



Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 07:51 am BST

PDB ID : 7ZP8 / pdb_00007zp8
EMDB ID : EMD-14850
Title : 70S E. coli ribosome with a stalled flamin domain 5 nascent chain
Authors : Mitropoulou, A.; Plessa, E.; Wlodarski, T.; Ahn, M.; Chan, S.H.S.; Becker, T.A.; Beckmann, R.; Cabrita, L.D.; Christodoulou, J.
Deposited on : 2022-04-26
Resolution : 2.20 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:

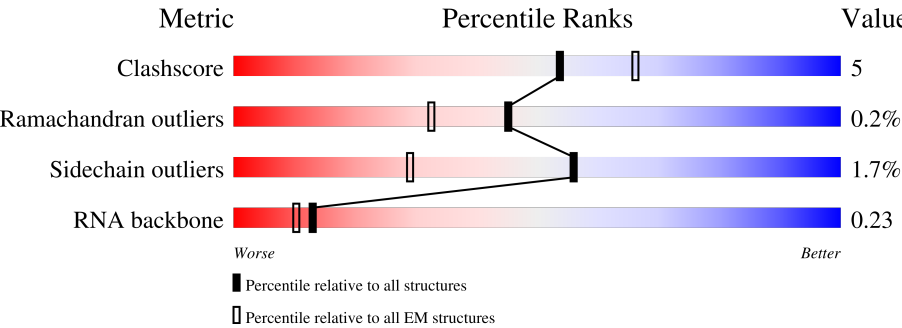
EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









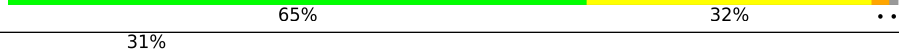
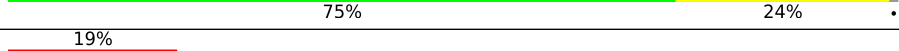
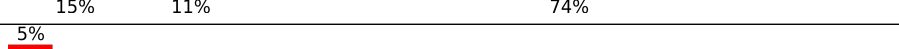
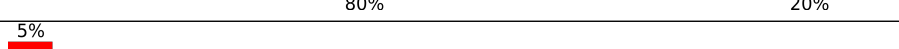
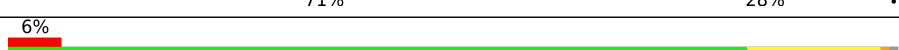

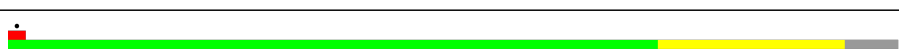

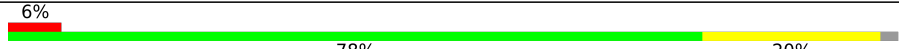





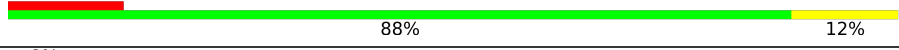
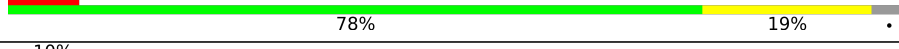
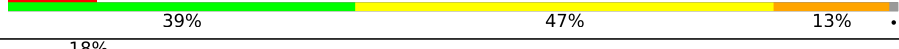


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	78	
2	1	63	
3	2	59	
4	3	57	
5	4	55	
6	6	46	
7	7	65	

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Mol	Chain	Length	Quality of chain
8	8	50	
9	a	120	
10	b	2904	
11	c	273	
12	d	209	
13	e	201	
14	f	179	
15	g	177	
16	h	149	
17	j	142	
18	k	123	
19	l	144	
20	m	136	
21	n	127	
22	o	117	
23	p	115	
24	q	118	
25	r	103	
26	s	110	
27	t	100	
28	u	104	
29	w	94	
30	y	85	
31	v	77	
32	z	148	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90951 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	2901	Total	C	N	O	P	0	0
			62281	27784	11464	20132	2901		

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

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

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

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

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	l	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	y	82	Total	C	N	O	S	0	0
			619	383	127	108	1		

- Molecule 31 is a RNA chain called Pro-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	v	76	Total	C	N	O	P	0	0
			1626	724	292	534	76		

- Molecule 32 is a protein called Gelation factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	z	33	Total	C	N	O	0	0
			277	186	44	47		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	20	MET	-	initiating methionine	UNP P13466
z	21	HIS	-	expression tag	UNP P13466
z	22	HIS	-	expression tag	UNP P13466
z	23	HIS	-	expression tag	UNP P13466
z	24	HIS	-	expression tag	UNP P13466
z	25	HIS	-	expression tag	UNP P13466
z	26	HIS	-	expression tag	UNP P13466
z	27	ALA	-	expression tag	UNP P13466
z	28	SER	-	expression tag	UNP P13466
z	149	GLU	-	expression tag	UNP P13466
z	150	LEU	-	expression tag	UNP P13466
z	151	PHE	-	expression tag	UNP P13466
z	152	SER	-	expression tag	UNP P13466

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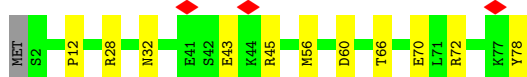
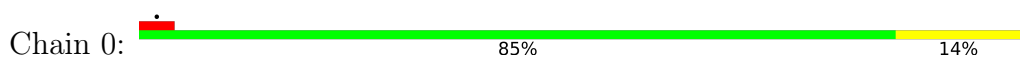
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Chain	Residue	Modelled	Actual	Comment	Reference
z	153	THR	-	expression tag	UNP P13466
z	154	PRO	-	expression tag	UNP P13466
z	155	VAL	-	expression tag	UNP P13466
z	156	TRP	-	expression tag	UNP P13466
z	157	ILE	-	expression tag	UNP P13466
z	158	TRP	-	expression tag	UNP P13466
z	159	TRP	-	expression tag	UNP P13466
z	160	TRP	-	expression tag	UNP P13466
z	161	PRO	-	expression tag	UNP P13466
z	162	ARG	-	expression tag	UNP P13466
z	163	ILE	-	expression tag	UNP P13466
z	164	ARG	-	expression tag	UNP P13466
z	165	GLY	-	expression tag	UNP P13466
z	166	PRO	-	expression tag	UNP P13466
z	167	PRO	-	expression tag	UNP P13466

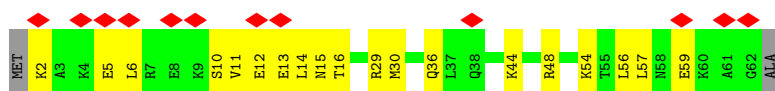
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

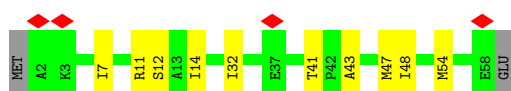
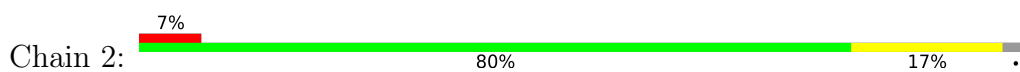
- Molecule 1: 50S ribosomal protein L28



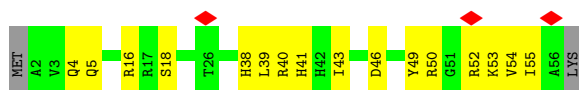
- Molecule 2: 50S ribosomal protein L29



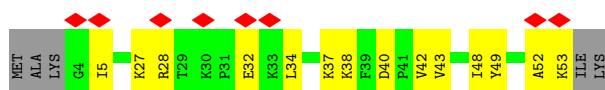
- Molecule 3: 50S ribosomal protein L30



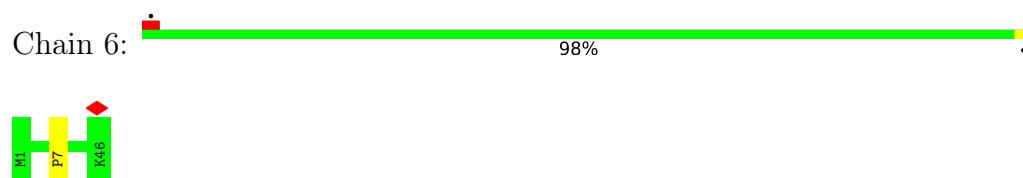
- Molecule 4: 50S ribosomal protein L32



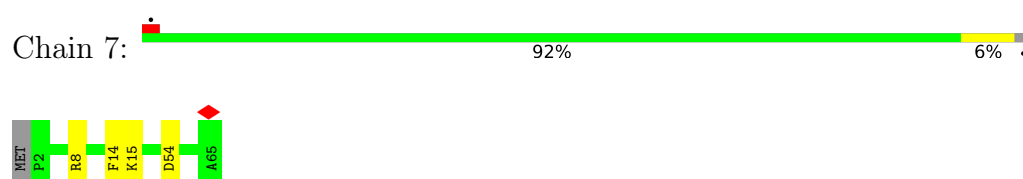
- Molecule 5: 50S ribosomal protein L33



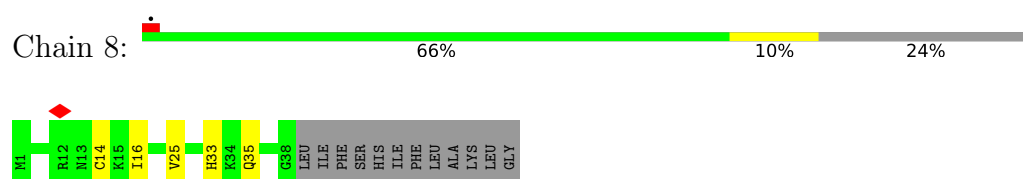
- Molecule 6: 50S ribosomal protein L34



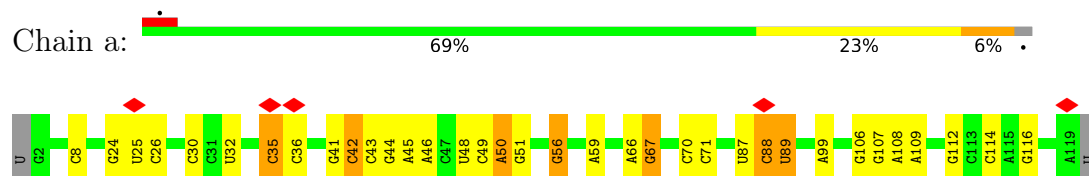
- Molecule 7: 50S ribosomal protein L35



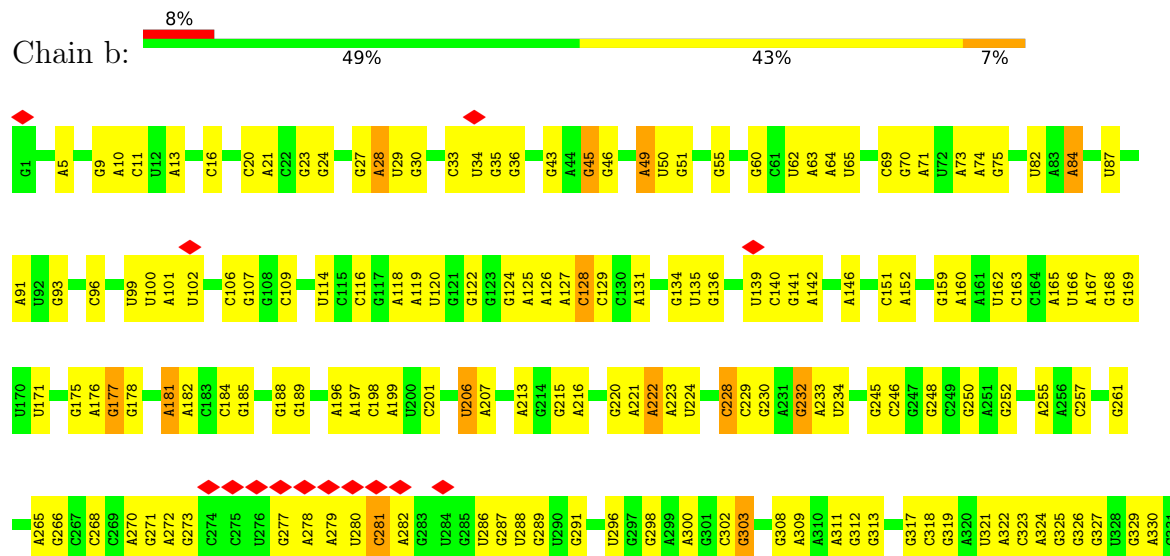
- Molecule 8: 50S ribosomal protein L36

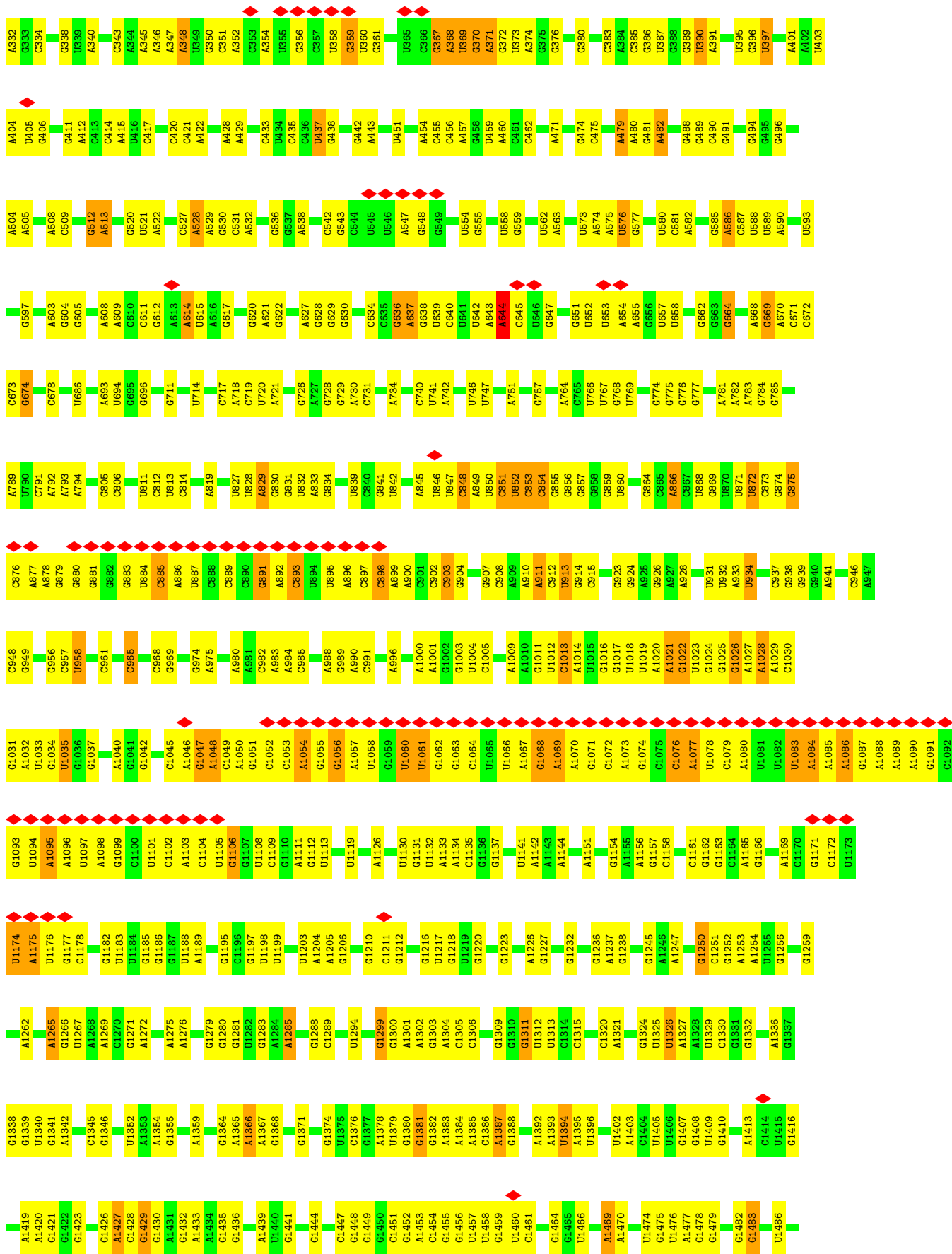


- Molecule 9: 5S rRNA

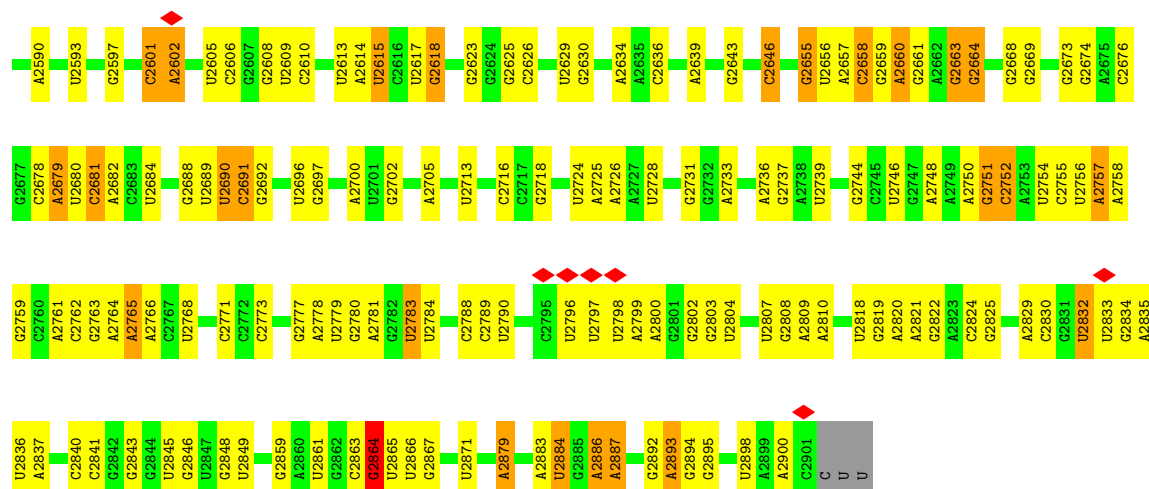


- Molecule 10: 23S rRNA

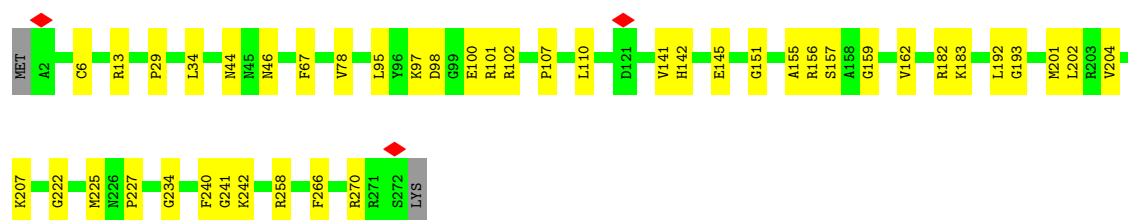
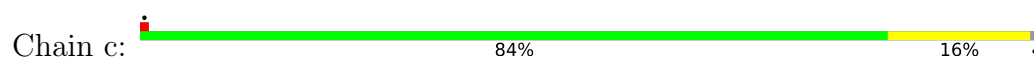




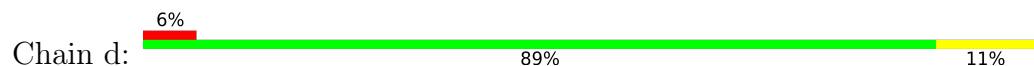
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A2503	C2427	G2337	A2267	C2174	A2114	A2033	U1946	G1857	G1756	G1674	C1576	G1491
U2504	G2428	C2338	A2268	C2175	G2115	U2034	A1952	A1858	U1757	C1675	C1577	C1492
G2505	G2429	C2339	A2269	C2176	G2116	G2035	G1953	G1862	A1759	G1681	G1578	C1493
U2506	U2430	A2340	A2273	C2177	A2117	A2036	G1954	G1863	A1762	G1682	G1581	A1494
G2507	U2431	A2341	A2274	C2178	U2118	G2038	G1955	U1864	G1763	G1683	C1582	A1495
G2508	A2432	A2342	A2275	C2179	U2119	U2039	U1956	U1865	C1764	G1684	C1583	A1496
A2513	A2433	C2343	A2276	C2180	A2120	G2040	C1957	G1869	A1773	U1584	U1497	U1497
U2514	A2434	C2344	C2282	U2181	G2121	A2041	C1958	C1870	A1776	C1585	C1586	C1498
G2515	G2350	C2345	C2283	U2182	U2122	A2042	G1961	A1871	G1776	A1690	A1503	A1503
A2516	G2351	A2352	G2286	U2183	G2123	C2051	C1962	A1872	U1779	U1693	U1588	U1506
G2517	G2352	G2353	A2287	A2184	G2124	C2055	U1963	C1873	U1782	C1694	U1589	C1507
U2518	C2354	A2355	A2288	U2185	G2125	G2056	G1964	C1874	A1783	A1593	A1508	A1508
C2520	G2355	G2356	U2291	G2186	A2126	A2059	A1966	A1875	U1784	U1700	A1509	A1509
G2526	G2361	G2362	U2292	U2187	G2127	A2060	C1967	U1882	A1785	G1702	G1600	G1516
C2527	C2364	C2365	G2293	U2188	C2128	G2061	A1970	U1883	A1786	G1703	C1601	G1517
U2528	U2293	G2366	G2294	U2189	U2129	A2062	G1971	G1884	A1787	C1704	G1602	G1518
G2529	G2294	G2367	G2295	G2190	G2130	C2063	G1972	U1887	G1792	C1705	U1603	G1519
U2533	G2295	G2368	G2296	A2191	U2131	U2068	G1973	C1887	C1793	G1706	A1603	G1523
A2534	U2296	G2369	A2297	U2192	A2132	G2069	G1974	A1889	A1794	G1707	C1606	G1524
G2535	G2297	G2370	G2298	G2193	G2133	U2074	G1975	A1890	C1800	U1713	C1607	G1529
C2536	U2298	G2371	G2299	U2197	A2134	U2075	G1980	C1895	A1809	U1714	A1608	G1530
U2537	C2300	G2372	G2301	A2198	G2135	U2076	A1981	C1985	A1810	G1715	A1609	G1531
G2543	G2302	G2373	G2302	A2199	A2136	A2077	C1986	A1989	C1804	U1716	A1610	A1532
A2468	G2303	U2384	G2303	U2203	G2137	C2078	A1987	A1900	A1805	G1721	C1612	C1533
G2469	U2304	G2385	U2305	G2204	U2138	U2079	U1991	G1906	A1808	C1725	C1613	U1534
A2471	G2305	C2386	G2306	G2204	U2139	A2080	U1992	A1913	A1809	G1726	A1618	A1535
G2472	G2306	G2387	G2307	U2208	G2140	U2081	U1993	C1914	A1810	A1727	G1622	C1536
U2473	G2307	U2388	G2308	A2211	G2141	U2085	C1996	U1915	G1811	C1728	G1626	G1537
A2474	G2308	G2389	A2309	A2212	A2142	U2086	C1997	A1916	C1816	U1729	A1627	G1538
C2475	G2310	G2390	G2310	U2213	C2143	G2087	A1998	U1917	U1817	U1730	G1627	U1539
A2476	G2311	U2391	G2311	G2214	G2144	G2093	C1999	G1921	U1818	G1731	A1630	A1544
G2477	A2312	G2392	U2312	C2214	C2145	A2094	G2002	G1922	A1819	C1732	A1634	C1547
U2478	G2313	U2393	G2313	A2215	C2146	A2095	C2008	C1923	U1820	U1733	A1635	A1552
A2479	A2314	G2394	A2314	U2216	U2147	C2096	A2009	C1924	A1821	G1734	G1642	U1553
G2480	G2315	U2395	U2315	C2217	G2148	U2098	G2010	U1925	C1822	U1735	G1643	G1555
C2481	G2316	G2396	G2316	C2218	U2149	G2099	U2011	A1927	G1823	G1736	U1647	C1558
A2482	A2317	U2397	G2317	G2219	C2150	G2100	G2012	A1928	U1827	G1737	U1559	U1560
G2483	G2318	U2398	G2318	U2220	U2151	A2101	G2013	G1929	G1828	G1738	G1648	U1563
A2484	G2319	G2399	G2319	G2221	G2152	G2102	A2020	U1930	A1829	U1740	G1649	C1564
G2485	U2320	U2399	U2320	U2222	A2153	C2104	G2021	U1931	C1833	A1744	A1664	G1665
C2486	G2321	G2400	G2321	U2223	U2155	U2105	U2022	G1935	C1836	A1745	A1665	C1566
A2487	A2322	U2401	U2322	G2224	G2156	U2106	C2023	A1937	A1848	G1749	G1666	C1567
G2488	G2323	U2402	U2323	U2225	U2157	G2107	G2024	A1938	G1849	U1751	A1667	G1568
U2489	U2324	U2403	U2324	G2226	G2158	A2108	G2029	U1939	A1853	G1752	A1669	G1569
G2490	G2325	C2404	G2325	U2227	A2159	U2109	A2031	U1940		A1754		A1571
U2491	C2326	U2405	G2326	A2228	G2160	U2110		U1944				
U2492	A2327	U2406	A2327	U2229	C2161	U2111						
G2493	G2328	U2407	U2328	U2230	G2162	G2112						
A2494	U2329	U2408	U2329	U2231	A2163							
G2495	G2330	U2409	G2330	U2232	A2164							
C2496	G2331	U2410	G2331	U2233	A2165							
U2497	U2332	U2411	U2332	U2234	U2167							
G2498	G2333	U2412	G2333	U2235	G2168							
C2499	U2334	U2413	U2334	U2236	A2169							
U2506	A2335	A2425	A2335	C2261	A2170							
					A2171							
					U2172							



