



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:41 AM UTC

PDB ID : 7NSO / pdb_00007nso
EMDB ID : EMD-12573
Title : Structure of ErmDL-Erythromycin-stalled 70S E. coli ribosomal complex with P-tRNA
Authors : Beckert, B.; Wilson, D.N.
Deposited on : 2021-03-08
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

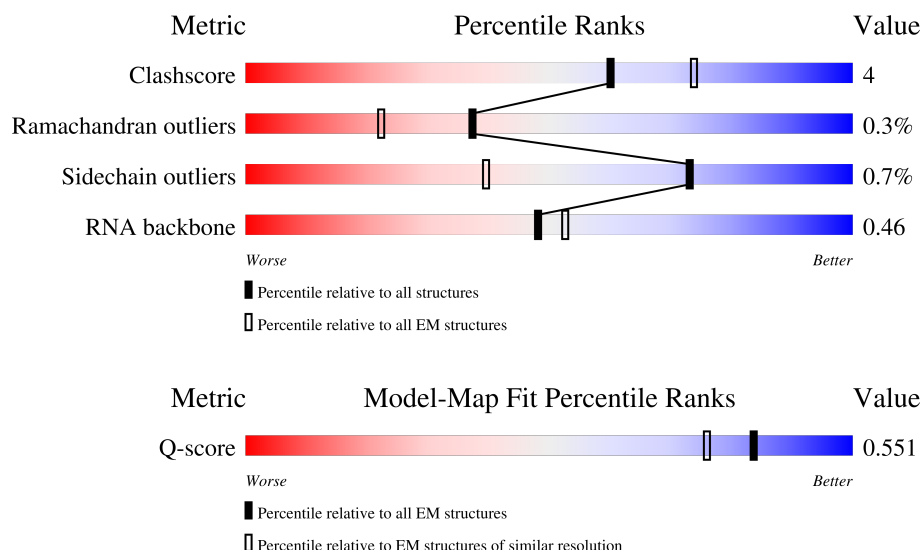
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	A	2903	
2	B	120	
3	C	271	

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	201	
6	F	177	
7	G	174	
8	H	149	
9	J	142	
10	K	122	
11	L	144	
12	M	136	
13	N	118	
14	O	116	
15	P	114	
16	Q	117	
17	R	103	
18	S	110	
19	T	89	
20	U	102	
21	V	94	
22	W	75	
23	X	77	
24	Y	63	
25	Z	58	
26	0	55	
27	1	50	
28	2	46	

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Mol	Chain	Length	Quality of chain
29	3	64	
30	4	38	
31	5	65	
32	6	3	
33	7	7	
34	8	87	
35	a	1540	
36	b	224	
37	c	206	
38	d	205	
39	e	157	
40	f	99	
41	g	151	
42	h	129	
43	i	127	
44	j	98	
45	k	117	
46	l	123	
47	m	114	
48	n	100	
49	o	88	
50	p	82	
51	q	80	
52	r	66	
53	s	83	

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Mol	Chain	Length	Quality of chain
54	t	86	14% 85% 15%
55	u	70	83% 86% 14%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 144454 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 RNA chain called 23S rRNA (2903-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	114	Total	C	N	O	S	0
			917	574	179	163	1	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	117	Total	C	N	O		0
			947	604	192	151		0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	103	Total	C	N	O	S	0
			816	516	153	145	2	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	110	Total	C	N	O	S	0
			857	532	166	156	3	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	T	89	Total	C	N	O	S	0
			709	449	133	125	2	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	U	102	Total	C	N	O		0
			779	492	146	141		0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	65	Total	C	N	O	S	0	0
			514	317	98	93	6		

- Molecule 32 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

- Molecule 33 is a protein called ermDL.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	7	Total	C	N	O	S	1	0
			69	41	16	10	2		

- Molecule 34 is a RNA chain called PtRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	87	Total	C	N	O	P	0	0
			1861	829	333	612	87		

- Molecule 35 is a RNA chain called 16S rRNA (1540-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	1540	Total	C	N	O	P	0	0
			33037	14735	6057	10705	1540		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	99	Total	C	N	O	S	0	0
			811	512	147	146	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	n	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r	66	Total	C	N	O	S	0	0
			545	344	102	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

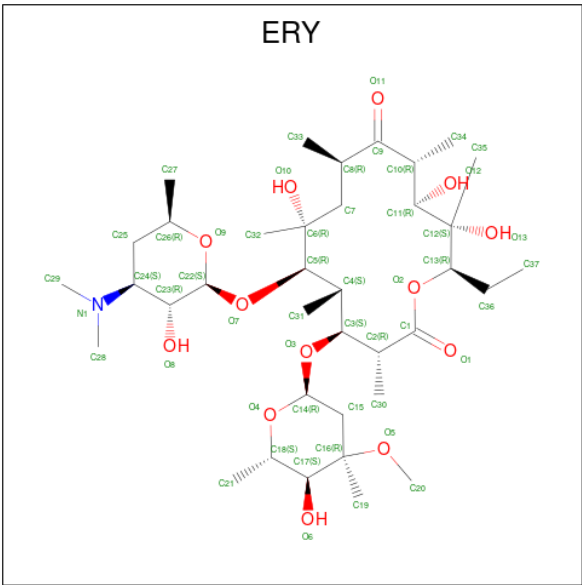
- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	u	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 56 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).

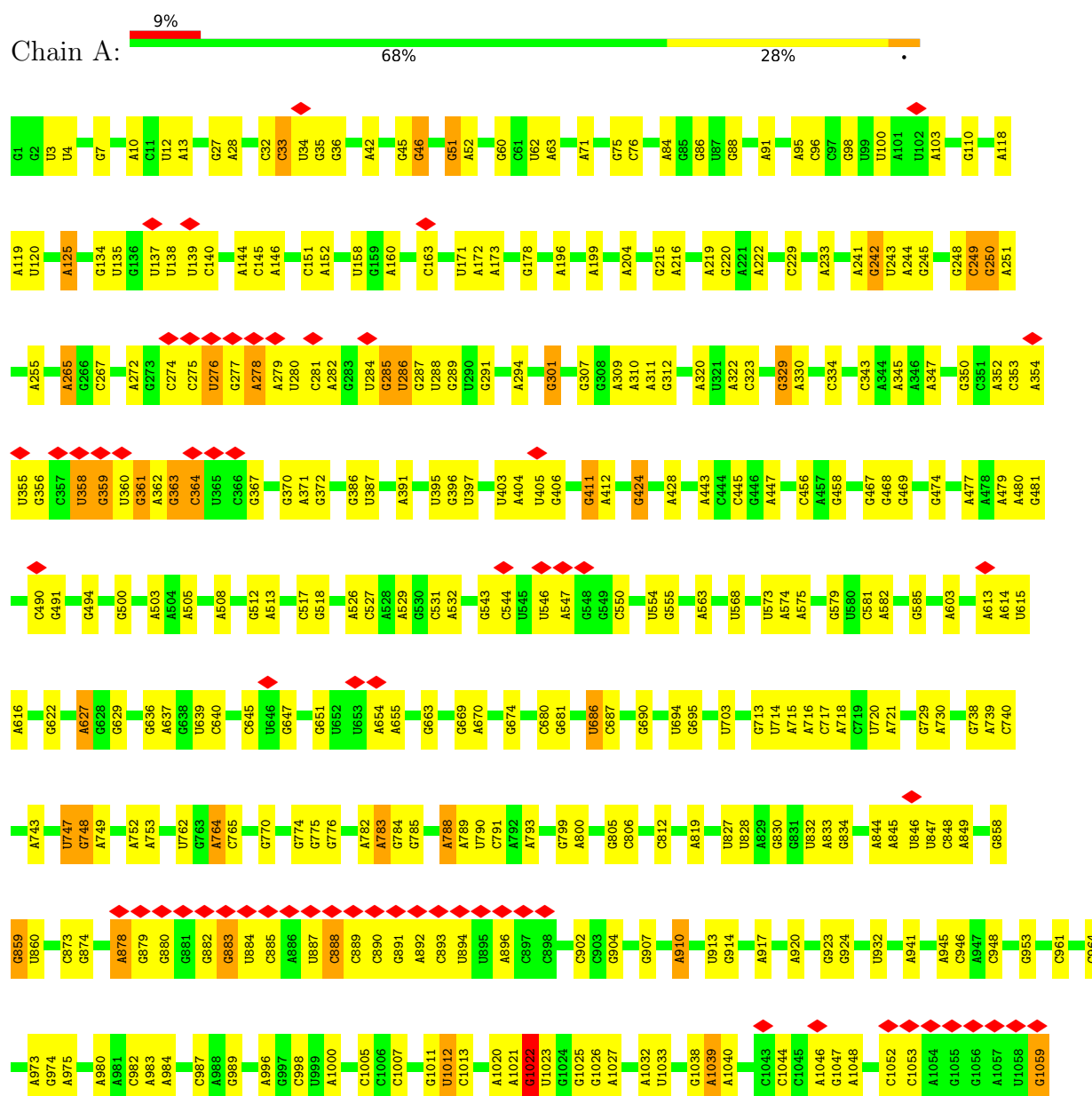


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
56	7	1	51	37	1	13	0

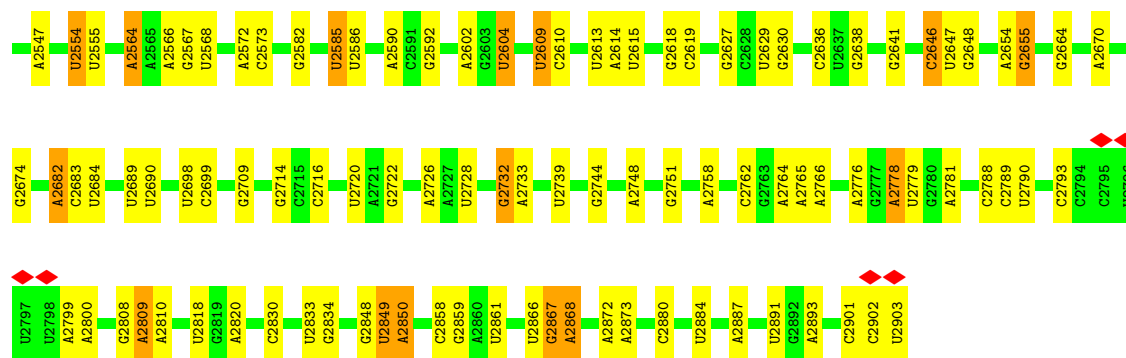
3 Residue-property plots

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.

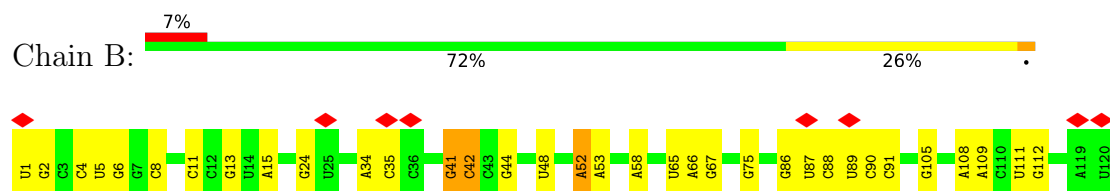
• Molecule 1: 23S rRNA (2903-MER)



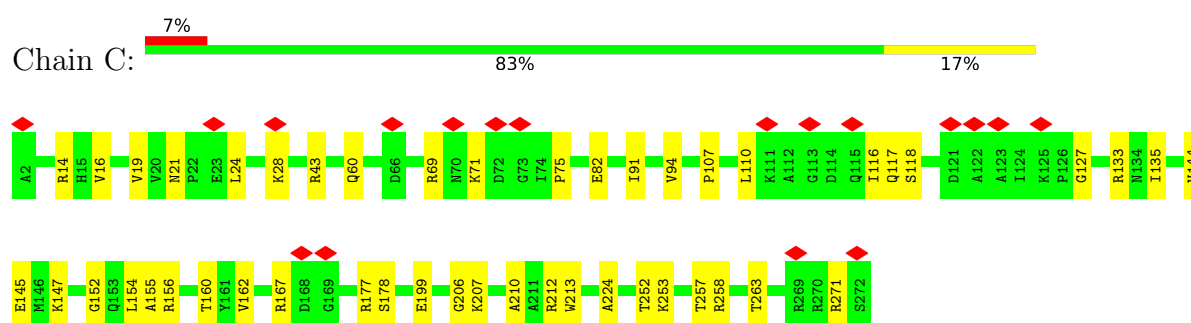
G2410	U2423	C2424	A2425	G2426	C2427	G2428	G2429	A2430	A2434	U2441	G2445	G2446	G2447	A2448	A2451	C2452	G2467	A2468	A2469	A2476	G2481	U2489	G2490	U2491	C2496	A2497	C2498	C2499	U2500	G2501	A2503	U2504	G2505	U2506	U2514	A2515	A2516	C2517	A2518	U2519	C2520	C2521	U2522	G2529	A2542														
G2304	U2305	C2306	G2307	G2308	A2309	U2312	G2313	A2314	U2320	G2325	C2326	A2327	A2328	U2329	G2330	C2331	A2333	U2334	A2340	G2345	A2346	C2347	U2348	G2349	C2350	C2354	G2361	C2362	G2370	C2374	C2380	G2383	U2384	C2385	A2386	C2391	A2392	G2396	U2402	C2403	A2406																		
G2186	U2187	U2188	U2189	G2190	A2191	U2192	G2193	A2198	A2199	U2203	G2204	A2211	A2212	U2213	G2223	G2224	A2225	C2226	G2230	U2233	G2234	G2238	U2245	G2246	A2247	G2250	C2258	A2268	G2271	U2272	A2273	A2274	G2275	G2276	G2277	A2278	C2283	A2287	A2288	U2291	U2292	G2293	A2298																
A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	G2141	A2142	C2143	G2144	C2145	C2146	A2147	G2148	U2149	C2150	U2151	G2152	C2153	U2154	U2155	G2156	G2157	A2158	C2159	C2160	C2161	G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	G2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	A2183	A2184	U2185
A2030	A2031	G2032	A2033	U2034	G2035	C2036	C2043	G2049	A2052	C2055	G2056	A2060	G2061	A2062	G2069	A2077	G2087	A2088	G2093	C2096	A2097	U2098	U2099	G2100	A2101	G2102	C2103	C2104	U2105	U2106	A2107	C2108	U2109	G2110	U2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	U2125										
G1906	G1907	A1912	A1913	A1914	C1914	U1917	A1927	A1928	G1929	G1930	U1931	A1936	A1937	U1938	U1940	C1941	G1942	U1943	U1944	U1955	C1962	U1963	G1964	C1965	A1966	C1967	A1970	U1971	G1972	A1981	U1982	U1991	G1992	C1997	C2006	G2012	A2013	A2014	A2015	A2019	A2020	C2021	U2022	C2023															
G1776	U1779	A1780	U1781	U1782	A1783	A1784	A1786	A1787	C1788	U1796	U1797	U1798	G1799	C1800	A1801	A1802	A1803	A1808	G1811	C1816	G1817	U1818	A1819	U1820	G1826	A1829	C1833	U1834	G1835	A1853	A1854	A1858	U1864	G1869	C1870	A1871	A1872	G1873	G1884	A1889	A1890	A1900	A1901																
G1645	C1646	U1647	U1648	G1649	A1650	G1651	A1652	G1659	A1664	G1667	A1668	A1669	C1670	G1674	C1675	A1689	A1690	U1693	C1694	G1695	A1713	U1714	G1715	G1721	G1724	U1725	G1728	U1729	G1731	G1732	A1735	U1736	G1737	G1738	A1739	A1744	A1745	A1746	U1747	A1757	G1764	A1773																	
G1516	G1517	U1523	G1524	A1528	G1529	G1530	C1531	A1532	C1533	U1534	A1535	C1536	G1537	G1538	U1539	G1540	C1541	U1542	G1543	A1544	U1554	G1555	C1558	U1559	G1560	A1566	G1567	G1568	A1569	A1570	U1578	G1581	C1582	A1583	U1584	C1585	A1590	C1607	A1608	A1609	A1610	C1611	U1621	G1622	G1631	A1634													
A1403	U1411	C1414	U1415	G1416	A1420	G1421	A1427	G1428	G1429	G1432	A1433	A1434	G1435	G1436	C1437	G1445	C1446	C1447	C1454	G1459	U1460	C1461	U1466	A1469	A1470	G1475	G1478	G1482	G1483	U1484	A1490	C1493	A1504	A1505	U1506	C1507	A1508	A1509	G1510	G1511	A1515																		
U1130	G1131	U1132	A1133	A1134	C1135	G1139	A1142	A1143	A1144	C1153	G1154	G1168	G1171	C1172	U1174	A1175	U1176	G1177	C1178	U1179	U1180	U1181	G1182	G1187	U1188	A1189	G1190	A1204	A1205	G1206	C1211	G1212	G1223	G1236	G1250	A1253	G1256	G1266	U1267	A1268	G1271																		
A1272	U1273	A1274	A1275	C1278	G1279	G1296	G1300	A1301	C1306	A1307	G1310	G1311	U1312	U1313	A1322	C1323	G1324	U1329	G1333	G1338	G1339	U1340	G1341	A1342	C1345	U1352	A1353	A1359	A1365	G1368	A1378	U1379	A1383	C1386	A1387	A1392	A1395	C1398	C1399																				
U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075	C1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	C1114	G1115	U1119	G1122		



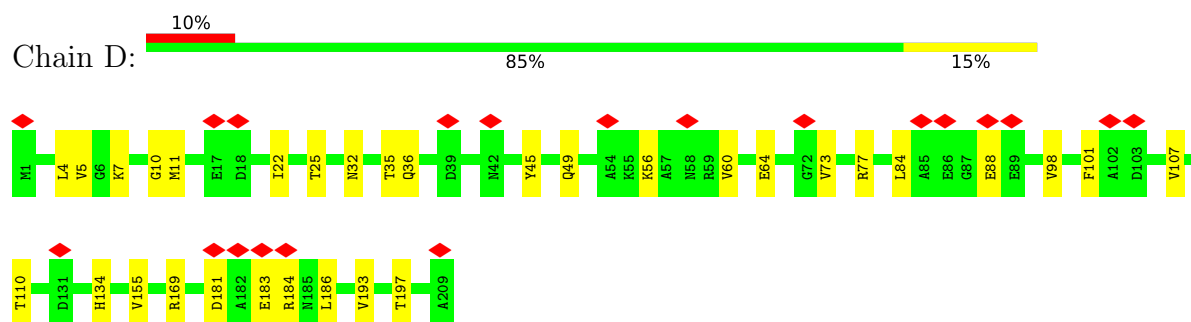
- Molecule 2: 5S rRNA



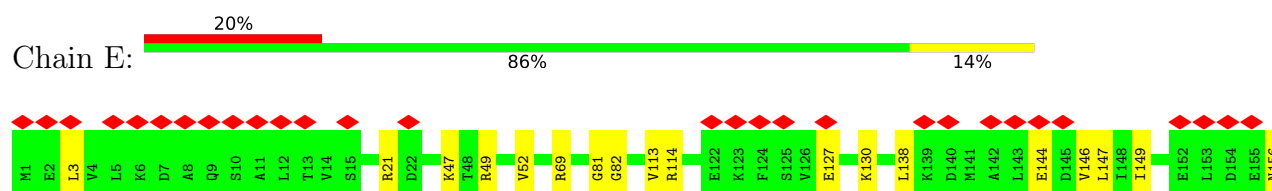
- Molecule 3: 50S ribosomal protein L2

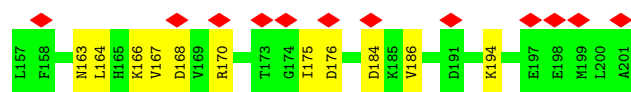


- Molecule 4: 50S ribosomal protein L3

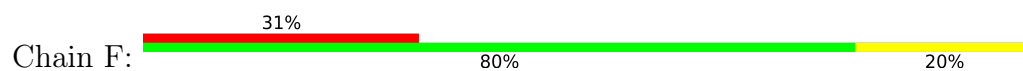


- Molecule 5: 50S ribosomal protein L4

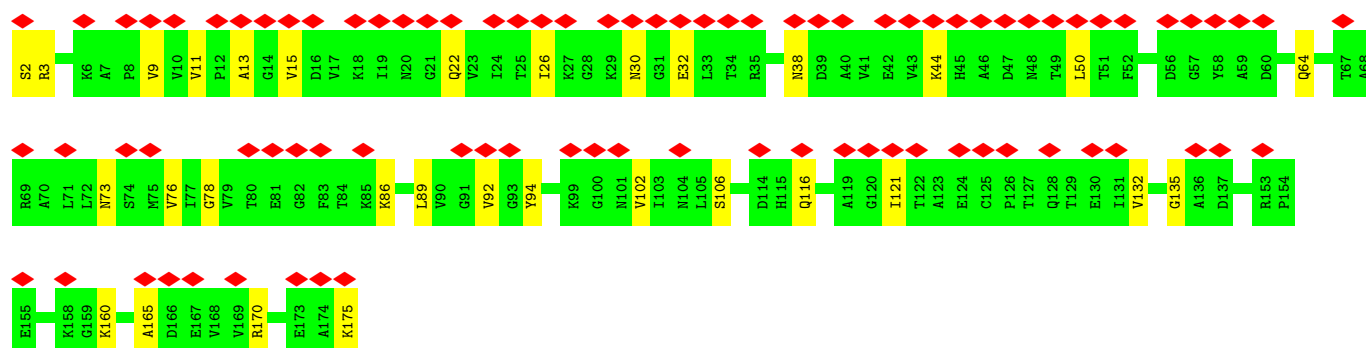
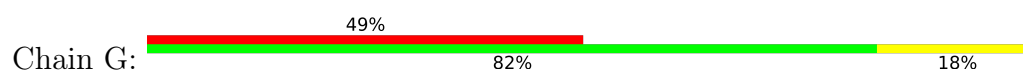




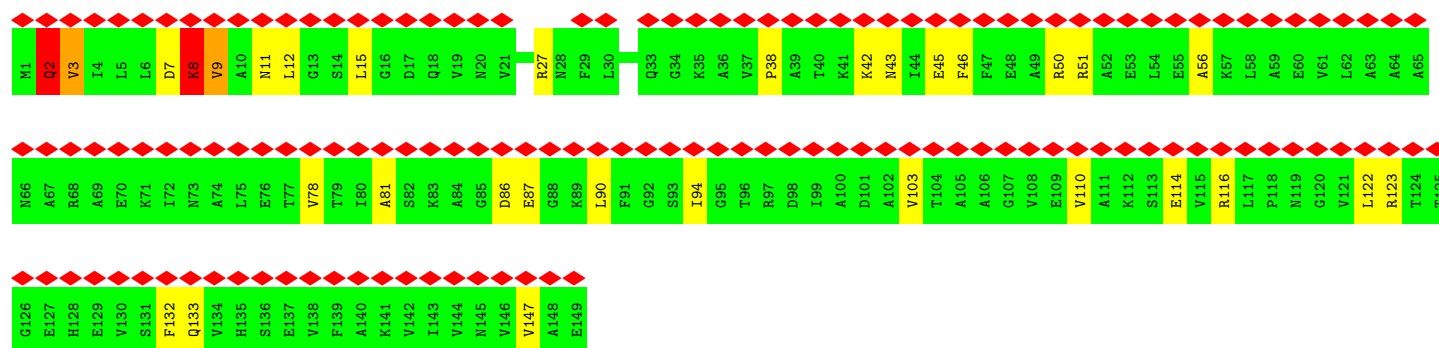
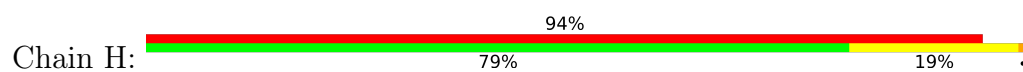
- Molecule 6: 50S ribosomal protein L5



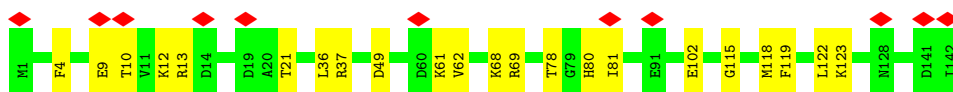
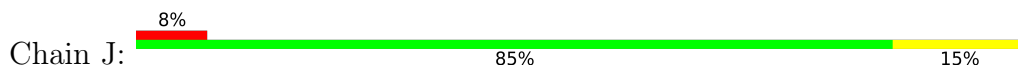
- Molecule 7: 50S ribosomal protein L6



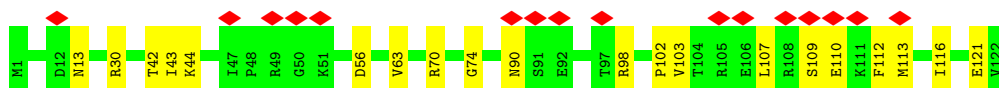
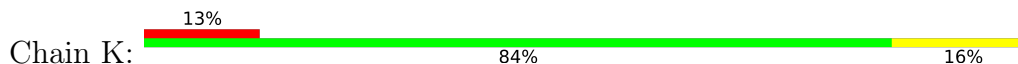
- Molecule 8: 50S ribosomal protein L9



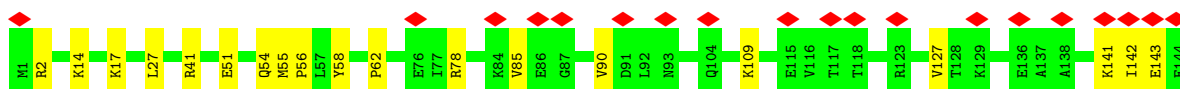
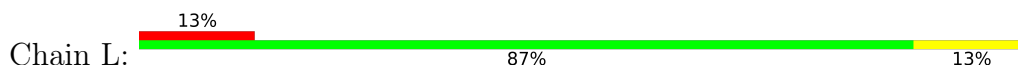
- Molecule 9: 50S ribosomal protein L13



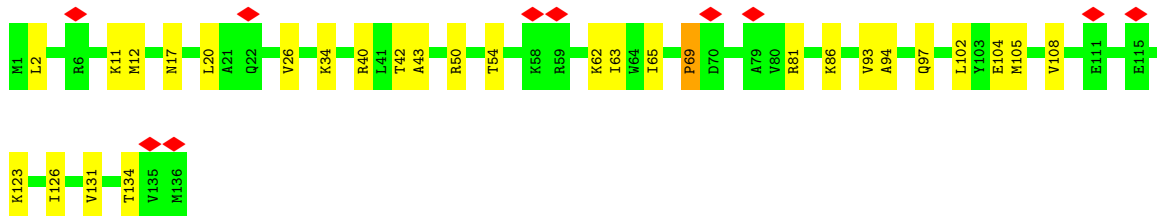
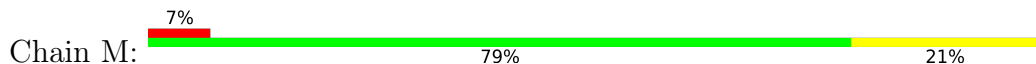
- Molecule 10: 50S ribosomal protein L14



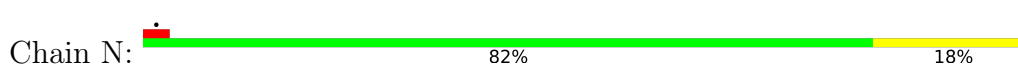
- Molecule 11: 50S ribosomal protein L15



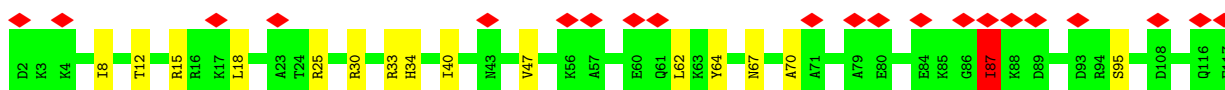
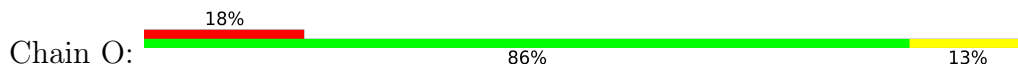
- Molecule 12: 50S ribosomal protein L16



