



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:04 PM UTC

PDB ID : 5MMI / pdb_00005mmi
EMDB ID : EMD-3531
Title : Structure of the large subunit of the chloroplast ribosome
Authors : Bieri, P.; Leibundgut, M.; Saurer, M.; Boehringer, D.; Ban, N.
Deposited on : 2016-12-10
Resolution : 3.20 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:

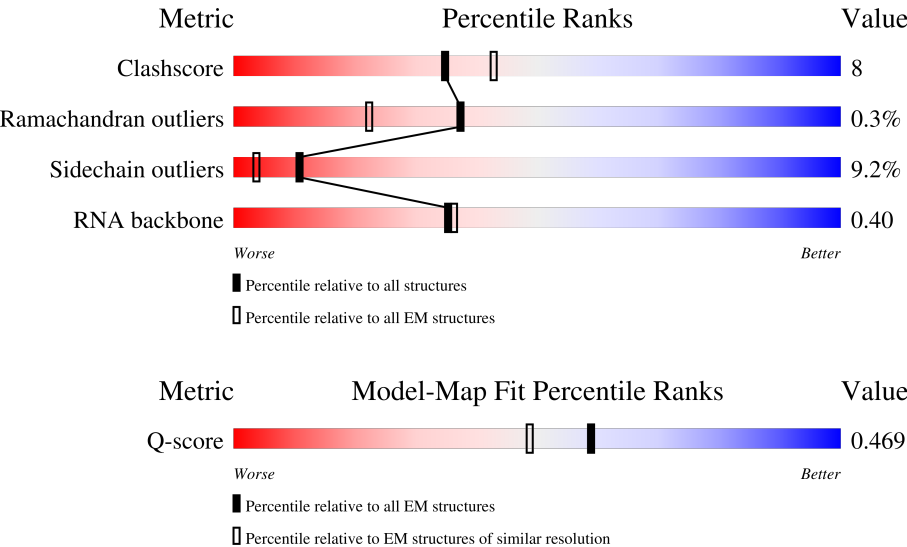
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	130	
2	1	57	
3	2	66	

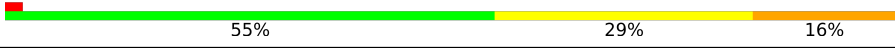
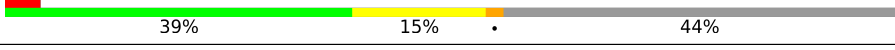
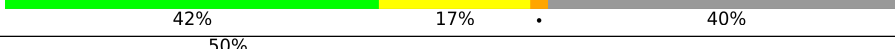
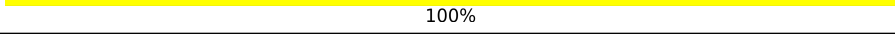
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Mol	Chain	Length	Quality of chain
4	3	152	
5	4	159	
6	5	37	
7	6	142	
8	7	116	
9	A	2810	
10	B	121	
11	C	272	
12	D	305	
13	E	293	
14	F	258	
15	G	220	
16	H	196	
17	I	232	
18	J	224	
19	K	250	
20	L	121	
21	M	271	
22	N	135	
23	O	126	
24	P	166	
25	Q	233	
26	R	128	
27	S	256	
28	T	199	

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Mol	Chain	Length	Quality of chain
29	U	198	
30	V	192	
31	W	106	
32	X	194	
33	Y	148	
34	Z	168	
35	z	2	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 95397 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 L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	44	Total	C	N	O	S	0	0
			359	226	61	70	2		

- Molecule 2 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	48	Total	C	N	O	0	0
			396	261	75	60		

- Molecule 3 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	60	Total	C	N	O	S	0	0
			489	304	98	83	4		

- Molecule 4 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	60	Total	C	N	O	S	0	0
			467	282	107	75	3		

- Molecule 5 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	72	Total	C	N	O	S	0	0
			588	370	124	93	1		

- Molecule 6 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	37	Total	C	N	O	S	0	0
			305	186	70	45	4		

- Molecule 7 is a protein called plastid ribosomal protein cL37, PSRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	49	Total	C	N	O	S	0	0
			422	268	92	57	5		

- Molecule 8 is a protein called 50S ribosomal protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	46	Total	C	N	O	S	0	0
			368	237	71	59	1		

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	2798	Total	C	N	O	P	0	0
			60083	26804	11116	19365	2798		

- Molecule 10 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	121	Total	C	N	O	P	0	0
			2584	1154	466	843	121		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	253	Total	C	N	O	S	0	0
			1952	1209	401	336	6		

- Molecule 12 is a protein called plastid ribosomal protein uL3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	221	Total	C	N	O	S	0	0
			1686	1066	308	301	11		

- Molecule 13 is a protein called plastid ribosomal protein uL4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	212	Total	C	N	O	S	0	0
			1676	1061	312	300	3		

- Molecule 14 is a protein called plastid ribosomal protein uL5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	193	Total	C	N	O	S	0	0
			1454	923	255	268	8		

- Molecule 15 is a protein called plastid ribosomal protein uL6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	178	Total	C	N	O	S	0	0
			1391	878	256	253	4		

- Molecule 16 is a protein called plastid ribosomal protein bL9c.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	H	48	Total	C	N	O	0	0
			382	251	69	62		

- Molecule 17 is a protein called plastid ribosomal protein uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	137	Total	C	N	O	S	0	0
			1106	711	186	203	6		

- Molecule 18 is a protein called 50S ribosomal protein L11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	133	Total	C	N	O	S	0	0
			977	624	161	186	6		

- Molecule 19 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	203	Total	C	N	O	S	0	0
			1648	1047	307	289	5		

- Molecule 20 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	121	Total	C	N	O	S	0	0
			942	588	179	170	5		

- Molecule 21 is a protein called plastid ribosomal protein uL15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	185	Total	C	N	O	S	0	0
			1410	879	280	245	6		

- Molecule 22 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	135	Total	C	N	O	S	0	0
			1075	677	218	174	6		

- Molecule 23 is a protein called plastid ribosomal protein bL17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	116	Total	C	N	O	S	0	0
			944	592	193	155	4		

- Molecule 24 is a protein called plastid ribosomal protein uL18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	122	Total	C	N	O	S	0	0
			962	598	186	173	5		

- Molecule 25 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	118	Total	C	N	O	S	0	0
			953	611	186	155	1		

- Molecule 26 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	119	Total	C	N	O	S	0	0
			1029	652	213	162	2		

- Molecule 27 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	S	170	Total	C	N	O	0	0
			1310	844	227	239		

- Molecule 28 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	172	Total	C	N	O	S	0	0
			1395	892	257	237	9		

- Molecule 29 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	96	Total	C	N	O	S	0	0
			776	503	135	136	2		

- Molecule 30 is a protein called plastid ribosomal protein uL24c.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	134	Total	C	N	O	S	0	0
			1078	677	203	195	3		

- Molecule 31 is a RNA chain called 4.5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	106	Total	C	N	O	P	0	0
			2277	1017	423	731	106		

- Molecule 32 is a protein called plastid ribosomal protein bL27c.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	X	109	Total	C	N	O	0	0
			888	560	175	153		

- Molecule 33 is a protein called plastid ribosomal protein bL28c.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	77	Total	C	N	O	S	0	0
			634	402	128	103	1		

- Molecule 34 is a protein called plastid ribosomal protein uL29c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	101	Total	C	N	O	S	0	0
			846	529	167	147	3		

- Molecule 35 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
36	2	1	Total	Zn	0
			1	1	
36	5	1	Total	Zn	0
			1	1	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	4	1	Total	Mg	0
			1	1	
37	6	1	Total	Mg	0
			1	1	
37	7	1	Total	Mg	0
			1	1	
37	A	453	Total	Mg	0
			453	453	
37	B	15	Total	Mg	0
			15	15	
37	C	1	Total	Mg	0
			1	1	
37	D	2	Total	Mg	0
			2	2	
37	E	1	Total	Mg	0
			1	1	
37	H	1	Total	Mg	0
			1	1	
37	M	2	Total	Mg	0
			2	2	
37	N	1	Total	Mg	0
			1	1	
37	P	1	Total	Mg	0
			1	1	
37	R	1	Total	Mg	0
			1	1	
37	T	1	Total	Mg	0
			1	1	
37	U	1	Total	Mg	0
			1	1	

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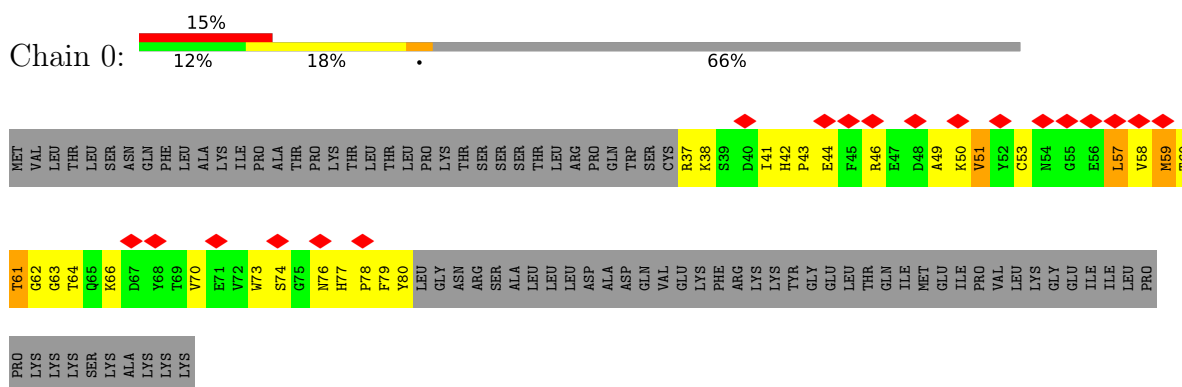
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Mol	Chain	Residues	Atoms		AltConf
37	V	2	Total 2	Mg 2	0
37	W	14	Total 14	Mg 14	0
37	X	1	Total 1	Mg 1	0
37	Y	1	Total 1	Mg 1	0

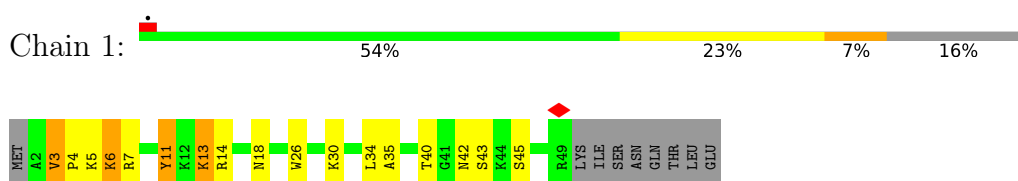
3 Residue-property plots [i](#)

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

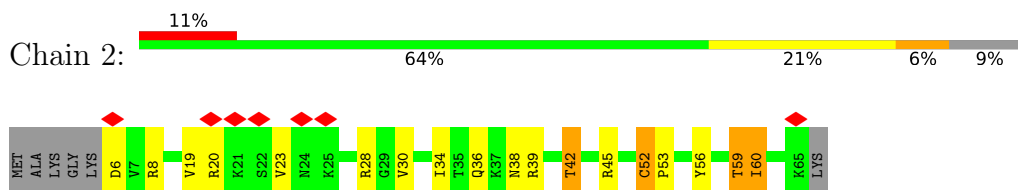
- Molecule 1: 50S ribosomal protein L31



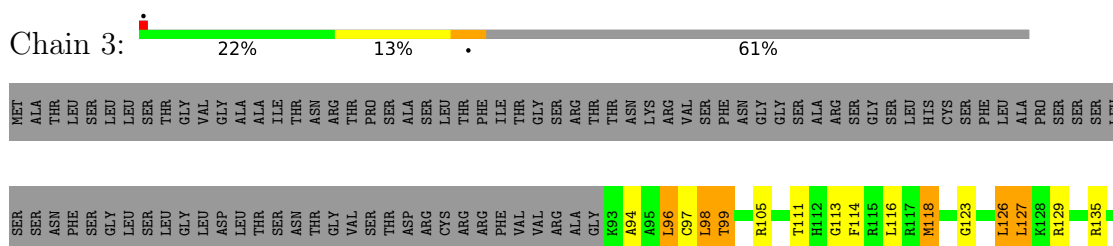
- Molecule 2: 50S ribosomal protein L32, chloroplastic



- Molecule 3: 50S ribosomal protein L33, chloroplastic



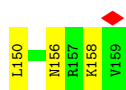
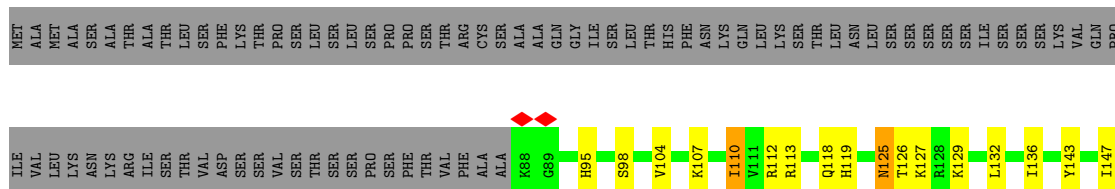
- Molecule 4: 50S ribosomal protein L34, chloroplastic





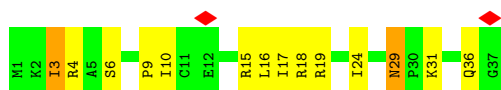
- Molecule 5: 50S ribosomal protein L35, chloroplastic

Chain 4: 33% 11% 55%



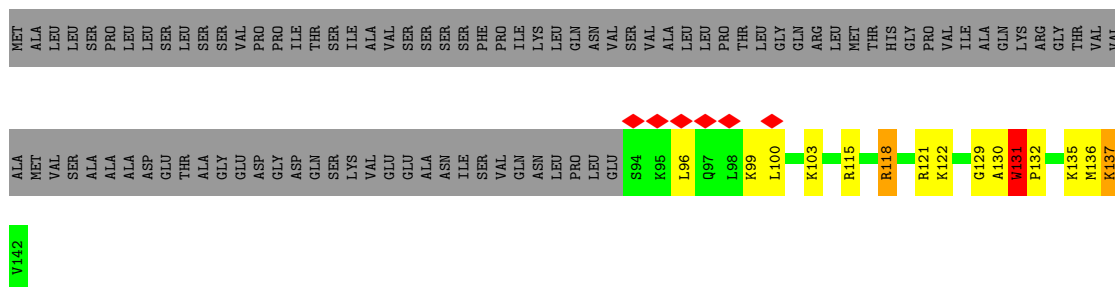
- Molecule 6: 50S ribosomal protein L36, chloroplastic