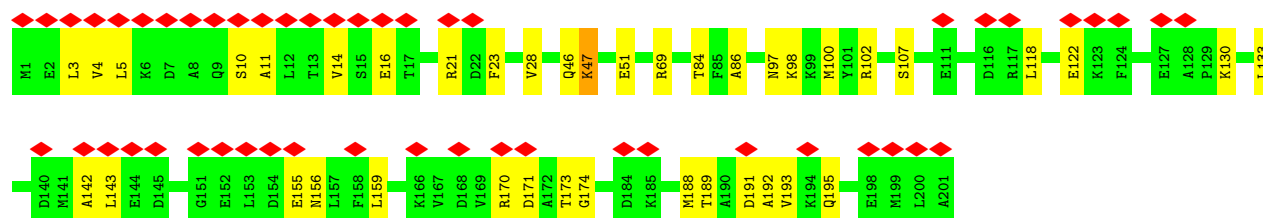
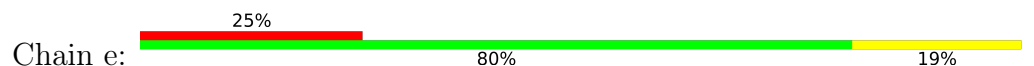
• Molecule 11: 50S ribosomal protein L2



• Molecule 12: 50S ribosomal protein L3

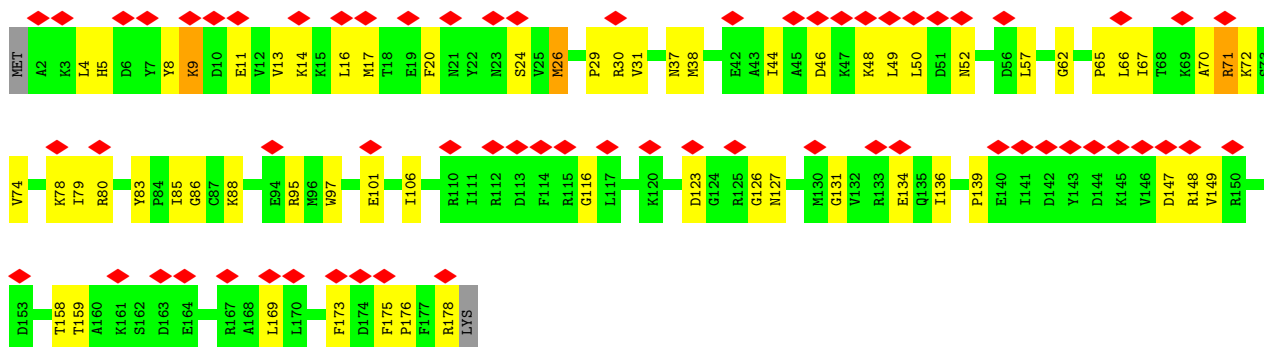


• Molecule 13: 50S ribosomal protein L4

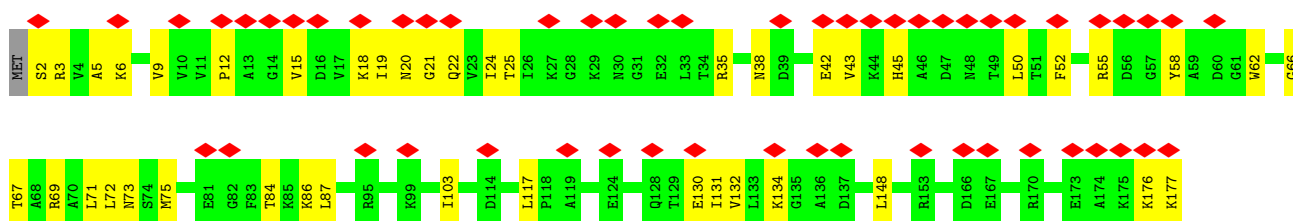
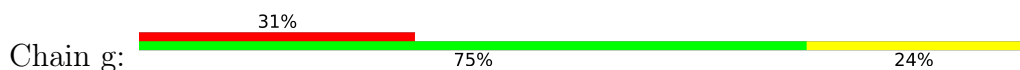


• Molecule 14: 50S ribosomal protein L5

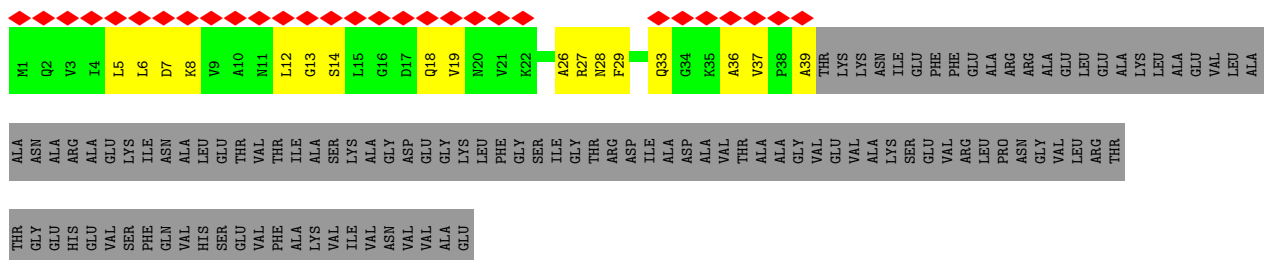




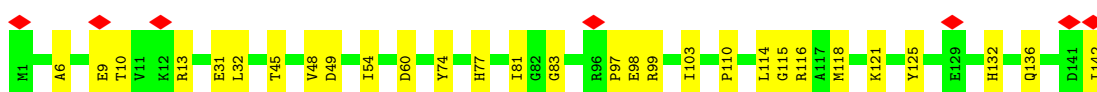
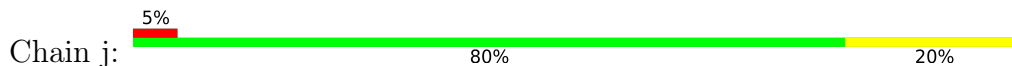
• Molecule 15: 50S ribosomal protein L6



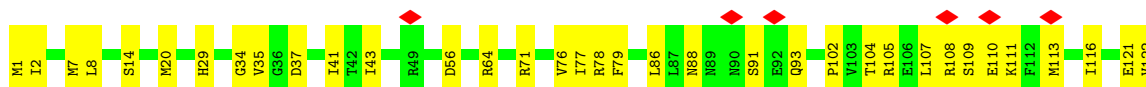
• Molecule 16: 50S ribosomal protein L9



• Molecule 17: 50S ribosomal protein L13




• Molecule 18: 50S ribosomal protein L14



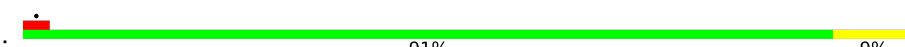
LEU

- Molecule 19: 50S ribosomal protein L15

Chain l:  6% 83% 15% ..



- Molecule 20: 50S ribosomal protein L16

Chain m:  91% 9%




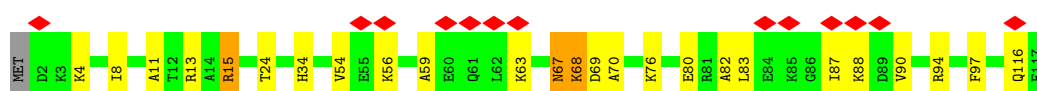
- Molecule 21: 50S ribosomal protein L17

Chain n:  73% 21% 6%




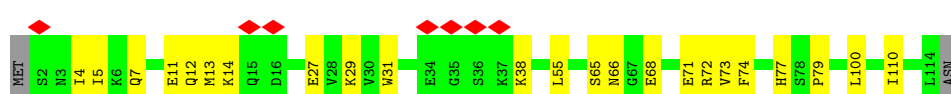
- Molecule 22: 50S ribosomal protein L18

Chain o:  11% 78% 19% ..




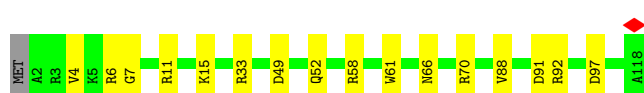
- Molecule 23: 50S ribosomal protein L19

Chain p:  6% 78% 20% .

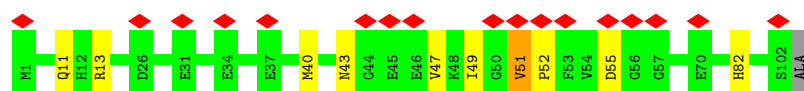
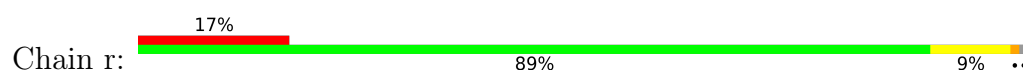


- Molecule 24: 50S ribosomal protein L20

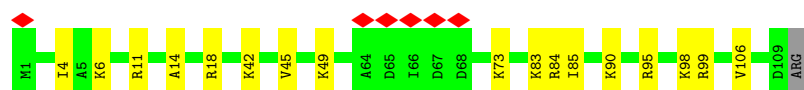
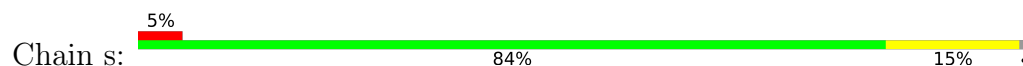
Chain q:  86% 14%



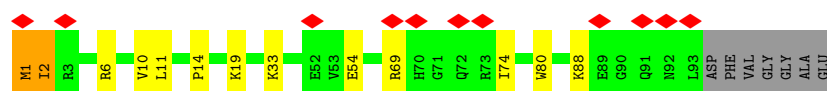
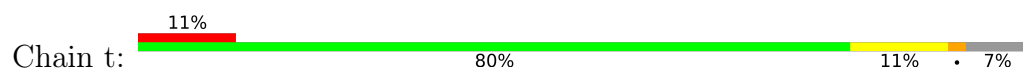
- Molecule 25: 50S ribosomal protein L21



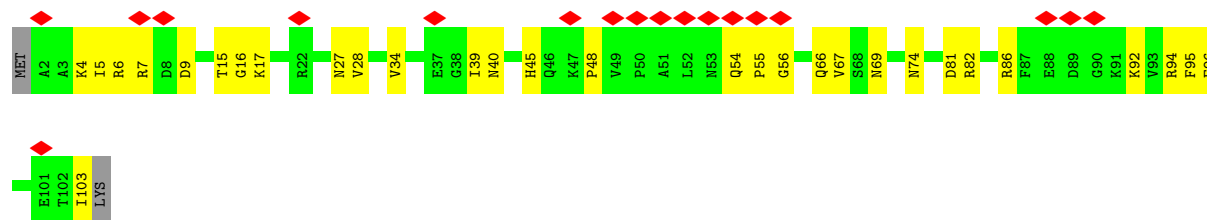
- Molecule 26: 50S ribosomal protein L22



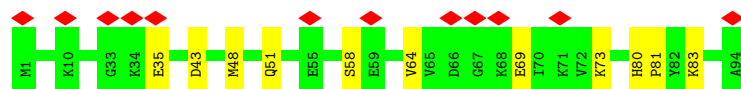
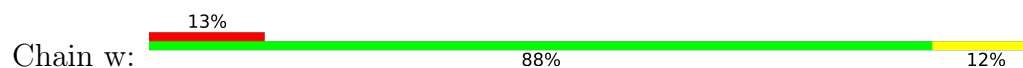
- Molecule 27: 50S ribosomal protein L23



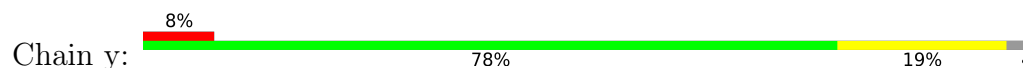
- Molecule 28: 50S ribosomal protein L24



- Molecule 29: 50S ribosomal protein L25

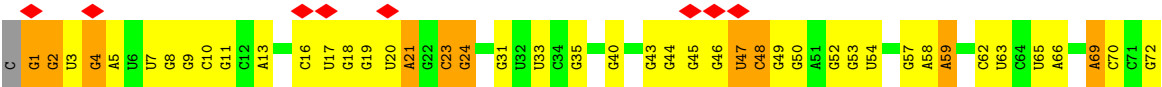


- Molecule 30: 50S ribosomal protein L27

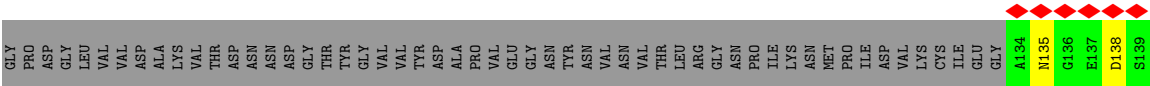
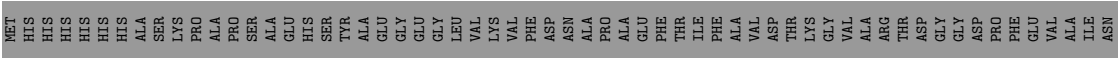


- Molecule 31: Pro-tRNA





● Molecule 32: Gelation factor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	614463	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	14.45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02965	Depositor
Map size (Å)	411.648, 411.648, 411.648	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.39	0/635	0.52	0/848
2	1	0.31	0/496	0.46	0/660
3	2	0.35	0/443	0.40	0/593
4	3	0.46	0/440	0.72	0/588
5	4	0.47	0/416	0.65	0/554
6	6	0.38	0/380	0.48	0/498
7	7	0.46	0/513	0.57	0/676
8	8	0.39	0/302	0.48	0/397
9	a	0.38	0/2828	0.36	0/4410
10	b	0.51	0/69757	0.72	19/108827 (0.0%)
11	c	0.37	0/2121	0.48	0/2852
12	d	0.40	0/1586	0.48	0/2134
13	e	0.33	0/1571	0.43	1/2113 (0.0%)
14	f	0.40	0/1434	0.62	0/1926
15	g	0.35	0/1343	0.51	0/1816
16	h	0.28	0/290	0.62	0/392
17	j	0.42	0/1152	0.47	1/1551 (0.1%)
18	k	0.40	0/947	0.47	0/1268
19	l	0.63	0/1052	0.82	1/1401 (0.1%)
20	m	0.36	0/1093	0.50	0/1460
21	n	0.40	0/973	0.52	0/1301
22	o	0.42	0/902	0.60	0/1209
23	p	0.38	0/920	0.43	0/1231
24	q	0.41	0/960	0.47	0/1278
25	r	0.53	0/823	0.65	0/1100
26	s	0.37	0/852	0.41	0/1142
27	t	0.39	0/744	0.53	0/994
28	u	0.39	0/787	0.57	0/1051
29	w	0.33	0/766	0.43	0/1025
30	y	0.39	0/627	0.55	0/829
31	v	0.52	0/1817	0.75	1/2832 (0.0%)
32	z	0.99	0/291	1.13	1/400 (0.2%)
All	All	0.48	0/99261	0.68	24/149356 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	b	2864	G	C2'-C3'-O3'	8.66	126.69	113.70
10	b	390	U	C2'-C3'-O3'	8.34	122.01	109.50
10	b	1595	C	C2'-C3'-O3'	7.92	125.58	113.70
10	b	2832	U	C4'-C3'-O3'	7.74	121.01	109.40
10	b	1626	A	C2'-C3'-O3'	7.08	124.33	113.70
10	b	228	C	C4'-C3'-O3'	6.95	119.83	109.40
10	b	2334	U	C1'-C2'-O2'	-6.79	101.62	111.80
10	b	9	G	C2'-C3'-O3'	6.62	123.63	113.70
10	b	479	A	C2'-C3'-O3'	-6.41	99.89	109.50
10	b	1538	G	C2'-C3'-O3'	6.24	123.06	113.70
10	b	2655	G	C4'-C3'-O3'	6.14	118.61	109.40
31	v	1	G	C2'-C3'-O3'	6.09	122.83	113.70
10	b	1930	G	C4'-C3'-O3'	5.93	118.30	109.40
10	b	45	G	C2'-C3'-O3'	-5.68	105.18	113.70
10	b	1762	A	C4'-C3'-O3'	-5.57	104.64	113.00
32	z	144	PHE	N-CA-C	-5.45	106.00	113.30
17	j	136	GLN	CA-C-O	-5.38	116.34	120.48
10	b	644	A	O4'-C1'-C2'	-5.37	102.23	107.60
19	l	100	ILE	N-CA-C	-5.32	106.61	111.67
10	b	2655	G	C2'-C3'-O3'	5.32	117.48	109.50
10	b	2055	C	C4'-C3'-O3'	5.29	120.93	113.00
10	b	1299	G	C2'-C3'-O3'	5.14	121.42	113.70
10	b	2055	C	C3'-C2'-O2'	5.10	118.35	110.70
13	e	47	LYS	CB-CG-CD	5.04	122.89	111.30

There are no chirality outliers.

There are no planarity outliers.

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	0	625	0	652	7	0
2	1	495	0	526	15	0
3	2	439	0	482	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	434	0	445	12	0
5	4	409	0	440	8	0
6	6	377	0	418	1	0
7	7	504	0	572	3	0
8	8	301	0	341	3	0
9	a	2529	0	1281	15	0
10	b	62281	0	31323	387	0
11	c	2082	0	2154	27	0
12	d	1565	0	1616	21	0
13	e	1552	0	1619	24	0
14	f	1410	0	1444	44	0
15	g	1323	0	1371	26	0
16	h	287	0	307	12	0
17	j	1129	0	1162	21	0
18	k	938	0	1012	25	0
19	l	1043	0	1123	10	0
20	m	1074	0	1157	9	0
21	n	960	0	1000	19	0
22	o	892	0	923	18	0
23	p	908	0	956	21	0
24	q	947	0	1019	15	0
25	r	810	0	834	5	0
26	s	845	0	909	15	0
27	t	738	0	807	9	0
28	u	779	0	831	22	0
29	w	753	0	780	7	0
30	y	619	0	642	14	0
31	v	1626	0	821	11	0
32	z	277	0	250	3	0
All	All	90951	0	59217	755	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 5.