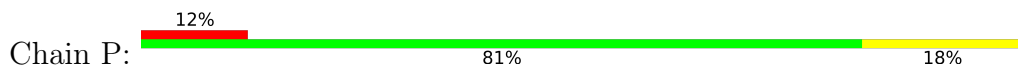
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

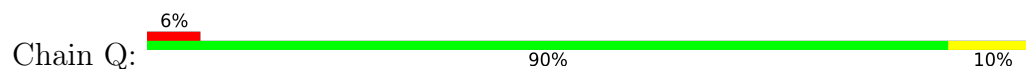


- Molecule 15: 50S ribosomal protein L19

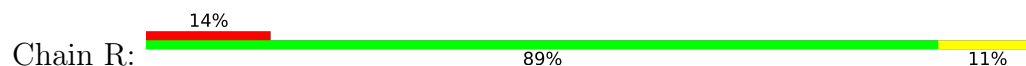




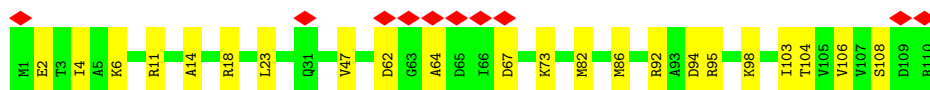
- Molecule 16: 50S ribosomal protein L20



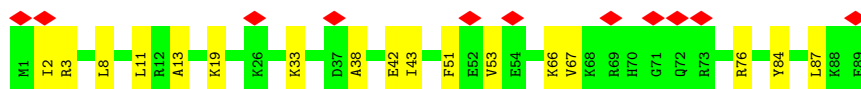
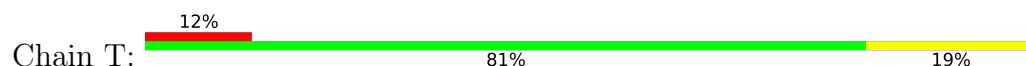
- Molecule 17: 50S ribosomal protein L21



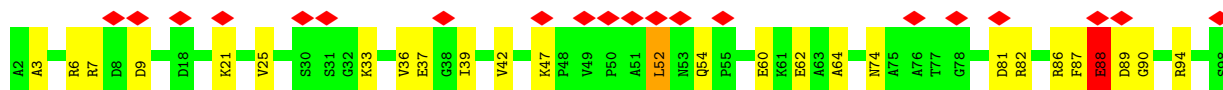
- Molecule 18: 50S ribosomal protein L22



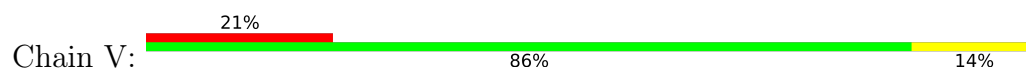
- Molecule 19: 50S ribosomal protein L23

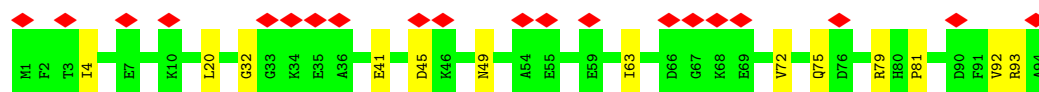


- Molecule 20: 50S ribosomal protein L24

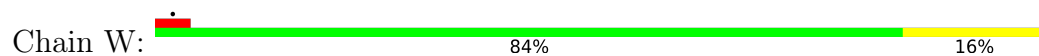


- Molecule 21: 50S ribosomal protein L25

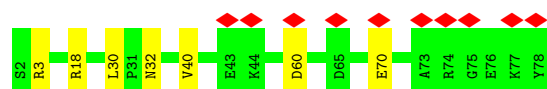




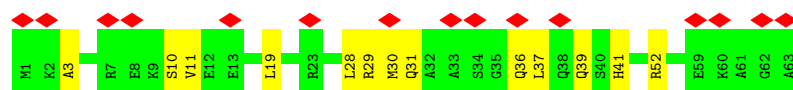
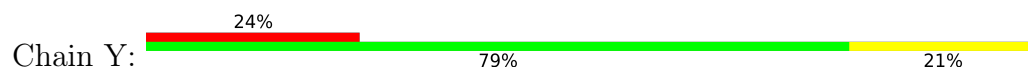
- Molecule 22: 50S ribosomal protein L27



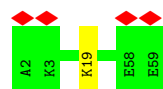
- Molecule 23: 50S ribosomal protein L28



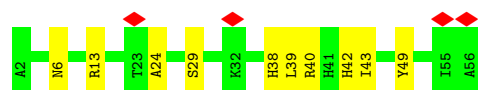
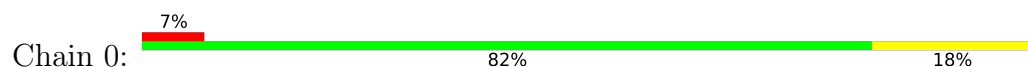
- Molecule 24: 50S ribosomal protein L29



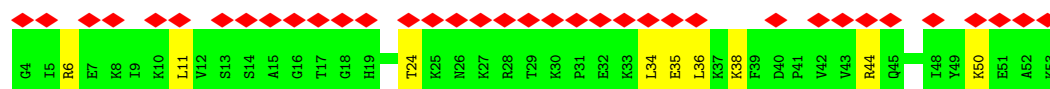
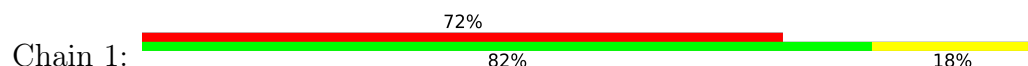
- Molecule 25: 50S ribosomal protein L30



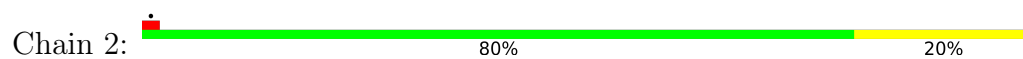
- Molecule 26: 50S ribosomal protein L32



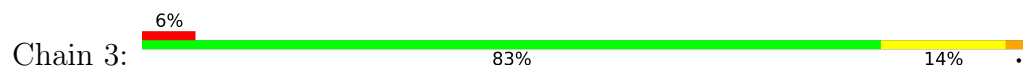
- Molecule 27: 50S ribosomal protein L33



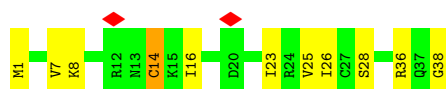
- Molecule 28: 50S ribosomal protein L34



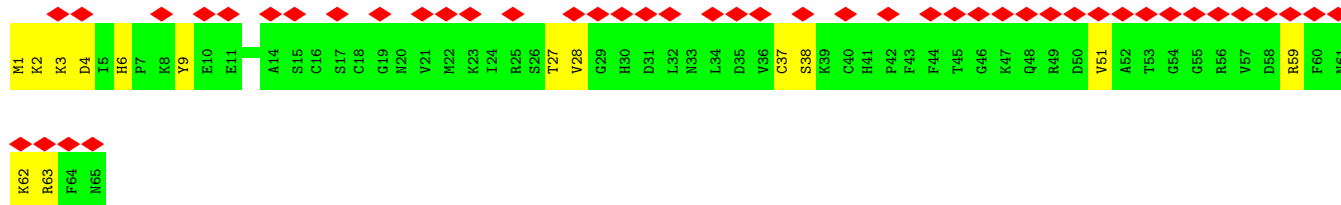
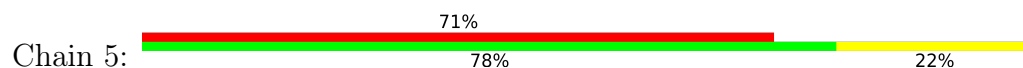
- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



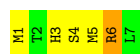
- Molecule 31: 50S ribosomal protein L31



- Molecule 32: mRNA



- Molecule 33: ermDL

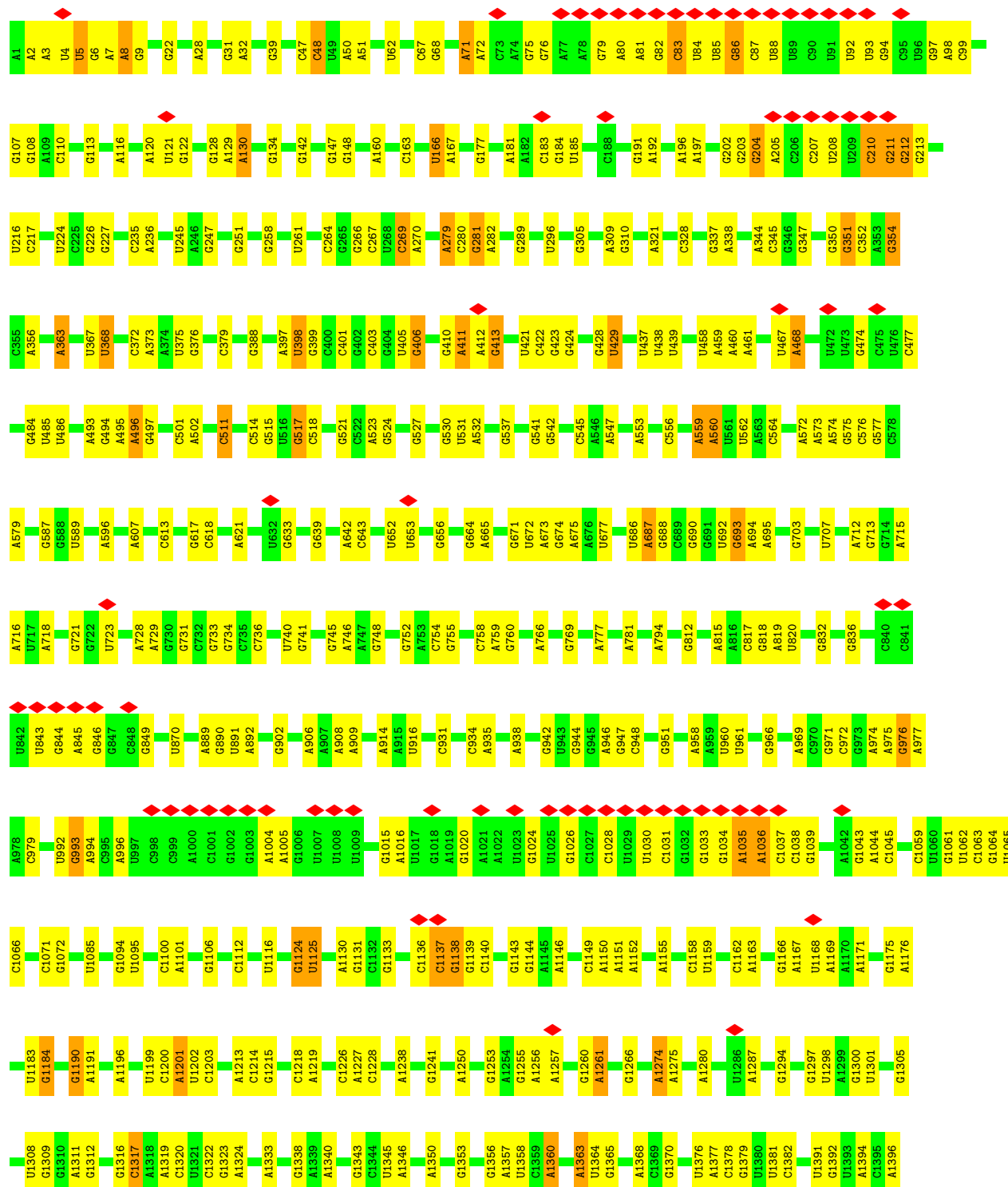


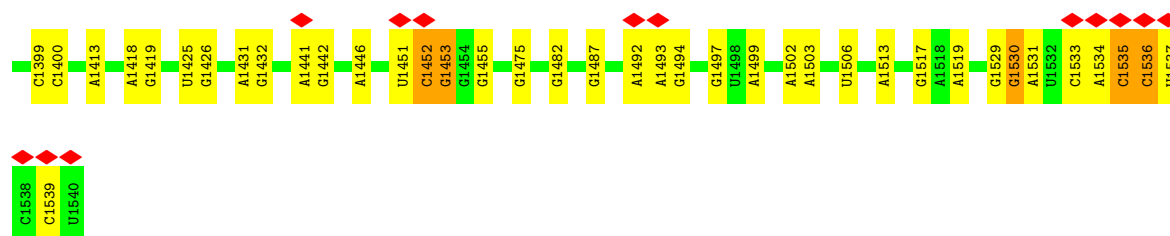
- Molecule 34: PtRNA-Leu



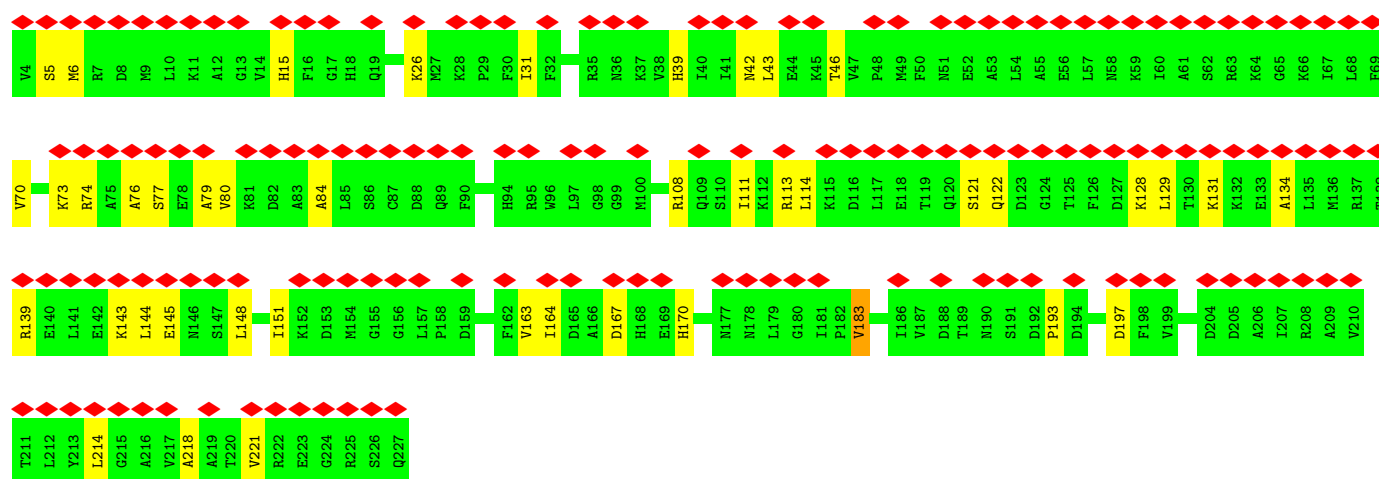
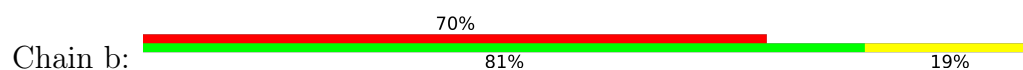


• Molecule 35: 16S rRNA (1540-MER)

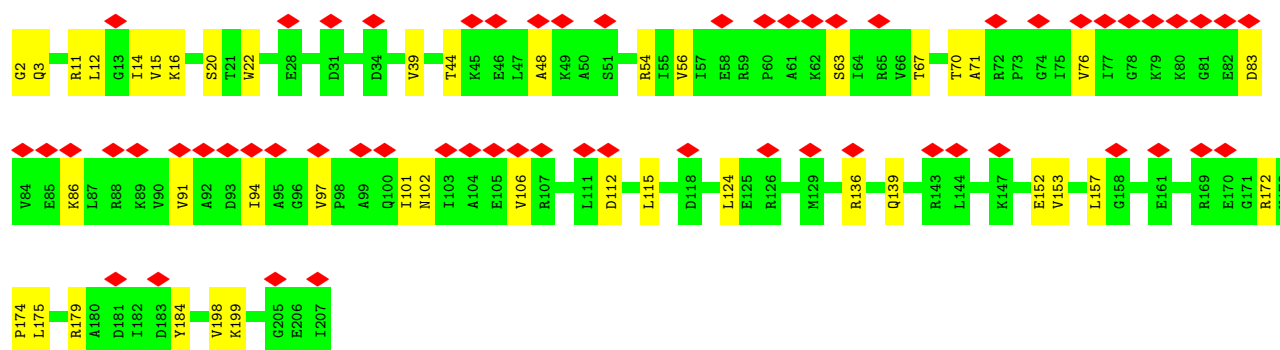
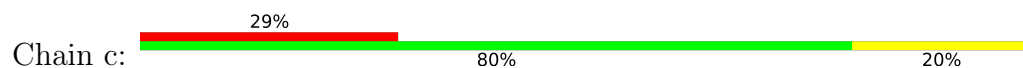




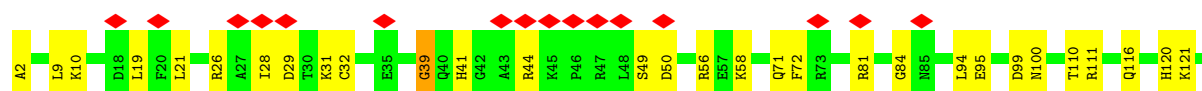
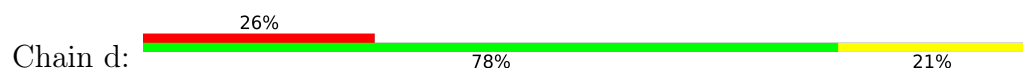
• Molecule 36: 30S ribosomal protein S2

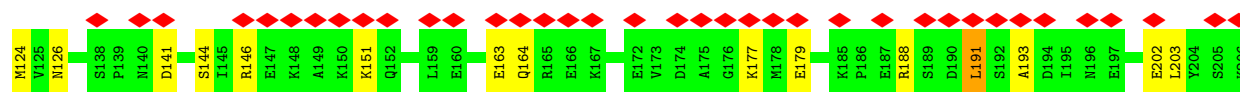


• Molecule 37: 30S ribosomal protein S3

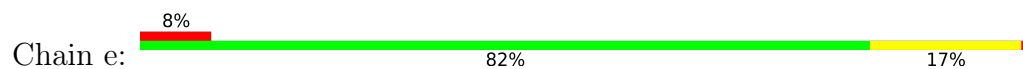


• Molecule 38: 30S ribosomal protein S4

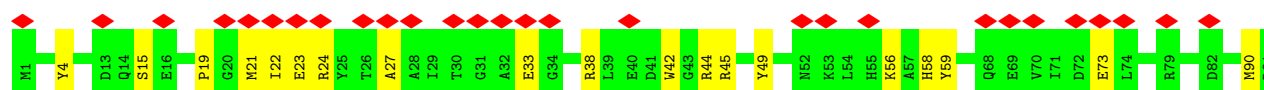
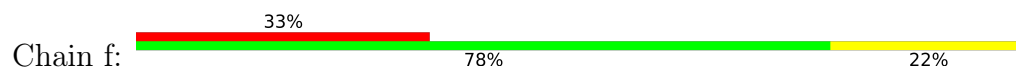




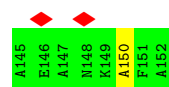
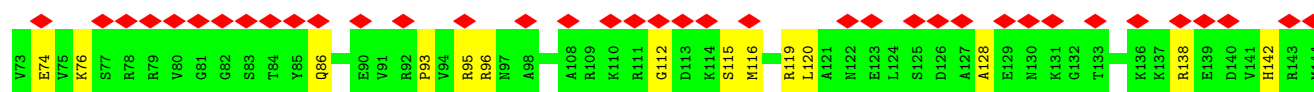
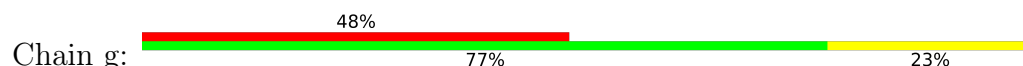
- Molecule 39: 30S ribosomal protein S5



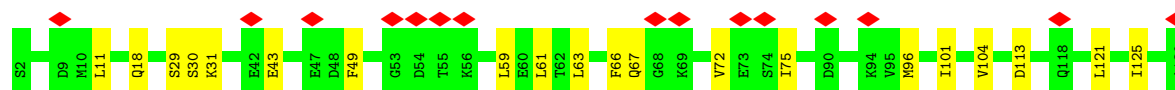
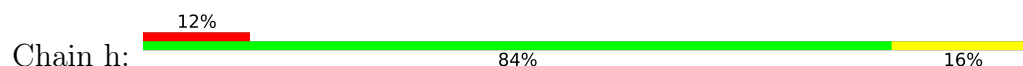
- Molecule 40: 30S ribosomal protein S6



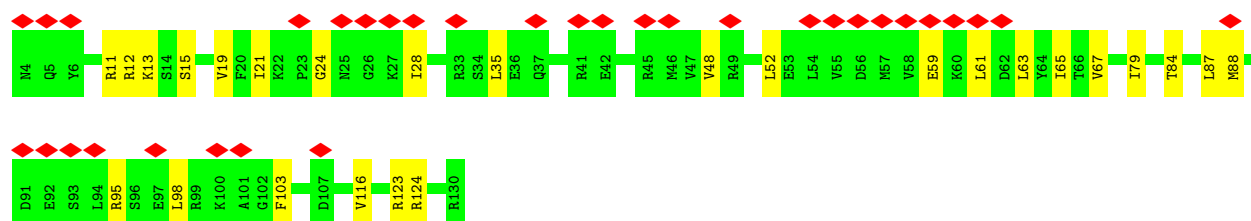
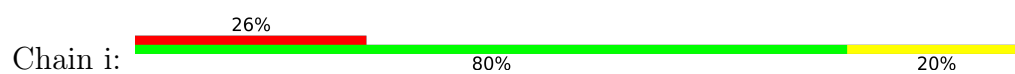
- Molecule 41: 30S ribosomal protein S7



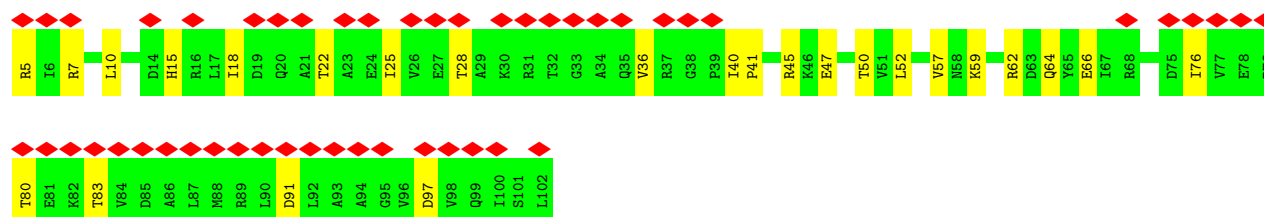
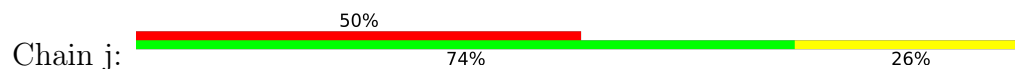
- Molecule 42: 30S ribosomal protein S8



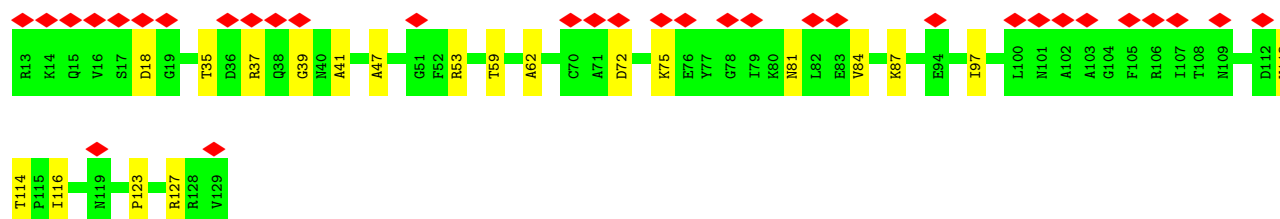
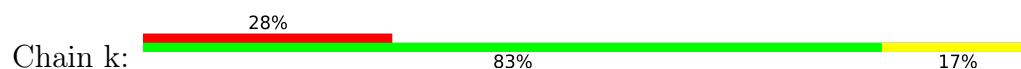
- Molecule 43: 30S ribosomal protein S9



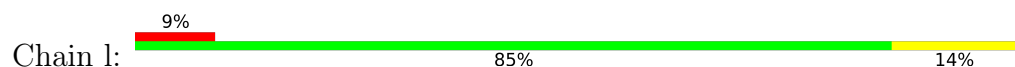
- Molecule 44: 30S ribosomal protein S10



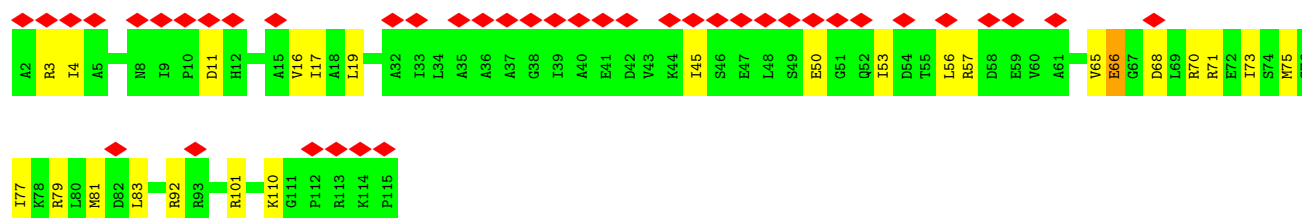
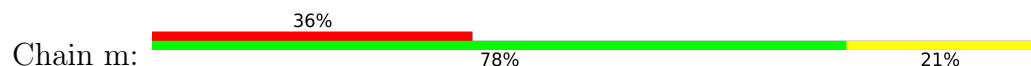
- Molecule 45: 30S ribosomal protein S11



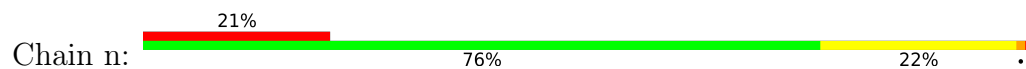
- Molecule 46: 30S ribosomal protein S12



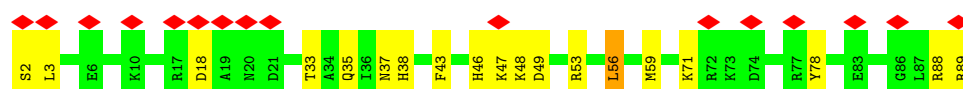
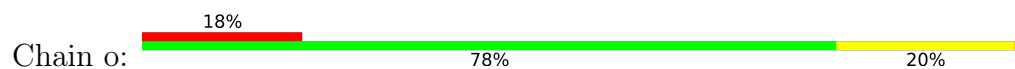
- Molecule 47: 30S ribosomal protein S13



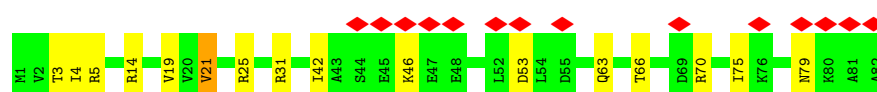
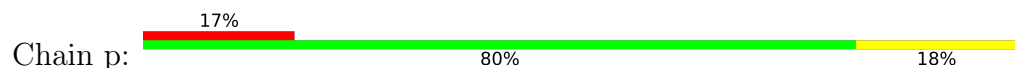
- Molecule 48: 30S ribosomal protein S14