Chain 5: 5% 62% 32% 5%



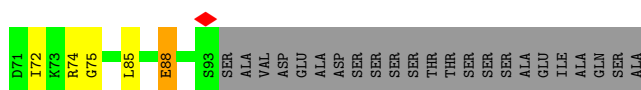
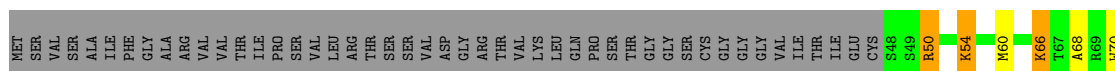
- Molecule 7: plastid ribosomal protein cL37, PSRP5

Chain 6: 23% 8% 65%

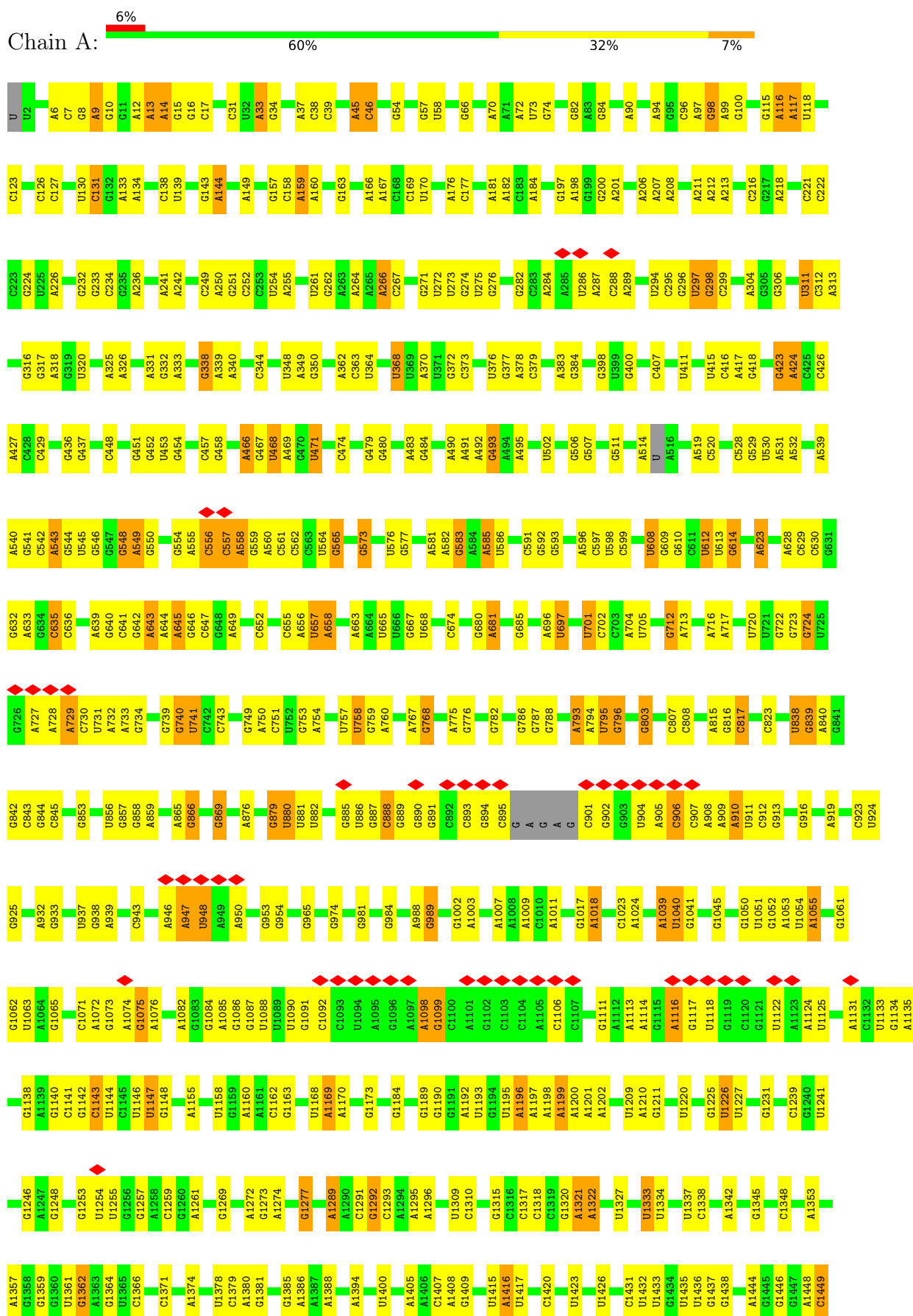


- Molecule 8: 50S ribosomal protein 6, chloroplastic

Chain 7: 30% 6% 60%



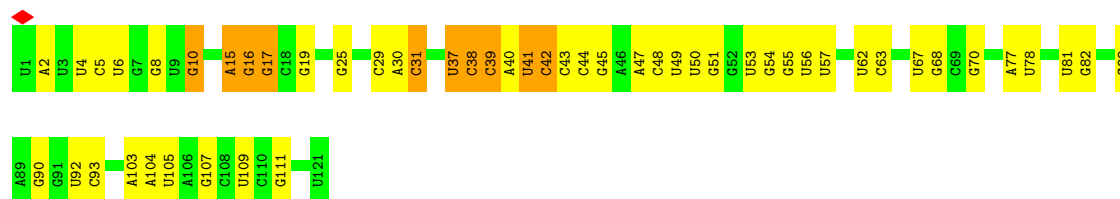
- Molecule 9: 23S ribosomal RNA



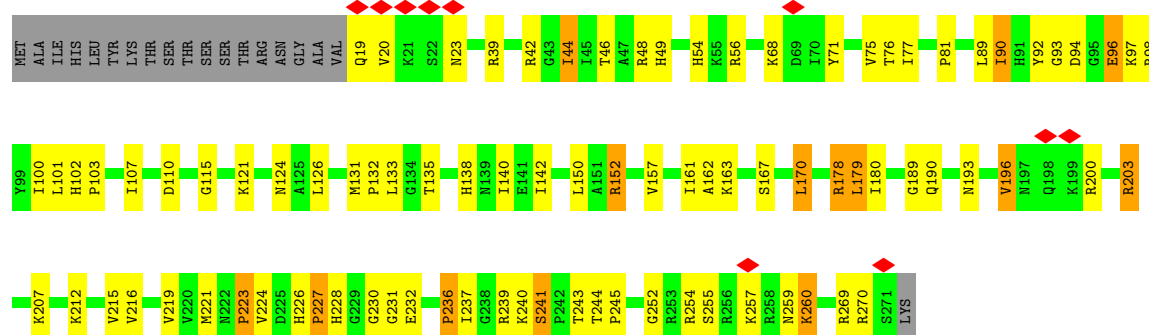
U2602	C2483	G2400	U2309	G2218	C2156	C2087	A1984	A1864	C1762	G1631	G1530	G1450
C2603	A2486	C2401	U2310	U2219	U2157	U2088	A1985	G1865	G1766	U1632	A1531	G1454
A2619	G2487	C2402	G2315	G2220	U2158	U2089	G1986	G1866	A1769	A1633	G1532	A1455
G2690	U2403	A2223	G2316	A2223	C2159	G2094	A1992	G1869	A1772	C1635	A1534	G1456
U2621	G2406	C2227	G2320	C2227	C2160	U2093	U2005	U1870	A1773	U1638	A1536	C1458
G2625	U2407	C2226	G2321	C2226	G2161	G2101	G2006	C1877	G1774	C1642	G1543	A1465
U2626	G2408	U2229	A2322	U2229	G2162	G2102	U2007	A1881	G1778	G1643	A1544	A1472
C2627	A2409	A2230	C2323	A2230	G2163	A2103	G2011	G1880	A1783	A1644	G1546	A1473
C2628	U2410	C2231	G2324	C2231	G2164	A2104	A2015	G1882	C1784	A1645	C1547	A1474
C2629	C2411	G2232	G2325	G2232	G2165	U2106	G2016	G1883	U1785	U1672	A1548	U1475
U2630	A2414	A2237	U2329	A2237	G2166	G2107	A2016	A1884	A1783	A1673	A1549	G1477
U2646	C2415	A2238	U2330	A2238	G2167	G2108	G2017	C1885	C1784	A1673	U1550	
A2649	G2416	A2242	G2331	A2242	C2168	U2112	A2027	A1886	C1791	G1678	C1554	A1480
U2653	U2418	U2245	G2332	U2245	C2169	G2113	A2028	G1887	C1800	G1679		
	G2419	U2246	C2333	U2246	C2170	U2114	A2029	G1888	A1801			
	A2423	C2249	A2339	C2249	G2171	C2115	U2030	G1889	C1807			
G2657	U2427	C2252	G2340	C2252	G2172	U2116	C2034	A1913	A1810	G1682	G1557	G1483
A2658	A2428	U2253	U2341	U2253	G2173	U2117	G2039	A1914	A1811	G1683	U1558	G1484
G2659	A2429	A2254	G2342	A2254	C2174	U2118	U2040	A1917	A1812	C1684	A1559	U1486
A2661	G2430	G2255	A2344	G2255	A2176	U2119	G2041	G1917	A1813	C1689	C1560	C1487
C2662	U2523	A2256	A2345	A2256	U2177	U2120	A2045	G1917	A1814	A1690	G1563	A1488
	U2523	C2257	A2346	C2257	C2178	G2121	U2046	G1920	A1815	U1693	G1566	G1491
	G2432	A2258	A2347	A2258	C2179	U2122	G2049	A1921	A1816	C1694	C1567	A1492
A2671	U2436	U2259	C2349	U2259	G2180	U2123	A2055	A1922	A1817	U1695	U1568	C1493
G2672	A2442	U2260	A2350	U2260	U2181	G2124	C2057	A1930	U1818	A1701	C1570	G1494
G2680	A2443	U2261	A2352	U2261	G2182	C2125	A2046	U1931	A1826	G1702	A1582	A1497
A2688	G2444	G2266	A2353	G2266	C2183	U2126	U2047	A1932	A1827	G1703	G1572	G1498
A2689	G2445	U2267	G2354	U2267	A2184	C2127	G2054	A1933	A1828	A1704	C1573	G1499
U2699	A2446	C2268	U2361	C2268	G2185	U2128	A2055	A1934	U1829	C1710	G1574	U1500
C2700	U2448	G2269	G2362	G2269	A2186	C2130	U2056	A1934	G1832	G1715	A1588	C1503
U2701	A2449	G2270	A2363	G2270	U2187	U2131	C2057	A1934	U1833	A1716	U1588	C1504
G2702	A2452	C2271	G2364	C2271	C2188	U2132	U2065	C1934	G1834	G1717	U1593	C1505
U2706	U2458	A2284	U2367	A2284	C2189	C2133	G2066	C1938	A1835	A1717	A1594	U1506
A2707	C2459	A2285	A2368	A2285	A2190	G2134	G2066	G1939	G1836	G1733	A1600	G1507
C2709	U2460	A2290	A2369	U2290	C2191	U2135	C2069	U1940	U1837	A1734	U1603	U1508
A2710	A2461	A2291	G2370	A2291	U2192	U2136	A2070	G1943	G1838	G1739	A1604	U1509
U2714	G2462	G2296	C2373	G2296	U2194	C2137	A2073	G1944	C1840	C1746	A1605	U1511
C2716	A2463	C2297	A2374	C2297	G2195	A2138	A2074	A1951	U1844	C1750	A1612	C1513
G2717	G2464	C2298	C2375	C2298	C2196	A2139	G2075	A1952	A1845	A	G1615	U1518
U2718	A2465	C2299	G2376	C2299	A2197	A2140	A2076	U1953	A1849	C	A1616	A1519
C2719	U2466	U2300	C2377	U2300	A2198	G2142	C2077	U1969	G1850	A	A1616	A1520
U2720	A2467	G2301	G2378	G2301	G2199	C2143	C2078	C1975	A1854	A	U1620	G1521
C2721	C2468	A2302	C2381	A2302	A2200	G2144	A2081	C1976	C1854	A	C1621	A1522
G2722	A2469	A2303	G2382	A2303	G2201	U2145	U2082	C1977	A1857	G1760	G1629	A1523
A2723	U2470	A2305	A2382	A2305	C2202	A2146	G2083	G1978	A1858	G1761	G1526	G1525
C2724	C2473	G2307	A2393	G2307	U2203	A2145	G2086	C1981			G1630	G1527
G2725	A2481	U2308	G2396	U2308	U2204	A2148						
C2726	C2482		U2397		G2205	A2149						
					A2206	G2150						
					A2207	G2151						
					U2208	C2152						
					U2209	C2153						
					C2210	C2154						
					U2211	C2155						
					A2212							
					A2213							
					U2217							



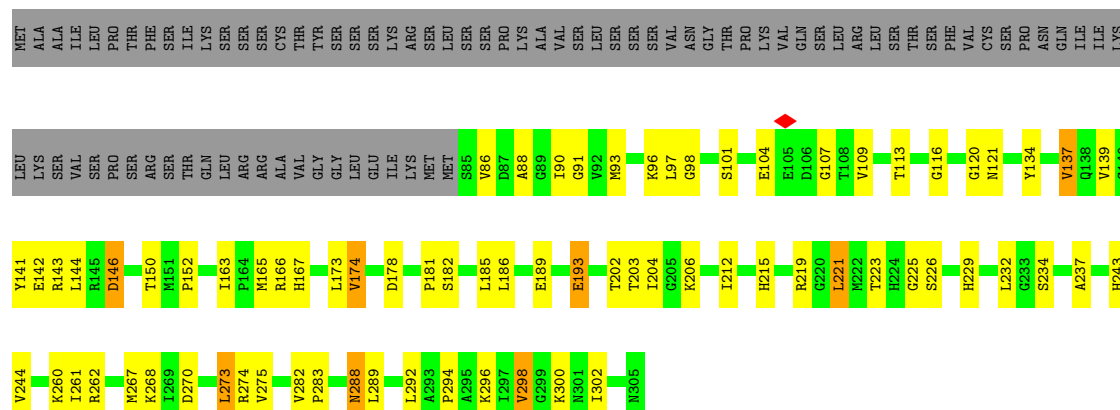
• Molecule 10: 5S ribosomal RNA



• Molecule 11: 50S ribosomal protein L2, chloroplastic



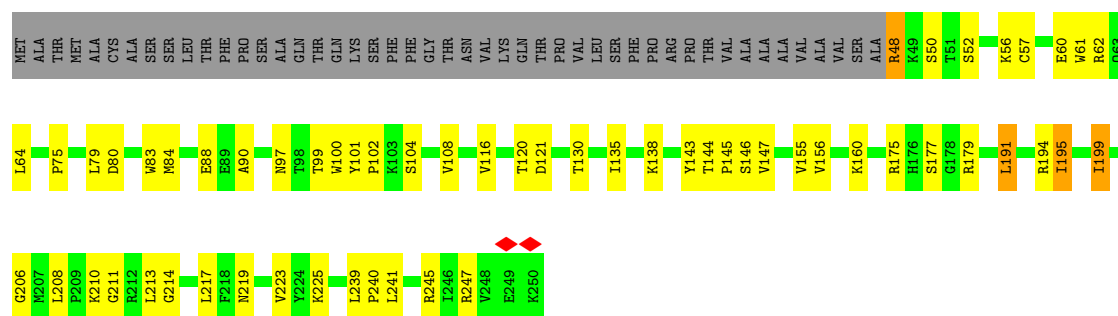
• Molecule 12: plastid ribosomal protein uL3c



