



Full wwPDB EM Validation Report ⓘ

Oct 12, 2026 – 03:19 pm BST

PDB ID : 9SY6 / pdb_00009sy6
EMDB ID : EMD-55345
Title : Structural characterization of hibernating ribosomes in the Gram-negative pathogen *Pseudomonas aeruginosa*
Authors : Vasanthakrishnan, R.K.B.S.; Olivier, D.; Sophie, C.; Yann, L.C.; Sylvie, G.D.; Sassi, M.; Emmanuel, G.; Reynald, G.
Deposited on : 2025-10-10
Resolution : 2.60 Å (reported)
Based on initial model : 7UNW

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:

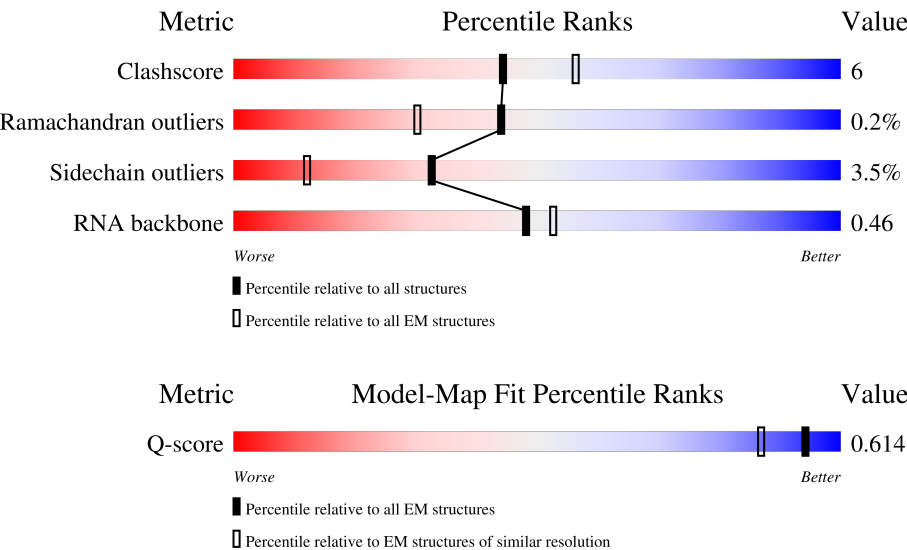
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	0	51	
2	1	44	
3	2	64	

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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	71	
6	A	1536	
7	B	246	
8	C	228	
9	D	206	
10	E	166	
11	F	139	
12	G	156	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	123	
18	M	118	
19	N	101	
20	O	89	
21	P	83	
22	Q	88	
23	R	76	
24	S	91	
25	T	91	
26	W	15	
27	X	102	
28	a	2891	

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Mol	Chain	Length	Quality of chain
29	b	120	
30	c	273	
31	d	211	
32	e	200	
33	f	179	
34	g	177	
35	h	148	
36	i	142	
37	j	122	
38	k	144	
39	l	137	
40	m	129	
41	n	116	
42	o	116	
43	p	118	
44	q	103	
45	r	110	
46	s	99	
47	t	104	
48	u	204	
49	v	85	
50	w	78	
51	x	63	
52	y	58	
53	z	60	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 143096 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 bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			426	272	78	75	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			365	222	87	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			307	186	69	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	68	Total	C	N	O	S	0	0
			531	334	95	96	6		

- Molecule 6 is a RNA chain called 16S rRNA (1535-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1535	Total	C	N	O	P	0	0
			32945	14701	6039	10670	1535		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	224	Total	C	N	O	S	0	0
			1763	1112	322	319	10		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	208	Total	C	N	O	S	0	0
			1664	1052	315	292	5		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	205	Total	C	N	O	S	0	0
			1627	1003	316	303	5		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	154	Total	C	N	O	S	0	0
			1134	711	210	207	6		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	106	Total	C	N	O	S	0	0
			868	539	159	164	6		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1199	752	232	210	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	129	Total	C	N	O	S	0	0
			982	618	173	185	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	127	Total	C	N	O	S	0	0
			1010	625	203	181	1		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	99	Total	C	N	O	S	0	0
			793	496	150	146	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	119	Total	C	N	O	S	0	0
			881	546	171	162	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP E2RXU4

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	122	Total	C	N	O	S	0	0
			961	589	198	169	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	113	Total	C	N	O	S	0	0
			883	541	178	160	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	100	Total	C	N	O	S	0	0
			804	496	167	138	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	88	Total	C	N	O	S	0	0
			703	434	139	129	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			637	398	125	113	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	80	Total	C	N	O	S	0	0
			645	404	124	115	2		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	R	62	Total	C	N	O		
			494	316	86	92	0	0

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	83	Total	C	N	O	S	0	0
			663	422	129	109	3		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	87	Total	C	N	O	S	0	0
			671	414	138	117	2		

- Molecule 26 is a RNA chain called non-STOP mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	10	Total	C	N	O	P	0	0
			219	97	41	71	10		

- Molecule 27 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	98	Total	C	N	O	S	0	0
			796	498	143	152	3		

- Molecule 28 is a RNA chain called 23S rRNA (2890-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2890	Total	C	N	O	P	0	0
			62019	27677	11363	20089	2890		

- Molecule 29 is a RNA chain called 5S rRNA (117-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	117	Total	C	N	O	P	0	0
			2495	1114	448	816	117		

- Molecule 30 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	272	Total	C	N	O	S	0	0
			2072	1276	426	364	6		

- Molecule 31 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	211	Total	C	N	O	S	0	0
			1589	982	304	297	6		

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	200	Total	C	N	O	S	0	0
			1524	956	283	282	3		

- Molecule 33 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	177	Total	C	N	O	S	0	0
			1418	905	253	256	4		

- Molecule 34 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	175	Total	C	N	O	S	0	0
			1326	835	244	245	2		

- Molecule 35 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	72	Total	C	N	O	S	0	0
			533	334	98	100	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	142	Total	C	N	O	S	0	0
			1130	718	206	202	4		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	144	Total	C	N	O	S	0	0
			1066	654	215	194	3		

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	137	Total	C	N	O	S	0	0
			1086	689	211	181	5		

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	120	Total	C	N	O	S	0	0
			959	600	192	162	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	114	Total	C	N	O	S	0	0
			902	568	171	162	1		

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	117	Total	C	N	O	S	0	0
			936	592	196	148			

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	103	Total	C	N	O	S	0	0
			822	521	156	143	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	110	Total	C	N	O	S	0	0
			833	515	161	153	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	94	Total	C	N	O	S	0	0
			739	472	134	132	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	103	Total	C	N	O	S	0	0
			800	503	152	143	2		

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	190	Total	C	N	O	S	0	0
			1446	915	262	266	3		

- Molecule 49 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	76	Total	C	N	O		0	0
			575	364	111	100			

- Molecule 50 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	77	Total	C	N	O	S	0	0
			630	391	134	103	2		

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	61	Total	C	N	O	S	0	0
			490	301	96	91	2		

- Molecule 52 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	57	Total	C	N	O	S	0	0
			445	277	87	79	2		

- Molecule 53 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	55	Total	C	N	O	S	0	0
			440	264	93	82	1		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	94	Total 94	Mg 94	0
55	X	1	Total 1	Mg 1	0
55	a	249	Total 249	Mg 249	0
55	b	5	Total 5	Mg 5	0
55	c	1	Total 1	Mg 1	0
55	p	2	Total 2	Mg 2	0
55	v	1	Total 1	Mg 1	0
55	z	1	Total 1	Mg 1	0

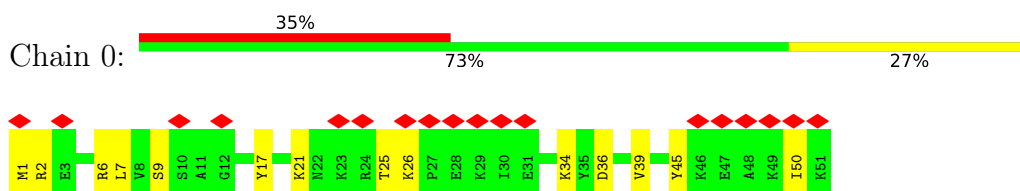
- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	A	48	Total 48	K 48	0
56	X	1	Total 1	K 1	0
56	a	113	Total 113	K 113	0
56	b	1	Total 1	K 1	0
56	c	4	Total 4	K 4	0
56	e	1	Total 1	K 1	0
56	f	1	Total 1	K 1	0

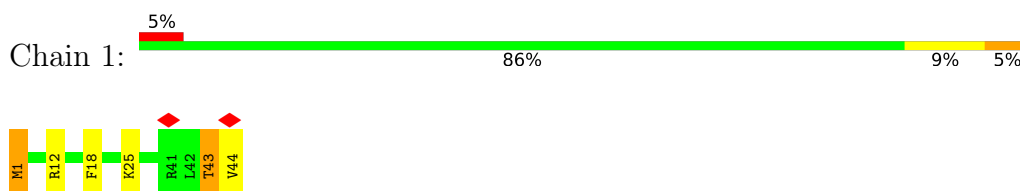
3 Residue-property plots [i](#)

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.

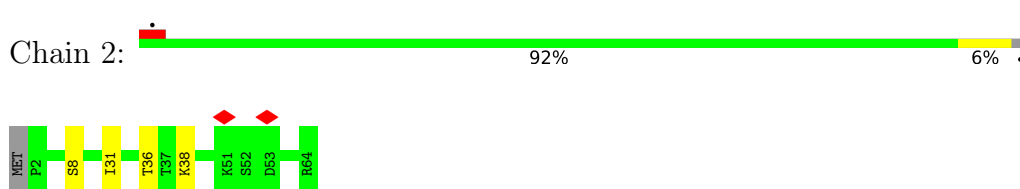
- Molecule 1: Large ribosomal subunit protein bL33



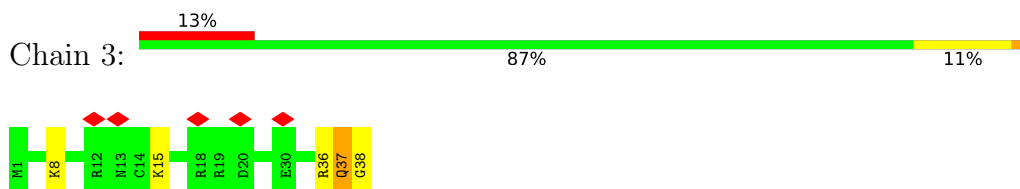
- Molecule 2: Large ribosomal subunit protein bL34



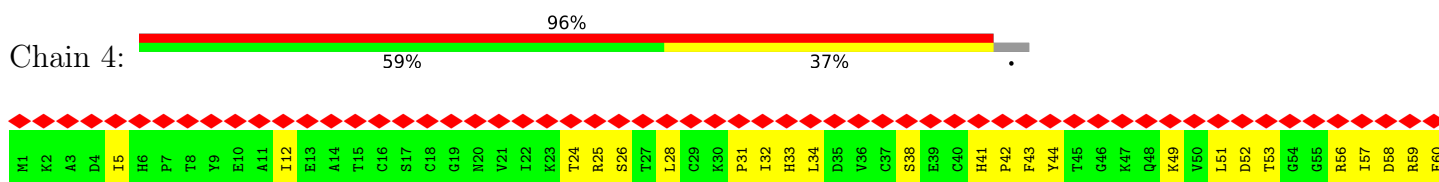
- Molecule 3: Large ribosomal subunit protein bL35



- Molecule 4: Large ribosomal subunit protein bL36

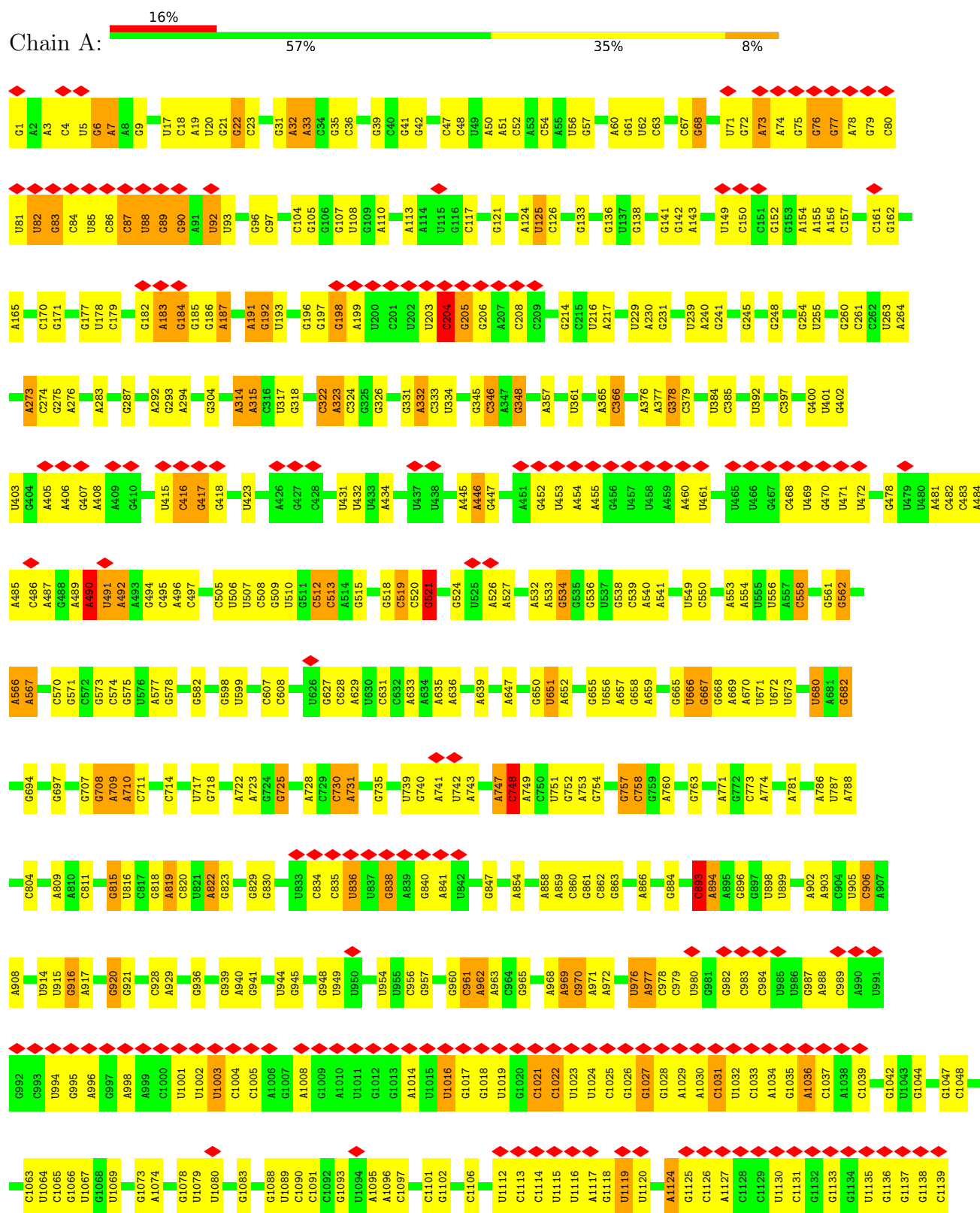


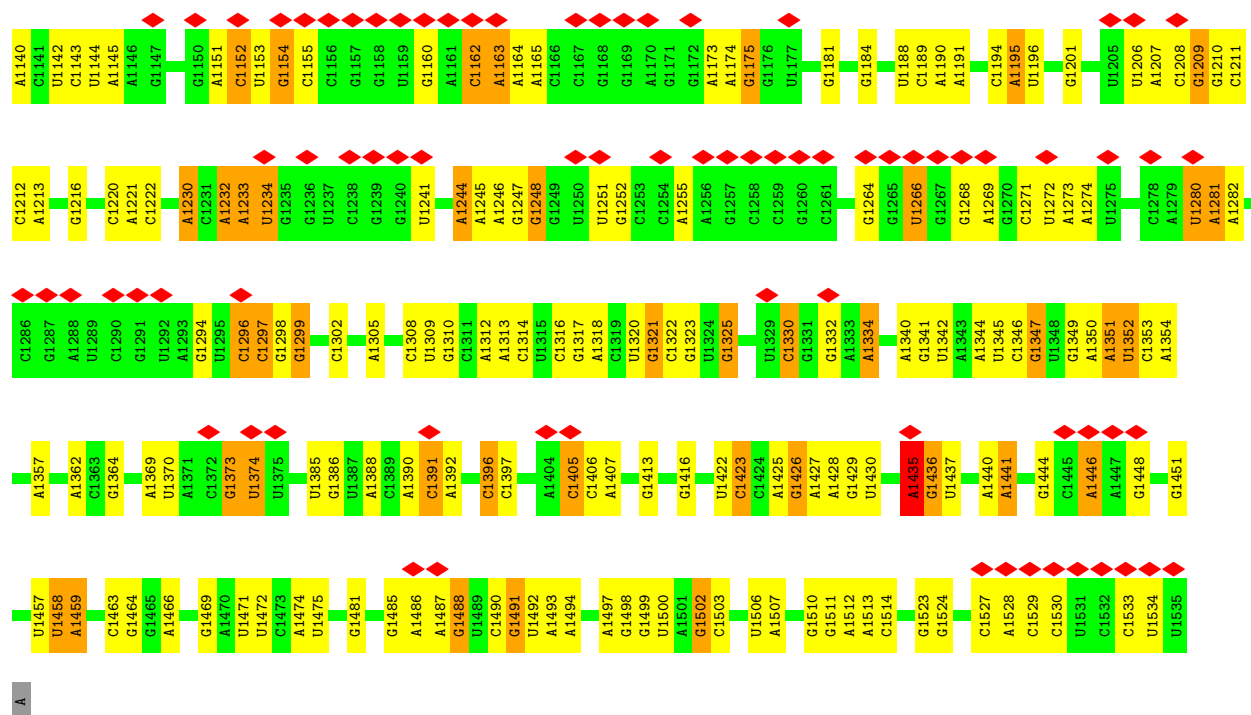
- Molecule 5: Large ribosomal subunit protein bL31



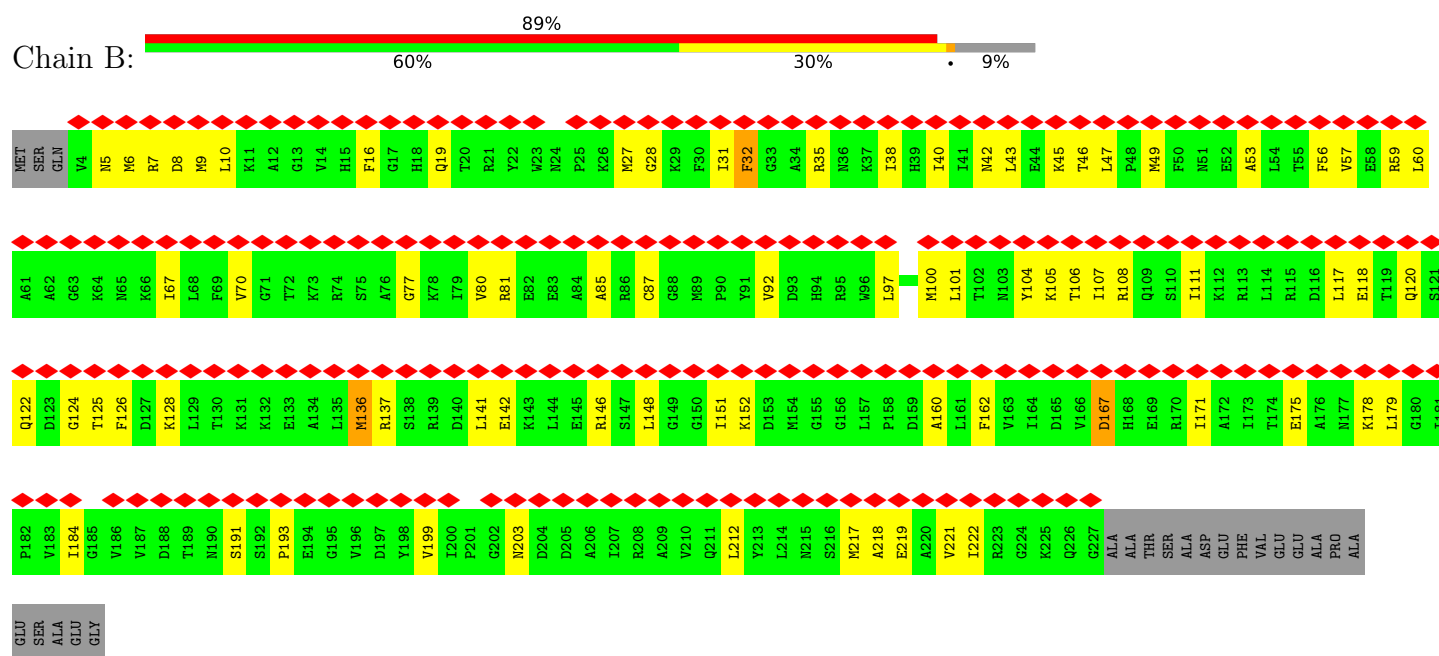


• Molecule 6: 16S rRNA (1535-MER)

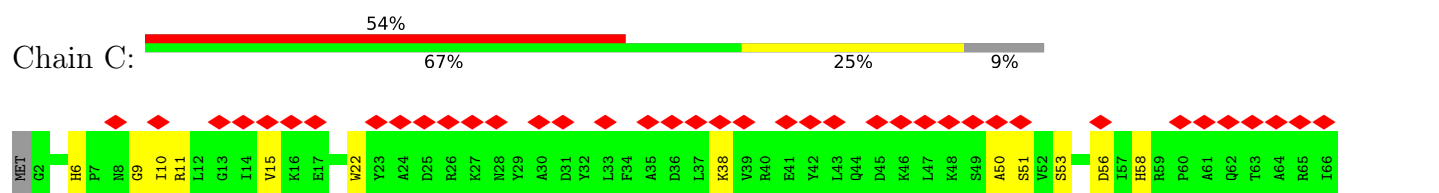


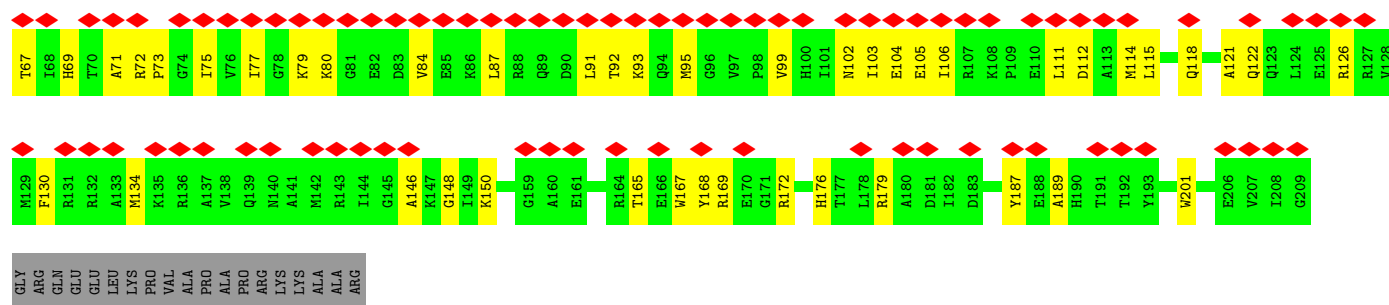


• Molecule 7: Small ribosomal subunit protein uS2

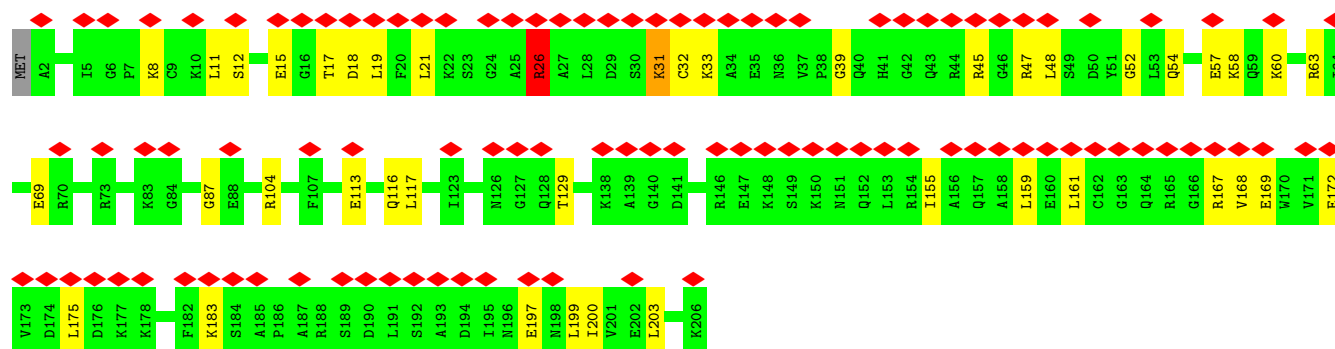
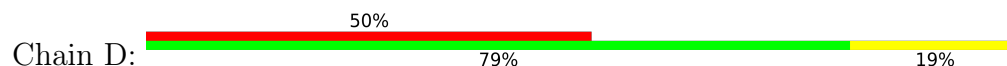


• Molecule 8: Small ribosomal subunit protein uS3

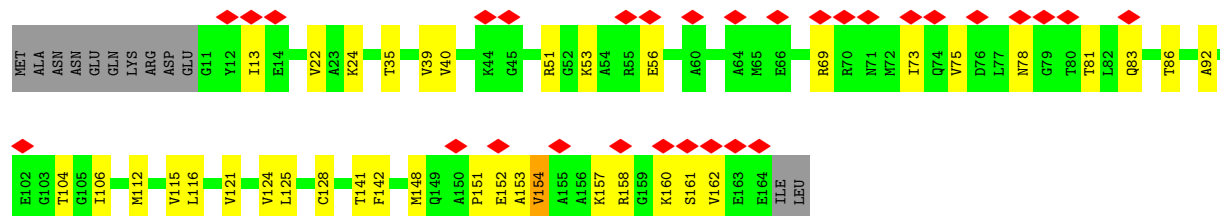




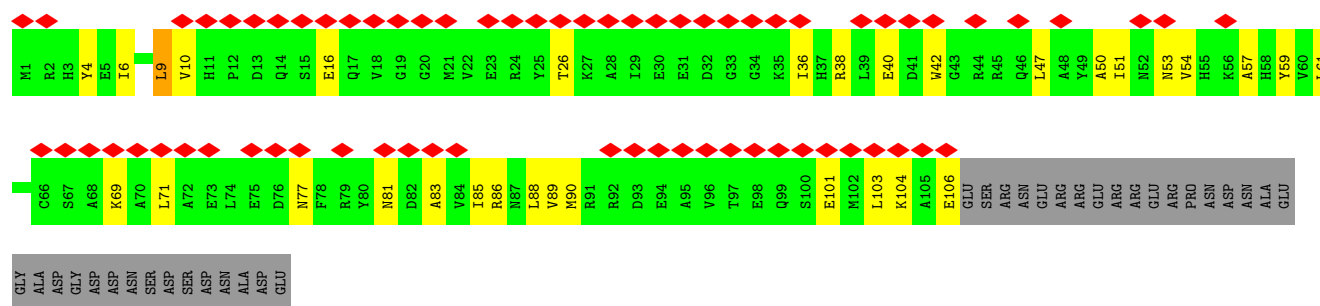
• Molecule 9: Small ribosomal subunit protein uS4



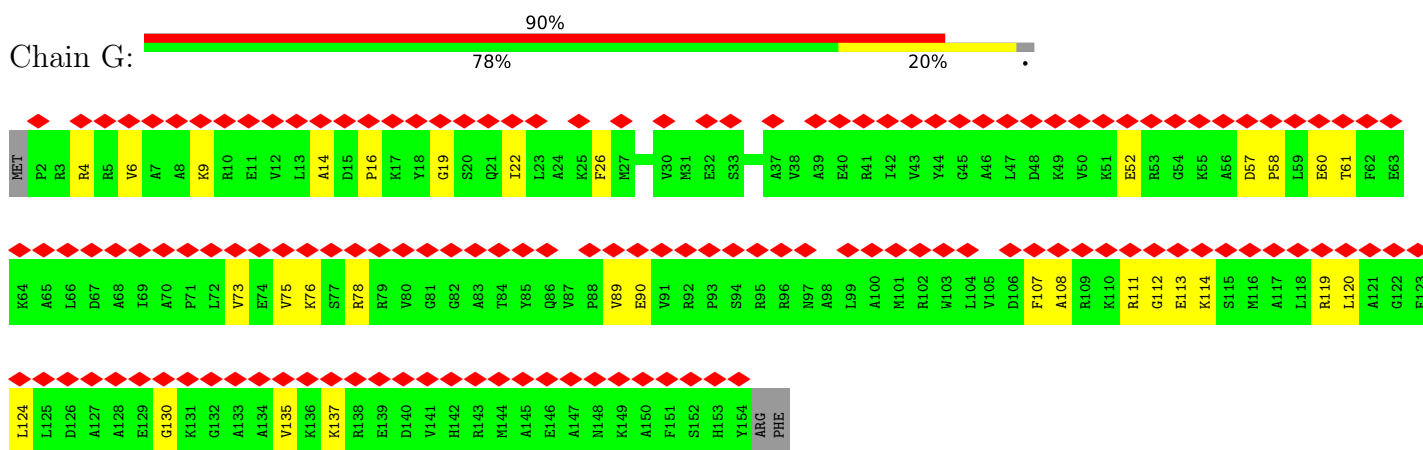
• Molecule 10: Small ribosomal subunit protein uS5



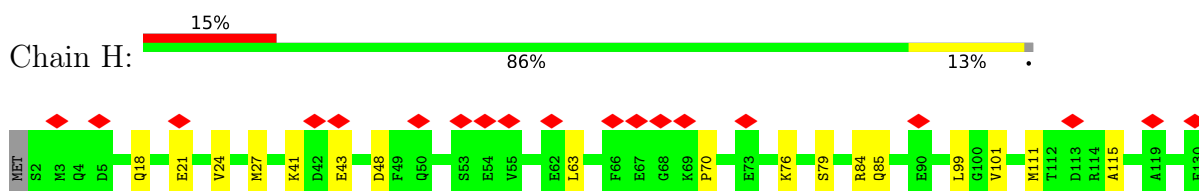
• Molecule 11: Small ribosomal subunit protein bS6



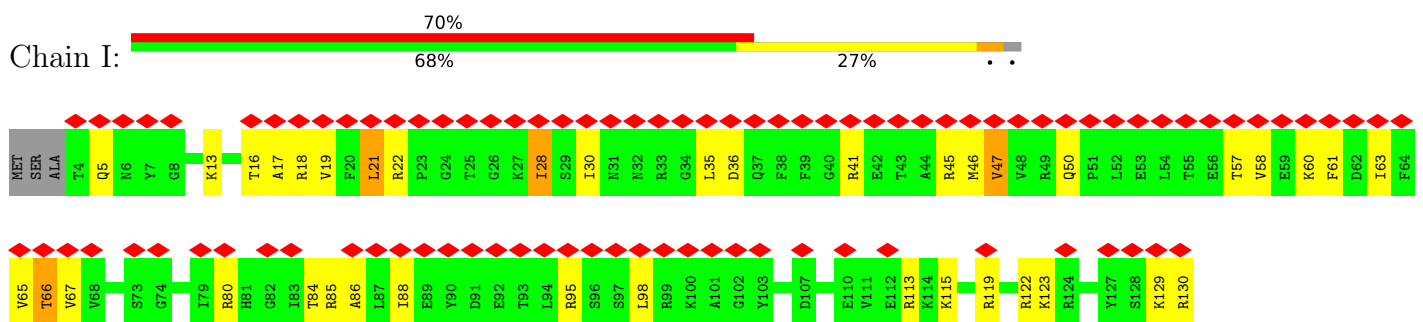
• Molecule 12: Small ribosomal subunit protein uS7



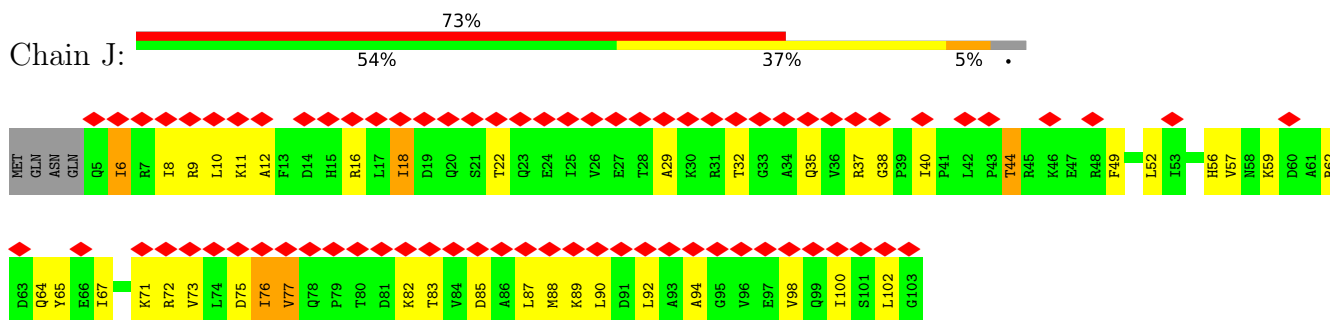
- Molecule 13: Small ribosomal subunit protein uS8



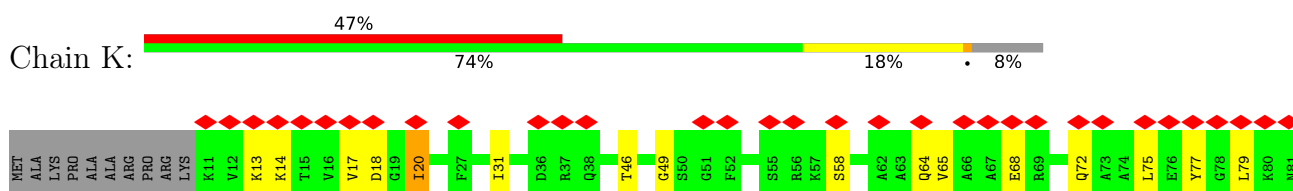
- Molecule 14: Small ribosomal subunit protein uS9

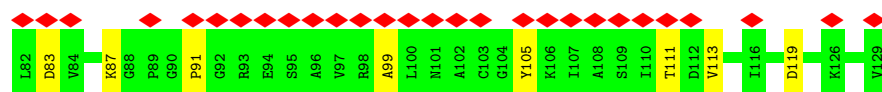


- Molecule 15: Small ribosomal subunit protein uS10



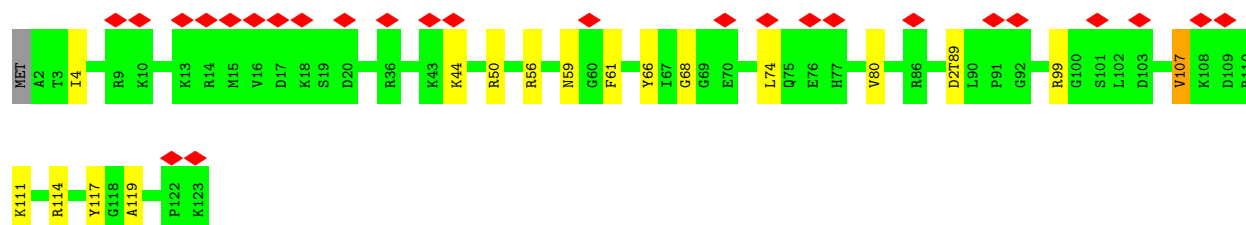
- Molecule 16: Small ribosomal subunit protein uS11





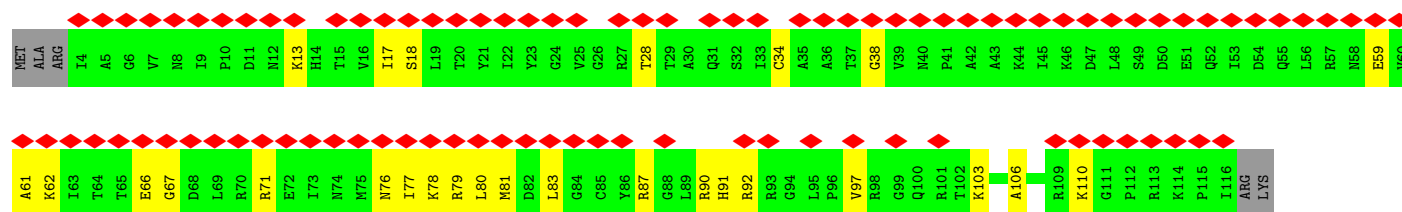
- Molecule 17: Small ribosomal subunit protein uS12

Chain L: 21% 85% 13% ..



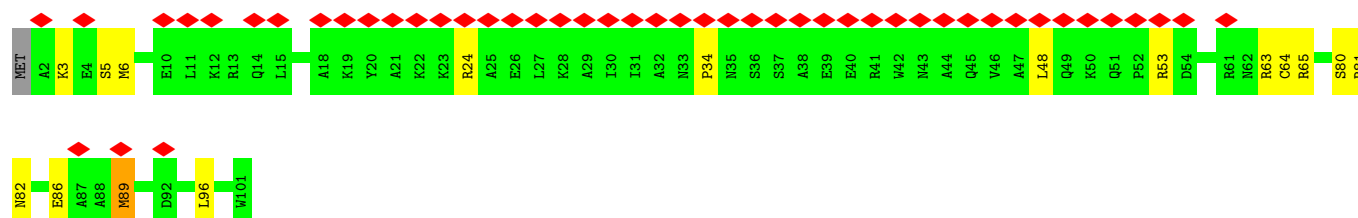
- Molecule 18: Small ribosomal subunit protein uS13

Chain M: 80% 73% 23% .



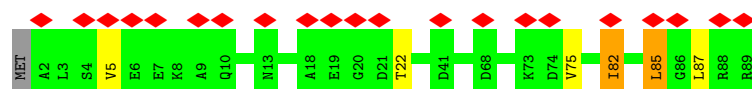
- Molecule 19: Small ribosomal subunit protein uS14

Chain N: 48% 83% 15% ..



- Molecule 20: Small ribosomal subunit protein uS15

Chain O: 24% 92% 14% ..

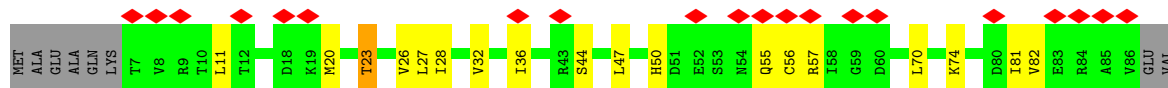


- Molecule 21: Small ribosomal subunit protein bS16

Chain P: 14% 83% 14% .



