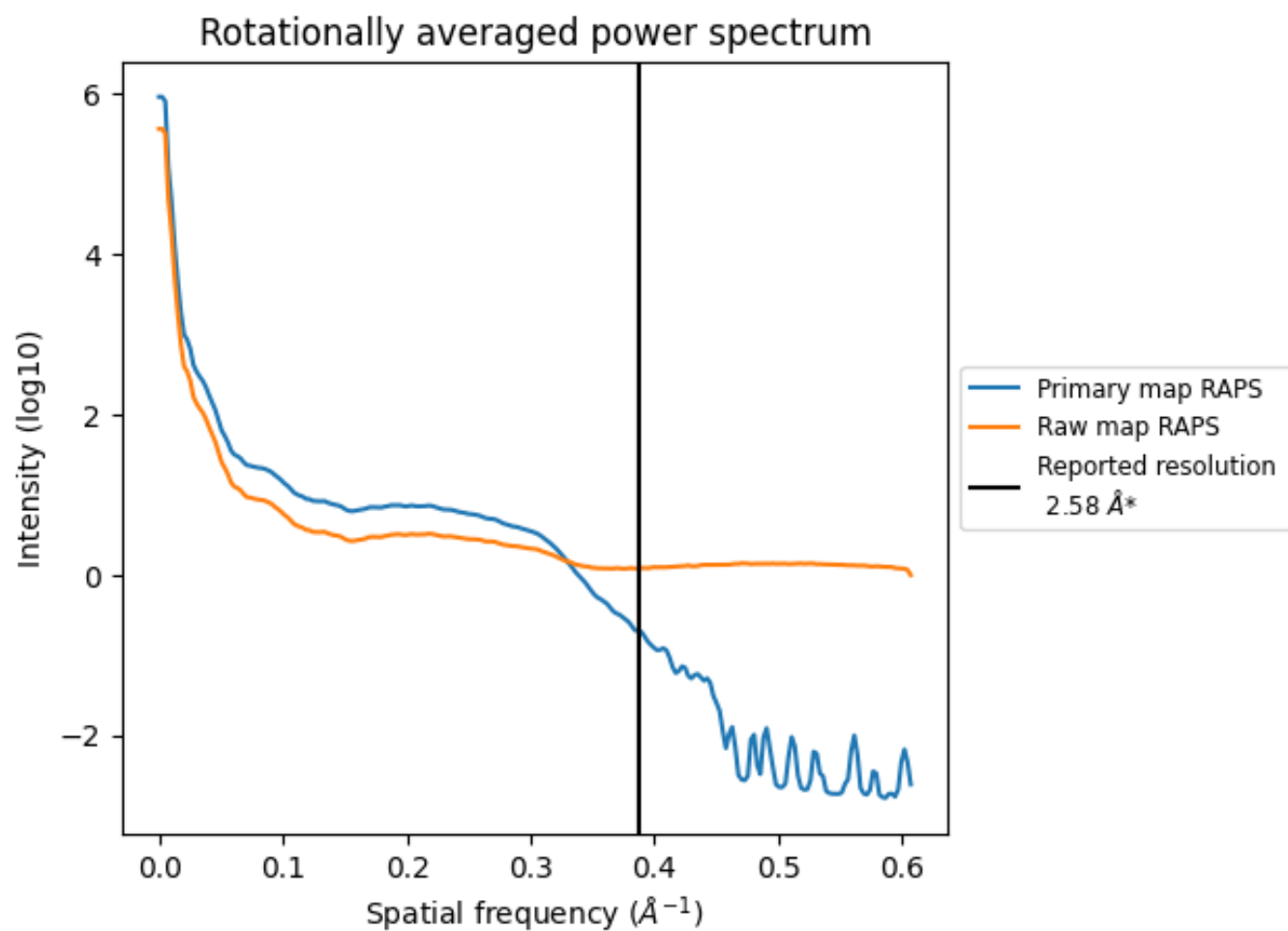
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 985 nm³; this corresponds to an approximate mass of 889 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