• Molecule 13: plastid ribosomal protein uL4c

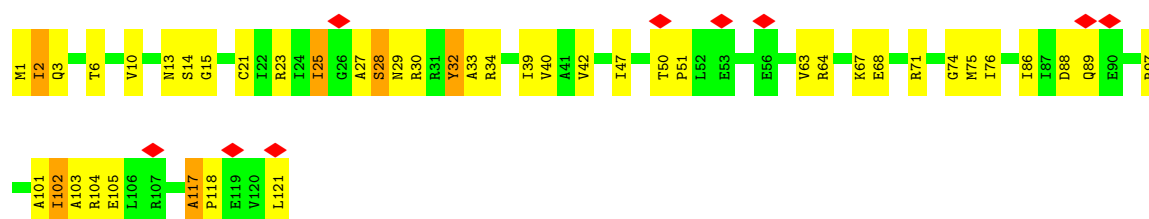


Chain K: 



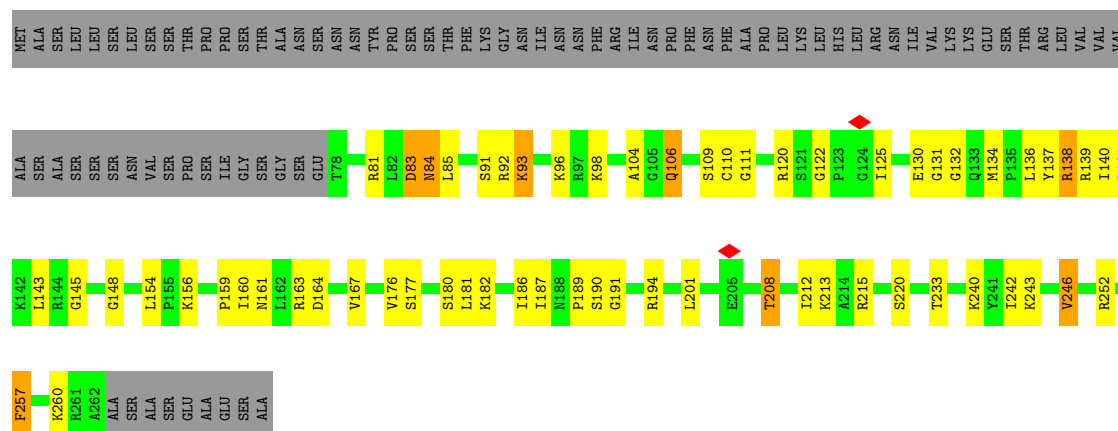
- Molecule 20: 50S ribosomal protein L14, chloroplastic

Chain L: 



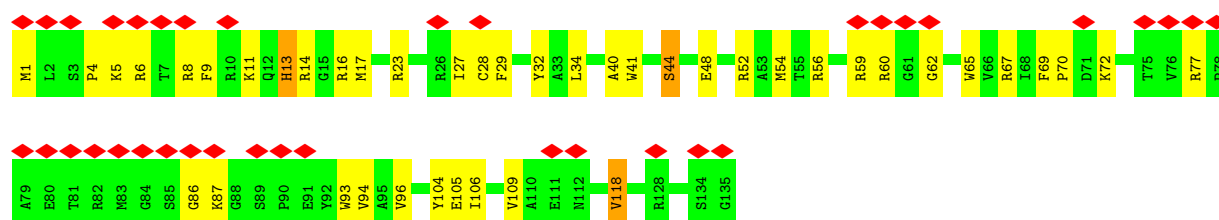
- Molecule 21: plastid ribosomal protein uL15c

Chain M: 



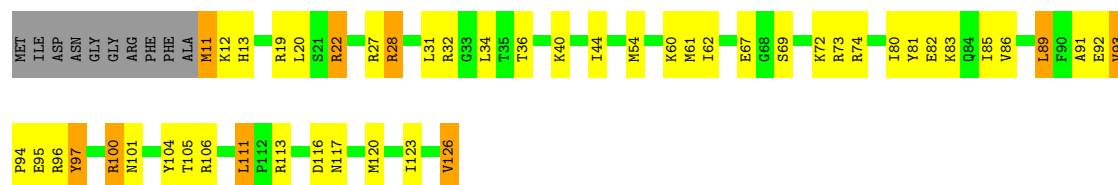
- Molecule 22: 50S ribosomal protein L16, chloroplastic

Chain N: 



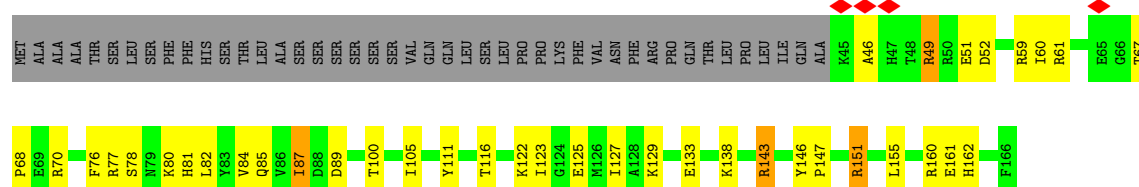
- Molecule 23: plastid ribosomal protein bL17c

Chain O: 



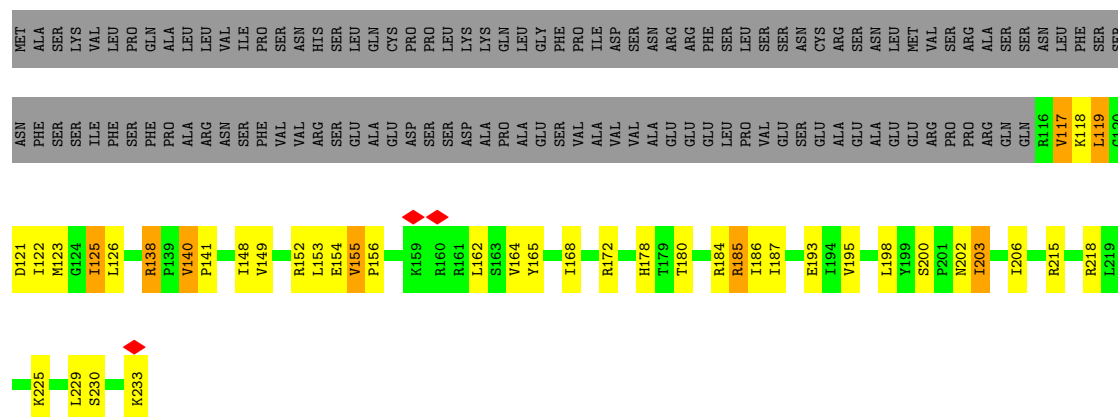
- Molecule 24: plastid ribosomal protein uL18c

Chain P: 



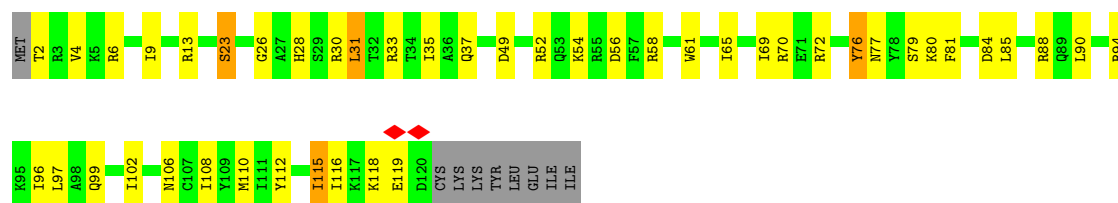
- Molecule 25: 50S ribosomal protein L19, chloroplastic

Chain Q: 

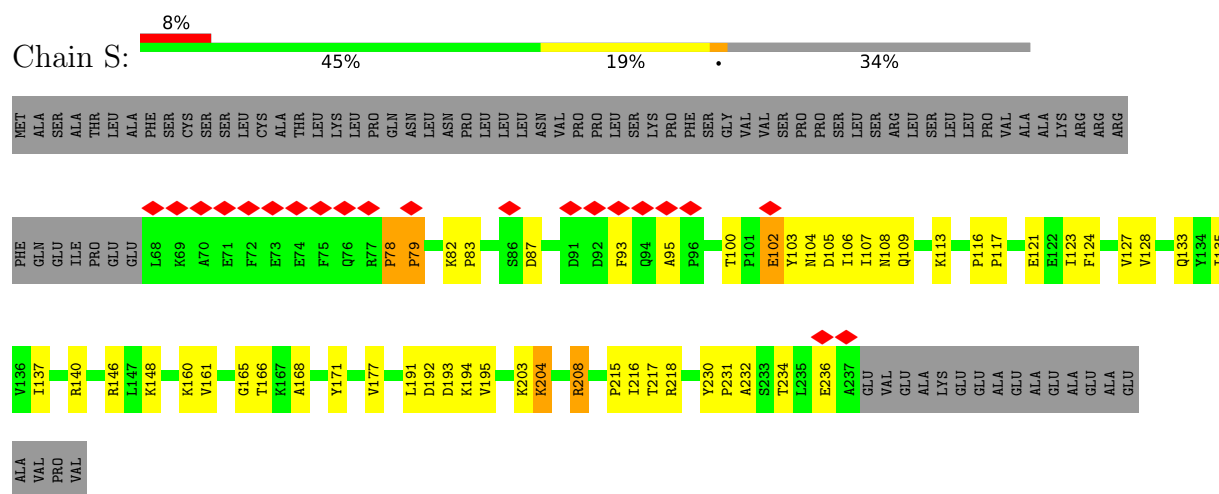


- Molecule 26: 50S ribosomal protein L20, chloroplastic

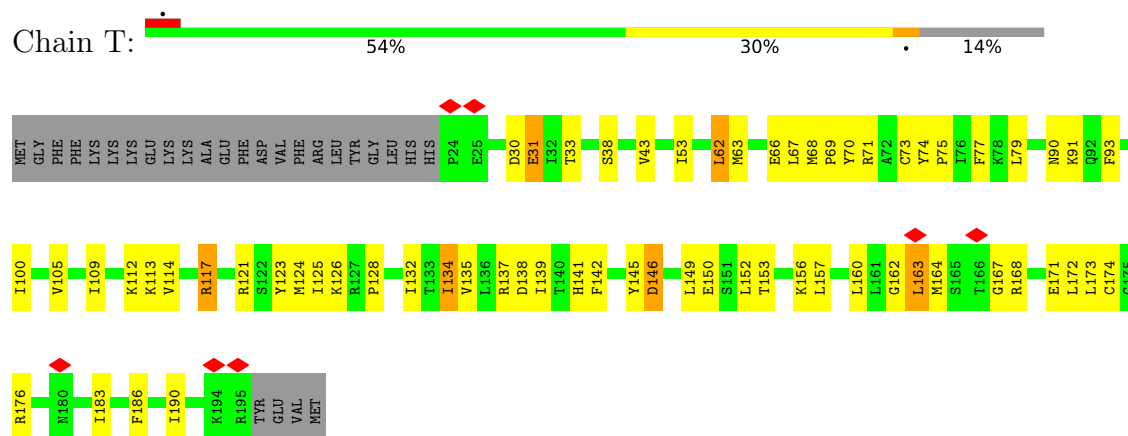
Chain R: 



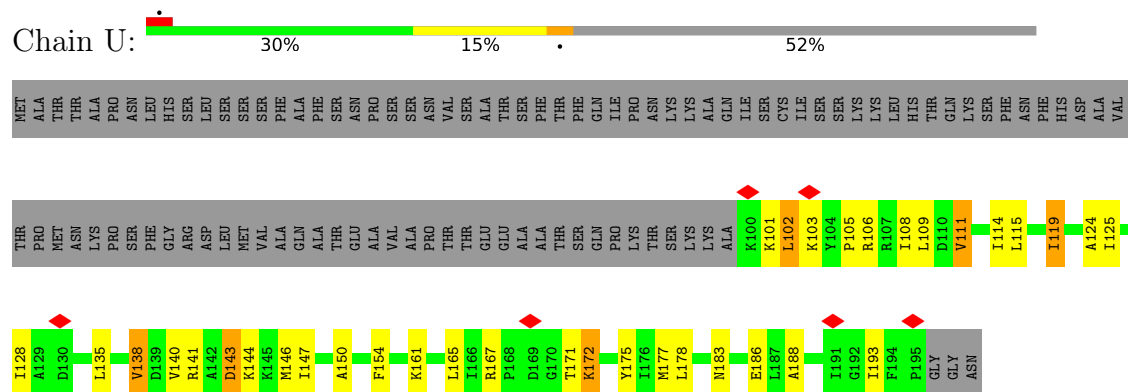
- Molecule 27: 50S ribosomal protein L21, chloroplastic



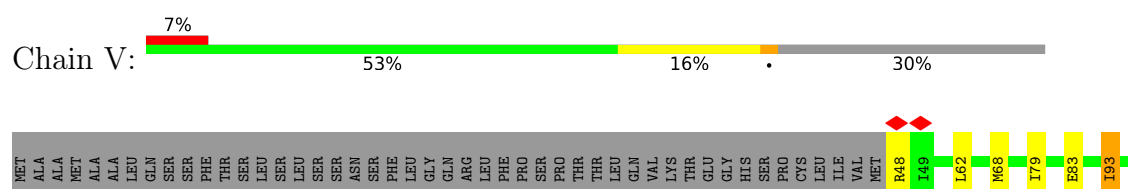
- Molecule 28: 50S ribosomal protein L22, chloroplastic