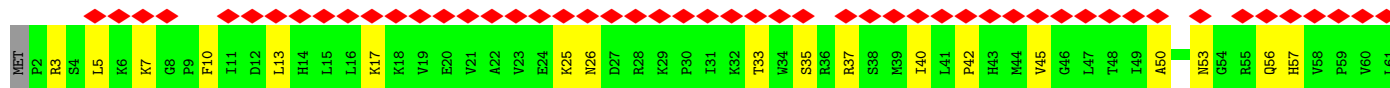
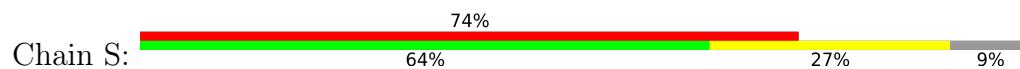
- Molecule 22: Small ribosomal subunit protein uS17



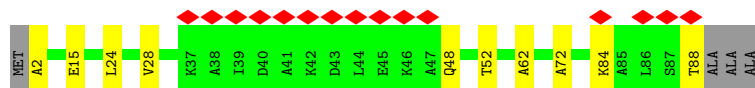
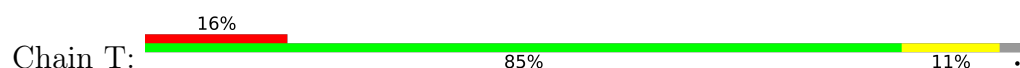
- Molecule 23: Small ribosomal subunit protein bS18



- Molecule 24: Small ribosomal subunit protein uS19



- Molecule 25: Small ribosomal subunit protein bS20



- Molecule 26: non-STOP mRNA

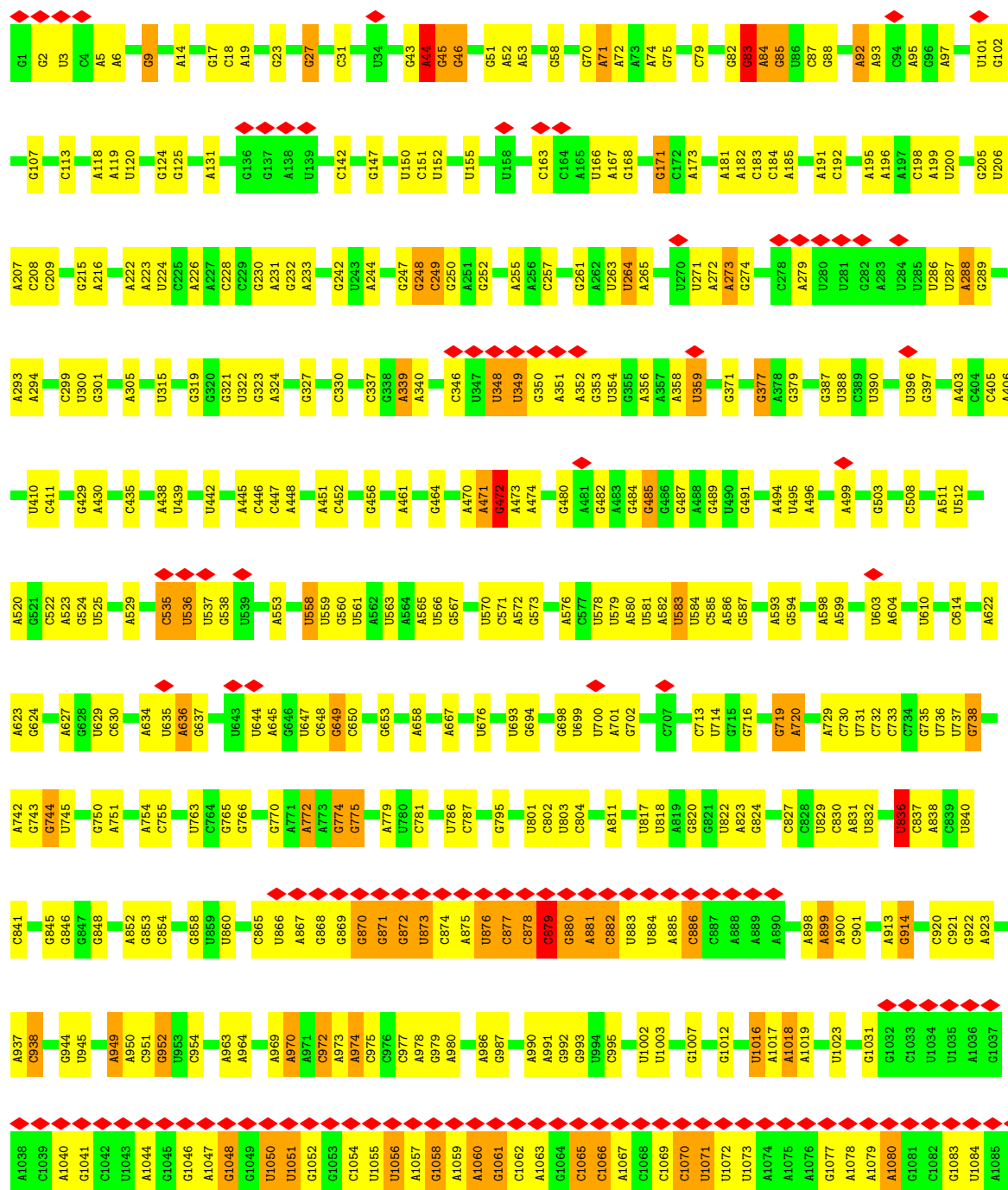


- Molecule 27: Ribosome hibernation promoting factor

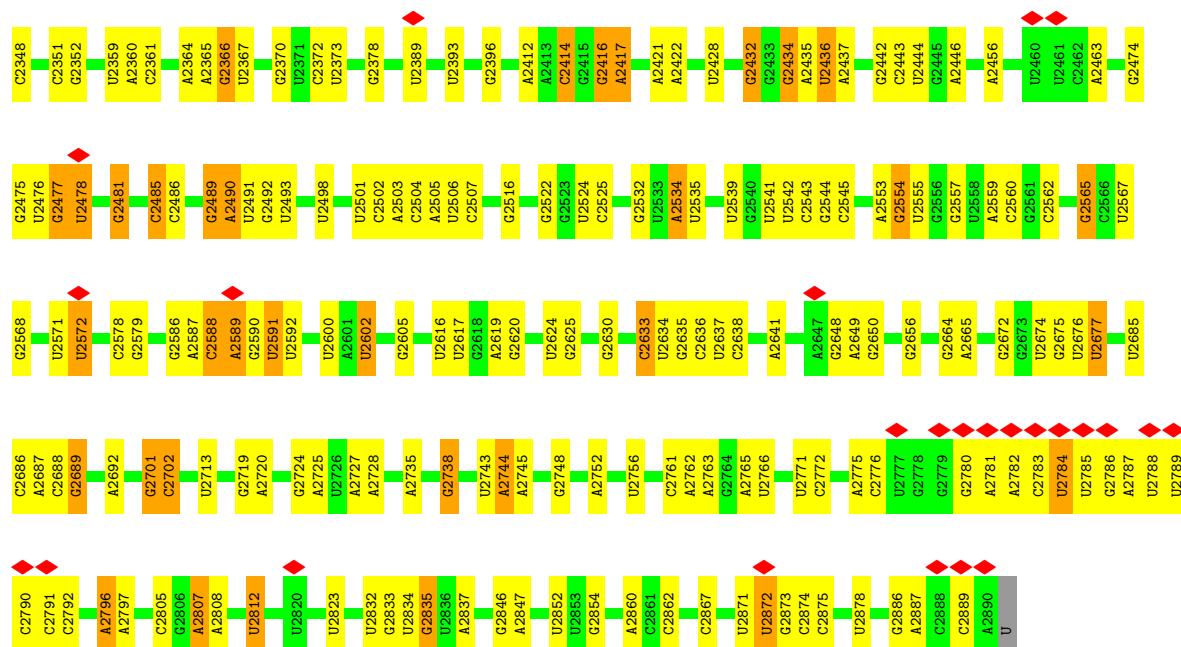




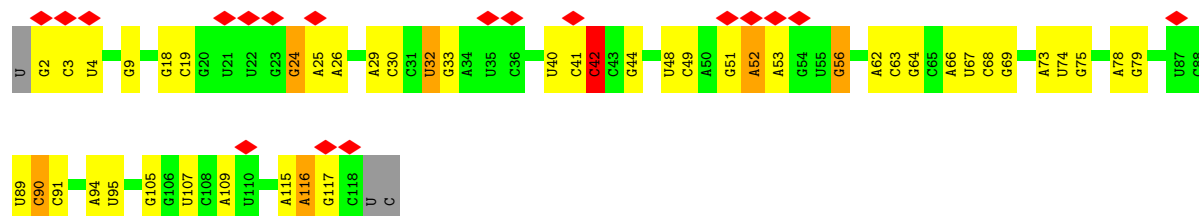
• Molecule 28: 23S rRNA (2890-MER)



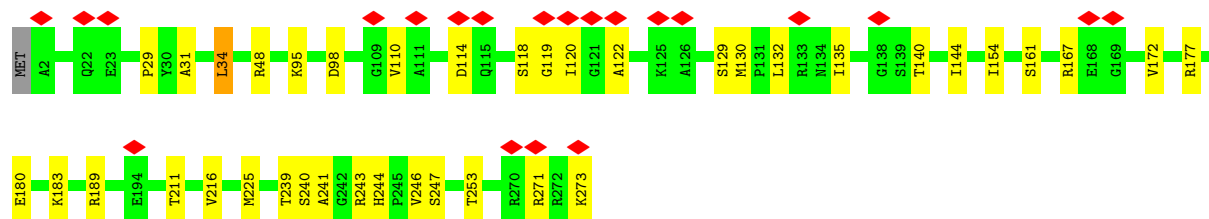
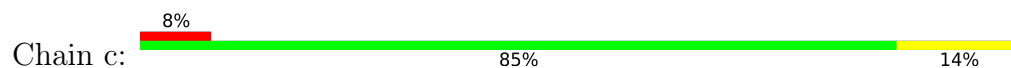
A2265	U2270	A2274	A2275	U2278	G2279	C2282	U2283	A2285	G2286	A2287	C2288	C2289	G2290	C2291	U2292	C2293	G2294	G2295	A2296	A2297	U2298	U2299	G2302	U2303	C2304	G2305	U2306	A2307	A2308	A2309	A2312	U2313	A2314	A2315	A2316	G2317	A2321	A2322	A2323	U2330	U2331	G2332	A2333	C2334	C2337	A2343	G2344																																																			
U2167	G2168	G2169	C2170	A2171	U2172	G2173	C2174	U2175	U2176	G2177	A2178	U2179	G2180	U2181	C2182	U2183	A2184	A2185	A2186	C2187	G2191	C2194	C2195	G2198	U2200	C2201	C2202	G2203	G2204	A2212	U2220	G2221	G2225	G2226	C2227	A2228	G2229	U2230	U2231	A2234	C2235	G2236	A2255	G2258	A2259	A2260	A2261																																																			
G2107	G2108	U2109	G2110	G2111	G2112	A2113	G2114	G2115	G2116	U2117	U2118	U2119	G2120	A2121	A2122	G2123	C2124	G2125	U2126	G2127	G2128	G2129	C2130	G2131	C2132	U2203	A2134	G2135	U2136	U2137	C2138	G2139	C2140	G2141	U2142	G2143	G2144	A2145	G2146	C2147	C2148	A2149	U2150	C2151	C2152	U2153	U2154	G2155	A2156	A2157	U2158	U2159	A2160	C2161	C2162	A2163	C2164	C2165	C2166																																							
C1912	A1915	G1916	G1917	A1924	A1925	U1926	U1927	C1928	U1933	C1934	A1939	U1942	C1945	C1949	U1950	G1951	C1954	A1957	U1958	G1959	G1967	C1977	U1978	G1979	U1980	G1984	A2001	A2002	A2008	U2009	C2010	G2011	C2012	U2013	G2014	U2015	G2016	A2017	A2018	C2019	A2020	U2021	G2022	C2023	A2024	G2025	U2026	G2027	U2030	G2031	C2032	U2038	A2039	G2040	A2041	C2042	G2043	A2047	G2048	A2049	C2050	C2051	C2052	G2053	U2055	G2056	A2057	A2058	C2059	U2060	U2061	U2062	G2067	G2080	C2083	U2084	U2085	U2086	G2087	A2088	G2089	C2090	C2091	U2092	G2093	C2094	U2095	U2096	G2097	U2098	G2099	U2100	A2101	G2102	U2103	A2104	U2105	A2106
U1814	G1815	A1816	G1822	A1834	A1835	A1841	U1842	U1843	G1844	A1845	U1846	G1849	G1850	U1851	U1852	C1855	G1856	C1857	A1858	A1859	G1860	C1861	G1862	G1865	G1866	U1867	C1868	U1870	G1871	A1876	A1877	G1893	G1894	C1895	C1896	G1897	U1898	A1899	A1900	C1901	3TD1902	A1903	U1904	A1905	A1906	G1909	U1910	C1911																																																		
U1720	C1721	C1722	G1723	U1724	A1725	G1733	C1734	U1738	U1739	G1740	A1741	G1743	A1744	U1745	G1750	G1751	A1760	C1761	U1762	G1763	U1766	U1769	A1770	A1771	U1772	A1773	A1774	C1775	A1776	C1777	A1778	A1781	C1782	U1783	C1784	C1787	A1788	A1789	A1790	A1795	A1796	U1797	G1798	C1803	U1807	G1811																																																				
U1814	G1815	A1816	G1822	A1834	A1835	A1841	U1842	U1843	G1844	A1845	U1846	G1849	G1850	U1851	U1852	C1855	G1856	C1857	A1858	A1859	G1860	C1861	G1862	G1865	G1866	U1867	C1868	U1870	G1871	A1876	A1877	G1893	G1894	C1895	C1896	G1897	U1898	A1899	A1900	C1901	3TD1902	A1903	U1904	A1905	A1906	G1909	U1910	C1911																																																		
C1912	A1915	G1916	G1917	A1924	A1925	U1926	U1927	C1928	U1933	C1934	A1939	U1942	C1945	C1949	U1950	G1951	C1954	A1957	U1958	G1959	G1967	C1977	U1978	G1979	U1980	G1984	A2001	A2002	A2008	U2009	C2010	G2011	C2012	U2013	G2014	U2015	G2016	A2017	A2018	C2019	A2020	U2021	G2022	C2023	A2024	G2025	U2026	G2027	U2030	G2031	C2032	U2038	A2039	G2040	A2041	C2042	G2043	A2047	G2048	A2049	C2050	C2051	C2052	G2053	U2055	G2056	A2057	A2058	C2059	U2060	U2061	U2062	G2067	G2080	C2083	U2084	U2085	U2086	G2087	A2088	G2089	C2090	C2091	U2092	G2093	C2094	U2095	U2096	G2097	U2098	G2099	U2100	A2101	G2102	U2103	A2104	U2105	A2106
G2107	G2108	U2109	G2110	G2111	G2112	A2113	G2114	G2115	G2116	U2117	U2118	U2119	G2120	A2121	A2122	G2123	C2124	G2125	U2126	G2127	G2128	G2129	C2130	G2131	C2132	U2203	A2134	G2135	U2136	U2137	C2138	G2139	C2140	G2141	U2142	G2143	G2144	A2145	G2146	C2147	C2148	A2149	U2150	C2151	C2152	U2153	U2154	G2155	A2156	A2157	U2158	U2159	A2160	C2161	C2162	A2163	C2164	C2165	C2166																																							
U2167	G2168	G2169	C2170	A2171	U2172	G2173	C2174	U2175	U2176	G2177	A2178	U2179	G2180	U2181	C2182	U2183	A2184	A2185	A2186	C2187	G2191	C2194	C2195	G2198	U2200	C2201	C2202	G2203	G2204	A2212	U2220	G2221	G2225	G2226	C2227	A2228	G2229	U2230	U2231	A2234	C2235	G2236	A2255	G2258	A2259	A2260	A2261																																																			
A2265	U2270	A2274	A2275	U2278	G2279	C2282	U2283	A2285	G2286	A2287	C2288	C2289	G2290	C2291	U2292	C2293	G2294	G2295	A2296	A2297	U2298	U2299	G2302	U2303	C2304	G2305	U2306	A2307	A2308	A2309	A2312	U2313	A2314	A2315	A2316	G2317	A2321	A2322	A2323	U2330	U2331	G2332	A2333	C2334	C2337	A2343	G2344																																																			



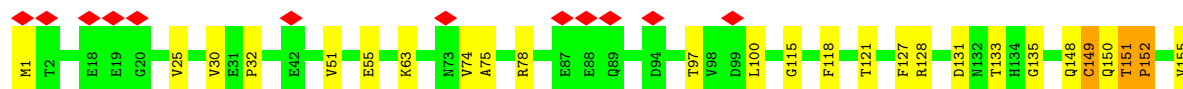
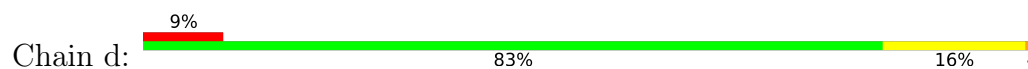
• Molecule 29: 5S rRNA (117-MER)

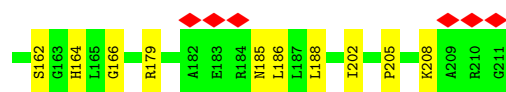


• Molecule 30: Large ribosomal subunit protein uL2

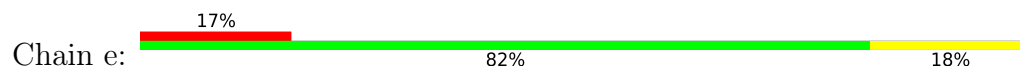


• Molecule 31: Large ribosomal subunit protein uL3

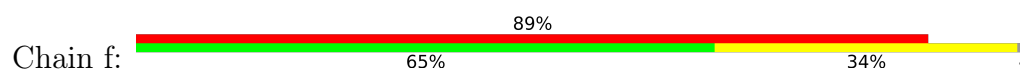




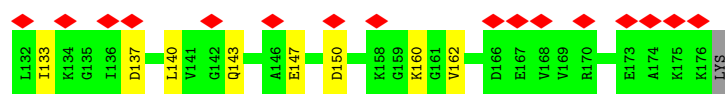
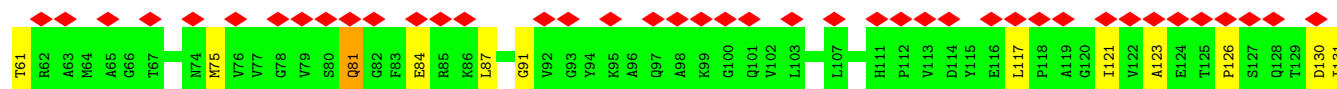
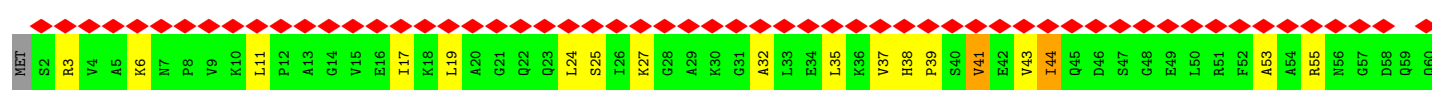
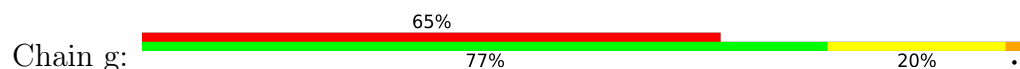
- Molecule 32: Large ribosomal subunit protein uL4



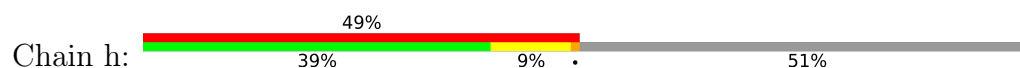
- Molecule 33: Large ribosomal subunit protein uL5

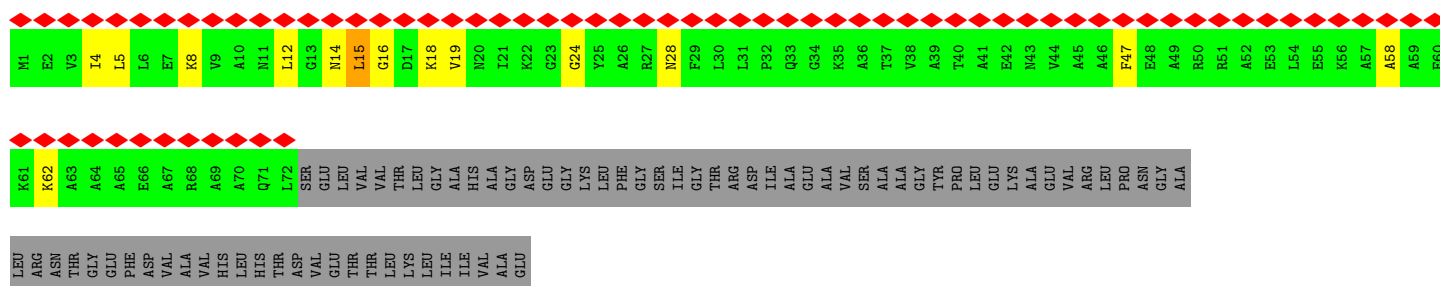


- Molecule 34: Large ribosomal subunit protein uL6

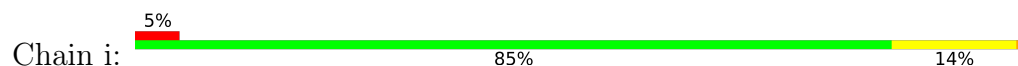


- Molecule 35: Large ribosomal subunit protein bL9

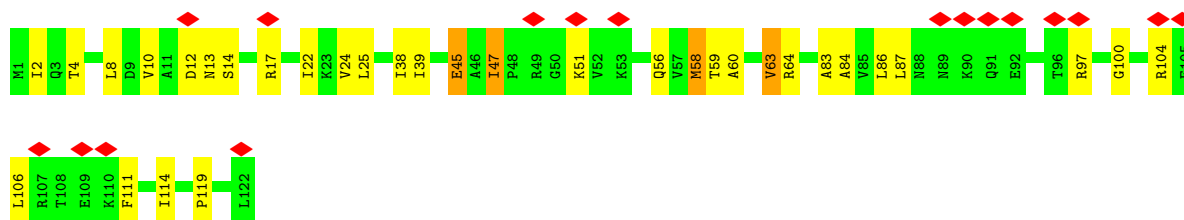




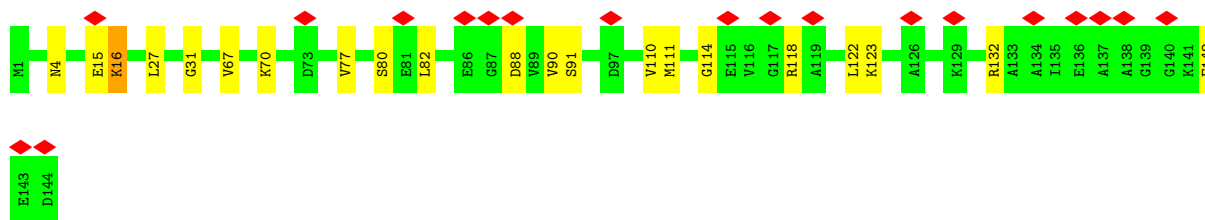
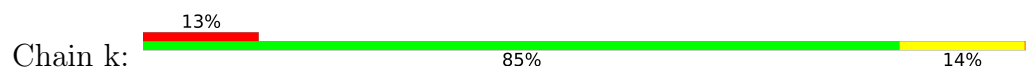
- Molecule 36: Large ribosomal subunit protein uL13



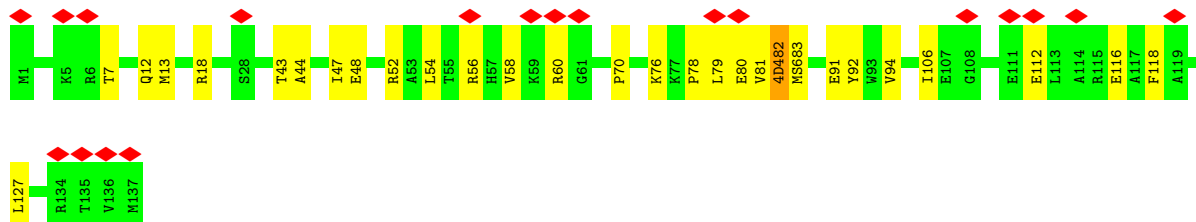
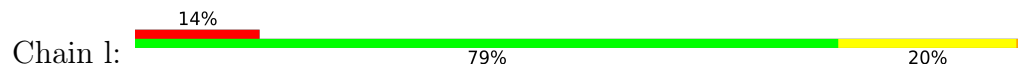
- Molecule 37: Large ribosomal subunit protein uL14



- Molecule 38: Large ribosomal subunit protein uL15



- Molecule 39: Large ribosomal subunit protein uL16



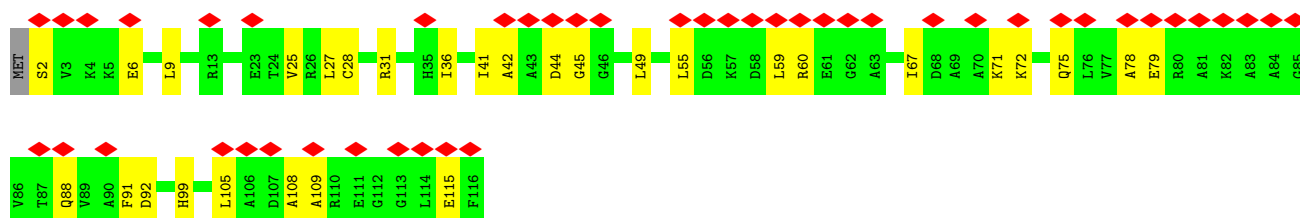
- Molecule 40: Large ribosomal subunit protein bL17

Chain m:  78% 15% 7%



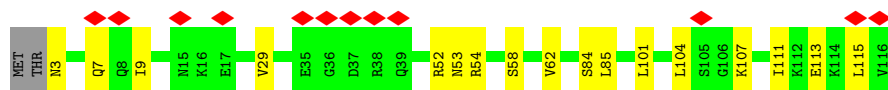
- Molecule 41: Large ribosomal subunit protein uL18

Chain n:  40% 73% 26%



- Molecule 42: Large ribosomal subunit protein bL19

Chain o:  10% 84% 15%



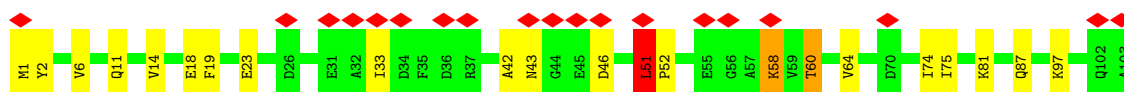
- Molecule 43: Large ribosomal subunit protein bL20

Chain p:  6% 82% 17%



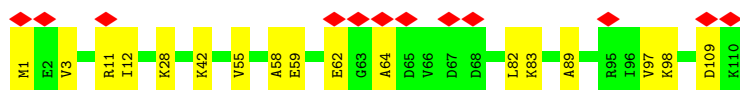
- Molecule 44: Large ribosomal subunit protein bL21

Chain q:  18% 79% 18%

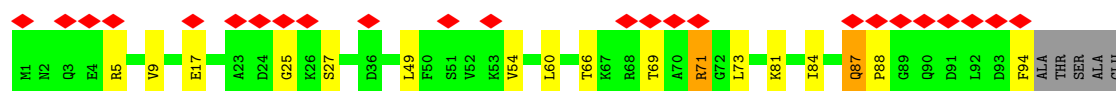
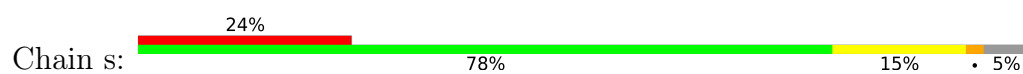


- Molecule 45: Large ribosomal subunit protein uL22

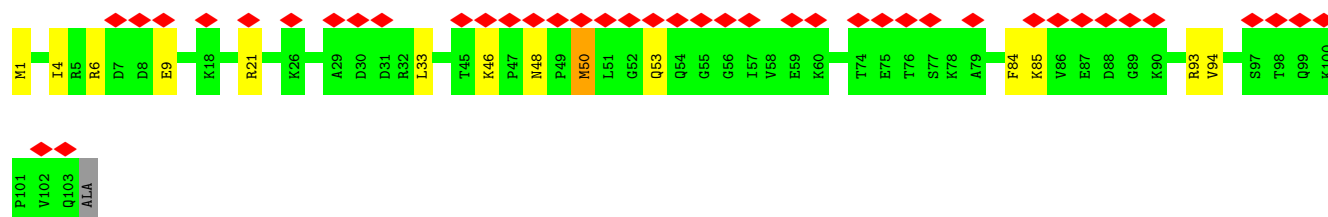
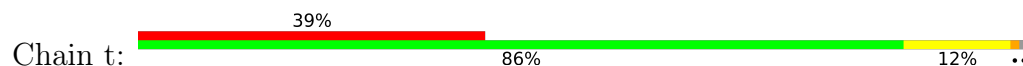
Chain r:  11% 85% 15%



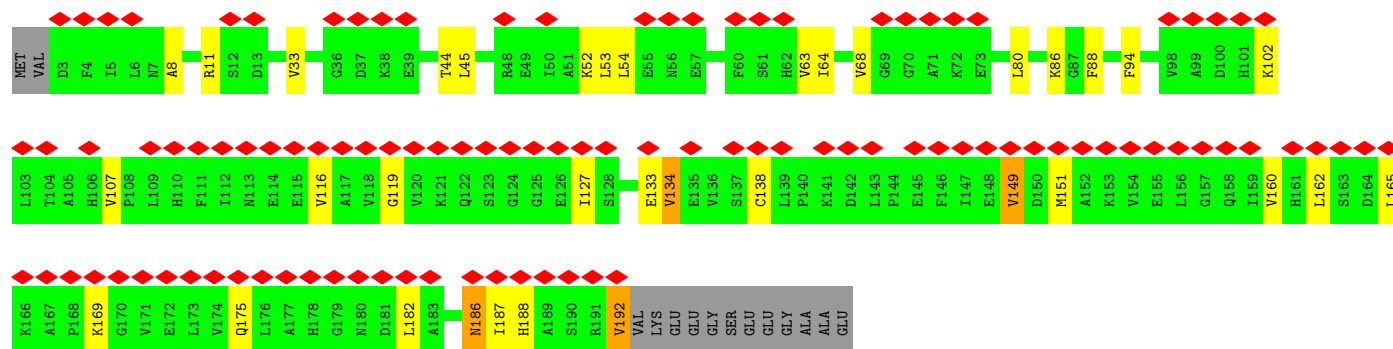
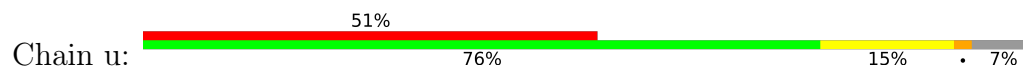
- Molecule 46: Large ribosomal subunit protein uL23



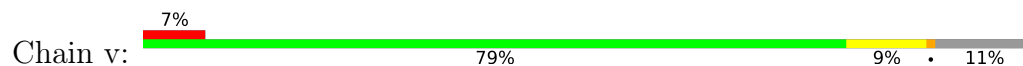
- Molecule 47: Large ribosomal subunit protein uL24



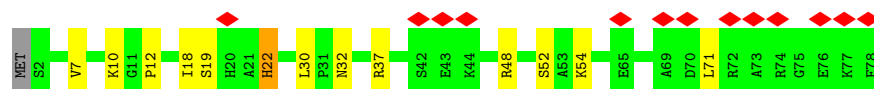
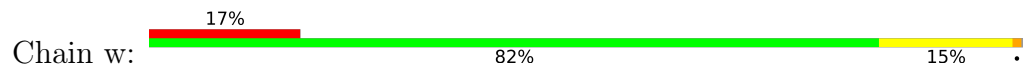
- Molecule 48: Large ribosomal subunit protein bL25



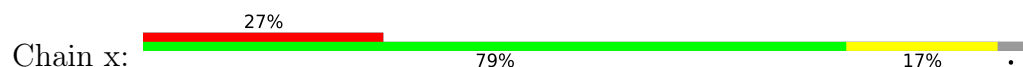
- Molecule 49: Large ribosomal subunit protein bL27

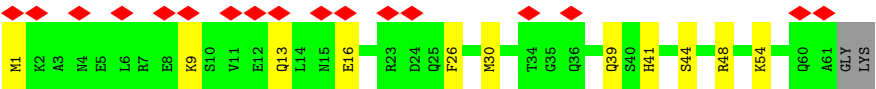


- Molecule 50: Large ribosomal subunit protein bL28

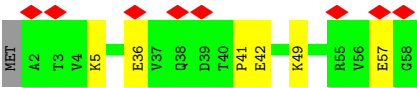
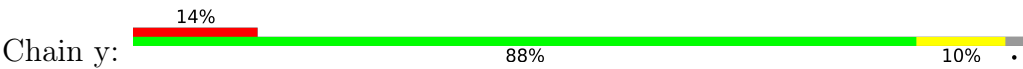


- Molecule 51: Large ribosomal subunit protein uL29

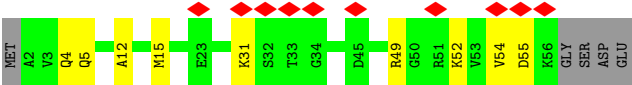
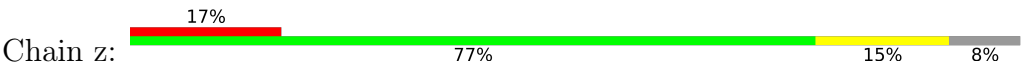




• Molecule 52: Large ribosomal subunit protein uL30



• Molecule 53: Large ribosomal subunit protein bL32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131785	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.134	Depositor
Minimum map value	-1.499	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, MEQ, 1MG, MG, IAS, 6MZ, ZN, 2MG, D2T, MS6, 4D4, G7M, 2MA, OMU, K, 3TD, 5MU, OMG, MA6, 5MC, UR3, PSU, OMC, 4OC

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	0	0.28	0/433	0.41	0/576
2	1	0.40	0/368	0.44	0/482
3	2	0.33	0/511	0.38	0/668
4	3	0.35	0/308	0.40	0/404
5	4	0.18	0/542	0.45	0/728
6	A	0.78	0/36632	0.85	21/57140 (0.0%)
7	B	0.20	0/1791	0.41	0/2405
8	C	0.26	0/1693	0.38	0/2279
9	D	0.26	0/1646	0.47	2/2201 (0.1%)
10	E	0.31	0/1148	0.48	0/1544
11	F	0.25	0/882	0.41	0/1186
12	G	0.21	0/1217	0.36	0/1627
13	H	0.30	0/993	0.39	0/1332
14	I	0.24	0/1022	0.41	0/1365
15	J	0.27	0/803	0.45	0/1083
16	K	0.26	0/889	0.33	0/1199
17	L	0.31	0/964	0.39	0/1289
18	M	0.22	0/892	0.42	0/1199
19	N	0.25	0/816	0.39	1/1087 (0.1%)
20	O	0.29	0/710	0.27	0/947
21	P	0.31	0/648	0.43	0/872
22	Q	0.29	0/653	0.43	0/881
23	R	0.26	0/502	0.32	0/677
24	S	0.22	0/678	0.34	0/912
25	T	0.31	0/678	0.33	0/904
26	W	0.50	0/245	0.86	0/381
27	X	0.24	0/803	0.42	0/1075
28	a	0.94	0/68901	0.88	50/107478 (0.0%)
29	b	0.72	0/2789	0.78	1/4345 (0.0%)
30	c	0.39	0/2108	0.43	0/2831
31	d	0.39	0/1601	0.46	0/2152

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.35	0/1544	0.37	0/2079
33	f	0.24	0/1439	0.42	0/1932
34	g	0.24	0/1344	0.40	0/1809
35	h	0.16	0/536	0.34	0/719
36	i	0.35	0/1156	0.42	0/1559
37	j	0.35	0/947	0.40	0/1268
38	k	0.34	0/1078	0.43	0/1436
39	l	0.34	0/1085	0.42	0/1449
40	m	0.38	0/975	0.41	0/1304
41	n	0.29	0/888	0.38	0/1183
42	o	0.35	0/911	0.39	0/1218
43	p	0.39	0/946	0.38	0/1257
44	q	0.33	0/835	0.43	0/1117
45	r	0.34	0/837	0.38	0/1114
46	s	0.33	0/749	0.42	0/1002
47	t	0.28	0/808	0.38	0/1079
48	u	0.26	0/1469	0.34	0/1988
49	v	0.38	0/583	0.45	0/774
50	w	0.34	0/641	0.35	0/854
51	x	0.28	0/491	0.36	0/654
52	y	0.32	0/449	0.40	0/602
53	z	0.38	0/446	0.45	0/594
All	All	0.76	0/154023	0.78	75/230240 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
31	d	0	1
44	q	0	1
46	s	0	1
All	All	0	3

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2087	G	OP1-P-O3'	-10.67	76.00	108.00
28	a	2087	G	OP2-P-O3'	-10.46	76.62	108.00
28	a	503	G	O4'-C1'-N9	9.10	115.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	879	C	O4'-C1'-N1	8.58	114.51	108.50
9	D	26	ARG	CA-C-N	-8.02	112.90	122.44
9	D	26	ARG	C-N-CA	-8.02	112.90	122.44
28	a	1300	U	C2-N1-C1'	7.22	126.36	117.70
6	A	1022	C	N3-C2-O2	-6.96	117.03	121.90
6	A	1435	A	O4'-C1'-N9	6.87	113.69	108.20
28	a	1382	A	O4'-C1'-N9	6.71	113.20	108.50
28	a	359	U	C2-N1-C1'	6.70	125.75	117.70
28	a	2158	A	O4'-C1'-N9	6.65	113.52	108.20
6	A	490	A	O4'-C1'-N9	6.42	112.99	108.50
6	A	1021	C	N1-C2-O2	6.22	122.63	118.90
28	a	2161	C	C2-N1-C1'	6.19	125.61	118.80
28	a	321	G	O4'-C1'-N9	6.17	113.14	108.20
28	a	2835	G	O4'-C1'-N9	6.16	113.13	108.20
6	A	1021	C	C2-N1-C1'	6.15	125.57	118.80
28	a	860	U	O5'-C5'-C4'	6.04	114.23	109.40
28	a	1573	U	O5'-C5'-C4'	5.95	114.16	109.40
28	a	83	G	C4-N9-C1'	5.92	134.19	126.50
6	A	1022	C	C6-N1-C2	-5.91	117.94	120.30
28	a	2162	C	C2-N1-C1'	5.89	125.28	118.80
28	a	1597	C	N3-C4-C5	5.84	124.24	121.90
28	a	471	A	O5'-C5'-C4'	5.76	114.01	109.40
6	A	322	C	P-O3'-C3'	5.75	126.60	119.70
28	a	359	U	N1-C2-O2	5.75	126.83	122.80
6	A	323	A	O5'-C5'-C4'	5.75	114.00	109.40
28	a	1225	G	O5'-C5'-C4'	5.74	114.00	109.40
28	a	2812	U	N3-C2-O2	-5.67	118.23	122.20
6	A	786	A	O4'-C1'-N9	5.65	112.72	108.20
28	a	249	C	O5'-C5'-C4'	5.65	113.92	109.40
28	a	348	U	C2-N1-C1'	5.58	124.39	117.70
28	a	2159	U	O5'-C5'-C4'	5.54	113.83	109.40
28	a	877	C	O4'-C1'-N1	5.53	112.37	108.50
28	a	2124	C	C5-C6-N1	5.52	123.76	121.00
28	a	920	C	P-O3'-C3'	5.50	126.31	119.70
28	a	2568	G	O4'-C1'-N9	5.50	112.60	108.20
6	A	893	C	C6-N1-C2	-5.48	118.11	120.30
28	a	2136	U	C5-C6-N1	5.46	125.43	122.70
28	a	44	A	O4'-C1'-N9	5.43	112.55	108.20
6	A	1021	C	C6-N1-C1'	-5.43	114.29	120.80
28	a	9	G	O4'-C1'-N9	5.42	112.54	108.20
28	a	1016	U	O5'-C5'-C4'	5.42	113.73	109.40
28	a	1146	A	O5'-C5'-C4'	5.41	113.73	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	748	C	C2-N1-C1'	5.41	124.75	118.80
28	a	1240	A	O5'-C5'-C4'	5.39	113.71	109.40
28	a	1300	U	N3-C2-O2	-5.35	118.45	122.20
28	a	738	G	O4'-C1'-N9	5.33	112.23	108.50
6	A	651	U	C2-N1-C1'	5.32	124.08	117.70
28	a	359	U	N3-C2-O2	-5.30	118.49	122.20
28	a	2434	G	O4'-C1'-N9	5.24	112.39	108.20
28	a	2677	U	O5'-C5'-C4'	5.23	113.59	109.40
28	a	27	G	O4'-C1'-N9	5.23	112.39	108.20
19	N	89	MET	CB-CG-SD	5.23	128.39	112.70
6	A	1405	C	C2-N1-C1'	5.22	124.54	118.80
28	a	472	G	O4'-C1'-N9	5.19	112.35	108.20
28	a	288	A	O4'-C1'-N9	5.18	112.34	108.20
28	a	1939	A	N9-C1'-C2'	5.17	117.69	112.00
28	a	836	U	C2-N1-C1'	5.17	123.90	117.70
6	A	631	C	C2-N1-C1'	5.16	124.48	118.80
6	A	984	C	C2-N1-C1'	5.16	124.47	118.80
6	A	1195	A	P-O3'-C3'	5.12	125.84	119.70
29	b	42	C	C2-N1-C1'	5.11	124.42	118.80
28	a	1373	C	O5'-C5'-C4'	5.09	113.47	109.40
28	a	2274	A	P-O3'-C3'	5.08	125.80	119.70
28	a	1502	A	O5'-C5'-C4'	5.08	113.46	109.40
6	A	204	C	N1-C2-O2	5.08	121.94	118.90
28	a	932	G	N1-C6-O6	-5.07	116.86	119.90
28	a	83	G	C8-N9-C1'	-5.07	120.41	127.00
6	A	680	U	O4'-C1'-N1	5.06	112.25	108.20
28	a	1261	A	O5'-C5'-C4'	5.05	113.44	109.40
6	A	1503	C	C2-N1-C1'	5.02	124.32	118.80
6	A	1126	C	C2-N1-C1'	5.01	124.31	118.80
28	a	970	A	N9-C1'-C2'	5.01	117.51	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	d	151	THR	Peptide
44	q	51	LEU	Peptide
46	s	25	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	426	0	457	10	0
2	1	365	0	409	4	0
3	2	506	0	569	1	0
4	3	307	0	342	4	0
5	4	531	0	528	23	0
6	A	32945	0	16588	354	0
7	B	1763	0	1811	44	0
8	C	1664	0	1723	40	0
9	D	1627	0	1665	25	0
10	E	1134	0	1181	27	0
11	F	868	0	846	23	0
12	G	1199	0	1253	18	0
13	H	982	0	1036	9	0
14	I	1010	0	1052	33	0
15	J	793	0	833	30	0
16	K	881	0	897	11	0
17	L	961	0	1010	9	0
18	M	883	0	929	21	0
19	N	804	0	841	15	0
20	O	703	0	727	3	0
21	P	637	0	648	7	0
22	Q	645	0	689	11	0
23	R	494	0	514	9	0
24	S	663	0	697	23	0
25	T	671	0	722	5	0
26	W	219	0	108	4	0
27	X	796	0	818	8	0
28	a	62019	0	31188	522	0
29	b	2495	0	1263	21	0
30	c	2072	0	2152	28	0
31	d	1589	0	1605	20	0
32	e	1524	0	1582	24	0
33	f	1418	0	1486	45	0
34	g	1326	0	1388	23	0
35	h	533	0	560	8	0
36	i	1130	0	1160	14	0
37	j	938	0	1012	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	k	1066	0	1112	13	0
39	l	1086	0	1145	19	0
40	m	959	0	1005	11	0
41	n	881	0	920	18	0
42	o	902	0	960	12	0
43	p	936	0	1025	13	0
44	q	822	0	858	15	0
45	r	833	0	897	9	0
46	s	739	0	788	9	0
47	t	800	0	863	9	0
48	u	1446	0	1486	19	0
49	v	575	0	598	5	0
50	w	630	0	653	8	0
51	x	490	0	520	8	0
52	y	445	0	472	4	0
53	z	440	0	437	9	0
54	3	1	0	0	0	0
54	4	1	0	0	0	0
55	A	94	0	0	0	0
55	X	1	0	0	0	0
55	a	249	0	0	0	0
55	b	5	0	0	0	0
55	c	1	0	0	0	0
55	p	2	0	0	0	0
55	v	1	0	0	0	0
55	z	1	0	0	0	0
56	A	48	0	0	0	0
56	X	1	0	0	0	0
56	a	113	0	0	0	0
56	b	1	0	0	0	0
56	c	4	0	0	0	0
56	e	1	0	0	0	0
56	f	1	0	0	0	0
All	All	143096	0	96028	1534	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 6.