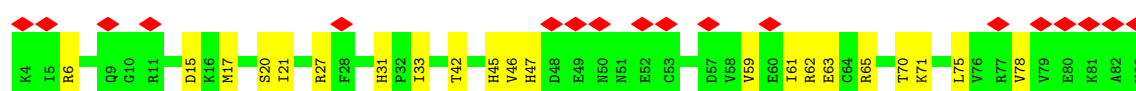
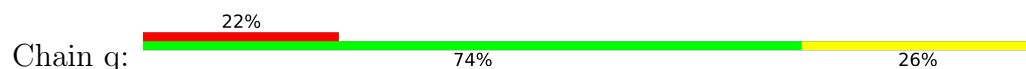
- Molecule 49: 30S ribosomal protein S15



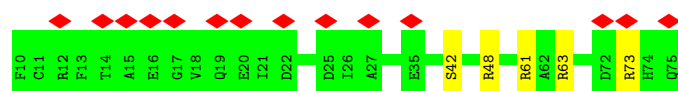
- Molecule 50: 30S ribosomal protein S16



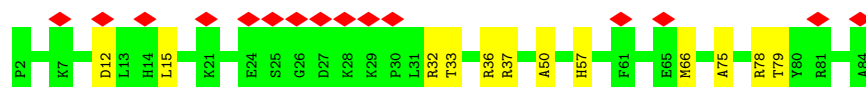
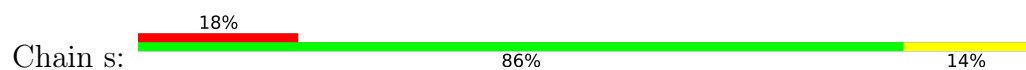
- Molecule 51: 30S ribosomal protein S17



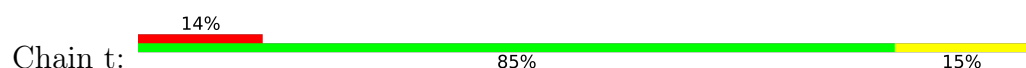
- Molecule 52: 30S ribosomal protein S18

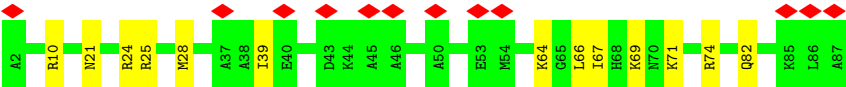


- Molecule 53: 30S ribosomal protein S19

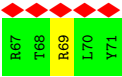
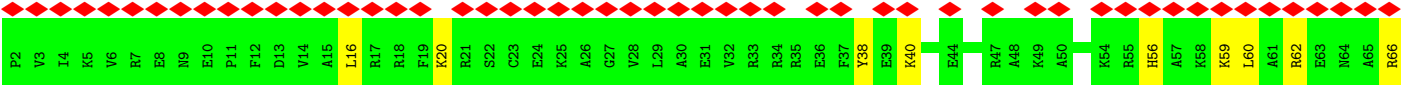
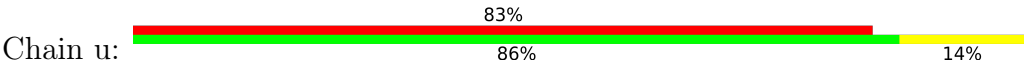


- Molecule 54: 30S ribosomal protein S20





• Molecule 55: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	172175	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.748	Depositor
Minimum map value	-0.390	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	398.88, 398.88, 398.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	0.41	1/69800 (0.0%)	0.46	8/108892 (0.0%)
2	B	0.28	0/2873	0.43	0/4478
3	C	0.41	0/2121	0.70	2/2852 (0.1%)
4	D	0.38	0/1586	0.64	0/2134
5	E	0.31	0/1571	0.61	0/2113
6	F	0.29	0/1434	0.69	0/1926
7	G	0.27	0/1324	0.70	1/1794 (0.1%)
8	H	0.30	0/1122	0.85	4/1515 (0.3%)
9	J	0.34	0/1152	0.55	0/1551
10	K	0.37	0/947	0.71	0/1268
11	L	0.35	0/1062	0.73	0/1413
12	M	0.34	0/1093	0.62	0/1460
13	N	0.38	0/958	0.65	0/1281
14	O	0.28	0/902	0.67	2/1209 (0.2%)
15	P	0.35	0/929	0.61	0/1242
16	Q	0.40	0/960	0.55	0/1278
17	R	0.35	0/829	0.71	0/1107
18	S	0.35	0/864	0.63	0/1156
19	T	0.29	0/715	0.63	1/955 (0.1%)
20	U	0.33	0/787	0.76	3/1051 (0.3%)
21	V	0.29	0/766	0.58	0/1025
22	W	0.34	0/582	0.57	0/769
23	X	0.34	0/635	0.60	0/848
24	Y	0.29	0/510	0.61	0/677
25	Z	0.30	0/453	0.51	0/605
26	0	0.38	0/440	0.61	0/588
27	1	0.31	0/416	0.76	0/554
28	2	0.39	0/380	0.64	0/498
29	3	0.37	0/513	0.78	3/676 (0.4%)
30	4	0.39	0/303	0.73	0/397
31	5	0.27	0/523	0.80	1/698 (0.1%)
32	6	0.38	0/65	0.46	0/98

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	7	0.30	0/69	0.94	0/89
34	8	0.25	0/2080	0.40	0/3242
35	a	0.44	0/36991	0.46	1/57705 (0.0%)
36	b	0.33	0/1784	0.77	0/2403
37	c	0.36	0/1651	0.74	1/2225 (0.0%)
38	d	0.34	0/1665	0.73	0/2227
39	e	0.41	0/1169	0.75	0/1573
40	f	0.35	0/829	0.73	0/1120
41	g	0.32	0/1195	0.79	1/1602 (0.1%)
42	h	0.41	0/989	0.66	0/1326
43	i	0.38	0/1034	0.79	0/1375
44	j	0.36	0/796	0.77	0/1077
45	k	0.34	0/893	0.66	0/1205
46	l	0.43	0/969	0.79	3/1300 (0.2%)
47	m	0.35	0/892	0.79	3/1193 (0.3%)
48	n	0.40	0/817	0.70	0/1088
49	o	0.36	0/722	0.67	0/964
50	p	0.39	0/659	0.76	0/884
51	q	0.37	0/657	0.79	1/881 (0.1%)
52	r	0.32	0/554	0.61	0/743
53	s	0.31	0/680	0.61	0/915
54	t	0.34	0/676	0.57	0/895
55	u	0.28	0/598	0.66	0/792
All	All	0.40	1/156984 (0.0%)	0.53	35/234932 (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
5	E	0	1
8	H	0	2
14	O	0	1
17	R	0	3
18	S	0	2
20	U	0	2
27	1	0	1
29	3	0	1
33	7	0	1
36	b	0	1
38	d	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	e	0	1
40	f	0	1
41	g	0	1
42	h	0	1
43	i	0	1
44	j	0	1
47	m	0	1
48	n	0	3
50	p	0	1
51	q	0	1
52	r	0	2
All	All	0	32

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2604	U	N3-C4	-5.73	1.26	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	g	65	ALA	N-CA-C	-8.15	104.21	114.56
47	m	4	ILE	CA-C-N	6.63	130.77	120.82
47	m	4	ILE	C-N-CA	6.63	130.77	120.82
19	T	2	ILE	N-CA-C	-6.20	105.32	111.77
8	H	8	LYS	CA-C-N	6.20	133.12	121.97
8	H	8	LYS	C-N-CA	6.20	133.12	121.97
8	H	2	GLN	CA-C-N	5.82	132.44	121.97
8	H	2	GLN	C-N-CA	5.82	132.44	121.97
46	l	15	LYS	CA-C-N	5.77	132.35	121.97
46	l	15	LYS	C-N-CA	5.77	132.35	121.97
29	3	32	ILE	N-CA-C	5.73	121.26	109.34
14	O	87	ILE	CA-C-N	5.64	129.27	120.82
14	O	87	ILE	C-N-CA	5.64	129.27	120.82
20	U	88	GLU	CA-C-N	5.64	132.31	121.54
20	U	88	GLU	C-N-CA	5.64	132.31	121.54
51	q	70	THR	N-CA-C	-5.63	100.30	108.07
1	A	1130	U	P-O3'-C3'	5.44	128.36	120.20
29	3	31	HIS	CA-C-N	5.44	131.76	121.97
29	3	31	HIS	C-N-CA	5.44	131.76	121.97
20	U	88	GLU	N-CA-C	-5.40	102.29	110.28
1	A	242	G	P-O3'-C3'	5.28	128.12	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	m	66	GLU	N-CA-CB	-5.26	101.59	110.49
7	G	13	ALA	N-CA-C	5.25	117.06	110.91
35	a	1190	G	P-O3'-C3'	5.23	128.05	120.20
1	A	51	G	C2'-C3'-O3'	5.22	117.32	109.50
1	A	859	G	P-O3'-C3'	5.18	127.97	120.20
3	C	14	ARG	CA-C-N	-5.18	114.86	122.83
3	C	14	ARG	C-N-CA	-5.18	114.86	122.83
1	A	1930	G	P-O3'-C3'	5.17	127.95	120.20
1	A	1022	G	P-O3'-C3'	5.14	127.92	120.20
37	c	157	LEU	N-CA-CB	-5.14	108.31	114.17
1	A	1062	G	P-O3'-C3'	5.12	127.88	120.20
46	l	47	SER	N-CA-C	5.08	116.85	110.91
1	A	1173	U	P-O3'-C3'	5.05	127.78	120.20
31	5	3	LYS	N-CA-C	5.03	116.46	110.97

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	1	34	LEU	Peptide
29	3	31	HIS	Peptide
33	7	6[A]	ARG	Sidechain
5	E	82	GLY	Peptide
8	H	2	GLN	Peptide
8	H	8	LYS	Peptide
14	O	87	ILE	Peptide
17	R	50	GLY	Peptide
17	R	51	VAL	Peptide
17	R	53	PHE	Peptide
18	S	62	ASP	Peptide
18	S	64	ALA	Peptide
20	U	87	PHE	Peptide
20	U	88	GLU	Peptide
36	b	73	LYS	Peptide
38	d	191	LEU	Peptide
38	d	31	LYS	Peptide
38	d	39	GLY	Peptide
39	e	98	PRO	Peptide
40	f	33	GLU	Peptide
41	g	64	VAL	Peptide
42	h	66	PHE	Peptide
43	i	59	GLU	Peptide

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Mol	Chain	Res	Type	Group
44	j	91	ASP	Peptide
47	m	65	VAL	Peptide
48	n	33	ASP	Peptide
48	n	34	VAL	Peptide
48	n	54	ASP	Peptide
50	p	42	ILE	Peptide
51	q	15	ASP	Peptide
52	r	48	ARG	Peptide
52	r	73	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62321	0	31343	296	0
2	B	2570	0	1301	10	0
3	C	2082	0	2154	31	0
4	D	1565	0	1616	17	0
5	E	1552	0	1619	18	0
6	F	1410	0	1444	21	0
7	G	1304	0	1345	18	0
8	H	1111	0	1148	20	0
9	J	1129	0	1162	14	0
10	K	938	0	1012	13	0
11	L	1053	0	1129	13	0
12	M	1074	0	1157	18	0
13	N	945	0	989	14	0
14	O	892	0	923	10	0
15	P	917	0	962	14	0
16	Q	947	0	1019	11	0
17	R	816	0	839	5	0
18	S	857	0	922	15	0
19	T	709	0	779	11	0
20	U	779	0	831	16	0
21	V	753	0	780	8	0
22	W	575	0	592	9	0
23	X	625	0	652	5	0
24	Y	509	0	543	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Z	449	0	488	1	0
26	0	434	0	445	7	0
27	1	409	0	440	5	0
28	2	377	0	418	7	0
29	3	504	0	572	8	0
30	4	302	0	340	7	0
31	5	514	0	509	10	0
32	6	60	0	32	0	0
33	7	69	0	75	17	0
34	8	1861	0	937	12	0
35	a	33037	0	16628	169	0
36	b	1753	0	1780	22	0
37	c	1624	0	1696	28	0
38	d	1643	0	1707	32	0
39	e	1156	0	1199	16	0
40	f	811	0	803	15	0
41	g	1181	0	1238	21	0
42	h	979	0	1031	12	0
43	i	1022	0	1070	15	0
44	j	786	0	828	16	0
45	k	877	0	887	19	0
46	l	955	0	1016	11	0
47	m	883	0	941	14	0
48	n	805	0	844	21	0
49	o	714	0	734	12	0
50	p	649	0	666	13	0
51	q	648	0	691	13	0
52	r	545	0	560	3	0
53	s	663	0	688	11	0
54	t	670	0	719	10	0
55	u	590	0	629	7	0
56	7	51	0	67	11	0
All	All	144454	0	96939	973	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 4.