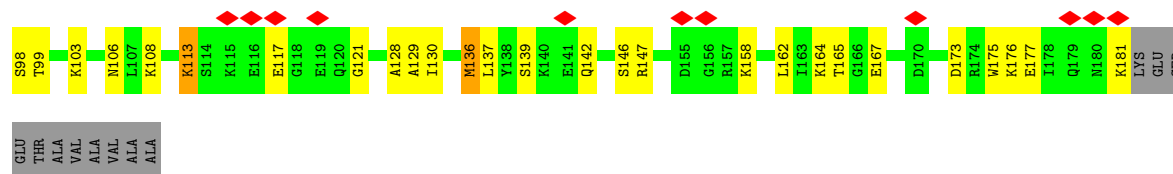


- Molecule 29: 50S ribosomal protein L23, chloroplastic

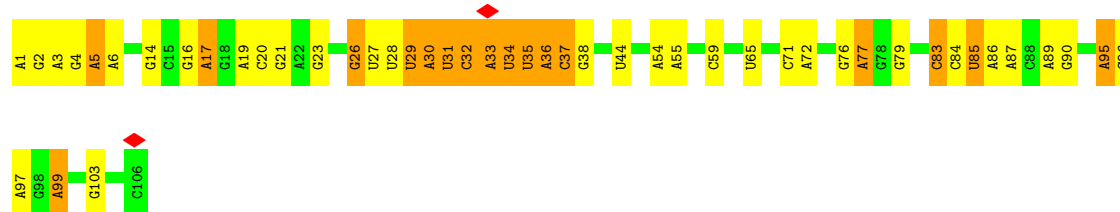


- Molecule 30: plastid ribosomal protein uL24c

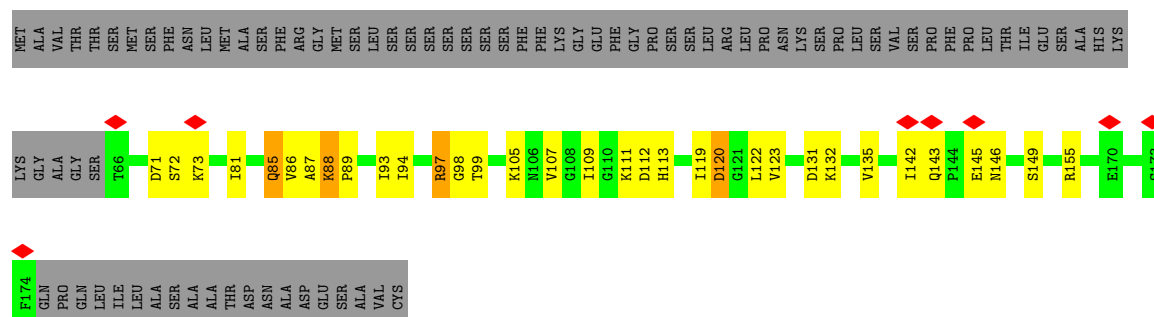




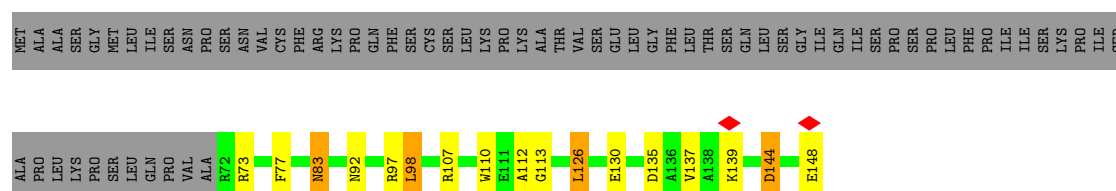
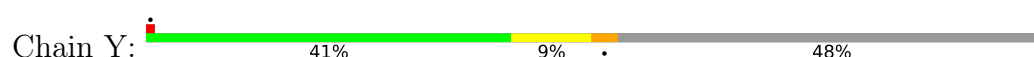
• Molecule 31: 4.5S ribosomal RNA



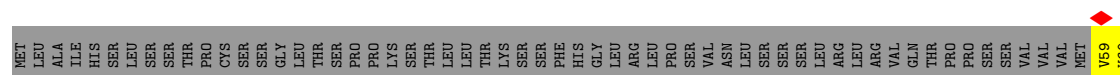
• Molecule 32: plastid ribosomal protein bL27c

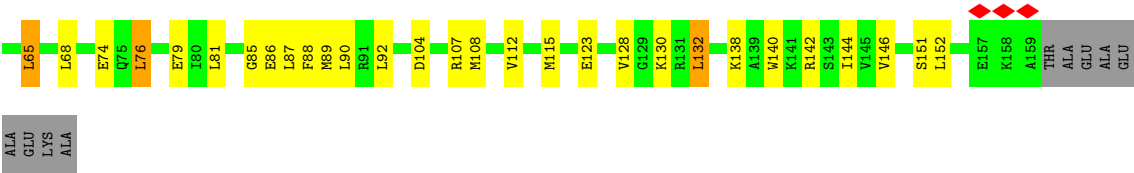


• Molecule 33: plastid ribosomal protein bL28c



• Molecule 34: plastid ribosomal protein uL29c





● Molecule 35: E-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	154332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.616	Depositor
Minimum map value	-0.270	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.63	0/369	0.97	2/499 (0.4%)
2	1	0.73	0/405	1.01	2/537 (0.4%)
3	2	0.60	0/497	1.04	5/664 (0.8%)
4	3	0.81	0/470	1.12	4/619 (0.6%)
5	4	0.71	0/594	1.11	0/784
6	5	0.52	0/307	0.92	0/403
7	6	0.62	0/425	1.47	5/551 (0.9%)
8	7	0.66	0/382	0.89	2/520 (0.4%)
9	A	0.40	0/67297	0.47	0/104984
10	B	0.24	0/2890	0.39	0/4503
11	C	0.65	0/1986	1.12	9/2666 (0.3%)
12	D	0.71	0/1713	1.08	3/2291 (0.1%)
13	E	0.69	0/1707	1.12	8/2298 (0.3%)
14	F	0.57	0/1475	1.04	10/1990 (0.5%)
15	G	0.50	0/1412	1.00	3/1898 (0.2%)
16	H	0.57	0/386	0.98	1/514 (0.2%)
17	I	0.77	0/1129	0.90	1/1521 (0.1%)
18	J	0.85	1/992 (0.1%)	0.99	3/1343 (0.2%)
19	K	0.67	1/1688 (0.1%)	0.96	2/2279 (0.1%)
20	L	0.64	0/951	1.13	4/1282 (0.3%)
21	M	0.65	0/1430	1.08	1/1896 (0.1%)
22	N	0.68	2/1097 (0.2%)	1.03	2/1471 (0.1%)
23	O	0.73	0/959	1.11	7/1280 (0.5%)
24	P	0.47	0/978	0.88	1/1311 (0.1%)
25	Q	0.70	0/967	1.14	8/1299 (0.6%)
26	R	0.79	0/1046	1.04	1/1395 (0.1%)
27	S	0.65	0/1339	1.13	4/1826 (0.2%)
28	T	0.65	0/1420	0.96	1/1900 (0.1%)
29	U	0.64	0/787	1.02	0/1056
30	V	0.55	0/1093	1.03	1/1457 (0.1%)
31	W	0.36	0/2551	0.48	0/3977
32	X	0.57	0/905	0.97	3/1204 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Y	0.64	0/644	0.93	0/856
34	Z	0.48	0/854	0.84	0/1131
35	z	0.55	0/46	1.01	0/69
All	All	0.49	4/103191 (0.0%)	0.67	93/154274 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	M	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	13	HIS	ND1-CE1	-8.30	1.24	1.32
22	N	13	HIS	CG-ND1	7.11	1.46	1.38
18	J	93	PRO	CA-C	5.46	1.57	1.52
19	K	108	VAL	CA-CB	5.11	1.60	1.54

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	6	131	TRP	CA-C-N	-16.13	103.76	120.38
7	6	131	TRP	C-N-CA	-16.13	103.76	120.38
11	C	231	GLY	N-CA-C	-8.92	98.84	113.02
20	L	117	ALA	CA-C-N	8.32	128.01	119.19
20	L	117	ALA	C-N-CA	8.32	128.01	119.19
27	S	78	PRO	N-CA-CB	8.01	110.85	103.08
12	D	215	HIS	N-CA-C	7.88	123.05	112.88
11	C	241	SER	CA-C-N	7.86	128.15	119.90
11	C	241	SER	C-N-CA	7.86	128.15	119.90
14	F	171	ASN	CA-C-N	7.85	127.48	119.56
14	F	171	ASN	C-N-CA	7.85	127.48	119.56
13	E	112	GLY	N-CA-C	-7.42	99.44	110.87
25	Q	155	VAL	CA-C-N	7.38	127.09	119.56
25	Q	155	VAL	C-N-CA	7.38	127.09	119.56
27	S	82	LYS	CA-C-N	7.35	127.11	119.76
27	S	82	LYS	C-N-CA	7.35	127.11	119.76
12	D	300	LYS	N-CA-C	7.19	122.22	113.38
7	6	129	GLY	CA-C-N	-7.12	112.38	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	6	129	GLY	C-N-CA	-7.12	112.38	122.41
20	L	74	GLY	N-CA-C	-6.95	105.47	115.27
27	S	79	PRO	N-CA-CB	6.92	110.52	103.25
18	J	93	PRO	N-CA-C	6.87	119.08	110.70
13	E	126	ARG	N-CA-C	6.86	118.83	111.36
22	N	40	ALA	N-CA-C	6.85	118.91	109.18
11	C	259	ASN	N-CA-C	6.78	121.62	112.88
13	E	172	SER	N-CA-C	6.42	119.28	110.24
15	G	70	GLY	N-CA-C	6.39	118.56	110.38
13	E	230	THR	CA-C-N	-6.36	113.14	119.56
13	E	230	THR	C-N-CA	-6.36	113.14	119.56
23	O	100	ARG	CA-C-N	-6.34	113.99	122.42
23	O	100	ARG	C-N-CA	-6.34	113.99	122.42
11	C	236	PRO	CA-C-N	-6.29	114.51	122.43
11	C	236	PRO	C-N-CA	-6.29	114.51	122.43
21	M	177	SER	CB-CA-C	-6.20	108.42	115.79
23	O	44	ILE	N-CA-C	6.08	116.92	108.23
14	F	191	PHE	CA-C-N	5.98	125.86	119.28
14	F	191	PHE	C-N-CA	5.98	125.86	119.28
14	F	74	SER	N-CA-C	5.90	119.53	111.39
30	V	103	LYS	N-CA-C	5.87	118.15	111.11
7	6	131	TRP	N-CA-C	5.85	122.75	109.81
25	Q	218	ARG	CA-C-N	-5.81	114.78	122.85
25	Q	218	ARG	C-N-CA	-5.81	114.78	122.85
4	3	143	ASN	CA-C-N	5.75	125.76	119.90
4	3	143	ASN	C-N-CA	5.75	125.76	119.90
3	2	42	THR	CA-C-N	5.68	125.30	119.56
3	2	42	THR	C-N-CA	5.68	125.30	119.56
25	Q	119	LEU	N-CA-C	5.65	118.64	111.69
23	O	93	VAL	CB-CA-C	-5.64	108.37	114.35
13	E	203	GLU	N-CA-C	5.60	119.86	113.19
14	F	195	LYS	CA-C-N	5.59	125.43	119.28
14	F	195	LYS	C-N-CA	5.59	125.43	119.28
2	1	3	VAL	CA-C-N	5.55	126.78	119.84
2	1	3	VAL	C-N-CA	5.55	126.78	119.84
4	3	99	THR	CA-C-N	-5.54	115.05	122.42
4	3	99	THR	C-N-CA	-5.54	115.05	122.42
15	G	67	GLY	CA-C-N	5.51	125.61	119.32
15	G	67	GLY	C-N-CA	5.51	125.61	119.32
14	F	190	VAL	N-CA-C	5.51	116.24	110.62
23	O	116	ASP	N-CA-C	5.49	120.66	113.30
23	O	97	TYR	N-CA-C	5.49	120.08	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	88	LYS	CA-C-N	-5.47	114.08	119.99
32	X	88	LYS	C-N-CA	-5.47	114.08	119.99
18	J	90	THR	CA-C-N	-5.44	114.38	120.14
18	J	90	THR	C-N-CA	-5.44	114.38	120.14
22	N	62	GLY	N-CA-C	5.43	126.04	113.18
14	F	93	ILE	N-CA-C	5.40	116.16	107.73
32	X	98	GLY	N-CA-C	-5.40	105.17	112.57
8	7	75	GLY	CA-C-N	5.39	125.39	119.90
8	7	75	GLY	C-N-CA	5.39	125.39	119.90
11	C	227	PRO	CA-C-N	-5.37	115.39	122.85
11	C	227	PRO	C-N-CA	-5.37	115.39	122.85
26	R	56	ASP	N-CA-C	5.35	117.11	111.28
24	P	87	ILE	N-CA-C	5.32	115.56	108.11
19	K	195	ILE	CA-C-N	5.32	124.99	119.56
19	K	195	ILE	C-N-CA	5.32	124.99	119.56
1	0	63	GLY	N-CA-C	-5.17	104.22	111.09
17	I	96	LEU	N-CA-C	5.16	119.27	112.35
14	F	230	PHE	N-CA-C	5.12	117.11	108.96
3	2	23	VAL	CB-CA-C	-5.12	102.89	111.29
12	D	229	HIS	CB-CA-C	-5.11	110.28	117.23
1	0	61	THR	N-CA-C	-5.11	102.01	108.45
28	T	31	GLU	N-CA-C	5.11	117.30	109.07
3	2	52	CYS	CA-C-N	5.08	124.75	119.56
3	2	52	CYS	C-N-CA	5.08	124.75	119.56
13	E	142	GLY	CA-C-N	5.06	124.97	119.76
13	E	142	GLY	C-N-CA	5.06	124.97	119.76
23	O	13	HIS	N-CA-C	-5.06	101.16	109.40
11	C	93	GLY	N-CA-C	-5.05	108.71	115.32
25	Q	220	TYR	N-CA-C	-5.04	107.17	113.38
16	H	87	VAL	N-CA-C	5.02	115.07	107.80
20	L	32	TYR	N-CA-C	5.01	116.69	108.52
25	Q	140	VAL	CA-C-N	5.01	124.99	120.03
25	Q	140	VAL	C-N-CA	5.01	124.99	120.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	M	104	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	359	0	330	25	0
2	1	396	0	437	15	0
3	2	489	0	507	10	0
4	3	467	0	526	15	0
5	4	588	0	658	12	0
6	5	305	0	344	9	0
7	6	422	0	508	16	0
8	7	368	0	386	6	0
9	A	60083	0	30260	544	0
10	B	2584	0	1305	38	0
11	C	1952	0	2038	56	0
12	D	1686	0	1772	51	0
13	E	1676	0	1737	39	0
14	F	1454	0	1488	52	0
15	G	1391	0	1458	38	0
16	H	382	0	437	5	0
17	I	1106	0	1122	41	0
18	J	977	0	1027	29	0
19	K	1648	0	1684	43	0
20	L	942	0	996	27	0
21	M	1410	0	1495	46	0
22	N	1075	0	1134	29	0
23	O	944	0	1004	34	0
24	P	962	0	984	28	0
25	Q	953	0	1050	27	0
26	R	1029	0	1092	34	0
27	S	1310	0	1315	38	0
28	T	1395	0	1482	44	0
29	U	776	0	837	25	0
30	V	1078	0	1144	24	0
31	W	2277	0	1146	28	0
32	X	888	0	923	15	0
33	Y	634	0	684	12	0
34	Z	846	0	918	20	0
35	z	42	0	23	1	0
36	2	1	0	0	0	0
36	5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	4	1	0	0	0	0
37	6	1	0	0	0	0
37	7	1	0	0	0	0
37	A	453	0	0	0	0
37	B	15	0	0	0	0
37	C	1	0	0	0	0
37	D	2	0	0	0	0
37	E	1	0	0	0	0
37	H	1	0	0	0	0
37	M	2	0	0	0	0
37	N	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	T	1	0	0	0	0
37	U	1	0	0	0	0
37	V	2	0	0	0	0
37	W	14	0	0	0	0
37	X	1	0	0	0	0
37	Y	1	0	0	0	0
All	All	95397	0	64251	1245	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 8.