All (1534) 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)
6:A:74:A:H62	6:A:89:G:N2	1.47	1.12
28:a:2126:U:H3	28:a:2139:G:H1	1.04	1.03
6:A:74:A:N6	6:A:89:G:H21	1.56	1.01
10:E:83:GLN:H	10:E:148:MET:HE1	1.36	0.91
28:a:1834:A:HO2'	28:a:1835:A:H8	0.92	0.90
7:B:100:MET:HA	7:B:107:ILE:HG13	1.60	0.84
28:a:2414:C:H5''	28:a:2416:G:H5'	1.61	0.82
28:a:1095:U:H2'	28:a:1096:A:H8	1.44	0.82
28:a:2292:U:H5''	33:f:131:GLY:HA3	1.60	0.82
6:A:1299:G:H22	6:A:1325:G:H2'	1.46	0.80
28:a:1519:G:H1	28:a:1529:U:H3	1.29	0.80
28:a:2097:G:H5'	28:a:2105:U:H3	1.45	0.80
15:J:37:ARG:HB2	15:J:75:ASP:HB2	1.64	0.80
6:A:1350:A:H2'	6:A:1351:A:H8	1.48	0.79
6:A:667:G:H2'	6:A:668:G:C8	2.18	0.79
28:a:845:G:H2'	28:a:846:G:C8	2.17	0.79
6:A:1080:U:H3	6:A:1093:G:H22	1.29	0.79
6:A:74:A:H62	6:A:89:G:H21	0.79	0.78
28:a:2456:A:H4'	39:I:56:ARG:HD2	1.67	0.77
6:A:1124:A:H2'	6:A:1125:G:H8	1.50	0.77
6:A:1534:U:O4	26:W:6:G:O6	2.02	0.77
9:D:159:LEU:HD13	9:D:175:LEU:HG	1.65	0.77
33:f:58:GLU:HG3	33:f:65:PRO:HD3	1.67	0.76
14:I:21:LEU:HD22	14:I:86:ALA:HB1	1.66	0.76
6:A:86:C:H2'	6:A:87:C:H6	1.50	0.76
14:I:84:THR:HG23	14:I:98:LEU:HD13	1.67	0.75
28:a:2315:A:H2'	28:a:2316:A:C8	2.21	0.75
6:A:1350:A:H2'	6:A:1351:A:C8	2.22	0.74
6:A:1342:U:H4'	14:I:122:ARG:HG3	1.71	0.73
28:a:2135:G:H2'	28:a:2136:U:C6	2.22	0.73
6:A:86:C:H2'	6:A:87:C:C6	2.24	0.73
51:x:1:MET:HE2	51:x:1:MET:HA	1.68	0.73
6:A:248:G:H4'	22:Q:23:THR:HG21	1.69	0.73
8:C:67:THR:HG22	8:C:102:ASN:HB2	1.71	0.72
10:E:151:PRO:O	10:E:152:GLU:HG2	1.89	0.72
9:D:58:LYS:HG3	9:D:200:ILE:HG23	1.72	0.72
15:J:12:ALA:HB3	15:J:18:ILE:HG12	1.70	0.72
28:a:2131:G:H21	28:a:2134:A:H2	1.38	0.71
1:O:25:THR:HG22	1:O:26:LYS:HD3	1.72	0.71
3:2:36:THR:HG22	3:2:38:LYS:H	1.56	0.71
10:E:157:LYS:HE2	10:E:157:LYS:H	1.56	0.71
28:a:1018:A:H2'	28:a:1019:A:C8	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:263:U:H2'	6:A:264:A:C8	2.26	0.70
12:G:113:GLU:HB2	12:G:119:ARG:HG2	1.73	0.70
6:A:1027:G:H2'	6:A:1028:G:C8	2.26	0.70
6:A:1487:A:H5''	28:a:1900:A:H62	1.57	0.70
30:c:120:ILE:H	30:c:120:ILE:HD12	1.55	0.70
48:u:11:ARG:HB2	48:u:44:THR:HG23	1.74	0.69
7:B:118:GLU:HG2	7:B:141:LEU:HD11	1.74	0.69
6:A:73:A:H8	6:A:90:G:H21	1.39	0.69
15:J:82:LYS:HE2	15:J:85:ASP:HB3	1.74	0.69
28:a:558:U:H1'	28:a:2017:6MZ:H9C1	1.72	0.69
28:a:1048:G:N1	28:a:1071:U:N3	2.40	0.69
37:j:25:LEU:HD12	37:j:38:ILE:HG22	1.75	0.69
24:S:45:VAL:HG13	24:S:63:ASN:HA	1.73	0.69
28:a:1672:G:H2'	28:a:1673:C:C6	2.27	0.69
28:a:2092:U:H2'	28:a:2093:G:C8	2.28	0.69
6:A:75:G:O6	6:A:88:U:O4	2.11	0.68
31:d:118:PHE:HA	31:d:164:HIS:H	1.59	0.68
5:4:56:ARG:HB2	5:4:59:ARG:HB3	1.74	0.68
6:A:969:A:H4'	6:A:970:G:H5''	1.74	0.68
30:c:122:ALA:HB3	30:c:130:MET:HE2	1.75	0.68
33:f:107:SER:HB3	33:f:137:ILE:HG12	1.75	0.67
7:B:16:PHE:HB2	7:B:203:ASN:HD22	1.59	0.67
34:g:143:GLN:O	34:g:147:GLU:HG3	1.94	0.67
28:a:2088:A:H3'	28:a:2089:G:H8	1.58	0.67
28:a:2299:U:H5'	33:f:85:ILE:HD11	1.75	0.67
9:D:197:GLU:HA	9:D:200:ILE:HD12	1.77	0.67
32:e:11:ILE:HD11	32:e:189:VAL:HG13	1.77	0.67
6:A:454:A:H2'	6:A:455:A:H8	1.60	0.67
28:a:2571:U:H2'	28:a:2572:U:H2'	1.77	0.67
2:1:12:ARG:HE	2:1:44:VAL:HG22	1.60	0.66
28:a:371:G:H5'	50:w:18:ILE:HD12	1.77	0.66
15:J:65:TYR:HB3	19:N:96:LEU:HD11	1.78	0.66
30:c:211:THR:HG22	30:c:216:VAL:HB	1.76	0.66
38:k:15:GLU:O	38:k:16:LYS:HB3	1.95	0.66
27:X:93:LEU:O	27:X:97:GLN:HB3	1.95	0.66
7:B:117:LEU:HB3	7:B:141:LEU:HD13	1.78	0.66
8:C:130:PHE:HD1	8:C:134:MET:HE2	1.60	0.66
13:H:43:GLU:HG3	13:H:101:VAL:HG11	1.77	0.66
6:A:940:A:H2'	6:A:941:G:C8	2.30	0.66
15:J:6:ILE:HG23	15:J:76:ILE:HG23	1.78	0.66
21:P:54:GLN:O	21:P:58:THR:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2278:U:H2'	28:a:2279:G:C8	2.31	0.66
35:h:8:LYS:HG2	35:h:14:ASN:HA	1.78	0.65
52:y:5:LYS:HB2	52:y:57:GLU:HB2	1.78	0.65
6:A:84:C:H2'	6:A:85:U:C6	2.32	0.65
7:B:57:VAL:HG21	7:B:217:MET:SD	2.36	0.65
7:B:70:VAL:HG12	7:B:92:VAL:HB	1.77	0.65
28:a:1116:A:H4'	28:a:1117:A:H5''	1.77	0.65
13:H:18:GLN:HE21	13:H:63:LEU:HB3	1.62	0.65
15:J:88:MET:HE1	15:J:92:LEU:HD11	1.78	0.65
28:a:1095:U:H2'	28:a:1096:A:C8	2.31	0.65
6:A:1255:A:N6	6:A:1268:G:H1'	2.12	0.65
28:a:2154:U:H2'	28:a:2155:G:O4'	1.97	0.65
28:a:200:U:H4'	50:w:22:HIS:HB3	1.79	0.64
16:K:64:GLN:HG2	16:K:99:ALA:HB2	1.79	0.64
28:a:1766:U:H5	28:a:1771:A:N7	1.95	0.64
5:4:12:ILE:HD11	5:4:28:LEU:HD12	1.78	0.64
9:D:8:LYS:HG3	9:D:21:LEU:HD22	1.79	0.64
16:K:20:ILE:HG23	16:K:83:ASP:HB2	1.78	0.64
16:K:31:ILE:HG12	16:K:46:THR:HG22	1.80	0.64
16:K:72:GLN:HA	16:K:75:LEU:HD12	1.78	0.64
50:w:10:LYS:HE3	50:w:54:LYS:HD2	1.80	0.64
7:B:97:LEU:H	7:B:100:MET:HE2	1.62	0.64
7:B:111:ILE:HG13	7:B:148:LEU:HD13	1.77	0.64
28:a:1635:G:H5''	28:a:1636:C:H5'	1.80	0.64
28:a:1783:U:H2'	28:a:1784:C:C6	2.33	0.64
45:r:55:VAL:O	45:r:59:GLU:HG3	1.98	0.64
15:J:35:GLN:HB2	15:J:77:VAL:HG22	1.80	0.64
28:a:1233:A:H4'	32:e:39:ARG:HH12	1.63	0.64
9:D:47:ARG:HG3	9:D:47:ARG:HH11	1.61	0.63
6:A:722:A:H2'	6:A:723:A:C8	2.34	0.63
18:M:87:ARG:HG3	18:M:97:VAL:HB	1.80	0.63
27:X:74:ILE:O	27:X:78:ILE:HG12	1.98	0.63
5:4:51:LEU:HD23	5:4:53:THR:H	1.63	0.63
6:A:1212:C:H2'	6:A:1213:A:C8	2.34	0.63
8:C:130:PHE:O	8:C:134:MET:HG2	1.98	0.63
6:A:1028:G:H2'	6:A:1029:A:H8	1.62	0.63
24:S:53:ASN:HD21	24:S:56:GLN:HG2	1.62	0.63
24:S:33:THR:HG22	24:S:35:SER:H	1.64	0.63
28:a:2096:U:H2'	28:a:2097:G:C8	2.34	0.63
6:A:1244:A:H2'	6:A:1245:A:C8	2.34	0.62
27:X:50:ILE:HG23	27:X:77:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2123:G:H2'	28:a:2124:C:C6	2.34	0.62
33:f:34:ILE:HG13	33:f:96:MET:HG3	1.81	0.62
28:a:879:C:H5'	28:a:880:G:N7	2.14	0.62
6:A:1255:A:H61	6:A:1268:G:H1'	1.63	0.62
14:I:28:ILE:HG22	14:I:35:LEU:HB2	1.81	0.62
6:A:204:C:H4'	6:A:205:G:H21	1.64	0.62
6:A:893:C:H2'	6:A:894:A:C8	2.35	0.62
28:a:963:A:H5''	44:q:81:LYS:HD2	1.80	0.62
6:A:1426:G:H5''	42:o:107:LYS:HG3	1.82	0.62
12:G:16:PRO:HB3	14:I:46:MET:HG3	1.81	0.62
28:a:1420:A:H2'	28:a:1421:A:C8	2.35	0.62
6:A:658:G:H22	6:A:735:G:H1	1.48	0.62
7:B:28:GLY:HA2	7:B:31:ILE:HD12	1.81	0.62
24:S:3:ARG:HH12	24:S:7:LYS:HE2	1.65	0.62
28:a:5:A:H2'	28:a:6:A:C8	2.35	0.62
6:A:1533:C:N3	26:W:7:U:O4	2.34	0.61
8:C:114:MET:O	8:C:118:GLN:HG3	2.00	0.61
19:N:89:MET:HA	19:N:89:MET:HE3	1.81	0.61
14:I:47:VAL:HA	14:I:50:GLN:HG3	1.83	0.61
32:e:3:LEU:HB2	32:e:11:ILE:HG22	1.82	0.61
35:h:16:GLY:HA2	35:h:47:PHE:CZ	2.35	0.61
1:0:6:ARG:HG3	1:0:50:ILE:HA	1.81	0.61
6:A:1124:A:H2'	6:A:1125:G:C8	2.34	0.61
7:B:32:PHE:HB2	7:B:42:ASN:HB3	1.82	0.61
28:a:1340:A:H2'	28:a:1341:A:C8	2.35	0.61
28:a:2873:G:H2'	28:a:2874:C:C6	2.36	0.61
18:M:106:ALA:HB3	18:M:110:LYS:HD2	1.83	0.61
33:f:136:ILE:HG21	33:f:143:TYR:HD1	1.65	0.61
6:A:1390:A:H4'	6:A:1391:C:H5''	1.82	0.61
28:a:1288:A:H2	28:a:1616:G:H21	1.48	0.61
46:s:5:ARG:O	46:s:9:VAL:HG23	2.01	0.61
12:G:9:LYS:HD2	12:G:9:LYS:N	2.16	0.60
48:u:53:LEU:HD21	48:u:64:ILE:HD13	1.82	0.60
10:E:160:LYS:NZ	10:E:161:SER:H	1.98	0.60
28:a:2146:G:H2'	28:a:2147:C:H6	1.65	0.60
33:f:3:ARG:NE	33:f:3:ARG:HA	2.16	0.60
28:a:873:U:O2	28:a:880:G:O6	2.19	0.60
28:a:2146:G:H2'	28:a:2147:C:C6	2.36	0.60
11:F:40:GLU:HB3	11:F:103:LEU:HD12	1.82	0.60
28:a:2105:U:OP2	28:a:2135:G:H4'	2.02	0.60
6:A:454:A:H2'	6:A:455:A:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:60:LEU:HD13	7:B:67:ILE:HD11	1.82	0.60
8:C:6:HIS:HB3	19:N:89:MET:HE2	1.83	0.60
28:a:571:C:H2'	28:a:572:A:C8	2.37	0.60
28:a:2126:U:O4	28:a:2139:G:O6	2.18	0.60
6:A:1034:A:H2'	6:A:1035:G:H8	1.66	0.60
12:G:76:LYS:HD3	12:G:89:VAL:HG21	1.83	0.60
12:G:108:ALA:HA	12:G:111:ARG:HG3	1.82	0.60
12:G:130:GLY:HA2	12:G:135:VAL:HG21	1.83	0.60
28:a:1789:A:H2'	28:a:1790:A:C8	2.36	0.59
35:h:58:ALA:O	35:h:62:LYS:HG3	2.02	0.59
40:m:37:THR:HG22	40:m:39:PRO:HD2	1.83	0.59
8:C:92:THR:O	8:C:95:MET:O	2.20	0.59
28:a:786:U:H2'	28:a:787:C:C6	2.36	0.59
28:a:2605:G:H21	31:d:155:VAL:HG21	1.67	0.59
17:L:114:ARG:HG2	17:L:119:ALA:HB3	1.84	0.59
28:a:1641:G:H5'	40:m:39:PRO:HG2	1.82	0.59
37:j:111:PHE:HB3	37:j:114:ILE:HD12	1.84	0.59
6:A:1440:A:HO2'	6:A:1441:A:H8	1.48	0.59
6:A:1487:A:H3'	6:A:1488:G:H5''	1.85	0.59
10:E:40:VAL:HG11	10:E:69:ARG:HG2	1.83	0.59
6:A:1216:G:H5''	24:S:78:ARG:HE	1.67	0.59
6:A:1034:A:H2'	6:A:1035:G:C8	2.38	0.59
18:M:90:ARG:HB2	18:M:97:VAL:HG12	1.83	0.59
47:t:4:ILE:HG21	47:t:33:LEU:HD11	1.84	0.59
34:g:38:HIS:CD2	34:g:39:PRO:HD2	2.38	0.59
16:K:79:LEU:HB3	16:K:105:TYR:HE2	1.68	0.59
6:A:707:G:H2'	6:A:708:G:C8	2.38	0.59
47:t:48:ASN:H	47:t:53:GLN:HA	1.66	0.59
6:A:1135:U:H2'	6:A:1136:G:H8	1.68	0.58
8:C:92:THR:HG23	8:C:99:VAL:HG22	1.85	0.58
6:A:77:G:H2'	6:A:78:A:C8	2.38	0.58
28:a:2260:A:H2'	28:a:2261:A:C8	2.38	0.58
46:s:60:LEU:HD11	46:s:81:LYS:HE2	1.86	0.58
6:A:453:U:H2'	6:A:454:A:C8	2.39	0.58
6:A:1406:C:H2'	6:A:1407:A:C8	2.37	0.58
22:Q:56:CYS:O	22:Q:57:ARG:HD2	2.04	0.58
28:a:1184:G:H2'	28:a:1185:U:H6	1.67	0.58
28:a:629:U:H2'	28:a:630:C:C6	2.39	0.58
8:C:150:LYS:HG2	8:C:201:TRP:CE3	2.39	0.58
22:Q:28:ILE:HD12	22:Q:47:LEU:HD12	1.85	0.58
23:R:26:LEU:HD11	23:R:67:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2038:U:H3'	28:a:2565:G:H5''	1.84	0.58
6:A:85:U:H2'	6:A:86:C:C6	2.39	0.58
6:A:1002:U:H4'	6:A:1003:U:C5	2.39	0.57
28:a:1708:U:H2'	28:a:1709:G:O4'	2.03	0.57
29:b:90:C:H5'	39:l:18:ARG:HG2	1.86	0.57
28:a:2290:G:H2'	28:a:2291:G:O4'	2.03	0.57
6:A:1002:U:H1'	6:A:1016:U:H5	1.69	0.57
44:q:6:VAL:HG22	44:q:11:GLN:HG2	1.86	0.57
11:F:101:GLU:HA	11:F:104:LYS:HB2	1.85	0.57
28:a:2113:A:H4'	28:a:2114:G:H5'	1.85	0.57
32:e:160:ALA:HA	32:e:163:LEU:HB2	1.86	0.57
5:4:61:LYS:HG2	24:S:42:PRO:HG3	1.86	0.57
6:A:763:G:H4'	6:A:1507:A:H4'	1.86	0.57
21:P:20:THR:HG22	21:P:35:ARG:HG2	1.85	0.57
28:a:2775:A:H2'	28:a:2776:C:C6	2.38	0.57
6:A:1220:C:N4	18:M:103:LYS:HD2	2.19	0.57
11:F:38:ARG:HH22	23:R:24:LYS:NZ	2.02	0.57
28:a:1083:G:H2'	28:a:1084:U:C6	2.40	0.57
38:k:80:SER:HB3	38:k:114:GLY:HA3	1.87	0.57
6:A:125:U:H2'	6:A:126:C:C6	2.40	0.57
12:G:57:ASP:HB3	12:G:60:GLU:HG2	1.87	0.57
14:I:28:ILE:CG2	14:I:35:LEU:HB2	2.35	0.57
28:a:1044:A:H62	28:a:1095:U:H3	1.52	0.57
33:f:3:ARG:HA	33:f:3:ARG:HE	1.69	0.57
8:C:111:LEU:HD22	8:C:146:ALA:HB2	1.87	0.57
28:a:647:U:H2'	28:a:648:C:C6	2.40	0.57
28:a:1069:C:H2'	28:a:1070:C:O4'	2.05	0.57
28:a:1186:U:H2'	28:a:1187:C:H6	1.70	0.57
28:a:1811:G:O2'	30:c:253:THR:HG21	2.05	0.57
28:a:2160:A:C5	28:a:2161:C:H1'	2.39	0.57
6:A:730:C:H2'	6:A:731:A:H8	1.70	0.57
6:A:1352:U:H5'	6:A:1353:C:OP2	2.05	0.57
14:I:19:VAL:HG22	14:I:65:VAL:HG12	1.87	0.57
28:a:2088:A:H3'	28:a:2089:G:C8	2.39	0.57
34:g:126:PRO:HD2	34:g:130:ASP:HB3	1.87	0.57
5:4:38:SER:OG	33:f:105:SER:HA	2.04	0.56
6:A:978:C:H2'	6:A:979:C:H6	1.69	0.56
28:a:272:A:H2'	28:a:273:A:C8	2.38	0.56
28:a:822:U:H2'	28:a:823:A:C8	2.40	0.56
28:a:2788:U:H2'	28:a:2789:U:C6	2.40	0.56
42:o:101:LEU:HD11	42:o:111:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1016:U:H2'	6:A:1017:G:O4'	2.05	0.56
10:E:154:VAL:HG11	13:H:99:LEU:HD13	1.86	0.56
5:4:42:PRO:HG3	5:4:49:LYS:HG3	1.86	0.56
6:A:88:U:H2'	6:A:89:G:C8	2.40	0.56
6:A:1268:G:HO2'	6:A:1269:A:H8	1.54	0.56
7:B:6:MET:HB3	7:B:7:ARG:HH12	1.70	0.56
9:D:12:SER:HA	9:D:19:LEU:HD13	1.87	0.56
28:a:470:A:N3	28:a:472:G:H5''	2.20	0.56
28:a:2121:A:H2'	28:a:2122:A:H8	1.71	0.56
48:u:86:LYS:HE3	48:u:88:PHE:HE2	1.69	0.56
6:A:83:G:H2'	6:A:84:C:C6	2.41	0.56
28:a:1373:C:H2'	28:a:1374:A:C8	2.41	0.56
28:a:2121:A:H2'	28:a:2122:A:C8	2.41	0.56
6:A:840:G:H2'	6:A:841:A:H8	1.70	0.56
6:A:957:G:N2	15:J:57:VAL:HG11	2.20	0.56
28:a:244:A:H5''	38:k:67:VAL:HG11	1.88	0.56
28:a:2578:C:H2'	28:a:2579:G:C8	2.40	0.56
37:j:63:VAL:HG23	37:j:106:LEU:HD11	1.87	0.56
39:l:78:PRO:HG2	39:l:81:VAL:HG21	1.87	0.56
8:C:91:LEU:HB2	8:C:99:VAL:HG21	1.88	0.56
6:A:549:U:H2'	6:A:550:C:C6	2.41	0.56
9:D:11:LEU:HB3	9:D:63:ARG:HD3	1.86	0.56
6:A:1230:A:H4'	6:A:1298:G:H4'	1.88	0.56
6:A:1281:A:H2'	6:A:1282:A:C8	2.40	0.56
18:M:34:CYS:O	18:M:38:GLY:HA2	2.06	0.56
28:a:339:A:H1'	28:a:340:A:C2	2.40	0.56
28:a:491:G:H22	28:a:494:A:H5'	1.70	0.56
28:a:2287:A:H2'	28:a:2288:C:C6	2.41	0.56
6:A:920:G:C6	27:X:87:LYS:HG3	2.41	0.56
28:a:2291:G:H5'	28:a:2292:U:OP2	2.06	0.56
28:a:1186:U:H2'	28:a:1187:C:C6	2.41	0.55
6:A:1002:U:H1'	6:A:1016:U:C5	2.41	0.55
34:g:41:VAL:HB	34:g:61:THR:HG23	1.89	0.55
6:A:730:C:H2'	6:A:731:A:C8	2.41	0.55
28:a:995:C:O2'	36:i:30:THR:HG21	2.07	0.55
41:n:27:LEU:HD23	41:n:91:PHE:HD1	1.71	0.55
8:C:112:ASP:OD1	8:C:115:LEU:HB2	2.07	0.55
28:a:1520:U:H2'	28:a:1521:C:C6	2.42	0.55
28:a:2109:U:H2'	28:a:2110:G:C8	2.41	0.55
28:a:898:A:H2'	28:a:901:C:C5	2.41	0.55
28:a:2067:G:H5'	50:w:19:SER:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:16:GLY:HA2	35:h:47:PHE:HZ	1.70	0.55
28:a:1084:U:H1'	28:a:1087:U:H5	1.72	0.55
28:a:1807:U:H5	30:c:177:ARG:HH12	1.53	0.55
28:a:2051:C:H2'	28:a:2052:C:C6	2.42	0.55
29:b:3:C:H2'	29:b:4:U:H6	1.72	0.55
34:g:137:ASP:HB3	34:g:140:LEU:HB2	1.88	0.55
7:B:19:GLN:HA	7:B:38:ILE:HA	1.88	0.55
7:B:67:ILE:HG13	7:B:160:ALA:HB3	1.89	0.55
8:C:148:GLY:HA3	8:C:172:ARG:O	2.07	0.55
12:G:107:PHE:HZ	12:G:137:LYS:HD3	1.72	0.55
15:J:59:LYS:O	15:J:62:ARG:HD3	2.07	0.55
51:x:26:PHE:CE1	51:x:30:MET:HE3	2.42	0.55
6:A:1385:U:H2'	6:A:1386:G:C8	2.42	0.55
28:a:263:U:H2'	28:a:264:U:O4'	2.06	0.55
28:a:1481:A:H2'	28:a:1482:A:C8	2.42	0.55
14:I:18:ARG:HH21	14:I:66:THR:HG21	1.72	0.54
18:M:67:GLY:O	18:M:71:ARG:HG3	2.07	0.54
30:c:244:HIS:O	30:c:246:VAL:HG23	2.07	0.54
6:A:67:C:H2'	6:A:68:G:C8	2.42	0.54
7:B:43:LEU:HA	7:B:46:THR:HB	1.89	0.54
8:C:9:GLY:HA3	19:N:89:MET:HE3	1.89	0.54
28:a:772:A:C2	30:c:225:MET:HG2	2.42	0.54
29:b:48:U:H2'	29:b:49:C:C6	2.42	0.54
46:s:69:THR:HG23	46:s:71:ARG:H	1.72	0.54
6:A:651:U:H5	6:A:743:A:N1	2.06	0.54
28:a:629:U:H2'	28:a:630:C:H6	1.73	0.54
30:c:29:PRO:HG2	30:c:34:LEU:HD21	1.89	0.54
33:f:38:MET:HE2	33:f:57:LEU:HD22	1.90	0.54
6:A:17:U:H2'	6:A:18:C:C6	2.42	0.54
6:A:77:G:H2'	6:A:78:A:H8	1.72	0.54
6:A:263:U:H2'	6:A:264:A:H8	1.69	0.54
8:C:51:SER:HB2	8:C:71:ALA:HB3	1.89	0.54
15:J:8:ILE:HG23	15:J:98:VAL:HG13	1.89	0.54
17:L:59:ASN:OD1	17:L:61:PHE:HD1	1.90	0.54
28:a:2489:G:H5''	28:a:2490:2MA:H5''	1.88	0.54
6:A:229:U:H2'	6:A:230:A:C8	2.42	0.54
6:A:1021:C:H2'	6:A:1022:C:C6	2.42	0.54
8:C:134:MET:HE3	8:C:168:TYR:HE1	1.71	0.54
22:Q:11:LEU:HD13	22:Q:28:ILE:HD13	1.90	0.54
28:a:1018:A:N6	28:a:1115:G:H2'	2.23	0.54
28:a:1670:U:H2'	28:a:1671:G:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2687:A:H2'	28:a:2688:C:C6	2.43	0.54
29:b:3:C:H2'	29:b:4:U:C6	2.42	0.54
18:M:76:ASN:O	18:M:79:ARG:HG3	2.07	0.54
28:a:899:A:H2'	28:a:900:A:C8	2.43	0.54
28:a:2559:A:N7	31:d:150:MEQ:HB3	2.23	0.54
33:f:24:ASN:HB3	33:f:27:GLU:HG3	1.88	0.54
40:m:45:ARG:HB3	40:m:95:LEU:HD11	1.89	0.54
6:A:532:A:H2'	6:A:533:A:C8	2.43	0.54
6:A:834:C:H2'	6:A:835:C:C6	2.42	0.54
28:a:990:A:H2'	28:a:991:A:C8	2.43	0.54
28:a:1721:C:H2'	28:a:1722:C:C6	2.43	0.54
30:c:239:THR:HG22	30:c:240:SER:H	1.73	0.54
6:A:1436:G:H2'	6:A:1437:U:C6	2.43	0.54
7:B:217:MET:O	7:B:221:VAL:HG23	2.08	0.54
36:i:56:VAL:HB	36:i:124:VAL:HG13	1.89	0.54
7:B:85:ALA:C	7:B:87:CYS:H	2.14	0.53
8:C:134:MET:HE3	8:C:168:TYR:CE1	2.44	0.53
28:a:949:A:H2'	28:a:950:A:C8	2.44	0.53
28:a:1781:A:H2'	28:a:1782:C:C6	2.43	0.53
28:a:2135:G:H2'	28:a:2136:U:H6	1.69	0.53
28:a:2562:C:H5'	31:d:149:CYS:HB2	1.91	0.53
48:u:151:MET:HE1	48:u:160:VAL:HG21	1.89	0.53
6:A:365:A:H2'	6:A:366:C:O4'	2.08	0.53
6:A:1008:A:C2	6:A:1213:A:H1'	2.44	0.53
15:J:9:ARG:HH12	15:J:71:LYS:HE2	1.72	0.53
36:i:21:ALA:HA	36:i:61:GLN:HB2	1.90	0.53
38:k:82:LEU:HD22	38:k:90:VAL:HG11	1.90	0.53
33:f:4:LEU:HG	33:f:101:ASP:HB3	1.90	0.53
39:l:48:GLU:HG3	39:l:52:ARG:HH22	1.72	0.53
6:A:1528:A:H2'	6:A:1529:C:C6	2.44	0.53
28:a:583:U:H2'	28:a:584:U:C6	2.44	0.53
28:a:2685:U:H2'	28:a:2686:C:C6	2.43	0.53
28:a:2727:A:H2'	28:a:2728:A:C8	2.44	0.53
6:A:1114:C:H2'	6:A:1115:U:C6	2.43	0.53
6:A:1135:U:H2'	6:A:1136:G:C8	2.43	0.53
9:D:48:LEU:HD22	9:D:52:GLY:HA3	1.91	0.53
13:H:18:GLN:HG2	13:H:70:PRO:HB3	1.91	0.53
28:a:852:A:H2'	28:a:853:G:C8	2.44	0.53
33:f:38:MET:HG3	33:f:152:LEU:HD23	1.89	0.53
6:A:1308:C:H2'	6:A:1309:U:C6	2.43	0.53
28:a:1522:U:H2'	28:a:1523:U:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:43:VAL:HB	34:g:53:ALA:HB3	1.90	0.53
6:A:346:C:H4'	6:A:348:G:OP1	2.09	0.53
10:E:157:LYS:HE2	10:E:157:LYS:N	2.23	0.53
24:S:3:ARG:HE	24:S:10:PHE:HB2	1.73	0.53
28:a:1519:G:H2'	28:a:1520:U:C6	2.43	0.53
28:a:2158:A:H1'	28:a:2159:U:C6	2.44	0.53
30:c:132:LEU:HA	30:c:135:ILE:HG13	1.91	0.53
2:l:1:MET:HE1	28:a:742:A:H3'	1.90	0.53
28:a:191:A:H2'	28:a:192:C:C6	2.44	0.53
48:u:107:VAL:HG12	48:u:134:VAL:HG12	1.91	0.53
6:A:141:G:H2'	6:A:142:G:C8	2.44	0.53
6:A:331:G:H2'	6:A:332:A:C8	2.44	0.53
22:Q:50:HIS:HB2	22:Q:70:LEU:HD13	1.91	0.53
24:S:25:LYS:CD	24:S:26:ASN:H	2.22	0.53
28:a:1518:C:H2'	28:a:1519:G:C8	2.44	0.53
28:a:1773:A:H1'	28:a:1925:A:N6	2.23	0.53
6:A:1069:U:H5''	7:B:178:LYS:HE2	1.91	0.53
28:a:1099:C:H3'	28:a:1100:G:C8	2.44	0.53
28:a:1157:G:H2'	28:a:1158:U:C6	2.44	0.53
28:a:2498:U:H5''	31:d:128:ARG:HG3	1.91	0.53
42:o:3:ASN:O	42:o:7:GLN:HG3	2.09	0.53
44:q:19:PHE:CE2	44:q:64:VAL:HG21	2.44	0.53
5:4:12:ILE:HD12	5:4:26:SER:OG	2.09	0.52
6:A:512:C:H4'	6:A:513:C:O5'	2.07	0.52
7:B:27:MET:HG2	7:B:193:PRO:HD3	1.90	0.52
11:F:38:ARG:HG2	11:F:40:GLU:HG2	1.90	0.52
28:a:1456:A:H2'	28:a:1457:A:C8	2.44	0.52
35:h:5:LEU:HD11	35:h:12:LEU:HD23	1.90	0.52
16:K:65:VAL:O	16:K:68:GLU:HG3	2.09	0.52
28:a:831:A:H2'	28:a:832:U:C6	2.43	0.52
41:n:78:ALA:HB2	41:n:109:ALA:HA	1.90	0.52
6:A:940:A:H2'	6:A:941:G:H8	1.73	0.52
25:T:48:GLN:O	25:T:52:THR:HG22	2.09	0.52
28:a:2738:G:C4	34:g:3:ARG:HD3	2.44	0.52
36:i:11:VAL:HG11	36:i:50:THR:HA	1.91	0.52
6:A:87:C:H2'	6:A:88:U:H6	1.75	0.52
6:A:672:U:H2'	6:A:673:U:C6	2.45	0.52
6:A:1220:C:H41	18:M:103:LYS:HD2	1.74	0.52
7:B:53:ALA:O	7:B:57:VAL:HG23	2.09	0.52
15:J:6:ILE:HD13	15:J:102:LEU:HA	1.91	0.52
28:a:2292:U:H2'	28:a:2293:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:n:31:ARG:HG3	41:n:36:ILE:HD12	1.92	0.52
5:4:60:PHE:CZ	6:A:1305:A:H5''	2.45	0.52
6:A:41:G:H2'	6:A:42:G:C8	2.45	0.52
6:A:905:U:H2'	6:A:906:C:C6	2.43	0.52
6:A:1346:C:H2'	6:A:1347:G:C8	2.45	0.52
28:a:1080:A:N1	28:a:1092:C:H1'	2.24	0.52
28:a:1933:U:H2'	28:a:1934:C:C6	2.45	0.52
6:A:1152:C:C5	6:A:1154:G:H1'	2.44	0.52
6:A:1181:G:H5'	14:I:115:LYS:HZ2	1.75	0.52
6:A:1506:U:H2'	6:A:1507:A:C8	2.44	0.52
11:F:42:TRP:HB2	11:F:59:TYR:HB2	1.92	0.52
28:a:1348:G:H2'	28:a:1349:C:C6	2.45	0.52
34:g:41:VAL:HA	34:g:55:ARG:HB2	1.90	0.52
39:l:48:GLU:HG3	39:l:52:ARG:NH2	2.23	0.52
6:A:725:G:H5'	6:A:760:A:H4'	1.92	0.52
19:N:64:CYS:HB2	19:N:80:SER:HB2	1.92	0.52
28:a:5:A:H2'	28:a:6:A:H8	1.73	0.52
39:l:44:ALA:HB2	39:l:70:PRO:HG2	1.91	0.52
43:p:43:GLY:HA3	44:q:75:ILE:HD12	1.91	0.52
28:a:1858:A:H2'	28:a:1859:A:C8	2.45	0.52
28:a:1876:A:H2'	28:a:1877:A:C8	2.45	0.52
28:a:2173:G:H2'	28:a:2174:C:C6	2.44	0.52
28:a:2554:G:H2'	28:a:2555:U:C6	2.44	0.52
6:A:384:U:H2'	6:A:385:C:C6	2.45	0.52
16:K:87:LYS:HB2	16:K:113:VAL:HG23	1.92	0.52
28:a:1094:C:H2'	28:a:1095:U:C6	2.45	0.52
28:a:1424:C:H2'	28:a:1425:U:C6	2.44	0.52
28:a:2302:G:H2'	28:a:2303:U:C6	2.44	0.52
39:l:79:LEU:HD12	39:l:80:GLU:N	2.25	0.52
6:A:198:G:H2'	6:A:199:A:C8	2.45	0.52
11:F:47:LEU:HD13	11:F:51:ILE:HD12	1.91	0.52
15:J:10:LEU:HD13	15:J:22:THR:HG22	1.91	0.52
28:a:1980:U:H4'	31:d:133:THR:OG1	2.09	0.52
28:a:2088:A:H4'	28:a:2088:A:OP1	2.09	0.52
28:a:2091:C:H2'	28:a:2092:U:C6	2.45	0.52
46:s:17:GLU:CD	46:s:17:GLU:H	2.17	0.52
6:A:1028:G:H2'	6:A:1029:A:C8	2.44	0.51
9:D:17:THR:HG22	9:D:18:ASP:H	1.73	0.51
14:I:19:VAL:HA	14:I:65:VAL:HG12	1.91	0.51
44:q:51:LEU:H	44:q:51:LEU:HD22	1.76	0.51
47:t:9:GLU:OE1	47:t:21:ARG:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2481:G:H4'	39:l:80:GLU:HG2	1.91	0.51
34:g:35:LEU:HB3	34:g:75:MET:HE1	1.92	0.51
6:A:1120:U:O4	15:J:73:VAL:HG21	2.11	0.51
33:f:80:ARG:HG3	33:f:83:TRP:CH2	2.45	0.51
39:l:58:VAL:HG11	39:l:106:ILE:HD11	1.91	0.51
50:w:37:ARG:HG2	50:w:48:ARG:HB2	1.91	0.51
1:0:36:ASP:HB3	1:0:39:VAL:HG22	1.93	0.51
6:A:484:A:H2'	6:A:485:A:H8	1.76	0.51
28:a:1527:G:H2'	28:a:1528:A:C8	2.45	0.51
34:g:84:GLU:HA	34:g:133:ILE:O	2.11	0.51
11:F:6:ILE:HG12	11:F:89:VAL:HG22	1.93	0.51
28:a:2026:U:H2'	28:a:2027:G:C8	2.45	0.51
28:a:2846:G:H2'	28:a:2847:A:C8	2.46	0.51
29:b:48:U:H4'	41:n:99:HIS:HD2	1.75	0.51
32:e:167:ASP:HB2	32:e:182:TYR:CZ	2.45	0.51
28:a:1482:A:H2'	28:a:1483:A:C8	2.46	0.51
28:a:1783:U:H2'	28:a:1784:C:H6	1.73	0.51
34:g:11:LEU:HD21	34:g:17:ILE:HD11	1.93	0.51
6:A:978:C:H2'	6:A:979:C:C6	2.45	0.51
6:A:1533:C:H2'	6:A:1534:U:C6	2.46	0.51
9:D:172:GLU:OE2	9:D:183:LYS:HD3	2.11	0.51
15:J:83:THR:O	15:J:87:LEU:HB2	2.11	0.51
28:a:584:U:H2'	28:a:585:C:C6	2.45	0.51
28:a:1574:U:H4'	28:a:1575:C:O5'	2.10	0.51
28:a:2097:G:H5'	28:a:2105:U:N3	2.20	0.51
6:A:532:A:H5''	17:L:111:LYS:HB2	1.93	0.51
6:A:1030:A:H2'	6:A:1031:C:O4'	2.11	0.51
6:A:1188:U:H2'	6:A:1189:C:C6	2.46	0.51
6:A:1435:A:O2'	6:A:1436:G:C8	2.62	0.51
7:B:105:LYS:HG2	7:B:106:THR:N	2.24	0.51
14:I:85:ARG:O	14:I:88:ILE:HG13	2.10	0.51
21:P:72:ALA:O	21:P:76:LYS:HG3	2.11	0.51
28:a:1721:C:H2'	28:a:1722:C:H6	1.75	0.51
28:a:2012:C:H2'	28:a:2013:U:C6	2.46	0.51
28:a:2149:A:H4'	28:a:2160:A:H5'	1.93	0.51
41:n:28:CYS:HA	41:n:92:ASP:HB3	1.93	0.51
43:p:49:ASP:HA	43:p:52:GLN:HB2	1.93	0.51
6:A:19:A:H5''	10:E:92:ALA:HB3	1.93	0.51
6:A:149:U:H2'	6:A:150:C:C6	2.46	0.51
6:A:1160:G:H3'	6:A:1162:C:H42	1.75	0.51
6:A:1528:A:H2'	6:A:1529:C:H6	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2085:U:H2'	28:a:2086:U:O4'	2.11	0.51
37:j:13:ASN:ND2	37:j:97:ARG:HB2	2.26	0.51
6:A:1534:U:H3	26:W:6:G:H1	0.81	0.51
12:G:58:PRO:HA	12:G:61:THR:HG22	1.92	0.51
28:a:82:G:O2'	28:a:83:G:H5'	2.11	0.51
28:a:649:G:H4'	32:e:94:LYS:HG2	1.92	0.51
28:a:1050:U:H5''	28:a:1051:U:H5'	1.92	0.51
28:a:1060:A:C6	28:a:1087:U:H4'	2.46	0.51
28:a:1834:A:O2'	28:a:1835:A:H8	1.74	0.51
28:a:2057:A:H2'	28:a:2058:A:C8	2.46	0.51
28:a:2534:A:H2'	28:a:2535:U:C6	2.46	0.51
6:A:216:U:H2'	6:A:217:A:C8	2.46	0.50
27:X:3:VAL:HG22	27:X:37:VAL:HG12	1.92	0.50
28:a:2138:C:H2'	28:a:2139:G:H8	1.76	0.50
6:A:574:C:H2'	6:A:575:G:O4'	2.10	0.50
28:a:1519:G:O6	28:a:1529:U:O4	2.30	0.50
28:a:2624:U:H2'	28:a:2625:G:O4'	2.10	0.50
28:a:2790:C:H2'	28:a:2791:C:C6	2.47	0.50
40:m:33:LEU:HD13	40:m:114:GLU:HB3	1.92	0.50
6:A:401:U:O2'	9:D:113:GLU:HG3	2.11	0.50
6:A:533:A:H2'	6:A:534:G:C8	2.47	0.50
6:A:835:C:H2'	6:A:836:U:C2	2.46	0.50
7:B:120:GLN:HA	7:B:124:GLY:HA3	1.93	0.50
10:E:112:MET:HE2	10:E:128:CYS:HB3	1.93	0.50
28:a:1058:G:H2'	28:a:1059:A:O4'	2.11	0.50
34:g:11:LEU:HD21	34:g:17:ILE:CD1	2.41	0.50
37:j:58:MET:SD	37:j:86:LEU:HD13	2.50	0.50
38:k:88:ASP:H	38:k:118:ARG:HH12	1.58	0.50
6:A:671:U:H3	6:A:707:G:H22	1.59	0.50
6:A:1494:A:H5''	6:A:1502:G:H5'	1.92	0.50
28:a:1392:U:H2'	28:a:1393:U:C6	2.46	0.50
28:a:1627:A:H2'	28:a:1628:C:C6	2.46	0.50
37:j:17:ARG:HB2	37:j:45:GLU:HB3	1.94	0.50
6:A:56:U:H2'	6:A:57:G:C8	2.46	0.50
6:A:471:U:H2'	6:A:472:U:C6	2.47	0.50
6:A:1245:A:H2'	6:A:1246:A:C8	2.46	0.50
9:D:54:GLN:HB3	9:D:203:LEU:HB2	1.94	0.50
28:a:2230:U:H2'	28:a:2231:U:C6	2.46	0.50
28:a:339:A:H1'	28:a:340:A:H2	1.77	0.50
28:a:586:A:H2'	28:a:587:G:C8	2.47	0.50
28:a:1450:A:H2'	28:a:1451:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:e:11:ILE:HG23	32:e:13:VAL:HG13	1.94	0.50
48:u:149:VAL:HG22	48:u:151:MET:HE3	1.94	0.50
6:A:709:A:H2'	6:A:710:A:C8	2.47	0.50
8:C:102:ASN:O	8:C:104:GLU:HG2	2.11	0.50
6:A:840:G:H2'	6:A:841:A:C8	2.47	0.50
15:J:52:LEU:HD23	15:J:62:ARG:HD2	1.92	0.50
28:a:300:U:H2'	28:a:301:G:O4'	2.12	0.50
28:a:2724:G:H2'	28:a:2725:A:C8	2.47	0.50
29:b:29:A:H2'	29:b:30:C:C6	2.46	0.50
6:A:87:C:H2'	6:A:88:U:C6	2.47	0.50
7:B:56:PHE:HA	7:B:59:ARG:HE	1.77	0.50
11:F:42:TRP:HZ2	11:F:61:LEU:HD22	1.77	0.50
14:I:17:ALA:HB2	14:I:67:VAL:HG23	1.92	0.50
28:a:45:G:H5'	28:a:46:G:OP1	2.12	0.50
28:a:1185:U:H2'	28:a:1186:U:C6	2.46	0.50
28:a:2544:G:H2'	28:a:2545:C:C6	2.47	0.50
28:a:2832:U:H5''	42:o:53:ASN:O	2.10	0.50
6:A:155:A:H2'	6:A:156:A:C8	2.46	0.49
6:A:484:A:H2'	6:A:485:A:C8	2.47	0.49
6:A:1056:U:H2'	6:A:1057:C:C6	2.47	0.49
9:D:26:ARG:HG3	9:D:31:LYS:HD2	1.94	0.49
10:E:160:LYS:HZ3	10:E:161:SER:H	1.58	0.49
19:N:6:MET:HE2	19:N:63:ARG:HH22	1.77	0.49
24:S:62:VAL:HA	24:S:66:MET:SD	2.52	0.49
28:a:729:A:H1'	28:a:730:C:H5	1.78	0.49
28:a:2315:A:H2'	28:a:2316:A:H8	1.74	0.49
28:a:2790:C:H2'	28:a:2791:C:H6	1.77	0.49
34:g:87:LEU:HB2	34:g:131:ILE:HB	1.94	0.49
6:A:553:A:H4'	6:A:554:A:H3'	1.94	0.49
28:a:2024:A:H2'	28:a:2025:G:C8	2.47	0.49
40:m:45:ARG:HD3	40:m:97:ILE:HD11	1.94	0.49
28:a:2:G:H2'	28:a:3:U:C6	2.47	0.49
28:a:598:A:H2'	28:a:599:A:C8	2.48	0.49
28:a:1525:U:H2'	28:a:1526:A:O4'	2.12	0.49
28:a:2084:U:H2'	28:a:2085:U:C6	2.47	0.49
28:a:2145:A:H1'	28:a:2146:G:C8	2.47	0.49
30:c:119:GLY:HA2	30:c:189:ARG:HH12	1.77	0.49
6:A:317:U:H2'	6:A:318:G:O4'	2.12	0.49
6:A:470:G:H2'	6:A:471:U:C6	2.47	0.49
6:A:1042:G:H1'	6:A:1209:G:H5''	1.94	0.49
7:B:35:ARG:HG3	7:B:40:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:38:ARG:HH22	23:R:24:LYS:HZ3	1.59	0.49
28:a:803:U:H2'	28:a:804:C:C6	2.48	0.49
30:c:167:ARG:HG3	30:c:172:VAL:HG22	1.95	0.49
31:d:30:VAL:O	31:d:185:ASN:HB3	2.13	0.49
6:A:230:A:H5''	22:Q:47:LEU:HD21	1.94	0.49
6:A:491:U:H2'	6:A:492:A:C8	2.47	0.49
6:A:532:A:H2'	6:A:533:A:H8	1.77	0.49
6:A:1232:A:H5'	6:A:1330:C:H41	1.77	0.49
7:B:136:MET:HE3	7:B:137:ARG:HG3	1.95	0.49
28:a:853:G:H2'	28:a:854:C:C6	2.48	0.49
28:a:2140:C:H2'	28:a:2141:G:C8	2.47	0.49
28:a:2788:U:H2'	28:a:2789:U:H6	1.77	0.49
32:e:142:LEU:HD13	32:e:145:VAL:HG21	1.93	0.49
34:g:27:LYS:HG2	34:g:32:ALA:HB2	1.93	0.49
37:j:56:GLN:NE2	37:j:58:MET:HE3	2.28	0.49
45:r:83:LYS:HD3	45:r:97:VAL:HG12	1.95	0.49
48:u:175:GLN:HG3	48:u:182:LEU:HD11	1.95	0.49
5:4:24:THR:HA	33:f:3:ARG:HH22	1.77	0.49
7:B:104:TYR:O	7:B:108:ARG:HG3	2.13	0.49
9:D:15:GLU:HB2	9:D:19:LEU:HD11	1.95	0.49
10:E:158:ARG:HG3	10:E:162:VAL:HG23	1.94	0.49
28:a:1870:U:H2'	28:a:1871:G:O4'	2.12	0.49
28:a:2258:G:OP1	49:v:18:SER:HB3	2.13	0.49
6:A:273:A:H5''	6:A:275:G:O4'	2.12	0.49
6:A:293:G:H2'	6:A:294:A:C8	2.47	0.49
6:A:1299:G:N2	6:A:1325:G:H2'	2.20	0.49
28:a:71:A:OP2	28:a:113:C:H5'	2.13	0.49
28:a:535:C:H2'	28:a:536:U:H5''	1.93	0.49
28:a:2130:C:H2'	28:a:2131:G:O4'	2.13	0.49
39:l:54:LEU:HD11	39:l:118:PHE:HE1	1.78	0.49
44:q:19:PHE:CZ	44:q:97:LYS:HG3	2.48	0.49
46:s:54:VAL:HG21	46:s:84:ILE:HG23	1.95	0.49
6:A:1210:G:H5'	19:N:5:SER:CB	2.43	0.49
9:D:57:GLU:HG2	9:D:199:LEU:HB2	1.95	0.49
28:a:1103:U:H2'	28:a:1104:C:C6	2.48	0.49
28:a:1276:C:H2'	28:a:1277:A:C8	2.48	0.49
28:a:2149:A:H5''	28:a:2159:U:O2'	2.12	0.49
28:a:2834:U:H2'	28:a:2835:G:O4'	2.12	0.49
41:n:2:SER:O	41:n:6:GLU:HB2	2.13	0.49
48:u:8:ALA:HB3	48:u:68:VAL:HG22	1.95	0.49
5:4:56:ARG:HD2	5:4:60:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:19:VAL:HG22	14:I:65:VAL:CG1	2.42	0.49
14:I:57:THR:HG23	14:I:60:LYS:HD3	1.95	0.49
18:M:13:LYS:HB3	18:M:18:SER:OG	2.12	0.49
28:a:1184:G:H2'	28:a:1185:U:C6	2.46	0.49
28:a:2637:U:H2'	28:a:2638:C:H6	1.78	0.49
41:n:55:LEU:HA	41:n:60:ARG:HD2	1.94	0.49
43:p:27:ALA:HB1	43:p:31:VAL:HG22	1.94	0.49
48:u:119:GLY:HA3	48:u:187:ILE:HG21	1.95	0.49
51:x:13:GLN:O	51:x:16:GLU:HG3	2.13	0.49
6:A:1048:C:O2'	27:X:45:LYS:HE3	2.13	0.48
8:C:58:HIS:HB3	15:J:94:ALA:HB2	1.95	0.48
28:a:2128:G:N2	28:a:2137:U:O2	2.39	0.48
40:m:87:TYR:OH	40:m:115:LEU:HB3	2.11	0.48
6:A:1115:U:H2'	6:A:1116:U:C6	2.49	0.48
15:J:56:HIS:CD2	15:J:57:VAL:HG22	2.47	0.48
15:J:89:LYS:H	15:J:89:LYS:HD2	1.77	0.48
28:a:700:U:H2'	28:a:701:A:C8	2.48	0.48
28:a:744:G:H2'	28:a:745:U:C6	2.48	0.48
28:a:2084:U:H2'	28:a:2085:U:H6	1.78	0.48
41:n:67:ILE:O	41:n:71:LYS:HG3	2.13	0.48
28:a:273:A:H2'	28:a:274:G:O4'	2.12	0.48
28:a:750:G:H2'	28:a:751:A:O4'	2.14	0.48
28:a:1843:U:H2'	28:a:1844:G:O4'	2.13	0.48
28:a:2061:U:H2'	28:a:2062:U:C6	2.48	0.48
4:3:36:ARG:O	4:3:37:GLN:HB2	2.13	0.48
6:A:446:A:H4'	21:P:73:GLN:NE2	2.28	0.48
6:A:1065:C:H2'	6:A:1066:G:H8	1.78	0.48
7:B:85:ALA:C	7:B:87:CYS:N	2.72	0.48
28:a:1163:U:H1'	28:a:1164:A:H5''	1.95	0.48
28:a:2688:C:H3'	28:a:2689:G:H5''	1.96	0.48
28:a:2873:G:H2'	28:a:2874:C:H6	1.77	0.48
44:q:74:ILE:HB	44:q:87:GLN:HB3	1.94	0.48
6:A:757:G:H2'	6:A:758:C:C6	2.48	0.48
10:E:151:PRO:C	10:E:153:ALA:H	2.21	0.48
28:a:85:G:OP2	47:t:6:ARG:HB2	2.14	0.48
28:a:2092:U:H2'	28:a:2093:G:H8	1.76	0.48
28:a:2314:A:H2'	28:a:2315:A:C8	2.48	0.48
30:c:144:ILE:HB	30:c:154:ILE:HB	1.95	0.48
32:e:96:ASN:HB2	32:e:99:MET:HG3	1.96	0.48
43:p:82:GLY:HA2	43:p:118:ALA:HB3	1.95	0.48
44:q:1:MET:SD	44:q:43:ASN:HB3	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:x:44:SER:O	51:x:48:ARG:HG2	2.14	0.48
6:A:107:G:H1'	6:A:348:G:H5'	1.96	0.48
6:A:656:U:H2'	6:A:657:A:C8	2.48	0.48
10:E:39:VAL:HG11	10:E:115:VAL:HG22	1.96	0.48
17:L:107:VAL:HG13	17:L:117:TYR:HB3	1.94	0.48
28:a:1529:U:H2'	28:a:1530:G:C8	2.49	0.48
6:A:198:G:H2'	6:A:199:A:H8	1.78	0.48
10:E:73:ILE:HD13	10:E:142:PHE:CE2	2.48	0.48
28:a:1017:A:C2	28:a:2475:G:H5'	2.48	0.48
28:a:2287:A:H2'	28:a:2288:C:H6	1.78	0.48
28:a:2674:U:H2'	28:a:2675:G:O4'	2.14	0.48
29:b:66:A:H61	29:b:107:U:H2'	1.79	0.48
39:l:47:ILE:HD12	39:l:70:PRO:HG3	1.96	0.48
6:A:496:A:H2'	6:A:497:C:O4'	2.13	0.48
6:A:961:5MC:H2'	6:A:962:A:C2	2.48	0.48
6:A:1181:G:H5'	14:I:115:LYS:NZ	2.28	0.48
7:B:6:MET:HE2	7:B:47:LEU:HD22	1.95	0.48
7:B:27:MET:HB3	7:B:193:PRO:HG3	1.96	0.48
10:E:160:LYS:C	10:E:162:VAL:H	2.22	0.48
28:a:1626:U:H2'	28:a:1627:A:C8	2.49	0.48
28:a:1720:U:HO2'	28:a:1721:C:H6	1.60	0.48
30:c:246:VAL:HG12	30:c:247:SER:O	2.13	0.48
11:F:10:VAL:HG13	11:F:83:ALA:HB1	1.95	0.48
28:a:2129:A:H2'	28:a:2130:C:C6	2.49	0.48
28:a:2360:A:H2'	28:a:2361:C:C6	2.48	0.48
38:k:91:SER:HB3	38:k:123:LYS:HE3	1.96	0.48
42:o:52:ARG:O	42:o:58:SER:HA	2.13	0.48
10:E:112:MET:HG2	10:E:141:THR:OG1	2.14	0.48
24:S:50:ALA:HB1	24:S:57:HIS:HB3	1.95	0.48
28:a:1529:U:H2'	28:a:1530:G:H8	1.79	0.48
28:a:2138:C:H2'	28:a:2139:G:C8	2.49	0.48
30:c:118:SER:HA	30:c:129:SER:O	2.14	0.48
33:f:132:VAL:HG11	33:f:137:ILE:HG21	1.95	0.48
34:g:117:LEU:HD21	34:g:123:ALA:HB2	1.96	0.48
45:r:1:MET:HG2	45:r:109:ASP:HB3	1.95	0.48
5:4:49:LYS:HD3	18:M:61:ALA:HB1	1.95	0.47
6:A:740:G:H2'	6:A:741:A:C8	2.49	0.47
6:A:1151:A:C2	6:A:1175:G:C4	3.02	0.47
34:g:19:LEU:HG	34:g:24:LEU:HD13	1.96	0.47
6:A:944:U:H2'	6:A:945:G:C8	2.49	0.47
8:C:122:GLN:O	8:C:126:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:87:GLY:HA3	9:D:197:GLU:HG3	1.96	0.47
15:J:29:ALA:HA	15:J:32:THR:HG22	1.96	0.47
28:a:247:G:H4'	28:a:377:G:C5	2.49	0.47
32:e:82:THR:HB	32:e:85:ALA:HB2	1.95	0.47
40:m:55:ALA:HA	40:m:80:PHE:CE1	2.49	0.47
6:A:486:C:H2'	6:A:487:A:C8	2.50	0.47
6:A:1117:A:H4'	15:J:38:GLY:HA3	1.95	0.47
28:a:559:U:H5''	28:a:811:A:C2	2.48	0.47
28:a:580:A:H2'	28:a:581:U:C6	2.49	0.47
28:a:2862:C:H4'	42:o:3:ASN:HB3	1.95	0.47
14:I:119:ARG:HB2	14:I:123:LYS:HD3	1.97	0.47
28:a:570:U:H2'	28:a:571:C:C6	2.50	0.47
28:a:2172:U:H2'	28:a:2173:G:C8	2.50	0.47
28:a:2228:A:H2'	28:a:2229:G:C8	2.50	0.47
28:a:2664:G:H2'	28:a:2665:A:C8	2.50	0.47
12:G:111:ARG:HB2	12:G:119:ARG:HB3	1.96	0.47
28:a:31:C:O3'	28:a:1225:G:H5''	2.14	0.47
28:a:231:A:H2'	28:a:232:G:O4'	2.14	0.47
28:a:950:A:H2'	28:a:952:G:H5'	1.96	0.47
28:a:1055:U:H2'	28:a:1056:U:O4'	2.15	0.47
6:A:56:U:H2'	6:A:57:G:H8	1.78	0.47
6:A:183:A:H4'	6:A:184:G:O5'	2.15	0.47
6:A:453:U:H2'	6:A:454:A:H8	1.79	0.47
6:A:1266:U:H5'	19:N:34:PRO:HG3	1.95	0.47
15:J:49:PHE:HE2	15:J:67:ILE:HG13	1.80	0.47
25:T:24:LEU:O	25:T:28:VAL:HG23	2.14	0.47
28:a:529:A:H4'	36:i:7:LYS:HG2	1.96	0.47
28:a:571:C:H2'	28:a:572:A:H8	1.78	0.47
28:a:1416:G:H2'	28:a:1417:G:H8	1.79	0.47
28:a:2578:C:H2'	28:a:2579:G:H8	1.78	0.47
34:g:91:GLY:HA2	34:g:160:LYS:HD2	1.96	0.47
39:l:79:LEU:HD12	39:l:80:GLU:H	1.78	0.47
5:4:12:ILE:O	5:4:31:PRO:HA	2.15	0.47
5:4:61:LYS:HG2	24:S:42:PRO:CG	2.45	0.47
6:A:32:A:H2'	6:A:33:A:C8	2.50	0.47
6:A:41:G:H2'	6:A:42:G:H8	1.79	0.47
6:A:75:G:H1	6:A:88:U:H3	0.73	0.47
6:A:518:G:H2'	6:A:519:C:C6	2.50	0.47
6:A:747:A:H4'	6:A:748:C:O5'	2.15	0.47
6:A:1112:U:H2'	6:A:1113:C:H6	1.80	0.47
6:A:1317:G:H2'	6:A:1318:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1322:C:H5'	18:M:28:THR:OG1	2.14	0.47
7:B:118:GLU:HA	7:B:141:LEU:HD21	1.96	0.47
7:B:142:GLU:O	7:B:146:ARG:HG2	2.15	0.47
7:B:162:PHE:HD1	7:B:184:ILE:HB	1.80	0.47
11:F:69:LYS:HB2	11:F:69:LYS:HE2	1.66	0.47
16:K:14:LYS:HE2	16:K:77:TYR:HE1	1.79	0.47
24:S:13:LEU:O	24:S:17:LYS:HG2	2.15	0.47
28:a:823:A:H2'	28:a:824:G:C8	2.49	0.47
28:a:1084:U:H1'	28:a:1087:U:C5	2.50	0.47
28:a:1426:A:H2'	28:a:1427:G:O4'	2.14	0.47
28:a:1856:G:N2	28:a:1858:A:H3'	2.30	0.47
29:b:51:G:H2'	29:b:52:A:C8	2.49	0.47
43:p:74:LEU:HD22	43:p:78:ARG:HB2	1.97	0.47
9:D:159:LEU:HD23	9:D:159:LEU:HA	1.76	0.47
28:a:184:C:H2'	28:a:185:A:C8	2.50	0.47
28:a:470:A:H1'	28:a:471:A:H5''	1.96	0.47
28:a:991:A:H2'	28:a:992:G:O4'	2.15	0.47
28:a:2220:U:H2'	28:a:2221:G:C8	2.49	0.47
6:A:506:U:H2'	6:A:507:U:C6	2.50	0.47
6:A:607:C:H2'	6:A:608:C:C6	2.49	0.47
6:A:1073:G:H5'	10:E:51:ARG:CZ	2.45	0.47
6:A:1090:C:H2'	6:A:1091:C:H6	1.79	0.47
28:a:774:G:H5'	28:a:775:G:OP1	2.14	0.47
28:a:2123:G:H2'	28:a:2124:C:H6	1.75	0.47
28:a:2182:U:H2'	28:a:2183:C:H6	1.80	0.47
39:l:76:LYS:HB2	39:l:91:GLU:HG3	1.96	0.47
5:4:25:ARG:HB2	33:f:98:GLU:OE1	2.14	0.47
6:A:739:U:H5'	6:A:829:G:N2	2.29	0.47
6:A:1322:C:OP1	18:M:28:THR:HG21	2.15	0.47
6:A:1529:C:H2'	6:A:1530:C:C6	2.50	0.47
14:I:129:LYS:HG3	27:X:60:GLU:OE2	2.15	0.47
15:J:18:ILE:HG23	15:J:72:ARG:HG3	1.97	0.47
22:Q:27:LEU:HD11	22:Q:44:SER:HB2	1.97	0.47
28:a:87:C:H5''	28:a:88:G:H5'	1.96	0.47
28:a:151:C:H2'	28:a:152:U:C6	2.50	0.47
28:a:1344:C:H2'	28:a:1345:G:O4'	2.14	0.47
28:a:2442:G:H2'	28:a:2443:C:C6	2.50	0.47
36:i:13:ARG:HG2	36:i:51:GLY:O	2.15	0.47
46:s:66:THR:HB	46:s:73:LEU:HD22	1.97	0.47
6:A:376:A:H2'	6:A:377:A:C8	2.50	0.46
6:A:468:C:H2'	6:A:469:U:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:598:G:H2'	6:A:599:U:O4'	2.14	0.46
6:A:1119:U:O2'	6:A:1120:U:H2'	2.15	0.46
10:E:24:LYS:HB2	10:E:24:LYS:HE2	1.72	0.46
28:a:1845:A:H2'	28:a:1846:U:O4'	2.15	0.46
28:a:1867:U:H2'	28:a:1868:C:C6	2.50	0.46
28:a:2182:U:H2'	28:a:2183:C:C6	2.50	0.46
28:a:2619:A:H2'	28:a:2620:G:C8	2.50	0.46
32:e:133:LEU:CD2	32:e:160:ALA:HB2	2.44	0.46
37:j:60:ALA:HB1	37:j:84:ALA:HB1	1.97	0.46
1:0:9:SER:HB3	1:0:45:TYR:CZ	2.50	0.46
5:4:32:ILE:HG13	5:4:33:HIS:N	2.30	0.46
7:B:171:ILE:O	7:B:175:GLU:HG3	2.16	0.46
20:O:82:ILE:HD12	20:O:87:LEU:HB2	1.97	0.46
28:a:151:C:H2'	28:a:152:U:H6	1.80	0.46