All (755) 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)
10:b:892:A:C8	10:b:893:C:C6	1.96	1.54
10:b:892:A:H8	10:b:893:C:C6	1.26	1.52
10:b:892:A:C8	10:b:893:C:C5	2.13	1.34
10:b:370:G:OP2	10:b:370:G:C8	1.81	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1871:A:H5''	10:b:1872:A:C2	1.74	1.22
10:b:1871:A:H5''	10:b:1872:A:N3	1.55	1.20
10:b:851:C:O2'	10:b:852:U:H5'	1.41	1.17
10:b:892:A:H8	10:b:893:C:C5	1.57	1.11
10:b:1997:C:H4'	10:b:1997:C:OP1	1.54	1.08
10:b:644:A:H8	10:b:644:A:C5'	1.69	1.05
10:b:368:A:H2'	10:b:369:U:O5'	1.57	1.04
10:b:368:A:C2'	10:b:369:U:O5'	2.11	0.98
10:b:643:A:H2'	10:b:644:A:H5''	1.43	0.98
10:b:644:A:H8	10:b:644:A:H5'	1.28	0.96
10:b:644:A:H5'	10:b:644:A:C8	2.03	0.93
10:b:892:A:H8	10:b:893:C:H6	1.12	0.93
10:b:851:C:C2'	10:b:852:U:H5'	1.97	0.93
10:b:2601:C:O2'	10:b:2602:A:OP1	1.88	0.92
10:b:644:A:C5'	10:b:644:A:C8	2.54	0.91
10:b:852:U:H2'	10:b:853:C:H6	1.35	0.91
10:b:851:C:H2'	10:b:852:U:C6	2.06	0.91
10:b:851:C:H2'	10:b:852:U:H6	1.34	0.91
10:b:643:A:C2'	10:b:644:A:H5''	2.02	0.89
10:b:892:A:N7	10:b:893:C:C6	2.42	0.88
10:b:874:G:H2'	10:b:875:G:H5'	1.56	0.87
10:b:1871:A:C5'	10:b:1872:A:C2	2.57	0.86
10:b:2041:U:H2'	10:b:2042:A:C8	2.10	0.86
10:b:1997:C:OP1	10:b:1997:C:C4'	2.24	0.86
10:b:370:G:OP2	10:b:370:G:N7	2.10	0.85
10:b:2783:U:H2'	10:b:2784:U:C6	2.12	0.85
18:k:110:GLU:H	18:k:113:MET:HE3	1.42	0.84
10:b:270:A:C2	10:b:369:U:H4'	2.15	0.82
10:b:892:A:N7	10:b:893:C:C5	2.47	0.82
10:b:673:C:O2'	10:b:674:G:H5'	1.80	0.81
15:g:18:LYS:HB3	15:g:25:THR:HB	1.64	0.80
10:b:1875:G:H8	10:b:1875:G:H5''	1.46	0.80
10:b:852:U:H2'	10:b:853:C:C6	2.16	0.80
10:b:874:G:C2'	10:b:875:G:H5'	2.12	0.79
10:b:2690:U:H4'	10:b:2691:C:OP1	1.83	0.79
10:b:948:C:O4'	10:b:984:A:C2	2.36	0.78
10:b:643:A:C3'	10:b:644:A:H5''	2.14	0.78
12:d:15:PHE:H	23:p:12:GLN:HE22	1.32	0.77
10:b:494:G:H4'	26:s:6:LYS:HB2	1.67	0.77
10:b:2657:A:C2'	10:b:2658:C:H5'	2.16	0.76
10:b:2682:A:H61	10:b:2728:U:H1'	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1875:G:H5''	10:b:1875:G:C8	2.21	0.74
10:b:1954:G:H5'	10:b:2550:G:H21	1.53	0.74
13:e:130:LYS:HB2	13:e:133:LEU:HD13	1.70	0.73
10:b:586:A:H5'	13:e:84:THR:HG21	1.69	0.73
4:3:54:VAL:HG23	4:3:55:ILE:HG12	1.70	0.73
10:b:281:C:H2'	10:b:282:A:C8	2.23	0.73
10:b:370:G:OP2	10:b:370:G:H8	1.64	0.73
28:u:15:THR:OG1	28:u:69:ASN:ND2	2.22	0.72
10:b:851:C:O2'	10:b:852:U:C5'	2.32	0.72
10:b:1992:G:N2	10:b:1996:C:O2'	2.22	0.72
30:y:43:THR:O	30:y:45:PHE:N	2.24	0.71
10:b:1964:G:H4'	10:b:1965:C:OP2	1.89	0.71
10:b:637:A:H4'	10:b:638:G:O5'	1.91	0.71
20:m:41:LEU:HA	20:m:45:GLN:HE21	1.54	0.70
10:b:1997:C:H2'	10:b:1998:A:H5'	1.72	0.70
10:b:612:G:C6	10:b:614:A:C8	2.79	0.70
10:b:2111:U:H2'	10:b:2143:C:H5''	1.74	0.70
10:b:2758:A:H2'	10:b:2759:G:H5'	1.74	0.70
10:b:1889:A:H8	10:b:1889:A:OP2	1.73	0.70
22:o:67:ASN:H	22:o:70:ALA:HB3	1.57	0.70
10:b:1250:G:H5''	24:q:6:ARG:HD3	1.74	0.69
17:j:118:MET:HA	17:j:121:LYS:HZ3	1.57	0.69
10:b:2293:G:H5''	22:o:94:ARG:HH22	1.55	0.69
10:b:852:U:C2	10:b:853:C:C5	2.80	0.69
10:b:612:G:N2	10:b:617:G:C6	2.61	0.69
10:b:1283:G:N2	10:b:1285:A:H3'	2.08	0.69
10:b:2690:U:C4'	10:b:2691:C:OP1	2.41	0.69
14:f:48:LYS:O	14:f:52:ASN:ND2	2.26	0.69
10:b:612:G:C2	10:b:617:G:O6	2.47	0.68
15:g:35:ARG:HG2	15:g:75:MET:HE1	1.74	0.68
4:3:40:ARG:HG3	4:3:41:HIS:ND1	2.08	0.68
10:b:1871:A:C5'	10:b:1872:A:N3	2.45	0.68
10:b:1870:C:O2'	10:b:1871:A:H5'	1.94	0.68
10:b:644:A:H8	10:b:644:A:H5''	1.58	0.67
23:p:7:GLN:NE2	23:p:11:GLU:OE1	2.25	0.67
14:f:116:GLY:O	14:f:178:ARG:NH2	2.27	0.67
10:b:272:A:H2'	10:b:273:G:C8	2.29	0.66
10:b:612:G:C5	10:b:614:A:C8	2.84	0.66
21:n:37:THR:HG22	21:n:110:MET:HE1	1.76	0.66
15:g:42:GLU:OE1	15:g:55:ARG:NE	2.28	0.66
21:n:12:ARG:HD3	21:n:16:HIS:CD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:51:G:OP1	22:o:63:LYS:NZ	2.28	0.66
10:b:1889:A:OP2	10:b:1889:A:C8	2.48	0.66
24:q:91:ASP:HB2	25:r:11:GLN:NE2	2.11	0.66
10:b:2830:C:OP1	12:d:59:ARG:HG3	1.95	0.65
10:b:2041:U:H2'	10:b:2042:A:H8	1.59	0.65
14:f:46:ASP:HB3	14:f:49:LEU:HD23	1.77	0.65
16:h:12:LEU:HD13	16:h:19:VAL:HG21	1.79	0.65
10:b:1997:C:C2'	10:b:1998:A:H5'	2.26	0.65
17:j:49:ASP:OD2	17:j:121:LYS:NZ	2.29	0.65
10:b:2758:A:C2'	10:b:2759:G:H5'	2.26	0.65
10:b:902:C:C4	10:b:903:C:C5	2.85	0.64
11:c:182:ARG:NH2	11:c:183:LYS:O	2.30	0.64
2:1:2:LYS:HE3	2:1:6:LEU:HD11	1.79	0.64
2:1:11:VAL:O	2:1:15:ASN:ND2	2.30	0.64
10:b:612:G:C2	10:b:617:G:C6	2.85	0.64
10:b:2617:U:C2'	10:b:2618:G:H5'	2.28	0.64
29:w:64:VAL:HG22	29:w:69:GLU:HG2	1.79	0.64
15:g:176:LYS:HG3	15:g:177:LYS:HG3	1.79	0.64
10:b:2110:G:H22	10:b:2179:C:H2'	1.61	0.64
11:c:67:PHE:CE1	11:c:156:ARG:HD2	2.32	0.64
10:b:948:C:O4'	10:b:984:A:H2	1.80	0.64
10:b:2543:G:H21	10:b:2646:C:H5''	1.61	0.64
7:7:54:ASP:HB3	19:l:57:LEU:HD22	1.80	0.64
10:b:852:U:C2	10:b:853:C:C6	2.86	0.64
10:b:892:A:C8	10:b:893:C:H6	1.90	0.64
15:g:103:ILE:HG13	15:g:117:LEU:HD11	1.80	0.64
10:b:1935:G:H1'	10:b:1964:G:N2	2.13	0.63
26:s:11:ARG:NH2	26:s:98:LYS:HD3	2.14	0.63
19:l:79:LEU:HB2	19:l:114:GLY:H	1.63	0.63
17:j:114:LEU:HG	17:j:118:MET:HE3	1.81	0.63
28:u:34:VAL:HG13	28:u:67:VAL:HG12	1.79	0.63
18:k:78:ARG:NH2	23:p:71:GLU:OE2	2.26	0.63
10:b:1199:U:H1'	24:q:4:VAL:HG22	1.80	0.62
10:b:272:A:H2'	10:b:273:G:H8	1.63	0.62
13:e:21:ARG:NH2	13:e:107:SER:OG	2.33	0.62
10:b:851:C:C2	10:b:852:U:C5	2.88	0.62
13:e:98:LYS:HB3	13:e:102:ARG:HH22	1.64	0.62
2:1:36:GLN:N	2:1:36:GLN:OE1	2.33	0.62
10:b:636:G:OP2	19:l:128:THR:HG22	2.00	0.62
15:g:43:VAL:HG23	15:g:52:PHE:HE1	1.64	0.62
10:b:628:G:O2'	10:b:629:G:H5'	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:148:GLN:HB2	12:d:152:PRO:HG2	1.82	0.62
10:b:2657:A:H2'	10:b:2658:C:H5'	1.82	0.61
11:c:227:PRO:HG3	11:c:234:GLY:H	1.65	0.61
10:b:933:A:C5'	10:b:934:U:OP2	2.48	0.61
10:b:2834:G:H2'	10:b:2879:A:H61	1.65	0.61
24:q:91:ASP:HB2	25:r:11:GLN:HE21	1.64	0.61
28:u:39:ILE:HG13	28:u:40:ASN:N	2.15	0.61
10:b:674:G:H1'	13:e:69:ARG:HD3	1.83	0.61
10:b:1269:A:H61	10:b:2011:U:H3	1.48	0.61
14:f:66:LEU:O	14:f:67:ILE:HD13	1.99	0.61
9:a:89:U:O2	10:b:958:U:H2'	2.01	0.61
11:c:155:ALA:HB2	11:c:162:VAL:HG23	1.82	0.60
2:l:10:SER:N	2:l:13:GLU:OE2	2.25	0.60
30:y:43:THR:C	30:y:45:PHE:H	2.10	0.60
28:u:94:ARG:HB3	28:u:103:ILE:HD12	1.83	0.60
8:8:16:ILE:HD13	8:8:25:VAL:HG22	1.84	0.60
10:b:373:U:H2'	10:b:374:A:H8	1.67	0.60
10:b:671:C:H2'	10:b:672:C:C6	2.36	0.59
10:b:2128:G:H1'	10:b:2174:C:H1'	1.83	0.59
10:b:874:G:O2'	10:b:875:G:H5'	2.02	0.59
21:n:86:ARG:HH21	21:n:117:ASP:HB2	1.65	0.59
14:f:134:GLU:OE1	14:f:136:ILE:HG22	2.02	0.59
28:u:7:ARG:NH1	28:u:28:VAL:HG23	2.18	0.59
10:b:2074:U:H2'	10:b:2075:U:C6	2.36	0.59
21:n:96:ARG:HG3	21:n:116:VAL:HG12	1.83	0.59
10:b:370:G:C8	10:b:370:G:P	2.94	0.59
18:k:107:LEU:HB2	18:k:116:ILE:HD11	1.84	0.59
21:n:114:GLU:HB2	21:n:118:ARG:HD2	1.85	0.59
10:b:669:G:H2'	10:b:669:G:N3	2.16	0.58
15:g:35:ARG:HG2	15:g:75:MET:CE	2.33	0.58
23:p:14:LYS:HD2	23:p:77:HIS:HA	1.84	0.58
10:b:28:A:N6	10:b:512:G:H1'	2.19	0.58
10:b:1820:U:C4	11:c:159:GLY:HA3	2.37	0.58
24:q:66:ASN:O	24:q:70:ARG:HG3	2.04	0.58
14:f:31:VAL:HG12	14:f:158:THR:HG22	1.85	0.58
18:k:76:VAL:HG12	23:p:73:VAL:HB	1.86	0.58
14:f:147:ASP:OD1	14:f:148:ARG:N	2.37	0.57
31:v:4:G:H1	31:v:69:A:H2	1.51	0.57
2:l:30:MET:HE1	27:t:14:PRO:HD3	1.85	0.57
10:b:581:C:H2'	10:b:582:A:C8	2.39	0.57
10:b:956:G:H2'	10:b:957:C:H2'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:29:VAL:O	21:n:78:LYS:NZ	2.30	0.57
10:b:673:C:C2'	10:b:674:G:H5'	2.34	0.57
17:j:118:MET:HA	17:j:121:LYS:NZ	2.19	0.57
10:b:2140:G:H3'	10:b:2141:G:H8	1.69	0.57
15:g:43:VAL:HG23	15:g:52:PHE:CE1	2.40	0.57
17:j:125:TYR:OH	17:j:132:HIS:NE2	2.36	0.57
10:b:833:A:H2'	10:b:834:G:C8	2.40	0.57
10:b:2547:G:H4'	18:k:29:HIS:CE1	2.40	0.57
10:b:2617:U:H2'	10:b:2618:G:H5'	1.86	0.57
10:b:898:C:C2'	10:b:899:A:O5'	2.53	0.56
11:c:78:VAL:HG21	11:c:110:LEU:HD11	1.87	0.56
10:b:368:A:O2'	10:b:369:U:O5'	2.22	0.56
2:l:29:ARG:NH2	27:t:11:LEU:O	2.38	0.56
10:b:2659:G:H2'	10:b:2660:A:H2'	1.88	0.56
14:f:57:LEU:HD23	14:f:65:PRO:HB3	1.87	0.56
10:b:933:A:H5'	10:b:934:U:OP2	2.06	0.56
12:d:46:ARG:NH1	12:d:85:ALA:O	2.39	0.56
22:o:56:LYS:O	22:o:59:ALA:N	2.39	0.56
31:v:1:G:H3'	31:v:2:G:H8	1.71	0.56
10:b:1384:A:H1'	10:b:1405:U:H1'	1.88	0.56
10:b:2324:U:H1'	10:b:2337:G:H5''	1.86	0.56
9:a:42:C:C4	14:f:66:LEU:HD21	2.41	0.56
14:f:126:GLY:O	14:f:158:THR:OG1	2.20	0.56
10:b:2751:G:H3'	10:b:2752:C:H6	1.70	0.56
5:4:32:GLU:OE2	5:4:32:GLU:N	2.28	0.55
10:b:866:A:H61	10:b:913:U:H1'	1.71	0.55
10:b:1469:A:H2'	10:b:1470:A:C8	2.42	0.55
15:g:22:GLN:NE2	15:g:38:ASN:O	2.40	0.55
15:g:9:VAL:HG12	15:g:50:LEU:HB2	1.87	0.55
10:b:898:C:H2'	10:b:899:A:O5'	2.06	0.55
10:b:2845:U:H2'	10:b:2846:G:C8	2.41	0.55
13:e:98:LYS:HB3	13:e:102:ARG:NH2	2.20	0.55
2:l:12:GLU:O	2:l:16:THR:HG23	2.07	0.55
2:l:44:LYS:O	2:l:48:ARG:HG2	2.06	0.55
10:b:2273:A:H2'	10:b:2274:A:C8	2.42	0.55
10:b:2829:A:C6	10:b:2830:C:C4	2.95	0.55
24:q:92:ARG:HG3	24:q:92:ARG:HH11	1.71	0.55
28:u:81:ASP:OD1	28:u:82:ARG:N	2.40	0.55
30:y:77:ARG:HG3	30:y:77:ARG:HH11	1.70	0.55
9:a:87:U:O2'	9:a:88:C:O5'	2.24	0.54
12:d:9:VAL:HG11	23:p:4:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:38:MET:HE2	14:f:57:LEU:HD13	1.89	0.54
16:h:6:LEU:HD13	16:h:36:ALA:HA	1.89	0.54
1:o:60:ASP:OD2	16:h:27:ARG:NH2	2.41	0.54
10:b:948:C:C4'	10:b:984:A:C2	2.89	0.54
10:b:1095:A:H5'	10:b:1096:A:H5''	1.89	0.54
22:o:88:LYS:NZ	22:o:116:GLN:HE22	2.05	0.54
26:s:4:ILE:HG13	26:s:106:VAL:HG22	1.88	0.54
28:u:39:ILE:HG13	28:u:40:ASN:H	1.72	0.54
10:b:2074:U:H2'	10:b:2075:U:O4'	2.08	0.54
21:n:37:THR:OG1	21:n:40:LYS:HG3	2.08	0.54
10:b:874:G:C2'	10:b:875:G:C5'	2.85	0.54
1:o:72:ARG:NH1	1:o:78:TYR:OH	2.38	0.54
10:b:643:A:H2'	10:b:644:A:C5'	2.28	0.54
10:b:644:A:C8	10:b:644:A:C4'	2.91	0.54
10:b:2333:A:H4'	10:b:2334:U:H3'	1.89	0.54
5:4:5:ILE:HG21	5:4:28:ARG:NH2	2.23	0.54
8:8:14:CYS:SG	8:8:33:HIS:ND1	2.81	0.54
10:b:2086:U:H2'	10:b:2087:G:C8	2.43	0.54
13:e:97:ASN:HB2	13:e:100:MET:HG3	1.89	0.54
10:b:852:U:N3	10:b:853:C:C5	2.76	0.53
10:b:2233:U:H2'	10:b:2234:G:C8	2.43	0.53
17:j:99:ARG:HE	17:j:103:ILE:HG23	1.74	0.53
19:l:110:VAL:HB	19:l:127:VAL:HG22	1.90	0.53
10:b:720:U:H2'	10:b:721:A:C8	2.43	0.53
11:c:240:PHE:O	11:c:242:LYS:HE3	2.09	0.53
19:l:141:LYS:NZ	19:l:143:GLU:OE2	2.42	0.53
13:e:191:ASP:OD1	13:e:192:ALA:N	2.42	0.53
11:c:201:MET:HG3	11:c:202:LEU:HD23	1.89	0.53
10:b:605:G:H1'	10:b:657:U:O2'	2.09	0.53
10:b:2547:G:H1	10:b:2561:U:H3	1.57	0.53
14:f:37:ASN:OD1	14:f:38:MET:N	2.42	0.53
18:k:121:GLU:HG2	18:k:122:VAL:HG23	1.89	0.53
4:3:4:GLN:HA	10:b:2615:U:C2	2.43	0.53
10:b:2575:C:H5'	12:d:149:ASN:HD22	1.73	0.53
11:c:95:LEU:HD13	11:c:101:ARG:HG3	1.89	0.53
11:c:141:VAL:HG12	11:c:192:LEU:HD23	1.91	0.53
14:f:80:ARG:HB3	14:f:83:TYR:CZ	2.43	0.53
26:s:83:LYS:HB3	26:s:95:ARG:HD2	1.91	0.53
28:u:66:GLN:HB2	28:u:69:ASN:OD1	2.08	0.53
11:c:182:ARG:NH2	11:c:266:PHE:HB3	2.24	0.53
12:d:156:PHE:CE1	17:j:81:ILE:HD13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:55:ARG:HB2	15:g:58:TYR:HD2	1.73	0.53
15:g:69:ARG:NH1	15:g:73:ASN:HB2	2.24	0.53
21:n:57:THR:HG23	21:n:62:ASN:ND2	2.23	0.53
17:j:31:GLU:HG2	17:j:142:ILE:HD12	1.92	0.52
18:k:121:GLU:OE1	23:p:65:SER:OG	2.26	0.52
10:b:850:U:H2'	10:b:851:C:C6	2.43	0.52
10:b:1752:C:H2'	10:b:1753:G:C8	2.44	0.52
10:b:1964:G:C4'	10:b:1965:C:OP2	2.58	0.52
11:c:258:ARG:HD3	11:c:270:ARG:NH1	2.24	0.52
14:f:50:LEU:HD21	14:f:67:ILE:HG23	1.92	0.52
15:g:67:THR:O	15:g:71:LEU:HG	2.10	0.52
10:b:2618:G:H21	12:d:155:VAL:HG21	1.75	0.52
4:3:46:ASP:O	4:3:53:LYS:NZ	2.41	0.52
10:b:2010:G:H5''	26:s:42:LYS:HB2	1.92	0.52
10:b:1000:A:H2'	10:b:1001:A:C8	2.45	0.51
10:b:2663:G:C6	10:b:2664:G:C5	2.98	0.51
28:u:5:ILE:C	28:u:6:ARG:HD2	2.36	0.51
4:3:40:ARG:HG3	4:3:41:HIS:CE1	2.46	0.51
5:4:38:LYS:HB2	5:4:49:TYR:CD2	2.45	0.51
10:b:1047:G:HO2'	10:b:1048:A:H8	1.57	0.51
10:b:2125:G:H2'	10:b:2126:A:H4'	1.91	0.51
13:e:47:LYS:HG3	13:e:51:GLU:HB2	1.93	0.51
14:f:49:LEU:HA	14:f:52:ASN:HD22	1.75	0.51
15:g:84:THR:HG22	15:g:134:LYS:HG2	1.93	0.51
22:o:94:ARG:HD2	22:o:97:PHE:O	2.10	0.51
23:p:72:ARG:HD2	23:p:74:PHE:CZ	2.44	0.51
1:0:12:PRO:HG2	1:0:28:ARG:HH21	1.76	0.51
10:b:29:U:H2'	10:b:30:G:C8	2.45	0.51
10:b:1490:A:H62	11:c:97:LYS:HG2	1.76	0.51
12:d:37:VAL:HG22	12:d:48:ILE:HG22	1.92	0.51
10:b:2601:C:O2'	10:b:2602:A:P	2.68	0.51
10:b:28:A:H61	10:b:512:G:H1'	1.76	0.51
10:b:2291:U:H2'	10:b:2292:U:C6	2.46	0.51
24:q:88:VAL:HA	25:r:49:ILE:HD12	1.91	0.51
21:n:41:ALA:HB1	21:n:97:ILE:HD13	1.92	0.51
21:n:103:ARG:HB2	21:n:110:MET:HE3	1.93	0.51
10:b:2663:G:C4	10:b:2664:G:C8	2.99	0.51
10:b:367:G:C2'	10:b:368:A:H5'	2.41	0.51
10:b:612:G:N2	10:b:617:G:O6	2.43	0.51
10:b:1047:G:O2'	10:b:1048:A:C8	2.61	0.51
10:b:1311:G:H21	10:b:1603:A:H62	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2783:U:H2'	10:b:2784:U:H6	1.70	0.51
5:4:27:LYS:NZ	5:4:53:LYS:O	2.34	0.50
14:f:85:ILE:HG13	14:f:86:GLY:N	2.26	0.50
18:k:14:SER:OG	18:k:86:LEU:HD12	2.11	0.50
30:y:43:THR:C	30:y:45:PHE:N	2.69	0.50
10:b:1408:G:H1	10:b:1594:U:H3	1.58	0.50
16:h:6:LEU:HD11	16:h:37:VAL:HG22	1.92	0.50
10:b:1802:A:H2'	10:b:1803:A:C8	2.46	0.50
28:u:82:ARG:HH21	28:u:82:ARG:HG3	1.77	0.50
10:b:853:C:H2'	10:b:853:C:O2	2.11	0.50
10:b:854:C:H2'	10:b:854:C:O2	2.12	0.50
10:b:2886:A:H3'	10:b:2887:A:H8	1.75	0.50
14:f:62:GLY:HA3	14:f:95:ARG:NH2	2.26	0.50
16:h:26:ALA:O	16:h:27:ARG:HG2	2.12	0.50
24:q:11:ARG:O	24:q:15:LYS:HG2	2.11	0.50
26:s:95:ARG:HH11	32:z:150:LEU:HB2	1.77	0.50
28:u:96:PHE:CE1	28:u:103:ILE:HG12	2.46	0.50
10:b:1884:G:H5''	10:b:1884:G:H8	1.77	0.50
10:b:2764:A:N6	10:b:2766:A:C6	2.79	0.50
11:c:6:CYS:SG	11:c:13:ARG:NH2	2.84	0.50
10:b:2756:U:H1'	10:b:2757:A:H5''	1.94	0.50
20:m:20:LEU:HD13	29:w:81:PRO:HG2	1.94	0.50
10:b:612:G:N2	10:b:617:G:C5	2.80	0.50
28:u:16:GLY:O	28:u:17:LYS:HG3	2.11	0.50
10:b:1028:A:H2'	10:b:1029:A:C8	2.46	0.50
10:b:1721:G:H2'	10:b:1738:G:H22	1.77	0.50
10:b:2312:U:H5'	14:f:85:ILE:HD11	1.94	0.49
10:b:2339:C:H2'	10:b:2340:A:C8	2.47	0.49
12:d:34:VAL:HG12	12:d:92:VAL:HA	1.93	0.49
26:s:73:LYS:HB2	26:s:106:VAL:HB	1.94	0.49
30:y:26:PHE:N	30:y:29:GLU:HG3	2.26	0.49
3:2:12:SER:OG	3:2:14:ILE:HG12	2.13	0.49
9:a:45:A:C4	9:a:46:A:C8	3.00	0.49
10:b:373:U:H2'	10:b:374:A:C8	2.46	0.49
10:b:2151:U:H5''	10:b:2152:G:H8	1.76	0.49
20:m:42:THR:OG1	20:m:45:GLN:HG2	2.12	0.49
23:p:13:MET:HE2	23:p:55:LEU:N	2.28	0.49
27:t:54:GLU:HG2	27:t:88:LYS:HB2	1.94	0.49
10:b:639:U:H2'	10:b:640:C:C6	2.47	0.49
2:1:54:LYS:HA	2:1:57:LEU:HB2	1.94	0.49
5:4:40:ASP:HB3	5:4:43:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1265:A:H61	10:b:2013:A:H3'	1.76	0.49
21:n:41:ALA:O	21:n:42:LYS:HB2	2.11	0.49
28:u:4:LYS:O	28:u:5:ILE:HD13	2.13	0.49
10:b:965:C:H4'	10:b:2273:A:H1'	1.94	0.49
10:b:1174:U:H5''	10:b:1175:A:H8	1.77	0.49
10:b:2241:A:H2'	10:b:2242:G:C8	2.48	0.49
10:b:1339:G:H5''	27:t:19:LYS:HD3	1.95	0.49
10:b:2408:U:H2'	10:b:2409:G:C8	2.48	0.49
11:c:29:PRO:HG2	11:c:34:LEU:HD11	1.92	0.49
13:e:3:LEU:HD12	13:e:14:VAL:HG11	1.95	0.49
14:f:13:VAL:O	14:f:17:MET:HG2	2.13	0.49
20:m:42:THR:HG22	20:m:93:VAL:HG12	1.95	0.49
10:b:589:U:H2'	10:b:590:A:C8	2.47	0.49
10:b:1061:U:H1'	10:b:1068:G:H1'	1.95	0.49
18:k:105:ARG:O	18:k:108:ARG:HG3	2.12	0.49
31:v:21:A:H62	31:v:47:U:H5'	1.78	0.49
10:b:853:C:C2	10:b:854:C:C5	3.01	0.49
10:b:2840:C:H2'	10:b:2841:C:C6	2.48	0.49
16:h:7:ASP:OD1	16:h:8:LYS:N	2.46	0.49
16:h:8:LYS:NZ	16:h:14:SER:HA	2.27	0.49
19:l:85:VAL:HG21	19:l:90:VAL:HA	1.94	0.49
20:m:75:GLU:HB2	20:m:90:GLU:HG3	1.94	0.49
17:j:6:ALA:HB3	17:j:48:VAL:HG11	1.94	0.49
4:3:43:ILE:HD11	21:n:98:LEU:HB3	1.95	0.48
10:b:558:U:H2'	10:b:559:G:H8	1.77	0.48
10:b:1483:G:H1	10:b:1506:U:H3	1.60	0.48
5:4:38:LYS:HB2	5:4:49:TYR:CE2	2.47	0.48
10:b:184:C:H2'	10:b:185:G:C8	2.48	0.48
10:b:184:C:H2'	10:b:185:G:H8	1.78	0.48
10:b:1664:A:H2	18:k:1:MET:HE1	1.78	0.48
14:f:9:LYS:HB2	14:f:9:LYS:HE2	1.59	0.48
20:m:47:GLU:OE2	20:m:51:ARG:NH1	2.46	0.48
10:b:27:G:H22	10:b:512:G:H2'	1.79	0.48
10:b:1429:G:H2'	10:b:1430:G:C8	2.48	0.48
10:b:1927:A:H2'	10:b:1928:A:C8	2.48	0.48
10:b:2458:G:H8	10:b:2459:A:H62	1.62	0.48
10:b:2543:G:H21	10:b:2646:C:C5'	2.25	0.48
21:n:72:ASP:OD2	21:n:75:ILE:HG12	2.13	0.48
26:s:14:ALA:O	26:s:18:ARG:HG3	2.14	0.48
10:b:1818:U:H5''	11:c:157:SER:HB2	1.94	0.48
10:b:2305:U:H5''	14:f:131:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2543:G:N2	10:b:2646:C:H5''	2.28	0.48
14:f:5:HIS:HB2	14:f:97:TRP:CD1	2.48	0.48
15:g:2:SER:HB2	15:g:62:TRP:HB3	1.96	0.48
10:b:871:U:H2'	10:b:872:U:C6	2.49	0.48
10:b:875:G:H3'	10:b:875:G:C8	2.49	0.48
10:b:2061:G:H5'	10:b:2502:G:H5'	1.96	0.48
10:b:2515:C:H2'	10:b:2516:A:H8	1.78	0.48
10:b:1021:A:H2'	10:b:1022:G:H4'	1.95	0.48
10:b:1326:U:H2'	10:b:1327:A:H8	1.78	0.48
10:b:2432:A:H2'	10:b:2433:A:C8	2.48	0.48
22:o:34:HIS:CE1	22:o:54:VAL:HA	2.49	0.48
17:j:74:TYR:CE1	17:j:103:ILE:HD11	2.48	0.48
10:b:856:G:H2'	10:b:857:G:C8	2.49	0.48
10:b:2829:A:C5	10:b:2830:C:C5	3.01	0.48
31:v:1:G:H1	31:v:72:G:H22	1.61	0.48
10:b:151:C:H2'	10:b:152:A:C8	2.49	0.47
10:b:358:U:H2'	10:b:359:G:C8	2.49	0.47
10:b:368:A:O2'	10:b:369:U:C5'	2.63	0.47
10:b:1056:G:H1'	10:b:1086:A:H62	1.78	0.47
10:b:1991:U:H2'	10:b:1992:G:C5'	2.43	0.47
10:b:2497:A:H1'	10:b:2498:C:H5	1.80	0.47
10:b:437:U:H2'	10:b:438:G:C8	2.49	0.47
10:b:2008:C:H2'	10:b:2009:A:C8	2.49	0.47
10:b:2335:A:H5'	22:o:13:ARG:HH12	1.78	0.47
30:y:37:ILE:HG21	30:y:80:ILE:HG21	1.94	0.47
10:b:585:G:N7	24:q:6:ARG:NH1	2.62	0.47
10:b:2173:A:H5''	10:b:2174:C:H5	1.80	0.47
10:b:2308:G:H2'	10:b:2310:C:H5	1.80	0.47
13:e:118:LEU:HD11	13:e:188:MET:HE3	1.96	0.47
10:b:852:U:N3	10:b:853:C:C4	2.82	0.47
15:g:24:ILE:HD13	15:g:72:LEU:HD11	1.96	0.47
10:b:903:C:H4'	10:b:903:C:OP1	2.14	0.47
14:f:30:ARG:H	14:f:159:THR:HB	1.79	0.47
17:j:9:GLU:HG2	17:j:10:THR:HG23	1.96	0.47
18:k:88:ASN:HB3	18:k:91:SER:O	2.14	0.47
24:q:58:ARG:HA	24:q:61:TRP:CE3	2.50	0.47
4:3:52:ARG:CZ	4:3:54:VAL:HG12	2.45	0.47
11:c:222:GLY:O	11:c:225:MET:HG3	2.15	0.47
2:1:56:LEU:HA	2:1:59:GLU:HG2	1.95	0.47
10:b:206:U:H2'	10:b:207:A:H8	1.79	0.47
10:b:272:A:C2	10:b:273:G:C5	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:38:MET:HE2	14:f:57:LEU:HB2	1.95	0.47
18:k:102:PRO:HD2	23:p:68:GLU:OE2	2.14	0.47
19:l:77:ILE:HD12	19:l:108:ALA:HB1	1.96	0.47
10:b:2331:G:H4'	30:y:43:THR:H	1.79	0.47
18:k:102:PRO:HD3	23:p:66:ASN:HB2	1.97	0.47
3:2:41:THR:HG22	3:2:43:ALA:H	1.79	0.47
10:b:1469:A:H2'	10:b:1470:A:H8	1.79	0.47
17:j:77:HIS:CE1	17:j:83:GLY:HA3	2.50	0.47
30:y:26:PHE:H	30:y:29:GLU:HG3	1.79	0.47
30:y:68:LYS:HD2	30:y:83:GLU:OE2	2.13	0.47
10:b:850:U:H3'	10:b:851:C:C5	2.50	0.47
10:b:459:U:H2'	10:b:460:A:H8	1.80	0.46
10:b:669:G:N3	10:b:669:G:C2'	2.77	0.46
10:b:839:U:H3	10:b:939:G:H1	1.63	0.46
18:k:71:ARG:HA	18:k:71:ARG:HD3	1.67	0.46
30:y:25:ARG:HH11	30:y:31:VAL:HG12	1.78	0.46
14:f:8:TYR:HB2	14:f:173:PHE:HZ	1.79	0.46
10:b:513:A:H2	10:b:582:A:H4'	1.79	0.46
9:a:42:C:C5	14:f:66:LEU:HD21	2.50	0.46
10:b:903:C:H2'	10:b:903:C:O2	2.15	0.46
27:t:1:MET:HB3	27:t:1:MET:HE3	1.70	0.46
10:b:1340:U:H4'	10:b:1394:U:H4'	1.97	0.46
21:n:8:ARG:HG3	21:n:43:GLU:OE2	2.15	0.46
24:q:97:ASP:OD2	25:r:13:ARG:NE	2.49	0.46
26:s:84:ARG:O	26:s:95:ARG:HD3	2.16	0.46
18:k:77:ILE:HG12	23:p:72:ARG:HE	1.80	0.46
4:3:43:ILE:HD13	4:3:49:TYR:HB2	1.98	0.46
10:b:848:C:H2'	10:b:849:A:C8	2.51	0.46
10:b:1716:U:H2'	10:b:1717:A:H8	1.80	0.46
10:b:2346:A:H3'	10:b:2347:C:H5''	1.97	0.46
12:d:184:ARG:NH2	23:p:11:GLU:OE1	2.34	0.46
14:f:44:ILE:HD12	14:f:78:LYS:HB2	1.98	0.46
13:e:5:LEU:HD13	13:e:10:SER:O	2.15	0.46
18:k:34:GLY:N	18:k:37:ASP:OD2	2.45	0.46
10:b:580:U:H2'	10:b:581:C:C6	2.50	0.46
10:b:1076:C:H2'	10:b:1077:A:C8	2.51	0.46
10:b:1923:U:H4'	31:v:24:G:H21	1.81	0.46
10:b:414:C:H2'	10:b:415:A:C8	2.50	0.45
10:b:482:A:H5''	28:u:45:HIS:HB2	1.96	0.45
10:b:581:C:H2'	10:b:582:A:H8	1.79	0.45
10:b:2657:A:O2'	10:b:2658:C:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:5:LEU:HD11	16:h:13:GLY:HA2	1.98	0.45
29:w:35:GLU:OE1	29:w:35:GLU:N	2.44	0.45
10:b:82:U:H5''	10:b:296:U:H5'	1.98	0.45
10:b:368:A:O2'	10:b:369:U:H5'	2.17	0.45
10:b:643:A:H3'	10:b:644:A:H5''	1.94	0.45
10:b:741:U:H2'	10:b:742:A:C8	2.52	0.45
10:b:891:G:O2'	10:b:893:C:N4	2.49	0.45
10:b:1689:A:H2'	10:b:1690:A:C8	2.51	0.45
10:b:1996:C:O2	10:b:1997:C:H1'	2.16	0.45
10:b:2208:C:H2'	10:b:2209:G:C8	2.51	0.45
1:0:43:GLU:HB3	1:0:45:ARG:HG2	1.98	0.45
5:4:34:LEU:HB3	5:4:52:ALA:HB2	1.98	0.45
10:b:222:A:H3'	10:b:421:C:H5'	1.97	0.45
10:b:1035:U:O2	10:b:1035:U:H2'	2.17	0.45
28:u:48:PRO:HB3	28:u:55:PRO:O	2.15	0.45
10:b:657:U:H2'	10:b:658:U:C6	2.51	0.45
10:b:2765:A:N3	10:b:2765:A:H2'	2.31	0.45
10:b:2830:C:H3'	12:d:59:ARG:HH11	1.82	0.45
18:k:43:ILE:HD12	18:k:56:ASP:HB2	1.99	0.45
26:s:45:VAL:O	26:s:49:LYS:HG2	2.16	0.45
9:a:48:U:H2'	9:a:49:C:C6	2.52	0.45
10:b:1026:G:H2'	10:b:1027:A:C8	2.51	0.45
10:b:1493:C:H3'	10:b:1494:A:H8	1.81	0.45
16:h:26:ALA:C	16:h:28:ASN:H	2.23	0.45
18:k:91:SER:O	18:k:93:GLN:N	2.48	0.45
23:p:31:TRP:CE3	23:p:38:LYS:HG2	2.51	0.45
31:v:1:G:H22	31:v:72:G:H22	1.65	0.45
2:1:12:GLU:HG2	2:1:13:GLU:N	2.30	0.45
13:e:155:GLU:O	13:e:159:LEU:HG	2.17	0.45
16:h:29:PHE:O	16:h:33:GLN:HG2	2.17	0.45
22:o:88:LYS:HZ2	22:o:116:GLN:HE22	1.65	0.45
9:a:8:C:H5''	22:o:15:ARG:HH12	1.82	0.45
10:b:948:C:H2'	10:b:949:G:C8	2.51	0.45
10:b:2134:A:H1'	10:b:2161:C:H5'	1.98	0.45
12:d:35:THR:HG22	12:d:73:VAL:HG21	1.99	0.45
17:j:110:PRO:O	17:j:115:GLY:HA3	2.17	0.45
12:d:47:ALA:HA	12:d:84:LEU:HD13	1.99	0.45
15:g:45:HIS:HA	15:g:50:LEU:HD23	1.99	0.45
17:j:60:ASP:HB3	17:j:97:PRO:HB3	1.98	0.45
18:k:2:ILE:HD12	18:k:8:LEU:HD21	1.99	0.45
19:l:23:ILE:HG12	25:r:82:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:41:ALA:C	21:n:43:GLU:H	2.25	0.45
28:u:54:GLN:CD	28:u:56:GLY:H	2.24	0.45
1:0:66:THR:O	1:0:70:GLU:HG3	2.17	0.45
6:6:7:PRO:HB2	10:b:1309:G:H4'	1.99	0.45
10:b:581:C:OP1	24:q:33:ARG:HG3	2.16	0.45
10:b:1683:U:H2'	10:b:1684:G:C8	2.52	0.45
10:b:2789:C:H2'	10:b:2893:A:N7	2.31	0.45
11:c:145:GLU:HG2	11:c:151:GLY:C	2.42	0.45
4:3:38:HIS:ND1	4:3:39:LEU:O	2.41	0.44
8:8:33:HIS:O	8:8:35:GLN:HG3	2.17	0.44
10:b:2331:G:H21	10:b:2336:A:H8	1.66	0.44
11:c:44:ASN:OD1	11:c:46:ASN:N	2.49	0.44
14:f:134:GLU:HG2	14:f:149:VAL:HB	2.00	0.44
10:b:1394:U:H5'	10:b:1603:A:H4'	1.99	0.44
28:u:74:ASN:HA	28:u:96:PHE:CE2	2.52	0.44
30:y:70:GLU:CD	30:y:72:LYS:HE2	2.43	0.44
10:b:106:C:H2'	10:b:107:G:H8	1.82	0.44
10:b:371:A:H61	10:b:401:A:H3'	1.83	0.44
10:b:2428:G:H5''	10:b:2429:G:H5'	1.98	0.44
18:k:41:ILE:HD11	18:k:86:LEU:CD2	2.48	0.44
24:q:7:GLY:O	24:q:11:ARG:HG2	2.18	0.44
4:3:5:GLN:NE2	10:b:2056:G:H4'	2.33	0.44
10:b:488:G:H4'	26:s:49:LYS:HE3	1.99	0.44
10:b:593:U:H3	10:b:664:G:H1	1.65	0.44
10:b:2096:C:H2'	10:b:2097:A:C8	2.53	0.44
12:d:151:THR:HB	12:d:152:PRO:HD3	1.99	0.44
10:b:2327:A:H2'	10:b:2328:A:C8	2.53	0.44
10:b:2788:C:H2'	10:b:2789:C:C6	2.52	0.44
15:g:18:LYS:NZ	15:g:20:ASN:OD1	2.51	0.44
10:b:829:A:N7	10:b:2248:C:H5'	2.32	0.44
15:g:3:ARG:HA	15:g:6:LYS:HG2	2.00	0.44
15:g:12:PRO:HD2	15:g:15:VAL:HG11	1.99	0.44
16:h:18:GLN:HE22	16:h:39:ALA:HB2	1.82	0.44
10:b:1306:C:H5''	10:b:1606:C:N4	2.33	0.44
10:b:2036:C:H2'	10:b:2037:A:H8	1.82	0.44
14:f:4:LEU:HD13	14:f:101:GLU:HB2	1.98	0.44
18:k:109:SER:C	18:k:111:LYS:H	2.24	0.44
3:2:47:MET:HE3	10:b:850:U:O2'	2.17	0.44
10:b:167:A:H2	10:b:2209:G:H4'	1.82	0.44
10:b:832:U:H2'	10:b:833:A:C8	2.53	0.44
10:b:875:G:C8	10:b:875:G:C3'	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:m:41:LEU:HA	20:m:45:GLN:NE2	2.29	0.44
23:p:100:LEU:HD11	23:p:110:ILE:HD11	2.00	0.44
9:a:106:G:H2'	9:a:107:G:O4'	2.18	0.44
10:b:521:U:H2'	10:b:522:A:C8	2.53	0.44
27:t:69:ARG:HG2	27:t:74:ILE:HD13	1.99	0.44
14:f:29:PRO:HB2	14:f:169:LEU:HD22	2.01	0.43
19:l:19:LEU:HD12	19:l:27:LEU:HD13	2.00	0.43
22:o:4:LYS:O	22:o:8:ILE:HG12	2.18	0.43
10:b:767:U:H2'	10:b:768:G:H8	1.84	0.43
10:b:2313:C:H2'	10:b:2314:A:C8	2.52	0.43
10:b:2810:A:H5''	12:d:62:LYS:NZ	2.32	0.43
11:c:100:GLU:OE2	11:c:102:ARG:NE	2.48	0.43
14:f:70:ALA:O	14:f:72:LYS:N	2.52	0.43
10:b:751:A:H5'	26:s:90:LYS:HA	2.00	0.43
10:b:813:U:H2'	10:b:814:C:C6	2.53	0.43
10:b:885:C:H2'	10:b:886:A:C8	2.54	0.43
10:b:1013:C:H2'	10:b:1014:A:H8	1.83	0.43
10:b:1426:G:H2'	10:b:1427:A:C8	2.52	0.43
10:b:1924:C:H4'	31:v:13:A:H4'	1.99	0.43
13:e:189:THR:O	13:e:193:VAL:HG23	2.17	0.43
14:f:123:ASP:OD2	14:f:127:ASN:HB2	2.18	0.43
10:b:1490:A:H8	11:c:98:ASP:HB3	1.83	0.43
10:b:1508:A:H5'	10:b:1509:A:C4	2.54	0.43
14:f:16:LEU:HD22	14:f:20:PHE:HE2	1.84	0.43
14:f:134:GLU:CD	14:f:136:ILE:H	2.26	0.43
3:2:12:SER:HB2	3:2:32:ILE:HD11	2.00	0.43
10:b:222:A:H61	10:b:232:G:H1'	1.83	0.43
10:b:1869:G:H22	10:b:1872:A:H1'	1.83	0.43
10:b:2601:C:HO2'	10:b:2602:A:P	2.40	0.43
11:c:107:PRO:HD2	11:c:110:LEU:HD22	2.00	0.43
12:d:9:VAL:HG21	23:p:4:ILE:HD11	2.00	0.43
10:b:851:C:H2'	10:b:852:U:H5'	1.92	0.43
15:g:24:ILE:HD12	15:g:43:VAL:HG21	2.01	0.43
22:o:83:LEU:HD23	22:o:83:LEU:HA	1.76	0.43
26:s:11:ARG:HA	26:s:11:ARG:HD2	1.89	0.43
10:b:1494:A:HO2'	10:b:1495:A:H8	1.63	0.43
10:b:1700:A:H3'	10:b:1701:A:H8	1.83	0.43
10:b:1915:U:H3'	10:b:1916:A:H8	1.84	0.43
15:g:86:LYS:HG2	15:g:132:VAL:HG22	2.01	0.43
17:j:13:ARG:NH1	17:j:49:ASP:O	2.52	0.43
10:b:576:U:H2'	10:b:577:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2233:U:H2'	10:b:2234:G:H8	1.81	0.43
13:e:46:GLN:HB2	13:e:86:ALA:HB1	1.99	0.43
10:b:874:G:O2'	10:b:875:G:C5'	2.66	0.43
10:b:911:A:C8	20:m:9:PHE:CE2	3.07	0.43
10:b:2765:A:N3	10:b:2765:A:C2'	2.82	0.43
14:f:70:ALA:C	14:f:72:LYS:H	2.27	0.43
17:j:60:ASP:OD1	17:j:60:ASP:N	2.35	0.43
22:o:82:ALA:HB1	22:o:87:ILE:HB	2.01	0.43
5:4:37:LYS:HG2	5:4:48:ILE:HD13	2.00	0.43
10:b:588:U:H2'	10:b:589:U:C6	2.54	0.43
10:b:1381:G:H3'	10:b:1382:G:H21	1.83	0.43
10:b:2114:A:H5''	10:b:2146:C:H41	1.84	0.43
18:k:35:VAL:HG11	18:k:104:THR:HG21	2.00	0.43
10:b:1047:G:O2'	10:b:1048:A:H8	2.00	0.42
10:b:2313:C:H5''	14:f:88:LYS:HD3	2.01	0.42
15:g:5:ALA:HB2	15:g:66:GLY:HA2	2.00	0.42
30:y:77:ARG:HG3	30:y:77:ARG:NH1	2.34	0.42
9:a:49:C:H2'	9:a:50:A:C8	2.54	0.42
10:b:222:A:N6	10:b:232:G:H1'	2.35	0.42
10:b:272:A:N1	10:b:273:G:C6	2.87	0.42
10:b:611:C:O2'	10:b:612:G:H5'	2.19	0.42
18:k:35:VAL:HG11	18:k:104:THR:CG2	2.49	0.42
21:n:96:ARG:O	21:n:113:ILE:HA	2.19	0.42
1:0:32:ASN:HB2	10:b:397:U:H5''	2.01	0.42
3:2:11:ARG:HB2	3:2:54:MET:HB2	2.01	0.42
10:b:1004:U:H2'	10:b:1011:G:H2'	2.02	0.42
10:b:1792:G:H5'	11:c:204:VAL:HG13	2.00	0.42
10:b:2099:U:H3	10:b:2190:G:H1	1.65	0.42
10:b:2863:C:H2'	10:b:2864:G:C8	2.54	0.42
10:b:608:A:H2'	10:b:609:A:C8	2.54	0.42
10:b:2075:U:H1'	10:b:2597:G:H21	1.84	0.42
12:d:9:VAL:HG12	23:p:5:ILE:HD11	2.02	0.42
14:f:106:ILE:HG21	14:f:139:PRO:HG3	2.02	0.42
17:j:98:GLU:H	17:j:98:GLU:CD	2.26	0.42
32:z:165:GLY:O	32:z:166:PRO:C	2.62	0.42
10:b:351:C:H2'	10:b:352:A:C8	2.55	0.42
10:b:1013:C:H2'	10:b:1014:A:C8	2.55	0.42
10:b:1049:C:H1'	10:b:1113:U:H4'	2.02	0.42
9:a:50:A:H5''	22:o:67:ASN:HD21	1.85	0.42
10:b:220:G:H1'	10:b:234:U:H1'	2.01	0.42
10:b:318:C:H2'	10:b:319:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1432:G:H2'	10:b:1433:A:C8	2.55	0.42
10:b:2261:C:C5	30:y:16:SER:HB3	2.55	0.42
12:d:25:THR:HG21	12:d:193:VAL:HG22	2.01	0.42
12:d:184:ARG:NH2	23:p:7:GLN:OE1	2.53	0.42
13:e:191:ASP:O	13:e:195:GLN:HG3	2.19	0.42
22:o:24:THR:HG23	22:o:90:VAL:HG12	2.02	0.42
10:b:696:G:H1	10:b:766:U:H3	1.67	0.42
10:b:2605:U:H2'	10:b:2606:C:C6	2.54	0.42
21:n:12:ARG:HD3	21:n:16:HIS:HD2	1.78	0.42
23:p:100:LEU:HD23	23:p:100:LEU:HA	1.84	0.42
10:b:302:C:H2'	10:b:303:G:C8	2.54	0.42
10:b:367:G:H2'	10:b:368:A:H5'	2.02	0.42
10:b:1054:A:H1'	10:b:1106:G:H22	1.85	0.42
10:b:1704:C:H2'	10:b:1705:A:C8	2.55	0.42
10:b:1884:G:H5''	10:b:1884:G:C8	2.53	0.42
10:b:2751:G:H3'	10:b:2752:C:C6	2.50	0.42
28:u:81:ASP:OD2	28:u:96:PHE:HB3	2.20	0.42
1:0:56:MET:HG2	16:h:27:ARG:NH2	2.35	0.42
2:1:5:GLU:H	2:1:5:GLU:CD	2.27	0.42
10:b:49:A:H61	10:b:177:G:H2'	1.85	0.42
31:v:62:C:H2'	31:v:63:U:C6	2.55	0.42
10:b:729:G:C6	11:c:207:LYS:HB2	2.55	0.42
24:q:92:ARG:HG3	24:q:92:ARG:NH1	2.34	0.42
28:u:86:ARG:HG2	28:u:95:PHE:CD1	2.55	0.42
10:b:107:G:H21	10:b:346:A:H62	1.68	0.41
10:b:109:C:H5'	10:b:348:A:H4'	2.02	0.41
10:b:528:A:H8	17:j:116:ARG:NH2	2.17	0.41
10:b:2302:U:H2'	10:b:2303:G:C8	2.55	0.41
10:b:2739:U:H5''	10:b:2763:G:O6	2.20	0.41
10:b:2809:A:H2'	10:b:2810:A:C8	2.55	0.41
14:f:175:PHE:HA	14:f:176:PRO:HD3	1.87	0.41
18:k:64:ARG:HD2	18:k:79:PHE:CD2	2.55	0.41
29:w:80:HIS:CE1	29:w:83:LYS:HD2	2.55	0.41
31:v:48:C:H2'	31:v:59:A:H1'	2.02	0.41
9:a:70:C:H2'	9:a:71:C:H6	1.85	0.41
10:b:1972:G:H2'	10:b:1973:G:C8	2.55	0.41
13:e:4:VAL:HA	13:e:11:ALA:HA	2.02	0.41
10:b:181:A:H1'	10:b:435:C:H5'	2.02	0.41
10:b:281:C:H2'	10:b:282:A:H8	1.81	0.41
10:b:1744:A:H3'	10:b:1745:A:H8	1.84	0.41
10:b:2377:A:H2'	10:b:2378:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:122:GLU:OE1	13:e:122:GLU:N	2.47	0.41
15:g:87:LEU:HB2	15:g:131:ILE:HB	2.01	0.41
9:a:66:A:H4'	9:a:67:G:OP1	2.19	0.41
10:b:20:C:H2'	10:b:21:A:C8	2.55	0.41
10:b:128:C:H2'	10:b:129:C:C6	2.56	0.41
13:e:170:ARG:NH2	13:e:174:GLY:O	2.53	0.41
22:o:68:LYS:HB2	22:o:68:LYS:HE2	1.78	0.41
7:7:14:PHE:O	7:7:15:LYS:HD3	2.20	0.41
10:b:308:G:H2'	10:b:309:A:C8	2.56	0.41
10:b:2125:G:C6	10:b:2126:A:H1'	2.55	0.41
10:b:2173:A:H5''	10:b:2174:C:C5	2.55	0.41
10:b:2301:C:H2'	10:b:2302:U:C6	2.56	0.41
10:b:2678:C:H2'	10:b:2679:A:C8	2.55	0.41
10:b:2680:U:H2'	10:b:2681:C:C6	2.56	0.41
20:m:111:GLU:HG2	20:m:112:LEU:N	2.36	0.41
3:2:7:ILE:HD11	3:2:48:ILE:HD11	2.02	0.41
10:b:1069:A:C2	10:b:1095:A:H5''	2.54	0.41
19:l:131:ALA:O	19:l:135:ILE:HG13	2.21	0.41
2:1:14:LEU:HD23	2:1:14:LEU:HA	1.90	0.41
10:b:558:U:H2'	10:b:559:G:C8	2.54	0.41
10:b:1026:G:H2'	10:b:1027:A:H8	1.85	0.41
10:b:1060:U:H4'	10:b:1061:U:H4'	2.03	0.41
10:b:2116:G:H1'	10:b:2148:G:H21	1.85	0.41
13:e:171:ASP:C	13:e:173:THR:H	2.29	0.41
22:o:76:LYS:HG2	22:o:80:GLU:OE1	2.20	0.41
27:t:33:LYS:HG2	27:t:80:TRP:CZ3	2.56	0.41
28:u:6:ARG:N	28:u:9:ASP:OD2	2.39	0.41
30:y:7:GLY:HA3	31:v:2:G:H4'	2.03	0.41
10:b:1386:C:H2'	10:b:1387:A:C8	2.56	0.41
10:b:1808:A:H3'	10:b:1809:A:C8	2.56	0.41
10:b:1986:C:H2'	10:b:1987:A:O5'	2.20	0.41
10:b:2334:U:O2'	10:b:2335:A:H4'	2.20	0.41
10:b:2663:G:N2	10:b:2664:G:H1'	2.36	0.41
14:f:74:VAL:HB	14:f:79:ILE:HD11	2.03	0.41
26:s:99:ARG:HG2	26:s:99:ARG:HH11	1.85	0.41
28:u:7:ARG:NH1	28:u:27:ASN:HA	2.36	0.41
2:1:11:VAL:HG12	2:1:15:ASN:HD21	1.86	0.41
4:3:40:ARG:HH12	10:b:2884:U:H2'	1.86	0.41
7:7:8:ARG:HA	7:7:8:ARG:HD2	1.90	0.41
10:b:1083:U:H2'	10:b:1084:A:H2'	2.02	0.41
10:b:1364:G:H5'	10:b:1809:A:H1'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1965:C:H2'	10:b:1966:A:C8	2.56	0.41
10:b:2300:C:H2'	10:b:2301:C:C6	2.56	0.41
10:b:2507:C:H2'	10:b:2508:G:C8	2.56	0.41
10:b:2597:G:H5'	11:c:241:GLY:HA3	2.03	0.41
10:b:2696:U:H2'	10:b:2697:G:C8	2.56	0.41
11:c:142:HIS:ND1	11:c:193:GLY:O	2.29	0.41
14:f:38:MET:CE	14:f:57:LEU:HB2	2.51	0.41
22:o:11:ALA:HB1	22:o:15:ARG:HE	1.85	0.41
23:p:27:GLU:OE1	23:p:29:LYS:HE3	2.21	0.41
26:s:85:ILE:HD11	32:z:149:GLU:O	2.21	0.41
29:w:48:MET:O	29:w:51:GLN:NE2	2.47	0.41
2:1:12:GLU:HA	2:1:15:ASN:HD22	1.86	0.41
10:b:1998:A:C2'	10:b:1999:C:O5'	2.69	0.41
12:d:19:GLY:HA2	23:p:79:PRO:HG2	2.03	0.41
13:e:142:ALA:O	13:e:143:LEU:HD23	2.20	0.41
14:f:8:TYR:HB2	14:f:173:PHE:CZ	2.56	0.41
14:f:26:MET:HB3	14:f:26:MET:HE2	1.86	0.41
21:n:12:ARG:CD	21:n:16:HIS:CD2	3.02	0.41
27:t:6:ARG:O	27:t:10:VAL:HG13	2.20	0.41
31:v:23:C:H2'	31:v:24:G:C8	2.55	0.41
10:b:1938:A:C6	10:b:2590:A:H1'	2.56	0.40
10:b:2783:U:H2'	10:b:2784:U:C5	2.55	0.40
10:b:2829:A:H2'	10:b:2830:C:O4'	2.20	0.40
14:f:14:LYS:HE3	14:f:14:LYS:HB3	1.95	0.40
17:j:45:THR:HB	17:j:48:VAL:CG1	2.51	0.40
21:n:56:LYS:HE2	21:n:87:PHE:O	2.21	0.40
29:w:43:ASP:OD1	29:w:43:ASP:C	2.64	0.40
10:b:1366:A:H3'	10:b:1367:A:H8	1.86	0.40
10:b:1600:C:H2'	10:b:1601:G:C8	2.56	0.40
10:b:2824:C:H2'	10:b:2825:G:O4'	2.20	0.40
15:g:148:LEU:HD23	15:g:148:LEU:HA	1.93	0.40
17:j:31:GLU:CG	17:j:142:ILE:HD12	2.51	0.40
27:t:2:ILE:H	27:t:2:ILE:HG12	1.53	0.40
4:3:50:ARG:O	4:3:50:ARG:HG2	2.21	0.40
10:b:84:A:H5''	28:u:6:ARG:HG3	2.03	0.40
10:b:360:U:H2'	10:b:361:G:C4	2.56	0.40
10:b:1188:U:H2'	10:b:1189:A:H8	1.85	0.40
10:b:1518:C:H2'	10:b:1519:G:C8	2.57	0.40
13:e:155:GLU:HG2	13:e:156:ASN:N	2.35	0.40
18:k:7:MET:SD	18:k:20:MET:HB2	2.61	0.40
10:b:1161:C:H2'	10:b:1162:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2036:C:H2'	10:b:2037:A:C8	2.56	0.40
11:c:44:ASN:OD1	11:c:44:ASN:C	2.64	0.40
13:e:16:GLU:HA	13:e:16:GLU:OE1	2.21	0.40
13:e:23:PHE:HE1	13:e:28:VAL:HG21	1.87	0.40
14:f:70:ALA:O	14:f:71:ARG:HG2	2.20	0.40
29:w:58:SER:O	29:w:73:LYS:NZ	2.54	0.40
9:a:24:G:N7	9:a:56:G:H2'	2.37	0.40
9:a:35:C:H2'	9:a:36:C:O4'	2.22	0.40
10:b:1447:C:H2'	10:b:1448:G:C8	2.56	0.40
10:b:2115:G:N2	10:b:2119:A:H62	2.18	0.40
15:g:19:ILE:HG22	15:g:21:GLY:H	1.86	0.40
17:j:32:LEU:HD22	17:j:54:ILE:HG21	2.03	0.40
24:q:49:ASP:HA	24:q:52:GLN:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	1	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
3	2	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
4	3	53/57 (93%)	49 (92%)	4 (8%)	0	100	100
5	4	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
6	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
7	7	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
8	8	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
11	c	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
12	d	207/209 (99%)	197 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
14	f	175/179 (98%)	164 (94%)	10 (6%)	1 (1%)	22	23
15	g	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
16	h	37/149 (25%)	32 (86%)	5 (14%)	0	100	100
17	j	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
18	k	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
19	l	141/144 (98%)	132 (94%)	9 (6%)	0	100	100
20	m	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
21	n	118/127 (93%)	111 (94%)	7 (6%)	0	100	100
22	o	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
23	p	111/115 (96%)	110 (99%)	1 (1%)	0	100	100
24	q	115/118 (98%)	115 (100%)	0	0	100	100
25	r	100/103 (97%)	93 (93%)	5 (5%)	2 (2%)	6	4
26	s	107/110 (97%)	100 (94%)	7 (6%)	0	100	100
27	t	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
28	u	100/104 (96%)	83 (83%)	17 (17%)	0	100	100
29	w	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
30	y	80/85 (94%)	76 (95%)	3 (4%)	1 (1%)	10	8
32	z	31/148 (21%)	23 (74%)	6 (19%)	2 (6%)	1	0
All	All	3087/3427 (90%)	2937 (95%)	144 (5%)	6 (0%)	45	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	r	52	PRO
32	z	148	VAL
25	r	51	VAL
30	y	44	LYS
14	f	71	ARG
32	z	147	THR