All (1245) 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)
9:A:652:C:N4	9:A:657:U:O4	1.86	1.08
9:A:2077:C:H42	9:A:2464:G:H1	1.10	0.98
20:L:15:GLY:HA3	20:L:50:THR:HG21	1.51	0.90
9:A:817:C:OP2	21:M:120:ARG:NH1	2.06	0.89
9:A:540:A:H62	9:A:2055:U:H3	1.18	0.88
9:A:550:G:H5'	19:K:104:SER:HB2	1.56	0.88
12:D:143:ARG:HD2	12:D:163:ILE:HD12	1.59	0.85
9:A:1828:U:OP2	11:C:152:ARG:NH1	2.08	0.85
19:K:75:PRO:HD2	19:K:88:GLU:HG2	1.61	0.83
12:D:93:MET:H	12:D:121:ASN:HD21	1.23	0.82
9:A:1485:U:H5'	9:A:1486:U:H5'	1.62	0.81
17:I:139:GLU:HB3	17:I:141:PRO:HD2	1.62	0.81
2:1:6:LYS:NZ	9:A:2033:A:N7	2.26	0.81
27:S:208:ARG:HG3	27:S:208:ARG:HH11	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:894:G:N2	9:A:901:C:O2	2.14	0.81
32:X:93:ILE:HG22	32:X:94:ILE:HG13	1.61	0.81
1:O:60:THR:HB	14:F:52:GLU:HA	1.63	0.80
9:A:2464:G:N7	9:A:2518:C:H2'	1.96	0.80
25:Q:138:ARG:HH12	25:Q:203:ILE:HB	1.47	0.80
9:A:2142:G:H1	9:A:2174:C:H42	1.29	0.80
9:A:2345:A:H2'	9:A:2346:A:C8	2.17	0.79
9:A:2125:C:O2	9:A:2161:G:N2	2.15	0.78
2:1:13:LYS:NZ	9:A:528:C:OP1	2.17	0.78
9:A:2726:G:OP1	23:O:28:ARG:NH1	2.16	0.78
10:B:8:G:H21	24:P:85:GLN:HE22	1.32	0.77
11:C:75:VAL:HG13	11:C:76:THR:HG22	1.65	0.77
14:F:107:ILE:HG23	14:F:118:PRO:HD2	1.67	0.77
7:6:118:ARG:NH1	9:A:1491:G:OP2	2.14	0.76
9:A:2657:G:OP2	19:K:194:ARG:NH2	2.18	0.76
13:E:128:SER:HB2	13:E:134:ARG:HH22	1.51	0.76
9:A:888:C:H3'	9:A:889:G:H8	1.49	0.76
9:A:1810:C:OP2	11:C:178:ARG:NH2	2.18	0.75
9:A:468:U:O2	9:A:471:U:O2'	2.04	0.75
3:2:6:ASP:O	3:2:39:ARG:NH2	2.20	0.75
7:6:132:PRO:O	7:6:135:LYS:N	2.16	0.75
9:A:2601:U:H5'	9:A:2602:U:H5'	1.69	0.75
9:A:2075:G:N2	9:A:2076:A:N1	2.36	0.74
10:B:44:C:O2	14:F:145:ARG:NH1	2.21	0.74
17:I:122:ILE:HD12	17:I:165:CYS:HB2	1.67	0.74
18:J:129:ILE:HD11	18:J:137:PHE:HB2	1.69	0.74
28:T:112:LYS:HB3	28:T:124:MET:HE1	1.70	0.74
9:A:182:A:N6	9:A:2447:A:O2'	2.21	0.74
9:A:2719:G:OP1	23:O:83:LYS:NZ	2.21	0.74
9:A:2077:C:N4	9:A:2464:G:H1	1.83	0.74
28:T:164:MET:HB2	28:T:168:ARG:HB2	1.70	0.73
9:A:596:A:H62	9:A:1272:A:H2	1.37	0.73
9:A:2486:A:N6	9:A:2498:G:O2'	2.20	0.73
26:R:76:TYR:OH	26:R:84:ASP:OD2	2.07	0.73
9:A:646:G:OP2	21:M:156:LYS:NZ	2.21	0.73
20:L:88:ASP:OD1	20:L:89:GLN:N	2.20	0.73
9:A:13:A:H2'	9:A:14:A:C8	2.23	0.73
24:P:81:HIS:HD2	24:P:100:THR:HB	1.52	0.73
9:A:2767:A:H3'	9:A:2768:A:H5''	1.71	0.72
9:A:723:G:H2'	9:A:724:G:H5''	1.71	0.72
11:C:157:VAL:HB	11:C:190:GLN:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2069:C:H5'	9:A:2070:A:H5''	1.71	0.72
20:L:13:ASN:HD21	20:L:97:ARG:HB3	1.53	0.72
9:A:869:G:O2'	9:A:925:G:O6	2.08	0.71
9:A:757:U:O2'	9:A:2628:C:O2'	2.08	0.71
10:B:15:A:H4'	10:B:16:G:H5''	1.72	0.71
17:I:63:VAL:HG13	17:I:113:ALA:HB2	1.71	0.71
13:E:128:SER:HB2	13:E:134:ARG:NH2	2.06	0.70
9:A:545:U:H2'	9:A:546:G:C8	2.26	0.70
17:I:77:ALA:HB3	17:I:133:LEU:HB3	1.74	0.70
27:S:192:ASP:OD1	27:S:193:ASP:N	2.25	0.70
9:A:2073:A:N6	9:A:2520:A:O5'	2.25	0.70
19:K:206:GLY:O	19:K:210:LYS:NZ	2.24	0.70
9:A:376:U:O2'	9:A:378:A:N1	2.24	0.70
9:A:879:G:O3'	22:N:6:ARG:NH1	2.26	0.69
14:F:55:ASN:HA	14:F:59:THR:HB	1.74	0.69
9:A:1408:A:H5'	9:A:1488:A:H1'	1.74	0.69
1:O:77:HIS:CG	1:O:78:PRO:HD2	2.28	0.69
14:F:160:ALA:HB1	14:F:190:VAL:HB	1.75	0.68
6:5:19:ARG:HG2	9:A:2774:U:H5''	1.76	0.68
13:E:230:THR:HG22	13:E:231:PRO:HD2	1.74	0.68
21:M:182:LYS:HE2	21:M:189:PRO:HG2	1.74	0.68
9:A:844:G:H1'	21:M:130:GLU:HB3	1.76	0.68
10:B:54:G:HO2'	10:B:55:G:H8	1.41	0.68
1:O:37:ARG:N	10:B:45:G:OP1	2.26	0.68
22:N:13:HIS:O	22:N:72:LYS:NZ	2.26	0.68
9:A:1531:A:N6	11:C:94:ASP:OD2	2.27	0.67
18:J:79:VAL:HG22	18:J:130:THR:HG23	1.76	0.67
9:A:1385:G:H5''	33:Y:73:ARG:HH21	1.58	0.67
10:B:10:G:O5'	24:P:61:ARG:NH1	2.28	0.67
4:3:105:ARG:NH1	4:3:149:ARG:O	2.28	0.67
13:E:103:LEU:HB3	13:E:107:GLU:HB2	1.75	0.67
9:A:1086:G:H21	18:J:198:ILE:HG12	1.60	0.67
9:A:2345:A:H2'	9:A:2346:A:H8	1.60	0.67
4:3:111:THR:O	4:3:116:LEU:HD23	1.94	0.66
9:A:2310:U:H5''	24:P:143:ARG:HH12	1.58	0.66
9:A:1978:G:O2'	9:A:1981:C:OP2	2.13	0.66
9:A:1844:U:H5''	9:A:1845:G:H5'	1.77	0.66
9:A:45:A:H2'	9:A:46:C:H5'	1.76	0.66
7:6:121:ARG:NH2	9:A:1549:A:OP1	2.29	0.66
17:I:54:ILE:HG23	17:I:58:LYS:HD3	1.78	0.66
17:I:123:LYS:HA	17:I:126:MET:HE3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:133:LEU:HD21	11:C:163:LYS:HG2	1.78	0.66
15:G:126:LYS:HE3	15:G:205:VAL:HG11	1.78	0.66
9:A:1832:G:H2'	9:A:1833:G:H5''	1.78	0.65
7:6:121:ARG:HH22	9:A:1549:A:P	2.20	0.65
9:A:1769:A:HO2'	9:A:2732:G:HO2'	1.40	0.65
9:A:2464:G:H4'	9:A:2465:A:H5'	1.78	0.65
15:G:48:ILE:HB	15:G:90:LEU:HB2	1.79	0.65
19:K:100:TRP:H	26:R:99:GLN:HE22	1.43	0.65
11:C:167:SER:HB2	11:C:179:LEU:HG	1.77	0.65
9:A:1812:A:H2'	9:A:1813:A:C8	2.31	0.65
15:G:74:ILE:HG21	15:G:115:MET:HE1	1.78	0.65
20:L:2:ILE:HB	20:L:33:ALA:HB3	1.78	0.65
9:A:312:C:OP1	30:V:164:LYS:NZ	2.30	0.65
9:A:1817:G:H5'	9:A:1818:U:OP2	1.96	0.65
13:E:207:PHE:HB2	13:E:228:LEU:HD22	1.78	0.65
9:A:1091:G:O2'	18:J:160:SER:O	2.14	0.65
9:A:2078:C:C2	9:A:2464:G:N2	2.65	0.65
9:A:2105:U:OP1	16:H:47:LYS:NZ	2.18	0.65
6:5:15:ARG:NH1	9:A:2771:A:O2'	2.30	0.64
12:D:166:ARG:NH1	31:W:26:G:OP1	2.29	0.64
9:A:232:G:OP2	9:A:234:C:N4	2.30	0.64
9:A:2256:A:OP1	11:C:239:ARG:NH2	2.31	0.64
9:A:2320:G:H1	9:A:2330:U:H3	1.45	0.64
8:7:85:LEU:HD13	27:S:160:LYS:HE3	1.80	0.64
9:A:1604:A:H2'	9:A:1605:A:C8	2.32	0.64
9:A:96:C:OP1	34:Z:60:LYS:NZ	2.31	0.64
19:K:99:THR:HA	26:R:99:GLN:NE2	2.12	0.64
12:D:202:THR:HG22	12:D:288:ASN:HD21	1.63	0.64
2:1:40:THR:HG23	2:1:42:ASN:H	1.61	0.64
1:0:61:THR:HG22	1:0:62:GLY:H	1.63	0.63
29:U:108:ILE:HD13	34:Z:138:LYS:HD2	1.80	0.63
9:A:9:A:C2	31:W:99:A:H1'	2.33	0.63
13:E:104:THR:HG22	13:E:107:GLU:HG2	1.78	0.63
34:Z:90:LEU:HD21	34:Z:104:ASP:HB3	1.80	0.63
4:3:123:GLY:O	4:3:126:LEU:HB2	1.99	0.63
9:A:2089:U:OP1	11:C:239:ARG:NH1	2.31	0.63
9:A:2628:C:H5'	9:A:2629:A:OP2	1.98	0.63
9:A:1886:A:H2'	9:A:1887:G:H8	1.63	0.63
1:0:43:PRO:HG3	14:F:111:ALA:HB1	1.78	0.63
9:A:642:G:N2	9:A:645:A:OP2	2.24	0.63
9:A:2147:G:H21	9:A:2172:A:H61	1.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:207:LYS:HD2	11:C:212:LYS:HD3	1.80	0.63
15:G:76:TYR:OH	15:G:112:THR:HG21	1.99	0.63
9:A:548:G:HO2'	9:A:549:A:P	2.21	0.63
24:P:129:LYS:O	24:P:133:GLU:HG2	1.99	0.63
9:A:176:A:H2'	9:A:177:C:C6	2.34	0.62
25:Q:186:ILE:HG12	25:Q:230:SER:HB3	1.80	0.62
9:A:495:A:O2'	30:V:121:GLY:HA3	1.99	0.62
12:D:221:LEU:O	12:D:226:SER:OG	2.17	0.62
20:L:102:ILE:HG22	20:L:103:ALA:H	1.64	0.62
21:M:159:PRO:O	21:M:160:ILE:HD13	1.99	0.62
13:E:243:GLU:OE1	21:M:81:ARG:NH2	2.32	0.62
23:O:101:ASN:OD1	31:W:44:U:O2'	2.18	0.62
28:T:113:LYS:HG3	28:T:125:ILE:HB	1.82	0.62
23:O:67:GLU:OE1	23:O:72:LYS:HE3	1.99	0.62
9:A:1090:U:H1'	18:J:205:ASN:HD21	1.64	0.62
9:A:1111:G:N1	9:A:1114:A:OP2	2.31	0.62
12:D:93:MET:H	12:D:121:ASN:ND2	1.97	0.62
9:A:98:G:H2'	30:V:175:TRP:CZ2	2.35	0.61
14:F:110:LEU:HA	14:F:113:ILE:HD12	1.82	0.61
23:O:34:LEU:HB3	23:O:54:MET:SD	2.40	0.61
4:3:148:LYS:NZ	9:A:1638:U:OP2	2.30	0.61
9:A:1883:G:H2'	9:A:1884:A:O4'	2.00	0.61
23:O:113:ARG:HD3	23:O:120:MET:HE2	1.80	0.61
20:L:76:ILE:HB	25:Q:195:VAL:HB	1.83	0.61
9:A:1082:A:H4'	17:I:83:GLY:HA2	1.82	0.61
20:L:30:ARG:HG2	20:L:32:TYR:H	1.65	0.61
13:E:116:TYR:CZ	13:E:130:ARG:HD3	2.35	0.61
19:K:121:ASP:O	19:K:247:ARG:NH1	2.34	0.61
9:A:2467:A:OP1	9:A:2514:A:O2'	2.09	0.61
17:I:100:THR:HG22	17:I:135:VAL:HG12	1.82	0.61
27:S:208:ARG:HG3	27:S:208:ARG:NH1	2.10	0.61
26:R:112:TYR:CZ	26:R:116:ILE:HD11	2.36	0.61
13:E:60:PHE:O	13:E:196:ARG:NH1	2.33	0.61
9:A:2662:C:O2'	9:A:2750:G:O2'	2.13	0.60
11:C:243:THR:HG22	11:C:244:THR:O	2.01	0.60
21:M:98:LYS:HE2	21:M:106:GLN:HG3	1.83	0.60
4:3:118:MET:HE1	4:3:127:LEU:HD12	1.82	0.60
9:A:58:U:H1'	9:A:72:A:H2'	1.82	0.60
3:2:20:ARG:HG2	3:2:30:VAL:HG21	1.83	0.60
6:5:31:LYS:HE2	9:A:2495:A:H5'	1.83	0.60