28:a:2366:G:H2'	28:a:2367:U:C6	2.50	0.46
40:m:55:ALA:HB2	40:m:79:LEU:HB3	1.98	0.46
42:o:101:LEU:HD23	42:o:104:LEU:HD12	1.97	0.46
9:D:58:LYS:HE2	9:D:58:LYS:HB3	1.84	0.46
11:F:26:THR:HG23	11:F:36:ILE:HD13	1.97	0.46
28:a:1018:A:H2'	28:a:1019:A:H8	1.77	0.46
28:a:1357:C:H2'	28:a:1358:G:O4'	2.16	0.46
31:d:32:PRO:HB3	31:d:97:THR:HG22	1.97	0.46
41:n:36:ILE:HG12	41:n:105:LEU:HD12	1.97	0.46
6:A:79:G:H2'	6:A:80:C:C6	2.51	0.46
6:A:561:G:H2'	6:A:562:G:O4'	2.16	0.46
6:A:751:U:H2'	6:A:752:G:O4'	2.16	0.46
9:D:104:ARG:HG3	9:D:168:VAL:HG11	1.97	0.46
10:E:35:THR:HG22	10:E:53:LYS:HG3	1.97	0.46
13:H:76:LYS:HB2	13:H:76:LYS:HE2	1.73	0.46
28:a:881:A:H1'	28:a:883:U:OP2	2.15	0.46
28:a:1071:U:H2'	28:a:1072:U:C6	2.51	0.46
28:a:1642:A:H2'	28:a:1643:G:O4'	2.16	0.46
30:c:140:THR:HG23	30:c:161:SER:HB2	1.96	0.46
6:A:914:U:H2'	6:A:915:U:C6	2.50	0.46
11:F:77:ASN:O	11:F:81:ASN:HB2	2.16	0.46
12:G:26:PHE:HE2	12:G:120:LEU:HD21	1.80	0.46
13:H:79:SER:HB2	13:H:85:GLN:HB2	1.97	0.46
28:a:19:A:H5''	43:p:22:LYS:HG2	1.97	0.46
28:a:1861:C:H2'	28:a:1862:G:O4'	2.16	0.46
28:a:2094:C:H2'	28:a:2095:U:C6	2.51	0.46
28:a:2100:U:H2'	28:a:2101:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2102:G:O2'	28:a:2154:U:H1'	2.15	0.46
28:a:2791:C:H2'	28:a:2792:C:H6	1.81	0.46
36:i:64:VAL:HB	36:i:68:LYS:HE3	1.97	0.46
40:m:103:ARG:HG3	40:m:110:MET:SD	2.55	0.46
47:t:84:PHE:CE1	47:t:93:ARG:HG2	2.51	0.46
6:A:862:C:H2'	6:A:863:G:O4'	2.16	0.46
6:A:939:G:C2	6:A:940:A:C8	3.04	0.46
15:J:52:LEU:HB2	19:N:81:ARG:HD2	1.98	0.46
18:M:81:MET:HE3	18:M:91:HIS:HB3	1.97	0.46
28:a:226:A:H5'	28:a:257:C:O2'	2.15	0.46
28:a:840:U:H2'	28:a:841:C:C6	2.51	0.46
28:a:2097:G:C2	28:a:2167:U:C2	3.04	0.46
38:k:132:ARG:HG3	38:k:142:PHE:CE1	2.51	0.46
1:0:1:MET:HG3	1:0:2:ARG:N	2.31	0.46
1:0:21:LYS:HE3	1:0:21:LYS:HB2	1.61	0.46
5:4:34:LEU:HD13	33:f:106:ILE:HG23	1.96	0.46
6:A:216:U:H2'	6:A:217:A:H8	1.80	0.46
9:D:33:LYS:O	9:D:33:LYS:HG3	2.15	0.46
17:L:44:LYS:HD2	17:L:44:LYS:HA	1.72	0.46
28:a:1567:C:H2'	28:a:1568:U:O4'	2.15	0.46
28:a:2783:C:H4'	28:a:2784:U:OP1	2.16	0.46
31:d:151:THR:HG22	31:d:152:PRO:CD	2.46	0.46
31:d:186:LEU:HD13	42:o:9:ILE:HD11	1.97	0.46
36:i:98:GLU:CD	36:i:98:GLU:H	2.23	0.46
39:l:60:ARG:HB3	48:u:192:VAL:HG12	1.97	0.46
6:A:652:A:H1'	20:O:22:THR:HG21	1.97	0.46
6:A:672:U:H2'	6:A:673:U:H6	1.80	0.46
6:A:708:G:H2'	6:A:709:A:C8	2.51	0.46
6:A:916:G:H2'	6:A:917:A:C8	2.51	0.46
6:A:1101:C:C4	6:A:1102:G:C8	3.03	0.46
12:G:78:ARG:HE	12:G:78:ARG:HB2	1.58	0.46
14:I:113:ARG:HG3	14:I:115:LYS:HZ3	1.80	0.46
21:P:44:THR:H	21:P:47:GLU:HB2	1.81	0.46
28:a:623:A:H5'	38:k:70:LYS:HD3	1.98	0.46
28:a:786:U:OP1	32:e:56:LYS:HE2	2.16	0.46
28:a:963:A:H5'	28:a:1175:U:H1'	1.97	0.46
28:a:1518:C:H2'	28:a:1519:G:H8	1.78	0.46
32:e:163:LEU:HD23	32:e:163:LEU:HA	1.70	0.46
33:f:73:SER:O	33:f:79:ILE:HG13	2.15	0.46
6:A:902:A:H2'	6:A:903:A:C8	2.51	0.46
6:A:1090:C:H2'	6:A:1091:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1320:U:O2'	6:A:1321:G:H5'	2.16	0.46
6:A:1349:G:H2'	6:A:1350:A:C8	2.51	0.46
8:C:56:ASP:HB2	8:C:67:THR:OG1	2.16	0.46
10:E:116:LEU:HD22	10:E:124:VAL:HG21	1.97	0.46
28:a:388:U:H5''	50:w:32:ASN:HB2	1.98	0.46
32:e:6:ASN:HB3	32:e:120:VAL:HG12	1.98	0.46
8:C:22:TRP:HA	15:J:94:ALA:O	2.16	0.46
15:J:88:MET:HE2	15:J:88:MET:HA	1.97	0.46
28:a:1048:G:N1	28:a:1071:U:C2	2.84	0.46
28:a:1277:A:H2'	28:a:1278:C:C6	2.51	0.46
28:a:1781:A:H2'	28:a:1782:C:H6	1.81	0.46
28:a:1866:C:H2'	28:a:1867:U:O4'	2.17	0.46
28:a:2114:G:O5'	28:a:2114:G:H8	2.00	0.46
6:A:1032:U:H2'	6:A:1033:C:C6	2.51	0.45
8:C:114:MET:HE1	8:C:187:TYR:HD2	1.82	0.45
18:M:59:GLU:HA	18:M:62:LYS:HE2	1.98	0.45
28:a:1056:U:H2'	28:a:1058:G:N7	2.31	0.45
28:a:2791:C:H2'	28:a:2792:C:C6	2.50	0.45
34:g:6:LYS:HA	34:g:6:LYS:HD3	1.72	0.45
39:l:76:LYS:HB2	39:l:76:LYS:HE2	1.69	0.45
53:z:52:LYS:HE2	53:z:55:ASP:HA	1.98	0.45
5:4:56:ARG:HD3	5:4:59:ARG:HG2	1.98	0.45
6:A:196:G:H21	6:A:460:A:H61	1.65	0.45
6:A:773:C:H2'	6:A:774:A:O4'	2.16	0.45
6:A:1248:G:O4'	6:A:1350:A:H5''	2.17	0.45
28:a:52:A:H2'	28:a:53:A:C8	2.51	0.45
28:a:1530:G:C6	28:a:1531:A:C5	3.05	0.45
33:f:128:TYR:CE2	33:f:130:MET:HB3	2.50	0.45
39:l:112:GLU:O	39:l:116:GLU:HG2	2.17	0.45
6:A:452:G:H2'	6:A:453:U:C6	2.51	0.45
6:A:1498:G:H4'	6:A:1499:G:C4	2.52	0.45
21:P:56:ARG:HD2	21:P:56:ARG:HA	1.65	0.45
28:a:1250:U:C4	28:a:1251:G:C6	3.05	0.45
28:a:1540:U:H2'	28:a:1541:U:C6	2.52	0.45
28:a:1684:C:H4'	28:a:1685:G:O5'	2.16	0.45
6:A:73:A:H8	6:A:90:G:N2	2.12	0.45
6:A:944:U:H2'	6:A:945:G:H8	1.80	0.45
6:A:1310:G:N2	6:A:1312:A:H3'	2.30	0.45
7:B:77:GLY:O	7:B:81:ARG:HG3	2.16	0.45
12:G:4:ARG:NH1	12:G:4:ARG:HA	2.32	0.45
28:a:572:A:H2'	28:a:573:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1541:U:H2'	28:a:1542:G:O4'	2.17	0.45
28:a:2351:C:H2'	28:a:2352:G:O4'	2.16	0.45
38:k:110:VAL:HG21	38:k:122:LEU:HD21	1.99	0.45
6:A:483:C:H2'	6:A:484:A:C8	2.51	0.45
6:A:1142:U:H2'	6:A:1143:C:O4'	2.15	0.45
28:a:150:U:H2'	28:a:151:C:C6	2.50	0.45
28:a:1434:U:H2'	28:a:1435:U:C6	2.52	0.45
28:a:1702:C:H2'	28:a:1703:U:O4'	2.17	0.45
28:a:2001:A:H2'	28:a:2002:A:C8	2.52	0.45
28:a:2107:G:H2'	28:a:2108:G:C8	2.51	0.45
34:g:81:GLN:H	34:g:81:GLN:HG2	1.70	0.45
41:n:42:ALA:HA	41:n:49:LEU:HD11	1.98	0.45
6:A:483:C:H2'	6:A:484:A:H8	1.80	0.45
6:A:1143:C:H2'	6:A:1144:U:C6	2.52	0.45
7:B:167:ASP:HB2	7:B:191:SER:OG	2.16	0.45
8:C:9:GLY:HA3	19:N:89:MET:CE	2.46	0.45
8:C:38:LYS:HD2	8:C:38:LYS:HA	1.56	0.45
28:a:840:U:H5''	52:y:49:LYS:HE3	1.99	0.45
28:a:938:C:H1'	28:a:974:A:C8	2.52	0.45
28:a:969:A:H2'	28:a:972:C:H42	1.80	0.45
28:a:2137:U:H2'	28:a:2138:C:C6	2.51	0.45
28:a:2417:A:H2'	28:a:2417:A:N3	2.31	0.45
28:a:2832:U:H2'	28:a:2833:G:C8	2.51	0.45
40:m:112:TYR:CZ	53:z:54:VAL:HG21	2.51	0.45
6:A:20:U:H2'	6:A:21:G:O4'	2.17	0.45
6:A:96:G:H2'	6:A:97:C:H6	1.82	0.45
6:A:1066:G:H2'	6:A:1067:U:C6	2.52	0.45
8:C:77:ILE:HA	8:C:84:VAL:HG23	1.99	0.45
28:a:1140:A:H2'	28:a:1141:C:C6	2.50	0.45
28:a:1795:A:H3'	28:a:1796:A:C8	2.52	0.45
28:a:2304:C:H2'	28:a:2305:G:O4'	2.16	0.45
29:b:78:A:H2'	29:b:79:G:O4'	2.17	0.45
42:o:113:GLU:HG2	42:o:115:LEU:HD23	1.98	0.45
6:A:192:G:H2'	6:A:193:U:C6	2.52	0.45
6:A:507:U:H2'	6:A:508:C:C6	2.52	0.45
6:A:858:A:H2'	6:A:859:A:C8	2.51	0.45
6:A:859:A:H2'	6:A:860:C:C6	2.52	0.45
6:A:1271:C:H2'	6:A:1272:U:H5''	1.98	0.45
6:A:1436:G:H2'	6:A:1437:U:H6	1.79	0.45
19:N:53:ARG:HH21	24:S:37:ARG:NH2	2.15	0.45
28:a:272:A:H2'	28:a:273:A:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:351:A:H2'	28:a:352:A:C8	2.52	0.45
28:a:693:U:H2'	28:a:694:G:O4'	2.16	0.45
28:a:1144:C:H2'	28:a:1145:G:O4'	2.16	0.45
28:a:2807:A:N3	28:a:2807:A:H2'	2.31	0.45
33:f:20:LEU:HD11	33:f:168:ALA:HB3	1.99	0.45
33:f:93:SER:OG	33:f:94:ASP:N	2.49	0.45
48:u:54:LEU:HD13	48:u:80:LEU:HD21	1.98	0.45
6:A:92:U:H2'	6:A:93:U:C6	2.51	0.45
6:A:178:U:H2'	6:A:179:C:H6	1.82	0.45
6:A:741:A:H2'	6:A:742:U:C6	2.52	0.45
6:A:1316:C:P	24:S:78:ARG:HH12	2.40	0.45
8:C:93:LYS:HA	8:C:93:LYS:HD3	1.70	0.45
24:S:25:LYS:HD3	24:S:26:ASN:H	1.82	0.45
28:a:207:A:H2'	28:a:208:C:O4'	2.17	0.45
28:a:353:G:H2'	28:a:354:U:O4'	2.17	0.45
28:a:2637:U:H2'	28:a:2638:C:C6	2.52	0.45
34:g:87:LEU:HD22	34:g:162:VAL:HG12	1.98	0.45
6:A:104:C:H2'	6:A:105:G:O4'	2.17	0.45
8:C:167:TRP:HZ3	8:C:169:ARG:HG2	1.81	0.45
28:a:1128:G:H2'	28:a:1129:G:O4'	2.17	0.45
28:a:2057:A:H2'	28:a:2058:A:H8	1.82	0.45
28:a:2498:U:OP1	31:d:128:ARG:HD2	2.17	0.45
35:h:24:GLY:O	35:h:28:ASN:HB2	2.17	0.45
37:j:2:ILE:HG13	37:j:8:LEU:HD21	1.99	0.45
5:4:64:PHE:CG	24:S:5:LEU:HD13	2.53	0.44
6:A:1008:A:N3	6:A:1213:A:H1'	2.32	0.44
7:B:101:LEU:HB3	7:B:179:LEU:HD12	1.99	0.44
12:G:14:ALA:HB1	12:G:19:GLY:HA2	1.98	0.44
28:a:451:A:H2'	28:a:452:C:O4'	2.16	0.44
28:a:1477:A:H2'	30:c:98:ASP:HB3	1.99	0.44
32:e:54:GLY:HA3	32:e:73:ARG:HG2	1.99	0.44
47:t:48:ASN:HD22	47:t:50:MET:HE3	1.81	0.44
6:A:968:A:H5'	6:A:970:G:OP1	2.18	0.44
6:A:1435:A:C4	42:o:115:LEU:HD11	2.52	0.44
14:I:30:ILE:HG13	14:I:65:VAL:CG2	2.46	0.44
26:W:11:G:H2'	26:W:12:U:C6	2.52	0.44
28:a:566:U:H2'	28:a:567:G:C8	2.52	0.44
28:a:1761:C:O2	28:a:1761:C:H2'	2.18	0.44
30:c:183:LYS:HB3	30:c:183:LYS:HE2	1.63	0.44
33:f:149:LEU:HD12	33:f:149:LEU:H	1.82	0.44
43:p:94:VAL:O	43:p:98:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:u:186:ASN:HD21	48:u:188:HIS:HB3	1.81	0.44
6:A:82:U:H4'	6:A:83:G:C8	2.52	0.44
6:A:84:C:H2'	6:A:85:U:H6	1.81	0.44
6:A:815:G:H2'	6:A:816:U:C6	2.52	0.44
6:A:1137:G:H2'	6:A:1138:G:H8	1.82	0.44
6:A:1302:C:H5''	18:M:97:VAL:HG22	1.99	0.44
6:A:1308:C:H2'	6:A:1309:U:H6	1.81	0.44
14:I:28:ILE:HD12	14:I:28:ILE:HG23	1.66	0.44
18:M:77:ILE:HA	18:M:80:LEU:HD12	1.98	0.44
18:M:83:LEU:HD11	24:S:65:ASP:HB3	1.99	0.44
28:a:837:C:H2'	28:a:838:A:H8	1.83	0.44
28:a:1065:C:H2'	28:a:1066:C:C6	2.53	0.44
28:a:1163:U:O4'	28:a:1164:A:H8	2.00	0.44
28:a:1287:A:H4'	28:a:1288:A:H5''	1.99	0.44
28:a:1419:G:O2'	28:a:1420:A:H5'	2.17	0.44
28:a:2364:A:H2'	28:a:2365:A:C8	2.53	0.44
29:b:42:C:H5	33:f:90:THR:HB	1.82	0.44
52:y:5:LYS:HG2	52:y:36:GLU:OE2	2.17	0.44
6:A:508:C:H2'	6:A:509:G:H8	1.81	0.44
6:A:1396:4OC:H6	6:A:1396:4OC:O5'	2.17	0.44
7:B:49:MET:HE2	7:B:199:VAL:HB	2.00	0.44
11:F:51:ILE:O	11:F:54:VAL:HG22	2.16	0.44
15:J:87:LEU:HD13	15:J:90:LEU:HD22	2.00	0.44
28:a:405:C:H2'	28:a:406:A:C8	2.52	0.44
28:a:2100:U:H2'	28:a:2101:A:C8	2.52	0.44
30:c:271:ARG:HD3	30:c:273:LYS:NZ	2.32	0.44
36:i:39:LYS:HE2	36:i:39:LYS:HB3	1.76	0.44
5:4:51:LEU:HD23	5:4:52:ASP:H	1.82	0.44
6:A:536:G:H5'	9:D:39:GLY:HA3	1.99	0.44
6:A:1119:U:HO2'	6:A:1120:U:H2'	1.83	0.44
6:A:1280:U:H2'	6:A:1281:A:H5'	2.00	0.44
6:A:1352:U:H5''	6:A:1353:C:C5	2.53	0.44
6:A:1429:G:H2'	6:A:1430:U:C6	2.52	0.44
6:A:1463:C:H2'	6:A:1464:G:O4'	2.17	0.44
7:B:218:ALA:O	7:B:222:ILE:HG13	2.18	0.44
28:a:578:U:H2'	28:a:579:U:C6	2.52	0.44
28:a:871:G:H2'	28:a:872:G:H8	1.82	0.44
28:a:2128:G:H1	28:a:2137:U:H3	1.64	0.44
37:j:10:VAL:HG12	37:j:12:ASP:HB2	1.99	0.44
47:t:85:LYS:HE3	47:t:94:VAL:HG11	1.99	0.44
2:1:25:LYS:HB3	2:1:25:LYS:HE3	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:495:C:H2'	6:A:496:A:C8	2.52	0.44
6:A:822:A:H2'	6:A:823:G:O4'	2.17	0.44
6:A:836:U:C2	6:A:838:G:O6	2.70	0.44
8:C:73:PRO:HG3	8:C:105:GLU:HB2	1.99	0.44
28:a:634:A:H2'	28:a:636:A:C8	2.52	0.44
28:a:763:U:O2'	30:c:48:ARG:HD3	2.18	0.44
28:a:880:G:N2	28:a:882:C:H41	2.16	0.44
28:a:1061:G:H1'	28:a:1079:A:H2'	2.00	0.44
28:a:2032:C:H5''	53:z:15:MET:HE3	1.99	0.44
28:a:2168:G:C6	28:a:2169:G:C6	3.05	0.44
28:a:2743:U:H1'	28:a:2744:A:H5''	1.99	0.44
32:e:12:GLU:HG3	32:e:12:GLU:O	2.17	0.44
40:m:77:GLY:O	40:m:81:ASN:HB2	2.18	0.44
48:u:52:LYS:HB2	48:u:52:LYS:HE3	1.83	0.44
6:A:668:G:H2'	6:A:669:A:H8	1.83	0.44
6:A:972:A:H2	6:A:1354:A:H61	1.66	0.44
6:A:1096:A:H2'	6:A:1097:C:C6	2.53	0.44
28:a:107:G:H4'	28:a:288:A:H5''	2.00	0.44
28:a:182:A:H2'	28:a:183:C:H6	1.81	0.44
28:a:195:A:H61	28:a:198:C:H3'	1.81	0.44
28:a:484:G:H2'	28:a:485:G:O4'	2.18	0.44
28:a:650:C:H5''	32:e:93:GLN:HB3	1.98	0.44
28:a:713:C:H2'	28:a:714:U:O4'	2.17	0.44
28:a:2123:G:C6	28:a:2143:G:C2	3.06	0.44
28:a:2633:C:H2'	28:a:2634:U:O4'	2.18	0.44
33:f:57:LEU:HD11	33:f:152:LEU:HD21	2.00	0.44
44:q:43:ASN:OD1	44:q:46:ASP:HB3	2.18	0.44
44:q:58:LYS:HE2	44:q:60:THR:HG23	1.98	0.44
6:A:494:G:H2'	6:A:495:C:C6	2.52	0.44
24:S:3:ARG:NH1	24:S:7:LYS:HE2	2.32	0.44
28:a:1083:G:H2'	28:a:1084:U:H6	1.81	0.44
28:a:2141:G:H2'	28:a:2142:U:O4'	2.18	0.44
29:b:2:G:H2'	29:b:3:C:C6	2.53	0.44
33:f:120:LYS:N	33:f:120:LYS:HD2	2.33	0.44
37:j:17:ARG:HE	37:j:47:ILE:HD11	1.83	0.44
41:n:27:LEU:HD23	41:n:91:PHE:CD1	2.52	0.44
44:q:23:GLU:OE1	44:q:23:GLU:HA	2.18	0.44
45:r:1:MET:HE3	45:r:64:ALA:HB2	1.99	0.44
51:x:9:LYS:HB3	51:x:13:GLN:HB2	2.00	0.44
4:3:8:LYS:HB3	4:3:8:LYS:HE2	1.74	0.44
6:A:154:A:H2'	6:A:155:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:240:A:C2	6:A:276:A:C5	3.06	0.44
6:A:818:G:O2'	6:A:819:A:H5'	2.18	0.44
6:A:1373:G:O2'	6:A:1374:U:H5'	2.18	0.44
11:F:4:TYR:CZ	11:F:71:LEU:HD22	2.53	0.44
28:a:84:A:H8	28:a:84:A:OP2	2.01	0.44
28:a:286:U:H2'	28:a:287:U:C6	2.53	0.44
28:a:614:C:O2'	28:a:647:U:H5''	2.17	0.44
28:a:1186:U:H1'	43:p:4:VAL:HG22	1.98	0.44
28:a:2112:G:H2'	28:a:2113:A:C5	2.53	0.44
28:a:2152:C:H2'	28:a:2153:U:O4'	2.18	0.44
31:d:115:GLY:HA2	31:d:166:GLY:O	2.17	0.44
33:f:65:PRO:HA	33:f:89:VAL:HG22	1.99	0.44
34:g:37:VAL:HG21	34:g:44:ILE:HG12	2.00	0.44
46:s:49:LEU:HD13	51:x:26:PHE:CE1	2.53	0.44
6:A:489:A:H4'	6:A:490:A:OP1	2.17	0.43
6:A:1112:U:H2'	6:A:1113:C:C6	2.53	0.43
6:A:1312:A:H5''	24:S:3:ARG:NH2	2.33	0.43
10:E:56:GLU:N	10:E:56:GLU:OE1	2.51	0.43
11:F:10:VAL:HA	11:F:83:ALA:O	2.17	0.43
12:G:112:GLY:H	12:G:119:ARG:HD3	1.83	0.43
14:I:13:LYS:HE3	14:I:13:LYS:HB3	1.66	0.43
28:a:987:G:OP1	43:p:92:ARG:HD2	2.18	0.43
28:a:1910:U:H2'	28:a:1911:C:C6	2.53	0.43
28:a:2343:A:H2'	28:a:2344:G:O4'	2.18	0.43
6:A:35:G:H2'	6:A:36:C:C6	2.53	0.43
6:A:1471:U:H2'	6:A:1472:U:C6	2.53	0.43
8:C:179:ARG:HE	8:C:179:ARG:HB3	1.56	0.43
11:F:47:LEU:HD21	11:F:57:ALA:HB3	2.00	0.43
28:a:770:G:H2'	28:a:772:A:N7	2.33	0.43
28:a:1673:C:H2'	28:a:1674:A:C8	2.52	0.43
28:a:1720:U:C2	28:a:1721:C:C5	3.06	0.43
51:x:39:GLN:HB3	51:x:41:HIS:CE1	2.54	0.43
6:A:62:U:H2'	6:A:63:C:C6	2.53	0.43
6:A:83:G:H2'	6:A:84:C:H6	1.80	0.43
6:A:520:C:C4	6:A:521:G7M:H1'	2.53	0.43
6:A:742:U:H2'	6:A:743:A:C8	2.52	0.43
11:F:106:GLU:CD	11:F:106:GLU:H	2.26	0.43
13:H:41:LYS:HD2	13:H:48:ASP:HA	1.99	0.43
23:R:15:ALA:O	23:R:19:LYS:HE3	2.18	0.43
28:a:43:G:C2'	28:a:44:A:H5'	2.48	0.43
28:a:586:A:H2'	28:a:587:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1373:C:H2'	28:a:1374:A:H8	1.80	0.43
28:a:1414:A:H4'	28:a:1415:C:O5'	2.18	0.43
28:a:1433:C:H2'	28:a:1434:U:C6	2.53	0.43
28:a:1552:U:H2'	28:a:1553:U:O4'	2.19	0.43
28:a:1615:C:H2'	28:a:1616:G:O4'	2.18	0.43
2:1:18:PHE:HA	2:1:43:THR:HG21	2.00	0.43
6:A:898:U:H2'	6:A:899:U:C6	2.53	0.43
7:B:8:ASP:HB2	7:B:212:LEU:HD11	2.00	0.43
28:a:1519:G:C2	28:a:1520:U:C4	3.07	0.43
53:z:12:ALA:HA	53:z:15:MET:HG3	2.01	0.43
4:3:15:LYS:HB3	4:3:15:LYS:HE2	1.70	0.43
6:A:314:A:H2'	6:A:315:A:O4'	2.19	0.43
6:A:1334:A:N3	14:I:130:ARG:HD3	2.34	0.43
10:E:148:MET:HE3	10:E:148:MET:HB3	1.81	0.43
12:G:4:ARG:HA	12:G:4:ARG:HH11	1.83	0.43
19:N:82:ASN:O	19:N:86:GLU:HG3	2.19	0.43
28:a:92:A:H2'	28:a:93:A:C8	2.53	0.43
28:a:167:A:H2'	28:a:168:G:O4'	2.19	0.43
28:a:634:A:H2'	28:a:636:A:N7	2.34	0.43
28:a:1104:C:H2'	28:a:1105:G:C8	2.54	0.43
28:a:1190:U:H1'	38:k:4:ASN:HB3	2.01	0.43
28:a:1672:G:H2'	28:a:1673:C:H6	1.80	0.43
28:a:1915:A:H2'	28:a:1916:G:O4'	2.17	0.43
28:a:2059:C:H2'	28:a:2060:C:H6	1.84	0.43
28:a:2087:G:C6	28:a:2177:G:C5	3.06	0.43
28:a:2122:A:C5	28:a:2123:G:H1'	2.53	0.43
49:v:25:LEU:HD13	49:v:31:VAL:HG22	1.99	0.43
6:A:21:G:H2'	6:A:22:G:C8	2.53	0.43
6:A:75:G:H2'	6:A:76:G:C8	2.54	0.43
6:A:667:G:H5''	11:F:86:ARG:NH2	2.34	0.43
6:A:1173:A:H2'	6:A:1174:A:O4'	2.18	0.43
6:A:1422:U:H2'	6:A:1423:C:O4'	2.18	0.43
7:B:148:LEU:HD22	7:B:151:ILE:HG21	2.00	0.43
18:M:92:ARG:HG3	28:a:876:U:H1'	1.99	0.43
28:a:1276:C:H2'	28:a:1277:A:H8	1.82	0.43
28:a:2234:A:H2'	28:a:2235:C:H6	1.84	0.43
28:a:2501:U:H2'	28:a:2502:C:C6	2.54	0.43
28:a:2781:A:H2'	28:a:2782:A:C8	2.53	0.43
30:c:241:ALA:C	30:c:243:ARG:H	2.25	0.43
33:f:57:LEU:HD23	33:f:89:VAL:HG23	2.00	0.43
6:A:74:A:N6	6:A:89:G:N2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:107:G:H2'	6:A:108:U:C6	2.53	0.43
6:A:1138:G:N2	6:A:1140:A:H62	2.16	0.43
6:A:1352:U:H5''	6:A:1353:C:H5	1.83	0.43
12:G:61:THR:HG23	12:G:124:LEU:HD21	2.01	0.43
14:I:36:ASP:HA	14:I:45:ARG:HE	1.83	0.43
28:a:1395:U:H2'	28:a:1396:G:H8	1.82	0.43
28:a:2113:A:N6	28:a:2150:U:H5'	2.33	0.43
28:a:2149:A:C5	28:a:2150:U:C5	3.07	0.43
28:a:2156:A:H2'	28:a:2157:A:C8	2.54	0.43
29:b:24:G:N7	29:b:56:G:H2'	2.34	0.43
6:A:31:G:H3'	6:A:32:A:H5''	2.00	0.43
9:D:8:LYS:HG3	9:D:21:LEU:HB3	2.01	0.43
10:E:13:ILE:HD12	10:E:13:ILE:N	2.34	0.43
28:a:1098:U:H2'	28:a:1099:C:C6	2.53	0.43
28:a:1376:G:H2'	28:a:1377:U:O4'	2.19	0.43
28:a:1394:C:H2'	28:a:1395:U:H6	1.83	0.43
28:a:2635:G:H2'	28:a:2636:C:C6	2.54	0.43
33:f:135:GLN:HG3	33:f:141:ILE:HD13	2.01	0.43
41:n:75:GLN:HG3	41:n:108:ALA:HB1	2.01	0.43
43:p:74:LEU:HD23	43:p:74:LEU:HA	1.87	0.43
48:u:127:ILE:HG12	48:u:187:ILE:CD1	2.49	0.43
6:A:378:G:H2'	6:A:379:C:C6	2.54	0.43
28:a:2151:C:H2'	28:a:2152:C:O4'	2.19	0.43
28:a:2587:A:O2'	28:a:2588:C:H5'	2.18	0.43
28:a:2781:A:H2'	28:a:2782:A:H8	1.83	0.43
33:f:8:TYR:OH	33:f:30:ARG:HB3	2.18	0.43
36:i:15:TRP:CE2	36:i:135:GLN:HG2	2.54	0.43
5:4:41:HIS:CD2	5:4:43:PHE:H	2.37	0.43
6:A:1:G:N2	6:A:608:C:H4'	2.33	0.43
6:A:6:G:O2'	6:A:7:A:H8	2.02	0.43
10:E:116:LEU:HD13	10:E:124:VAL:HG11	2.01	0.43
14:I:47:VAL:HG13	14:I:80:ARG:HE	1.84	0.43
17:L:50:ARG:HB3	17:L:66:TYR:HE1	1.84	0.43
19:N:24:ARG:HG3	19:N:48:LEU:HD11	2.01	0.43
28:a:248:G:H5'	28:a:250:G:N7	2.33	0.43
28:a:410:U:H2'	28:a:411:C:C6	2.54	0.43
28:a:2305:G:H5''	28:a:2306:U:OP2	2.19	0.43
28:a:2771:U:H2'	28:a:2772:C:C6	2.54	0.43
46:s:87:GLN:HG3	46:s:88:PRO:HD2	2.00	0.43
6:A:445:A:H4'	6:A:446:A:O5'	2.18	0.42
6:A:566:A:H5'	6:A:567:A:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1027:G:O5'	6:A:1027:G:H8	2.02	0.42
28:a:865:C:H2'	28:a:866:U:O4'	2.19	0.42
38:k:123:LYS:HE3	38:k:123:LYS:HB3	1.80	0.42
44:q:2:TYR:CE2	44:q:42:ALA:HB3	2.54	0.42
6:A:507:U:H2'	6:A:508:C:H6	1.83	0.42
6:A:1529:C:H2'	6:A:1530:C:H6	1.83	0.42
8:C:67:THR:HG22	8:C:102:ASN:CB	2.45	0.42
9:D:117:LEU:HD11	9:D:155:ILE:HD11	2.01	0.42
14:I:5:GLN:HA	14:I:22:ARG:HG2	2.01	0.42
28:a:869:G:H22	28:a:886:C:H2'	1.84	0.42
32:e:144:ASP:HB3	32:e:183:ASP:HB2	2.00	0.42
33:f:12:ILE:HG12	33:f:172:ALA:HB1	2.00	0.42
33:f:152:LEU:HD23	33:f:152:LEU:HA	1.85	0.42
37:j:24:VAL:HA	37:j:39:ILE:HG22	2.01	0.42
43:p:85:LYS:HE2	43:p:85:LYS:HB2	1.81	0.42
45:r:28:LYS:HA	45:r:28:LYS:HD2	1.89	0.42
47:t:1:MET:HG3	47:t:84:PHE:CE1	2.54	0.42
49:v:38:VAL:HG12	49:v:40:GLN:HG2	2.00	0.42
1:0:2:ARG:HA	1:0:21:LYS:O	2.18	0.42
6:A:1004:C:H2'	6:A:1005:C:C6	2.55	0.42
6:A:1021:C:H2'	6:A:1022:C:O4'	2.19	0.42
6:A:1029:A:C6	6:A:1030:A:C6	3.07	0.42
6:A:1032:U:H2'	6:A:1033:C:H6	1.84	0.42
7:B:6:MET:HE2	7:B:6:MET:HB2	1.91	0.42
28:a:299:C:H2'	28:a:300:U:C6	2.53	0.42
28:a:836:U:H5	28:a:923:A:N7	2.18	0.42
28:a:977:C:H2'	28:a:978:A:O4'	2.19	0.42
28:a:1738:U:H2'	28:a:1739:C:C6	2.54	0.42
28:a:2164:C:H2'	28:a:2165:C:O4'	2.19	0.42
30:c:95:LYS:HB3	30:c:95:LYS:HE2	1.90	0.42
31:d:1:MET:O	31:d:205:PRO:HD2	2.19	0.42
36:i:106:LYS:HB2	36:i:106:LYS:HE3	1.69	0.42
41:n:41:ILE:HG21	41:n:45:GLY:HA2	2.01	0.42
48:u:169:LYS:HB3	48:u:169:LYS:HE3	1.66	0.42
6:A:170:C:H2'	6:A:171:G:N3	2.35	0.42
6:A:468:C:H2'	6:A:469:U:C6	2.54	0.42
6:A:481:A:H2'	6:A:482:C:O4'	2.18	0.42
6:A:1114:C:H2'	6:A:1115:U:H6	1.82	0.42
8:C:121:ALA:HB1	8:C:189:ALA:HB2	2.00	0.42
14:I:28:ILE:HD13	14:I:63:ILE:HB	2.01	0.42
17:L:74:LEU:HD21	17:L:80:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:875:A:H8	28:a:878:C:C5	2.37	0.42
28:a:1855:C:H2'	28:a:1856:G:O4'	2.19	0.42
28:a:2220:U:H2'	28:a:2221:G:H8	1.84	0.42
6:A:682:G:H5'	16:K:49:GLY:HA2	2.01	0.42
6:A:1074:A:H5''	10:E:22:VAL:HG11	2.00	0.42
6:A:1233:A:H4'	6:A:1234:U:O5'	2.19	0.42
6:A:1446:A:H8	6:A:1446:A:OP2	2.03	0.42
20:O:85:LEU:HD13	20:O:85:LEU:HA	1.86	0.42
22:Q:55:GLN:HG3	22:Q:81:ILE:HD11	2.02	0.42
28:a:1475:U:H2'	28:a:1476:U:C6	2.55	0.42
28:a:1553:U:H2'	28:a:1554:C:C6	2.55	0.42
28:a:2124:C:H2'	28:a:2125:G:C8	2.55	0.42
28:a:2761:C:H2'	28:a:2762:A:O4'	2.20	0.42
28:a:2796:A:H2'	28:a:2797:A:C8	2.54	0.42
30:c:110:VAL:HA	30:c:114:ASP:OD2	2.19	0.42
33:f:136:ILE:HA	33:f:141:ILE:HD11	2.00	0.42
45:r:3:VAL:HG21	45:r:58:ALA:HA	2.00	0.42
48:u:33:VAL:HG22	48:u:94:PHE:HB2	2.01	0.42
6:A:972:A:C4	6:A:1313:A:C2	3.07	0.42
8:C:87:LEU:O	8:C:91:LEU:HG	2.20	0.42
28:a:511:A:H2'	28:a:512:U:C6	2.54	0.42
28:a:837:C:H2'	28:a:838:A:C8	2.55	0.42
28:a:1673:C:H2'	28:a:1674:A:H8	1.85	0.42
28:a:2872:U:H5	53:z:49:ARG:HH21	1.67	0.42
30:c:273:LYS:H	30:c:273:LYS:HG2	1.54	0.42
43:p:86:ALA:HB2	43:p:116:SER:OG	2.20	0.42
6:A:401:U:H2'	6:A:402:G:C8	2.53	0.42
6:A:1349:G:O2'	6:A:1350:A:H5'	2.19	0.42
8:C:15:VAL:HG11	8:C:179:ARG:O	2.20	0.42
28:a:1200:A:H2'	28:a:1201:A:O4'	2.18	0.42
28:a:1857:C:H3'	28:a:1858:A:H8	1.85	0.42
29:b:115:A:H2'	29:b:116:A:C8	2.54	0.42
30:c:132:LEU:HD23	30:c:135:ILE:HD12	2.01	0.42
32:e:47:THR:O	32:e:51:VAL:HG23	2.18	0.42
32:e:133:LEU:HD23	32:e:160:ALA:HB2	2.01	0.42
33:f:78:LYS:HE3	33:f:78:LYS:HB3	1.82	0.42
33:f:132:VAL:HB	33:f:152:LEU:HB2	2.02	0.42
48:u:162:LEU:HD23	48:u:162:LEU:HA	1.89	0.42
28:a:17:G:H2'	28:a:18:C:C6	2.55	0.42
28:a:1065:C:C4	28:a:1066:C:N4	2.87	0.42
28:a:2602:U:C2	53:z:4:GLN:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2782:A:H2'	28:a:2783:C:C6	2.54	0.42
36:i:4:TYR:CD2	43:p:100:VAL:HG11	2.55	0.42
44:q:2:TYR:CZ	44:q:42:ALA:HB3	2.55	0.42
6:A:230:A:H2'	6:A:231:G:C8	2.55	0.42
6:A:1309:U:H2'	6:A:1310:G:O4'	2.20	0.42
11:F:38:ARG:NH2	11:F:61:LEU:HD21	2.34	0.42
14:I:30:ILE:HA	14:I:65:VAL:HG23	2.01	0.42
28:a:560:G:H2'	28:a:2017:6MZ:N7	2.35	0.42
28:a:822:U:H2'	28:a:823:A:H8	1.84	0.42
28:a:2373:U:H4'	49:v:56:ASP:HA	2.00	0.42
28:a:2588:C:H4'	28:a:2589:A:N1	2.35	0.42
30:c:31:ALA:HA	30:c:34:LEU:HD22	2.01	0.42
41:n:9:LEU:HD23	41:n:9:LEU:HA	1.80	0.42
5:4:41:HIS:HB3	5:4:44:TYR:CD1	2.55	0.42
5:4:64:PHE:CE1	24:S:5:LEU:HB3	2.55	0.42
6:A:86:C:O2'	6:A:87:C:H5'	2.20	0.42
6:A:191:A:H4'	6:A:192:G:OP1	2.20	0.42
6:A:416:C:H4'	6:A:417:G:C4	2.55	0.42
6:A:1021:C:N4	6:A:1029:A:H61	2.18	0.42
6:A:1210:G:H5'	19:N:5:SER:HB2	2.02	0.42
11:F:88:LEU:HG	11:F:90:MET:HE2	2.02	0.42
18:M:92:ARG:HG3	28:a:876:U:C1'	2.49	0.42
28:a:869:G:C5	28:a:870:G:H1'	2.55	0.42
28:a:937:A:H2'	28:a:938:C:C6	2.55	0.42
28:a:1733:G:H2'	28:a:1734:C:C6	2.55	0.42
28:a:2174:C:H2'	28:a:2175:U:O4'	2.19	0.42
6:A:22:G:H2'	6:A:23:C:C6	2.54	0.41
6:A:304:G:H5''	21:P:31:ARG:HB2	2.02	0.41
6:A:326:G:OP2	25:T:2:ALA:HA	2.20	0.41
6:A:714:C:OP1	23:R:41:PRO:HG3	2.20	0.41
11:F:9:LEU:HD22	11:F:59:TYR:CE2	2.55	0.41
28:a:803:U:H2'	28:a:804:C:H6	1.84	0.41
28:a:1665:C:O2	31:d:133:THR:HB	2.20	0.41
28:a:1777:C:H2'	28:a:1778:A:C5	2.55	0.41
28:a:1933:U:H2'	28:a:1934:C:H6	1.84	0.41
28:a:2015:U:H2'	28:a:2016:G:O4'	2.20	0.41
28:a:2152:C:C4	28:a:2153:U:C4	3.07	0.41
28:a:2282:C:H2'	28:a:2283:U:C6	2.55	0.41
29:b:68:C:H2'	29:b:69:G:O4'	2.20	0.41
33:f:93:SER:N	33:f:96:MET:HE2	2.35	0.41
33:f:134:GLU:O	33:f:137:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:56:ARG:HB3	5:4:59:ARG:HE	1.85	0.41
6:A:254:G:H2'	6:A:255:U:C6	2.55	0.41
6:A:628:C:H2'	6:A:629:A:H8	1.85	0.41
6:A:976:U:H4'	6:A:977:A:O5'	2.19	0.41
6:A:1527:C:H2'	6:A:1528:A:C8	2.56	0.41
8:C:79:LYS:O	8:C:80:LYS:HB2	2.20	0.41
22:Q:20:MET:HE3	22:Q:20:MET:HB2	1.95	0.41
23:R:36:THR:HG22	23:R:72:ASP:OD2	2.20	0.41
25:T:84:LYS:O	25:T:88:THR:HG23	2.18	0.41
28:a:579:U:H2'	28:a:580:A:C8	2.55	0.41
28:a:1553:U:O2'	28:a:1554:C:H5'	2.20	0.41
28:a:2039:A:H4'	31:d:148:GLN:O	2.20	0.41
32:e:149:THR:O	32:e:170:ASP:HA	2.21	0.41
34:g:121:ILE:HD11	34:g:140:LEU:HB3	2.03	0.41
1:0:17:TYR:CD1	1:0:34:LYS:HD3	2.56	0.41
6:A:902:A:H2'	6:A:903:A:H8	1.85	0.41
6:A:979:C:H2'	6:A:980:U:C6	2.55	0.41
16:K:13:LYS:HG3	16:K:14:LYS:H	1.85	0.41
28:a:829:U:H2'	28:a:830:C:C6	2.55	0.41
28:a:867:A:H2'	28:a:868:G:O4'	2.20	0.41
28:a:944:G:O3'	39:l:13:MET:HG2	2.20	0.41
28:a:2052:C:H2'	28:a:2053:C:H6	1.83	0.41
28:a:2107:G:H2'	28:a:2108:G:H8	1.85	0.41
28:a:2285:A:OP1	33:f:71:ARG:HD2	2.20	0.41
30:c:271:ARG:HD3	30:c:273:LYS:HZ1	1.84	0.41
35:h:4:ILE:HG22	35:h:18:LYS:HG3	2.01	0.41
45:r:82:LEU:HB2	45:r:98:LYS:HB2	2.01	0.41
4:3:37:GLN:HB3	4:3:38:GLY:H	1.75	0.41
6:A:186:G:C2'	6:A:187:A:H5'	2.51	0.41
6:A:558:C:C5	22:Q:36:ILE:HD11	2.56	0.41
6:A:1036:A:H8	6:A:1036:A:OP2	2.03	0.41
18:M:92:ARG:HE	18:M:92:ARG:HB2	1.64	0.41
28:a:247:G:H4'	28:a:377:G:C6	2.56	0.41
28:a:1393:U:H2'	28:a:1394:C:H6	1.86	0.41
28:a:1814:U:H2'	28:a:1815:G:O4'	2.19	0.41
28:a:2278:U:H2'	28:a:2279:G:H8	1.81	0.41
29:b:18:G:H2'	29:b:19:C:C6	2.56	0.41
31:d:179:ARG:HB3	31:d:188:LEU:HB2	2.02	0.41
32:e:62:LYS:HE3	32:e:62:LYS:HB3	1.82	0.41
33:f:140:GLU:H	33:f:140:GLU:CD	2.28	0.41
39:l:82:4D4:H14	39:l:82:4D4:H10	1.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:q:97:LYS:HB3	44:q:97:LYS:HE3	1.80	0.41
6:A:1137:G:H2'	6:A:1138:G:C8	2.55	0.41
11:F:50:ALA:HB1	11:F:53:ASN:HA	2.02	0.41
23:R:21:ILE:HD13	23:R:55:LEU:HB2	2.03	0.41
25:T:62:ALA:HB2	25:T:72:ALA:HB2	2.02	0.41
28:a:1400:A:H2'	28:a:1401:C:C6	2.56	0.41
28:a:1597:C:N4	28:a:1612:G:OP2	2.53	0.41
28:a:1722:C:H2'	28:a:1723:G:O4'	2.20	0.41
28:a:2019:G:C5	31:d:150:MEQ:HE3	2.55	0.41
28:a:2052:C:H2'	28:a:2053:C:C6	2.55	0.41
29:b:62:A:H2'	29:b:63:C:C6	2.55	0.41
31:d:63:LYS:HE3	31:d:63:LYS:HB3	1.74	0.41
32:e:124:ALA:O	32:e:136:LYS:HE2	2.20	0.41
36:i:59:ALA:HB2	36:i:124:VAL:HG12	2.01	0.41
41:n:88:GLN:H	41:n:115:GLU:HB2	1.85	0.41
53:z:31:LYS:HA	53:z:31:LYS:HD2	1.82	0.41
6:A:401:U:H2'	6:A:402:G:H8	1.86	0.41
13:H:111:MET:HB2	13:H:115:ALA:HB3	2.02	0.41
14:I:22:ARG:O	14:I:61:PHE:HD1	2.03	0.41
17:L:99:ARG:CZ	17:L:107:VAL:HG12	2.51	0.41
23:R:21:ILE:HG21	23:R:55:LEU:HA	2.03	0.41
28:a:474:A:H5''	47:t:46:LYS:HG2	2.02	0.41
28:a:744:G:H2'	28:a:745:U:H6	1.86	0.41
28:a:1693:G:H2'	28:a:1694:U:C6	2.55	0.41
28:a:2201:C:H2'	28:a:2202:C:O4'	2.21	0.41
28:a:2541:U:H2'	28:a:2542:U:C6	2.56	0.41
28:a:2701:G:C2'	28:a:2702:C:H5'	2.50	0.41
33:f:57:LEU:HA	33:f:57:LEU:HD12	1.79	0.41
37:j:64:ARG:HG2	37:j:83:ALA:HB3	2.02	0.41
41:n:59:LEU:HD21	41:n:72:LYS:CB	2.51	0.41
42:o:29:VAL:HG22	42:o:85:LEU:HD13	2.03	0.41
6:A:96:G:H2'	6:A:97:C:C6	2.56	0.41
6:A:192:G:H2'	6:A:193:U:H6	1.85	0.41
6:A:577:A:H2'	6:A:578:G:O4'	2.21	0.41
6:A:1369:A:H2'	6:A:1370:U:O4'	2.21	0.41
7:B:16:PHE:CB	7:B:203:ASN:HD22	2.30	0.41
28:a:871:G:H2'	28:a:872:G:C8	2.55	0.41
28:a:2090:C:C2	28:a:2091:C:C5	3.09	0.41
28:a:2294:G:N7	28:a:2295:G:C5	2.89	0.41
28:a:2478:U:H5''	28:a:2557:G:H5'	2.03	0.41
41:n:25:VAL:HA	41:n:42:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:948:G:H2'	6:A:949:U:C6	2.56	0.41
6:A:1017:G:O5'	6:A:1017:G:H8	2.04	0.41
6:A:1027:G:H2'	6:A:1028:G:H8	1.81	0.41
6:A:1145:A:H5''	15:J:44:THR:HG22	2.03	0.41
6:A:1296:C:C5	18:M:17:ILE:HG13	2.55	0.41
7:B:125:THR:HG23	7:B:128:LYS:CB	2.51	0.41
14:I:129:LYS:HA	14:I:129:LYS:HD2	1.78	0.41
16:K:58:SER:O	16:K:91:PRO:HG2	2.21	0.41
22:Q:23:THR:HB	22:Q:74:LYS:HD2	2.03	0.41
23:R:48:LYS:HA	23:R:48:LYS:HD2	1.95	0.41
28:a:731:U:H2'	28:a:732:C:C6	2.55	0.41
28:a:1395:U:H2'	28:a:1396:G:C8	2.55	0.41
28:a:1679:A:H2'	28:a:1680:A:C8	2.56	0.41
29:b:66:A:N6	29:b:107:U:H2'	2.35	0.41
31:d:121:THR:HB	31:d:127:PHE:CD2	2.56	0.41
33:f:108:LEU:HA	33:f:108:LEU:HD23	1.71	0.41
38:k:77:VAL:O	38:k:110:VAL:HA	2.21	0.41
50:w:32:ASN:O	50:w:52:SER:HA	2.21	0.41
1:0:7:LEU:HB3	1:0:45:TYR:HB3	2.03	0.41
1:0:26:LYS:HD2	1:0:26:LYS:HA	1.80	0.41
6:A:540:A:P	9:D:69:GLU:HB3	2.61	0.41
6:A:666:U:H2'	6:A:667:G:H8	1.86	0.41
6:A:1063:C:H2'	6:A:1064:U:O4'	2.21	0.41
6:A:1154:G:C2	6:A:1155:C:C6	3.09	0.41
6:A:1162:C:H1'	6:A:1163:A:OP2	2.21	0.41
6:A:1184:G:H5'	8:C:176:HIS:NE2	2.36	0.41
6:A:1232:A:N7	6:A:1297:C:H1'	2.36	0.41
6:A:1344:A:H2'	6:A:1345:U:C6	2.56	0.41
8:C:10:ILE:HG23	8:C:11:ARG:HG3	2.01	0.41
8:C:69:HIS:HB3	8:C:106:ILE:HD11	2.01	0.41
9:D:15:GLU:HB3	9:D:60:LYS:HG3	2.03	0.41
10:E:78:ASN:O	10:E:81:THR:HG22	2.20	0.41
13:H:27:MET:HE2	13:H:27:MET:HB3	1.80	0.41
15:J:9:ARG:HD2	15:J:73:VAL:HG22	2.03	0.41
28:a:208:C:H2'	28:a:209:C:C6	2.56	0.41
28:a:529:A:H5''	36:i:7:LYS:HZ2	1.86	0.41
28:a:732:C:H2'	28:a:733:C:O4'	2.21	0.41
28:a:733:C:OP1	31:d:135:GLY:HA2	2.20	0.41
28:a:827:C:N3	28:a:931:A:N6	2.67	0.41
28:a:829:U:H1'	28:a:1178:A:H1'	2.03	0.41
28:a:852:A:H2'	28:a:853:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1166:G:OP1	28:a:1166:G:H4'	2.21	0.41
28:a:1573:U:H5'	28:a:1574:U:OP1	2.20	0.41
28:a:1777:C:H2'	28:a:1778:A:C8	2.56	0.41
28:a:1867:U:H2'	28:a:1868:C:H6	1.86	0.41
28:a:1958:U:C2	30:c:240:SER:HB3	2.56	0.41
28:a:2123:G:C4	28:a:2124:C:C5	3.09	0.41
28:a:2162:C:H3'	28:a:2163:A:H8	1.85	0.41
28:a:2292:U:C2	33:f:151:GLY:HA3	2.56	0.41
28:a:2503:A:O2'	28:a:2504:C:H5'	2.21	0.41
28:a:2524:U:H2'	28:a:2525:C:C6	2.56	0.41
28:a:2874:C:H2'	28:a:2875:C:C6	2.56	0.41
32:e:68:ARG:H	32:e:68:ARG:HG2	1.64	0.41
37:j:4:THR:HG23	37:j:22:ILE:HA	2.03	0.41
37:j:100:GLY:O	37:j:119:PRO:HD2	2.21	0.41
39:l:43:THR:HG23	39:l:92:TYR:CD2	2.56	0.41
41:n:67:ILE:HG22	41:n:71:LYS:HE2	2.03	0.41
6:A:1458:U:H2'	6:A:1459:A:H8	1.86	0.41
19:N:6:MET:HE3	19:N:6:MET:HB3	1.78	0.41
28:a:155:U:H3	28:a:171:G:H1	1.69	0.41
28:a:738:G:C8	45:r:89:ALA:HB1	2.56	0.41
28:a:1166:G:H2'	28:a:1167:U:C6	2.56	0.41
28:a:2590:G:H2'	28:a:2591:PSU:O4'	2.20	0.41
29:b:2:G:H2'	29:b:3:C:H6	1.86	0.41
46:s:71:ARG:N	46:s:71:ARG:HD3	2.36	0.41
48:u:127:ILE:HG12	48:u:187:ILE:HD13	2.03	0.41
6:A:89:G:OP2	6:A:89:G:H8	2.04	0.40
6:A:292:A:H2'	6:A:293:G:O4'	2.21	0.40
6:A:331:G:H2'	6:A:332:A:H8	1.85	0.40
6:A:670:A:H2'	6:A:671:U:H6	1.86	0.40
6:A:1490:C:H2'	6:A:1491:G:O4'	2.21	0.40
15:J:8:ILE:HG13	15:J:100:ILE:HG22	2.03	0.40
27:X:10:LEU:HD22	27:X:43:VAL:HG23	2.02	0.40
28:a:72:A:C8	51:x:54:LYS:HD3	2.56	0.40
28:a:970:A:N7	28:a:1126:G:H5'	2.36	0.40
28:a:1077:G:C6	28:a:1079:A:C4	3.09	0.40
28:a:1121:G:O2'	28:a:2013:U:H5'	2.21	0.40
28:a:1270:G:N2	28:a:1272:A:H3'	2.36	0.40
28:a:2017:6MZ:C2	28:a:2486:C:H5''	2.51	0.40
28:a:2041:A:H2'	53:z:5:GLN:NE2	2.36	0.40
28:a:2050:C:O2	28:a:2437:A:N1	2.53	0.40
28:a:2126:U:H3'	28:a:2127:G:H8	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2648:G:H2'	28:a:2649:A:C8	2.55	0.40
28:a:2886:G:H2'	28:a:2887:A:C8	2.56	0.40
29:b:94:A:H2'	29:b:95:U:O4'	2.20	0.40
33:f:48:LYS:HA	33:f:48:LYS:HD2	1.73	0.40
37:j:59:THR:HG22	37:j:87:LEU:HD12	2.02	0.40
42:o:54:ARG:HA	42:o:54:ARG:HD3	1.92	0.40
45:r:12:ILE:HD12	45:r:42:LYS:HE2	2.03	0.40
53:z:52:LYS:NZ	53:z:55:ASP:HA	2.37	0.40
6:A:995:G:H2'	6:A:996:A:H8	1.86	0.40
6:A:1115:U:H2'	6:A:1116:U:H6	1.86	0.40
6:A:1396:4OC:H2'	6:A:1397:C:O4'	2.21	0.40
7:B:5:ASN:C	7:B:7:ARG:H	2.29	0.40
8:C:95:MET:O	8:C:95:MET:HG2	2.20	0.40
12:G:76:LYS:HB3	12:G:76:LYS:HE2	1.67	0.40
14:I:41:ARG:HD2	14:I:41:ARG:HA	1.79	0.40
14:I:88:ILE:HD13	14:I:95:ARG:NH2	2.36	0.40
28:a:913:A:H2'	28:a:914:G:C8	2.56	0.40
28:a:1164:A:H4'	28:a:1165:A:O5'	2.21	0.40
28:a:1977:C:H2'	28:a:1978:U:O4'	2.21	0.40
29:b:32:U:H2'	29:b:33:G:H8	1.87	0.40
49:v:19:LYS:HD3	49:v:19:LYS:HA	1.85	0.40
6:A:1312:A:H1'	24:S:37:ARG:HH11	1.87	0.40
6:A:1474:A:H2'	6:A:1475:U:O4'	2.20	0.40
8:C:50:ALA:HA	8:C:72:ARG:HD3	2.03	0.40
24:S:79:THR:HG21	24:S:81:ARG:HH21	1.87	0.40
28:a:184:C:H2'	28:a:185:A:H8	1.85	0.40
28:a:473:A:H1'	28:a:489:G:N2	2.36	0.40
28:a:719:G:H5''	28:a:720:A:H5''	2.03	0.40
28:a:2476:U:H2'	28:a:2477:G:O4'	2.21	0.40
33:f:162:THR:HG23	33:f:165:GLU:H	1.86	0.40
35:h:15:LEU:H	35:h:15:LEU:HG	1.46	0.40
6:A:1021:C:C4	6:A:1022:C:N4	2.90	0.40
6:A:1349:G:H2'	6:A:1350:A:H8	1.87	0.40
10:E:106:ILE:HA	10:E:124:VAL:HG12	2.03	0.40
24:S:40:ILE:HG21	24:S:62:VAL:HG11	2.03	0.40
28:a:524:G:H2'	28:a:525:U:C6	2.56	0.40
28:a:2316:A:H2'	28:a:2317:G:C8	2.56	0.40
29:b:74:U:H2'	29:b:75:G:O4'	2.22	0.40
33:f:147:ASP:HB3	33:f:150:ARG:HH12	1.87	0.40
37:j:12:ASP:HB3	37:j:14:SER:H	1.86	0.40
44:q:19:PHE:CE1	44:q:97:LYS:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1113:C:H2'	6:A:1114:C:H6	1.85	0.40
8:C:53:SER:HB2	8:C:115:LEU:HG	2.04	0.40
14:I:57:THR:HA	14:I:60:LYS:HD3	2.04	0.40
17:L:68:GLY:O	17:L:99:ARG:HD3	2.22	0.40
28:a:348:U:H2'	28:a:349:U:H5'	2.04	0.40
28:a:429:G:H2'	28:a:430:A:C8	2.57	0.40
28:a:698:G:H2'	28:a:699:U:C6	2.56	0.40
28:a:1394:C:H2'	28:a:1395:U:C6	2.56	0.40
28:a:2156:A:H2'	28:a:2157:A:O4'	2.21	0.40
28:a:2234:A:H2'	28:a:2235:C:C6	2.57	0.40
28:a:2238:OMG:HM23	28:a:2238:OMG:H1'	1.68	0.40
34:g:35:LEU:CB	34:g:75:MET:HE1	2.52	0.40
38:k:27:LEU:O	38:k:31:GLY:HA2	2.22	0.40
48:u:102:LYS:HG3	48:u:138:CYS:C	2.46	0.40
50:w:12:PRO:HB3	50:w:30:LEU:HD23	2.03	0.40
52:y:41:PRO:HG2	52:y:42:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/51 (96%)	49 (100%)	0	0	100	100
2	1	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	6
5	4	66/71 (93%)	55 (83%)	10 (15%)	1 (2%)	8	18
7	B	222/246 (90%)	198 (89%)	23 (10%)	1 (0%)	24	46
8	C	206/228 (90%)	186 (90%)	20 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	D	203/206 (98%)	188 (93%)	15 (7%)	0	100	100
10	E	152/166 (92%)	139 (91%)	13 (9%)	0	100	100
11	F	104/139 (75%)	100 (96%)	3 (3%)	1 (1%)	12	28
12	G	151/156 (97%)	141 (93%)	10 (7%)	0	100	100
13	H	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	34
14	I	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	16	34
15	J	97/103 (94%)	88 (91%)	9 (9%)	0	100	100
16	K	115/129 (89%)	108 (94%)	6 (5%)	1 (1%)	14	30
17	L	119/123 (97%)	110 (92%)	9 (8%)	0	100	100
18	M	111/118 (94%)	100 (90%)	11 (10%)	0	100	100
19	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
20	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	P	79/83 (95%)	79 (100%)	0	0	100	100
22	Q	78/88 (89%)	77 (99%)	1 (1%)	0	100	100
23	R	60/76 (79%)	55 (92%)	5 (8%)	0	100	100
24	S	81/91 (89%)	78 (96%)	3 (4%)	0	100	100
25	T	85/91 (93%)	85 (100%)	0	0	100	100
27	X	96/102 (94%)	92 (96%)	4 (4%)	0	100	100
30	c	270/273 (99%)	258 (96%)	12 (4%)	0	100	100
31	d	208/211 (99%)	192 (92%)	13 (6%)	3 (1%)	9	19
32	e	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	24	46
33	f	175/179 (98%)	154 (88%)	20 (11%)	1 (1%)	21	42
34	g	173/177 (98%)	159 (92%)	14 (8%)	0	100	100
35	h	70/148 (47%)	63 (90%)	7 (10%)	0	100	100
36	i	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
37	j	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
38	k	142/144 (99%)	132 (93%)	9 (6%)	1 (1%)	18	38
39	l	133/137 (97%)	129 (97%)	4 (3%)	0	100	100
40	m	118/129 (92%)	113 (96%)	5 (4%)	0	100	100
41	n	113/116 (97%)	103 (91%)	10 (9%)	0	100	100
42	o	112/116 (97%)	103 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
44	q	101/103 (98%)	100 (99%)	0	1 (1%)	12	28
45	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
46	s	92/99 (93%)	85 (92%)	7 (8%)	0	100	100
47	t	101/104 (97%)	93 (92%)	8 (8%)	0	100	100
48	u	188/204 (92%)	184 (98%)	4 (2%)	0	100	100
49	v	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
50	w	75/78 (96%)	75 (100%)	0	0	100	100
51	x	59/63 (94%)	59 (100%)	0	0	100	100
52	y	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
53	z	53/60 (88%)	51 (96%)	2 (4%)	0	100	100
All	All	5642/6039 (93%)	5314 (94%)	314 (6%)	14 (0%)	44	66