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	67/68 (98%)	67 (100%)	0	100	100
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	47/49 (96%)	47 (100%)	0	100	100
4	3	46/48 (96%)	44 (96%)	2 (4%)	25	32
5	4	45/49 (92%)	44 (98%)	1 (2%)	47	61
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	51 (100%)	0	100	100
8	8	34/44 (77%)	34 (100%)	0	100	100
11	c	216/218 (99%)	216 (100%)	0	100	100
12	d	164/164 (100%)	164 (100%)	0	100	100
13	e	165/165 (100%)	165 (100%)	0	100	100
14	f	148/150 (99%)	144 (97%)	4 (3%)	40	53
15	g	137/138 (99%)	136 (99%)	1 (1%)	81	90
16	h	30/114 (26%)	30 (100%)	0	100	100
17	j	116/116 (100%)	116 (100%)	0	100	100
18	k	103/104 (99%)	103 (100%)	0	100	100
19	l	102/103 (99%)	94 (92%)	8 (8%)	10	11
20	m	109/109 (100%)	109 (100%)	0	100	100
21	n	100/103 (97%)	100 (100%)	0	100	100
22	o	86/87 (99%)	82 (95%)	4 (5%)	22	29
23	p	98/100 (98%)	98 (100%)	0	100	100
24	q	89/90 (99%)	89 (100%)	0	100	100
25	r	84/84 (100%)	79 (94%)	5 (6%)	16	19
26	s	92/93 (99%)	92 (100%)	0	100	100
27	t	80/84 (95%)	78 (98%)	2 (2%)	42	56
28	u	83/85 (98%)	82 (99%)	1 (1%)	67	80
29	w	78/78 (100%)	78 (100%)	0	100	100
30	y	61/63 (97%)	61 (100%)	0	100	100
32	z	29/121 (24%)	14 (48%)	15 (52%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2552/2772 (92%)	2509 (98%)	43 (2%)	56 71