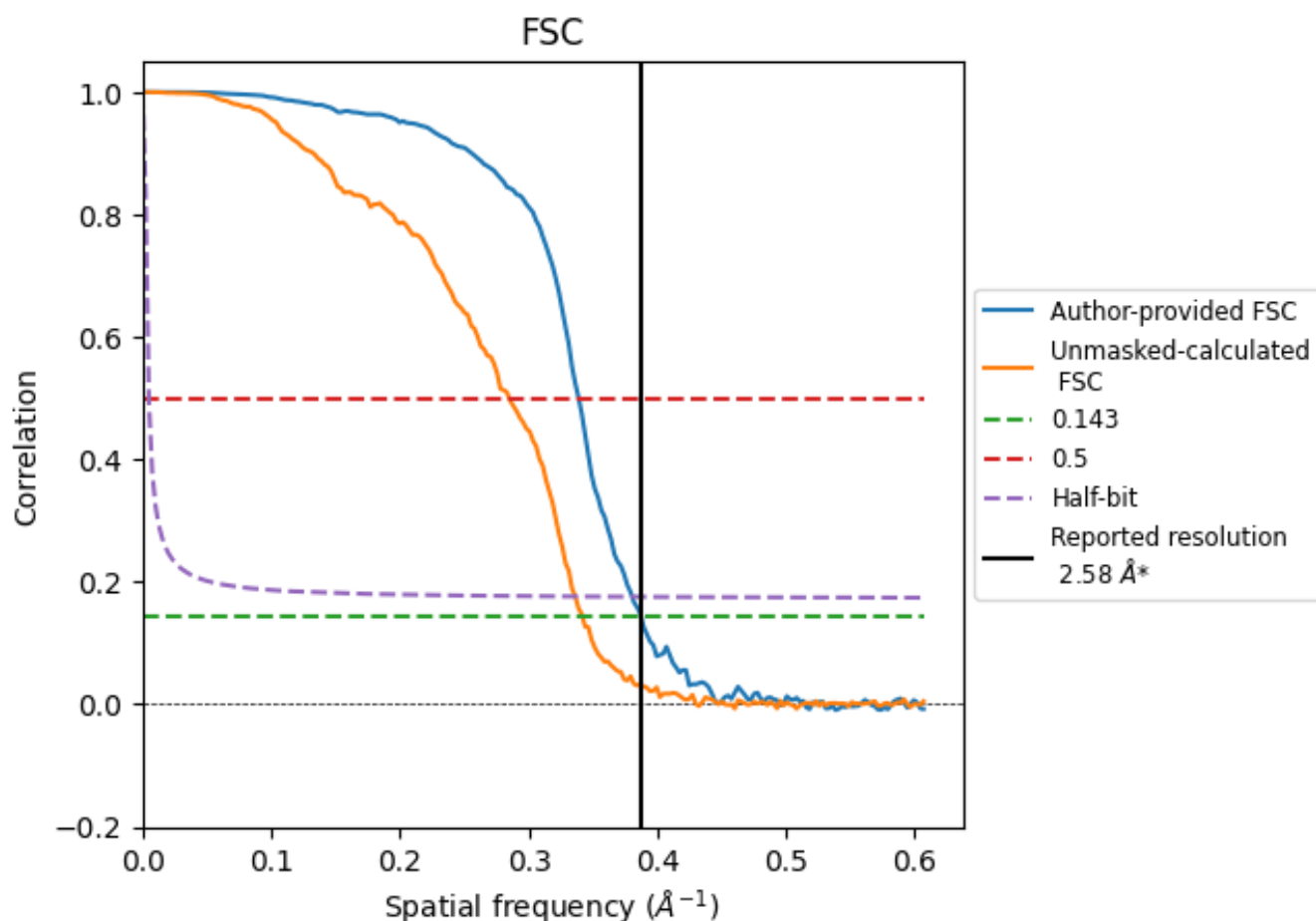


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.388 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

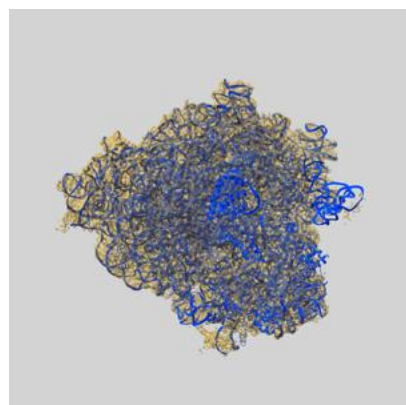
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	2.95	2.63
Unmasked-calculated*	2.92	3.51	2.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.92 differs from the reported value 2.58 by more than 10 %

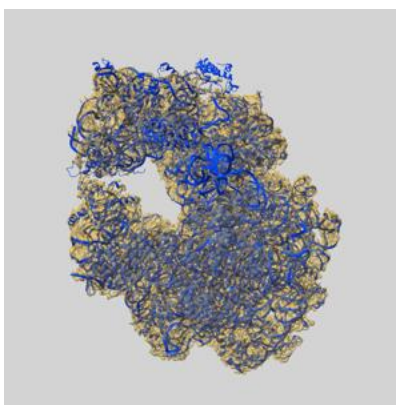
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38875 and PDB model 8Y38. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

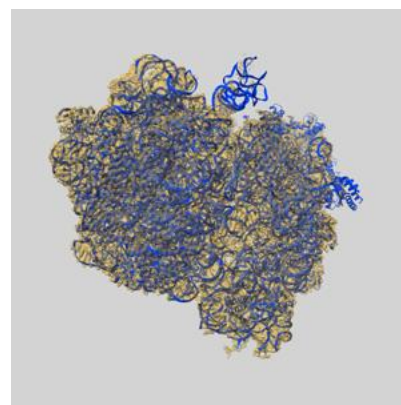
9.1 Map-model overlay [i](#)