All (973) 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)
33:7:5:MET:SD	56:7:101:ERY:H273	1.58	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:7:5:MET:SD	56:7:101:ERY:C27	2.16	1.32
33:7:6[B]:ARG:NH1	33:7:6[B]:ARG:HB3	1.55	1.21
33:7:6[B]:ARG:HB3	33:7:6[B]:ARG:HH11	1.06	1.05
33:7:5:MET:SD	56:7:101:ERY:H271	2.01	1.00
33:7:1:MET:HE3	56:7:101:ERY:H152	1.42	0.99
1:A:284:U:H3	1:A:356:G:H1	0.97	0.96
33:7:6[B]:ARG:HH11	33:7:6[B]:ARG:CB	1.83	0.91
8:H:86:ASP:CG	40:f:24:ARG:HH11	1.86	0.83
1:A:1530:G:H8	1:A:1530:G:H5''	1.47	0.80
8:H:86:ASP:CG	40:f:24:ARG:NH1	2.40	0.79
31:5:59:ARG:NH1	35:a:1311:A:OP1	2.16	0.78
1:A:1912:A:N7	1:A:1917:U:O4	2.18	0.77
1:A:2590:A:N1	1:A:2604:U:H5	1.84	0.76
1:A:2590:A:N1	1:A:2604:U:C5	2.55	0.75
35:a:83:C:O2	35:a:86:G:N2	2.19	0.74
33:7:6[B]:ARG:HB3	33:7:6[B]:ARG:CZ	2.18	0.74
35:a:207:C:O2	35:a:212:G:N2	2.20	0.74
35:a:76:G:H1	35:a:93:U:H3	1.36	0.74
35:a:107:G:N7	54:t:10:ARG:NH2	2.36	0.73
1:A:2099:U:H3	1:A:2190:G:H1	1.33	0.73
1:A:1530:G:H5''	1:A:1530:G:C8	2.23	0.73
35:a:664:G:H22	35:a:741:G:H1	1.36	0.73
18:S:14:ALA:O	18:S:18:ARG:HB2	1.89	0.73
35:a:207:C:N3	35:a:212:G:N1	2.37	0.72
33:7:1:MET:CE	56:7:101:ERY:H152	2.19	0.72
8:H:86:ASP:OD2	40:f:24:ARG:NH1	2.23	0.71
1:A:2590:A:N6	1:A:2604:U:O4	2.19	0.71
1:A:27:G:N2	1:A:512:G:O2'	2.19	0.71
1:A:1517:G:N2	1:A:1732:C:O2	2.25	0.70
1:A:2451:A:C2	33:7:6[B]:ARG:NH1	2.59	0.70
1:A:95:A:HO2'	24:Y:41:HIS:HD1	1.40	0.69
37:c:67:THR:HA	37:c:102:ASN:O	1.93	0.69
34:8:13:G:H21	34:8:23:A:H62	1.40	0.69
35:a:1200:C:H5''	35:a:1201:A:H3'	1.75	0.69
8:H:3:VAL:HA	8:H:38:PRO:HA	1.76	0.68
44:j:10:LEU:HA	44:j:97:ASP:O	1.94	0.68
37:c:83:ASP:O	37:c:86:LYS:HB3	1.94	0.67
33:7:5:MET:CE	56:7:101:ERY:H273	2.25	0.67
35:a:310:G:H5''	50:p:31:ARG:HB2	1.77	0.66
34:8:8:U:H3	34:8:14:A:H62	1.41	0.66
1:A:1858:A:N6	1:A:1884:G:O2'	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2848:G:O2'	1:A:2867:G:N2	2.28	0.66
1:A:716:A:OP1	49:o:88:ARG:NH1	2.27	0.65
30:4:16:ILE:HG12	30:4:25:VAL:HG22	1.79	0.64
1:A:2304:G:H22	1:A:2312:U:H3	1.45	0.64
1:A:1069:A:H2'	1:A:1073:A:H62	1.61	0.64
1:A:1724:G:H1	1:A:1736:U:H3	1.44	0.64
19:T:67:VAL:HG22	19:T:76:ARG:HG3	1.80	0.63
47:m:83:LEU:HD11	53:s:66:MET:HG2	1.81	0.63
43:i:28:ILE:HG12	43:i:63:LEU:HD13	1.81	0.63
1:A:806:C:OP2	11:L:41:ARG:NH2	2.31	0.63
53:s:36:ARG:NH2	53:s:75:ALA:O	2.31	0.63
12:M:20:LEU:HD13	21:V:81:PRO:HG2	1.80	0.62
47:m:19:LEU:HD21	47:m:56:LEU:HD21	1.81	0.62
7:G:22:GLN:NE2	7:G:38:ASN:O	2.32	0.62
35:a:501:C:OP1	46:l:114:ARG:NH2	2.32	0.62
35:a:1106:G:H5''	37:c:172:ARG:HB3	1.80	0.62
48:n:24:ARG:O	48:n:28:LYS:HB2	1.99	0.62
48:n:49:GLN:NE2	53:s:12:ASP:OD1	2.33	0.62
35:a:261:U:OP2	54:t:74:ARG:NH1	2.33	0.62
1:A:883:G:H1	1:A:893:C:H42	1.47	0.62
37:c:44:THR:O	37:c:48:ALA:HB2	1.99	0.62
1:A:910:A:H62	12:M:12:MET:HA	1.65	0.62
22:W:65:GLY:HA3	22:W:83:GLU:O	2.00	0.61
10:K:109:SER:O	10:K:113:MET:N	2.32	0.61
35:a:356:A:N3	35:a:368:U:O2'	2.34	0.61
35:a:556:C:OP1	46:l:14:ARG:NH1	2.34	0.61
35:a:972:C:OP2	44:j:59:LYS:NZ	2.33	0.61
1:A:2312:U:O2	6:F:37:ASN:ND2	2.34	0.61
8:H:87:GLU:OE1	40:f:21:MET:SD	2.59	0.61
1:A:1105:U:H2'	1:A:1106:G:H8	1.66	0.61
3:C:19:VAL:HG21	3:C:199:GLU:HG3	1.83	0.61
28:2:24:THR:HG23	28:2:27:GLY:H	1.65	0.60
24:Y:31:GLN:HG2	24:Y:36:GLN:HE21	1.67	0.60
1:A:2117:A:H61	1:A:2170:A:H61	1.49	0.60
35:a:951:G:OP2	47:m:101:ARG:NH2	2.35	0.60
51:q:59:VAL:HG22	51:q:78:VAL:HG22	1.82	0.60
1:A:2469:A:N6	1:A:2481:G:O2'	2.34	0.60
20:U:86:ARG:NH1	20:U:100:SER:OG	2.35	0.60
1:A:585:G:N7	16:Q:6:ARG:NH1	2.48	0.60
1:A:1798:U:OP2	3:C:271:ARG:NH2	2.35	0.60
1:A:284:U:O2	1:A:356:G:N2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2849:U:O4	15:P:21:ARG:NH2	2.34	0.60
41:g:28:ASN:OD1	41:g:36:LYS:NZ	2.34	0.60
35:a:31:G:O2'	35:a:48:C:N4	2.34	0.60
38:d:100:ASN:OD1	38:d:111:ARG:NH1	2.35	0.59
1:A:1721:G:O2'	1:A:1739:A:N6	2.35	0.59
44:j:59:LYS:HE2	44:j:62:ARG:HH21	1.66	0.59
35:a:8:A:N6	38:d:202:GLU:O	2.33	0.59
1:A:2452:C:C6	33:7:6[B]:ARG:NH2	2.69	0.59
14:O:40:ILE:HG12	14:O:47:VAL:HG12	1.84	0.59
30:4:14:CYS:HA	30:4:26:ILE:O	2.03	0.59
1:A:948:C:O2	1:A:984:A:O2'	2.20	0.59
33:7:3:HIS:HB2	56:7:101:ERY:H191	1.85	0.59
1:A:517:C:OP1	26:0:13:ARG:NH2	2.36	0.59
53:s:15:LEU:HD13	53:s:33:THR:HG21	1.85	0.58
3:C:135:ILE:O	3:C:167:ARG:NH2	2.36	0.58
35:a:690:G:O6	45:k:53:ARG:NH2	2.36	0.58
21:V:4:ILE:HD11	21:V:63:ILE:HG12	1.85	0.58
35:a:1064:G:O2'	35:a:1190:G:N2	2.36	0.58
37:c:20:SER:OG	37:c:22:TRP:NE1	2.37	0.58
41:g:112:GLY:HA2	41:g:119:ARG:HD3	1.85	0.58
44:j:5:ARG:HH21	44:j:7:ARG:HH21	1.51	0.58
1:A:2298:A:OP1	6:F:71:ARG:NH2	2.37	0.58
41:g:74:GLU:OE1	41:g:95:ARG:NH1	2.37	0.58
1:A:1154:G:OP2	16:Q:58:ARG:NH1	2.36	0.58
1:A:2683:C:OP1	15:P:51:ARG:NH2	2.36	0.58
7:G:86:LYS:HB3	7:G:165:ALA:HB2	1.85	0.58
48:n:27:LEU:HD21	48:n:47:LYS:HG3	1.84	0.58
48:n:44:ALA:HA	48:n:47:LYS:HG2	1.85	0.58
7:G:121:ILE:HG13	7:G:135:GLY:HA3	1.86	0.57
34:8:13:G:N2	34:8:23:A:H62	2.02	0.57
1:A:2683:C:O2	10:K:70:ARG:NH2	2.37	0.57
5:E:127:GLU:O	5:E:156:ASN:ND2	2.37	0.57
6:F:23:ASN:OD1	6:F:27:GLN:NE2	2.37	0.57
1:A:1059:G:H5''	1:A:1060:U:H5''	1.87	0.57
1:A:2182:U:H2'	1:A:2183:A:H8	1.68	0.57
39:e:38:VAL:HG11	39:e:114:VAL:HG22	1.85	0.57
17:R:60:LYS:NZ	17:R:99:THR:OG1	2.37	0.57
35:a:559:A:H4'	35:a:560:A:H3'	1.86	0.57
43:i:88:MET:HG2	43:i:95:ARG:HB3	1.86	0.57
48:n:49:GLN:HE22	53:s:12:ASP:HA	1.69	0.57
1:A:2305:U:H5''	6:F:131:GLY:HA3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:ASN:HB3	3:C:24:LEU:HG	1.87	0.57
35:a:740:U:OP1	49:o:38:HIS:NE2	2.38	0.57
1:A:1799:G:N7	3:C:178:SER:OG	2.36	0.57
35:a:1376:U:O4	41:g:10:ARG:NH1	2.37	0.57
38:d:188:ARG:NH1	38:d:191:LEU:O	2.37	0.57
45:k:72:ASP:HA	45:k:75:LYS:HG3	1.87	0.57
35:a:1320:C:O2	53:s:36:ARG:NH1	2.38	0.56
1:A:1607:C:N4	1:A:1622:G:OP2	2.35	0.56
12:M:134:THR:HG21	21:V:79:ARG:HH21	1.69	0.56
35:a:1112:C:O2'	37:c:179:ARG:NH1	2.38	0.56
7:G:2:SER:OG	7:G:3:ARG:N	2.38	0.56
35:a:979:C:O2	48:n:59:ARG:NH1	2.39	0.56
38:d:29:ASP:N	38:d:29:ASP:OD1	2.38	0.56
5:E:3:LEU:HD22	5:E:113:VAL:HG21	1.87	0.56
7:G:11:VAL:HG23	7:G:76:VAL:HG21	1.87	0.56
34:8:16:U:O4'	34:8:70:G:N2	2.39	0.56
35:a:993:G:O2'	35:a:994:A:N7	2.37	0.56
3:C:75:PRO:HA	3:C:117:GLN:HB3	1.86	0.56
27:1:36:LEU:HD13	27:1:38:LYS:HE2	1.88	0.56
1:A:636:G:N7	11:L:109:LYS:NZ	2.54	0.56
35:a:5:U:O2'	35:a:6:G:N2	2.39	0.56
35:a:227:G:O2'	50:p:63:GLN:NE2	2.35	0.56
35:a:1100:C:H5'	55:u:69:ARG:HH12	1.70	0.56
48:n:14:VAL:HG22	48:n:60:GLN:HE22	1.70	0.56
1:A:2128:G:N3	1:A:2173:A:O2'	2.36	0.56
6:F:4:LEU:HD23	6:F:101:GLU:HG2	1.87	0.56
6:F:74:VAL:HG12	6:F:76:GLY:H	1.70	0.56
20:U:3:ALA:O	20:U:6:ARG:NH2	2.38	0.56
1:A:494:G:H4'	18:S:6:LYS:HB2	1.88	0.56
1:A:663:G:H5''	11:L:17:LYS:HD3	1.88	0.56
1:A:2102:G:H1	1:A:2187:U:H3	1.54	0.56
34:8:1:G:H1	34:8:83:U:H3	1.53	0.56
16:Q:48:ARG:NH2	16:Q:52:GLN:OE1	2.38	0.56
48:n:31:ILE:O	48:n:41:ARG:NH1	2.38	0.56
37:c:91:VAL:HA	37:c:94:ILE:HG22	1.88	0.56
6:F:102:ARG:NH2	31:5:9:TYR:OH	2.39	0.55
18:S:4:ILE:HG22	18:S:106:VAL:HG22	1.87	0.55
1:A:2788:C:O2'	1:A:2809:A:N3	2.35	0.55
37:c:44:THR:O	37:c:48:ALA:CB	2.54	0.55
1:A:500:G:N1	1:A:503:A:OP2	2.38	0.55
6:F:140:GLU:HA	31:5:28:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:110:VAL:HG13	8:H:114:GLU:HB2	1.89	0.55
38:d:121:LYS:HB3	38:d:146:ARG:HH21	1.71	0.55
43:i:84:THR:HG21	43:i:103:PHE:HB3	1.88	0.55
1:A:2314:A:OP1	6:F:88:LYS:NZ	2.36	0.55
21:V:32:GLY:O	21:V:93:ARG:NH1	2.39	0.55
37:c:11:ARG:NH2	37:c:175:LEU:O	2.40	0.55
1:A:1428:C:OP2	3:C:28:LYS:NZ	2.40	0.55
35:a:1061:G:N7	37:c:2:GLY:N	2.53	0.55
13:N:24:MET:HE2	13:N:44:LEU:HD22	1.88	0.55
15:P:89:ARG:HB3	15:P:113:ARG:HD3	1.88	0.55
44:j:52:LEU:HD21	44:j:59:LYS:HD2	1.88	0.55
1:A:1053:C:H42	1:A:1106:G:H1	1.55	0.55
36:b:148:LEU:HD22	36:b:151:ILE:HD11	1.89	0.55
45:k:18:ASP:OD2	45:k:37:ARG:NH2	2.39	0.55
50:p:75:ILE:O	50:p:79:ASN:HB2	2.07	0.55
1:A:674:G:H1'	5:E:69:ARG:HD3	1.89	0.55
1:A:2306:C:N4	6:F:39:GLY:O	2.39	0.55
17:R:58:VAL:H	17:R:102:SER:HB3	1.72	0.55
19:T:8:LEU:O	24:Y:29:ARG:NH1	2.30	0.55
35:a:537:G:OP1	46:l:110:ARG:NH2	2.33	0.55
44:j:45:ARG:NH1	44:j:47:GLU:OE2	2.39	0.54
47:m:77:ILE:HG22	47:m:81:MET:HE2	1.88	0.54
1:A:2204:G:OP2	3:C:147:LYS:NZ	2.39	0.54
20:U:37:GLU:HA	20:U:62:GLU:HG2	1.89	0.54
35:a:83:C:O2'	35:a:86:G:N2	2.40	0.54
35:a:134:G:O6	50:p:25:ARG:NH2	2.40	0.54
35:a:736:C:OP1	52:r:61:ARG:NH2	2.40	0.54
48:n:54:ASP:OD1	48:n:54:ASP:N	2.40	0.54
1:A:84:A:OP1	20:U:6:ARG:NH1	2.40	0.54
9:J:13:ARG:NH1	9:J:49:ASP:O	2.37	0.54
20:U:74:ASN:ND2	20:U:81:ASP:OD2	2.40	0.54
51:q:62:ARG:NH1	51:q:63:GLU:O	2.40	0.54
1:A:1338:G:N7	19:T:66:LYS:NZ	2.51	0.54
40:f:45:ARG:O	40:f:56:LYS:HA	2.08	0.54
1:A:568:U:O4	17:R:81:LYS:NZ	2.40	0.54
6:F:60:ILE:O	6:F:102:ARG:NH1	2.40	0.54
6:F:105:THR:HA	31:5:38:SER:HB3	1.90	0.54
35:a:212:G:H2'	35:a:213:G:H8	1.73	0.54
41:g:70:ARG:H	41:g:138:ARG:HD3	1.72	0.54
1:A:276:U:O2'	1:A:278:A:N6	2.41	0.54
11:L:127:VAL:HG11	11:L:142:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:26:VAL:HG13	12:M:104:GLU:HG2	1.89	0.54
15:P:85:SER:OG	15:P:87:LYS:NZ	2.41	0.54
35:a:1124:G:N2	35:a:1125:U:O4	2.31	0.54
1:A:251:A:OP1	11:L:58:TYR:OH	2.26	0.54
1:A:920:A:OP1	25:Z:19:LYS:NZ	2.41	0.54
8:H:116:ARG:NH1	8:H:132:PHE:O	2.40	0.54
9:J:36:LEU:HD11	9:J:122:LEU:HB2	1.89	0.54
35:a:224:U:OP1	54:t:69:LYS:NZ	2.40	0.54
12:M:50:ARG:HD3	12:M:65:ILE:HD11	1.91	0.53
13:N:114:GLU:OE1	13:N:118:ARG:NH2	2.41	0.53
30:4:1:MET:HE2	30:4:36:ARG:HB2	1.89	0.53
1:A:2350:C:OP2	29:3:45:ARG:NH1	2.41	0.53
45:k:59:THR:HG23	45:k:62:ALA:H	1.73	0.53
3:C:82:GLU:HB2	3:C:91:ILE:HG13	1.91	0.53
8:H:78:VAL:HG21	8:H:103:VAL:HG12	1.90	0.53
1:A:1040:A:N1	1:A:1115:G:O6	2.41	0.53
41:g:5:ARG:HB3	41:g:7:ILE:HG23	1.89	0.53
51:q:47:HIS:HA	51:q:71:LYS:HE3	1.89	0.53
1:A:320:A:N3	5:E:163:ASN:ND2	2.52	0.53
35:a:264:C:H4'	51:q:65:ARG:HD2	1.89	0.53
36:b:131:LYS:O	36:b:134:ALA:HB3	2.08	0.53
12:M:54:THR:HG22	12:M:63:ILE:HG13	1.91	0.53
21:V:72:VAL:HG12	21:V:93:ARG:HA	1.91	0.53
1:A:2345:G:H5'	1:A:2347:C:H5'	1.91	0.53
1:A:2618:G:H21	4:D:155:VAL:HG21	1.74	0.53
42:h:113:ASP:OD1	42:h:113:ASP:N	2.41	0.53
54:t:39:ILE:HG21	54:t:82:GLN:HG3	1.89	0.53
1:A:2126:A:N6	1:A:2163:A:O2'	2.42	0.53
8:H:9:VAL:HG12	8:H:11:ASN:H	1.74	0.53
20:U:25:VAL:HG22	20:U:36:VAL:HG22	1.91	0.53
26:0:38:HIS:ND1	26:0:39:LEU:O	2.42	0.53
35:a:707:U:O2'	45:k:39:GLY:O	2.26	0.53
35:a:1317:C:OP2	48:n:28:LYS:NZ	2.31	0.53
37:c:14:ILE:HG22	37:c:15:VAL:HG23	1.89	0.53
44:j:22:THR:HA	44:j:25:ILE:HG12	1.91	0.53
1:A:1022:G:O6	9:J:68:LYS:NZ	2.39	0.53
35:a:403:C:OP2	38:d:71:GLN:NE2	2.42	0.53
1:A:627:A:OP1	11:L:78:ARG:NH1	2.42	0.52
3:C:69:ARG:NH2	3:C:127:GLY:O	2.42	0.52
1:A:2585:U:C5	34:8:87:A:H5'	2.44	0.52
7:G:9:VAL:HG13	7:G:73:ASN:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:c:152:GLU:HB3	37:c:199:LYS:HB2	1.90	0.52
1:A:713:G:H21	1:A:718:A:H62	1.58	0.52
2:B:11:C:OP1	22:W:72:LYS:NZ	2.42	0.52
35:a:363:A:N6	46:l:27:CYS:SG	2.81	0.52
35:a:677:U:H3	35:a:713:G:H22	1.56	0.52
35:a:1360:A:OP2	48:n:75:ARG:NH2	2.42	0.52
41:g:27:VAL:HG12	41:g:43:VAL:HG21	1.92	0.52
1:A:284:U:O4	1:A:356:G:O6	2.28	0.52
35:a:398:U:H2'	35:a:399:G:H8	1.75	0.52
1:A:1447:C:O2'	1:A:1544:A:N3	2.39	0.52
1:A:1834:U:H5'	1:A:1835:G:H5'	1.92	0.52
1:A:2370:G:O2'	27:1:44:ARG:NH1	2.41	0.52
35:a:1005:A:OP2	35:a:1024:G:N2	2.43	0.52
35:a:1255:G:OP2	44:j:45:ARG:NH2	2.43	0.52
37:c:184:TYR:OH	37:c:199:LYS:NZ	2.43	0.52
41:g:70:ARG:HD2	41:g:96:ARG:HG2	1.92	0.52
44:j:80:THR:O	44:j:83:THR:OG1	2.24	0.52
12:M:40:ARG:HD2	12:M:93:VAL:HG21	1.92	0.52
15:P:91:ALA:HB2	15:P:113:ARG:HA	1.91	0.52
35:a:692:U:H5''	45:k:127:ARG:HH12	1.75	0.52
35:a:1350:A:O2'	41:g:33:ASP:OD1	2.26	0.52
1:A:2682:A:H61	1:A:2728:U:H1'	1.75	0.52
12:M:17:ASN:OD1	12:M:97:GLN:NE2	2.42	0.52
19:T:38:ALA:HB1	19:T:43:ILE:HD11	1.92	0.52
35:a:1261:A:N6	35:a:1274:A:O2'	2.40	0.52
43:i:12:ARG:HD3	43:i:13:LYS:HB2	1.92	0.52
1:A:1796:U:H2'	1:A:1797:G:H8	1.74	0.52
2:B:52:A:N7	14:O:64:TYR:OH	2.38	0.52
4:D:84:LEU:HD22	4:D:88:GLU:HB2	1.90	0.52
35:a:1425:U:H2'	35:a:1426:G:H8	1.75	0.52
37:c:39:VAL:HG22	37:c:94:ILE:HG23	1.92	0.52
54:t:28:MET:HE1	54:t:67:ILE:HG21	1.92	0.52
2:B:8:C:O3'	14:O:25:ARG:NH2	2.42	0.52
7:G:30:ASN:ND2	7:G:78:GLY:O	2.38	0.52
49:o:3:LEU:HB2	49:o:35:GLN:HE21	1.75	0.52
1:A:2638:G:O2'	1:A:2778:A:N6	2.43	0.51
7:G:102:VAL:HG12	7:G:116:GLN:HA	1.92	0.51
20:U:86:ARG:HG3	20:U:88:GLU:H	1.75	0.51
4:D:10:GLY:H	4:D:197:THR:HG23	1.75	0.51
35:a:938:A:N3	35:a:1376:U:O2'	2.40	0.51
38:d:39:GLY:HA3	38:d:41:HIS:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:o:56:LEU:HA	49:o:59:MET:HE3	1.92	0.51
1:A:1062:G:C6	1:A:1077:A:C6	2.98	0.51
1:A:2140:G:H2'	1:A:2141:G:H8	1.75	0.51
2:B:111:U:H2'	2:B:112:G:H8	1.75	0.51
16:Q:72:ASN:HB3	16:Q:110:VAL:HG11	1.92	0.51
1:A:917:A:H5''	1:A:2268:A:H61	1.75	0.51
1:A:1340:U:OP1	19:T:19:LYS:NZ	2.39	0.51
1:A:2134:A:O2'	1:A:2159:G:N3	2.41	0.51
1:A:2271:G:H5'	22:W:20:ARG:HD3	1.93	0.51
8:H:116:ARG:NH2	8:H:133:GLN:OE1	2.43	0.51
38:d:163:GLU:OE2	38:d:164:GLN:NE2	2.43	0.51
39:e:115:LEU:HD13	39:e:123:VAL:HG11	1.93	0.51
1:A:1048:A:OP2	1:A:1110:G:N2	2.43	0.51
1:A:2107:G:H22	1:A:2182:U:H3	1.57	0.51
15:P:9:GLU:OE1	15:P:56:HIS:NE2	2.44	0.51
54:t:21:ASN:OD1	54:t:24:ARG:NH2	2.44	0.51
5:E:52:VAL:HG11	5:E:81:GLY:HA2	1.92	0.51
9:J:4:PHE:O	16:Q:64:ARG:NH2	2.43	0.51
11:L:51:GLU:OE1	11:L:54:GLN:NE2	2.43	0.51
35:a:207:C:N4	35:a:212:G:O6	2.43	0.51
40:f:19:PRO:O	40:f:22:ILE:HB	2.11	0.51
44:j:15:HIS:HA	44:j:18:ILE:HG22	1.92	0.51
11:L:141:LYS:NZ	11:L:143:GLU:O	2.42	0.51
35:a:401:C:O2'	35:a:621:A:N3	2.42	0.51
36:b:31:ILE:HD12	36:b:39:HIS:HB3	1.92	0.51
1:A:1558:C:H4'	1:A:1559:U:H5'	1.93	0.51
9:J:9:GLU:HG2	9:J:10:THR:HG23	1.93	0.51
35:a:28:A:O2'	35:a:296:U:OP1	2.24	0.51
44:j:50:THR:HG23	44:j:64:GLN:HG2	1.92	0.51
1:A:1066:U:N3	1:A:1069:A:OP2	2.38	0.51
1:A:2099:U:O2	1:A:2190:G:N2	2.35	0.51
1:A:2320:U:C2	1:A:2333:A:N6	2.79	0.51
1:A:2340:A:H5'	2:B:41:G:H21	1.76	0.51
49:o:71:LYS:HE2	49:o:89:ARG:HH22	1.75	0.51
1:A:1032:A:H1'	30:4:23:ILE:HD13	1.93	0.50
3:C:107:PRO:HD2	3:C:110:LEU:HD22	1.91	0.50
13:N:103:ARG:HB2	13:N:110:MET:HE3	1.93	0.50
30:4:7:VAL:HG22	30:4:38:GLY:HA3	1.92	0.50
38:d:99:ASP:OD1	38:d:99:ASP:N	2.43	0.50
47:m:50:GLU:HA	47:m:53:ILE:HG12	1.92	0.50
7:G:44:LYS:O	7:G:50:LEU:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:1144:G:H21	35:a:1146:A:H62	1.60	0.50
1:A:686:U:O4	28:2:12:ARG:NH2	2.38	0.50
35:a:437:U:O2'	38:d:120:HIS:ND1	2.39	0.50
44:j:36:VAL:HG12	44:j:76:ILE:HG12	1.93	0.50
1:A:1223:G:OP1	17:R:68:ARG:NH2	2.45	0.50
1:A:1819:A:H4'	1:A:1820:U:H5''	1.93	0.50
1:A:2245:U:H5''	1:A:2246:G:H5'	1.94	0.50
4:D:7:LYS:HE2	4:D:77:ARG:HH11	1.76	0.50
33:7:6[B]:ARG:HH11	33:7:6[B]:ARG:CA	2.25	0.50
36:b:5:SER:OG	36:b:6:MET:N	2.42	0.50
41:g:11:LYS:NZ	41:g:12:ILE:O	2.41	0.50
31:5:4:ASP:OD1	31:5:4:ASP:N	2.42	0.50
1:A:45:G:H5''	1:A:46:G:H5'	1.93	0.50
1:A:1038:G:H2'	1:A:1039:A:C8	2.47	0.50
19:T:3:ARG:HH12	19:T:42:GLU:HG2	1.77	0.50
39:e:105:ILE:O	39:e:112:ARG:NH2	2.45	0.50
2:B:48:U:OP1	14:O:30:ARG:NH2	2.33	0.49
35:a:693:G:OP1	45:k:127:ARG:NH2	2.44	0.49
1:A:788:A:OP1	1:A:791:C:N4	2.44	0.49
1:A:1306:C:H2'	1:A:1307:A:H8	1.76	0.49
27:1:11:LEU:HA	27:1:50:LYS:O	2.11	0.49
38:d:19:LEU:HB2	38:d:21:LEU:HD22	1.94	0.49
41:g:30:LEU:HD21	41:g:120:LEU:HD11	1.93	0.49
1:A:574:A:N6	1:A:2034:U:OP1	2.44	0.49
1:A:1365:A:OP1	23:X:3:ARG:NH1	2.42	0.49
38:d:124:MET:HE2	38:d:146:ARG:HA	1.94	0.49
39:e:149:SER:H	39:e:152:MET:HG2	1.77	0.49
1:A:1779:U:OP2	1:A:1784:A:N6	2.37	0.49
7:G:86:LYS:HG3	7:G:132:VAL:HG22	1.94	0.49
42:h:43:GLU:HG2	42:h:101:ILE:HG21	1.93	0.49
44:j:25:ILE:HA	44:j:28:THR:HG22	1.94	0.49
1:A:250:G:OP2	29:3:13:ARG:NH2	2.43	0.49
1:A:1296:G:OP1	1:A:2709:G:O2'	2.26	0.49
1:A:2641:G:H5''	9:J:78:THR:HB	1.94	0.49
1:A:2674:G:H4'	10:K:30:ARG:HG3	1.94	0.49
4:D:5:VAL:H	4:D:32:ASN:HD21	1.59	0.49
35:a:202:G:O2'	35:a:468:A:N3	2.43	0.49
35:a:405:U:O4	38:d:2:ALA:N	2.46	0.49
35:a:946:A:H2'	35:a:947:G:C8	2.48	0.49
47:m:68:ASP:HA	47:m:71:ARG:HB3	1.94	0.49
1:A:1433:A:H2'	1:A:1434:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2467:C:O2	12:M:123:LYS:NZ	2.39	0.49
38:d:188:ARG:HH12	38:d:193:ALA:H	1.59	0.49
50:p:3:THR:HG22	50:p:66:THR:HB	1.93	0.49
1:A:1168:G:H1	1:A:1181:U:H3	1.59	0.49
1:A:1826:G:O2'	1:A:1971:U:OP2	2.31	0.49
14:O:15:ARG:NH2	14:O:95:SER:OG	2.46	0.49
35:a:376:G:H5''	50:p:5:ARG:HB2	1.95	0.49
37:c:112:ASP:HB2	37:c:115:LEU:HD12	1.94	0.49
51:q:46:VAL:HG21	51:q:61:ILE:HD13	1.94	0.49
1:A:998:C:OP2	16:Q:58:ARG:NH2	2.46	0.49
1:A:1568:G:H5'	3:C:60:GLN:HA	1.93	0.49
2:B:42:C:OP2	31:5:2:LYS:NZ	2.41	0.49
12:M:42:THR:HG22	12:M:93:VAL:HG12	1.95	0.49
35:a:1308:U:H2'	35:a:1309:G:H8	1.78	0.49
35:a:1418:A:N6	35:a:1482:G:O2'	2.45	0.49
46:l:86:ARG:HA	46:l:94:ARG:HA	1.94	0.49
21:V:75:GLN:HB2	21:V:92:VAL:HG23	1.95	0.48
36:b:15:HIS:HB3	36:b:43:LEU:HD11	1.95	0.48
39:e:148:ASN:HD21	42:h:96:MET:HE1	1.77	0.48
49:o:2:SER:O	49:o:2:SER:OG	2.30	0.48
1:A:1310:G:H1'	1:A:1611:C:H5''	1.94	0.48
4:D:110:THR:HG21	4:D:169:ARG:HE	1.79	0.48
10:K:107:LEU:HG	10:K:112:PHE:HB3	1.94	0.48
22:W:19:LYS:O	22:W:39:ARG:NH2	2.46	0.48
22:W:25:ARG:HH12	22:W:35:SER:HB3	1.77	0.48
36:b:74:ARG:O	36:b:77:SER:OG	2.26	0.48
36:b:183:VAL:HG23	36:b:197:ASP:H	1.78	0.48
48:n:17:ALA:O	48:n:21:PHE:HB3	2.13	0.48
21:V:45:ASP:O	21:V:49:ASN:ND2	2.47	0.48
35:a:113:G:H1'	35:a:354:G:H5'	1.95	0.48
35:a:542:G:OP1	38:d:10:LYS:NZ	2.45	0.48
36:b:26:LYS:HD3	36:b:193:PRO:HD2	1.95	0.48
48:n:20:TYR:HB2	48:n:55:SER:HB2	1.94	0.48
1:A:1796:U:H2'	1:A:1797:G:C8	2.49	0.48
7:G:89:LEU:HD23	7:G:94:TYR:HB3	1.96	0.48
15:P:51:ARG:O	15:P:57:SER:HA	2.13	0.48
24:Y:10:SER:OG	24:Y:11:VAL:N	2.45	0.48
35:a:890:G:O2'	35:a:906:A:N6	2.45	0.48
35:a:908:A:H2'	35:a:909:A:C8	2.49	0.48
35:a:1316:G:N1	35:a:1319:A:OP2	2.42	0.48
35:a:1530:G:H2'	35:a:1531:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:54:ARG:HD2	46:l:64:THR:HG22	1.95	0.48
55:u:16:LEU:HD23	55:u:20:LYS:HE2	1.96	0.48
1:A:33:C:O2	1:A:447:A:N6	2.45	0.48
4:D:4:LEU:HB2	4:D:101:PHE:HE2	1.78	0.48
35:a:1137:C:O2'	35:a:1138:G:N2	2.46	0.48
36:b:42:ASN:O	36:b:46:THR:OG1	2.31	0.48
1:A:2349:G:OP1	29:3:45:ARG:NH2	2.46	0.48
1:A:2452:C:N1	33:7:6[B]:ARG:NH2	2.59	0.48
1:A:2590:A:C2	1:A:2604:U:H5	2.30	0.48
3:C:71:LYS:O	3:C:118:SER:OG	2.31	0.48
1:A:2087:G:H2'	1:A:2088:A:H8	1.79	0.48
5:E:149:ILE:HG21	5:E:175:ILE:HD11	1.96	0.48
10:K:74:GLY:O	15:P:75:GLN:NE2	2.47	0.48
45:k:87:LYS:NZ	45:k:113:VAL:O	2.47	0.48
50:p:70:ARG:HD2	50:p:70:ARG:HA	1.67	0.48
1:A:1153:C:OP1	16:Q:92:ARG:NH2	2.43	0.48
3:C:160:THR:HG23	3:C:177:ARG:HG2	1.95	0.48
19:T:51:PHE:HZ	24:Y:30:MET:HE2	1.79	0.48
1:A:715:A:N1	49:o:53:ARG:NH1	2.61	0.48
1:A:1645:G:H5''	1:A:1646:C:H5'	1.96	0.48
1:A:2809:A:H2'	1:A:2810:A:C8	2.49	0.48
3:C:94:VAL:HG21	3:C:116:ILE:HD11	1.96	0.48
8:H:81:ALA:HA	8:H:147:VAL:HB	1.96	0.48
1:A:882:G:H22	1:A:894:U:H3	1.61	0.47
8:H:43:ASN:HA	8:H:46:PHE:HB2	1.96	0.47
15:P:16:ASP:OD1	15:P:16:ASP:N	2.41	0.47
34:8:22:G:H5'	34:8:23:A:H5'	1.94	0.47
1:A:2496:C:OP2	12:M:81:ARG:NH1	2.46	0.47
4:D:25:THR:HG21	4:D:193:VAL:HG22	1.96	0.47
35:a:553:A:H5''	46:l:21:VAL:HG21	1.96	0.47
53:s:50:ALA:HB1	53:s:57:HIS:HB3	1.95	0.47
1:A:301:G:OP2	20:U:82:ARG:NH1	2.47	0.47
1:A:411:G:OP2	1:A:2406:A:O2'	2.31	0.47
10:K:13:ASN:HD21	10:K:98:ARG:H	1.63	0.47
13:N:101:GLY:H	26:0:42:HIS:HD2	1.62	0.47
37:c:11:ARG:O	37:c:15:VAL:N	2.46	0.47
1:A:848:C:H2'	1:A:849:A:H8	1.78	0.47
1:A:1278:C:H2'	1:A:1279:G:H8	1.80	0.47
1:A:1340:U:OP1	19:T:84:TYR:OH	2.32	0.47
1:A:2564:A:OP1	1:A:2648:G:O2'	2.32	0.47
38:d:126:ASN:ND2	38:d:141:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:i:12:ARG:O	43:i:15:SER:OG	2.29	0.47
1:A:468:G:N7	28:2:39:ARG:NH2	2.63	0.47
1:A:1864:U:OP1	1:A:2410:G:O2'	2.29	0.47
1:A:2014:A:H4'	18:S:92:ARG:HH22	1.79	0.47
1:A:2590:A:N1	1:A:2604:U:C4	2.82	0.47
14:O:8:ILE:O	14:O:12:THR:OG1	2.20	0.47
35:a:974:A:OP1	48:n:69:ARG:NH2	2.46	0.47
36:b:80:VAL:O	36:b:84:ALA:N	2.47	0.47
38:d:58:LYS:HD3	38:d:203:LEU:HD22	1.96	0.47
49:o:18:ASP:OD1	49:o:18:ASP:N	2.46	0.47
1:A:1508:A:O2'	1:A:1509:A:O4'	2.33	0.47
1:A:2500:U:HO2'	1:A:2504:U:H5	1.57	0.47
1:A:2722:G:O2'	13:N:3:HIS:O	2.30	0.47
35:a:309:A:O2'	35:a:607:A:N1	2.45	0.47
35:a:618:C:H1'	50:p:14:ARG:HH12	1.79	0.47
35:a:1059:C:O3'	48:n:85:ARG:NH2	2.46	0.47
1:A:651:G:H5'	29:3:19:LYS:HG2	1.95	0.47
1:A:1062:G:O6	1:A:1077:A:C6	2.67	0.47
1:A:1187:G:N2	1:A:1188:U:O4	2.47	0.47
1:A:1528:A:N6	1:A:1543:G:O2'	2.47	0.47
1:A:1530:G:C8	1:A:1530:G:C5'	2.96	0.47
1:A:2144:G:O2'	1:A:2147:A:N1	2.47	0.47
1:A:2258:C:O2'	1:A:2427:C:OP2	2.33	0.47
4:D:35:THR:HG22	4:D:73:VAL:HG21	1.97	0.47
5:E:176:ASP:OD1	5:E:176:ASP:N	2.36	0.47
8:H:50:ARG:HD3	8:H:51:ARG:HB3	1.95	0.47
15:P:32:VAL:HG13	15:P:39:ARG:HB3	1.96	0.47
35:a:643:C:OP1	42:h:31:LYS:NZ	2.47	0.47
35:a:1226:C:O2'	47:m:110:LYS:NZ	2.48	0.47
41:g:115:SER:OG	41:g:116:MET:N	2.46	0.47
1:A:2362:C:OP1	29:3:40:ARG:NH1	2.45	0.47
35:a:71:A:H61	35:a:99:C:H1'	1.79	0.47
35:a:1343:G:H4'	43:i:124:ARG:HB2	1.96	0.47
41:g:76:LYS:O	41:g:86:GLN:HA	2.14	0.47
1:A:764:A:OP1	3:C:207:LYS:NZ	2.48	0.47
1:A:1386:C:H2'	1:A:1387:A:C8	2.49	0.47
1:A:1797:G:O2'	3:C:257:THR:OG1	2.32	0.47
6:F:143:TYR:HA	6:F:146:VAL:HG13	1.97	0.47
26:0:43:ILE:HG22	26:0:49:TYR:HB2	1.96	0.47
37:c:136:ARG:HA	37:c:139:GLN:HG2	1.96	0.47
13:N:66:ALA:O	13:N:70:THR:OG1	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:128:LYS:HB3	36:b:129:LEU:HD12	1.96	0.47
47:m:11:ASP:HA	47:m:45:ILE:HB	1.97	0.47
1:A:345:A:O2'	1:A:347:A:N6	2.44	0.46
1:A:1068:G:H21	1:A:1096:A:H5'	1.79	0.46
1:A:2250:G:O2'	1:A:2496:C:OP1	2.33	0.46
1:A:2291:U:OP1	1:A:2380:C:O2'	2.33	0.46
1:A:2636:C:HO2'	4:D:45:TYR:HH	1.62	0.46
56:7:101:ERY:H312	56:7:101:ERY:H2	1.69	0.46
1:A:1445:G:O6	1:A:1466:U:O2	2.33	0.46
35:a:1308:U:H2'	35:a:1309:G:C8	2.50	0.46
37:c:12:LEU:HD11	48:n:91:GLY:HA2	1.96	0.46
24:Y:3:ALA:HB2	24:Y:52:ARG:HD3	1.98	0.46
35:a:686:U:O2'	35:a:687:A:O4'	2.34	0.46
40:f:49:TYR:OH	52:r:63:ARG:O	2.31	0.46
41:g:93:PRO:HA	41:g:96:ARG:HB3	1.97	0.46
1:A:783:A:O2'	1:A:1779:U:O2	2.33	0.46
1:A:2850:A:N7	1:A:2868:A:O2'	2.43	0.46
6:F:41:GLY:HA2	6:F:85:ILE:HG13	1.97	0.46
35:a:976:G:OP2	35:a:1358:U:O2'	2.33	0.46
35:a:1116:U:O2	35:a:1184:G:O6	2.33	0.46
37:c:172:ARG:HH21	37:c:174:PRO:HG3	1.80	0.46
1:A:687:C:H1'	28:2:4:THR:HG22	1.97	0.46
7:G:92:VAL:H	7:G:160:LYS:HZ1	1.63	0.46
8:H:15:LEU:HD23	8:H:56:ALA:HB1	1.98	0.46
35:a:1062:U:O4	37:c:3:GLN:NE2	2.49	0.46