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	3	16	ARG
4	3	18	SER
5	4	42	VAL
14	f	9	LYS
14	f	11	GLU
14	f	24	SER
14	f	26	MET
15	g	130	GLU
19	l	69	ARG
19	l	70	LYS
19	l	73	ILE
19	l	77	ILE
19	l	85	VAL
19	l	92	LEU
19	l	103	ILE
19	l	104	GLN
22	o	15	ARG
22	o	67	ASN
22	o	68	LYS
22	o	69	ASP
25	r	40	MET
25	r	43	ASN
25	r	47	VAL
25	r	51	VAL
25	r	55	ASP
27	t	1	MET
27	t	2	ILE
28	u	92	LYS
32	z	135	ASN
32	z	138	ASP
32	z	140	SER
32	z	144	PHE
32	z	145	THR
32	z	146	PHE
32	z	148	VAL
32	z	149	GLU
32	z	151	PHE

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Mol	Chain	Res	Type
32	z	152	SER
32	z	157	ILE
32	z	159	TRP
32	z	163	ILE
32	z	164	ARG
32	z	166	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	34	HIS
2	1	15	ASN
2	1	27	ASN
4	3	19	HIS
5	4	45	GLN
6	6	26	ASN
7	7	43	HIS
11	c	117	GLN
11	c	153	GLN
11	c	163	GLN
11	c	200	HIS
11	c	243	HIS
12	d	150	GLN
13	e	29	HIS
13	e	92	HIS
13	e	136	GLN
13	e	163	ASN
14	f	52	ASN
15	g	38	ASN
16	h	18	GLN
17	j	76	HIS
17	j	136	GLN
18	k	29	HIS
18	k	93	GLN
20	m	13	HIS
20	m	45	GLN
21	n	9	GLN
22	o	67	ASN
22	o	98	GLN
22	o	116	GLN
23	p	10	GLN
23	p	12	GLN

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Mol	Chain	Res	Type
23	p	66	ASN
24	q	44	GLN
24	q	72	ASN
24	q	81	ASN
25	r	11	GLN
26	s	7	HIS
27	t	28	ASN
27	t	70	HIS
28	u	46	GLN
28	u	69	ASN
30	y	3	HIS
32	z	135	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	2900/2904 (99%)	1200 (41%)	0
31	v	75/77 (97%)	41 (54%)	0
9	a	117/120 (97%)	21 (17%)	0
All	All	3092/3101 (99%)	1262 (40%)	0

All (1262) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	25	U
9	a	26	C
9	a	30	C
9	a	32	U
9	a	35	C
9	a	41	G
9	a	42	C
9	a	43	C
9	a	44	G
9	a	50	A
9	a	56	G
9	a	59	A
9	a	67	G
9	a	88	C
9	a	89	U
9	a	99	A
9	a	108	A

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Mol	Chain	Res	Type
9	a	109	A
9	a	112	G
9	a	114	C
9	a	116	G
10	b	5	A
10	b	10	A
10	b	11	C
10	b	13	A
10	b	16	C
10	b	23	G
10	b	24	G
10	b	28	A
10	b	33	C
10	b	34	U
10	b	35	G
10	b	36	G
10	b	43	G
10	b	45	G
10	b	46	G
10	b	49	A
10	b	50	U
10	b	51	G
10	b	55	G
10	b	60	G
10	b	62	U
10	b	63	A
10	b	64	A
10	b	65	U
10	b	69	C
10	b	70	G
10	b	71	A
10	b	73	A
10	b	74	A
10	b	75	G
10	b	84	A
10	b	87	U
10	b	91	A
10	b	93	G
10	b	96	C
10	b	99	U
10	b	100	U
10	b	101	A

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Mol	Chain	Res	Type
10	b	102	U
10	b	114	U
10	b	116	C
10	b	118	A
10	b	119	A
10	b	120	U
10	b	122	G
10	b	124	G
10	b	125	A
10	b	126	A
10	b	127	A
10	b	128	C
10	b	131	A
10	b	134	G
10	b	135	U
10	b	136	G
10	b	139	U
10	b	140	C
10	b	141	G
10	b	142	A
10	b	146	A
10	b	159	G
10	b	160	A
10	b	162	U
10	b	163	C
10	b	165	A
10	b	166	U
10	b	168	G
10	b	169	G
10	b	171	U
10	b	175	G
10	b	176	A
10	b	177	G
10	b	178	G
10	b	181	A
10	b	182	A
10	b	188	G
10	b	189	G
10	b	196	A
10	b	197	A
10	b	198	C
10	b	199	A