7:6:99:LYS:O	7:6:103:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:94:LYS:HB2	15:G:97:GLU:OE2	2.02	0.60
27:S:208:ARG:HH11	27:S:208:ARG:CG	2.12	0.60
9:A:1473:G:H5'	9:A:1474:A:H5''	1.84	0.60
9:A:2075:G:H5''	9:A:2519:G:H4'	1.83	0.60
32:X:89:PRO:HD3	32:X:120:ASP:OD1	2.01	0.60
1:O:37:ARG:HB3	1:O:42:HIS:HD2	1.66	0.60
9:A:1345:G:OP2	28:T:113:LYS:NZ	2.34	0.60
17:I:161:PHE:HE2	17:I:176:VAL:HG11	1.67	0.60
9:A:255:A:OP2	9:A:271:G:N1	2.19	0.60
9:A:2549:G:N2	9:A:2680:G:O2'	2.35	0.60
33:Y:97:ARG:HG2	33:Y:98:LEU:N	2.16	0.60
9:A:511:G:N1	9:A:514:A:OP2	2.35	0.60
12:D:88:ALA:O	12:D:294:PRO:HG2	2.02	0.60
19:K:239:LEU:HD12	19:K:240:PRO:HD2	1.82	0.60
27:S:104:ASN:HA	27:S:107:ILE:HG22	1.83	0.60
9:A:1689:C:O2'	23:O:19:ARG:NH2	2.35	0.60
9:A:2340:G:H2'	9:A:2341:U:H5'	1.84	0.59
9:A:984:G:N7	22:N:14:ARG:NH2	2.47	0.59
12:D:90:ILE:HD11	12:D:173:LEU:HD11	1.83	0.59
2:1:3:VAL:HG12	9:A:2029:A:C2	2.37	0.59
9:A:543:A:H2'	9:A:543:A:N3	2.17	0.59
9:A:1040:U:OP1	26:R:70:ARG:NH2	2.35	0.59
3:2:56:TYR:OH	9:A:655:C:O4'	2.18	0.59
9:A:1133:U:H2'	9:A:1134:G:H8	1.67	0.59
25:Q:138:ARG:NH1	25:Q:203:ILE:HB	2.16	0.59
9:A:2249:C:P	33:Y:97:ARG:HH22	2.26	0.59
29:U:183:ASN:HB3	29:U:186:GLU:HG3	1.85	0.59
19:K:191:LEU:HD13	19:K:199:ILE:HG13	1.84	0.59
23:O:60:LYS:HB3	23:O:61:MET:HE2	1.85	0.59
9:A:2340:G:C2'	9:A:2341:U:H5'	2.32	0.59
18:J:171:ILE:HG12	18:J:210:ILE:HG12	1.85	0.59
29:U:119:ILE:HG21	29:U:167:ARG:HH22	1.68	0.59
9:A:411:U:H1'	16:H:42:GLN:HE21	1.68	0.58
26:R:88:ARG:HG3	26:R:115:ILE:HD12	1.84	0.58
8:7:50:ARG:NH1	9:A:1055:A:O2'	2.36	0.58
22:N:67:ARG:NH1	22:N:105:GLU:OE1	2.31	0.58
19:K:61:TRP:HZ2	28:T:157:LEU:HD23	1.67	0.58
29:U:119:ILE:HG13	29:U:135:LEU:HB3	1.86	0.58
15:G:44:GLY:HA3	15:G:105:HIS:CD2	2.39	0.58
27:S:100:THR:HG22	27:S:102:GLU:H	1.68	0.58
9:A:1497:A:H2'	9:A:1497:A:N3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:72:LEU:HD13	15:G:115:MET:HB2	1.86	0.58
9:A:885:G:H1	9:A:911:U:H3	1.52	0.58
12:D:143:ARG:HG2	12:D:144:LEU:H	1.68	0.58
9:A:2047:A:O2'	9:A:2049:G:OP2	2.22	0.57
18:J:183:LYS:HE2	18:J:187:LEU:HD21	1.85	0.57
27:S:106:ILE:HD13	28:T:162:GLY:HA3	1.85	0.57
9:A:1220:U:H1'	26:R:4:VAL:HG22	1.85	0.57
9:A:1880:G:N7	21:M:252:ARG:NH1	2.52	0.57
11:C:138:HIS:ND1	11:C:189:GLY:O	2.31	0.57
11:C:223:PRO:HD3	11:C:230:GLY:H	1.69	0.57
9:A:886:U:H3	9:A:910:A:H61	1.52	0.57
9:A:1362:G:H21	29:U:177:MET:HE1	1.69	0.57
9:A:2706:U:H2'	9:A:2706:U:O2	2.05	0.57
9:A:426:C:H2'	9:A:427:A:C8	2.39	0.57
23:O:100:ARG:NH2	31:W:85:U:H5'	2.19	0.57
9:A:2761:U:OP2	9:A:2773:C:N4	2.37	0.57
18:J:189:CYS:SG	18:J:195:ALA:HB2	2.44	0.57
25:Q:153:LEU:HD12	25:Q:165:TYR:HE2	1.69	0.57
9:A:612:U:HO2'	9:A:614:G:HO2'	1.51	0.57
9:A:2321:G:H22	9:A:2329:U:H3	1.50	0.57
9:A:2332:G:H2'	9:A:2333:C:C6	2.40	0.57
6:5:6:SER:HB2	9:A:2483:C:H5''	1.86	0.57
15:G:41:SER:HG	15:G:105:HIS:CE1	2.22	0.57
23:O:11:MET:SD	23:O:11:MET:N	2.78	0.57
1:0:46:ARG:CZ	1:0:66:LYS:HB2	2.35	0.57
12:D:274:ARG:NH1	31:W:36:A:N1	2.52	0.57
22:N:44:SER:HB3	22:N:70:PRO:HG3	1.86	0.57
28:T:70:TYR:HB2	28:T:73:CYS:SG	2.45	0.57
1:0:53:CYS:HB3	1:0:57:LEU:HB3	1.86	0.56
9:A:681:A:H5''	21:M:122:GLY:HA2	1.87	0.56
9:A:1817:G:H5''	9:A:1817:G:H8	1.70	0.56
18:J:176:LEU:HB3	18:J:196:MET:HG3	1.86	0.56
1:0:42:HIS:CE1	14:F:116:GLN:HE22	2.22	0.56
5:4:98:SER:HB2	5:4:150:LEU:HD21	1.86	0.56
9:A:474:C:O2'	13:E:118:GLN:NE2	2.38	0.56
9:A:531:A:H2'	9:A:532:A:C8	2.40	0.56
9:A:1857:A:HO2'	9:A:1858:A:H8	1.50	0.56
9:A:2447:A:H2'	9:A:2447:A:N3	2.19	0.56
9:A:2469:C:H2'	9:A:2470:A:C8	2.39	0.56
11:C:56:ARG:HD3	11:C:81:PRO:HB2	1.86	0.56
19:K:97:ASN:HD21	27:S:135:ILE:H	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:89:LEU:HD22	23:O:93:VAL:HG23	1.87	0.56
8:7:68:ALA:HB1	8:7:70:TRP:CD1	2.40	0.56
9:A:13:A:H2'	9:A:14:A:H8	1.69	0.56
9:A:1106:C:O2'	9:A:1116:A:OP1	2.17	0.56
10:B:54:G:O6	24:P:80:LYS:NZ	2.32	0.56
20:L:3:GLN:O	20:L:6:THR:OG1	2.10	0.56
24:P:84:VAL:HG21	24:P:155:LEU:HD11	1.88	0.56
5:4:107:LYS:HB2	9:A:663:A:H5'	1.87	0.56
9:A:1098:A:N7	9:A:1124:A:O2'	2.31	0.56
9:A:1273:G:H1	26:R:37:GLN:HE21	1.53	0.56
4:3:99:THR:O	9:A:697:U:O2'	2.23	0.56
9:A:2206:A:H2'	9:A:2207:A:C8	2.41	0.56
18:J:200:ALA:HA	18:J:210:ILE:HD12	1.88	0.56
3:2:59:THR:HG22	3:2:60:ILE:H	1.70	0.56
9:A:1570:C:H4'	9:A:1571:G:C2	2.41	0.56
9:A:2122:C:O2	9:A:2195:G:N1	2.39	0.56
20:L:30:ARG:HD3	20:L:32:TYR:O	2.05	0.56
9:A:131:C:OP2	29:U:101:LYS:NZ	2.39	0.55
9:A:720:U:H3	9:A:733:A:H61	1.54	0.55
9:A:1211:G:H5''	21:M:111:GLY:HA2	1.87	0.55
12:D:142:GLU:HB3	12:D:166:ARG:HB3	1.88	0.55
19:K:52:SER:HB3	31:W:1:A:O4'	2.06	0.55
9:A:635:C:H2'	9:A:636:C:C6	2.41	0.55
15:G:166:GLU:HG3	15:G:168:ASN:HB2	1.87	0.55
31:W:32:C:H2'	31:W:33:A:H2'	1.87	0.55
6:5:29:ASN:HD21	6:5:31:LYS:HB2	1.72	0.55
13:E:243:GLU:HA	21:M:81:ARG:HH21	1.71	0.55
14:F:67:PRO:O	14:F:71:GLU:HG2	2.06	0.55
20:L:25:ILE:HD11	20:L:40:VAL:HG23	1.89	0.55
9:A:2203:U:H2'	9:A:2204:A:O4'	2.07	0.55
20:L:13:ASN:ND2	20:L:97:ARG:HB3	2.19	0.55
27:S:171:TYR:CE2	27:S:232:ALA:HB2	2.42	0.55
1:0:50:LYS:HG3	1:0:58:VAL:HG13	1.88	0.55
9:A:573:G:H21	26:R:37:GLN:HE22	1.54	0.55
20:L:121:LEU:HD22	25:Q:165:TYR:HE1	1.72	0.55
21:M:93:LYS:HZ3	21:M:93:LYS:HB3	1.72	0.55
9:A:2432:G:H5''	21:M:148:GLY:HA3	1.88	0.54
21:M:134:MET:O	21:M:139:ARG:NH1	2.39	0.54
9:A:704:A:O2'	9:A:1374:A:N3	2.39	0.54
28:T:62:LEU:HD22	28:T:77:PHE:CE1	2.42	0.54
32:X:143:GLN:O	32:X:145:GLU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1690:A:OP2	23:O:11:MET:HA	2.07	0.54
29:U:135:LEU:HD21	29:U:175:TYR:CD2	2.42	0.54
30:V:68:MET:HE1	30:V:98:SER:HA	1.90	0.54
9:A:1195:U:H3'	9:A:1196:A:H8	1.71	0.54
12:D:146:ASP:N	12:D:146:ASP:OD1	2.36	0.54
9:A:318:A:N3	9:A:338:G:O2'	2.41	0.54
9:A:1169:A:H5'	19:K:245:ARG:CZ	2.37	0.54
18:J:125:ILE:HG21	18:J:141:LEU:HD22	1.90	0.54
30:V:83:GLU:CD	30:V:106:ASN:H	2.16	0.54
31:W:29:U:H2'	31:W:83:C:H42	1.72	0.54
9:A:1520:A:H4'	9:A:1521:G:OP1	2.08	0.54
11:C:68:LYS:HD2	11:C:115:GLY:HA2	1.89	0.54
17:I:76:LEU:HD22	17:I:134:PHE:HD1	1.73	0.54
5:4:113:ARG:HB2	21:M:141:PRO:HG2	1.89	0.54
9:A:1090:U:H1'	18:J:205:ASN:ND2	2.22	0.54
9:A:1113:A:H61	17:I:86:VAL:HG11	1.71	0.54
19:K:155:VAL:HB	19:K:223:VAL:HG22	1.88	0.54
29:U:138:VAL:HG21	29:U:147:ILE:HD11	1.90	0.54
9:A:2414:A:H2'	9:A:2415:C:C6	2.43	0.54
12:D:113:THR:HG21	12:D:282:VAL:HG22	1.89	0.54
28:T:146:ASP:O	28:T:150:GLU:HG2	2.07	0.54
10:B:56:U:O2'	14:F:77:ASN:ND2	2.38	0.54
15:G:82:VAL:HG22	15:G:92:VAL:HG22	1.89	0.54
15:G:112:THR:HA	15:G:115:MET:HE3	1.89	0.54
19:K:130:THR:HG21	19:K:241:LEU:HD23	1.89	0.54
9:A:296:G:H2'	9:A:297:U:C5	2.43	0.53
9:A:2249:C:OP2	33:Y:97:ARG:NH2	2.38	0.53
1:0:44:GLU:O	1:0:64:THR:HG23	2.08	0.53
9:A:656:A:H2'	9:A:658:A:C8	2.44	0.53
9:A:740:G:C8	11:C:203:ARG:NH1	2.76	0.53
9:A:1088:U:O4	18:J:205:ASN:ND2	2.36	0.53
28:T:74:TYR:HB3	28:T:75:PRO:HD3	1.90	0.53
9:A:157:G:O2'	9:A:159:A:OP1	2.15	0.53
9:A:2198:A:H2'	9:A:2199:G:C8	2.43	0.53
13:E:85:HIS:HA	21:M:85:LEU:HD13	1.90	0.53
14:F:164:THR:HG22	14:F:165:ARG:H	1.72	0.53
17:I:151:GLN:HA	17:I:154:ARG:HB2	1.90	0.53
9:A:423:G:OP2	9:A:2423:A:O2'	2.26	0.53
9:A:947:A:H2'	9:A:948:U:H5''	1.90	0.53
9:A:1122:U:H1'	9:A:1125:U:H5	1.73	0.53
11:C:132:PRO:O	11:C:135:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:61:ARG:NH2	24:P:89:ASP:OD2	2.42	0.53
28:T:114:VAL:HG22	28:T:124:MET:SD	2.49	0.53
24:P:76:PHE:CE2	24:P:78:SER:HB3	2.44	0.53
9:A:953:G:H2'	9:A:954:G:H8	1.73	0.53
9:A:1074:A:N1	17:I:63:VAL:HG21	2.23	0.53
9:A:1854:C:H5'	11:C:252:GLY:O	2.09	0.53
14:F:114:THR:HG22	14:F:152:PHE:CE1	2.44	0.53
18:J:123:PHE:HE1	18:J:152:LYS:HD2	1.73	0.53
24:P:125:GLU:HG2	24:P:162:HIS:CD2	2.44	0.53
9:A:1693:U:H2'	9:A:1694:C:H6	1.74	0.53
14:F:155:ARG:HG2	14:F:159:LEU:HD23	1.91	0.53
9:A:548:G:O2'	9:A:549:A:O5'	2.23	0.53
9:A:1837:U:H5'	9:A:1985:A:H5'	1.91	0.53
9:A:1886:A:H2'	9:A:1887:G:C8	2.44	0.53