40:f:92:THR:OG1	40:f:93:LYS:N	2.49	0.46
47:m:66:GLU:OE2	47:m:70:ARG:NH2	2.45	0.46
1:A:629:G:N3	1:A:639:U:O2'	2.48	0.46
5:E:144:GLU:OE2	5:E:166:LYS:NZ	2.49	0.46
22:W:18:ALA:O	22:W:20:ARG:NH1	2.49	0.46
40:f:4:TYR:HA	40:f:90:MET:O	2.15	0.46
40:f:42:TRP:HB2	40:f:59:TYR:HB2	1.97	0.46
51:q:31:HIS:HD2	51:q:33:ILE:H	1.63	0.46
1:A:1434:A:H2'	1:A:1435:G:H8	1.80	0.46
1:A:2500:U:O2'	1:A:2504:U:H5	1.99	0.46
31:5:63:ARG:NH1	35:a:1312:G:OP2	2.48	0.46
35:a:1149:C:H2'	35:a:1150:A:C8	2.51	0.46
35:a:1218:C:H2'	35:a:1219:A:C8	2.51	0.46
35:a:1356:G:H2'	35:a:1357:A:C8	2.51	0.46
39:e:74:VAL:HG11	39:e:144:LEU:HB3	1.97	0.46
41:g:150:ALA:HB1	45:k:59:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:C:H2'	1:A:874:G:H8	1.80	0.46
1:A:1936:A:H2	1:A:1943:U:H3	1.63	0.46
8:H:27:ARG:NH1	23:X:60:ASP:OD2	2.49	0.46
20:U:21:LYS:HZ2	20:U:39:ILE:HG13	1.81	0.46
37:c:54:ARG:HH21	37:c:56:VAL:HG11	1.80	0.46
38:d:49:SER:OG	38:d:50:ASP:N	2.49	0.46
1:A:1434:A:H2'	1:A:1435:G:C8	2.51	0.46
18:S:47:VAL:HG12	18:S:103:ILE:HG21	1.97	0.46
35:a:410:G:H2'	35:a:429:U:C4	2.51	0.46
35:a:715:A:H2'	35:a:716:A:C8	2.50	0.46
40:f:38:ARG:HD3	40:f:96:VAL:HG23	1.98	0.46
45:k:123:PRO:HD2	55:u:38:TYR:HD1	1.81	0.46
1:A:964:C:O2'	1:A:2273:A:N3	2.43	0.46
1:A:2131:U:H5'	1:A:2132:U:H5''	1.97	0.46
22:W:44:LYS:HB3	22:W:44:LYS:HE2	1.72	0.46
35:a:110:C:O2'	50:p:25:ARG:O	2.32	0.46
51:q:27:ARG:NH2	51:q:42:THR:OG1	2.49	0.46
55:u:62:ARG:HA	55:u:66:ARG:HE	1.79	0.46
1:A:1652:A:N6	13:N:11:ASN:OD1	2.43	0.45
1:A:2012:G:OP1	18:S:11:ARG:NH2	2.41	0.45
1:A:2386:A:H4'	22:W:56:ASP:HA	1.98	0.45
1:A:2758:A:H1'	7:G:64:GLN:HE22	1.81	0.45
28:2:2:LYS:HE3	28:2:6:GLN:HG3	1.96	0.45
37:c:11:ARG:O	37:c:16:LYS:N	2.43	0.45
48:n:38:ASP:OD1	48:n:38:ASP:N	2.43	0.45
4:D:11:MET:HE2	4:D:11:MET:HB3	1.90	0.45
5:E:168:ASP:OD2	5:E:170:ARG:NE	2.50	0.45
5:E:184:ASP:OD1	11:L:2:ARG:NH1	2.38	0.45
12:M:69:PRO:HA	12:M:94:ALA:HB2	1.98	0.45
13:N:13:ASN:OD1	13:N:13:ASN:N	2.42	0.45
43:i:95:ARG:HA	43:i:98:LEU:HG	1.98	0.45
12:M:2:LEU:H	12:M:43:ALA:HB1	1.81	0.45
22:W:41:ARG:HA	22:W:41:ARG:HD3	1.69	0.45
35:a:147:G:H2'	35:a:148:G:C8	2.52	0.45
43:i:116:VAL:HG13	44:j:62:ARG:HH11	1.81	0.45
1:A:2164:C:H41	1:A:2171:A:H61	1.65	0.45
5:E:164:LEU:HD23	5:E:167:VAL:HG21	1.97	0.45
16:Q:104:VAL:HG11	17:R:45:GLU:HB2	1.99	0.45
39:e:81:LEU:HB2	39:e:98:PRO:HA	1.98	0.45
49:o:46:HIS:O	49:o:48:LYS:N	2.49	0.45
1:A:96:C:OP1	24:Y:39:GLN:NE2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:C:OP1	9:J:37:ARG:NH2	2.50	0.45
1:A:1026:G:H2'	1:A:1027:A:H8	1.82	0.45
1:A:1782:U:H1'	1:A:2609:U:H5''	1.98	0.45
3:C:144:VAL:HB	3:C:154:LEU:HB2	1.98	0.45
19:T:53:VAL:HG11	19:T:87:LEU:HD13	1.99	0.45
34:8:55:G:H2'	34:8:56:G:H8	1.80	0.45
1:A:2515:C:H2'	1:A:2516:A:H8	1.82	0.45
5:E:21:ARG:O	5:E:114:ARG:NH2	2.50	0.45
23:X:18:ARG:HD3	23:X:18:ARG:HA	1.76	0.45
35:a:652:U:O4	35:a:752:G:O2'	2.31	0.45
35:a:1350:A:OP1	43:i:123:ARG:NE	2.42	0.45
49:o:33:THR:O	49:o:37:ASN:ND2	2.49	0.45
1:A:1084:A:O2'	1:A:1105:U:O2'	2.30	0.45
1:A:1266:G:O2'	1:A:2012:G:O6	2.32	0.45
1:A:2327:A:H2'	1:A:2328:A:C8	2.52	0.45
35:a:458:U:H2'	35:a:459:A:C8	2.52	0.45
35:a:613:C:OP1	38:d:81:ARG:NH1	2.48	0.45
35:a:1144:G:N2	35:a:1146:A:H62	2.14	0.45
35:a:1413:A:H2	35:a:1487:G:H22	1.64	0.45
45:k:53:ARG:HA	45:k:53:ARG:HD2	1.75	0.45
1:A:286:U:H2'	1:A:287:G:H8	1.81	0.45
5:E:147:LEU:HB3	5:E:186:VAL:HG12	1.99	0.45
9:J:21:THR:HA	9:J:61:LYS:HB2	1.98	0.45
21:V:20:LEU:HD21	21:V:41:GLU:HG3	1.99	0.45
35:a:83:C:O2	35:a:86:G:C2	2.69	0.45
35:a:458:U:H2'	35:a:459:A:H8	1.81	0.45
35:a:745:G:H2'	35:a:746:A:C8	2.52	0.45
43:i:24:GLY:H	43:i:61:LEU:HA	1.80	0.45
1:A:370:G:O2'	1:A:424:G:OP1	2.32	0.45
18:S:67:ASP:OD1	18:S:67:ASP:N	2.49	0.45
35:a:204:G:H2'	35:a:205:A:H8	1.82	0.45
35:a:279:A:H5''	35:a:281:G:H5'	1.99	0.45
39:e:47:GLY:HA3	39:e:71:MET:HG2	1.99	0.45
1:A:1536:C:O2	1:A:1537:G:N2	2.51	0.44
35:a:494:G:H2'	35:a:496:A:H8	1.82	0.44
35:a:1391:U:H2'	35:a:1392:G:C8	2.53	0.44
44:j:47:GLU:O	44:j:66:GLU:HA	2.17	0.44
48:n:17:ALA:O	48:n:21:PHE:CB	2.64	0.44
1:A:172:A:H2'	1:A:173:A:C8	2.52	0.44
1:A:987:C:O2'	1:A:1000:A:N3	2.46	0.44
1:A:2329:U:H2'	1:A:2330:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5:59:ARG:HA	31:5:62:LYS:HE3	1.98	0.44
35:a:769:G:H4'	35:a:1513:A:H4'	1.99	0.44
35:a:1162:C:H2'	35:a:1163:A:C8	2.53	0.44
43:i:52:LEU:HD23	43:i:87:LEU:HD11	2.00	0.44
1:A:7:G:H5''	9:J:123:LYS:HE2	1.99	0.44
18:S:86:MET:HB3	18:S:94:ASP:HB3	1.99	0.44
35:a:617:G:OP1	50:p:46:LYS:NZ	2.50	0.44
38:d:177:LYS:HD3	38:d:179:GLU:HG3	1.99	0.44
42:h:29:SER:HB3	42:h:59:LEU:HB2	1.99	0.44
48:n:33:ASP:OD1	48:n:33:ASP:N	2.50	0.44
50:p:4:ILE:HG12	50:p:21:VAL:HB	1.98	0.44
1:A:2233:U:H2'	1:A:2234:G:C8	2.52	0.44
1:A:2273:A:H2'	1:A:2274:A:C8	2.52	0.44
4:D:60:VAL:HG13	4:D:64:GLU:HG3	1.99	0.44
35:a:5:U:O4	38:d:84:GLY:N	2.48	0.44
35:a:946:A:O2'	35:a:1333:A:N3	2.45	0.44
42:h:11:LEU:HD22	42:h:75:ILE:HD11	1.98	0.44
1:A:458:G:O2'	1:A:469:G:O6	2.33	0.44
1:A:1509:A:H2'	1:A:1510:G:C8	2.53	0.44
3:C:212:ARG:HD2	3:C:212:ARG:HA	1.82	0.44
24:Y:28:LEU:HD22	24:Y:37:LEU:HD21	1.99	0.44
1:A:2274:A:O2'	1:A:2276:G:OP1	2.31	0.44
5:E:138:LEU:HD13	5:E:146:VAL:HG21	1.99	0.44
35:a:62:U:O2'	35:a:379:C:O2	2.35	0.44
36:b:76:ALA:O	36:b:79:ALA:HB3	2.18	0.44
37:c:153:VAL:HG22	37:c:198:VAL:HG22	1.98	0.44
46:l:53:CYS:HB3	46:l:67:ILE:HD11	2.00	0.44
1:A:288:U:H2'	1:A:289:G:C8	2.53	0.44
1:A:320:A:OP1	5:E:130:LYS:NZ	2.46	0.44
1:A:1800:C:H5	1:A:1819:A:H62	1.66	0.44
6:F:62:GLY:HA3	6:F:95:ARG:HH21	1.82	0.44
10:K:113:MET:HA	10:K:116:ILE:HG22	1.99	0.44
31:5:51:VAL:HG12	47:m:75:MET:HE1	1.99	0.44
35:a:191:G:H2'	35:a:192:A:C8	2.52	0.44
35:a:541:G:O2'	38:d:39:GLY:O	2.32	0.44
35:a:686:U:O4	35:a:703:G:O2'	2.31	0.44
37:c:70:THR:HG21	37:c:76:VAL:HG21	2.00	0.44
51:q:59:VAL:HG11	51:q:75:LEU:HG	1.98	0.44
1:A:397:U:H5''	23:X:32:ASN:HB2	2.00	0.44
36:b:113:ARG:HA	36:b:113:ARG:HD2	1.77	0.44
45:k:116:ILE:HD13	45:k:116:ILE:HA	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:G:H2'	1:A:288:U:C6	2.52	0.44
1:A:307:G:N1	1:A:310:A:OP2	2.50	0.44
1:A:1432:G:H2'	1:A:1433:A:C8	2.53	0.44
1:A:1788:C:H5''	3:C:224:ALA:HB1	1.99	0.44
1:A:1962:C:O2'	1:A:1964:G:OP2	2.31	0.44
10:K:90:ASN:OD1	10:K:90:ASN:N	2.51	0.44
35:a:6:G:H22	39:e:103:THR:HG21	1.82	0.44
35:a:514:C:H2'	35:a:515:G:H8	1.81	0.44
39:e:102:GLY:O	39:e:122:ASN:ND2	2.51	0.44
40:f:15:SER:OG	40:f:44:ARG:NH2	2.51	0.44
1:A:28:A:N6	1:A:512:G:H1'	2.33	0.43
1:A:581:C:H2'	1:A:582:A:C8	2.53	0.43
1:A:1651:G:H5'	13:N:39:PRO:HG2	2.00	0.43
4:D:36:GLN:HB3	4:D:49:GLN:HE21	1.82	0.43
6:F:49:LEU:HD13	6:F:148:ARG:HH12	1.83	0.43
9:J:115:GLY:HA2	9:J:118:MET:HG2	2.00	0.43
20:U:9:ASP:OD1	20:U:94:ARG:NH2	2.43	0.43
20:U:47:LYS:HB2	20:U:47:LYS:HE3	1.78	0.43
35:a:501:C:H2'	35:a:502:A:C8	2.53	0.43
39:e:150:PRO:HA	39:e:153:VAL:HG12	2.00	0.43
7:G:11:VAL:HG22	7:G:15:VAL:HG12	2.00	0.43
19:T:13:ALA:HB3	19:T:33:LYS:HD3	1.99	0.43
35:a:1071:C:H2'	35:a:1072:G:C8	2.53	0.43
49:o:78:TYR:OH	49:o:89:ARG:NH1	2.50	0.43
51:q:17:MET:HE1	51:q:45:HIS:HD2	1.83	0.43
1:A:286:U:H2'	1:A:287:G:C8	2.54	0.43
1:A:1667:G:O2'	1:A:1991:U:O4	2.28	0.43
1:A:1802:A:H2'	1:A:1803:A:C8	2.53	0.43
1:A:2522:U:O2'	1:A:2647:U:OP1	2.27	0.43
10:K:110:GLU:H	10:K:110:GLU:HG3	1.48	0.43
56:7:101:ERY:H71	56:7:101:ERY:H4	1.73	0.43
35:a:6:G:H1	39:e:100:SER:HB3	1.82	0.43
35:a:672:U:H2'	35:a:673:A:C8	2.53	0.43
35:a:1071:C:H2'	35:a:1072:G:H8	1.84	0.43
46:l:10:LYS:HA	46:l:11:PRO:HD3	1.85	0.43
49:o:43:PHE:HE1	49:o:49:ASP:HB3	1.82	0.43
1:A:288:U:H2'	1:A:289:G:H8	1.83	0.43
1:A:309:A:N3	1:A:329:G:O2'	2.51	0.43
1:A:639:U:H2'	1:A:640:C:H6	1.83	0.43
1:A:888:C:C6	47:m:92:ARG:HG2	2.54	0.43
7:G:106:SER:O	7:G:106:SER:OG	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:42:VAL:O	20:U:60:GLU:HA	2.17	0.43
35:a:130:A:C8	51:q:65:ARG:HG3	2.53	0.43
36:b:167:ASP:O	36:b:170:HIS:ND1	2.50	0.43
39:e:11:LEU:HD23	39:e:11:LEU:HA	1.91	0.43
1:A:848:C:H2'	1:A:849:A:C8	2.54	0.43
2:B:1:U:H2'	2:B:2:G:H8	1.84	0.43
10:K:42:THR:HG23	10:K:44:LYS:HD3	2.01	0.43
11:L:85:VAL:HG21	11:L:90:VAL:HG22	2.00	0.43
1:A:639:U:H2'	1:A:640:C:C6	2.54	0.43
1:A:2115:G:OP1	1:A:2166:U:O2'	2.36	0.43
3:C:258:ARG:NH2	3:C:263:THR:OG1	2.44	0.43
8:H:94:ILE:HB	8:H:122:LEU:HB3	1.99	0.43
13:N:36:THR:OG1	13:N:37:THR:N	2.51	0.43
18:S:73:LYS:HB2	18:S:106:VAL:HB	2.00	0.43
36:b:114:LEU:HD11	36:b:145:GLU:HG3	2.00	0.43
38:d:72:PHE:HE1	38:d:94:LEU:HD11	1.83	0.43
41:g:70:ARG:HG3	41:g:96:ARG:HD3	2.01	0.43
45:k:87:LYS:HG3	45:k:114:THR:HA	1.99	0.43
47:m:16:VAL:HG23	47:m:17:ILE:HD12	2.01	0.43
1:A:1168:G:H2'	1:A:1169:A:H8	1.83	0.43
1:A:1176:U:H6	1:A:1176:U:H2'	1.71	0.43
8:H:7:ASP:OD2	8:H:8:LYS:N	2.52	0.43
24:Y:19:LEU:HD23	24:Y:19:LEU:HA	1.82	0.43
35:a:166:U:H2'	35:a:167:A:C8	2.53	0.43
35:a:337:G:H2'	35:a:338:A:C8	2.53	0.43
35:a:564:C:OP1	46:l:12:ARG:NH1	2.50	0.43
35:a:674:G:H2'	35:a:675:A:C8	2.54	0.43
35:a:766:A:OP2	35:a:812:G:N2	2.49	0.43
1:A:265:A:O2'	1:A:428:A:N6	2.52	0.43
1:A:1278:C:H2'	1:A:1279:G:C8	2.53	0.43
12:M:102:LEU:HD11	12:M:126:ILE:HD11	1.99	0.43
14:O:67:ASN:OD1	14:O:67:ASN:N	2.47	0.43
1:A:2646:C:OP2	1:A:2732:G:O2'	2.37	0.43
12:M:11:LYS:HD3	12:M:86:LYS:HG2	2.01	0.43
12:M:34:LYS:HD2	12:M:131:VAL:HG11	2.00	0.43
16:Q:15:LYS:HE3	16:Q:15:LYS:HB3	1.86	0.43
34:8:8:U:O4	34:8:14:A:N7	2.52	0.43
35:a:944:G:N1	35:a:1338:G:OP2	2.41	0.43
36:b:139:ARG:O	36:b:143:LYS:N	2.47	0.43
53:s:32:ARG:HA	53:s:50:ALA:HB3	2.01	0.43
1:A:125:A:H2	28:2:9:VAL:HG13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:U:H2'	1:A:172:A:C8	2.53	0.43
1:A:285:G:H1	1:A:355:U:H3	1.67	0.43
1:A:770:G:H5''	28:2:10:LEU:HD23	2.00	0.43
1:A:1090:A:H2'	1:A:1091:G:H8	1.84	0.43
1:A:1900:A:H1'	1:A:1970:A:H2'	2.01	0.43
7:G:175:LYS:HD2	7:G:175:LYS:HA	1.84	0.43
9:J:12:LYS:HD3	9:J:12:LYS:HA	1.85	0.43
11:L:62:PRO:HB2	29:3:30:ARG:HH11	1.84	0.43
35:a:108:G:N1	54:t:10:ARG:HG2	2.33	0.43
35:a:350:G:H2'	35:a:351:G:C8	2.53	0.43
1:A:1670:C:O2	4:D:134:HIS:NE2	2.49	0.42
1:A:2246:G:H2'	1:A:2247:A:C8	2.54	0.42
9:J:62:VAL:O	9:J:69:ARG:NH2	2.51	0.42
35:a:196:A:OP1	54:t:64:LYS:NZ	2.40	0.42
36:b:70:VAL:HB	36:b:163:VAL:HG23	2.00	0.42
55:u:62:ARG:HG2	55:u:66:ARG:HH11	1.84	0.42
1:A:743:A:O2'	1:A:1659:G:OP1	2.32	0.42
1:A:2192:U:H2'	1:A:2193:G:C8	2.53	0.42
8:H:42:LYS:O	8:H:45:GLU:HG2	2.19	0.42
9:J:102:GLU:HB3	9:J:119:PHE:HZ	1.83	0.42
13:N:73:ASN:HA	13:N:76:VAL:HG22	2.01	0.42
34:8:55:G:H2'	34:8:56:G:C8	2.54	0.42
35:a:511:C:H5'	38:d:44:ARG:HH22	1.83	0.42
35:a:523:A:N6	46:l:89:ASP:OD2	2.35	0.42
37:c:71:ALA:HA	37:c:106:VAL:HB	2.01	0.42
1:A:720:U:H2'	1:A:721:A:C8	2.54	0.42
1:A:1032:A:H2	1:A:1122:G:H22	1.68	0.42
4:D:181:ASP:HB2	4:D:186:LEU:HB2	2.02	0.42
11:L:14:LYS:HD2	11:L:14:LYS:HA	1.88	0.42
35:a:67:C:H2'	35:a:68:G:C8	2.54	0.42
35:a:142:G:O2'	35:a:196:A:N1	2.52	0.42
36:b:108:ARG:HA	36:b:111:ILE:HG22	2.02	0.42
38:d:56:ARG:HA	38:d:56:ARG:HD3	1.68	0.42
42:h:49:PHE:HB3	42:h:61:LEU:HD23	2.01	0.42
54:t:67:ILE:HB	54:t:71:LYS:HD3	2.00	0.42
1:A:1352:U:O2'	1:A:1570:A:N3	2.52	0.42
1:A:1693:U:H5''	1:A:1694:C:H5	1.83	0.42
38:d:9:LEU:HD11	38:d:28:ILE:HG23	2.00	0.42
1:A:878:A:H3'	1:A:879:G:H8	1.85	0.42
4:D:183:GLU:OE2	4:D:184:ARG:NH2	2.53	0.42
35:a:589:U:H5''	42:h:30:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:n:49:GLN:NE2	53:s:12:ASP:HA	2.34	0.42
51:q:21:ILE:HD11	51:q:75:LEU:HD11	2.01	0.42
1:A:729:G:C6	3:C:207:LYS:HB2	2.54	0.42
14:O:33:ARG:HG3	14:O:34:HIS:CD2	2.55	0.42
35:a:1322:C:OP1	53:s:78:ARG:NH2	2.50	0.42
51:q:6:ARG:HE	51:q:6:ARG:HB3	1.66	0.42
1:A:2627:G:O2'	1:A:2781:A:N1	2.45	0.42
35:a:6:G:N2	39:e:103:THR:HG21	2.34	0.42
35:a:517:G:N2	35:a:530:G:OP1	2.49	0.42
45:k:47:ALA:HB1	45:k:62:ALA:HB1	2.01	0.42
1:A:32:C:N4	1:A:447:A:OP2	2.52	0.42
1:A:98:G:H22	20:U:7:ARG:HH12	1.67	0.42
6:F:71:ARG:O	6:F:81:GLN:NE2	2.40	0.42
35:a:692:U:O2'	35:a:694:A:N7	2.45	0.42
35:a:1035:A:H3'	35:a:1036:A:H8	1.83	0.42
43:i:19:VAL:HG12	43:i:21:ILE:HG23	2.02	0.42
55:u:40:LYS:HB3	55:u:40:LYS:HE2	1.91	0.42
1:A:1090:A:H2'	1:A:1091:G:C8	2.55	0.42
1:A:2391:G:H2'	1:A:2424:C:H41	1.85	0.42
3:C:16:VAL:HG22	3:C:206:GLY:HA3	2.02	0.42
7:G:26:ILE:O	7:G:32:GLU:HA	2.20	0.42
7:G:170:ARG:NH1	30:4:28:SER:O	2.51	0.42
10:K:43:ILE:HD12	10:K:56:ASP:HB2	2.02	0.42
15:P:65:SER:O	15:P:67:GLY:N	2.53	0.42
20:U:99:ASN:OD1	20:U:99:ASN:N	2.52	0.42
29:3:51:SER:O	29:3:55:LEU:N	2.52	0.42
35:a:673:A:H2'	35:a:674:G:C8	2.55	0.42
35:a:1203:C:OP1	48:n:2:ALA:N	2.52	0.42
39:e:36:LEU:HD22	39:e:134:ILE:HG13	2.01	0.42
41:g:70:ARG:HD3	41:g:70:ARG:HA	1.68	0.42
42:h:104:VAL:HG22	42:h:125:ILE:HG12	2.02	0.42
1:A:2183:A:H2'	1:A:2184:A:C8	2.55	0.41
6:F:33:LYS:HG2	6:F:157:THR:HB	2.02	0.41
18:S:23:LEU:HD22	26:0:24:ALA:HB2	2.02	0.41
35:a:1062:U:H2'	35:a:1063:C:C6	2.55	0.41
35:a:1149:C:OP2	43:i:11:ARG:NH2	2.40	0.41
40:f:23:GLU:O	40:f:27:ALA:N	2.42	0.41
50:p:53:ASP:OD1	50:p:53:ASP:N	2.53	0.41
1:A:151:C:H2'	1:A:152:A:C8	2.55	0.41
1:A:171:U:H2'	1:A:172:A:H8	1.85	0.41
1:A:832:U:H2'	1:A:833:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:A:H2'	1:A:834:G:C8	2.55	0.41
1:A:1012:U:OP2	16:Q:70:ARG:NH1	2.50	0.41
1:A:1528:A:OP2	1:A:1543:G:N2	2.51	0.41
1:A:1631:G:N1	1:A:1634:A:OP2	2.45	0.41
1:A:2116:G:H1	1:A:2164:C:H42	1.68	0.41
6:F:65:PRO:HB3	6:F:89:VAL:HG22	2.02	0.41
9:J:80:HIS:HB3	9:J:81:ILE:H	1.71	0.41
39:e:106:ILE:HD11	39:e:124:LEU:HD22	2.01	0.41
54:t:25:ARG:HG3	54:t:66:LEU:HD11	2.02	0.41
1:A:355:U:H2'	1:A:356:G:H8	1.84	0.41
1:A:358:U:H2'	1:A:359:G:C8	2.56	0.41
2:B:1:U:H2'	2:B:2:G:C8	2.56	0.41
14:O:18:LEU:HD12	14:O:18:LEU:HA	1.82	0.41
15:P:14:LYS:HE2	15:P:77:HIS:HA	2.03	0.41
15:P:106:LYS:O	15:P:109:ARG:NH2	2.44	0.41
35:a:406:G:H21	38:d:116:GLN:HE22	1.68	0.41
35:a:1175:G:H2'	35:a:1176:A:H8	1.86	0.41
36:b:114:LEU:HD13	36:b:144:LEU:HB2	2.03	0.41
1:A:739:A:H1'	1:A:740:C:H5	1.85	0.41
1:A:747:U:H5'	1:A:748:G:H5'	2.02	0.41
1:A:923:G:H2'	1:A:924:G:H8	1.85	0.41
1:A:1744:A:H3'	1:A:1745:A:H8	1.84	0.41
1:A:1853:A:H2'	1:A:1854:A:C8	2.55	0.41
1:A:2830:C:H5''	4:D:56:LYS:HE2	2.01	0.41
10:K:63:VAL:HB	10:K:103:VAL:HG12	2.02	0.41
1:A:1040:A:H2	1:A:1115:G:H1	1.65	0.41
1:A:1469:A:H2'	1:A:1470:A:C8	2.56	0.41
1:A:1889:A:H2'	1:A:1890:A:C8	2.55	0.41
1:A:2655:G:O2'	1:A:2664:G:N1	2.51	0.41
13:N:75:ILE:HD13	13:N:75:ILE:HA	1.90	0.41
35:a:411:A:OP1	38:d:26:ARG:NH2	2.40	0.41
36:b:164:ILE:HD11	36:b:214:LEU:HD11	2.03	0.41
1:A:680:C:H2'	1:A:681:G:C8	2.56	0.41
1:A:690:G:H21	3:C:43:ARG:HH12	1.69	0.41
1:A:1746:A:H2'	1:A:1747:U:C6	2.56	0.41
1:A:2698:U:H2'	1:A:2699:C:C6	2.56	0.41
3:C:145:GLU:HA	3:C:152:GLY:HA2	2.03	0.41
3:C:155:ALA:HB2	3:C:162:VAL:HG23	2.01	0.41
3:C:252:THR:OG1	3:C:253:LYS:N	2.51	0.41
5:E:49:ARG:H	5:E:49:ARG:HG2	1.66	0.41
12:M:105:MET:HE2	12:M:108:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:52:LEU:O	20:U:54:GLN:NE2	2.44	0.41
26:0:29:SER:HB3	26:0:40:ARG:HD3	2.03	0.41
27:1:6:ARG:HB3	27:1:24:THR:HB	2.02	0.41
31:5:1:MET:HE2	31:5:6:HIS:CD2	2.55	0.41
33:7:4:SER:HB3	56:7:101:ERY:H24	2.02	0.41
37:c:91:VAL:HG21	37:c:101:ILE:HD11	2.03	0.41
1:A:151:C:H2'	1:A:152:A:H8	1.85	0.41
1:A:360:U:H2'	1:A:361:G:C4	2.55	0.41
1:A:554:U:H2'	1:A:555:G:O4'	2.20	0.41
11:L:55:MET:HA	11:L:56:PRO:HD3	1.93	0.41
13:N:19:ALA:O	13:N:23:ASN:ND2	2.45	0.41
27:1:50:LYS:HA	27:1:50:LYS:HD3	1.92	0.41
35:a:891:U:H2'	35:a:892:A:H8	1.84	0.41
35:a:1535:C:H2'	35:a:1536:C:H4'	2.02	0.41
38:d:151:LYS:HE2	38:d:151:LYS:HB2	1.90	0.41
55:u:56:HIS:HA	55:u:59:LYS:HB3	2.01	0.41
1:A:1820:U:H5	3:C:177:ARG:HH12	1.69	0.41
1:A:2101:A:H2'	1:A:2102:G:C8	2.55	0.41
10:K:102:PRO:HB3	10:K:121:GLU:HB2	2.03	0.41
14:O:62:LEU:HD22	14:O:70:ALA:HA	2.02	0.41
16:Q:17:ILE:HD13	16:Q:17:ILE:HA	1.91	0.41
35:a:216:U:H2'	35:a:217:C:C6	2.56	0.41
35:a:459:A:H2'	35:a:460:A:H8	1.86	0.41
51:q:20:SER:HB3	51:q:71:LYS:NZ	2.36	0.41
1:A:249:C:H4'	1:A:250:G:H5''	2.03	0.41
1:A:579:G:O2'	1:A:2019:A:OP1	2.38	0.41
1:A:1178:C:H2'	1:A:1179:G:C8	2.56	0.41
1:A:1323:C:OP1	18:S:98:LYS:NZ	2.53	0.41
1:A:2014:A:H2'	1:A:2015:A:C8	2.56	0.41
1:A:2020:A:H62	26:0:6:ASN:HD21	1.68	0.41
1:A:2230:G:H5''	23:X:30:LEU:HD12	2.02	0.41
5:E:194:LYS:HA	5:E:194:LYS:HD2	1.95	0.41
8:H:8:LYS:HD2	8:H:9:VAL:H	1.85	0.41
8:H:90:LEU:O	8:H:123:ARG:NH2	2.38	0.41
18:S:6:LYS:HG2	18:S:104:THR:HG23	2.03	0.41
19:T:11:LEU:O	24:Y:29:ARG:NH1	2.53	0.41
20:U:33:LYS:HB3	20:U:64:ALA:HB1	2.03	0.41
35:a:210:C:H4'	35:a:211:G:C2	2.55	0.41
35:a:235:C:H2'	35:a:236:A:C8	2.56	0.41
35:a:1005:A:N6	35:a:1024:G:O2'	2.54	0.41
35:a:1452:C:H4'	35:a:1453:G:C2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:218:ALA:HA	36:b:221:VAL:HG12	2.03	0.41
38:d:144:SER:HB3	38:d:179:GLU:HG2	2.01	0.41
41:g:35:LYS:HE2	41:g:35:LYS:HB3	1.89	0.41
42:h:18:GLN:HG2	42:h:63:LEU:HD13	2.02	0.41
43:i:65:ILE:HG12	43:i:79:ILE:HD11	2.03	0.41
45:k:84:VAL:HG11	45:k:97:ILE:HG22	2.02	0.41
47:m:79:ARG:O	47:m:83:LEU:HB2	2.21	0.41
1:A:2087:G:H2'	1:A:2088:A:C8	2.55	0.41
1:A:2514:U:H2'	1:A:2515:C:C6	2.56	0.41
5:E:47:LYS:HE2	5:E:47:LYS:HB3	1.93	0.41
6:F:56:ASP:OD2	6:F:150:ARG:NH1	2.48	0.41
29:3:52:LYS:HE2	29:3:52:LYS:HB2	1.93	0.41
35:a:675:A:O2'	45:k:116:ILE:O	2.38	0.41
37:c:124:LEU:HD23	37:c:124:LEU:HA	1.84	0.41
38:d:95:GLU:HG3	38:d:191:LEU:HD22	2.03	0.41
41:g:68:ASN:HD22	41:g:128:ALA:HA	1.86	0.41
41:g:71:PRO:HA	41:g:142:HIS:HE1	1.86	0.41
42:h:18:GLN:HE21	42:h:72:VAL:HB	1.85	0.41
42:h:67:GLN:H	42:h:67:GLN:HG2	1.71	0.41
45:k:18:ASP:OD1	45:k:18:ASP:N	2.54	0.41
52:r:42:SER:O	52:r:42:SER:OG	2.38	0.41
1:A:1322:A:H5''	18:S:82:MET:HE1	2.04	0.40
1:A:1689:A:H2'	1:A:1690:A:C8	2.56	0.40
2:B:5:U:H2'	2:B:6:G:H8	1.86	0.40
33:7:1:MET:HB2	56:7:101:ERY:H17	2.02	0.40
35:a:728:A:H2'	35:a:729:A:C8	2.55	0.40
35:a:1038:C:H2'	35:a:1039:G:C8	2.56	0.40
45:k:35:THR:HA	45:k:41:ALA:HA	2.03	0.40
1:A:2250:G:N3	1:A:2250:G:H5'	2.36	0.40
1:A:2467:C:OP1	30:4:8:LYS:NZ	2.51	0.40
6:F:164:GLU:OE1	6:F:167:ARG:NH1	2.53	0.40
18:S:2:GLU:HA	18:S:108:SER:HB3	2.02	0.40
34:8:36:A:H2'	34:8:37:G:H8	1.86	0.40
34:8:54:G:H2'	34:8:55:G:C8	2.56	0.40
35:a:1323:G:H2'	35:a:1324:A:C8	2.56	0.40
40:f:44:ARG:HA	40:f:58:HIS:HA	2.03	0.40
44:j:40:ILE:HA	44:j:41:PRO:HD3	1.91	0.40
47:m:3:ARG:O	47:m:57:ARG:NH2	2.54	0.40
1:A:2033:A:O2'	1:A:2035:G:OP1	2.36	0.40
1:A:2117:A:N6	1:A:2170:A:H61	2.17	0.40
1:A:2292:U:H2'	1:A:2293:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2328:A:H2'	1:A:2329:U:C6	2.56	0.40
3:C:133:ARG:O	3:C:167:ARG:NH1	2.55	0.40
12:M:62:LYS:O	12:M:105:MET:HA	2.21	0.40
13:N:72:ASP:HB3	13:N:75:ILE:HB	2.02	0.40
15:P:31:TRP:NE1	15:P:82:ASP:OD2	2.51	0.40
35:a:269:C:H2'	35:a:270:A:C8	2.56	0.40
35:a:413:G:O6	38:d:32:CYS:HB2	2.21	0.40
35:a:1317:C:O2	53:s:37:ARG:NH1	2.50	0.40
37:c:63:SER:HA	37:c:97:VAL:HB	2.03	0.40
40:f:93:LYS:HD3	40:f:93:LYS:HA	1.90	0.40
45:k:81:ASN:OD1	45:k:81:ASN:N	2.52	0.40
50:p:46:LYS:HE3	50:p:46:LYS:HB3	1.90	0.40
1:A:363:G:H2'	1:A:364:C:C6	2.56	0.40
1:A:1168:G:H2'	1:A:1169:A:C8	2.57	0.40
1:A:1817:G:OP2	3:C:156:ARG:NH2	2.55	0.40
1:A:2554:U:H2'	1:A:2555:U:C6	2.57	0.40
3:C:210:ALA:HA	3:C:213:TRP:CE2	2.57	0.40
36:b:121:SER:OG	36:b:122:GLN:N	2.54	0.40
41:g:2:PRO:HB2	41:g:3:ARG:H	1.69	0.40
43:i:28:ILE:HD12	43:i:35:LEU:HD22	2.04	0.40
1:A:1510:G:H2'	1:A:1511:G:H8	1.85	0.40
1:A:2127:G:H2'	1:A:2128:G:C8	2.57	0.40
1:A:2175:C:H2'	1:A:2176:A:C8	2.57	0.40
1:A:2291:U:O2'	1:A:2374:C:O2	2.37	0.40
18:S:94:ASP:OD1	18:S:95:ARG:N	2.50	0.40
35:a:398:U:H2'	35:a:399:G:C8	2.54	0.40
35:a:460:A:H2'	35:a:461:A:C8	2.56	0.40
35:a:1015:G:H2'	35:a:1016:A:C8	2.56	0.40
35:a:1363:A:O2'	35:a:1365:G:N7	2.45	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	
3	C	269/271 (99%)	251 (93%)	18 (7%)	0	100	100
4	D	207/209 (99%)	191 (92%)	16 (8%)	0	100	100
5	E	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
6	F	175/177 (99%)	162 (93%)	13 (7%)	0	100	100
7	G	172/174 (99%)	157 (91%)	15 (9%)	0	100	100
8	H	147/149 (99%)	126 (86%)	18 (12%)	3 (2%)	6	22
9	J	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
10	K	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	L	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
12	M	134/136 (98%)	131 (98%)	2 (2%)	1 (1%)	18	48
13	N	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	O	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
15	P	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
16	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
17	R	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	12	39
18	S	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
19	T	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
20	U	100/102 (98%)	88 (88%)	10 (10%)	2 (2%)	6	22
21	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
22	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
23	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
24	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
25	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
26	0	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
27	1	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	5	21
28	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
29	3	62/64 (97%)	54 (87%)	6 (10%)	2 (3%)	3	13
30	4	36/38 (95%)	36 (100%)	0	0	100	100
31	5	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
33	7	6/7 (86%)	6 (100%)	0	0	100	100
36	b	222/224 (99%)	204 (92%)	18 (8%)	0	100	100
37	c	204/206 (99%)	193 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	d	203/205 (99%)	178 (88%)	25 (12%)	0	100	100
39	e	155/157 (99%)	140 (90%)	13 (8%)	2 (1%)	9	32
40	f	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
41	g	149/151 (99%)	138 (93%)	11 (7%)	0	100	100
42	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
43	i	125/127 (98%)	112 (90%)	13 (10%)	0	100	100
44	j	96/98 (98%)	86 (90%)	9 (9%)	1 (1%)	12	39
45	k	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
46	l	121/123 (98%)	108 (89%)	12 (10%)	1 (1%)	16	44
47	m	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
48	n	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	12	39
49	o	86/88 (98%)	80 (93%)	5 (6%)	1 (1%)	10	34
50	p	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
51	q	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
52	r	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
53	s	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
54	t	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
55	u	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	5592/5691 (98%)	5179 (93%)	397 (7%)	16 (0%)	37	65