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Mol	Chain	Res	Type
10	b	201	C
10	b	206	U
10	b	213	A
10	b	215	G
10	b	216	A
10	b	221	A
10	b	222	A
10	b	223	A
10	b	224	U
10	b	228	C
10	b	229	C
10	b	230	G
10	b	232	G
10	b	233	A
10	b	245	G
10	b	246	C
10	b	248	G
10	b	250	G
10	b	252	G
10	b	255	A
10	b	257	C
10	b	261	G
10	b	265	A
10	b	266	G
10	b	268	C
10	b	271	G
10	b	277	G
10	b	278	A
10	b	279	A
10	b	280	U
10	b	281	C
10	b	286	U
10	b	287	G
10	b	288	U
10	b	289	G
10	b	291	G
10	b	298	G
10	b	300	A
10	b	303	G
10	b	311	A
10	b	312	G
10	b	313	G

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Mol	Chain	Res	Type
10	b	317	G
10	b	321	U
10	b	322	A
10	b	323	C
10	b	324	A
10	b	325	G
10	b	326	G
10	b	327	G
10	b	329	G
10	b	330	A
10	b	332	A
10	b	334	C
10	b	338	G
10	b	340	A
10	b	343	C
10	b	345	A
10	b	347	A
10	b	348	A
10	b	350	G
10	b	354	A
10	b	356	G
10	b	359	G
10	b	367	G
10	b	368	A
10	b	369	U
10	b	370	G
10	b	371	A
10	b	372	G
10	b	376	G
10	b	380	G
10	b	383	C
10	b	385	C
10	b	386	G
10	b	387	U
10	b	389	G
10	b	390	U
10	b	391	A
10	b	395	U
10	b	396	G
10	b	397	U
10	b	403	U
10	b	404	A

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Mol	Chain	Res	Type
10	b	405	U
10	b	406	G
10	b	411	G
10	b	412	A
10	b	417	C
10	b	420	C
10	b	422	A
10	b	428	A
10	b	429	A
10	b	433	C
10	b	437	U
10	b	442	G
10	b	443	A
10	b	451	U
10	b	454	A
10	b	455	C
10	b	456	C
10	b	457	A
10	b	462	C
10	b	471	A
10	b	474	G
10	b	475	C
10	b	479	A
10	b	480	A
10	b	481	G
10	b	482	A
10	b	489	G
10	b	490	C
10	b	491	G
10	b	496	G
10	b	504	A
10	b	505	A
10	b	508	A
10	b	509	C
10	b	512	G
10	b	513	A
10	b	520	G
10	b	527	C
10	b	528	A
10	b	529	A
10	b	530	G
10	b	531	C

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Mol	Chain	Res	Type
10	b	532	A
10	b	536	G
10	b	538	A
10	b	542	C
10	b	543	G
10	b	547	A
10	b	548	G
10	b	554	U
10	b	555	G
10	b	562	U
10	b	563	A
10	b	573	U
10	b	574	A
10	b	575	A
10	b	576	U
10	b	586	A
10	b	587	C
10	b	597	G
10	b	603	A
10	b	604	G
10	b	614	A
10	b	615	U
10	b	620	G
10	b	621	A
10	b	622	G
10	b	627	A
10	b	630	G
10	b	634	C
10	b	636	G
10	b	637	A
10	b	642	U
10	b	644	A
10	b	645	C
10	b	647	G
10	b	651	G
10	b	652	U
10	b	653	U
10	b	654	A
10	b	655	A
10	b	662	G
10	b	664	G
10	b	668	A

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Mol	Chain	Res	Type
10	b	669	G
10	b	670	A
10	b	674	G
10	b	678	C
10	b	686	U
10	b	693	A
10	b	694	U
10	b	711	G
10	b	714	U
10	b	717	C
10	b	718	A
10	b	719	C
10	b	726	G
10	b	728	G
10	b	730	A
10	b	731	C
10	b	734	A
10	b	740	C
10	b	746	U
10	b	747	U
10	b	757	G
10	b	764	A
10	b	769	U
10	b	774	G
10	b	775	G
10	b	776	G
10	b	777	G
10	b	781	A
10	b	782	A
10	b	783	A
10	b	784	G
10	b	785	G
10	b	789	A
10	b	791	C
10	b	792	A
10	b	793	A
10	b	794	A
10	b	805	G
10	b	806	C
10	b	811	U
10	b	812	C
10	b	819	A

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Mol	Chain	Res	Type
10	b	827	U
10	b	828	U
10	b	829	A
10	b	830	G
10	b	831	G
10	b	841	G
10	b	842	U
10	b	845	A
10	b	846	U
10	b	847	U
10	b	848	C
10	b	851	C
10	b	852	U
10	b	853	C
10	b	854	C
10	b	855	G
10	b	859	G
10	b	860	U
10	b	864	G
10	b	866	A
10	b	868	U
10	b	869	G
10	b	872	U
10	b	873	C
10	b	875	G
10	b	876	C
10	b	877	A
10	b	878	A
10	b	879	G
10	b	880	G
10	b	881	G
10	b	883	G
10	b	884	U
10	b	885	C
10	b	887	U
10	b	889	C
10	b	891	G
10	b	893	C
10	b	895	U
10	b	896	A
10	b	897	C
10	b	898	C

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Mol	Chain	Res	Type
10	b	900	A
10	b	903	C
10	b	904	G
10	b	907	G
10	b	908	C
10	b	910	A
10	b	911	A
10	b	912	C
10	b	913	U
10	b	914	G
10	b	915	C
10	b	923	G
10	b	924	G
10	b	926	G
10	b	928	A
10	b	931	U
10	b	932	U
10	b	934	U
10	b	937	C
10	b	938	G
10	b	941	A
10	b	946	C
10	b	958	U
10	b	961	C
10	b	965	C
10	b	968	C
10	b	969	G
10	b	974	G
10	b	975	A
10	b	980	A
10	b	982	C
10	b	983	A
10	b	985	C
10	b	988	A
10	b	989	G
10	b	990	A
10	b	991	C
10	b	996	A
10	b	1003	G
10	b	1005	C
10	b	1009	A
10	b	1012	U

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Mol	Chain	Res	Type
10	b	1013	C
10	b	1016	G
10	b	1017	G
10	b	1018	U
10	b	1019	U
10	b	1020	A
10	b	1021	A
10	b	1022	G
10	b	1023	U
10	b	1024	G
10	b	1025	G
10	b	1026	G
10	b	1028	A
10	b	1030	C
10	b	1031	G
10	b	1032	A
10	b	1033	U
10	b	1034	G
10	b	1035	U
10	b	1037	G
10	b	1040	A
10	b	1042	G
10	b	1045	C
10	b	1046	A
10	b	1047	G
10	b	1048	A
10	b	1050	A
10	b	1051	G
10	b	1052	C
10	b	1053	C
10	b	1054	A
10	b	1055	G
10	b	1056	G
10	b	1057	A
10	b	1058	U
10	b	1060	U
10	b	1061	U
10	b	1062	G
10	b	1063	G
10	b	1064	C
10	b	1066	U
10	b	1067	A

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Mol	Chain	Res	Type
10	b	1068	G
10	b	1069	A
10	b	1070	A
10	b	1071	G
10	b	1072	C
10	b	1073	A
10	b	1074	G
10	b	1076	C
10	b	1077	A
10	b	1078	U
10	b	1079	C
10	b	1080	A
10	b	1083	U
10	b	1084	A
10	b	1085	A
10	b	1086	A
10	b	1087	G
10	b	1088	A
10	b	1089	A
10	b	1090	A
10	b	1091	G
10	b	1093	G
10	b	1094	U
10	b	1095	A
10	b	1097	U
10	b	1098	A
10	b	1099	G
10	b	1101	U
10	b	1102	C
10	b	1103	A
10	b	1104	C
10	b	1105	U
10	b	1106	G
10	b	1108	U
10	b	1109	C
10	b	1111	A
10	b	1112	G
10	b	1119	U
10	b	1126	A
10	b	1130	U
10	b	1131	G
10	b	1132	U

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Mol	Chain	Res	Type
10	b	1133	A
10	b	1134	A
10	b	1135	C
10	b	1137	G
10	b	1141	U
10	b	1142	A
10	b	1144	A
10	b	1151	A
10	b	1154	G
10	b	1156	A
10	b	1157	G
10	b	1158	C
10	b	1163	G
10	b	1165	A
10	b	1166	G
10	b	1169	A
10	b	1171	G
10	b	1172	C
10	b	1174	U
10	b	1175	A
10	b	1176	U
10	b	1177	G
10	b	1178	C
10	b	1182	G
10	b	1183	U
10	b	1185	G
10	b	1186	G
10	b	1195	G
10	b	1197	G
10	b	1198	U
10	b	1203	U
10	b	1204	A
10	b	1205	A
10	b	1206	G
10	b	1210	G
10	b	1211	C
10	b	1212	G
10	b	1216	G
10	b	1217	U
10	b	1218	G
10	b	1220	G
10	b	1223	G

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Mol	Chain	Res	Type
10	b	1226	A
10	b	1227	G
10	b	1232	G
10	b	1236	G
10	b	1237	A
10	b	1238	G
10	b	1245	G
10	b	1247	A
10	b	1250	G
10	b	1251	C
10	b	1252	G
10	b	1253	A
10	b	1254	A
10	b	1256	G
10	b	1259	G
10	b	1262	A
10	b	1265	A
10	b	1266	G
10	b	1267	U
10	b	1271	G
10	b	1272	A
10	b	1275	A
10	b	1276	A
10	b	1279	G
10	b	1280	G
10	b	1281	G
10	b	1285	A
10	b	1288	G
10	b	1289	C
10	b	1294	U
10	b	1299	G
10	b	1300	G
10	b	1301	A
10	b	1302	A
10	b	1303	G
10	b	1304	A
10	b	1305	C
10	b	1311	G
10	b	1312	U
10	b	1313	U
10	b	1315	C
10	b	1320	C

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Mol	Chain	Res	Type
10	b	1321	A
10	b	1324	G
10	b	1325	U
10	b	1326	U
10	b	1329	U
10	b	1330	C
10	b	1332	G
10	b	1336	A
10	b	1338	G
10	b	1341	G
10	b	1342	A
10	b	1345	C
10	b	1346	G
10	b	1352	U
10	b	1354	A
10	b	1355	G
10	b	1359	A
10	b	1365	A
10	b	1366	A
10	b	1368	G
10	b	1371	G
10	b	1374	G
10	b	1376	C
10	b	1378	A
10	b	1379	U
10	b	1380	G
10	b	1381	G
10	b	1383	A
10	b	1385	A
10	b	1387	A
10	b	1388	G
10	b	1392	A
10	b	1393	A
10	b	1394	U
10	b	1395	A
10	b	1396	U
10	b	1402	U
10	b	1403	A
10	b	1407	G
10	b	1409	U
10	b	1410	G
10	b	1413	A

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Mol	Chain	Res	Type
10	b	1416	G
10	b	1419	A
10	b	1420	A
10	b	1421	G
10	b	1423	G
10	b	1427	A
10	b	1428	C
10	b	1429	G
10	b	1435	G
10	b	1436	G
10	b	1439	A
10	b	1441	G
10	b	1444	G
10	b	1449	G
10	b	1451	C
10	b	1452	G
10	b	1453	A
10	b	1454	C
10	b	1455	G
10	b	1456	G
10	b	1457	U
10	b	1458	U
10	b	1459	G
10	b	1460	U
10	b	1461	C
10	b	1464	G
10	b	1466	U
10	b	1469	A
10	b	1474	U
10	b	1475	G
10	b	1476	U
10	b	1477	A
10	b	1478	G
10	b	1479	G
10	b	1482	G
10	b	1483	G
10	b	1486	U
10	b	1492	G
10	b	1493	C
10	b	1494	A
10	b	1495	A
10	b	1496	A

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Mol	Chain	Res	Type
10	b	1498	C
10	b	1503	A
10	b	1508	A
10	b	1509	A
10	b	1510	G
10	b	1516	G
10	b	1517	G
10	b	1523	U
10	b	1524	G
10	b	1529	G
10	b	1530	G
10	b	1531	C
10	b	1532	A
10	b	1536	C
10	b	1537	G
10	b	1538	G
10	b	1539	U
10	b	1544	A
10	b	1547	C
10	b	1552	A
10	b	1554	U
10	b	1555	G
10	b	1558	C
10	b	1559	U
10	b	1560	G
10	b	1563	U
10	b	1565	C
10	b	1566	A
10	b	1567	G
10	b	1568	G
10	b	1569	A
10	b	1571	A
10	b	1575	C
10	b	1576	U
10	b	1578	U
10	b	1581	G
10	b	1582	C
10	b	1583	A
10	b	1584	U
10	b	1585	C
10	b	1588	G
10	b	1589	U

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Mol	Chain	Res	Type
10	b	1593	A
10	b	1595	C
10	b	1596	A
10	b	1607	C
10	b	1608	A
10	b	1610	A
10	b	1611	C
10	b	1613	G
10	b	1617	C
10	b	1618	A
10	b	1622	G
10	b	1627	G
10	b	1630	A
10	b	1634	A
10	b	1635	A
10	b	1642	G
10	b	1643	G
10	b	1647	U
10	b	1648	U
10	b	1649	G
10	b	1664	A
10	b	1665	A
10	b	1666	G
10	b	1667	G
10	b	1669	A
10	b	1673	G
10	b	1674	G
10	b	1675	C
10	b	1681	G
10	b	1689	A
10	b	1693	U
10	b	1694	C
10	b	1699	G
10	b	1700	A
10	b	1701	A
10	b	1703	G
10	b	1706	C
10	b	1707	G
10	b	1713	A
10	b	1714	U
10	b	1715	G
10	b	1716	U

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Mol	Chain	Res	Type
10	b	1721	G
10	b	1725	C
10	b	1726	G
10	b	1729	U
10	b	1731	G
10	b	1732	C
10	b	1733	U
10	b	1735	G
10	b	1736	U
10	b	1738	G
10	b	1740	G
10	b	1749	A
10	b	1750	G
10	b	1755	A
10	b	1756	G
10	b	1758	U
10	b	1759	A
10	b	1762	A
10	b	1763	G
10	b	1764	C
10	b	1773	A
10	b	1776	G
10	b	1779	U
10	b	1782	U
10	b	1784	A
10	b	1786	A
10	b	1787	A
10	b	1792	G
10	b	1794	A
10	b	1800	C
10	b	1801	A
10	b	1805	A
10	b	1808	A
10	b	1809	A
10	b	1811	G
10	b	1816	C
10	b	1818	U
10	b	1821	A
10	b	1823	G
10	b	1827	U
10	b	1829	A
10	b	1833	C

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Mol	Chain	Res	Type
10	b	1836	C
10	b	1848	A
10	b	1849	G
10	b	1853	A
10	b	1856	U
10	b	1857	G
10	b	1858	A
10	b	1862	G
10	b	1863	G
10	b	1864	U
10	b	1869	G
10	b	1872	A
10	b	1873	G
10	b	1875	G
10	b	1876	A
10	b	1882	U
10	b	1884	G
10	b	1887	C
10	b	1889	A
10	b	1890	A
10	b	1895	C
10	b	1899	A
10	b	1900	A
10	b	1906	G
10	b	1913	A
10	b	1917	U
10	b	1921	G
10	b	1922	G
10	b	1923	U
10	b	1924	C
10	b	1925	C
10	b	1927	A
10	b	1929	G
10	b	1930	G
10	b	1931	U
10	b	1937	A
10	b	1938	A
10	b	1939	U
10	b	1940	U
10	b	1944	U
10	b	1946	U
10	b	1952	A

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Mol	Chain	Res	Type
10	b	1953	A
10	b	1954	G
10	b	1955	U
10	b	1956	U
10	b	1958	C
10	b	1961	C
10	b	1964	G
10	b	1965	C
10	b	1966	A
10	b	1967	C
10	b	1970	A
10	b	1971	U
10	b	1972	G
10	b	1975	G
10	b	1980	G
10	b	1981	A
10	b	1985	C
10	b	1987	A
10	b	1991	U
10	b	1992	G
10	b	1993	U
10	b	1996	C
10	b	1997	C
10	b	1998	A
10	b	1999	C
10	b	2002	G
10	b	2020	A
10	b	2021	C
10	b	2022	U
10	b	2023	C
10	b	2024	G
10	b	2029	G
10	b	2030	A
10	b	2031	A
10	b	2032	G
10	b	2033	A
10	b	2034	U
10	b	2036	C
10	b	2039	U
10	b	2043	C
10	b	2051	A
10	b	2055	C

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Mol	Chain	Res	Type
10	b	2056	G
10	b	2059	A
10	b	2060	A
10	b	2061	G
10	b	2062	A
10	b	2063	C
10	b	2068	U
10	b	2069	G
10	b	2076	U
10	b	2077	A
10	b	2078	C
10	b	2080	A
10	b	2081	U
10	b	2085	U
10	b	2093	G
10	b	2095	A
10	b	2100	G
10	b	2101	A
10	b	2102	G
10	b	2104	C
10	b	2105	U
10	b	2106	U
10	b	2107	G
10	b	2109	U
10	b	2110	G
10	b	2111	U
10	b	2112	G
10	b	2113	U
10	b	2114	A
10	b	2115	G
10	b	2116	G
10	b	2117	A
10	b	2118	U
10	b	2119	A
10	b	2120	G
10	b	2121	G
10	b	2123	G
10	b	2124	G
10	b	2126	A
10	b	2127	G
10	b	2128	G
10	b	2129	C

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Mol	Chain	Res	Type
10	b	2130	U
10	b	2131	U
10	b	2133	G
10	b	2134	A
10	b	2135	A
10	b	2136	G
10	b	2137	U
10	b	2138	G
10	b	2139	U
10	b	2140	G
10	b	2142	A
10	b	2143	C
10	b	2144	G
10	b	2145	C
10	b	2146	C
10	b	2147	A
10	b	2148	G
10	b	2149	U
10	b	2150	C
10	b	2151	U
10	b	2152	G
10	b	2153	C
10	b	2154	A
10	b	2155	U
10	b	2157	G
10	b	2158	A
10	b	2159	G
10	b	2160	C
10	b	2161	C
10	b	2162	G
10	b	2163	A
10	b	2164	C
10	b	2165	C
10	b	2166	U
10	b	2169	A
10	b	2170	A
10	b	2171	A
10	b	2172	U
10	b	2174	C
10	b	2175	C
10	b	2176	A
10	b	2177	C

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Mol	Chain	Res	Type
10	b	2178	C
10	b	2180	U
10	b	2183	A
10	b	2186	G
10	b	2190	G
10	b	2192	U
10	b	2193	G
10	b	2197	U
10	b	2198	A
10	b	2199	A
10	b	2203	U
10	b	2204	G
10	b	2211	A
10	b	2212	A
10	b	2213	U
10	b	2214	C
10	b	2225	A
10	b	2228	G
10	b	2234	G
10	b	2238	G
10	b	2239	G
10	b	2243	U
10	b	2249	U
10	b	2250	G
10	b	2258	C
10	b	2259	U
10	b	2261	C
10	b	2266	A
10	b	2268	A
10	b	2273	A
10	b	2278	A
10	b	2282	G
10	b	2283	C
10	b	2286	G
10	b	2287	A
10	b	2288	A
10	b	2295	C
10	b	2297	A
10	b	2298	A
10	b	2305	U
10	b	2307	G
10	b	2308	G

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Mol	Chain	Res	Type
10	b	2309	A
10	b	2311	A
10	b	2312	U
10	b	2315	G
10	b	2316	G
10	b	2317	A
10	b	2319	G
10	b	2320	U
10	b	2321	U
10	b	2322	A
10	b	2325	G
10	b	2327	A
10	b	2333	A
10	b	2334	U
10	b	2335	A
10	b	2336	A
10	b	2337	G
10	b	2340	A
10	b	2345	G
10	b	2347	C
10	b	2350	C
10	b	2352	A
10	b	2354	C
10	b	2355	G
10	b	2361	G
10	b	2364	C
10	b	2367	G
10	b	2368	C
10	b	2379	G
10	b	2383	G
10	b	2385	C
10	b	2389	G
10	b	2391	G
10	b	2396	G
10	b	2397	G
10	b	2399	G
10	b	2402	U
10	b	2403	C
10	b	2405	G
10	b	2406	A
10	b	2407	A
10	b	2408	U

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Mol	Chain	Res	Type
10	b	2410	G
10	b	2416	C
10	b	2419	U
10	b	2420	C
10	b	2422	C
10	b	2423	U
10	b	2424	C
10	b	2425	A
10	b	2427	C
10	b	2428	G
10	b	2429	G
10	b	2430	A
10	b	2431	U
10	b	2435	A
10	b	2439	A
10	b	2441	U
10	b	2445	G
10	b	2447	G
10	b	2448	A
10	b	2454	G
10	b	2457	U
10	b	2458	G
10	b	2459	A
10	b	2464	G
10	b	2468	A
10	b	2470	G
10	b	2471	A
10	b	2473	U
10	b	2474	U
10	b	2475	C
10	b	2476	A
10	b	2478	A
10	b	2480	C
10	b	2482	A
10	b	2484	G
10	b	2485	G
10	b	2486	C
10	b	2488	G
10	b	2490	G
10	b	2491	U
10	b	2492	U
10	b	2494	G

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Mol	Chain	Res	Type
10	b	2497	A
10	b	2498	C
10	b	2499	C
10	b	2502	G
10	b	2503	A
10	b	2504	U
10	b	2505	G
10	b	2513	A
10	b	2518	A
10	b	2519	U
10	b	2520	C
10	b	2526	G
10	b	2528	U
10	b	2529	G
10	b	2533	U
10	b	2534	A
10	b	2535	G
10	b	2536	G
10	b	2537	U
10	b	2543	G
10	b	2546	U
10	b	2547	G
10	b	2550	G
10	b	2554	U
10	b	2556	C
10	b	2560	A
10	b	2562	U
10	b	2564	A
10	b	2566	A
10	b	2567	G
10	b	2572	A
10	b	2573	C
10	b	2574	G
10	b	2579	C
10	b	2581	G
10	b	2582	G
10	b	2583	G
10	b	2586	U
10	b	2593	U
10	b	2601	C
10	b	2602	A
10	b	2608	G

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Mol	Chain	Res	Type
10	b	2609	U
10	b	2610	C
10	b	2613	U
10	b	2614	A
10	b	2615	U
10	b	2618	G
10	b	2623	G
10	b	2625	G
10	b	2626	C
10	b	2629	U
10	b	2630	G
10	b	2634	A
10	b	2636	C
10	b	2639	A
10	b	2643	G
10	b	2646	C
10	b	2655	G
10	b	2656	U
10	b	2658	C
10	b	2660	A
10	b	2661	G
10	b	2663	G
10	b	2664	G
10	b	2668	G
10	b	2669	G
10	b	2673	G
10	b	2674	G
10	b	2676	C
10	b	2679	A
10	b	2681	C
10	b	2684	U
10	b	2688	G
10	b	2689	U
10	b	2690	U
10	b	2691	C
10	b	2692	G
10	b	2700	A
10	b	2702	G
10	b	2705	A
10	b	2713	U
10	b	2716	C
10	b	2718	G