X



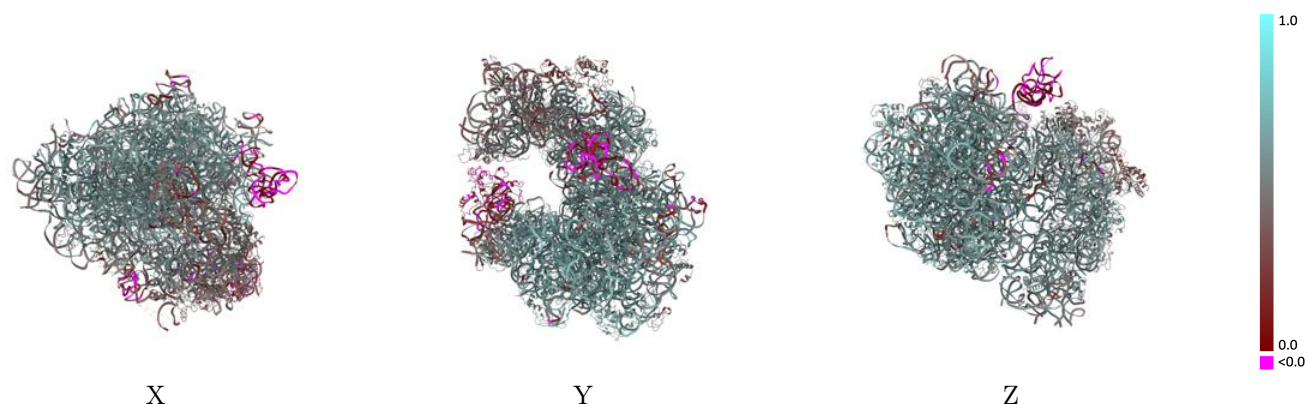
Y



Z

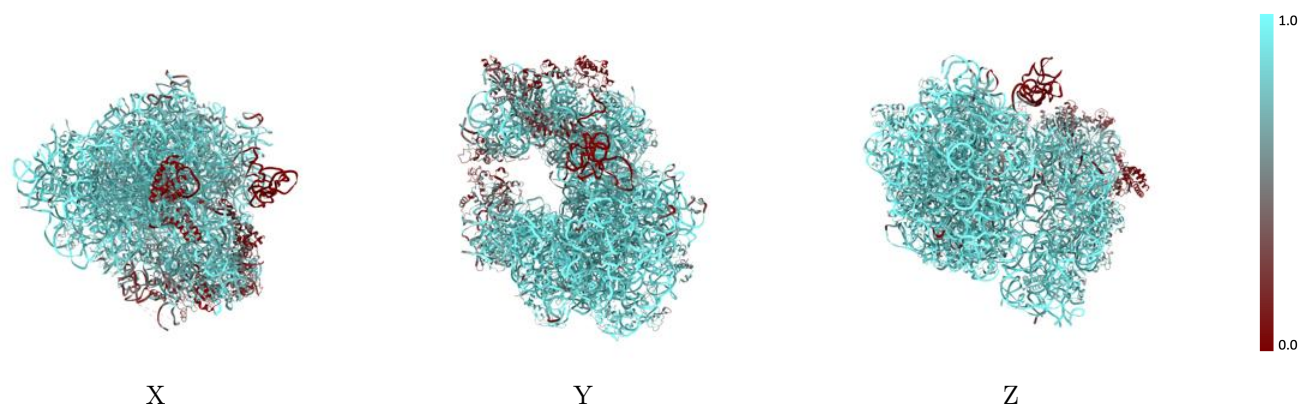
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