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	U	89	ASP
29	3	32	ILE
8	H	9	VAL
27	1	35	GLU
39	e	99	ALA
44	j	57	VAL
49	o	47	LYS
8	H	2	GLN
8	H	8	LYS
29	3	33	LEU
39	e	98	PRO
48	n	33	ASP
20	U	90	GLY

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Mol	Chain	Res	Type
46	I	15	LYS
12	M	69	PRO
17	R	54	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/216 (100%)	216 (100%)	0	100	100
4	D	164/164 (100%)	161 (98%)	3 (2%)	51	80
5	E	165/165 (100%)	165 (100%)	0	100	100
6	F	148/148 (100%)	145 (98%)	3 (2%)	48	78
7	G	135/135 (100%)	135 (100%)	0	100	100
8	H	114/114 (100%)	112 (98%)	2 (2%)	51	80
9	J	116/116 (100%)	116 (100%)	0	100	100
10	K	103/103 (100%)	103 (100%)	0	100	100
11	L	103/103 (100%)	102 (99%)	1 (1%)	68	89
12	M	109/109 (100%)	109 (100%)	0	100	100
13	N	98/98 (100%)	98 (100%)	0	100	100
14	O	86/86 (100%)	85 (99%)	1 (1%)	63	86
15	P	99/99 (100%)	98 (99%)	1 (1%)	68	89
16	Q	89/89 (100%)	89 (100%)	0	100	100
17	R	84/84 (100%)	84 (100%)	0	100	100
18	S	93/93 (100%)	93 (100%)	0	100	100
19	T	77/77 (100%)	77 (100%)	0	100	100
20	U	83/83 (100%)	82 (99%)	1 (1%)	63	86
21	V	78/78 (100%)	78 (100%)	0	100	100
22	W	57/57 (100%)	57 (100%)	0	100	100
23	X	67/67 (100%)	65 (97%)	2 (3%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y	55/55 (100%)	55 (100%)	0	100	100
25	Z	48/48 (100%)	48 (100%)	0	100	100
26	0	46/46 (100%)	46 (100%)	0	100	100
27	1	45/45 (100%)	45 (100%)	0	100	100
28	2	38/38 (100%)	38 (100%)	0	100	100
29	3	51/51 (100%)	51 (100%)	0	100	100
30	4	34/34 (100%)	33 (97%)	1 (3%)	37	71
31	5	58/58 (100%)	56 (97%)	2 (3%)	32	66
33	7	8/7 (114%)	8 (100%)	0	100	100
36	b	186/186 (100%)	185 (100%)	1 (0%)	81	93
37	c	170/170 (100%)	170 (100%)	0	100	100
38	d	172/172 (100%)	171 (99%)	1 (1%)	78	93
39	e	119/119 (100%)	118 (99%)	1 (1%)	73	90
40	f	86/86 (100%)	85 (99%)	1 (1%)	63	86
41	g	124/124 (100%)	124 (100%)	0	100	100
42	h	104/104 (100%)	103 (99%)	1 (1%)	68	89
43	i	105/105 (100%)	103 (98%)	2 (2%)	50	79
44	j	86/86 (100%)	86 (100%)	0	100	100
45	k	90/90 (100%)	90 (100%)	0	100	100
46	l	103/103 (100%)	102 (99%)	1 (1%)	68	89
47	m	92/92 (100%)	91 (99%)	1 (1%)	65	88
48	n	83/83 (100%)	83 (100%)	0	100	100
49	o	76/76 (100%)	75 (99%)	1 (1%)	61	86
50	p	65/65 (100%)	63 (97%)	2 (3%)	35	69
51	q	74/74 (100%)	74 (100%)	0	100	100
52	r	57/57 (100%)	57 (100%)	0	100	100
53	s	72/72 (100%)	71 (99%)	1 (1%)	59	85
54	t	65/65 (100%)	65 (100%)	0	100	100
55	u	60/60 (100%)	59 (98%)	1 (2%)	53	82
All	All	4656/4655 (100%)	4625 (99%)	31 (1%)	73	92

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	22	ILE
4	D	98	VAL
4	D	107	VAL
6	F	31	VAL
6	F	35	THR
6	F	91	LEU
8	H	3	VAL
8	H	12	LEU
11	L	27	LEU
14	O	87	ILE
15	P	32	VAL
20	U	52	LEU
23	X	40	VAL
23	X	70	GLU
30	4	14	CYS
31	5	27	THR
31	5	37	CYS
36	b	183	VAL
38	d	110	THR
39	e	94	VAL
40	f	73	GLU
42	h	121	LEU
43	i	48	VAL
43	i	67	VAL
46	l	16	VAL
47	m	73	ILE
49	o	56	LEU
50	p	19	VAL
50	p	21	VAL
53	s	79	THR
55	u	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	90	ASN
3	C	115	GLN
4	D	49	GLN
4	D	130	GLN
4	D	136	ASN
4	D	164	GLN
5	E	41	GLN
5	E	136	GLN

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Mol	Chain	Res	Type
5	E	195	GLN
6	F	27	GLN
6	F	63	GLN
6	F	127	ASN
7	G	22	GLN
7	G	64	GLN
7	G	73	ASN
8	H	66	ASN
8	H	128	HIS
9	J	47	HIS
9	J	58	ASN
9	J	80	HIS
9	J	138	GLN
10	K	13	ASN
13	N	3	HIS
16	Q	44	GLN
17	R	11	GLN
17	R	12	HIS
19	T	48	GLN
19	T	59	ASN
20	U	46	GLN
20	U	53	ASN
20	U	66	GLN
20	U	69	ASN
20	U	74	ASN
23	X	36	HIS
24	Y	27	ASN
24	Y	31	GLN
25	Z	20	HIS
26	0	5	GLN
26	0	6	ASN
26	0	42	HIS
27	1	26	ASN
27	1	45	GLN
36	b	58	ASN
36	b	227	GLN
37	c	123	GLN
38	d	85	ASN
38	d	196	ASN
39	e	122	ASN
39	e	146	ASN
40	f	14	GLN

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Mol	Chain	Res	Type
40	f	55	HIS
40	f	63	ASN
41	g	68	ASN
41	g	148	ASN
42	h	18	GLN
43	i	75	GLN
43	i	110	GLN
45	k	15	GLN
45	k	118	HIS
48	n	49	GLN
48	n	60	GLN
48	n	66	GLN
48	n	71	HIS
49	o	37	ASN
50	p	26	ASN
50	p	63	GLN
53	s	14	HIS
53	s	52	HIS
54	t	3	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2902/2903 (99%)	640 (22%)	47 (1%)
2	B	119/120 (99%)	23 (19%)	3 (2%)
32	6	2/3 (66%)	1 (50%)	0
34	8	86/87 (98%)	25 (29%)	1 (1%)
35	a	1539/1540 (99%)	310 (20%)	0
All	All	4648/4653 (99%)	999 (21%)	51 (1%)

All (999) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	U
1	A	10	A
1	A	12	U
1	A	13	A
1	A	33	C
1	A	34	U
1	A	35	G
1	A	36	G

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Mol	Chain	Res	Type
1	A	42	A
1	A	46	G
1	A	51	G
1	A	52	A
1	A	60	G
1	A	62	U
1	A	63	A
1	A	71	A
1	A	75	G
1	A	76	C
1	A	88	G
1	A	91	A
1	A	100	U
1	A	103	A
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	135	U
1	A	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	144	A
1	A	145	C
1	A	146	A
1	A	158	U
1	A	160	A
1	A	163	C
1	A	178	G
1	A	196	A
1	A	199	A
1	A	204	A
1	A	215	G
1	A	216	A
1	A	219	A
1	A	220	G
1	A	222	A
1	A	229	C
1	A	233	A
1	A	241	A

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Mol	Chain	Res	Type
1	A	242	G
1	A	243	U
1	A	244	A
1	A	245	G
1	A	248	G
1	A	249	C
1	A	250	G
1	A	255	A
1	A	265	A
1	A	267	C
1	A	272	A
1	A	274	C
1	A	275	C
1	A	276	U
1	A	278	A
1	A	279	A
1	A	280	U
1	A	281	C
1	A	282	A
1	A	285	G
1	A	286	U
1	A	291	G
1	A	294	A
1	A	301	G
1	A	311	A
1	A	312	G
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	334	C
1	A	343	C
1	A	350	G
1	A	352	A
1	A	353	C
1	A	354	A
1	A	358	U
1	A	359	G
1	A	361	G
1	A	362	A
1	A	363	G
1	A	364	C

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Mol	Chain	Res	Type
1	A	367	G
1	A	371	A
1	A	372	G
1	A	386	G
1	A	387	U
1	A	391	A
1	A	395	U
1	A	396	G
1	A	403	U
1	A	404	A
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	424	G
1	A	443	A
1	A	445	C
1	A	456	C
1	A	467	G
1	A	474	G
1	A	477	A
1	A	480	A
1	A	481	G
1	A	490	C
1	A	491	G
1	A	505	A
1	A	508	A
1	A	513	A
1	A	518	G
1	A	526	A
1	A	527	C
1	A	529	A
1	A	531	C
1	A	532	A
1	A	543	G
1	A	544	C
1	A	547	A
1	A	550	C
1	A	563	A
1	A	573	U
1	A	575	A
1	A	603	A

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Mol	Chain	Res	Type
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	622	G
1	A	627	A
1	A	637	A
1	A	645	C
1	A	647	G
1	A	654	A
1	A	655	A
1	A	669	G
1	A	670	A
1	A	686	U
1	A	694	U
1	A	695	G
1	A	703	U
1	A	714	U
1	A	717	C
1	A	730	A
1	A	738	G
1	A	747	U
1	A	748	G
1	A	749	A
1	A	752	A
1	A	753	A
1	A	762	U
1	A	764	A
1	A	765	C
1	A	774	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G
1	A	788	A
1	A	789	A
1	A	790	U
1	A	793	A
1	A	799	G
1	A	800	A

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Mol	Chain	Res	Type
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	844	A
1	A	845	A
1	A	846	U
1	A	847	U
1	A	858	G
1	A	859	G
1	A	860	U
1	A	878	A
1	A	880	G
1	A	883	G
1	A	884	U
1	A	885	C
1	A	887	U
1	A	888	C
1	A	889	C
1	A	890	C
1	A	891	G
1	A	892	A
1	A	896	A
1	A	902	C
1	A	904	G
1	A	907	G
1	A	910	A
1	A	913	U
1	A	914	G
1	A	932	U
1	A	941	A
1	A	945	A
1	A	946	C
1	A	953	G
1	A	961	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	980	A
1	A	982	C

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Mol	Chain	Res	Type
1	A	983	A
1	A	989	G
1	A	996	A
1	A	1005	C
1	A	1011	G
1	A	1012	U
1	A	1013	C
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1033	U
1	A	1039	A
1	A	1044	C
1	A	1046	A
1	A	1047	G
1	A	1052	C
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1063	G
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1073	A
1	A	1075	C
1	A	1076	C
1	A	1078	U
1	A	1079	C
1	A	1081	U
1	A	1084	A
1	A	1085	A
1	A	1088	A
1	A	1089	A
1	A	1090	A
1	A	1094	U

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Mol	Chain	Res	Type
1	A	1097	U
1	A	1098	A
1	A	1101	U
1	A	1104	C
1	A	1107	G
1	A	1111	A
1	A	1112	G
1	A	1113	U
1	A	1114	C
1	A	1115	G
1	A	1119	U
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1134	A
1	A	1135	C
1	A	1139	G
1	A	1142	A
1	A	1143	A
1	A	1144	A
1	A	1172	C
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1204	A
1	A	1206	G
1	A	1211	C
1	A	1212	G
1	A	1236	G
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1268	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1275	A
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1301	A
1	A	1311	G
1	A	1312	U
1	A	1313	U
1	A	1324	G
1	A	1329	U
1	A	1333	G
1	A	1340	U
1	A	1341	G
1	A	1342	A
1	A	1345	C
1	A	1352	U
1	A	1353	A
1	A	1359	A
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1386	C
1	A	1392	A
1	A	1395	A
1	A	1398	C
1	A	1403	A
1	A	1411	U
1	A	1414	C
1	A	1416	G
1	A	1420	A
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1437	C
1	A	1454	C
1	A	1459	G
1	A	1460	U
1	A	1461	C
1	A	1475	G
1	A	1478	G
1	A	1482	G
1	A	1483	G
1	A	1484	U

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Mol	Chain	Res	Type
1	A	1490	A
1	A	1504	A
1	A	1509	A
1	A	1515	A
1	A	1523	U
1	A	1524	G
1	A	1529	G
1	A	1530	G
1	A	1531	C
1	A	1532	A
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1539	U
1	A	1542	U
1	A	1554	U
1	A	1555	G
1	A	1558	C
1	A	1559	U
1	A	1560	G
1	A	1566	A
1	A	1567	G
1	A	1569	A
1	A	1578	U
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1590	A
1	A	1607	C
1	A	1608	A
1	A	1610	A
1	A	1611	C
1	A	1621	U
1	A	1634	A
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1651	G
1	A	1664	A

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Mol	Chain	Res	Type
1	A	1667	G
1	A	1669	A
1	A	1674	G
1	A	1675	C
1	A	1693	U
1	A	1695	G
1	A	1713	A
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1735	A
1	A	1738	G
1	A	1757	A
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1782	U
1	A	1784	A
1	A	1786	A
1	A	1788	C
1	A	1800	C
1	A	1801	A
1	A	1808	A
1	A	1811	G
1	A	1816	C
1	A	1820	U
1	A	1829	A
1	A	1833	C
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1873	G
1	A	1884	G
1	A	1900	A
1	A	1901	A
1	A	1906	G
1	A	1907	G
1	A	1912	A
1	A	1914	C
1	A	1917	U

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Mol	Chain	Res	Type
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1937	A
1	A	1938	A
1	A	1940	U
1	A	1941	C
1	A	1944	U
1	A	1955	U
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1981	A
1	A	1982	U
1	A	1991	U
1	A	1992	G
1	A	1997	C
1	A	2006	C
1	A	2021	C
1	A	2022	U
1	A	2023	C
1	A	2030	A
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2035	G
1	A	2036	C
1	A	2043	C
1	A	2049	G
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	G
1	A	2077	A
1	A	2093	G
1	A	2096	C

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Mol	Chain	Res	Type
1	A	2098	U
1	A	2100	G
1	A	2104	C
1	A	2105	U
1	A	2107	G
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2115	G
1	A	2118	U
1	A	2119	A
1	A	2120	G
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2145	C
1	A	2146	C
1	A	2147	A
1	A	2149	U
1	A	2158	A
1	A	2162	G
1	A	2163	A
1	A	2164	C
1	A	2165	C
1	A	2167	U
1	A	2168	G
1	A	2169	A
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2178	C
1	A	2181	U
1	A	2182	U
1	A	2186	G
1	A	2191	A
1	A	2198	A
1	A	2199	A
1	A	2203	U

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Mol	Chain	Res	Type
1	A	2204	G
1	A	2211	A
1	A	2212	A
1	A	2223	G
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2250	G
1	A	2278	A
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2305	U
1	A	2307	G
1	A	2309	A
1	A	2320	U
1	A	2325	G
1	A	2327	A
1	A	2331	G
1	A	2333	A
1	A	2334	U
1	A	2345	G
1	A	2350	C
1	A	2354	C
1	A	2361	G
1	A	2383	G
1	A	2385	C
1	A	2391	G
1	A	2392	A
1	A	2396	G
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2423	U
1	A	2426	A
1	A	2429	G
1	A	2430	A
1	A	2434	A
1	A	2441	U
1	A	2445	G
1	A	2447	G
1	A	2448	A

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Mol	Chain	Res	Type
1	A	2476	A
1	A	2489	U
1	A	2491	U
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2519	U
1	A	2520	C
1	A	2529	G
1	A	2542	A
1	A	2547	A
1	A	2554	U
1	A	2564	A
1	A	2567	G
1	A	2568	U
1	A	2572	A
1	A	2573	C
1	A	2582	G
1	A	2585	U
1	A	2586	U
1	A	2592	G
1	A	2602	A
1	A	2609	U
1	A	2610	C
1	A	2613	U
1	A	2614	A
1	A	2615	U
1	A	2619	C
1	A	2629	U
1	A	2630	G
1	A	2646	C
1	A	2654	A
1	A	2655	G
1	A	2670	A
1	A	2682	A
1	A	2684	U
1	A	2689	U
1	A	2690	U
1	A	2714	G

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Mol	Chain	Res	Type
1	A	2716	C
1	A	2720	U
1	A	2726	A
1	A	2732	G
1	A	2733	A
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2751	G
1	A	2762	C
1	A	2764	A
1	A	2765	A
1	A	2766	A
1	A	2776	A
1	A	2778	A
1	A	2779	U
1	A	2789	C
1	A	2790	U
1	A	2793	C
1	A	2799	A
1	A	2800	A
1	A	2808	G
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2833	U
1	A	2834	G
1	A	2849	U
1	A	2850	A
1	A	2858	C
1	A	2859	G
1	A	2861	U
1	A	2866	U
1	A	2867	G
1	A	2868	A
1	A	2872	A
1	A	2873	A
1	A	2880	C
1	A	2884	U
1	A	2887	A
1	A	2891	U
1	A	2893	A