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Mol	Chain	Res	Type
10	b	2724	U
10	b	2725	A
10	b	2726	A
10	b	2731	G
10	b	2733	A
10	b	2736	A
10	b	2737	G
10	b	2744	G
10	b	2746	U
10	b	2748	A
10	b	2750	A
10	b	2751	G
10	b	2752	C
10	b	2754	U
10	b	2755	C
10	b	2757	A
10	b	2761	A
10	b	2762	C
10	b	2765	A
10	b	2768	U
10	b	2771	C
10	b	2773	C
10	b	2777	G
10	b	2778	A
10	b	2779	U
10	b	2780	G
10	b	2781	A
10	b	2783	U
10	b	2790	U
10	b	2796	U
10	b	2797	U
10	b	2798	U
10	b	2799	A
10	b	2800	A
10	b	2802	G
10	b	2803	G
10	b	2804	U
10	b	2807	U
10	b	2808	G
10	b	2818	U
10	b	2819	G
10	b	2820	A

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Mol	Chain	Res	Type
10	b	2821	A
10	b	2822	G
10	b	2832	U
10	b	2833	U
10	b	2835	A
10	b	2836	U
10	b	2837	A
10	b	2843	G
10	b	2848	G
10	b	2849	U
10	b	2859	G
10	b	2861	U
10	b	2864	G
10	b	2865	U
10	b	2866	U
10	b	2867	G
10	b	2871	U
10	b	2879	A
10	b	2883	A
10	b	2884	U
10	b	2886	A
10	b	2887	A
10	b	2892	G
10	b	2893	A
10	b	2894	G
10	b	2895	G
10	b	2898	U
10	b	2900	A
31	v	2	G
31	v	3	U
31	v	4	G
31	v	5	A
31	v	7	U
31	v	8	G
31	v	9	G
31	v	10	C
31	v	11	G
31	v	16	C
31	v	17	U
31	v	18	G
31	v	19	G
31	v	20	U

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Mol	Chain	Res	Type
31	v	21	A
31	v	23	C
31	v	24	G
31	v	31	G
31	v	33	U
31	v	35	G
31	v	40	G
31	v	43	G
31	v	44	G
31	v	45	G
31	v	46	G
31	v	47	U
31	v	48	C
31	v	49	G
31	v	50	G
31	v	52	G
31	v	53	G
31	v	54	U
31	v	57	G
31	v	58	A
31	v	59	A
31	v	65	U
31	v	66	A
31	v	69	A
31	v	70	C
31	v	73	A
31	v	76	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

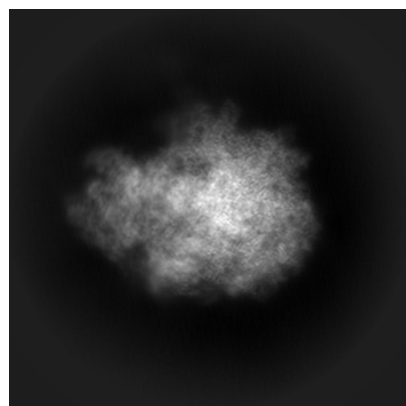
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14850. These allow visual inspection of the internal detail of the map and identification of artifacts.

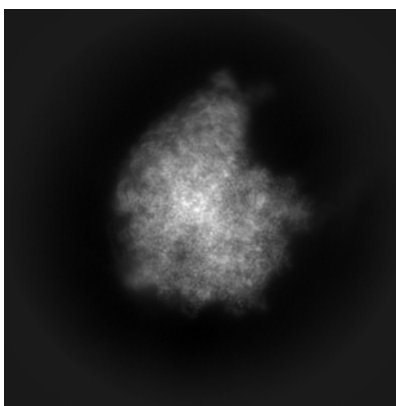
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

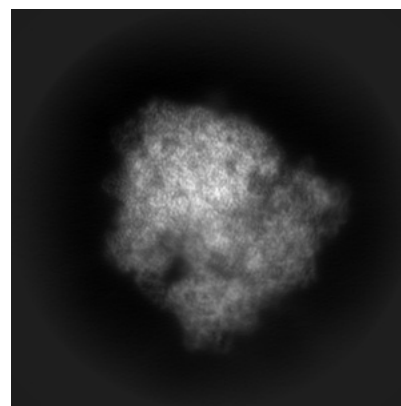
6.1.1 Primary map



X

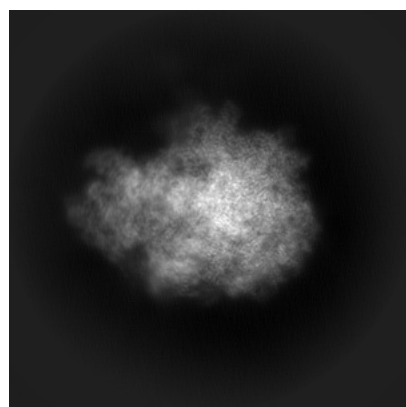


Y

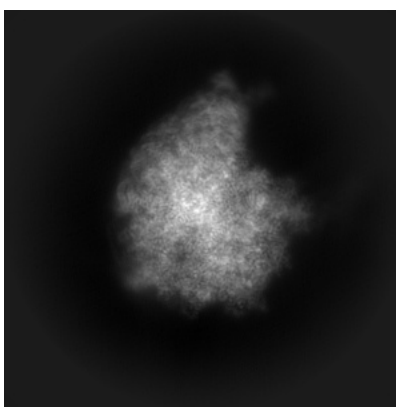


Z

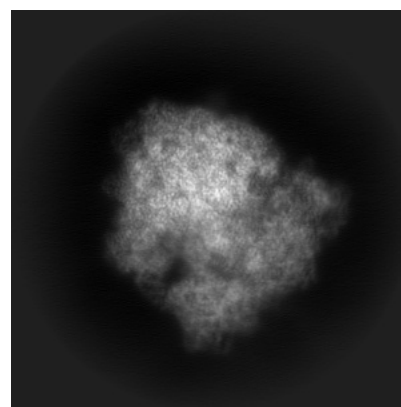
6.1.2 Raw map



X



Y

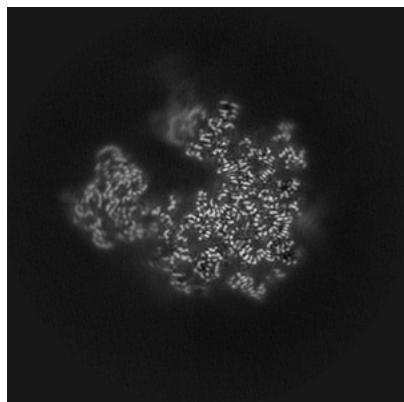


Z

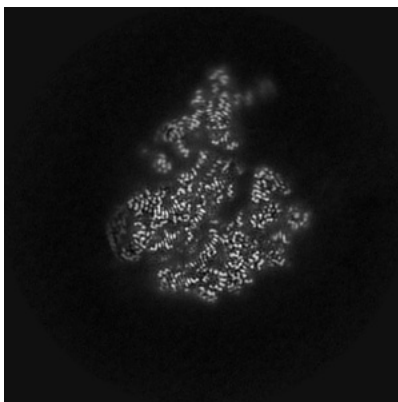
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

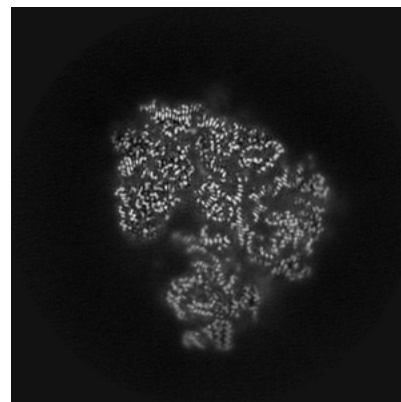
6.2.1 Primary map



X Index: 192

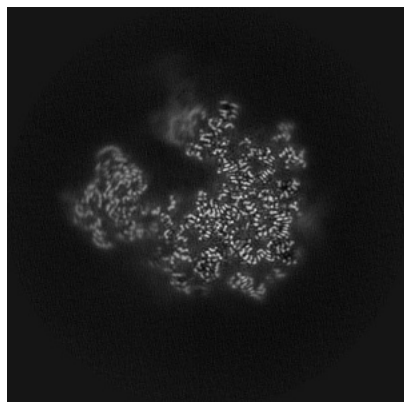


Y Index: 192

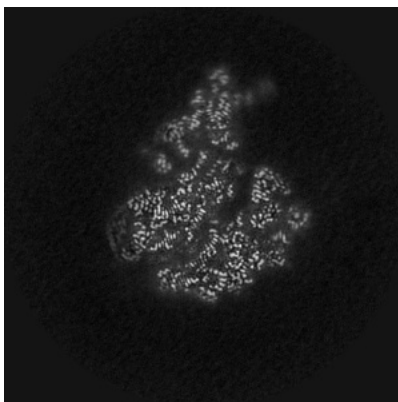


Z Index: 192

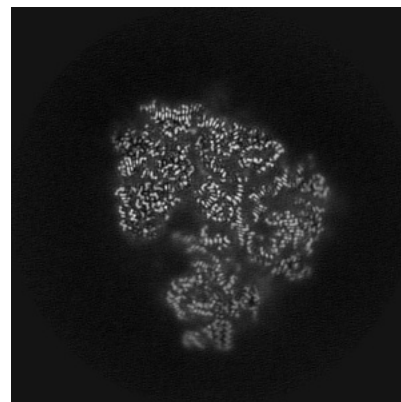
6.2.2 Raw map



X Index: 192



Y Index: 192

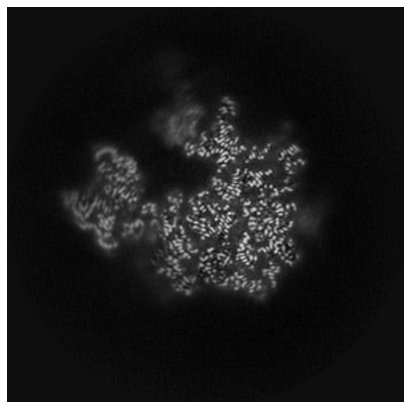


Z Index: 192

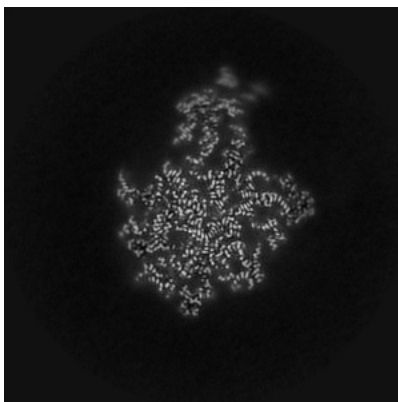
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

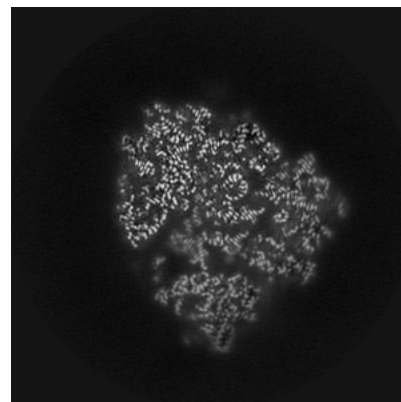
6.3.1 Primary map



X Index: 197

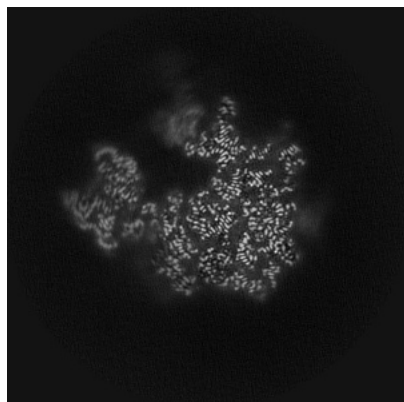


Y Index: 211

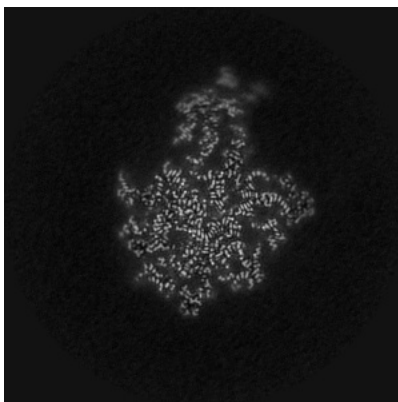


Z Index: 198

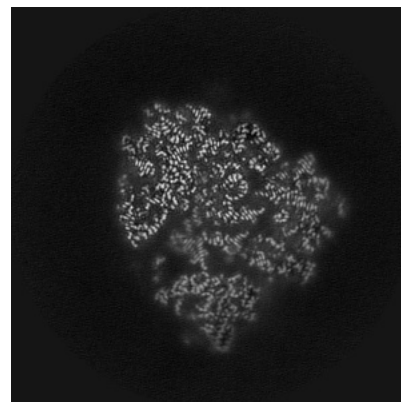
6.3.2 Raw map



X Index: 197



Y Index: 211

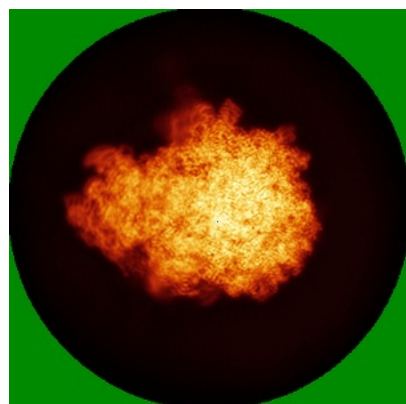


Z Index: 198

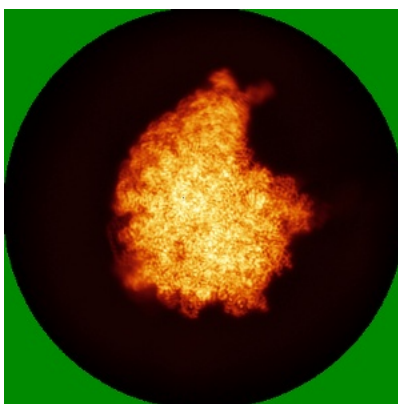
The images above show the largest variance slices of the map in three orthogonal directions.

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

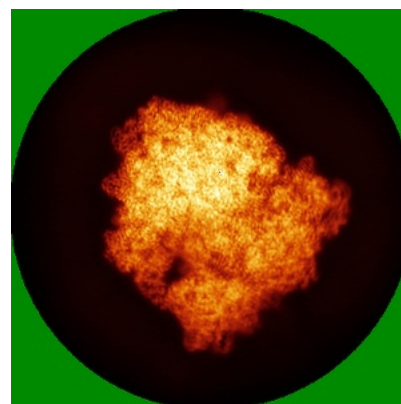
6.4.1 Primary map



X



Y

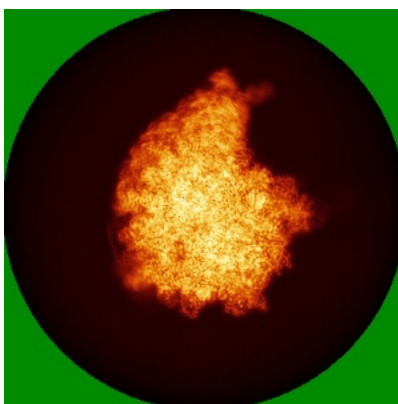


Z

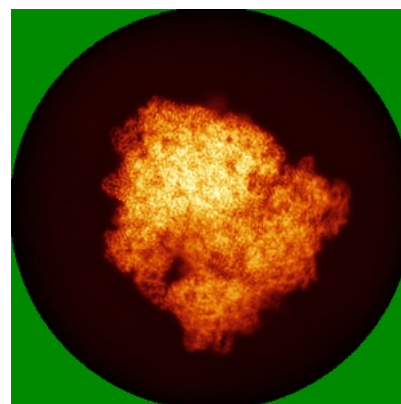
6.4.2 Raw map



X



Y

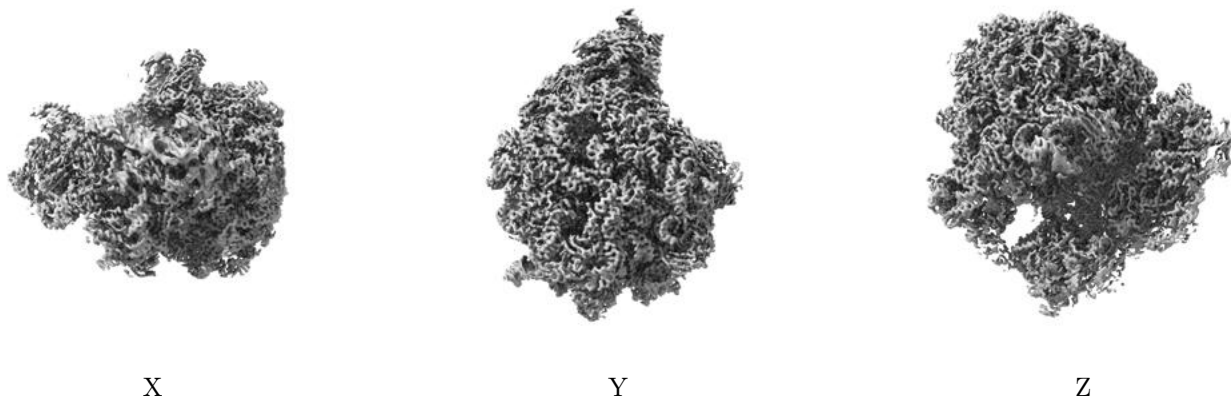


Z

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.

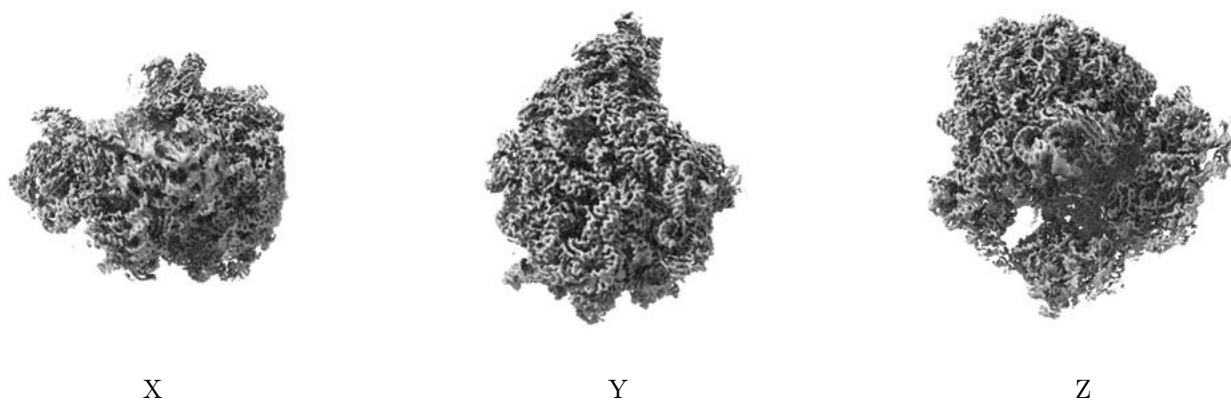
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02965. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

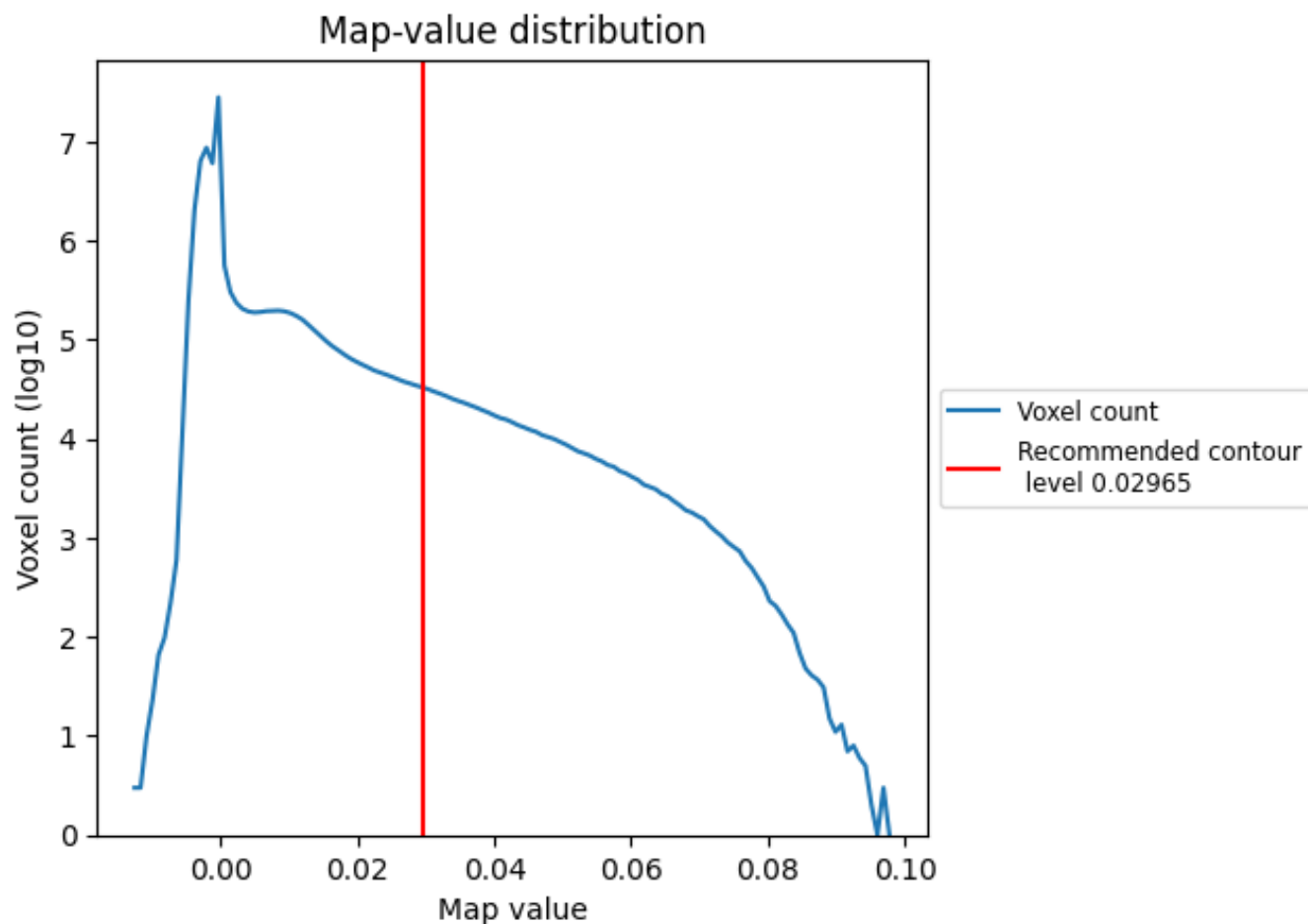
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