21:M:213:LYS:HD3	21:M:233:THR:HB	1.91	0.53
6:5:3:ILE:HD13	9:A:2556:C:H4'	1.91	0.52
9:A:2767:A:H3'	9:A:2768:A:C5'	2.38	0.52
24:P:60:ILE:HD13	24:P:143:ARG:HG3	1.91	0.52
9:A:490:A:O2'	30:V:108:LYS:NZ	2.42	0.52
9:A:2307:G:H2'	9:A:2308:U:O4'	2.09	0.52
17:I:75:LEU:HD21	17:I:144:ILE:HD11	1.91	0.52
22:N:34:LEU:HD13	22:N:118:VAL:HG13	1.90	0.52
33:Y:77:PHE:HD2	33:Y:137:VAL:HG12	1.75	0.52
9:A:1834:G:H5''	11:C:48:ARG:HH21	1.74	0.52
13:E:240:LEU:O	21:M:81:ARG:HD3	2.09	0.52
27:S:105:ASP:OD1	27:S:106:ILE:N	2.40	0.52
1:0:79:PHE:O	1:0:80:TYR:HD2	1.92	0.52
18:J:195:ALA:O	18:J:199:ILE:HG12	2.09	0.52
28:T:186:PHE:O	28:T:190:ILE:HG13	2.09	0.52
29:U:106:ARG:HB3	29:U:143:ASP:OD2	2.09	0.52
30:V:142:GLN:NE2	30:V:165:THR:OG1	2.42	0.52
9:A:1039:A:OP1	26:R:77:ASN:HB3	2.09	0.52
9:A:1135:A:H4'	17:I:129:MET:HG2	1.91	0.52
9:A:2762:G:H1	9:A:2778:U:H3	1.58	0.52
10:B:43:C:O2'	14:F:116:GLN:NE2	2.43	0.52
28:T:91:LYS:HB3	28:T:93:PHE:CE1	2.45	0.52
28:T:141:HIS:O	28:T:142:PHE:HB2	2.08	0.52
12:D:270:ASP:HB2	12:D:275:VAL:HG22	1.92	0.52
28:T:31:GLU:OE2	28:T:176:ARG:NH2	2.43	0.52
28:T:79:LEU:HB3	28:T:134:ILE:HD11	1.92	0.52
9:A:880:U:OP1	22:N:6:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1189:G:H5'	27:S:148:LYS:HE2	1.91	0.52
9:A:1273:G:OP2	26:R:13:ARG:NH2	2.41	0.52
11:C:254:ARG:NE	11:C:269:ARG:HH12	2.07	0.52
21:M:134:MET:SD	21:M:138:ARG:NH1	2.83	0.52
1:O:51:VAL:HB	1:O:59:MET:HG3	1.91	0.52
9:A:2204:A:H3'	9:A:2205:G:H8	1.75	0.52
9:A:2753:C:H5''	9:A:2753:C:H6	1.75	0.52
11:C:39:ARG:HA	11:C:44:ILE:O	2.10	0.52
9:A:576:U:H2'	9:A:577:G:O4'	2.10	0.52
9:A:2600:G:OP2	9:A:2600:G:N2	2.32	0.52
9:A:17:C:O2'	9:A:564:U:OP1	2.26	0.51
9:A:1291:C:H5''	9:A:1292:G:H5'	1.92	0.51
9:A:2519:G:O2'	9:A:2521:U:OP2	2.28	0.51
11:C:23:ASN:HD21	11:C:76:THR:HG21	1.75	0.51
19:K:80:ASP:OD1	19:K:80:ASP:N	2.42	0.51
28:T:117:ARG:HD3	28:T:123:TYR:CD1	2.46	0.51
34:Z:89:MET:HG2	34:Z:152:LEU:HB2	1.92	0.51
9:A:635:C:H2'	9:A:636:C:H6	1.74	0.51
9:A:1321:A:H4'	9:A:1322:A:H5''	1.92	0.51
12:D:150:THR:OG1	12:D:152:PRO:HD2	2.10	0.51
34:Z:108:MET:O	34:Z:112:VAL:HG23	2.10	0.51
9:A:144:A:N3	9:A:2223:A:O2'	2.43	0.51
9:A:297:U:C5	9:A:298:G:C8	2.99	0.51
9:A:407:C:O2'	33:Y:83:ASN:HB2	2.10	0.51
13:E:120:LYS:HG3	13:E:124:ALA:HB3	1.91	0.51
23:O:61:MET:HG3	23:O:80:ILE:HD11	1.92	0.51
1:O:57:LEU:HD21	1:O:59:MET:HG2	1.93	0.51
9:A:312:C:H2'	9:A:313:A:C8	2.45	0.51
9:A:548:G:O2'	9:A:549:A:H8	1.93	0.51
9:A:623:A:C6	13:E:233:SER:HB3	2.46	0.51
9:A:881:U:H4'	22:N:69:PHE:CE2	2.45	0.51
9:A:1269:G:OP1	26:R:2:THR:N	2.44	0.51
9:A:1530:G:H2'	9:A:1532:G:N7	2.26	0.51
9:A:2269:G:H2'	9:A:2270:G:C8	2.45	0.51
9:A:2329:U:H5'	14:F:138:LEU:HD12	1.91	0.51
14:F:108:ASN:O	14:F:112:LEU:HG	2.10	0.51
20:L:15:GLY:HA2	20:L:47:ILE:HD12	1.91	0.51
32:X:88:LYS:HB3	32:X:89:PRO:HD2	1.92	0.51
10:B:54:G:O2'	10:B:55:G:H8	1.91	0.51
14:F:153:LEU:HD21	14:F:226:MET:HE1	1.93	0.51
23:O:100:ARG:HH21	31:W:85:U:H5'	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:150:ALA:O	29:U:154:PHE:HB2	2.11	0.51
9:A:1932:A:O2'	9:A:1934:C:N4	2.44	0.51
9:A:2149:A:H1'	9:A:2173:G:O2'	2.11	0.51
9:A:2432:G:C5'	21:M:148:GLY:HA3	2.41	0.51
11:C:244:THR:HG22	11:C:245:PRO:HD2	1.93	0.51
9:A:1133:U:H2'	9:A:1134:G:C8	2.43	0.51
9:A:1615:G:H2'	9:A:1616:A:C8	2.46	0.51
11:C:94:ASP:HB3	11:C:96:GLU:CD	2.36	0.51
14:F:57:LEU:HD21	14:F:154:ASP:HB2	1.91	0.51
22:N:41:TRP:CZ2	22:N:72:LYS:HE2	2.46	0.51
28:T:123:TYR:HE2	28:T:125:ILE:HD11	1.75	0.51
33:Y:126:LEU:O	33:Y:130:GLU:HG3	2.11	0.51
9:A:2254:A:H2'	9:A:2256:A:N7	2.25	0.51
9:A:2155:C:N3	9:A:2165:G:N2	2.59	0.51
14:F:188:GLN:OE1	14:F:205:MET:HG3	2.11	0.51
15:G:99:ARG:O	15:G:103:GLN:HG3	2.11	0.51
27:S:93:PHE:CZ	27:S:95:ALA:HA	2.46	0.51
28:T:105:VAL:HG22	28:T:132:ILE:HG23	1.93	0.51
6:5:10:ILE:HG13	9:A:2494:C:N4	2.26	0.51
9:A:1408:A:H2'	9:A:1409:G:C8	2.46	0.51
9:A:1573:C:H2'	9:A:1574:G:C8	2.46	0.51
9:A:1953:U:OP1	9:A:2621:U:O2'	2.29	0.51
9:A:2331:G:H5'	14:F:88:VAL:HG11	1.92	0.51
21:M:176:VAL:O	21:M:180:SER:HB2	2.11	0.51
9:A:880:U:H5''	22:N:6:ARG:HG3	1.93	0.50
9:A:2066:G:H4'	12:D:237:ALA:O	2.12	0.50
10:B:42:C:C5	14:F:119:VAL:HG22	2.45	0.50
10:B:49:U:OP1	24:P:77:ARG:NH2	2.36	0.50
19:K:138:LYS:HD3	19:K:143:TYR:CE1	2.45	0.50
20:L:21:CYS:HB2	20:L:39:ILE:HD12	1.94	0.50
9:A:306:G:O3'	30:V:158:LYS:NZ	2.44	0.50
9:A:581:A:O2'	27:S:203:LYS:NZ	2.45	0.50
9:A:1582:A:H2'	9:A:1583:A:C8	2.46	0.50
21:M:240:LYS:HE3	21:M:242:ILE:HD11	1.92	0.50
1:0:41:ILE:HB	14:F:117:ARG:HH11	1.75	0.50
9:A:1976:C:H4'	9:A:1977:C:C5	2.45	0.50
9:A:2142:G:H1	9:A:2174:C:N4	2.04	0.50
9:A:2154:C:H42	9:A:2165:G:H1	1.60	0.50
9:A:2460:U:H2'	9:A:2461:A:C8	2.47	0.50
17:I:154:ARG:HD2	17:I:159:ASN:HB2	1.93	0.50
29:U:111:VAL:O	29:U:114:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:125:ASN:ND2	5:4:127:LYS:H	2.09	0.50
9:A:557:C:H5	27:S:218:ARG:HH12	1.60	0.50
9:A:1168:U:H4'	9:A:1169:A:O4'	2.12	0.50
9:A:1593:U:O2'	9:A:1594:A:OP1	2.25	0.50
14:F:73:PHE:CZ	14:F:221:LYS:HD2	2.47	0.50
25:Q:118:LYS:O	25:Q:121:ASP:HB2	2.12	0.50
9:A:1487:C:H5'	9:A:1488:A:OP1	2.12	0.50
9:A:1523:A:N3	9:A:1546:C:H4'	2.27	0.50
30:V:99:THR:HB	30:V:129:ALA:HB1	1.93	0.50
6:5:9:PRO:HD3	6:5:16:LEU:HD21	1.94	0.50
9:A:1394:A:H5'	9:A:2230:A:H1'	1.93	0.50
9:A:2330:U:H2'	9:A:2331:G:H8	1.77	0.50
9:A:2464:G:N2	9:A:2467:A:C6	2.80	0.50
9:A:126:C:H2'	9:A:127:C:H6	1.76	0.50
9:A:241:A:H2'	9:A:242:A:C8	2.46	0.50
9:A:1361:U:O2'	29:U:165:LEU:HD11	2.11	0.50
17:I:75:LEU:HD12	17:I:166:PHE:HB2	1.93	0.50
24:P:46:ALA:HB1	24:P:51:GLU:OE1	2.12	0.50
9:A:1714:A:H2'	9:A:1715:A:O4'	2.12	0.50
9:A:1823:C:O2'	11:C:46:THR:OG1	2.27	0.50
11:C:121:LYS:HG2	11:C:124:ASN:ND2	2.26	0.50
12:D:193:GLU:OE2	12:D:268:LYS:HA	2.12	0.50
14:F:132:VAL:HG13	14:F:136:MET:HE2	1.93	0.50
9:A:1003:A:H1'	9:A:1018:A:C2	2.47	0.50
9:A:1199:A:H3'	9:A:1200:A:H8	1.77	0.50
9:A:1535:A:H2'	9:A:1536:A:C8	2.47	0.50
11:C:75:VAL:HG11	11:C:89:LEU:HD23	1.93	0.50
9:A:37:A:H2'	9:A:38:C:C6	2.47	0.49
9:A:221:C:H2'	9:A:222:C:H6	1.77	0.49
9:A:984:G:OP2	22:N:14:ARG:NH1	2.44	0.49
9:A:1023:C:OP2	26:R:54:LYS:NZ	2.45	0.49
9:A:1074:A:O2'	17:I:59:LYS:HD2	2.12	0.49
9:A:2320:G:O2'	14:F:174:SER:O	2.29	0.49
9:A:865:A:H2'	9:A:866:G:H5''	1.94	0.49
14:F:123:ALA:HB2	14:F:138:LEU:HG	1.93	0.49
18:J:176:LEU:HD11	18:J:210:ILE:HG21	1.94	0.49
25:Q:153:LEU:HD12	25:Q:165:TYR:CE2	2.47	0.49
29:U:115:LEU:HB2	34:Z:88:PHE:HE2	1.76	0.49
9:A:1195:U:H5''	9:A:1196:A:H2'	1.93	0.49
9:A:1209:U:O2'	9:A:1210:A:H5'	2.11	0.49
9:A:1348:C:H5''	28:T:71:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:151:LEU:HG	18:J:206:MET:HE1	1.94	0.49
28:T:167:GLY:O	28:T:171:GLU:HG2	2.12	0.49
9:A:273:U:O2'	9:A:274:G:H5'	2.12	0.49
9:A:1084:G:H5''	9:A:1085:A:H5'	1.93	0.49
9:A:2729:A:N3	9:A:2729:A:H2'	2.28	0.49
12:D:90:ILE:HG22	12:D:91:GLY:O	2.12	0.49
9:A:843:C:H2'	9:A:844:G:C8	2.48	0.49
10:B:62:U:H2'	10:B:63:C:C6	2.47	0.49
14:F:97:SER:HB3	14:F:137:THR:O	2.13	0.49
14:F:211:THR:HG22	14:F:213:ALA:H	1.77	0.49
20:L:14:SER:OG	20:L:86:ILE:HD12	2.13	0.49
28:T:93:PHE:CD2	28:T:138:ASP:HB2	2.47	0.49
8:7:66:LYS:O	8:7:72:ILE:HD11	2.12	0.49
9:A:296:G:H2'	9:A:297:U:C6	2.47	0.49
9:A:530:U:H2'	9:A:531:A:H8	1.78	0.49
13:E:72:LEU:HD22	13:E:259:TYR:HB2	1.95	0.49
15:G:155:MET:SD	15:G:188:ILE:HD13	2.53	0.49
18:J:150:LEU:HD13	18:J:203:ALA:HB2	1.95	0.49
9:A:839:G:C2	9:A:840:A:N6	2.81	0.49
9:A:1088:U:H5	18:J:202:THR:HG23	1.78	0.49
9:A:1569:A:H2'	9:A:1569:A:N3	2.28	0.49
9:A:1693:U:H2'	9:A:1694:C:C6	2.48	0.49
12:D:104:GLU:OE2	12:D:267:MET:HE1	2.12	0.49
12:D:273:LEU:HD13	25:Q:126:LEU:HD21	1.94	0.49
17:I:154:ARG:HA	17:I:157:GLU:HB2	1.95	0.49
7:6:118:ARG:O	7:6:122:LYS:HG3	2.11	0.49
9:A:793:A:N7	11:C:216:VAL:HG21	2.27	0.49
9:A:1813:A:OP1	11:C:257:LYS:HE3	2.11	0.49
9:A:2715:U:H2'	9:A:2716:C:C6	2.48	0.49
19:K:211:GLY:O	19:K:214:GLY:N	2.46	0.49