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Mol	Chain	Res	Type
1	A	2902	C
1	A	2903	U
2	B	4	C
2	B	13	G
2	B	15	A
2	B	24	G
2	B	34	A
2	B	35	C
2	B	41	G
2	B	42	C
2	B	44	G
2	B	52	A
2	B	53	A
2	B	58	A
2	B	65	U
2	B	67	G
2	B	75	G
2	B	87	U
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	105	G
2	B	108	A
2	B	109	A
32	6	27	U
34	8	2	C
34	8	6	G
34	8	7	G
34	8	8	U
34	8	9	G
34	8	14	A
34	8	16	U
34	8	17	U
34	8	18	G
34	8	19	G
34	8	20	U
34	8	21	A
34	8	24	C
34	8	42	U
34	8	47	C
34	8	48	C

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Mol	Chain	Res	Type
34	8	49	C
34	8	50	A
34	8	53	A
34	8	60	A
34	8	64	G
34	8	68	A
34	8	69	A
34	8	72	C
34	8	87	A
35	a	2	A
35	a	3	A
35	a	4	U
35	a	5	U
35	a	7	A
35	a	8	A
35	a	9	G
35	a	22	G
35	a	32	A
35	a	39	G
35	a	47	C
35	a	48	C
35	a	50	A
35	a	51	A
35	a	71	A
35	a	72	A
35	a	75	G
35	a	79	G
35	a	80	A
35	a	81	A
35	a	82	G
35	a	83	C
35	a	84	U
35	a	85	U
35	a	86	G
35	a	87	C
35	a	88	U
35	a	92	U
35	a	94	G
35	a	97	G
35	a	98	A
35	a	116	A
35	a	120	A

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Mol	Chain	Res	Type
35	a	121	U
35	a	122	G
35	a	128	G
35	a	129	A
35	a	130	A
35	a	160	A
35	a	163	C
35	a	166	U
35	a	177	G
35	a	181	A
35	a	183	C
35	a	184	G
35	a	185	U
35	a	197	A
35	a	203	G
35	a	204	G
35	a	208	U
35	a	210	C
35	a	211	G
35	a	212	G
35	a	226	G
35	a	245	U
35	a	247	G
35	a	251	G
35	a	258	G
35	a	266	G
35	a	267	C
35	a	269	C
35	a	279	A
35	a	280	C
35	a	281	G
35	a	282	A
35	a	289	G
35	a	305	G
35	a	321	A
35	a	328	C
35	a	344	A
35	a	345	C
35	a	347	G
35	a	351	G
35	a	352	C
35	a	354	G

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Mol	Chain	Res	Type
35	a	363	A
35	a	367	U
35	a	368	U
35	a	372	C
35	a	373	A
35	a	375	U
35	a	388	G
35	a	397	A
35	a	398	U
35	a	406	G
35	a	411	A
35	a	412	A
35	a	413	G
35	a	421	U
35	a	422	C
35	a	423	G
35	a	424	G
35	a	428	G
35	a	429	U
35	a	438	U
35	a	439	U
35	a	467	U
35	a	468	A
35	a	474	G
35	a	477	C
35	a	484	G
35	a	485	U
35	a	486	U
35	a	493	A
35	a	495	A
35	a	496	A
35	a	497	G
35	a	511	C
35	a	517	G
35	a	518	C
35	a	521	G
35	a	524	G
35	a	527	G
35	a	531	U
35	a	532	A
35	a	545	C
35	a	547	A

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Mol	Chain	Res	Type
35	a	559	A
35	a	560	A
35	a	562	U
35	a	572	A
35	a	573	A
35	a	574	A
35	a	575	G
35	a	576	C
35	a	577	G
35	a	579	A
35	a	587	G
35	a	596	A
35	a	633	G
35	a	639	G
35	a	642	A
35	a	653	U
35	a	656	G
35	a	665	A
35	a	671	G
35	a	687	A
35	a	688	G
35	a	693	G
35	a	695	A
35	a	712	A
35	a	718	A
35	a	721	G
35	a	723	U
35	a	731	G
35	a	733	G
35	a	734	G
35	a	748	G
35	a	754	C
35	a	755	G
35	a	758	C
35	a	759	A
35	a	760	G
35	a	777	A
35	a	781	A
35	a	794	A
35	a	815	A
35	a	817	C
35	a	818	G

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Mol	Chain	Res	Type
35	a	819	A
35	a	820	U
35	a	832	G
35	a	836	G
35	a	843	U
35	a	844	G
35	a	845	A
35	a	846	G
35	a	849	G
35	a	870	U
35	a	889	A
35	a	902	G
35	a	914	A
35	a	916	U
35	a	931	C
35	a	934	C
35	a	935	A
35	a	942	G
35	a	948	C
35	a	958	A
35	a	960	U
35	a	961	U
35	a	966	G
35	a	969	A
35	a	971	G
35	a	975	A
35	a	976	G
35	a	977	A
35	a	992	U
35	a	993	G
35	a	996	A
35	a	1004	A
35	a	1020	G
35	a	1026	G
35	a	1028	C
35	a	1030	U
35	a	1031	C
35	a	1033	G
35	a	1034	G
35	a	1035	A
35	a	1036	A
35	a	1037	C

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Mol	Chain	Res	Type
35	a	1043	G
35	a	1044	A
35	a	1045	C
35	a	1065	U
35	a	1066	C
35	a	1085	U
35	a	1094	G
35	a	1095	U
35	a	1101	A
35	a	1124	G
35	a	1125	U
35	a	1130	A
35	a	1131	G
35	a	1133	G
35	a	1136	C
35	a	1137	C
35	a	1138	G
35	a	1139	G
35	a	1140	C
35	a	1143	G
35	a	1151	A
35	a	1152	A
35	a	1155	A
35	a	1158	C
35	a	1159	U
35	a	1166	G
35	a	1167	A
35	a	1168	U
35	a	1169	A
35	a	1171	A
35	a	1183	U
35	a	1184	G
35	a	1191	A
35	a	1196	A
35	a	1199	U
35	a	1201	A
35	a	1202	U
35	a	1213	A
35	a	1214	C
35	a	1215	G
35	a	1227	A
35	a	1228	C

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Mol	Chain	Res	Type
35	a	1238	A
35	a	1241	G
35	a	1250	A
35	a	1253	G
35	a	1256	A
35	a	1257	A
35	a	1260	G
35	a	1261	A
35	a	1266	G
35	a	1274	A
35	a	1275	A
35	a	1280	A
35	a	1287	A
35	a	1294	G
35	a	1297	G
35	a	1298	U
35	a	1300	G
35	a	1301	U
35	a	1305	G
35	a	1317	C
35	a	1340	A
35	a	1345	U
35	a	1346	A
35	a	1353	G
35	a	1360	A
35	a	1363	A
35	a	1364	U
35	a	1368	A
35	a	1370	G
35	a	1377	A
35	a	1378	C
35	a	1379	G
35	a	1381	U
35	a	1382	C
35	a	1394	A
35	a	1396	A
35	a	1399	C
35	a	1400	C
35	a	1419	G
35	a	1431	A
35	a	1432	G
35	a	1441	A

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Mol	Chain	Res	Type
35	a	1442	G
35	a	1446	A
35	a	1451	U
35	a	1452	C
35	a	1453	G
35	a	1455	G
35	a	1475	G
35	a	1492	A
35	a	1493	A
35	a	1494	G
35	a	1497	G
35	a	1499	A
35	a	1502	A
35	a	1503	A
35	a	1506	U
35	a	1517	G
35	a	1519	A
35	a	1529	G
35	a	1530	G
35	a	1533	C
35	a	1534	A
35	a	1535	C
35	a	1536	C
35	a	1537	U
35	a	1539	C

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	33	C
1	A	51	G
1	A	86	G
1	A	134	G
1	A	242	G
1	A	277	G
1	A	281	C
1	A	358	U
1	A	404	A
1	A	479	A
1	A	490	C
1	A	546	U

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Mol	Chain	Res	Type
1	A	655	A
1	A	748	G
1	A	752	A
1	A	827	U
1	A	858	G
1	A	859	G
1	A	890	C
1	A	1020	A
1	A	1022	G
1	A	1060	U
1	A	1062	G
1	A	1074	G
1	A	1111	A
1	A	1130	U
1	A	1171	G
1	A	1173	U
1	A	1179	G
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1399	C
1	A	1420	A
1	A	1508	A
1	A	1536	C
1	A	1541	C
1	A	1729	U
1	A	1930	G
1	A	1940	U
1	A	2326	C
1	A	2391	G
1	A	2566	A
1	A	2585	U
1	A	2808	G
1	A	2901	C
2	B	66	A
2	B	86	G
2	B	88	C
34	8	63	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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$
56	ERY	7	101	-	53,53,53	1.70	6 (11%)	82,82,82	1.62	16 (19%)

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
56	ERY	7	101	-	-	5/72/107/107	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	7	101	ERY	C10-C9	-7.36	1.40	1.52
56	7	101	ERY	C2-C1	-6.65	1.37	1.51
56	7	101	ERY	C8-C9	-3.17	1.42	1.52
56	7	101	ERY	C10-C11	2.61	1.57	1.54
56	7	101	ERY	O7-C22	2.19	1.47	1.41
56	7	101	ERY	C12-C13	-2.00	1.51	1.55

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	7	101	ERY	O5-C16-C17	4.59	110.52	103.86
56	7	101	ERY	C27-C26-C25	-3.97	107.26	113.27
56	7	101	ERY	C6-C5-C4	-3.49	108.83	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	7	101	ERY	C29-N1-C28	-3.42	100.45	110.49
56	7	101	ERY	O8-C23-C24	3.36	116.02	109.87
56	7	101	ERY	O7-C5-C6	3.05	110.04	106.40
56	7	101	ERY	C36-C13-C12	-2.52	110.60	115.20
56	7	101	ERY	C32-C6-C7	-2.49	107.06	111.09
56	7	101	ERY	O2-C13-C36	2.48	111.97	107.36
56	7	101	ERY	O13-C12-C11	2.38	113.49	108.88
56	7	101	ERY	C8-C9-C10	2.35	123.10	119.13
56	7	101	ERY	C22-O7-C5	2.31	120.20	116.26
56	7	101	ERY	C21-C18-C17	-2.31	108.75	112.58
56	7	101	ERY	C16-C15-C14	-2.14	111.38	114.99
56	7	101	ERY	C31-C4-C3	-2.13	107.65	111.40
56	7	101	ERY	C25-C24-C23	-2.11	106.98	110.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

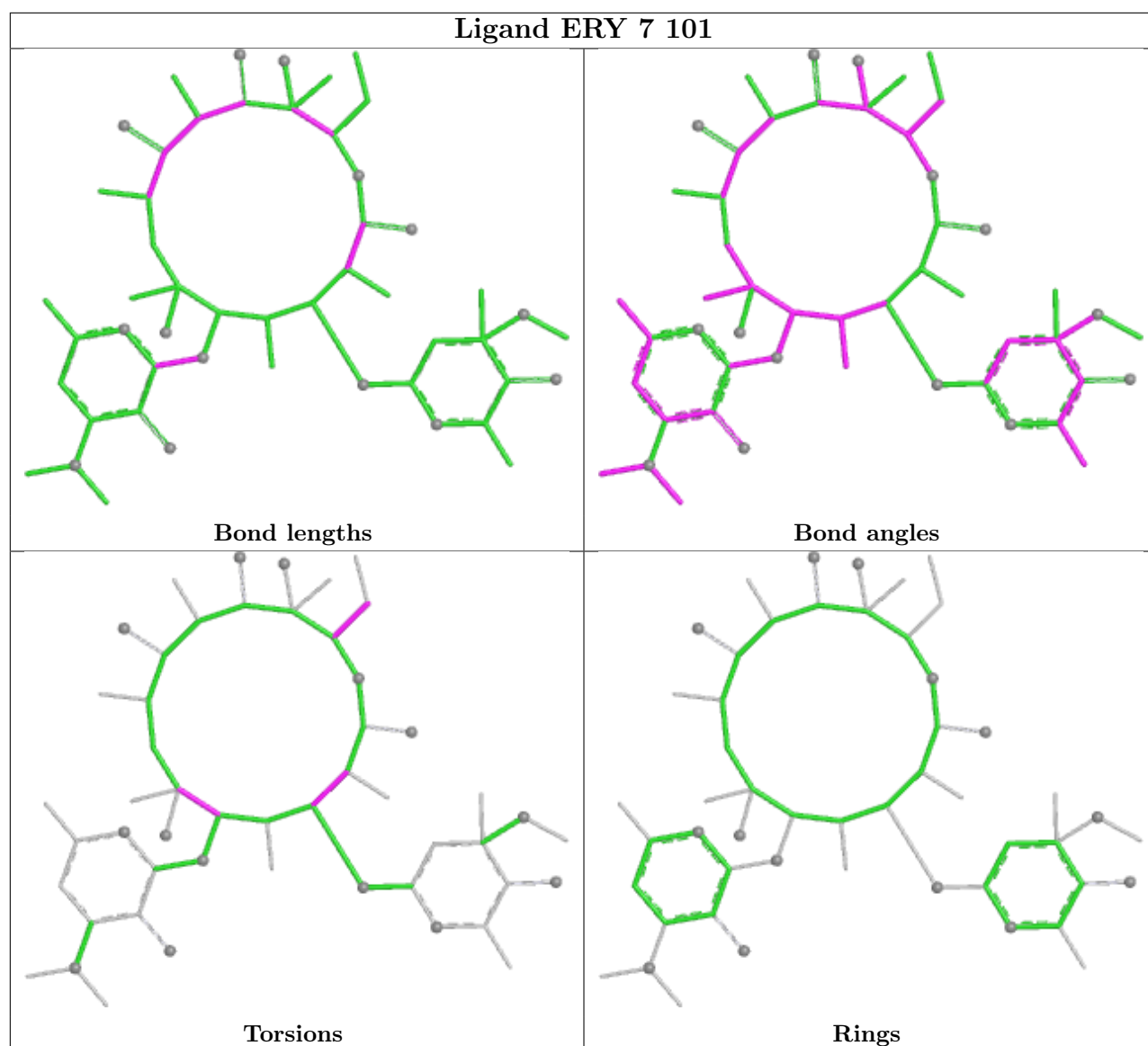
Mol	Chain	Res	Type	Atoms
56	7	101	ERY	C4-C5-C6-O10
56	7	101	ERY	O2-C13-C36-C37
56	7	101	ERY	C12-C13-C36-C37
56	7	101	ERY	C4-C5-C6-C32
56	7	101	ERY	C30-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	7	101	ERY	11	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

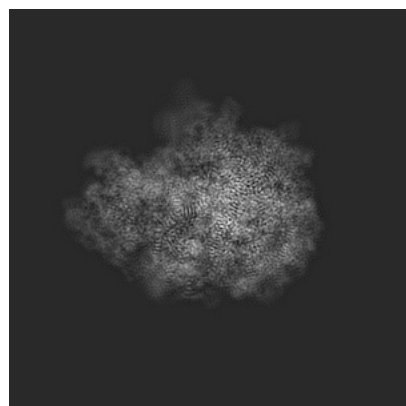
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12573. These allow visual inspection of the internal detail of the map and identification of artifacts.

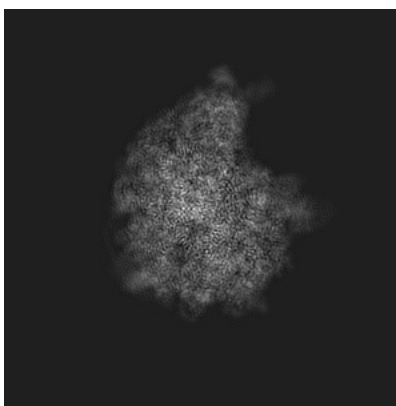
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

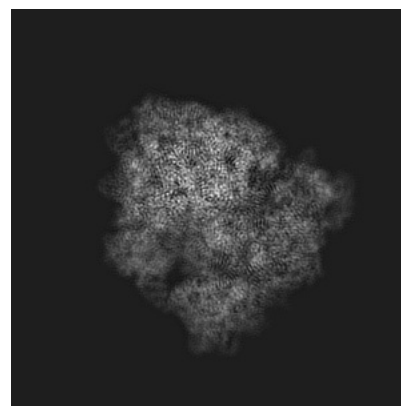
6.1.1 Primary map



X

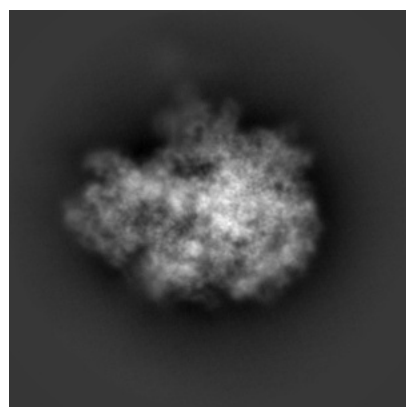


Y

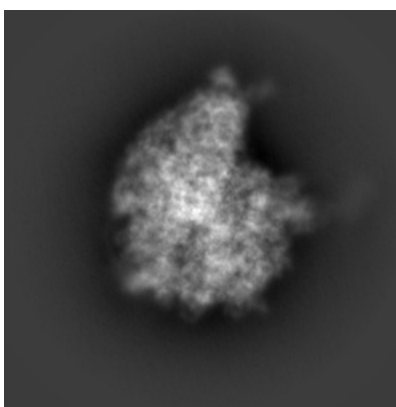


Z

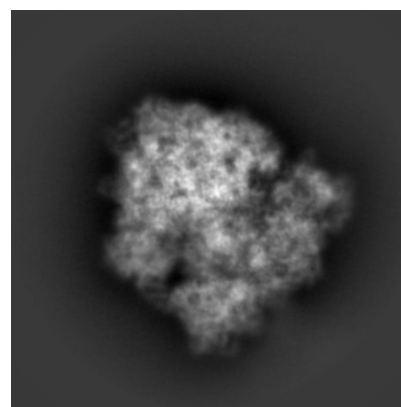
6.1.2 Raw map



X



Y

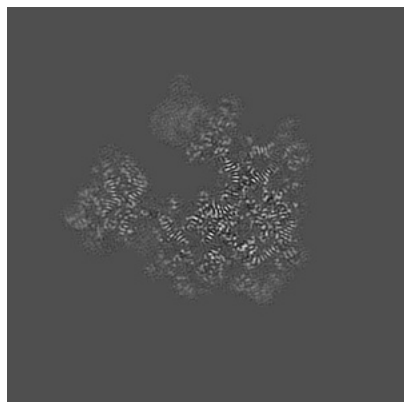


Z

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

6.2 Central slices [i](#)

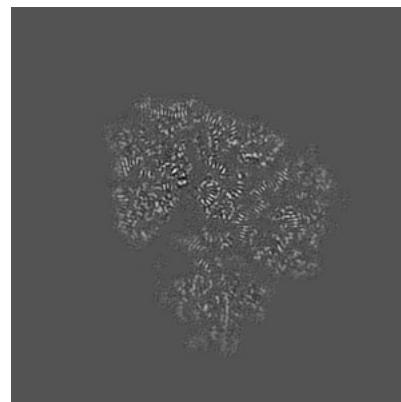
6.2.1 Primary map



X Index: 180

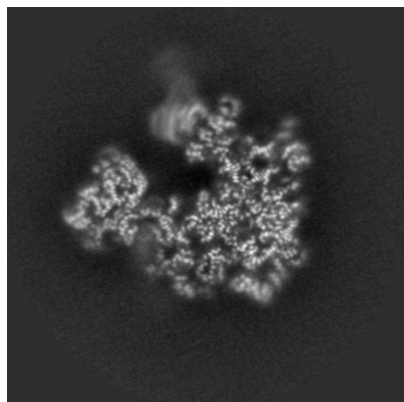


Y Index: 180

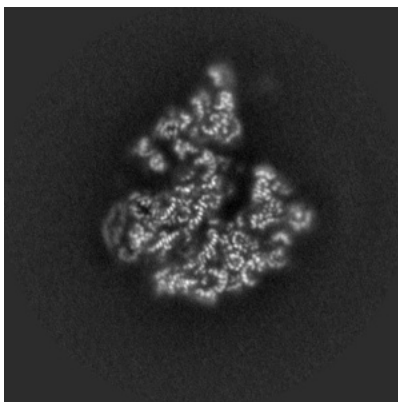


Z Index: 180

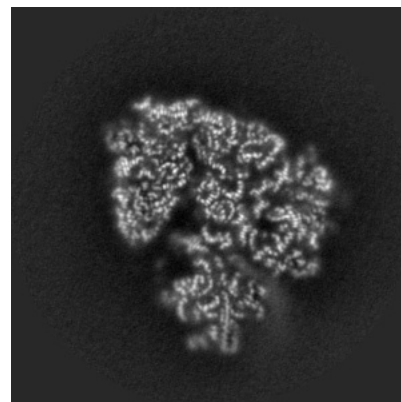
6.2.2 Raw map



X Index: 180



Y Index: 180

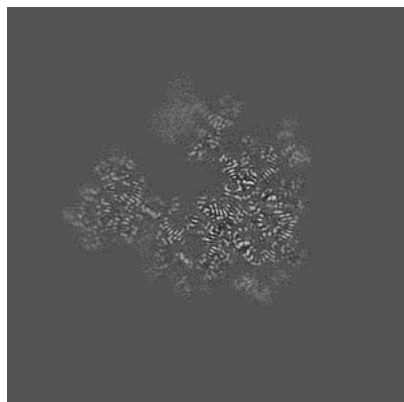


Z Index: 180

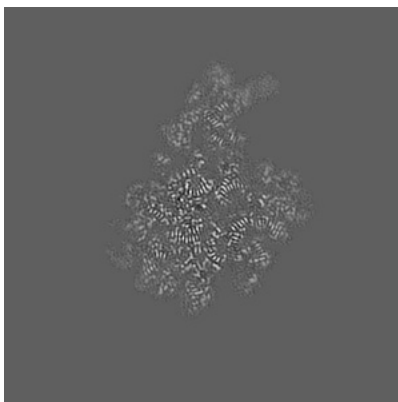
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

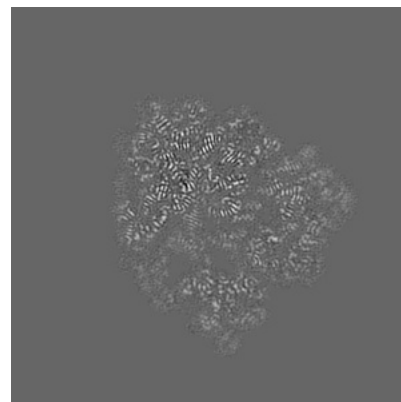
6.3.1 Primary map



X Index: 178

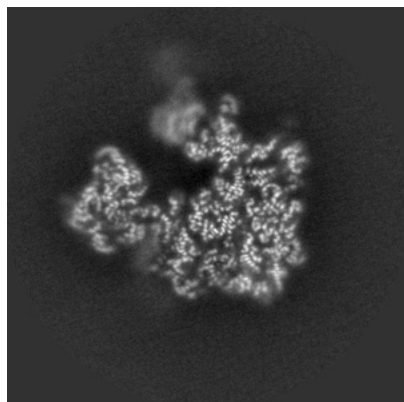


Y Index: 190

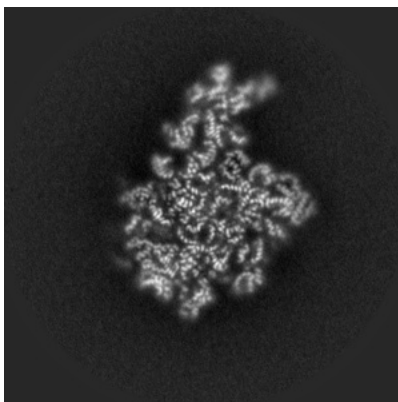


Z Index: 188

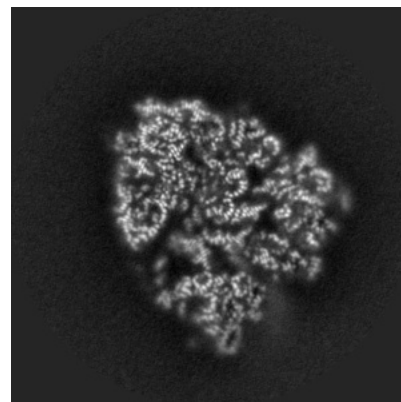
6.3.2 Raw map



X Index: 184



Y Index: 194

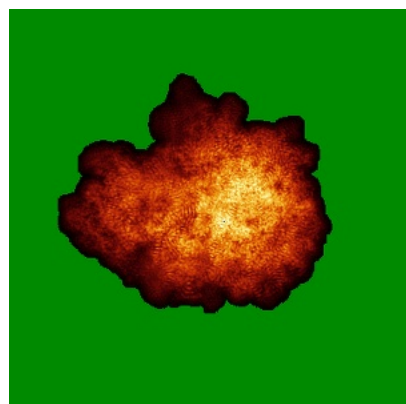


Z Index: 184

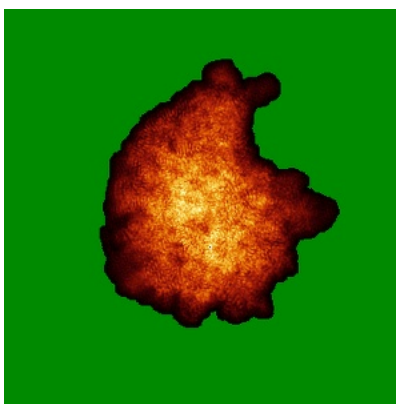
The images above show the largest variance slices of the map in three orthogonal directions.