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	d	152	PRO
38	k	16	LYS
44	q	52	PRO
4	3	37	GLN
7	B	126	PHE
31	d	149	CYS
11	F	85	ILE
16	K	18	ASP
32	e	122	ASP
33	f	74	ILE
13	H	84	ARG
31	d	75	ALA
14	I	28	ILE
5	4	57	ILE

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	47 (100%)	0	100	100
2	1	37/37 (100%)	35 (95%)	2 (5%)	20	42
3	2	54/55 (98%)	52 (96%)	2 (4%)	30	57
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	59/61 (97%)	57 (97%)	2 (3%)	32	60
7	B	187/202 (93%)	177 (95%)	10 (5%)	20	43
8	C	172/187 (92%)	169 (98%)	3 (2%)	53	78
9	D	173/174 (99%)	164 (95%)	9 (5%)	21	44
10	E	113/124 (91%)	107 (95%)	6 (5%)	20	43
11	F	91/119 (76%)	89 (98%)	2 (2%)	45	72
12	G	119/122 (98%)	112 (94%)	7 (6%)	18	38
13	H	108/109 (99%)	106 (98%)	2 (2%)	50	75
14	I	104/106 (98%)	99 (95%)	5 (5%)	23	47
15	J	88/92 (96%)	79 (90%)	9 (10%)	7	15
16	K	90/97 (93%)	87 (97%)	3 (3%)	33	61
17	L	105/106 (99%)	102 (97%)	3 (3%)	37	65
18	M	95/99 (96%)	93 (98%)	2 (2%)	47	73
19	N	81/82 (99%)	79 (98%)	2 (2%)	42	69
20	O	74/75 (99%)	70 (95%)	4 (5%)	20	42
21	P	64/65 (98%)	63 (98%)	1 (2%)	55	79
22	Q	73/79 (92%)	69 (94%)	4 (6%)	19	41
23	R	52/64 (81%)	50 (96%)	2 (4%)	29	56
24	S	72/78 (92%)	72 (100%)	0	100	100
25	T	69/70 (99%)	68 (99%)	1 (1%)	59	81
27	X	86/88 (98%)	82 (95%)	4 (5%)	23	48
30	c	212/213 (100%)	210 (99%)	2 (1%)	70	87
31	d	161/161 (100%)	151 (94%)	10 (6%)	16	36
32	e	158/158 (100%)	156 (99%)	2 (1%)	61	82
33	f	151/153 (99%)	145 (96%)	6 (4%)	28	55
34	g	139/141 (99%)	134 (96%)	5 (4%)	31	58
35	h	49/107 (46%)	47 (96%)	2 (4%)	27	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	i	119/119 (100%)	114 (96%)	5 (4%)	26	52
37	j	102/102 (100%)	96 (94%)	6 (6%)	18	38
38	k	106/106 (100%)	105 (99%)	1 (1%)	70	87
39	l	108/108 (100%)	104 (96%)	4 (4%)	30	57
40	m	99/104 (95%)	97 (98%)	2 (2%)	48	74
41	n	86/87 (99%)	84 (98%)	2 (2%)	44	71
42	o	96/98 (98%)	94 (98%)	2 (2%)	47	73
43	p	87/88 (99%)	85 (98%)	2 (2%)	44	71
44	q	86/86 (100%)	80 (93%)	6 (7%)	14	31
45	r	87/87 (100%)	85 (98%)	2 (2%)	44	71
46	s	79/82 (96%)	75 (95%)	4 (5%)	21	45
47	t	88/88 (100%)	87 (99%)	1 (1%)	65	84
48	u	155/165 (94%)	146 (94%)	9 (6%)	18	39
49	v	56/61 (92%)	53 (95%)	3 (5%)	20	42
50	w	66/67 (98%)	63 (96%)	3 (4%)	24	50
51	x	54/55 (98%)	54 (100%)	0	100	100
52	y	48/49 (98%)	48 (100%)	0	100	100
53	z	48/52 (92%)	48 (100%)	0	100	100
All	All	4687/4909 (96%)	4523 (96%)	164 (4%)	32	59