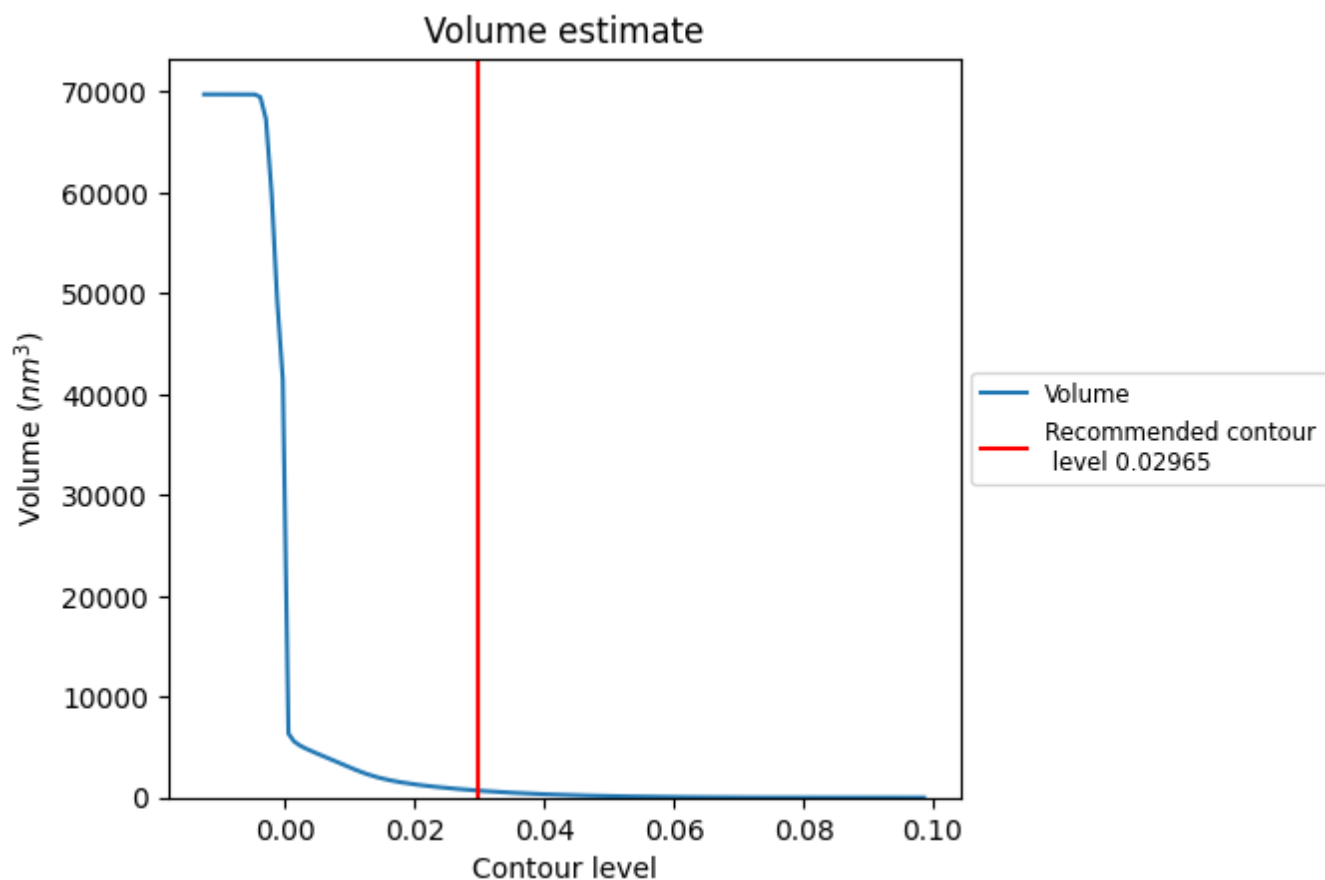
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

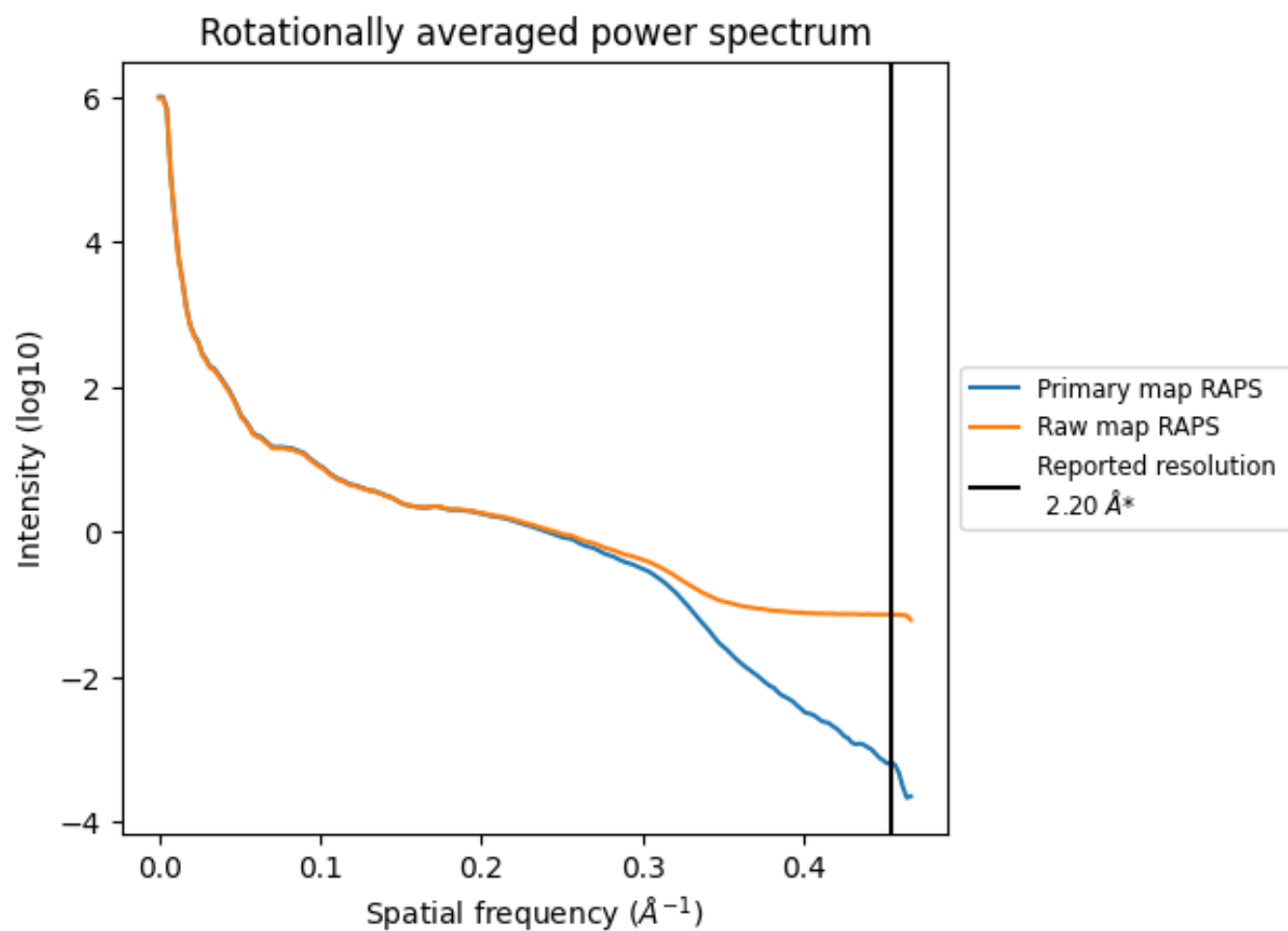
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 698 nm³; this corresponds to an approximate mass of 631 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 ⓘ

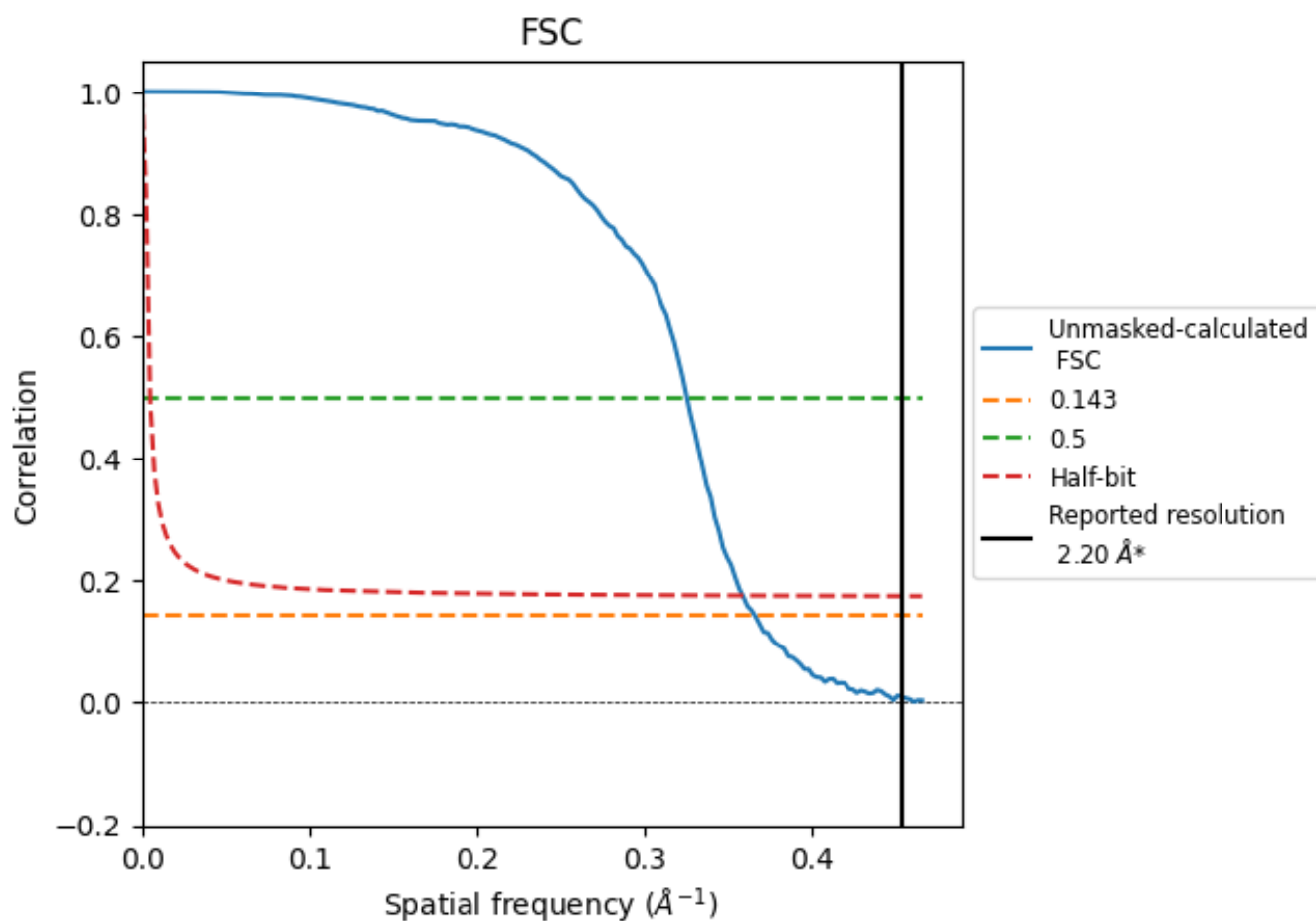


*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

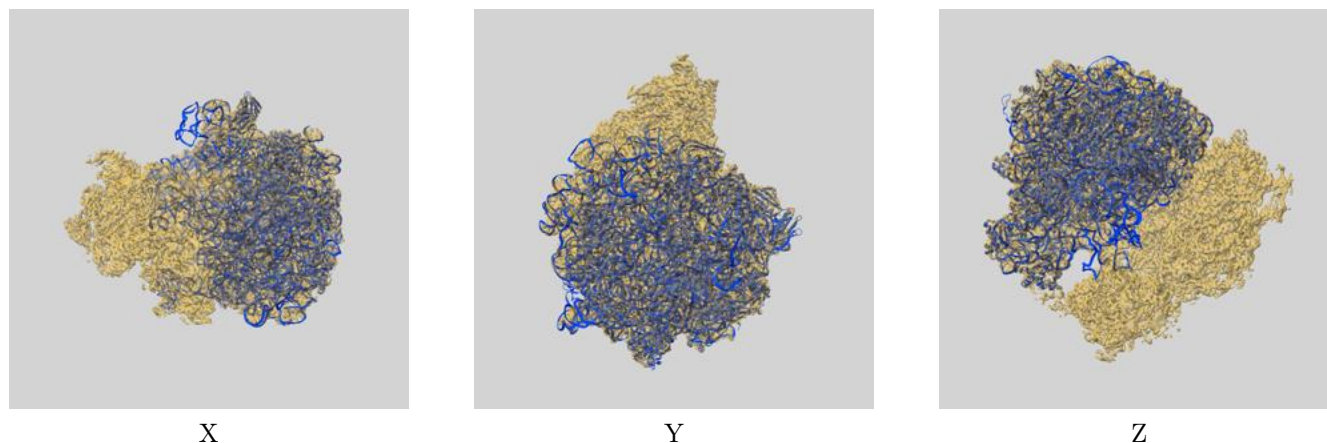
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.73	3.07	2.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.73 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

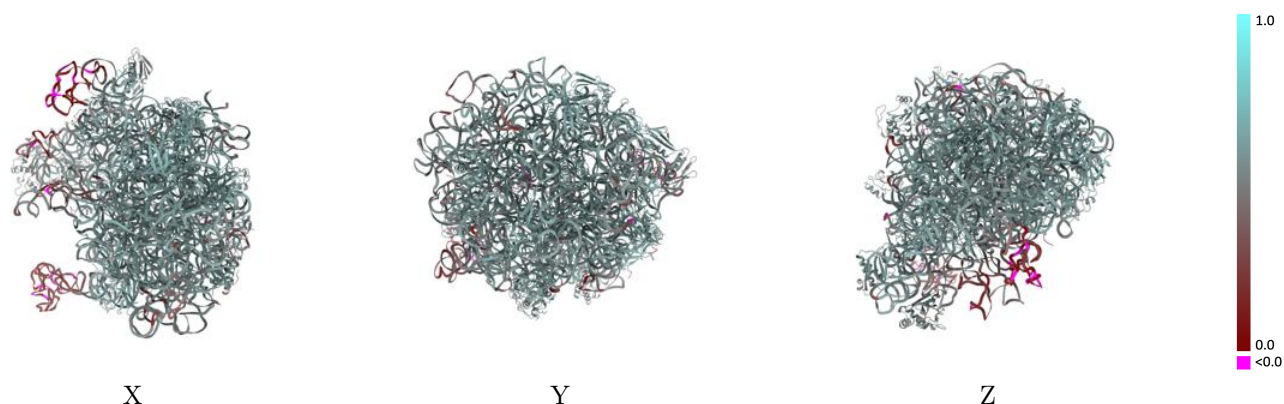
This section contains information regarding the fit between EMDB map EMD-14850 and PDB model 7ZP8. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



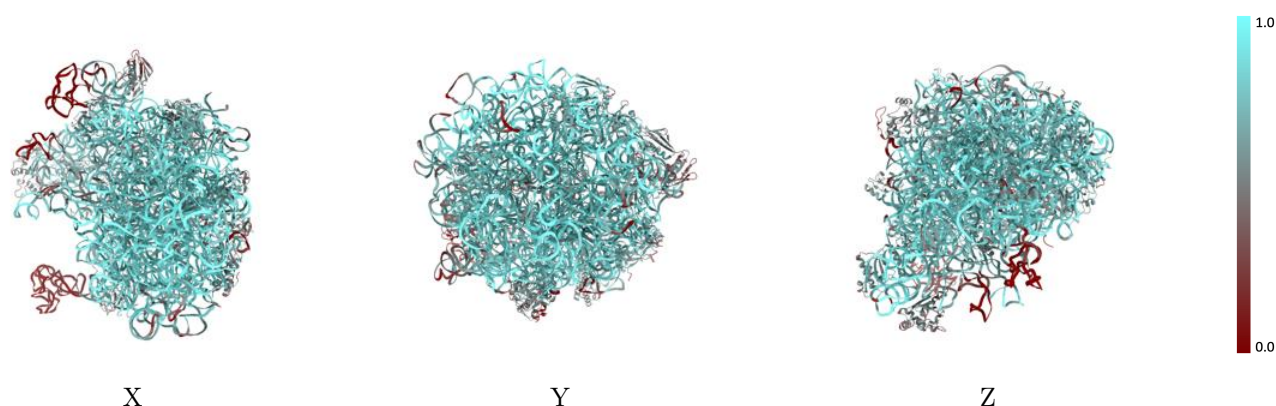
The images above show the 3D surface view of the map at the recommended contour level 0.02965 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



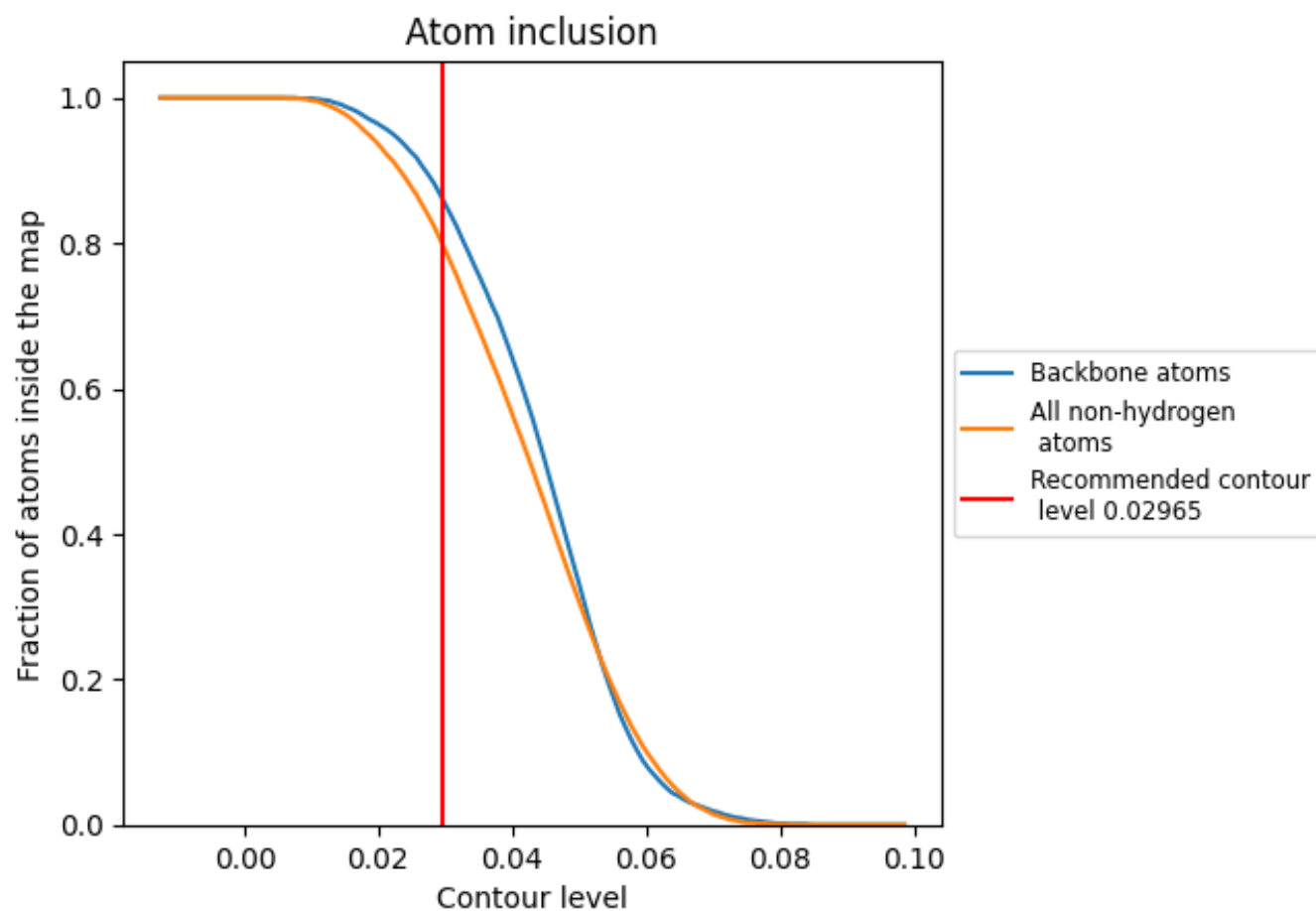
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02965).



































































9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.02965) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7970	 0.5450
0	 0.8050	 0.6060
1	 0.5900	 0.5440
2	 0.7490	 0.5970
3	 0.7490	 0.5780
4	 0.6230	 0.5630
6	 0.9150	 0.6310
7	 0.8660	 0.6240
8	 0.7770	 0.6060
a	 0.8650	 0.5650
b	 0.8380	 0.5330
c	 0.8400	 0.6180
d	 0.7650	 0.6110
e	 0.6060	 0.5800
f	 0.4740	 0.5080
g	 0.4990	 0.5400
h	 0.1970	 0.4970
j	 0.7710	 0.5980
k	 0.7360	 0.6060
l	 0.7310	 0.5870
m	 0.7730	 0.6040
n	 0.8080	 0.6130
o	 0.6360	 0.5540
p	 0.7530	 0.6060
q	 0.8090	 0.6100
r	 0.6570	 0.5740
s	 0.7590	 0.6060
t	 0.6510	 0.5780
u	 0.5500	 0.5500
v	 0.6440	 0.4040
w	 0.6580	 0.5880
y	 0.7550	 0.5950
z	 0.1780	 0.3270