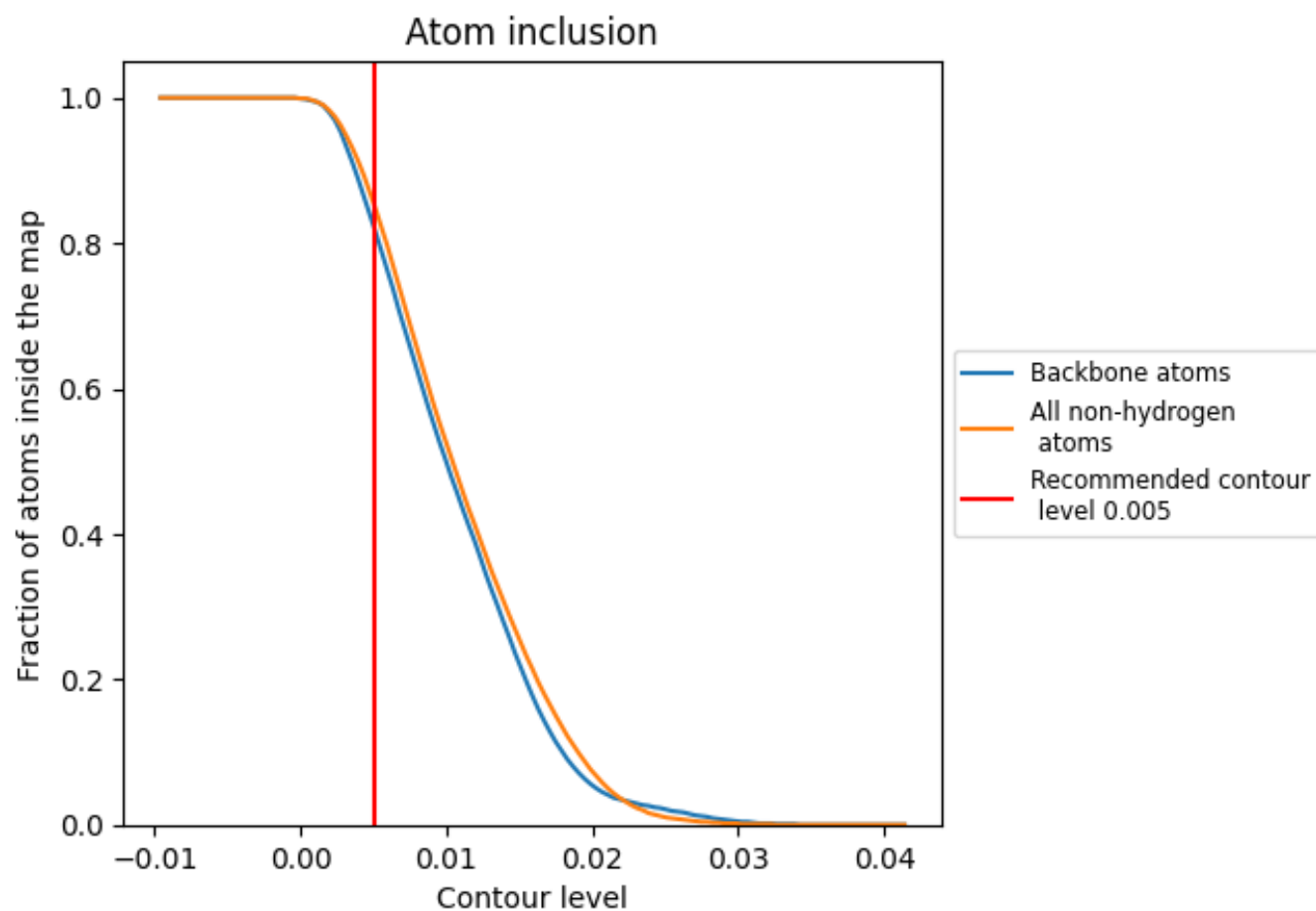
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.5370
1	 0.9150	 0.6010
2	 0.9650	 0.6280
3	 0.9780	 0.6410
4	 0.9520	 0.6130
A	 0.9110	 0.5610
B	 0.8620	 0.4350
C	 0.9310	 0.6040
D	 0.9300	 0.6140
E	 0.8810	 0.6110
F	 0.4590	 0.1610
G	 0.8080	 0.5210
H	 0.9380	 0.6060
I	 0.9210	 0.5850
J	 0.8810	 0.5700
K	 0.9490	 0.6130
L	 0.9080	 0.5820
M	 0.7370	 0.4210
N	 0.8660	 0.5210
O	 0.9490	 0.6200
P	 0.8820	 0.5940
Q	 0.9290	 0.6110
R	 0.8680	 0.5560
S	 0.7570	 0.5060
T	 0.7550	 0.5000
U	 0.9130	 0.5670
V	 0.9390	 0.5930
W	 0.7960	 0.5230
X	 0.9140	 0.5950
Y	 0.2280	 0.0600
Z	 0.9680	 0.6280
a	 0.9050	 0.5210
b	 0.1260	 0.3690
c	 0.4970	 0.4630
d	 0.7720	 0.5150



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Chain	Atom inclusion	Q-score
e	 0.8350	 0.5620
f	 0.7560	 0.5730
g	 0.2920	 0.4130
h	 0.8120	 0.5700
i	 0.2990	 0.3510
j	 0.3950	 0.3980
k	 0.5990	 0.4590
l	 0.8060	 0.5570
m	 0.3840	 0.4140
n	 0.6980	 0.4990
o	 0.8370	 0.5790
p	 0.8500	 0.5570
q	 0.8410	 0.5580
r	 0.7750	 0.5620
s	 0.3530	 0.4190
t	 0.8670	 0.5790