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	1	MET
2	1	43	THR
3	2	8	SER
3	2	31	ILE
5	4	5	ILE
5	4	58	ASP
7	B	9	MET
7	B	10	LEU
7	B	32	PHE
7	B	45	LYS
7	B	80	VAL
7	B	122	GLN
7	B	136	MET

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Mol	Chain	Res	Type
7	B	152	LYS
7	B	167	ASP
7	B	219	GLU
8	C	75	ILE
8	C	103	ILE
8	C	165	THR
9	D	26	ARG
9	D	31	LYS
9	D	32	CYS
9	D	45	ARG
9	D	116	GLN
9	D	129	THR
9	D	161	LEU
9	D	167	ARG
9	D	169	GLU
10	E	75	VAL
10	E	86	THR
10	E	104	THR
10	E	121	VAL
10	E	125	LEU
10	E	154	VAL
11	F	9	LEU
11	F	16	GLU
12	G	6	VAL
12	G	22	ILE
12	G	52	GLU
12	G	73	VAL
12	G	75	VAL
12	G	90	GLU
12	G	114	LYS
13	H	21	GLU
13	H	24	VAL
14	I	16	THR
14	I	21	LEU
14	I	47	VAL
14	I	58	VAL
14	I	66	THR
15	J	6	ILE
15	J	11	LYS
15	J	16	ARG
15	J	18	ILE
15	J	40	ILE

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Mol	Chain	Res	Type
15	J	44	THR
15	J	64	GLN
15	J	76	ILE
15	J	77	VAL
16	K	17	VAL
16	K	20	ILE
16	K	111	THR
17	L	4	ILE
17	L	56	ARG
17	L	107	VAL
18	M	66	GLU
18	M	78	LYS
19	N	3	LYS
19	N	65	ARG
20	O	5	VAL
20	O	75	VAL
20	O	82	ILE
20	O	85	LEU
21	P	11	SER
22	Q	23	THR
22	Q	26	VAL
22	Q	32	VAL
22	Q	82	VAL
23	R	22	ASP
23	R	29	LEU
25	T	15	GLU
27	X	11	ASP
27	X	35	THR
27	X	36	ASN
27	X	93	LEU
30	c	34	LEU
30	c	180	GLU
31	d	25	VAL
31	d	51	VAL
31	d	55	GLU
31	d	74	VAL
31	d	78	ARG
31	d	100	LEU
31	d	131	ASP
31	d	162	SER
31	d	202	ILE
31	d	208	LYS

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Mol	Chain	Res	Type
32	e	125	VAL
32	e	187	VAL
33	f	11	GLU
33	f	22	LEU
33	f	31	VAL
33	f	54	VAL
33	f	66	VAL
33	f	104	LEU
34	g	25	SER
34	g	41	VAL
34	g	44	ILE
34	g	81	GLN
34	g	150	ASP
35	h	15	LEU
35	h	19	VAL
36	i	30	THR
36	i	95	LYS
36	i	98	GLU
36	i	101	ILE
36	i	117	ASP
37	j	45	GLU
37	j	47	ILE
37	j	51	LYS
37	j	58	MET
37	j	63	VAL
37	j	104	ARG
38	k	111	MET
39	l	7	THR
39	l	12	GLN
39	l	94	VAL
39	l	127	LEU
40	m	78	LYS
40	m	120	VAL
41	n	44	ASP
41	n	79	GLU
42	o	62	VAL
42	o	84	SER
43	p	12	ARG
43	p	41	LYS
44	q	14	VAL
44	q	18	GLU
44	q	33	ILE

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Mol	Chain	Res	Type
44	q	51	LEU
44	q	58	LYS
44	q	60	THR
45	r	11	ARG
45	r	62	GLU
46	s	27	SER
46	s	71	ARG
46	s	87	GLN
46	s	94	PHE
47	t	50	MET
48	u	45	LEU
48	u	63	VAL
48	u	116	VAL
48	u	133	GLU
48	u	134	VAL
48	u	149	VAL
48	u	165	LEU
48	u	186	ASN
48	u	192	VAL
49	v	10	THR
49	v	31	VAL
49	v	82	ILE
50	w	7	VAL
50	w	22	HIS
50	w	71	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	50	ASN
7	B	19	GLN
8	C	3	GLN
8	C	58	HIS
8	C	123	GLN
9	D	157	GLN
10	E	62	GLN
10	E	133	ASN
10	E	136	ASN
11	F	55	HIS
11	F	58	HIS
11	F	77	ASN
11	F	87	ASN

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Mol	Chain	Res	Type
13	H	58	GLN
14	I	6	ASN
15	J	99	GLN
16	K	22	HIS
16	K	38	GLN
17	L	25	GLN
18	M	55	GLN
20	O	13	ASN
20	O	40	GLN
21	P	26	ASN
21	P	40	ASN
24	S	53	ASN
25	T	3	ASN
27	X	9	GLN
27	X	48	GLN
30	c	134	ASN
30	c	226	ASN
30	c	261	ASN
31	d	65	GLN
31	d	173	GLN
32	e	2	GLN
32	e	45	GLN
32	e	172	GLN
34	g	59	GLN
34	g	128	GLN
36	i	12	GLN
36	i	58	ASN
36	i	61	GLN
36	i	112	ASN
37	j	67	HIS
39	l	96	GLN
39	l	98	GLN
40	m	31	HIS
42	o	39	GLN
42	o	53	ASN
42	o	67	ASN
43	p	72	ASN
45	r	23	GLN
47	t	48	ASN
48	u	41	GLN
48	u	56	ASN
48	u	67	ASN

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Mol	Chain	Res	Type
50	w	22	HIS
50	w	36	HIS
51	x	15	ASN
51	x	31	GLN
51	x	39	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	W	9/15 (60%)	1 (11%)	0
28	a	2889/2891 (99%)	604 (20%)	0
29	b	116/120 (96%)	22 (18%)	0
6	A	1534/1536 (99%)	324 (21%)	22 (1%)
All	All	4548/4562 (99%)	951 (20%)	22 (0%)

All (951) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	3	A
6	A	4	C
6	A	5	U
6	A	6	G
6	A	7	A
6	A	9	G
6	A	22	G
6	A	32	A
6	A	33	A
6	A	39	G
6	A	47	C
6	A	48	C
6	A	50	A
6	A	51	A
6	A	52	C
6	A	54	C
6	A	60	A
6	A	61	G
6	A	68	G
6	A	71	U
6	A	72	G
6	A	73	A
6	A	76	G

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Mol	Chain	Res	Type
6	A	77	G
6	A	81	U
6	A	82	U
6	A	83	G
6	A	87	C
6	A	88	U
6	A	89	G
6	A	90	G
6	A	92	U
6	A	110	A
6	A	113	A
6	A	117	C
6	A	121	G
6	A	124	A
6	A	125	U
6	A	133	G
6	A	136	G
6	A	138	G
6	A	143	A
6	A	152	G
6	A	157	C
6	A	161	C
6	A	162	G
6	A	165	A
6	A	177	G
6	A	182	G
6	A	184	G
6	A	185	G
6	A	187	A
6	A	191	A
6	A	192	G
6	A	197	G
6	A	198	G
6	A	203	U
6	A	204	C
6	A	205	G
6	A	206	G
6	A	208	C
6	A	214	G
6	A	239	U
6	A	241	G
6	A	245	G

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Mol	Chain	Res	Type
6	A	260	G
6	A	261	C
6	A	274	C
6	A	283	A
6	A	287	G
6	A	315	A
6	A	322	C
6	A	323	A
6	A	324	C
6	A	333	C
6	A	334	U
6	A	345	G
6	A	346	C
6	A	348	G
6	A	357	A
6	A	361	U
6	A	366	C
6	A	378	G
6	A	392	U
6	A	397	C
6	A	400	G
6	A	403	U
6	A	405	A
6	A	406	A
6	A	407	G
6	A	408	A
6	A	415	U
6	A	416	C
6	A	417	G
6	A	418	G
6	A	423	U
6	A	431	U
6	A	432	U
6	A	446	A
6	A	447	G
6	A	461	U
6	A	478	G
6	A	490	A
6	A	492	A
6	A	505	C
6	A	513	C
6	A	515	G

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Mol	Chain	Res	Type
6	A	519	C
6	A	521	G7M
6	A	524	G
6	A	526	A
6	A	527	A
6	A	534	G
6	A	538	G
6	A	539	C
6	A	541	A
6	A	556	U
6	A	558	C
6	A	562	G
6	A	566	A
6	A	567	A
6	A	570	C
6	A	571	G
6	A	573	G
6	A	582	G
6	A	627	G
6	A	633	A
6	A	635	A
6	A	636	A
6	A	639	A
6	A	647	A
6	A	650	G
6	A	655	G
6	A	659	A
6	A	665	G
6	A	667	G
6	A	680	U
6	A	682	G
6	A	694	G
6	A	697	G
6	A	708	G
6	A	709	A
6	A	710	A
6	A	711	C
6	A	717	U
6	A	718	G
6	A	725	G
6	A	728	A
6	A	730	C

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Mol	Chain	Res	Type
6	A	731	A
6	A	747	A
6	A	748	C
6	A	749	A
6	A	753	A
6	A	754	G
6	A	758	C
6	A	771	A
6	A	781	A
6	A	787	U
6	A	788	A
6	A	804	C
6	A	809	A
6	A	811	C
6	A	815	G
6	A	819	A
6	A	820	C
6	A	822	A
6	A	830	G
6	A	836	U
6	A	838	G
6	A	847	G
6	A	854	A
6	A	861	G
6	A	866	A
6	A	884	G
6	A	893	C
6	A	894	A
6	A	896	G
6	A	906	C
6	A	908	A
6	A	916	G
6	A	920	G
6	A	921	G
6	A	928	C
6	A	929	A
6	A	936	G
6	A	954	U
6	A	956	C
6	A	962	A
6	A	963	A
6	A	965	G

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Mol	Chain	Res	Type
6	A	969	A
6	A	970	G
6	A	971	A
6	A	977	A
6	A	982	G
6	A	983	C
6	A	987	G
6	A	988	A
6	A	989	C
6	A	994	U
6	A	998	A
6	A	1001	U
6	A	1003	U
6	A	1014	A
6	A	1016	U
6	A	1018	G
6	A	1019	U
6	A	1023	U
6	A	1024	U
6	A	1025	C
6	A	1026	G
6	A	1027	G
6	A	1031	C
6	A	1036	A
6	A	1037	C
6	A	1039	C
6	A	1044	G
6	A	1047	G
6	A	1059	U
6	A	1078	G
6	A	1079	U
6	A	1083	G
6	A	1088	G
6	A	1089	U
6	A	1095	A
6	A	1106	C
6	A	1118	G
6	A	1119	U
6	A	1124	A
6	A	1127	A
6	A	1130	U
6	A	1131	C

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Mol	Chain	Res	Type
6	A	1133	G
6	A	1139	C
6	A	1152	C
6	A	1153	U
6	A	1154	G
6	A	1162	C
6	A	1163	A
6	A	1165	A
6	A	1175	G
6	A	1190	A
6	A	1191	A
6	A	1194	C
6	A	1196	U
6	A	1206	U
6	A	1207	A
6	A	1208	C
6	A	1209	G
6	A	1211	C
6	A	1221	A
6	A	1222	C
6	A	1230	A
6	A	1232	A
6	A	1234	U
6	A	1241	U
6	A	1244	A
6	A	1248	G
6	A	1251	U
6	A	1252	G
6	A	1264	G
6	A	1266	U
6	A	1273	A
6	A	1274	A
6	A	1280	U
6	A	1281	A
6	A	1294	G
6	A	1296	C
6	A	1297	C
6	A	1299	G
6	A	1314	C
6	A	1321	G
6	A	1323	G
6	A	1325	G

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Mol	Chain	Res	Type
6	A	1330	C
6	A	1332	G
6	A	1334	A
6	A	1340	A
6	A	1341	G
6	A	1347	G
6	A	1351	A
6	A	1352	U
6	A	1357	A
6	A	1362	A
6	A	1364	G
6	A	1373	G
6	A	1374	U
6	A	1388	A
6	A	1391	C
6	A	1392	A
6	A	1405	C
6	A	1413	G
6	A	1416	G
6	A	1423	C
6	A	1425	A
6	A	1426	G
6	A	1427	A
6	A	1428	A
6	A	1435	A
6	A	1436	G
6	A	1441	A
6	A	1444	G
6	A	1446	A
6	A	1448	G
6	A	1451	G
6	A	1457	U
6	A	1458	U
6	A	1459	A
6	A	1466	A
6	A	1469	G
6	A	1481	G
6	A	1485	G
6	A	1486	A
6	A	1488	G
6	A	1491	G
6	A	1493	A

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Mol	Chain	Res	Type
6	A	1497	A
6	A	1500	U
6	A	1502	G
6	A	1511	G
6	A	1514	C
6	A	1523	G
6	A	1524	G
26	W	15	G
28	a	9	G
28	a	14	A
28	a	23	G
28	a	27	G
28	a	44	A
28	a	45	G
28	a	46	G
28	a	51	G
28	a	58	G
28	a	70	G
28	a	71	A
28	a	74	A
28	a	75	G
28	a	79	C
28	a	83	G
28	a	84	A
28	a	85	G
28	a	92	A
28	a	95	A
28	a	97	A
28	a	101	U
28	a	102	G
28	a	118	A
28	a	119	A
28	a	120	U
28	a	124	G
28	a	125	G
28	a	131	A
28	a	142	C
28	a	147	G
28	a	163	C
28	a	166	U
28	a	171	G
28	a	173	A

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Mol	Chain	Res	Type
28	a	181	A
28	a	196	A
28	a	199	A
28	a	205	G
28	a	206	U
28	a	215	G
28	a	216	A
28	a	222	A
28	a	223	A
28	a	224	U
28	a	228	C
28	a	230	G
28	a	233	A
28	a	242	G
28	a	248	G
28	a	249	C
28	a	252	G
28	a	255	A
28	a	261	G
28	a	264	U
28	a	265	A
28	a	271	U
28	a	273	A
28	a	279	A
28	a	289	G
28	a	293	A
28	a	294	A
28	a	305	A
28	a	315	U
28	a	319	G
28	a	322	U
28	a	323	G
28	a	324	A
28	a	327	G
28	a	330	C
28	a	337	C
28	a	339	A
28	a	346	C
28	a	349	U
28	a	350	G
28	a	356	A
28	a	358	A

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Mol	Chain	Res	Type
28	a	359	U
28	a	377	G
28	a	379	G
28	a	387	G
28	a	390	U
28	a	396	U
28	a	397	G
28	a	403	A
28	a	435	C
28	a	438	A
28	a	439	U
28	a	442	U
28	a	445	A
28	a	446	C
28	a	447	C
28	a	448	A
28	a	456	G
28	a	461	A
28	a	464	G
28	a	472	G
28	a	480	G
28	a	482	G
28	a	485	G
28	a	487	G
28	a	495	U
28	a	496	A
28	a	499	A
28	a	508	C
28	a	520	A
28	a	522	C
28	a	523	A
28	a	535	C
28	a	536	U
28	a	537	U
28	a	538	G
28	a	553	A
28	a	558	U
28	a	561	U
28	a	563	U
28	a	565	A
28	a	576	A
28	a	582	A

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Mol	Chain	Res	Type
28	a	583	U
28	a	593	A
28	a	594	G
28	a	603	U
28	a	604	A
28	a	610	U
28	a	622	A
28	a	624	G
28	a	627	A
28	a	635	U
28	a	636	A
28	a	637	G
28	a	644	U
28	a	645	A
28	a	649	G
28	a	653	G
28	a	658	A
28	a	667	A
28	a	676	U
28	a	702	G
28	a	716	G
28	a	719	G
28	a	720	A
28	a	737	U
28	a	743	G
28	a	744	G
28	a	754	A
28	a	755	C
28	a	765	G
28	a	766	G
28	a	772	A
28	a	774	G
28	a	775	G
28	a	779	A
28	a	781	C
28	a	795	G
28	a	801	U
28	a	802	C
28	a	817	U
28	a	818	U
28	a	820	G
28	a	836	U

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Mol	Chain	Res	Type
28	a	848	G
28	a	858	G
28	a	870	G
28	a	871	G
28	a	872	G
28	a	873	U
28	a	874	C
28	a	876	U
28	a	877	C
28	a	878	C
28	a	879	C
28	a	880	G
28	a	881	A
28	a	882	C
28	a	884	U
28	a	885	A
28	a	886	C
28	a	899	A
28	a	914	G
28	a	921	C
28	a	922	G
28	a	931	A
28	a	935	A
28	a	936	C
28	a	938	C
28	a	949	A
28	a	951	C
28	a	952	G
28	a	954	C
28	a	964	A
28	a	972	C
28	a	973	A
28	a	974	A
28	a	975	C
28	a	979	G
28	a	980	A
28	a	986	A
28	a	993	G
28	a	1002	U
28	a	1003	U
28	a	1007	G
28	a	1012	G

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Mol	Chain	Res	Type
28	a	1016	U
28	a	1018	A
28	a	1023	U
28	a	1031	G
28	a	1040	A
28	a	1041	G
28	a	1046	G
28	a	1047	A
28	a	1048	G
28	a	1050	U
28	a	1051	U
28	a	1052	G
28	a	1054	C
28	a	1056	U
28	a	1057	A
28	a	1058	G
28	a	1060	A
28	a	1061	G
28	a	1062	C
28	a	1063	A
28	a	1065	C
28	a	1066	C
28	a	1067	A
28	a	1070	C
28	a	1071	U
28	a	1073	U
28	a	1078	A
28	a	1080	A
28	a	1093	A
28	a	1099	C
28	a	1100	G
28	a	1101	A
28	a	1102	G
28	a	1112	G
28	a	1117	A
28	a	1119	A
28	a	1120	U
28	a	1122	U
28	a	1123	A
28	a	1124	A
28	a	1125	C
28	a	1126	G

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Mol	Chain	Res	Type
28	a	1129	G
28	a	1133	A
28	a	1146	A
28	a	1147	A
28	a	1148	G
28	a	1162	G
28	a	1163	U
28	a	1164	A
28	a	1165	A
28	a	1166	G
28	a	1167	U
28	a	1193	G
28	a	1198	U
28	a	1199	G
28	a	1214	A
28	a	1223	G
28	a	1225	G
28	a	1234	A
28	a	1237	G
28	a	1238	C
28	a	1240	A
28	a	1242	U
28	a	1243	G
28	a	1249	A
28	a	1253	G
28	a	1258	G
28	a	1259	A
28	a	1261	A
28	a	1263	U
28	a	1275	A
28	a	1276	C
28	a	1287	A
28	a	1288	A
28	a	1301	C
28	a	1304	G
28	a	1307	C
28	a	1308	A
28	a	1316	U
28	a	1334	G
28	a	1339	U
28	a	1347	G
28	a	1352	A

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Mol	Chain	Res	Type
28	a	1354	A
28	a	1355	A
28	a	1361	G
28	a	1366	U
28	a	1370	A
28	a	1371	A
28	a	1372	A
28	a	1373	C
28	a	1379	A
28	a	1382	A
28	a	1403	G
28	a	1404	C
28	a	1408	G
28	a	1414	A
28	a	1415	C
28	a	1420	A
28	a	1421	A
28	a	1423	G
28	a	1428	G
28	a	1429	C
28	a	1438	C
28	a	1439	G
28	a	1445	U
28	a	1446	G
28	a	1447	U
28	a	1469	G
28	a	1480	U
28	a	1496	A
28	a	1497	G
28	a	1511	G
28	a	1524	U
28	a	1525	U
28	a	1529	U
28	a	1538	G
28	a	1548	A
28	a	1550	G
28	a	1556	A
28	a	1558	G
28	a	1559	A
28	a	1560	A
28	a	1568	U
28	a	1573	U

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Mol	Chain	Res	Type
28	a	1574	U
28	a	1575	C
28	a	1576	A
28	a	1580	A
28	a	1597	C
28	a	1598	A
28	a	1624	A
28	a	1627	A
28	a	1628	C
28	a	1629	C
28	a	1634	C
28	a	1637	U
28	a	1638	U
28	a	1639	G
28	a	1641	G
28	a	1650	G
28	a	1657	G
28	a	1664	G
28	a	1673	C
28	a	1685	G
28	a	1686	G
28	a	1690	A
28	a	1710	A
28	a	1717	U
28	a	1718	A
28	a	1719	C
28	a	1720	U
28	a	1721	C
28	a	1724	U
28	a	1725	A
28	a	1740	G
28	a	1741	A
28	a	1742	A
28	a	1744	A
28	a	1745	U
28	a	1750	G
28	a	1751	G
28	a	1760	A
28	a	1763	G
28	a	1769	U
28	a	1771	A
28	a	1773	A

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Mol	Chain	Res	Type
28	a	1775	C
28	a	1787	C
28	a	1788	A
28	a	1795	A
28	a	1798	G
28	a	1803	C
28	a	1807	U
28	a	1816	A
28	a	1841	A
28	a	1844	G
28	a	1849	G
28	a	1851	U
28	a	1852	U
28	a	1859	A
28	a	1860	G
28	a	1865	G
28	a	1871	G
28	a	1893	G
28	a	1906	A
28	a	1916	G
28	a	1917	G
28	a	1924	A
28	a	1925	A
28	a	1928	C
28	a	1942	U
28	a	1945	C
28	a	1951	G
28	a	1954	C
28	a	1957	A
28	a	1958	U
28	a	1959	G
28	a	1967	G
28	a	1978	U
28	a	1980	U
28	a	1984	C
28	a	2008	A
28	a	2010	C
28	a	2017	6MZ
28	a	2018	A
28	a	2019	G
28	a	2020	A
28	a	2022	G

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Mol	Chain	Res	Type
28	a	2023	C
28	a	2030	U
28	a	2042	C
28	a	2043	G
28	a	2047	A
28	a	2048	G
28	a	2049	A
28	a	2055	U
28	a	2056	G7M
28	a	2057	A
28	a	2058	A
28	a	2067	G
28	a	2080	G
28	a	2088	A
28	a	2091	C
28	a	2093	G
28	a	2095	U
28	a	2097	G
28	a	2098	U
28	a	2099	G
28	a	2100	U
28	a	2104	A
28	a	2105	U
28	a	2106	A
28	a	2107	G
28	a	2108	G
28	a	2111	G
28	a	2113	A
28	a	2114	G
28	a	2115	G
28	a	2116	C
28	a	2118	U
28	a	2119	U
28	a	2120	G
28	a	2121	A
28	a	2123	G
28	a	2125	G
28	a	2126	U
28	a	2127	G
28	a	2131	G
28	a	2132	C
28	a	2137	U

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Mol	Chain	Res	Type
28	a	2139	G
28	a	2144	G
28	a	2145	A
28	a	2146	G
28	a	2151	C
28	a	2153	U
28	a	2154	U
28	a	2155	G
28	a	2157	A
28	a	2160	A
28	a	2161	C
28	a	2162	C
28	a	2165	C
28	a	2169	G
28	a	2170	C
28	a	2173	G
28	a	2185	A
28	a	2186	A
28	a	2187	C
28	a	2191	G
28	a	2194	C
28	a	2195	C
28	a	2199	A
28	a	2200	U
28	a	2201	C
28	a	2204	G
28	a	2212	A
28	a	2225	G
28	a	2226	G
28	a	2238	OMG
28	a	2255	A
28	a	2260	A
28	a	2265	A
28	a	2270	U
28	a	2274	A
28	a	2275	A
28	a	2289	C
28	a	2290	G
28	a	2291	G
28	a	2292	U
28	a	2295	G
28	a	2296	A

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Mol	Chain	Res	Type
28	a	2297	A
28	a	2306	U
28	a	2307	A
28	a	2309	A
28	a	2312	A
28	a	2313	U
28	a	2314	A
28	a	2321	A
28	a	2323	A
28	a	2330	U
28	a	2332	G
28	a	2334	C
28	a	2337	C
28	a	2348	C
28	a	2359	U
28	a	2366	G
28	a	2370	G
28	a	2372	C
28	a	2378	G
28	a	2389	U
28	a	2393	U
28	a	2396	G
28	a	2412	A
28	a	2414	C
28	a	2416	G
28	a	2417	A
28	a	2421	A
28	a	2422	A
28	a	2428	U
28	a	2432	2MG
28	a	2434	G
28	a	2435	A
28	a	2436	H2U
28	a	2446	A
28	a	2463	A
28	a	2474	G
28	a	2477	G
28	a	2478	U
28	a	2481	G
28	a	2485	OMC
28	a	2489	G
28	a	2492	G

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Mol	Chain	Res	Type
28	a	2493	U
28	a	2505	A
28	a	2506	U
28	a	2507	C
28	a	2516	G
28	a	2522	G
28	a	2532	G
28	a	2534	A
28	a	2543	C
28	a	2553	A
28	a	2554	G
28	a	2560	C
28	a	2565	G
28	a	2572	U
28	a	2586	G
28	a	2588	C
28	a	2589	A
28	a	2600	U
28	a	2602	U
28	a	2616	U
28	a	2617	U
28	a	2630	G
28	a	2633	C
28	a	2641	A
28	a	2650	G
28	a	2656	G
28	a	2672	G
28	a	2676	U
28	a	2677	U
28	a	2689	G
28	a	2692	A
28	a	2701	G
28	a	2702	C
28	a	2713	U
28	a	2719	G
28	a	2720	A
28	a	2735	A
28	a	2738	G
28	a	2744	A
28	a	2745	A
28	a	2748	G
28	a	2752	A

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Mol	Chain	Res	Type
28	a	2756	U
28	a	2763	A
28	a	2765	A
28	a	2766	U
28	a	2780	G
28	a	2784	U
28	a	2785	U
28	a	2786	G
28	a	2787	A
28	a	2796	A
28	a	2805	C
28	a	2807	A
28	a	2808	A
28	a	2812	U
28	a	2823	U
28	a	2837	A
28	a	2852	U
28	a	2854	G
28	a	2860	A
28	a	2867	C
28	a	2871	U
28	a	2872	U
28	a	2878	U
28	a	2889	C
29	b	9	G
29	b	24	G
29	b	25	A
29	b	26	A
29	b	32	U
29	b	40	U
29	b	41	C
29	b	42	C
29	b	44	G
29	b	52	A
29	b	53	A
29	b	56	G
29	b	64	G
29	b	67	U
29	b	73	A
29	b	89	U
29	b	90	C
29	b	91	C

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Mol	Chain	Res	Type
29	b	105	G
29	b	109	A
29	b	116	A
29	b	117	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	5	U
6	A	83	G
6	A	87	C
6	A	183	A
6	A	273	A
6	A	314	A
6	A	322	C
6	A	332	A
6	A	434	A
6	A	491	U
6	A	512	C
6	A	666	U
6	A	757	G
6	A	893	C
6	A	976	U
6	A	1039	C
6	A	1162	C
6	A	1164	A
6	A	1195	A
6	A	1233	A
6	A	1247	G
6	A	1391	C