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

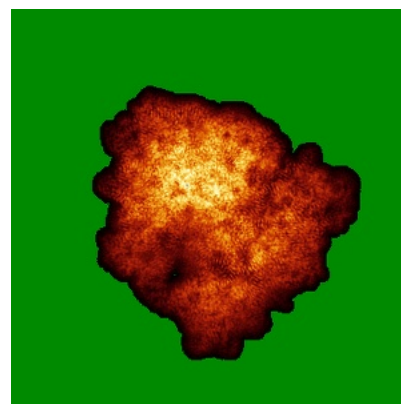
6.4.1 Primary map



X

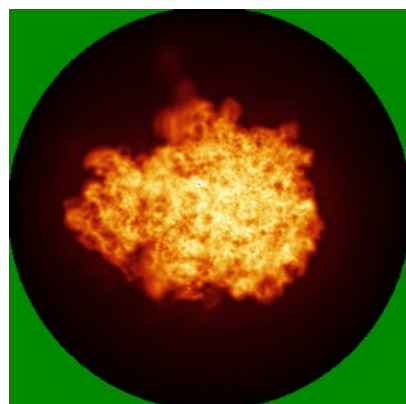


Y

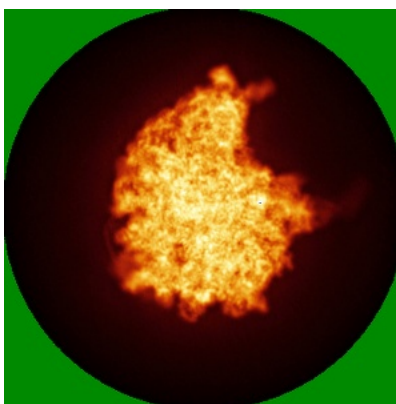


Z

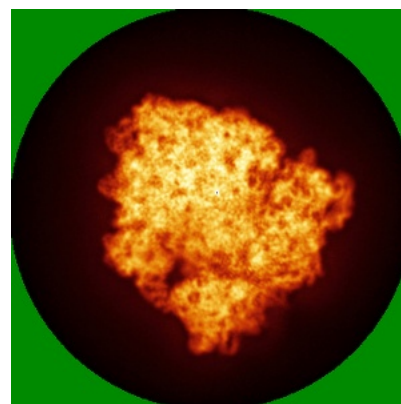
6.4.2 Raw map



X



Y

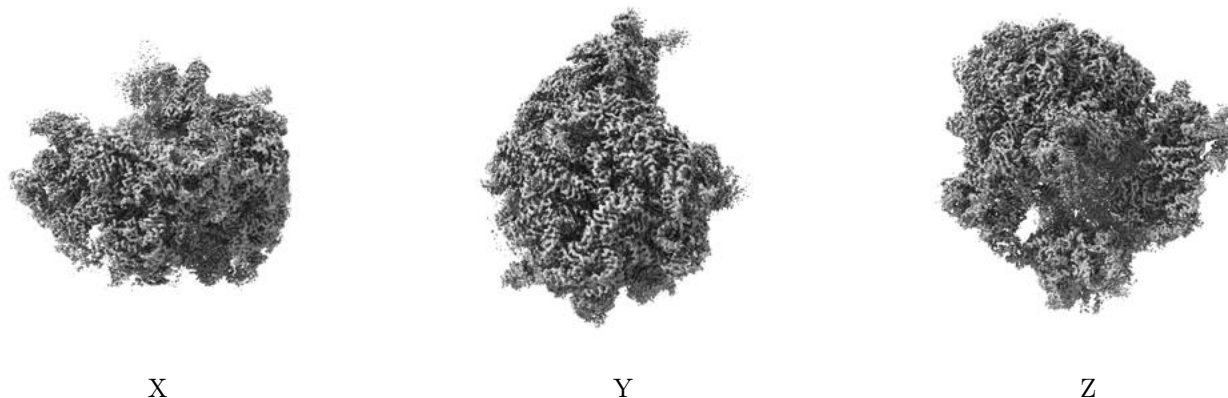


Z

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

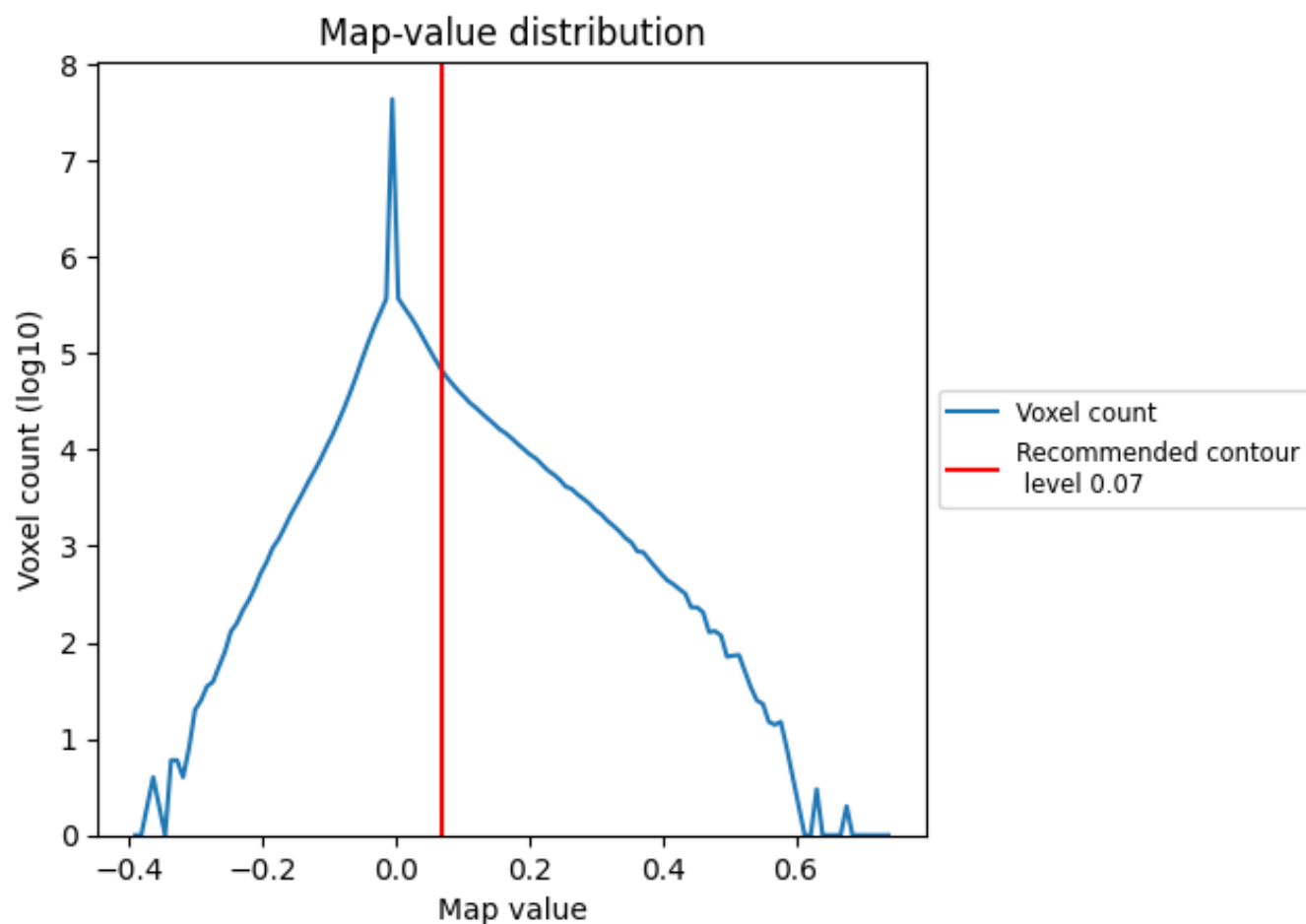
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

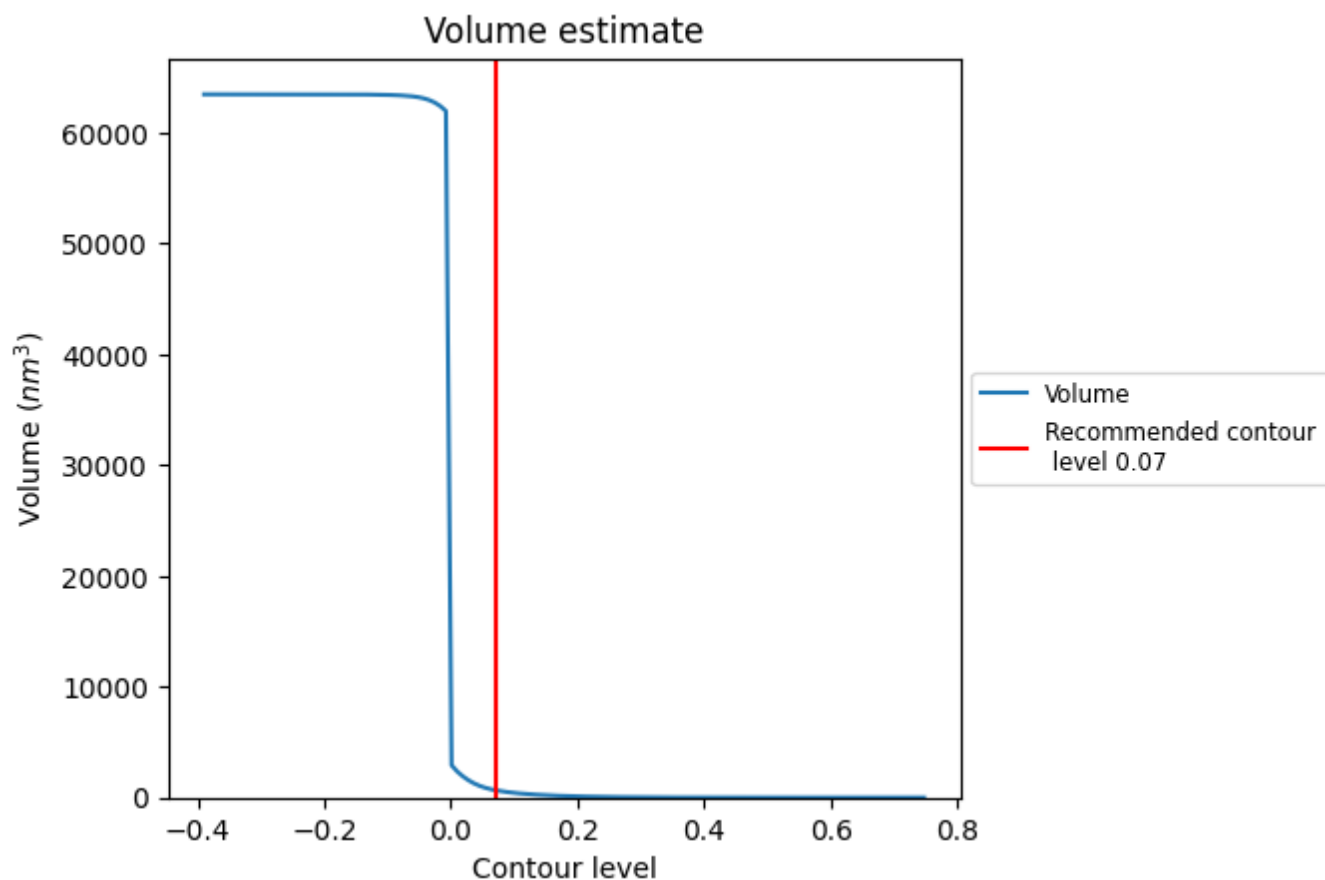
This section contains the results of statistical analysis of the map.

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.

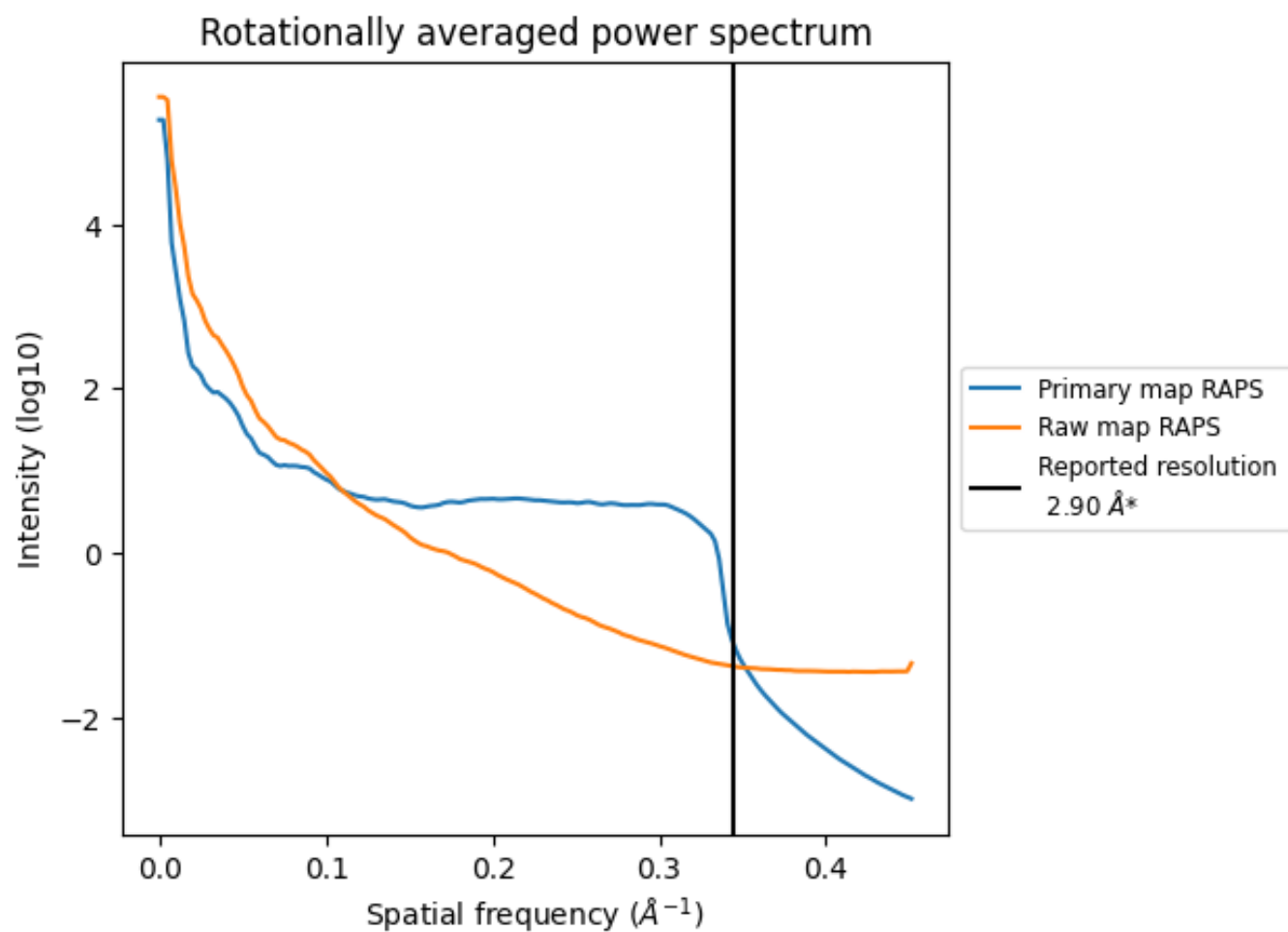
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 670 nm^3 ; this corresponds to an approximate mass of 605 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 ⓘ

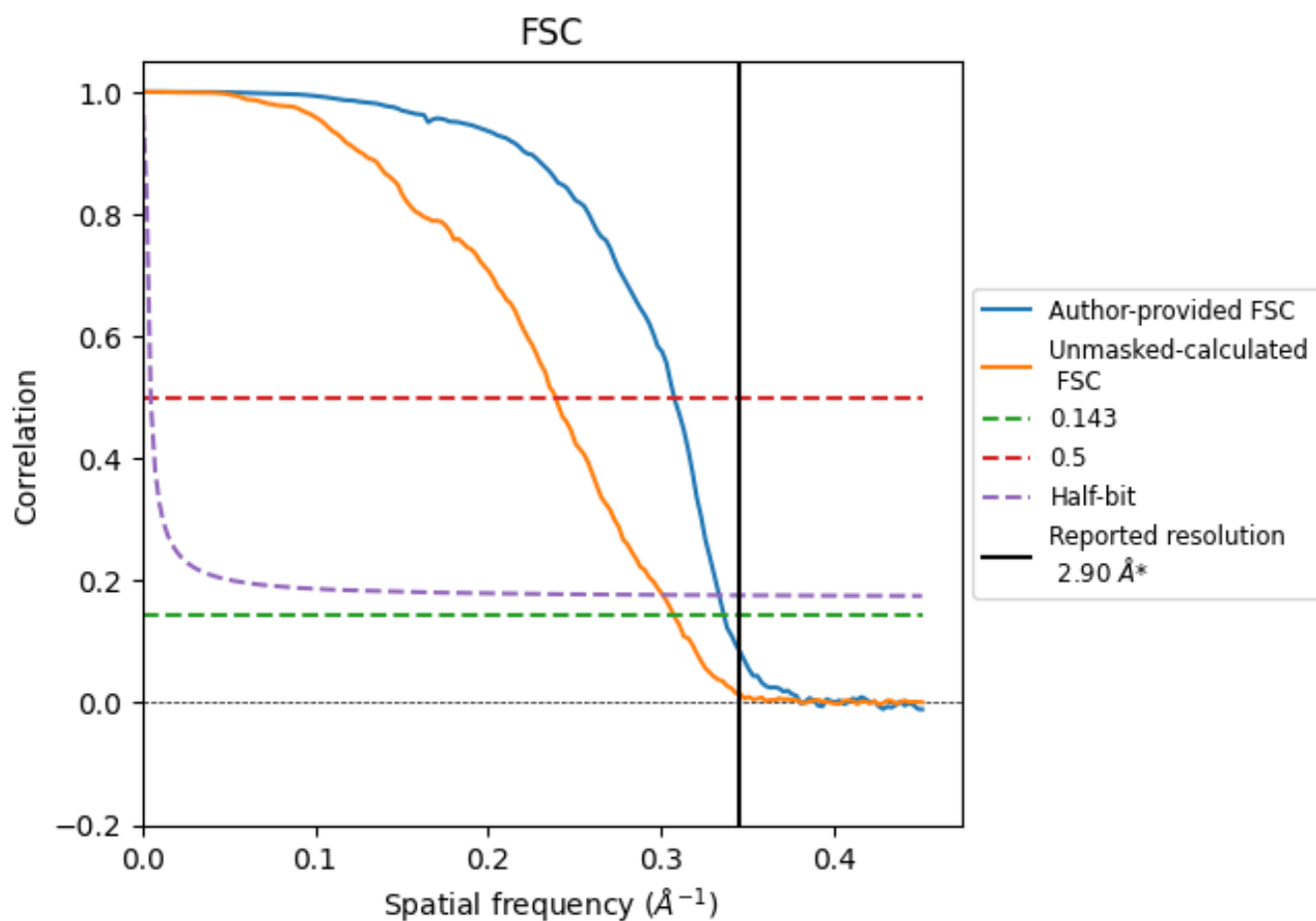


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

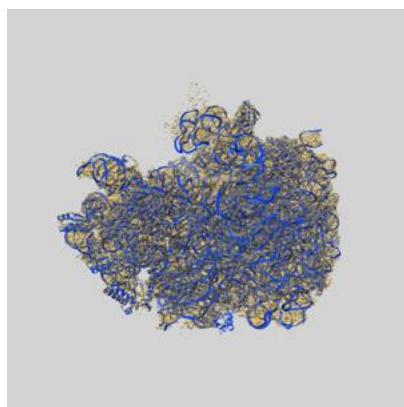
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.97	3.25	2.99
Unmasked-calculated*	3.25	4.18	3.32

*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 3.25 differs from the reported value 2.9 by more than 10 %

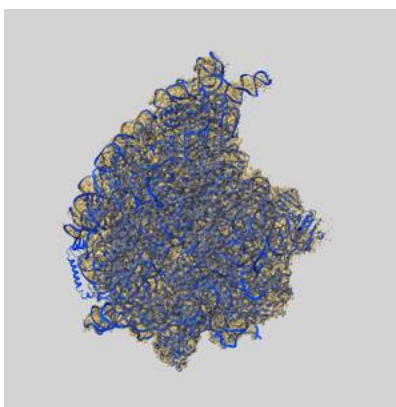
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12573 and PDB model 7NSO. Per-residue inclusion information can be found in section 3 on page 15.

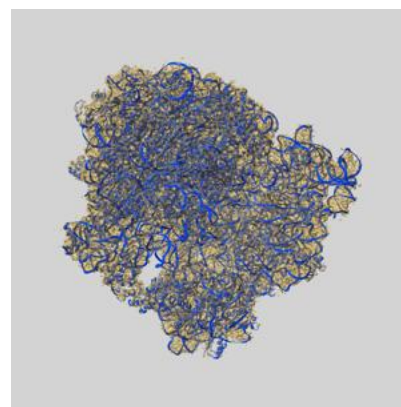
9.1 Map-model overlay [i](#)



X



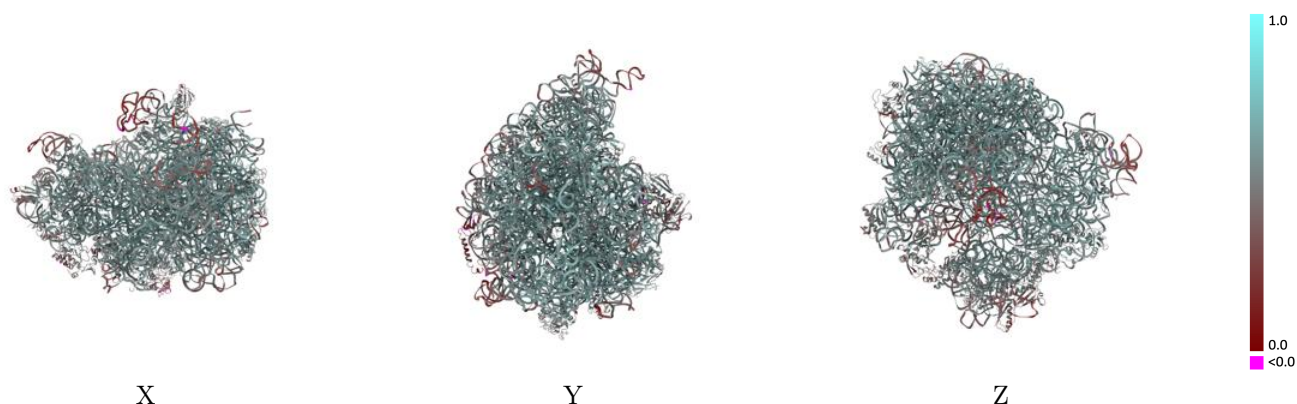
Y



Z

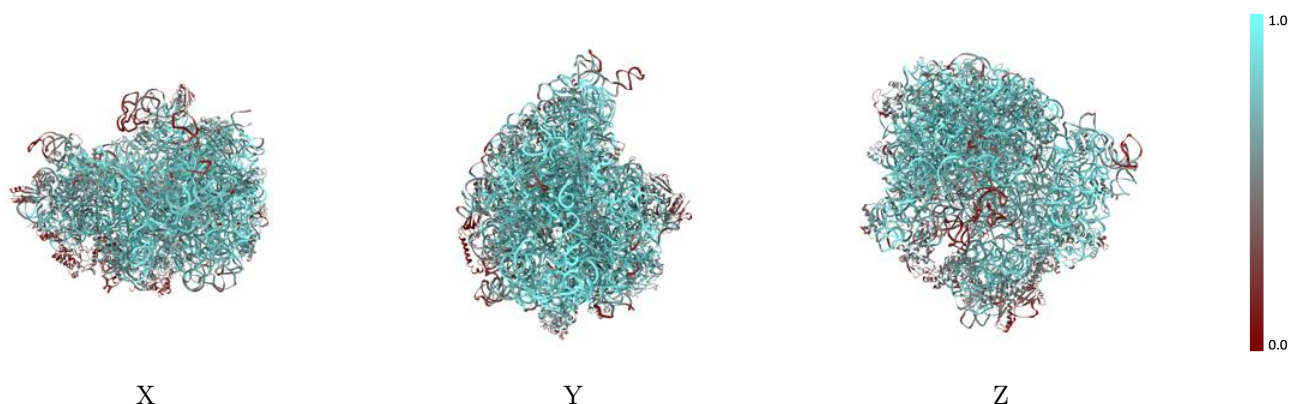
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



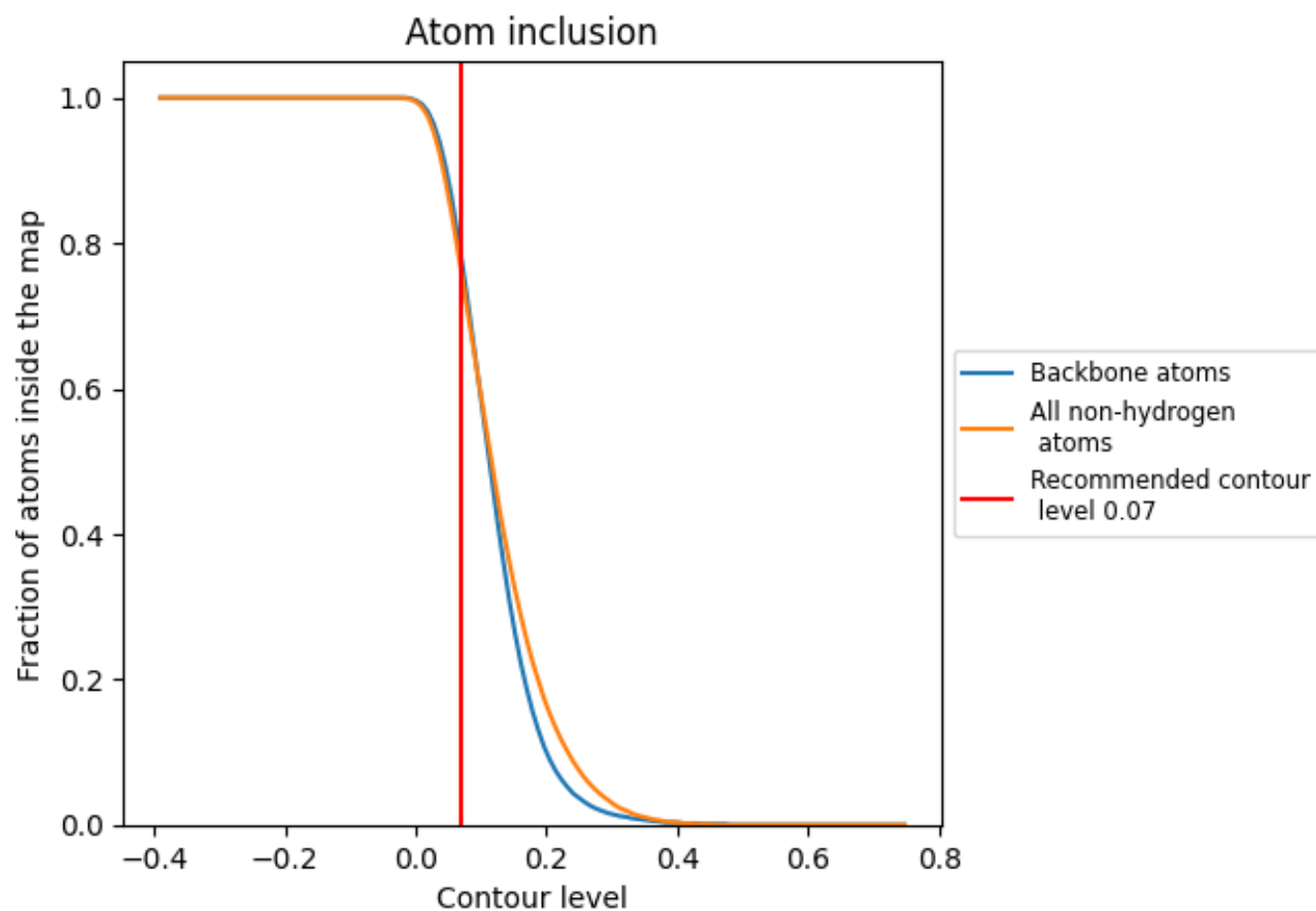
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.5510
0	 0.7560	 0.5810
1	 0.2740	 0.4920
2	 0.8390	 0.6160
3	 0.7900	 0.6010
4	 0.7430	 0.5660
5	 0.2840	 0.4000
6	 0.9330	 0.5950
7	 0.6730	 0.5630
8	 0.5780	 0.4730
A	 0.8420	 0.5670
B	 0.7840	 0.5230
C	 0.7720	 0.5890
D	 0.7280	 0.5760
E	 0.6370	 0.5410
F	 0.5110	 0.4870
G	 0.4350	 0.4710
H	 0.0740	 0.2870
J	 0.7330	 0.5690
K	 0.6990	 0.5710
L	 0.6880	 0.5570
M	 0.7260	 0.5770
N	 0.7830	 0.5830
O	 0.5940	 0.5080
P	 0.6820	 0.5580
Q	 0.7900	 0.5880
R	 0.6600	 0.5510
S	 0.7240	 0.5720
T	 0.6310	 0.5470
U	 0.6000	 0.5270
V	 0.6150	 0.5380
W	 0.7690	 0.5980
X	 0.6970	 0.5720
Y	 0.5590	 0.5070
Z	 0.7050	 0.5680



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Chain	Atom inclusion	Q-score
a	 0.8330	 0.5610
b	 0.2850	 0.4430
c	 0.5600	 0.5190
d	 0.5790	 0.5300
e	 0.6750	 0.5540
f	 0.4850	 0.4870
g	 0.4140	 0.4680
h	 0.6490	 0.5530
i	 0.5430	 0.4930
j	 0.4520	 0.4860
k	 0.5720	 0.5220
l	 0.6940	 0.5740
m	 0.5100	 0.4930
n	 0.6090	 0.5150
o	 0.6230	 0.5310
p	 0.6430	 0.5350
q	 0.6000	 0.5390
r	 0.5920	 0.5330
s	 0.5750	 0.5200
t	 0.6380	 0.5260
u	 0.1800	 0.4310