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

38 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
28	PSU	a	2591	28	18,21,22	2.25	8 (44%)	22,30,33	1.84	4 (18%)
28	PSU	a	2567	56,28	18,21,22	2.30	9 (50%)	22,30,33	1.93	4 (18%)
28	PSU	a	1904	28	18,21,22	2.08	7 (38%)	22,30,33	1.77	4 (18%)
28	5MC	a	1949	56,28	18,22,23	1.94	6 (33%)	26,32,35	1.23	2 (7%)
6	2MG	A	1201	6,56	23,26,27	2.56	6 (26%)	32,38,41	2.10	11 (34%)
6	2MG	A	1510	6,56	23,26,27	2.59	6 (26%)	32,38,41	2.18	10 (31%)
28	OMG	a	2238	56,28	23,26,27	2.40	6 (26%)	33,38,41	1.80	8 (24%)
28	PSU	a	2592	28	18,21,22	2.24	8 (44%)	22,30,33	1.89	3 (13%)
6	MA6	A	1512	6	23,26,27	1.28	3 (13%)	34,38,41	2.28	9 (26%)
28	6MZ	a	2017	28	22,25,26	2.37	3 (13%)	30,36,39	2.49	10 (33%)
28	OMU	a	2539	56,28	19,22,23	2.71	7 (36%)	26,31,34	1.76	5 (19%)
28	5MU	a	1926	56,28	19,22,23	2.65	7 (36%)	28,32,35	3.86	9 (32%)
28	PSU	a	2444	28	18,21,22	2.37	8 (44%)	22,30,33	1.85	3 (13%)
28	OMC	a	2485	28,55	19,22,23	1.83	5 (26%)	26,31,34	1.05	2 (7%)
6	MA6	A	1513	6	23,26,27	1.26	3 (13%)	34,38,41	2.27	9 (26%)
28	2MG	a	2432	28	23,26,27	2.57	7 (30%)	32,38,41	2.19	11 (34%)
6	4OC	A	1396	6	20,23,24	2.15	4 (20%)	26,32,35	1.04	3 (11%)
31	MEQ	d	150	31	8,9,10	0.90	0	5,10,12	0.66	0
28	6MZ	a	1608	28	22,25,26	2.41	4 (18%)	30,36,39	2.21	10 (33%)
28	PSU	a	1898	28	18,21,22	2.00	7 (38%)	22,30,33	1.85	3 (13%)
28	1MG	a	735	28	22,26,27	2.51	6 (27%)	33,39,42	2.00	8 (24%)
16	IAS	K	119	16	5,6,8	1.86	1 (20%)	3,6,10	3.52	1 (33%)
28	PSU	a	736	28,55	18,21,22	2.20	9 (50%)	22,30,33	1.93	4 (18%)
28	PSU	a	945	28	18,21,22	2.29	8 (44%)	22,30,33	1.96	4 (18%)
28	H2U	a	2436	28	18,21,22	4.04	5 (27%)	21,30,33	4.63	6 (28%)
6	2MG	A	960	6	23,26,27	2.58	5 (21%)	32,38,41	2.15	9 (28%)
28	3TD	a	1902	28	18,22,23	2.73	7 (38%)	22,32,35	1.75	2 (9%)
17	D2T	L	89	17	7,9,10	1.35	1 (14%)	6,11,13	1.41	1 (16%)
28	G7M	a	2056	56,28	23,26,27	2.22	5 (21%)	35,39,42	1.84	8 (22%)
28	PSU	a	2491	56,28	18,21,22	2.23	7 (38%)	22,30,33	1.87	3 (13%)
6	G7M	A	521	6,56	23,26,27	2.17	5 (21%)	35,39,42	1.89	7 (20%)
6	UR3	A	1492	6	19,22,23	2.54	5 (26%)	26,32,35	1.39	2 (7%)
39	4D4	l	82	39	9,11,12	0.80	0	8,13,15	1.70	2 (25%)
28	2MA	a	2490	56,28,55	22,25,26	1.37	4 (18%)	33,37,40	2.08	7 (21%)
6	5MC	A	961	6	18,22,23	1.91	6 (33%)	26,32,35	1.33	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	2MG	a	1822	28	23,26,27	2.59	7 (30%)	32,38,41	2.01	8 (25%)
39	MS6	l	83	39	5,7,8	0.64	0	2,7,9	1.53	1 (50%)
6	PSU	A	510	6,56,55	18,21,22	2.10	9 (50%)	22,30,33	1.81	5 (22%)

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
28	PSU	a	2591	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2567	56,28	-	0/7/25/26	0/2/2/2
28	PSU	a	1904	28	-	0/7/25/26	0/2/2/2
28	5MC	a	1949	56,28	-	0/7/25/26	0/2/2/2
6	2MG	A	1201	6,56	-	0/9/27/28	0/3/3/3
6	2MG	A	1510	6,56	-	0/9/27/28	0/3/3/3
28	OMG	a	2238	56,28	-	3/9/27/28	0/3/3/3
28	PSU	a	2592	28	-	0/7/25/26	0/2/2/2
6	MA6	A	1512	6	-	0/11/29/30	0/3/3/3
28	6MZ	a	2017	28	-	2/9/27/28	0/3/3/3
28	OMU	a	2539	56,28	-	0/9/27/28	0/2/2/2
28	5MU	a	1926	56,28	-	0/7/25/26	0/2/2/2
28	PSU	a	2444	28	-	0/7/25/26	0/2/2/2
28	OMC	a	2485	28,55	-	1/9/27/28	0/2/2/2
6	MA6	A	1513	6	-	2/11/29/30	0/3/3/3
28	2MG	a	2432	28	-	2/9/27/28	0/3/3/3
6	4OC	A	1396	6	-	1/9/29/30	0/2/2/2
31	MEQ	d	150	31	-	4/8/9/11	-
28	6MZ	a	1608	28	-	0/9/27/28	0/3/3/3
28	PSU	a	1898	28	-	0/7/25/26	0/2/2/2
28	1MG	a	735	28	-	0/7/25/26	0/3/3/3
16	IAS	K	119	16	-	1/3/5/8	-
28	PSU	a	736	28,55	-	1/7/25/26	0/2/2/2
28	PSU	a	945	28	-	0/7/25/26	0/2/2/2
28	H2U	a	2436	28	-	1/7/38/39	0/2/2/2
6	2MG	A	960	6	-	0/9/27/28	0/3/3/3
28	3TD	a	1902	28	-	3/7/25/26	0/2/2/2
17	D2T	L	89	17	-	4/7/12/14	-
28	G7M	a	2056	56,28	-	2/7/25/26	0/3/3/3
28	PSU	a	2491	56,28	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	G7M	A	521	6,56	-	3/7/25/26	0/3/3/3
6	UR3	A	1492	6	-	0/7/25/26	0/2/2/2
39	4D4	l	82	39	-	1/11/12/14	-
28	2MA	a	2490	56,28,55	-	2/7/25/26	0/3/3/3
6	5MC	A	961	6	-	0/7/25/26	0/2/2/2
28	2MG	a	1822	28	-	0/9/27/28	0/3/3/3
39	MS6	l	83	39	-	2/4/6/8	-
6	PSU	A	510	6,56,55	-	0/7/25/26	0/2/2/2

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2436	H2U	O4-C4	9.71	1.43	1.23
28	a	1608	6MZ	C6-N6	9.65	1.44	1.34
28	a	2017	6MZ	C6-N6	9.27	1.44	1.34
6	A	1201	2MG	O6-C6	9.00	1.40	1.23
6	A	1510	2MG	O6-C6	8.96	1.40	1.23
6	A	960	2MG	O6-C6	8.96	1.40	1.23
28	a	1822	2MG	O6-C6	8.72	1.40	1.23
6	A	1492	UR3	O4-C4	8.58	1.42	1.23
28	a	2432	2MG	O6-C6	8.48	1.39	1.23
28	a	2238	OMG	O6-C6	8.15	1.39	1.23
28	a	1902	3TD	O4-C4	8.10	1.40	1.23
28	a	2436	H2U	C2-N1	8.05	1.47	1.35
28	a	2436	H2U	O2-C2	7.98	1.37	1.23
28	a	735	1MG	O6-C6	7.85	1.39	1.23
6	A	521	G7M	O6-C6	7.76	1.38	1.23
28	a	2539	OMU	O4-C4	7.64	1.39	1.24
28	a	2056	G7M	O6-C6	7.59	1.38	1.23
28	a	2436	H2U	C2-N3	6.70	1.49	1.38
28	a	1926	5MU	C2-N1	-6.03	1.28	1.38
6	A	1396	4OC	O2-C2	5.93	1.34	1.23
6	A	960	2MG	C2-N2	5.86	1.46	1.33
6	A	1201	2MG	C2-N2	5.77	1.46	1.33
6	A	1510	2MG	C2-N2	5.72	1.46	1.33
28	a	735	1MG	C2-N2	5.68	1.44	1.34
28	a	1822	2MG	C2-N2	5.67	1.46	1.33
28	a	2432	2MG	C2-N2	5.54	1.45	1.33
28	a	1926	5MU	C2-N3	-5.30	1.28	1.38
6	A	1396	4OC	C4-N4	5.14	1.46	1.35
28	a	2436	H2U	C4-N3	4.70	1.45	1.37
28	a	2539	OMU	C2-N1	-4.60	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2485	OMC	C4-N4	4.55	1.44	1.33
28	a	1926	5MU	C6-N1	-4.55	1.30	1.38
28	a	2444	PSU	C2-N1	-4.53	1.30	1.36
28	a	2238	OMG	C6-N1	-4.51	1.30	1.38
28	a	2444	PSU	C4-N3	-4.41	1.30	1.38
28	a	2567	PSU	C2-N1	-4.33	1.30	1.36
28	a	945	PSU	C4-N3	-4.31	1.30	1.38
28	a	2490	2MA	C6-N6	4.26	1.44	1.34
28	a	2591	PSU	C4-N3	-4.26	1.30	1.38
28	a	2444	PSU	C2-N3	-4.24	1.30	1.37
28	a	736	PSU	C2-N1	-4.23	1.31	1.36
28	a	2485	OMC	C2-N1	-4.22	1.30	1.40
28	a	1902	3TD	C2-N1	-4.20	1.31	1.37
28	a	2591	PSU	C2-N3	-4.18	1.30	1.37
28	a	2539	OMU	C4-N3	-4.15	1.31	1.38
28	a	2491	PSU	C2-N1	-4.14	1.31	1.36
28	a	2567	PSU	C4-N3	-4.13	1.31	1.38
28	a	945	PSU	C2-N1	-4.09	1.31	1.36
28	a	2592	PSU	C4-N3	-4.07	1.31	1.38
6	A	961	5MC	C4-N4	4.07	1.44	1.34
28	a	735	1MG	C6-N1	-4.05	1.31	1.40
28	a	2491	PSU	C4-N3	-4.05	1.31	1.38
28	a	2539	OMU	C2-N3	-4.05	1.30	1.38
28	a	2592	PSU	C2-N3	-4.01	1.30	1.37
28	a	736	PSU	C4-N3	-4.00	1.31	1.38
28	a	2056	G7M	C5-N7	-4.00	1.34	1.39
28	a	1949	5MC	C2-N1	-3.99	1.31	1.40
28	a	945	PSU	C2-N3	-3.99	1.30	1.37
28	a	2238	OMG	C2-N2	3.95	1.43	1.34
28	a	2567	PSU	C2-N3	-3.95	1.30	1.37
6	A	1396	4OC	C2-N1	-3.93	1.31	1.40
28	a	1949	5MC	C4-N4	3.91	1.44	1.34
28	a	2591	PSU	C2-N1	-3.89	1.31	1.36
28	a	2491	PSU	C2-N3	-3.89	1.30	1.37
6	A	510	PSU	C2-N1	-3.87	1.31	1.36
28	a	2592	PSU	C2-N1	-3.82	1.31	1.36
6	A	510	PSU	C4-N3	-3.82	1.31	1.38
28	a	2432	2MG	C6-N1	-3.81	1.31	1.38
28	a	1904	PSU	C4-N3	-3.81	1.31	1.38
28	a	1904	PSU	C2-N1	-3.81	1.31	1.36
6	A	961	5MC	C2-N1	-3.77	1.31	1.40
28	a	1926	5MU	C4-N3	-3.75	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1898	PSU	C4-N3	-3.72	1.31	1.38
6	A	1492	UR3	C4-N3	-3.68	1.32	1.40
28	a	2017	6MZ	C8-N9	-3.66	1.31	1.37
6	A	521	G7M	C5-N7	-3.66	1.34	1.39
28	a	2056	G7M	C6-N1	-3.63	1.32	1.38
16	K	119	IAS	OD1-CG	3.63	1.40	1.19
28	a	1902	3TD	C4-N3	-3.61	1.32	1.40
28	a	1898	PSU	C2-N1	-3.58	1.31	1.36
6	A	1492	UR3	C2-N3	-3.57	1.32	1.39
28	a	1904	PSU	C2-N3	-3.54	1.31	1.37
6	A	1512	MA6	C8-N9	-3.54	1.31	1.37
28	a	736	PSU	C2-N3	-3.52	1.31	1.37
6	A	961	5MC	C6-N1	-3.52	1.32	1.38
28	a	1608	6MZ	C8-N9	-3.51	1.31	1.37
6	A	521	G7M	C6-N1	-3.50	1.32	1.38
28	a	1926	5MU	C6-C5	3.49	1.40	1.34
6	A	510	PSU	C2-N3	-3.47	1.31	1.37
28	a	1822	2MG	C6-N1	-3.39	1.32	1.38
28	a	1949	5MC	C6-N1	-3.36	1.32	1.38
28	a	1898	PSU	C2-N3	-3.31	1.31	1.37
6	A	1513	MA6	C6-N6	3.26	1.46	1.36
6	A	1513	MA6	C8-N9	-3.24	1.31	1.37
6	A	1510	2MG	C6-N1	-3.23	1.32	1.38
28	a	1902	3TD	C6-C5	3.21	1.39	1.35
6	A	960	2MG	C6-N1	-3.20	1.32	1.38
6	A	1512	MA6	C6-N6	3.16	1.46	1.36
28	a	1949	5MC	O2-C2	-3.15	1.17	1.23
28	a	2017	6MZ	C5-N7	-3.13	1.33	1.39
28	a	2444	PSU	O4-C4	-3.13	1.17	1.23
28	a	2567	PSU	O4-C4	-3.09	1.17	1.23
28	a	2592	PSU	O4-C4	-3.09	1.17	1.23
28	a	945	PSU	C6-N1	-3.09	1.31	1.36
28	a	1902	3TD	C2-N3	-3.07	1.31	1.38
28	a	1926	5MU	O4-C4	-3.07	1.17	1.23
28	a	945	PSU	O4-C4	-3.05	1.17	1.23
28	a	736	PSU	C6-N1	-3.03	1.31	1.36
6	A	1201	2MG	C6-N1	-3.02	1.33	1.38
28	a	2491	PSU	O4-C4	-3.02	1.17	1.23
28	a	1822	2MG	C5-N7	-3.02	1.33	1.39
28	a	2567	PSU	C6-N1	-3.01	1.31	1.36
6	A	960	2MG	C5-N7	-3.01	1.33	1.39
6	A	1492	UR3	C2-N1	-2.99	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	521	G7M	C2-N2	2.97	1.41	1.34
28	a	2592	PSU	C6-C5	2.94	1.38	1.35
28	a	2539	OMU	O2-C2	-2.93	1.17	1.23
28	a	2591	PSU	O4-C4	-2.93	1.18	1.23
28	a	1904	PSU	C6-C5	2.92	1.38	1.35
28	a	2238	OMG	C8-N9	-2.91	1.31	1.37
28	a	736	PSU	O4-C4	-2.90	1.18	1.23
28	a	2491	PSU	C6-N1	-2.90	1.31	1.36
28	a	1926	5MU	O2-C2	-2.88	1.17	1.23
28	a	1608	6MZ	C5-N7	-2.85	1.33	1.39
28	a	2432	2MG	C5-N7	-2.84	1.33	1.39
6	A	510	PSU	C6-C5	2.82	1.38	1.35
28	a	2056	G7M	C2-N2	2.80	1.40	1.34
28	a	2444	PSU	O2-C2	-2.80	1.17	1.23
28	a	2444	PSU	C6-N1	-2.79	1.31	1.36
6	A	961	5MC	O2-C2	-2.75	1.18	1.23
28	a	2238	OMG	C5-N7	-2.74	1.33	1.39
28	a	2591	PSU	C6-N1	-2.73	1.31	1.36
28	a	1898	PSU	O4-C4	-2.72	1.18	1.23
28	a	2591	PSU	C6-C5	2.71	1.38	1.35
28	a	2238	OMG	C2-N1	-2.70	1.31	1.37
28	a	1898	PSU	C6-C5	2.69	1.38	1.35
28	a	2491	PSU	O2-C2	-2.69	1.17	1.23
6	A	510	PSU	O4-C4	-2.67	1.18	1.23
28	a	2567	PSU	O2-C2	-2.65	1.17	1.23
28	a	945	PSU	O2-C2	-2.64	1.17	1.23
28	a	2592	PSU	C6-N1	-2.62	1.31	1.36
28	a	2539	OMU	C5-C4	-2.61	1.37	1.43
28	a	735	1MG	C8-N9	-2.61	1.31	1.37
28	a	1904	PSU	O4-C4	-2.60	1.18	1.23
6	A	510	PSU	C6-N1	-2.59	1.31	1.36
28	a	735	1MG	C5-N7	-2.59	1.34	1.39
6	A	1201	2MG	C5-N7	-2.59	1.34	1.39
28	a	2592	PSU	O2-C2	-2.59	1.18	1.23
28	a	2444	PSU	C6-C5	2.57	1.38	1.35
6	A	1510	2MG	C5-N7	-2.55	1.34	1.39
28	a	1902	3TD	O2-C2	-2.54	1.18	1.23
6	A	1510	2MG	C4-N9	-2.53	1.31	1.38
28	a	2591	PSU	O2-C2	-2.53	1.18	1.23
28	a	2539	OMU	C6-N1	-2.51	1.31	1.38
28	a	2056	G7M	C2-N1	-2.51	1.31	1.37
6	A	521	G7M	C2-N1	-2.47	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1904	PSU	C6-N1	-2.46	1.32	1.36
28	a	1898	PSU	C6-N1	-2.46	1.32	1.36
28	a	1902	3TD	C6-N1	-2.44	1.32	1.36
28	a	736	PSU	O2-C2	-2.41	1.18	1.23
17	L	89	D2T	CB-CG	2.39	1.56	1.52
28	a	2567	PSU	O4'-C1'	-2.37	1.40	1.43
28	a	1904	PSU	O2-C2	-2.36	1.18	1.23
28	a	945	PSU	C6-C5	2.36	1.38	1.35
28	a	736	PSU	C6-C5	2.35	1.38	1.35
6	A	1512	MA6	C5-N7	-2.34	1.34	1.39
28	a	2491	PSU	C6-C5	2.33	1.38	1.35
28	a	1898	PSU	O2-C2	-2.32	1.18	1.23
28	a	2485	OMC	C5-C4	-2.32	1.37	1.42
6	A	510	PSU	O2-C2	-2.31	1.18	1.23
6	A	1513	MA6	C5-N7	-2.30	1.34	1.39
28	a	1822	2MG	CM2-N2	-2.29	1.41	1.45
6	A	1510	2MG	CM2-N2	-2.26	1.41	1.45
28	a	2567	PSU	C6-C5	2.26	1.38	1.35
28	a	2490	2MA	C8-N9	-2.26	1.33	1.37
28	a	2432	2MG	CM2-N2	-2.26	1.41	1.45
28	a	945	PSU	C4-C5	-2.26	1.37	1.44
28	a	1822	2MG	C4-N9	-2.25	1.32	1.38
6	A	1492	UR3	C6-N1	-2.24	1.32	1.38
6	A	1396	4OC	C2-N3	-2.24	1.31	1.36
28	a	1822	2MG	C8-N9	-2.23	1.32	1.37
28	a	1608	6MZ	C6-N1	-2.22	1.31	1.35
28	a	1949	5MC	C2-N3	-2.21	1.31	1.36
28	a	2432	2MG	C4-N9	-2.20	1.32	1.38
6	A	961	5MC	C6-C5	2.20	1.38	1.34
6	A	1201	2MG	C4-N9	-2.20	1.32	1.38
28	a	2592	PSU	C4-C5	-2.19	1.37	1.44
28	a	2490	2MA	C5-N7	-2.19	1.34	1.39
28	a	2485	OMC	O2-C2	-2.18	1.19	1.23
28	a	2485	OMC	C2-N3	-2.18	1.31	1.36
28	a	2490	2MA	C4-N9	-2.17	1.32	1.37
28	a	1949	5MC	C6-C5	2.14	1.38	1.34
6	A	961	5MC	C2-N3	-2.14	1.32	1.36
28	a	735	1MG	C5-C6	-2.13	1.40	1.45
28	a	2444	PSU	C4-C5	-2.12	1.38	1.44
28	a	2591	PSU	C4-C5	-2.11	1.38	1.44
28	a	736	PSU	C4-C5	-2.10	1.38	1.44
28	a	736	PSU	O4'-C1'	-2.09	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2432	2MG	C8-N9	-2.08	1.32	1.37
6	A	510	PSU	C4-C5	-2.07	1.38	1.44
6	A	510	PSU	O4'-C1'	-2.05	1.41	1.43
28	a	2567	PSU	C4-C5	-2.04	1.38	1.44
6	A	960	2MG	C8-N9	-2.02	1.33	1.37
6	A	1201	2MG	CM2-N2	-2.02	1.42	1.45

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2436	H2U	C4-N3-C2	-12.41	115.49	125.79
28	a	2436	H2U	O2-C2-N1	-10.48	109.95	123.11
28	a	1926	5MU	C4-N3-C2	-8.63	116.17	127.35
28	a	1926	5MU	N3-C2-N1	8.63	126.34	114.89
28	a	1926	5MU	C5M-C5-C4	8.44	128.06	118.77
28	a	2436	H2U	O4-C4-N3	-7.72	108.05	120.28
28	a	2432	2MG	C2-N3-C4	7.60	121.46	112.04
28	a	1926	5MU	C5-C6-N1	-7.53	115.59	123.34
6	A	1510	2MG	C2-N3-C4	7.29	121.08	112.04
6	A	960	2MG	C2-N3-C4	7.26	121.05	112.04
28	a	2490	2MA	C5-C4-N3	-7.11	119.19	127.19
28	a	2436	H2U	O2-C2-N3	-7.09	108.29	121.50
6	A	1201	2MG	C2-N3-C4	7.03	120.75	112.04
28	a	1822	2MG	C2-N3-C4	6.92	120.62	112.04
28	a	1902	3TD	N1-C2-N3	6.74	121.46	116.14
28	a	2436	H2U	O4-C4-C5	-6.63	108.02	122.17
28	a	1926	5MU	C5-C4-N3	6.58	120.92	115.31
28	a	1926	5MU	C5M-C5-C6	-6.57	114.08	122.85
28	a	735	1MG	C5-C4-N3	-6.53	117.87	128.46
28	a	2017	6MZ	C9-N6-C6	-6.39	117.36	122.87
28	a	945	PSU	N1-C2-N3	6.11	122.05	115.13
16	K	119	IAS	OD1-CG-CB	-6.07	107.73	125.43
28	a	736	PSU	N1-C2-N3	5.94	121.86	115.13
6	A	1512	MA6	C5-C4-N3	-5.82	119.15	126.75
28	a	2592	PSU	N1-C2-N3	5.70	121.59	115.13
6	A	1513	MA6	C5-C4-N3	-5.69	119.33	126.75
28	a	2491	PSU	N1-C2-N3	5.65	121.53	115.13
28	a	2444	PSU	N1-C2-N3	5.62	121.49	115.13
28	a	2591	PSU	N1-C2-N3	5.61	121.48	115.13
28	a	2567	PSU	N1-C2-N3	5.60	121.47	115.13
28	a	1898	PSU	N1-C2-N3	5.48	121.34	115.13
28	a	2539	OMU	N3-C2-N1	5.48	122.16	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2432	2MG	C5-C4-N3	-5.48	119.57	128.46
6	A	960	2MG	C5-C4-N3	-5.47	119.58	128.46
6	A	510	PSU	N1-C2-N3	5.46	121.32	115.13
28	a	1608	6MZ	C5-C4-N3	-5.42	119.67	126.75
28	a	2017	6MZ	N1-C2-N3	-5.39	120.17	128.60
28	a	1904	PSU	N1-C2-N3	5.38	121.22	115.13
28	a	2490	2MA	N3-C4-N9	5.31	134.36	126.99
6	A	521	G7M	C2-N3-C4	5.27	121.68	112.30
28	a	2238	OMG	C5-C4-N3	-5.24	119.97	128.46
28	a	2017	6MZ	C5-C4-N3	-5.10	120.10	126.75
6	A	1513	MA6	N1-C2-N3	-5.07	120.68	128.60
28	a	735	1MG	C2-N3-C4	5.05	123.34	111.98
28	a	1608	6MZ	N1-C2-N3	-5.05	120.70	128.60
6	A	1512	MA6	N1-C2-N3	-5.04	120.72	128.60
28	a	2056	G7M	C2-N3-C4	5.02	121.24	112.30
28	a	2436	H2U	N3-C2-N1	-5.00	111.36	116.65
6	A	1492	UR3	C4-N3-C2	-4.99	119.86	124.56
28	a	1822	2MG	C5-C4-N3	-4.92	120.49	128.46
6	A	961	5MC	C5-C6-N1	-4.83	118.37	123.34
28	a	735	1MG	N9-C4-N3	4.71	135.39	125.94
6	A	1512	MA6	N3-C4-N9	4.70	134.83	127.08
6	A	1201	2MG	C5-C4-N3	-4.69	120.85	128.46
6	A	521	G7M	C5-C4-N3	-4.59	119.35	128.15
6	A	1510	2MG	C5-C4-N3	-4.52	121.14	128.46
28	a	2238	OMG	C2-N3-C4	4.48	120.27	112.30
28	a	2539	OMU	C4-N3-C2	-4.32	120.89	126.58
6	A	1512	MA6	C2-N3-C4	4.28	121.87	111.75
6	A	521	G7M	C5-C6-N1	4.26	120.68	111.79
6	A	1513	MA6	C2-N3-C4	4.24	121.76	111.75
28	a	1926	5MU	O4-C4-N3	-4.22	112.03	120.12
6	A	1513	MA6	C2-N1-C6	4.20	121.67	111.75
28	a	1949	5MC	C5-C6-N1	-4.20	119.02	123.34
28	a	2056	G7M	C5-C6-N1	4.13	120.41	111.79
6	A	1512	MA6	C2-N1-C6	4.11	121.46	111.75
28	a	2017	6MZ	C6-C5-N7	4.11	136.84	132.39
28	a	2017	6MZ	C2-N3-C4	4.07	121.38	111.75
6	A	1513	MA6	N3-C4-N9	4.04	133.74	127.08
28	a	736	PSU	O2-C2-N1	-4.00	118.39	122.79
28	a	2056	G7M	C5-C4-N3	-3.99	120.50	128.15
28	a	1608	6MZ	C2-N3-C4	3.99	121.18	111.75
28	a	2056	G7M	C6-C5-N7	3.99	137.07	132.25
28	a	736	PSU	C4-N3-C2	-3.97	120.61	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	1898	PSU	C4-N3-C2	-3.92	120.69	126.34
28	a	2491	PSU	C4-N3-C2	-3.92	120.70	126.34
6	A	1510	2MG	C6-C5-N7	3.90	137.50	130.25
28	a	945	PSU	C4-N3-C2	-3.87	120.76	126.34
6	A	960	2MG	N9-C4-N3	3.85	133.68	125.94
28	a	2592	PSU	C4-N3-C2	-3.82	120.84	126.34
28	a	2591	PSU	C4-N3-C2	-3.78	120.89	126.34
28	a	2567	PSU	C4-N3-C2	-3.74	120.95	126.34
6	A	1513	MA6	N9-C8-N7	-3.71	108.83	113.91
6	A	1512	MA6	N9-C8-N7	-3.71	108.85	113.91
6	A	1513	MA6	C5-N7-C8	3.69	108.75	103.51
28	a	2432	2MG	N9-C4-N3	3.63	133.22	125.94
28	a	2238	OMG	N9-C4-N3	3.62	133.21	125.94
28	a	1608	6MZ	N3-C4-N9	3.61	133.03	127.08
28	a	2017	6MZ	C4-C5-N7	-3.60	106.23	110.62
28	a	1926	5MU	O2-C2-N1	-3.59	118.01	122.79
6	A	1512	MA6	C4-N9-C8	3.55	109.58	105.73
6	A	521	G7M	C6-C5-N7	3.55	136.54	132.25
6	A	1512	MA6	C5-N7-C8	3.53	108.53	103.51
28	a	2444	PSU	C4-N3-C2	-3.53	121.25	126.34
6	A	521	G7M	O6-C6-C5	-3.53	120.09	128.06
28	a	2017	6MZ	C5-N7-C8	3.51	108.49	103.51
28	a	2056	G7M	O6-C6-C5	-3.47	120.23	128.06
28	a	2567	PSU	O2-C2-N1	-3.44	119.00	122.79
6	A	521	G7M	N9-C4-N3	3.43	132.84	125.94
6	A	1201	2MG	C6-C5-N7	3.43	136.62	130.25
28	a	2490	2MA	N9-C8-N7	-3.39	109.28	113.91
28	a	1608	6MZ	C6-C5-N7	3.38	136.05	132.39
6	A	1513	MA6	C4-C5-N7	-3.35	106.54	110.62
28	a	1904	PSU	C4-N3-C2	-3.34	121.52	126.34
28	a	1608	6MZ	C5-N7-C8	3.32	108.23	103.51
28	a	1822	2MG	N9-C4-N3	3.32	132.61	125.94
6	A	510	PSU	C4-N3-C2	-3.32	121.56	126.34
39	l	82	4D4	NE-CZ-NH2	3.27	126.45	120.70
28	a	1608	6MZ	C4-C5-N7	-3.23	106.69	110.62
28	a	2485	OMC	O2-C2-N3	-3.15	117.20	122.33
28	a	1926	5MU	O2-C2-N3	-3.14	115.65	121.50
28	a	2491	PSU	O2-C2-N1	-3.13	119.34	122.79
28	a	1898	PSU	O2-C2-N1	-3.12	119.36	122.79
28	a	2490	2MA	C5-N7-C8	3.11	107.93	103.51
28	a	2017	6MZ	N3-C4-N9	3.10	132.20	127.08
28	a	2056	G7M	N9-C4-N3	3.10	132.16	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2432	2MG	C6-C5-N7	3.04	135.90	130.25
28	a	2238	OMG	C6-C5-N7	3.03	135.88	130.25
28	a	2490	2MA	C4-N9-C8	2.99	108.96	105.73
28	a	1608	6MZ	N9-C8-N7	-2.98	109.83	113.91
6	A	510	PSU	O2-C2-N1	-2.96	119.53	122.79
6	A	1513	MA6	C4-N9-C8	2.96	108.94	105.73
28	a	1822	2MG	C6-C5-N7	2.95	135.74	130.25
28	a	945	PSU	O2-C2-N1	-2.94	119.55	122.79
6	A	1512	MA6	C4-C5-N7	-2.94	107.03	110.62
6	A	1201	2MG	N9-C4-N3	2.89	131.74	125.94
6	A	1510	2MG	C4-C5-N7	-2.88	106.17	110.72
28	a	2444	PSU	O2-C2-N1	-2.84	119.67	122.79
28	a	1904	PSU	O2-C2-N1	-2.82	119.68	122.79
6	A	521	G7M	C2-N1-C6	-2.81	119.97	125.10
28	a	2592	PSU	O2-C2-N1	-2.80	119.71	122.79
28	a	2539	OMU	C5-C4-N3	2.73	118.93	114.84
6	A	1201	2MG	C4-C5-N7	-2.72	106.42	110.72
28	a	2017	6MZ	N9-C8-N7	-2.71	110.21	113.91
6	A	1396	4OC	O2-C2-N3	-2.71	117.93	122.33
28	a	2591	PSU	O2-C2-N1	-2.70	119.81	122.79
28	a	2490	2MA	C4-C5-N7	-2.66	107.38	110.62
28	a	2539	OMU	O2-C2-N1	-2.64	119.28	122.79
28	a	735	1MG	C5-C6-N1	2.63	120.00	114.91
6	A	960	2MG	C2-N1-C6	-2.60	121.49	124.48
28	a	1902	3TD	C4-N3-C2	-2.58	121.81	124.61
28	a	945	PSU	C6-N1-C2	-2.54	120.08	122.68
6	A	960	2MG	O6-C6-C5	-2.54	119.87	126.60
6	A	960	2MG	C6-C5-N7	2.53	134.95	130.25
28	a	2567	PSU	O4'-C1'-C2'	2.50	108.67	105.14
39	l	82	4D4	NH1-CZ-NE	-2.50	113.44	119.19
28	a	2432	2MG	C4-C5-N7	-2.47	106.81	110.72
28	a	2238	OMG	C4-C5-N7	-2.47	106.82	110.72
28	a	735	1MG	C6-C5-N7	2.45	134.88	129.35
28	a	2238	OMG	C8-N7-C5	2.44	108.66	104.24
6	A	1510	2MG	N9-C4-N3	2.44	130.83	125.94
28	a	1949	5MC	C5-C4-N3	-2.43	119.05	121.67
6	A	1510	2MG	N1-C2-N3	-2.41	120.23	123.95
6	A	1201	2MG	C8-N7-C5	2.39	108.56	104.24
6	A	960	2MG	C5-C6-N1	2.36	119.19	113.19
28	a	2238	OMG	C5-C6-N1	2.35	119.17	113.19
28	a	2056	G7M	C2-N1-C6	-2.35	120.81	125.10
28	a	2539	OMU	O4-C4-C5	-2.34	121.04	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	510	PSU	C6-N1-C2	-2.34	120.29	122.68
28	a	2432	2MG	C5-C6-N1	2.34	119.13	113.19
17	L	89	D2T	OD1-CG-CB	-2.33	117.57	122.44
6	A	961	5MC	C5-C4-N3	-2.31	119.18	121.67
28	a	2485	OMC	N1-C2-N3	2.31	123.02	118.81
6	A	1201	2MG	N9-C8-N7	-2.30	109.06	113.39
6	A	1510	2MG	C5-C6-N1	2.28	118.99	113.19
6	A	1510	2MG	C8-N7-C5	2.27	108.36	104.24
28	a	2490	2MA	N3-C2-N1	-2.27	121.54	125.72
6	A	1492	UR3	C5-C6-N1	-2.26	118.02	121.81
28	a	1822	2MG	C4-C5-N7	-2.26	107.14	110.72
6	A	1510	2MG	N9-C8-N7	-2.25	109.14	113.39
6	A	1201	2MG	CM2-N2-C2	-2.25	118.88	123.86
28	a	735	1MG	C4-C5-N7	-2.21	107.23	110.72
28	a	2432	2MG	N1-C2-N3	-2.20	120.54	123.95
6	A	510	PSU	O4'-C1'-C2'	2.20	108.25	105.14
6	A	960	2MG	C4-C5-N7	-2.20	107.23	110.72
28	a	2432	2MG	CM2-N2-C2	-2.20	119.00	123.86
6	A	1510	2MG	CM2-N2-C2	-2.19	119.02	123.86
28	a	2238	OMG	N9-C8-N7	-2.18	109.29	113.39
28	a	1822	2MG	C5-C6-N1	2.17	118.71	113.19
28	a	2432	2MG	C2-N1-C6	-2.16	122.00	124.48
28	a	2591	PSU	C5-C6-N1	-2.15	118.88	122.11
6	A	1201	2MG	C5-C6-N1	2.15	118.65	113.19
39	l	83	MS6	CE-SD-CG	2.15	107.78	100.40
28	a	2017	6MZ	C2-N1-C6	2.14	122.44	115.25
6	A	1201	2MG	N1-C2-N3	-2.13	120.66	123.95
28	a	735	1MG	C8-N7-C5	2.11	108.05	104.24
28	a	735	1MG	N9-C8-N7	-2.10	109.43	113.39
28	a	1904	PSU	O4'-C1'-C2'	2.10	108.11	105.14
28	a	1608	6MZ	C9-N6-C6	-2.09	121.07	122.87
6	A	1396	4OC	CM4-N4-C4	-2.09	118.36	122.45
28	a	2432	2MG	O6-C6-C5	-2.08	121.07	126.60
28	a	2432	2MG	C8-N7-C5	2.08	108.01	104.24
6	A	960	2MG	C8-N7-C5	2.06	107.96	104.24
28	a	736	PSU	C6-N1-C2	-2.06	120.58	122.68
28	a	1608	6MZ	C4-N9-C8	2.05	107.95	105.73
6	A	961	5MC	O2-C2-N3	-2.04	119.01	122.33
6	A	1201	2MG	C2-N1-C6	-2.04	122.14	124.48
28	a	2056	G7M	N2-C2-N1	2.03	121.04	116.71
28	a	1822	2MG	CM2-N2-C2	-2.03	119.39	123.86
6	A	1396	4OC	C5-C4-N3	-2.02	119.35	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	1822	2MG	N1-C2-N3	-2.02	120.83	123.95

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	521	G7M	C3'-C4'-C5'-O5'
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
17	L	89	D2T	SB-CB-CG-OD2
31	d	150	MEQ	O-C-CA-CB
16	K	119	IAS	N-CA-CB-CG
28	a	1902	3TD	O4'-C1'-C5-C4
28	a	1902	3TD	C2'-C1'-C5-C6
28	a	1902	3TD	O4'-C1'-C5-C6
28	a	2238	OMG	O4'-C4'-C5'-O5'
28	a	2238	OMG	C1'-C2'-O2'-CM2
28	a	2432	2MG	C3'-C4'-C5'-O5'
28	a	2017	6MZ	O4'-C4'-C5'-O5'
28	a	2017	6MZ	C3'-C4'-C5'-O5'
28	a	2056	G7M	O4'-C4'-C5'-O5'
28	a	2056	G7M	C3'-C4'-C5'-O5'
28	a	2238	OMG	C3'-C4'-C5'-O5'
28	a	2491	PSU	C3'-C4'-C5'-O5'
28	a	2491	PSU	O4'-C4'-C5'-O5'
6	A	1513	MA6	O4'-C4'-C5'-O5'
28	a	2432	2MG	O4'-C4'-C5'-O5'
6	A	521	G7M	O4'-C4'-C5'-O5'
39	l	83	MS6	CB-CG-SD-CE
6	A	1513	MA6	C3'-C4'-C5'-O5'
39	l	83	MS6	CA-CB-CG-SD
17	L	89	D2T	CG-CB-SB-CB1
6	A	521	G7M	C4'-C5'-O5'-P
31	d	150	MEQ	N-CA-CB-CG
28	a	2436	H2U	C4'-C5'-O5'-P
6	A	1396	4OC	O4'-C4'-C5'-O5'
39	l	82	4D4	CG-CD-NE-CZ
31	d	150	MEQ	OE1-CD-CG-CB
28	a	736	PSU	O4'-C1'-C5-C6
28	a	2485	OMC	C4'-C5'-O5'-P
28	a	2490	2MA	C4'-C5'-O5'-P
31	d	150	MEQ	NE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
28	a	2490	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	2591	PSU	1	0
28	a	2238	OMG	1	0
28	a	2017	6MZ	3	0
6	A	1396	4OC	2	0
31	d	150	MEQ	2	0
6	A	521	G7M	1	0
39	l	82	4D4	1	0
28	a	2490	2MA	1	0
6	A	961	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 525 ligands modelled in this entry, 525 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

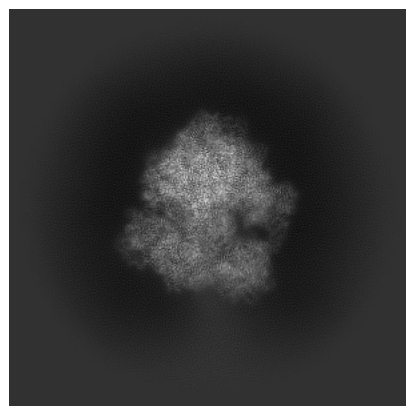
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55345. These allow visual inspection of the internal detail of the map and identification of artifacts.

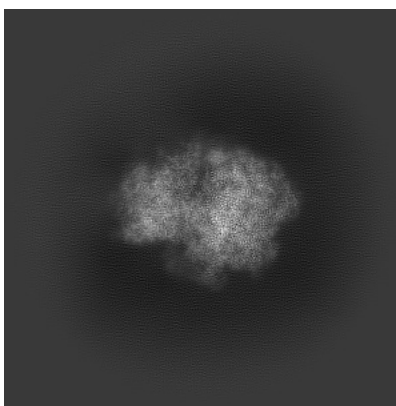
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

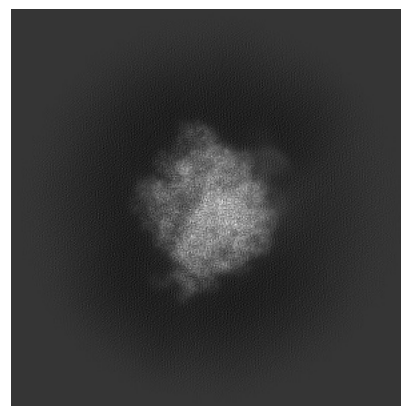
6.1.1 Primary map



X

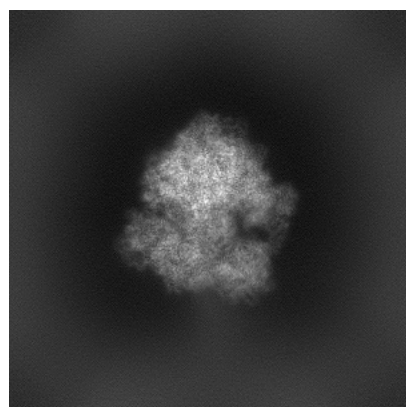


Y

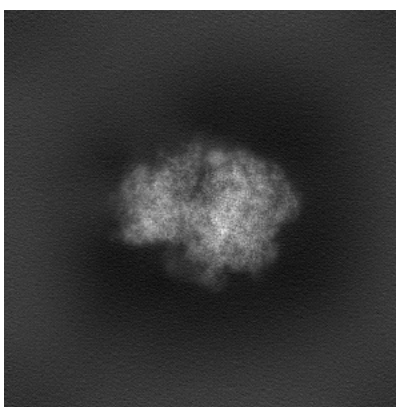


Z

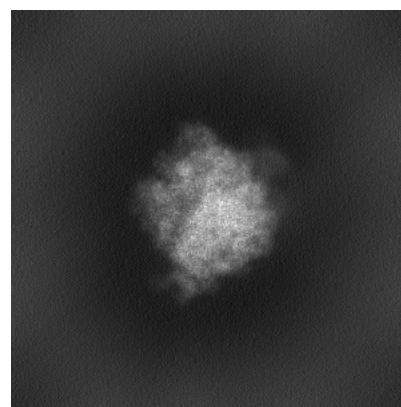
6.1.2 Raw map



X



Y

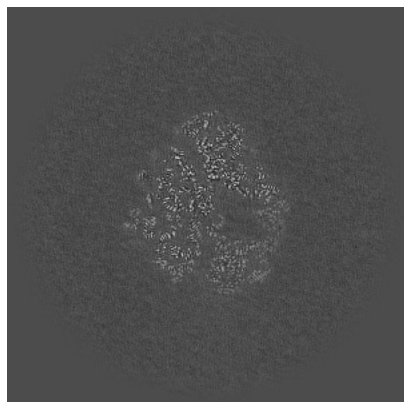


Z

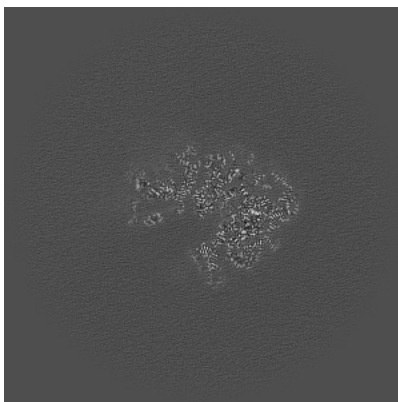
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

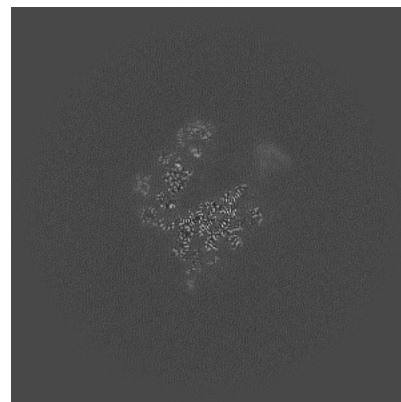
6.2.1 Primary map



X Index: 256

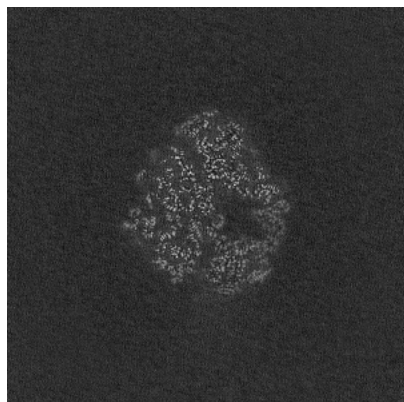


Y Index: 256

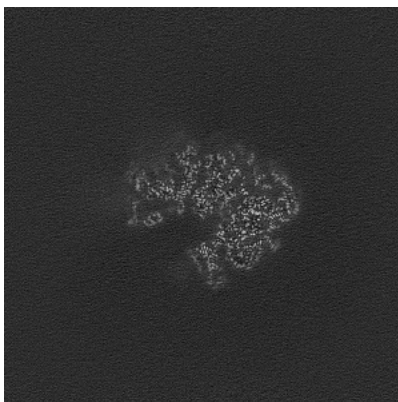


Z Index: 256

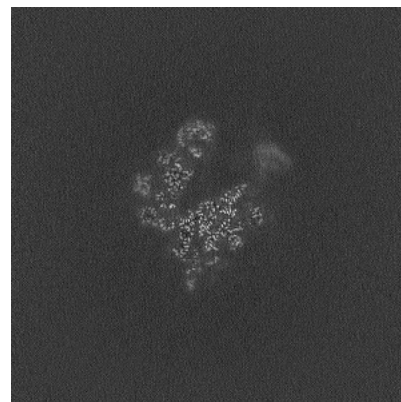
6.2.2 Raw map



X Index: 256



Y Index: 256

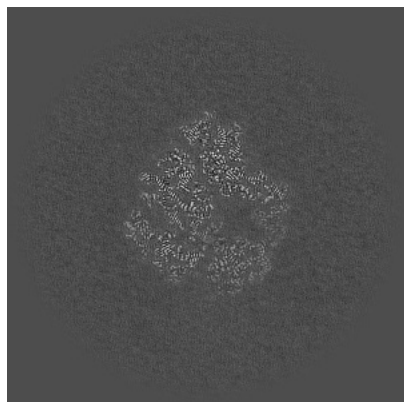


Z Index: 256

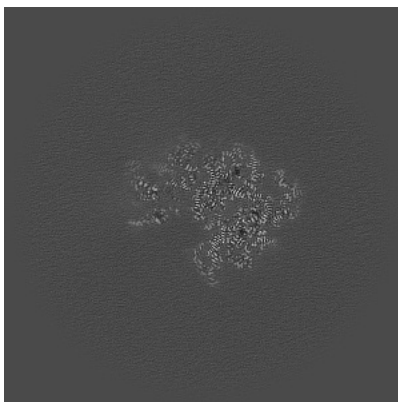
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

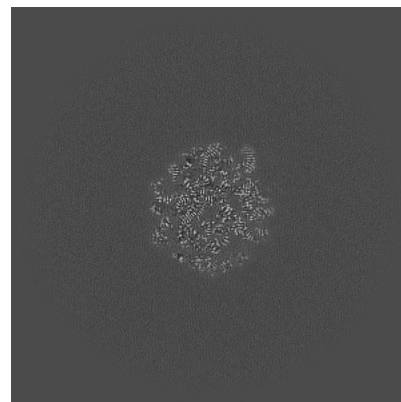
6.3.1 Primary map



X Index: 252

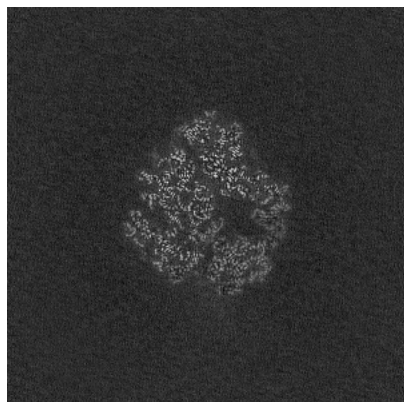


Y Index: 251

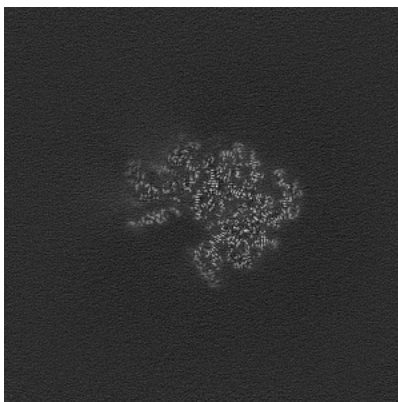


Z Index: 295

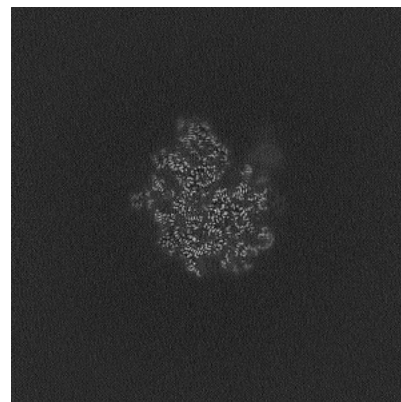
6.3.2 Raw map



X Index: 253



Y Index: 252

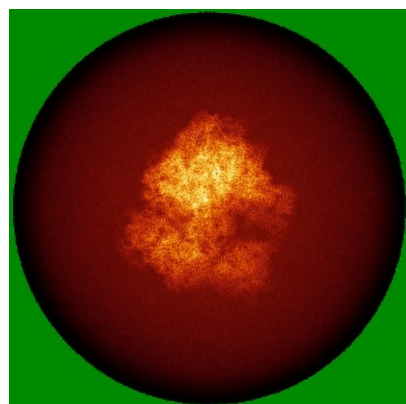


Z Index: 278

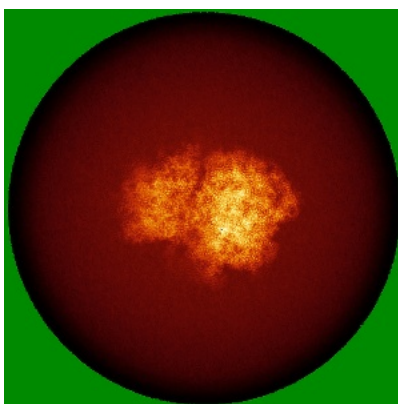
The images above show the largest variance slices of the map in three orthogonal directions.

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

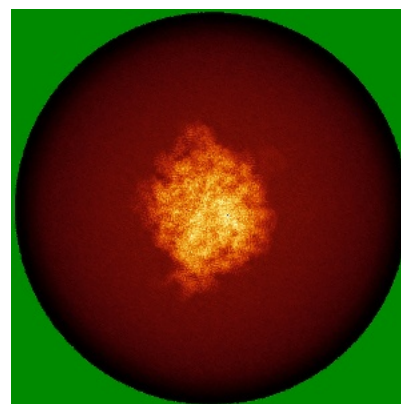
6.4.1 Primary map



X

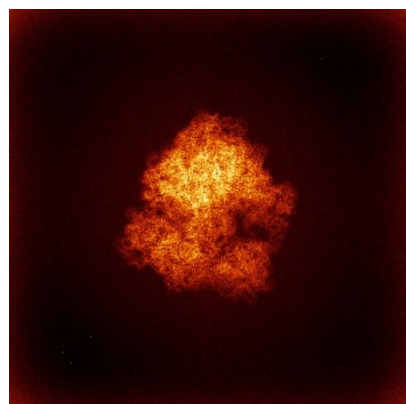


Y

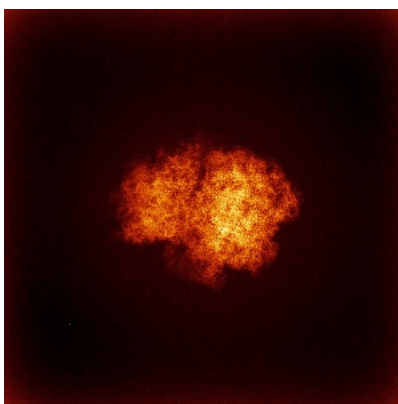


Z

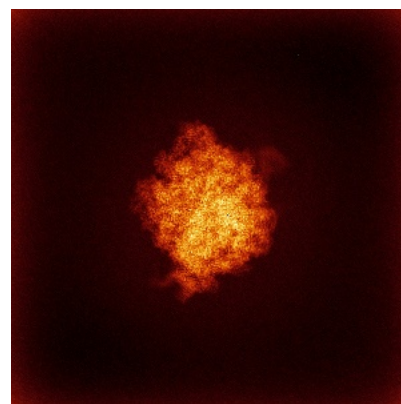
6.4.2 Raw map



X



Y

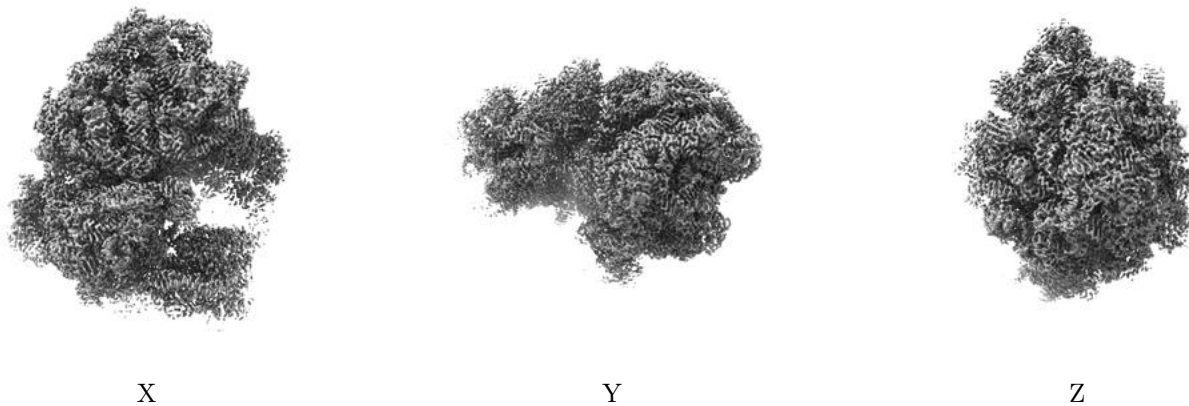


Z

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.

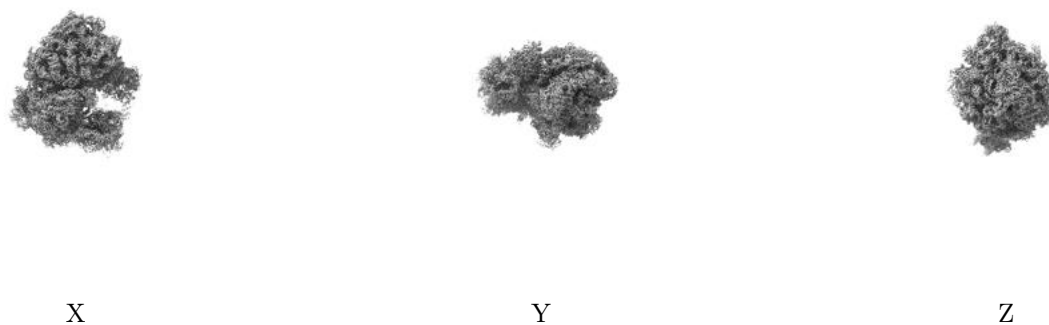
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

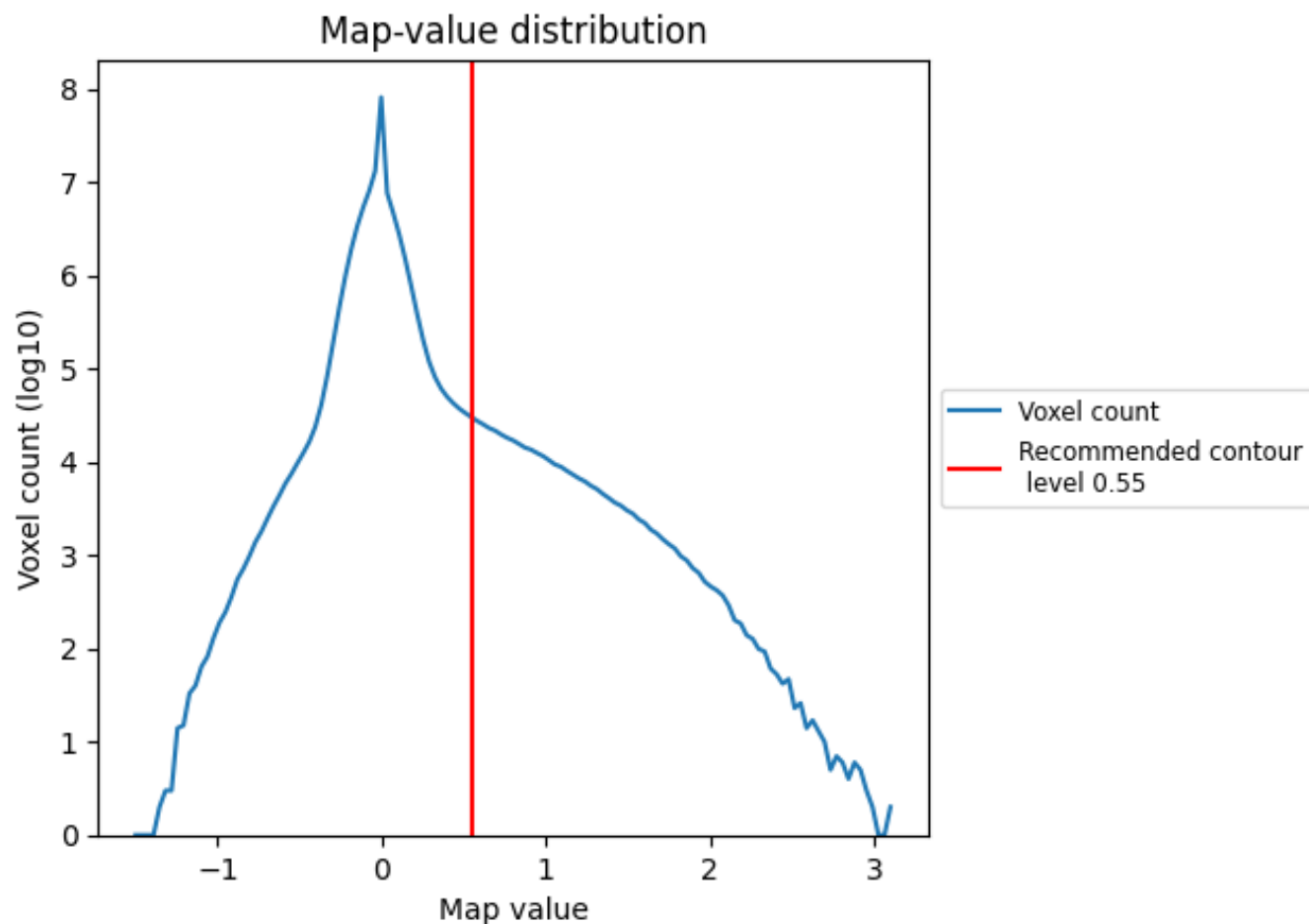
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

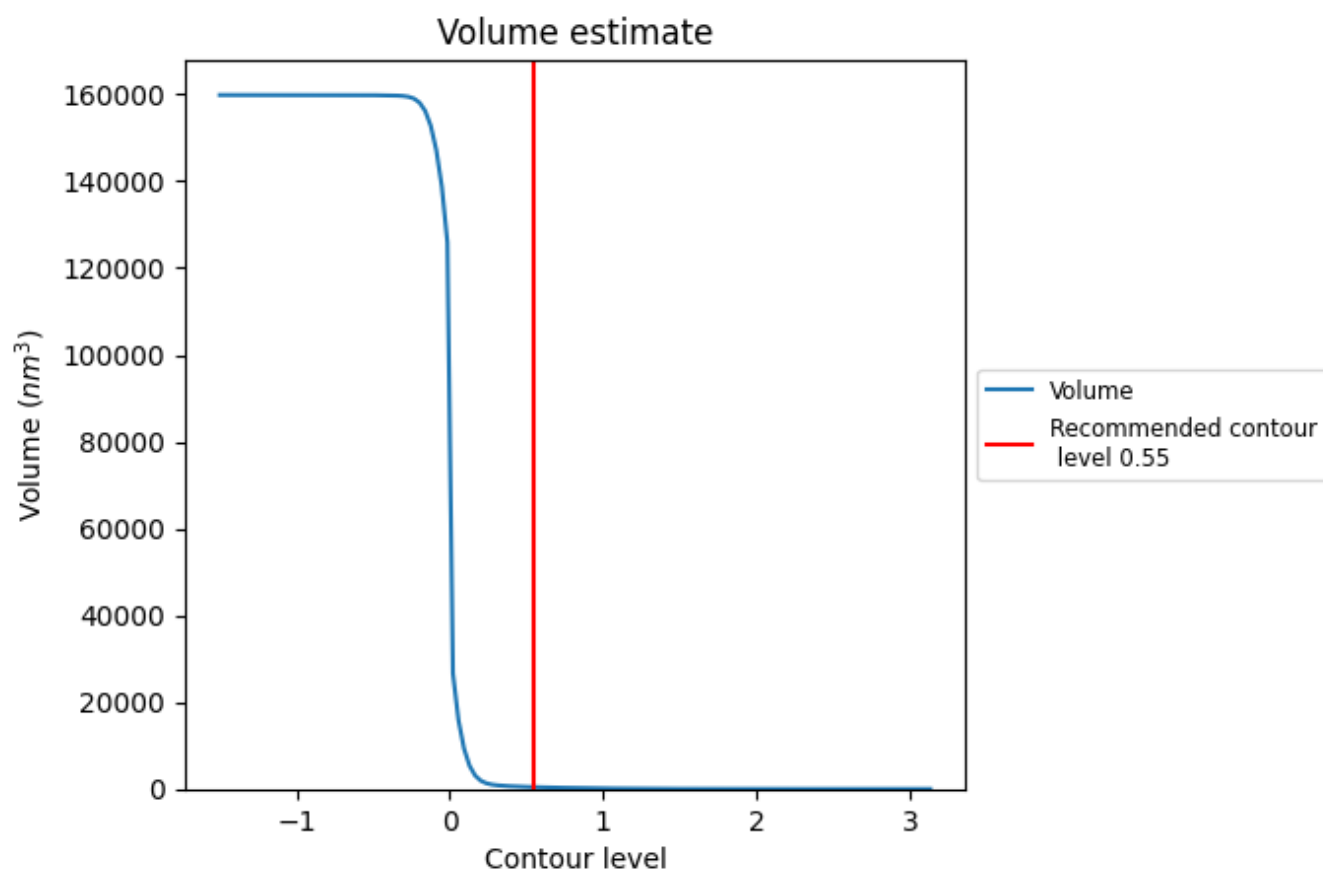
This section contains the results of statistical analysis of the map.

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.

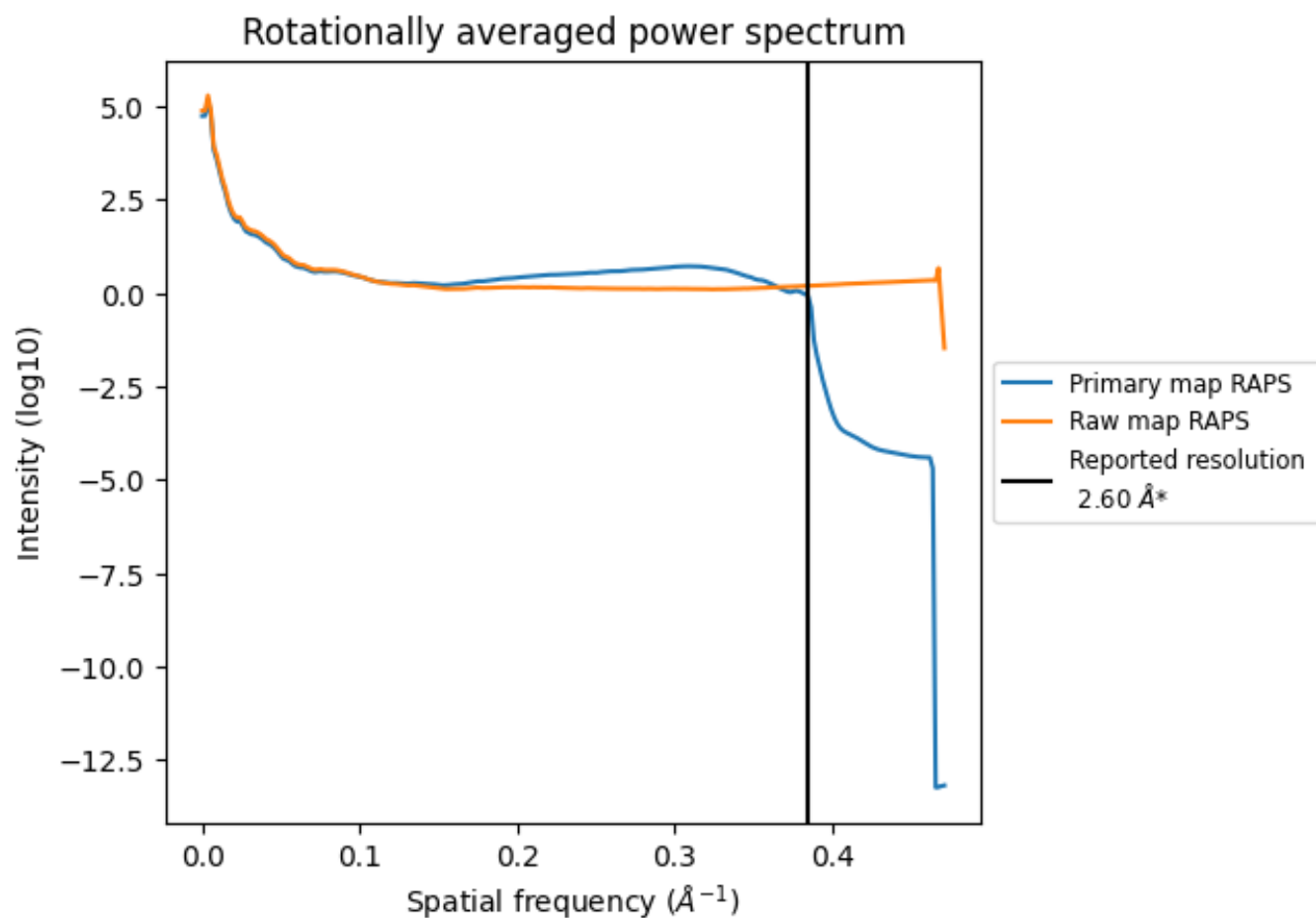
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 422 nm³; this corresponds to an approximate mass of 381 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 ⓘ

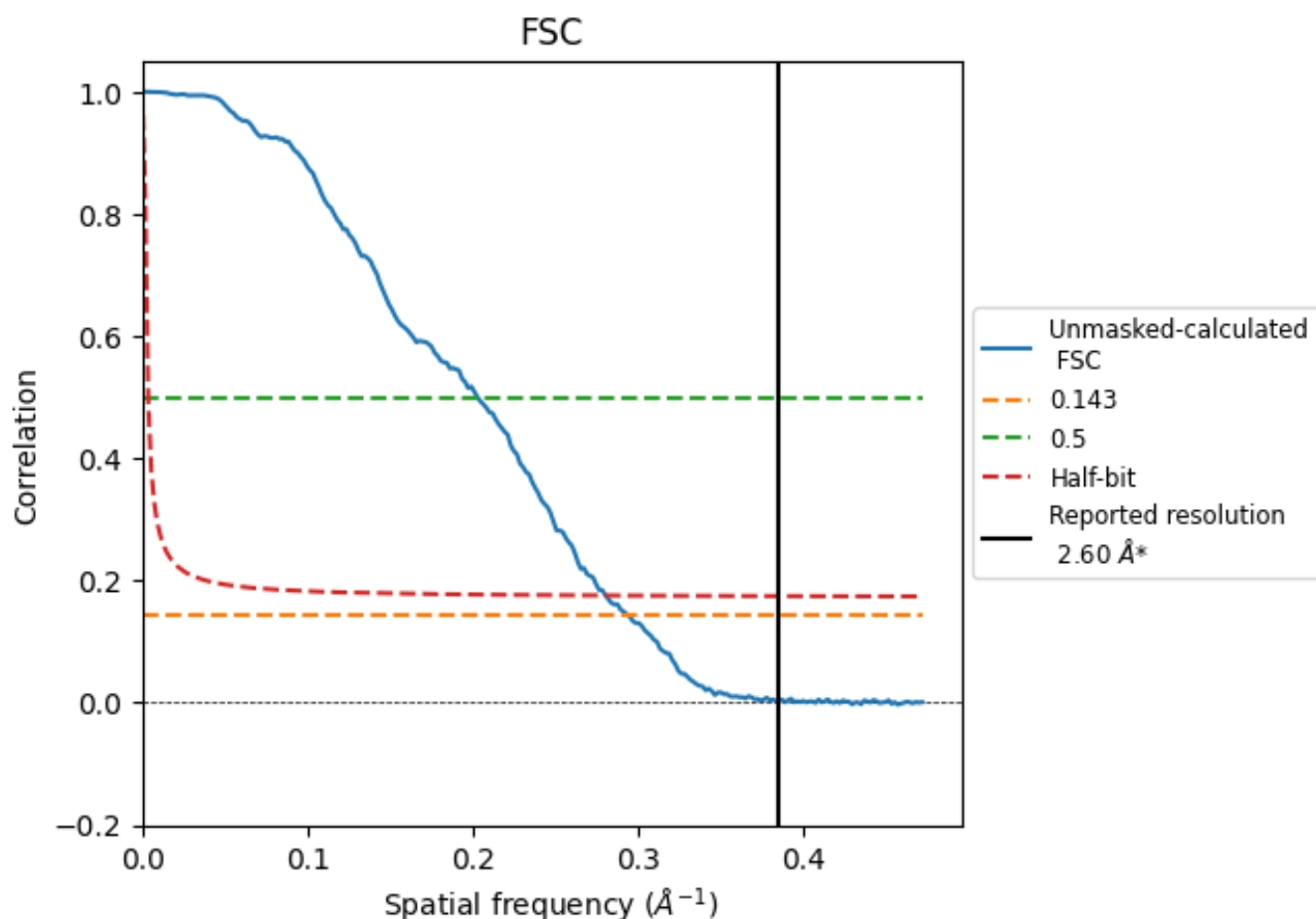


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

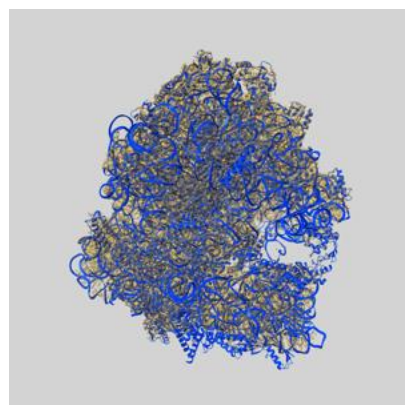
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	4.93	3.57

*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 3.40 differs from the reported value 2.6 by more than 10 %

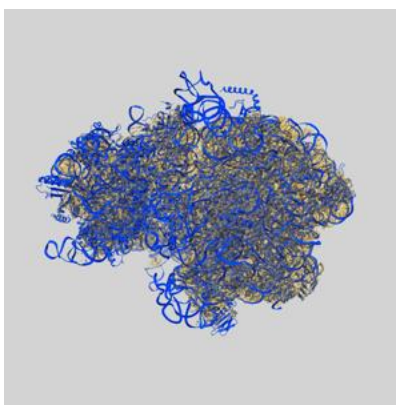
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55345 and PDB model 9SY6. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

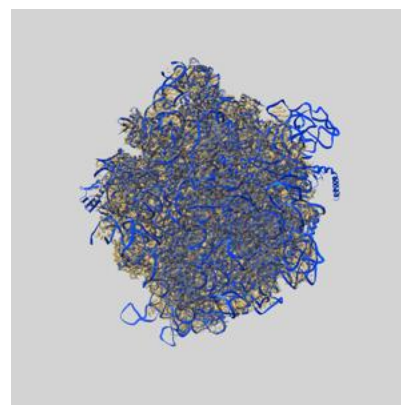
9.1 Map-model overlay [i](#)



X



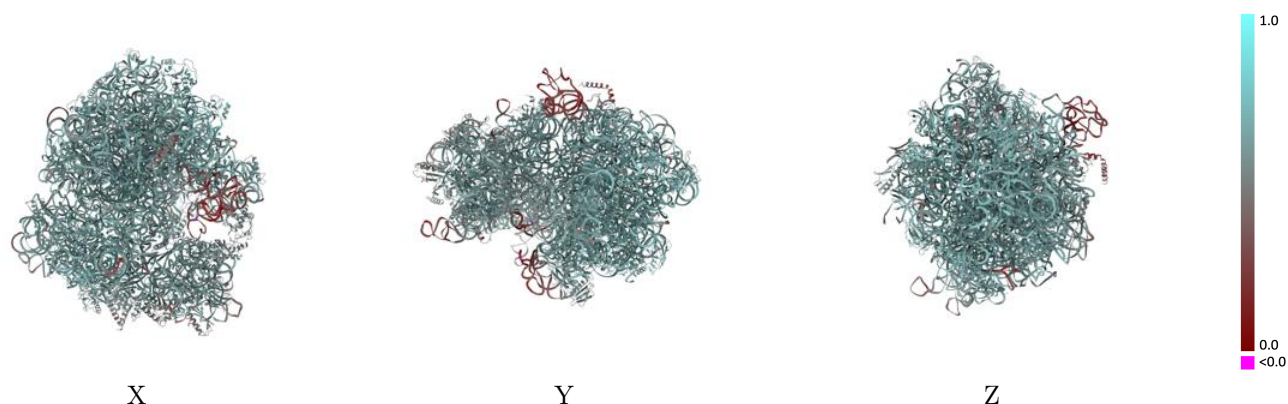
Y



Z

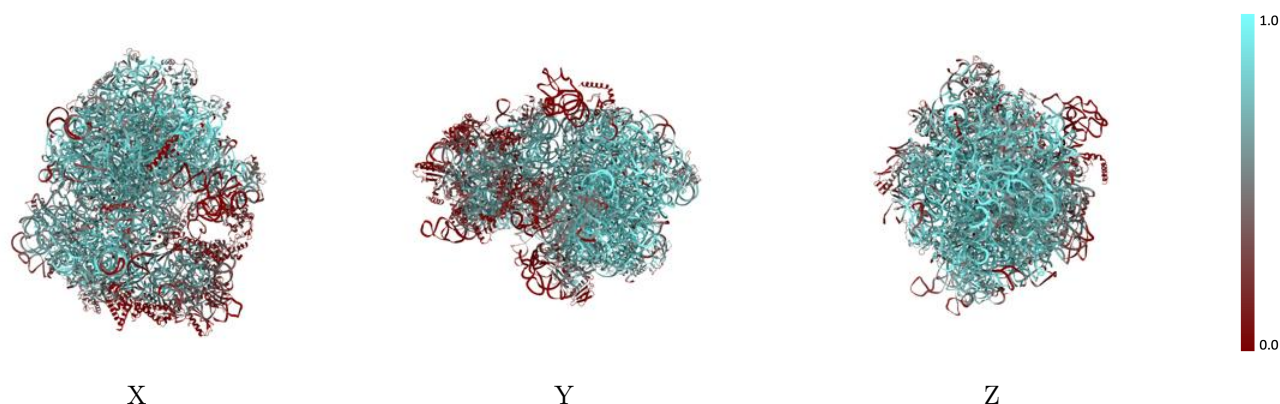
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



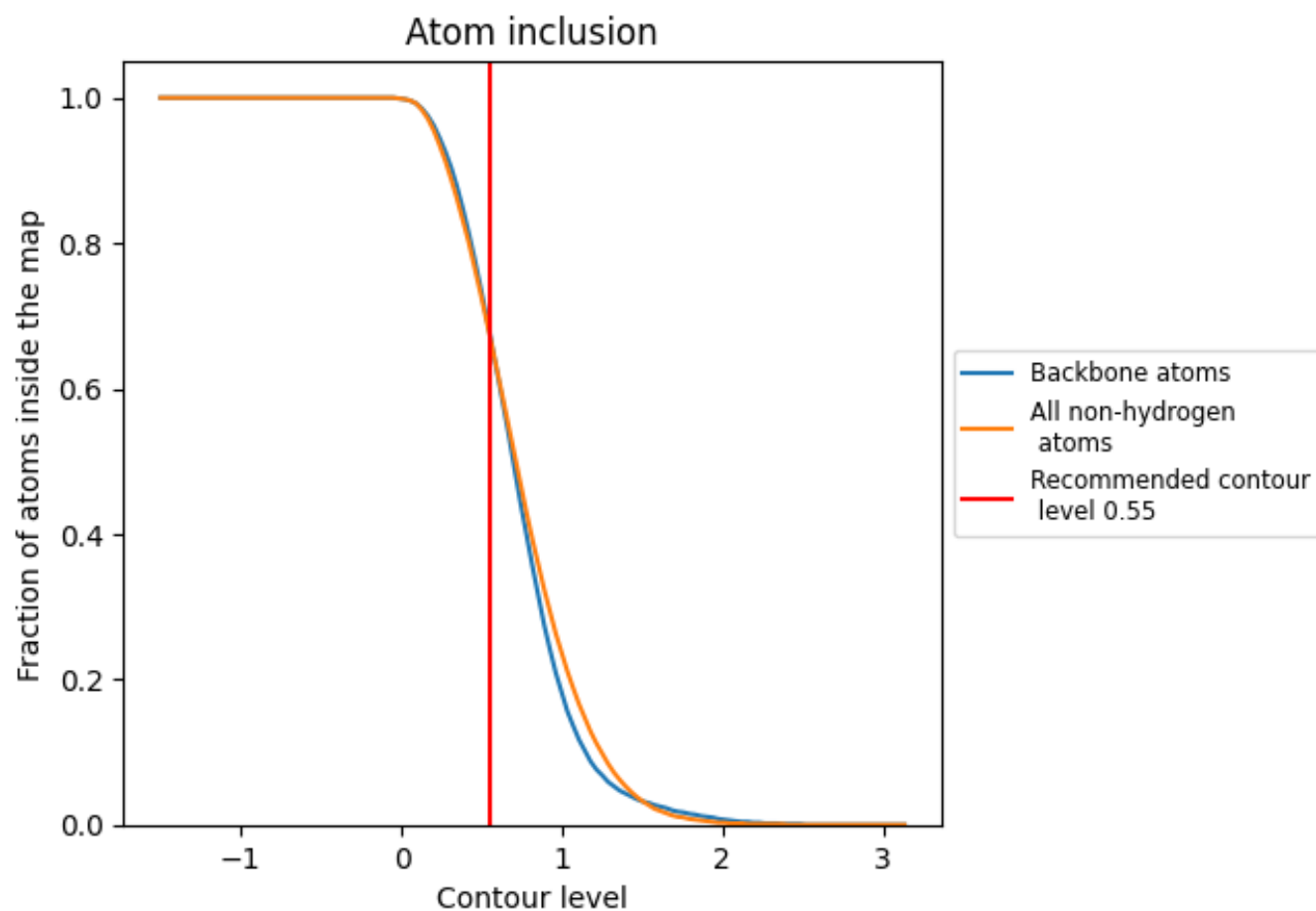
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6750	 0.6140
0	 0.4890	 0.6190
1	 0.8460	 0.6640
2	 0.8040	 0.6660
3	 0.6910	 0.6480
4	 0.0380	 0.4780
A	 0.6870	 0.6090
B	 0.0460	 0.5070
C	 0.3690	 0.5900
D	 0.4150	 0.6050
E	 0.5980	 0.6230
F	 0.3200	 0.5770
G	 0.1470	 0.5500
H	 0.6130	 0.6340
I	 0.2700	 0.5690
J	 0.2280	 0.5220
K	 0.4210	 0.5990
L	 0.6080	 0.6350
M	 0.2030	 0.5630
N	 0.3870	 0.5850
O	 0.5840	 0.6270
P	 0.6660	 0.6400
Q	 0.5480	 0.6240
R	 0.4530	 0.5900
S	 0.1930	 0.5520
T	 0.6060	 0.6310
W	 0.1280	 0.4930
X	 0.3190	 0.6010
a	 0.7890	 0.6190
b	 0.6490	 0.6090
c	 0.7690	 0.6600
d	 0.7740	 0.6520
e	 0.6920	 0.6430
f	 0.1660	 0.5450
g	 0.2980	 0.5790



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Chain	Atom inclusion	Q-score
h	 0.0020	 0.4060
i	 0.7600	 0.6530
j	 0.6930	 0.6470
k	 0.7240	 0.6500
l	 0.6850	 0.6500
m	 0.8070	 0.6550
n	 0.4780	 0.6090
o	 0.6890	 0.6510
p	 0.8000	 0.6620
q	 0.6590	 0.6470
r	 0.7300	 0.6550
s	 0.6010	 0.6270
t	 0.4820	 0.5980
u	 0.3880	 0.6100
v	 0.7460	 0.6540
w	 0.7040	 0.6500
x	 0.5580	 0.6180
y	 0.7140	 0.6490
z	 0.7110	 0.6420