28:T:186:PHE:CE2	28:T:190:ILE:HD11	2.48	0.49
9:A:880:U:P	22:N:6:ARG:HH11	2.35	0.49
9:A:2352:A:N7	9:A:2354:G:C5	2.81	0.49
9:A:2546:G:H5''	9:A:2547:U:H5''	1.95	0.49
20:L:71:ARG:HH12	20:L:104:ARG:HH11	1.60	0.49
9:A:2268:G:H1	9:A:2467:A:H4'	1.77	0.49
30:V:79:ILE:HD11	30:V:136:MET:HB2	1.95	0.49
9:A:838:U:H4'	9:A:839:G:C8	2.48	0.48
9:A:911:U:H2'	9:A:912:C:C6	2.48	0.48
3:2:20:ARG:HD3	9:A:2417:G:OP1	2.14	0.48
9:A:1195:U:H3'	9:A:1196:A:C8	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:97:LEU:HD11	12:D:116:GLY:HA3	1.96	0.48
30:V:165:THR:HG23	30:V:167:GLU:H	1.78	0.48
34:Z:65:LEU:HD12	34:Z:68:LEU:HD12	1.94	0.48
9:A:261:U:H3	9:A:266:A:H61	1.60	0.48
9:A:2028:A:H2'	9:A:2029:A:C8	2.48	0.48
28:T:112:LYS:HB3	28:T:124:MET:CE	2.41	0.48
5:4:110:ILE:HG13	5:4:143:TYR:CE2	2.48	0.48
9:A:266:A:OP2	33:Y:139:LYS:NZ	2.46	0.48
9:A:1333:U:H4'	9:A:1334:U:O5'	2.13	0.48
11:C:170:LEU:HD11	11:C:180:ILE:HD13	1.95	0.48
21:M:83:ASP:OD1	21:M:83:ASP:N	2.47	0.48
1:0:49:ALA:HA	1:0:66:LYS:O	2.13	0.48
15:G:104:MET:HA	15:G:104:MET:HE2	1.94	0.48
20:L:27:ALA:HB1	20:L:30:ARG:HD2	1.95	0.48
26:R:6:ARG:O	26:R:9:ILE:HG22	2.14	0.48
34:Z:140:TRP:O	34:Z:144:ILE:HG12	2.14	0.48
2:1:5:LYS:NZ	9:A:2069:C:OP1	2.29	0.48
9:A:795:U:C5	9:A:803:G:C5	3.02	0.48
9:A:2151:G:N2	9:A:2169:C:O2	2.46	0.48
9:A:2718:U:O2'	23:O:83:LYS:HE3	2.14	0.48
10:B:29:C:H2'	10:B:30:A:O4'	2.13	0.48
15:G:69:LEU:HD11	15:G:121:LYS:O	2.14	0.48
15:G:71:GLU:O	15:G:176:ARG:NH1	2.45	0.48
33:Y:110:TRP:NE1	33:Y:112:ALA:HB3	2.29	0.48
9:A:1087:G:O2'	18:J:202:THR:OG1	2.32	0.48
9:A:2714:A:H2'	9:A:2715:U:O4'	2.14	0.48
11:C:107:ILE:O	11:C:110:ASP:HB2	2.13	0.48
12:D:142:GLU:O	12:D:165:MET:HA	2.13	0.48
9:A:555:A:N6	9:A:558:A:O2'	2.37	0.48
9:A:2154:C:N4	9:A:2165:G:H22	2.12	0.48
9:A:2524:C:C2	9:A:2599:G:N2	2.82	0.48
12:D:296:LYS:HB3	12:D:302:ILE:HD11	1.95	0.48
20:L:71:ARG:HH12	20:L:104:ARG:NH1	2.12	0.48
21:M:243:LYS:O	21:M:246:VAL:HG23	2.14	0.48
10:B:67:U:C4	10:B:109:U:C4	3.01	0.48
13:E:172:SER:HA	13:E:245:LEU:O	2.14	0.48
23:O:31:LEU:HD23	23:O:31:LEU:HA	1.57	0.48
9:A:1454:G:H2'	9:A:1455:A:C8	2.49	0.48
9:A:2393:A:O2'	24:P:160:ARG:NH1	2.39	0.48
10:B:5:C:H2'	10:B:6:U:C6	2.48	0.48
19:K:177:SER:OG	19:K:179:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:126:THR:HA	5:4:129:LYS:HE3	1.94	0.47
9:A:1485:U:H5'	9:A:1486:U:C5'	2.40	0.47
9:A:1701:A:H2'	9:A:1702:G:O4'	2.14	0.47
9:A:2073:A:H2'	9:A:2519:G:H21	1.78	0.47
9:A:2308:U:H2'	9:A:2309:U:C6	2.48	0.47
18:J:92:ALA:HB3	18:J:93:PRO:HD3	1.96	0.47
23:O:20:LEU:O	23:O:22:ARG:HG2	2.14	0.47
28:T:117:ARG:HD3	28:T:123:TYR:CE1	2.49	0.47
9:A:138:C:H2'	9:A:139:U:H6	1.79	0.47
9:A:753:G:H2'	9:A:754:A:C8	2.49	0.47
11:C:42:ARG:CZ	11:C:44:ILE:HD11	2.44	0.47
19:K:213:LEU:HD12	19:K:213:LEU:HA	1.75	0.47
4:3:144:PRO:HG2	4:3:149:ARG:HB2	1.97	0.47
9:A:1272:A:OP1	26:R:13:ARG:NH1	2.48	0.47
9:A:2403:U:H4'	32:X:112:ASP:HA	1.96	0.47
9:A:2463:G:H2'	9:A:2464:G:O4'	2.14	0.47
9:A:2658:A:P	19:K:175:ARG:HH12	2.37	0.47
15:G:196:PRO:HG2	15:G:197:TYR:CD2	2.49	0.47
23:O:111:LEU:HD12	23:O:111:LEU:HA	1.61	0.47
26:R:72:ARG:HA	26:R:72:ARG:HD3	1.72	0.47
34:Z:86:GLU:HB3	34:Z:108:MET:HE1	1.96	0.47
9:A:635:C:OP2	21:M:190:SER:HB2	2.14	0.47
10:B:50:U:P	24:P:151:ARG:HE	2.37	0.47
26:R:79:SER:OG	26:R:80:LYS:N	2.47	0.47
9:A:555:A:C6	9:A:558:A:H1'	2.49	0.47
9:A:881:U:H2'	9:A:882:U:C6	2.49	0.47
9:A:1226:U:O5'	9:A:1226:U:H6	1.98	0.47
9:A:2206:A:H2'	9:A:2207:A:H8	1.78	0.47
9:A:2290:A:H2'	9:A:2291:A:C8	2.50	0.47
10:B:49:U:P	24:P:77:ARG:HH22	2.38	0.47
17:I:75:LEU:HD13	17:I:140:ILE:HB	1.96	0.47
19:K:90:ALA:O	27:S:140:ARG:HD3	2.14	0.47
31:W:5:A:H5'	31:W:6:A:OP2	2.14	0.47
9:A:947:A:H61	9:A:950:A:H61	1.61	0.47
10:B:30:A:H2'	10:B:31:C:C6	2.49	0.47
12:D:101:SER:CB	25:Q:178:HIS:HD2	2.28	0.47
15:G:177:ASP:O	15:G:181:VAL:HG12	2.13	0.47
26:R:61:TRP:O	26:R:65:ILE:HG13	2.13	0.47
9:A:646:G:H2'	9:A:647:C:C6	2.50	0.47
9:A:1494:G:H22	9:A:1550:U:H3	1.60	0.47
9:A:1567:C:H5'	9:A:1568:U:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1806:U:H2'	9:A:1807:C:C6	2.50	0.47
9:A:2406:G:H5''	9:A:2407:U:O4'	2.14	0.47
15:G:137:THR:HG22	15:G:139:GLU:HG3	1.96	0.47
17:I:161:PHE:CE2	17:I:176:VAL:HG11	2.49	0.47
23:O:36:THR:HG21	23:O:81:TYR:H	1.79	0.47
26:R:106:ASN:O	26:R:110:MET:HG3	2.15	0.47
28:T:79:LEU:HD23	28:T:79:LEU:HA	1.67	0.47
29:U:109:LEU:HB2	29:U:146:MET:HE1	1.96	0.47
9:A:724:G:H1'	9:A:729:A:H62	1.78	0.47
9:A:1415:U:C4	9:A:1416:A:C6	3.03	0.47
17:I:79:ILE:HG13	17:I:147:TYR:CE1	2.50	0.47
19:K:75:PRO:CD	19:K:88:GLU:HG2	2.39	0.47
26:R:49:ASP:HA	26:R:52:ARG:HB2	1.96	0.47
32:X:99:THR:HG22	32:X:113:HIS:HB3	1.97	0.47
34:Z:123:GLU:O	34:Z:128:VAL:HG22	2.13	0.47
7:6:122:LYS:NZ	9:A:1407:C:OP1	2.32	0.47
9:A:557:C:H41	27:S:218:ARG:NH1	2.13	0.47
13:E:206:LEU:HB3	13:E:245:LEU:HD22	1.97	0.47
14:F:105:ALA:O	14:F:109:GLU:HG2	2.15	0.47
22:N:59:ARG:HG3	22:N:60:ARG:H	1.79	0.47
23:O:82:GLU:HB2	23:O:85:ILE:HG13	1.96	0.47
9:A:7:C:N4	9:A:8:G:C6	2.83	0.47
9:A:583:G:H5''	9:A:585:A:N7	2.30	0.47
9:A:1497:A:O2'	9:A:1498:G:H5'	2.14	0.47
17:I:79:ILE:HD11	17:I:151:GLN:NE2	2.30	0.47
17:I:120:ALA:HB1	17:I:123:LYS:HE3	1.96	0.47
28:T:124:MET:HE3	28:T:124:MET:HB3	1.71	0.47
29:U:140:VAL:HA	29:U:172:LYS:HB2	1.97	0.47
6:5:17:ILE:HG22	6:5:18:ARG:H	1.79	0.46
9:A:932:A:H2'	9:A:933:G:C8	2.50	0.46
9:A:1407:C:H2'	9:A:1408:A:C8	2.50	0.46
9:A:1864:A:H2'	9:A:1865:G:O4'	2.15	0.46
9:A:2369:A:H2'	9:A:2370:G:O4'	2.15	0.46
9:A:2725:G:H4'	23:O:32:ARG:HH12	1.78	0.46
10:B:31:C:OP1	24:P:49:ARG:HD2	2.16	0.46
20:L:117:ALA:HA	20:L:118:PRO:HD3	1.75	0.46
29:U:161:LYS:O	29:U:177:MET:HG2	2.15	0.46
9:A:2307:G:N2	9:A:2360:U:H1'	2.29	0.46
9:A:2699:U:H2'	9:A:2700:C:H6	1.81	0.46
13:E:113:ARG:H	13:E:113:ARG:HG3	1.43	0.46
16:H:57:ILE:HD12	16:H:83:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:116:ILE:O	26:R:119:GLU:HG2	2.15	0.46
32:X:97:ARG:HA	32:X:97:ARG:HD3	1.51	0.46
9:A:608:U:O2'	21:M:91:SER:HB2	2.16	0.46
9:A:1277:G:H21	13:E:133:LEU:HB3	1.80	0.46
10:B:30:A:P	24:P:78:SER:HB2	2.55	0.46
15:G:63:LEU:HD21	15:G:84:LYS:HZ2	1.80	0.46
15:G:196:PRO:O	15:G:211:ARG:HA	2.15	0.46
23:O:106:ARG:NH1	23:O:126:VAL:HG21	2.30	0.46
9:A:6:A:H2'	9:A:7:C:O4'	2.16	0.46
15:G:123:PHE:O	15:G:174:SER:HA	2.16	0.46
18:J:84:LEU:HD21	18:J:95:VAL:HB	1.97	0.46
20:L:101:ALA:C	20:L:102:ILE:HG12	2.40	0.46
22:N:77:ARG:NH2	22:N:86:GLY:O	2.40	0.46
30:V:108:LYS:HD2	30:V:128:ALA:HB2	1.97	0.46
1:O:74:SER:HB2	14:F:158:ASN:HA	1.98	0.46
9:A:221:C:H2'	9:A:222:C:C6	2.51	0.46
9:A:1557:G:N3	9:A:1557:G:H2'	2.31	0.46
9:A:1836:C:OP1	11:C:219:VAL:HG23	2.15	0.46
9:A:2660:G:H2'	9:A:2661:A:O4'	2.14	0.46
10:B:16:G:N3	10:B:16:G:H2'	2.29	0.46
14:F:226:MET:HE2	14:F:226:MET:HB3	1.78	0.46
23:O:32:ARG:HH21	23:O:81:TYR:HE1	1.62	0.46
25:Q:138:ARG:HH22	25:Q:203:ILE:CG2	2.28	0.46
9:A:126:C:H2'	9:A:127:C:C6	2.51	0.46
9:A:564:U:C2'	9:A:565:G:H5'	2.46	0.46
9:A:1074:A:H3'	9:A:1075:G:C5'	2.45	0.46
12:D:96:LYS:HD2	12:D:282:VAL:HG23	1.96	0.46
19:K:135:ILE:HG22	19:K:217:LEU:HD22	1.98	0.46
20:L:67:LYS:HG3	20:L:68:GLU:H	1.81	0.46
27:S:105:ASP:O	27:S:109:GLN:HG2	2.16	0.46
9:A:17:C:O3'	26:R:23:SER:HA	2.15	0.46
9:A:169:C:H2'	9:A:170:U:C6	2.50	0.46
9:A:1225:G:P	13:E:204:LYS:HZ1	2.38	0.46
10:B:92:U:OP1	22:N:16:ARG:HG3	2.16	0.46
11:C:178:ARG:HG2	11:C:179:LEU:N	2.31	0.46
11:C:239:ARG:C	11:C:241:SER:H	2.24	0.46
22:N:8:ARG:H	22:N:8:ARG:HD2	1.81	0.46
23:O:106:ARG:HH11	23:O:126:VAL:HG21	1.80	0.46
30:V:175:TRP:H	30:V:175:TRP:CD1	2.32	0.46
9:A:750:A:H1'	9:A:751:C:H5	1.80	0.46
9:A:1073:G:H4'	9:A:1074:A:H5''	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:45:SER:HB3	31:W:87:A:OP1	2.16	0.46
9:A:685:G:P	13:E:105:ARG:HH22	2.39	0.46
9:A:2396:G:H2'	9:A:2397:U:C6	2.51	0.46
34:Z:108:MET:HB3	34:Z:108:MET:HE2	1.52	0.46
4:3:135:ARG:NH2	9:A:480:G:N7	2.61	0.46
9:A:348:U:O5'	9:A:348:U:H6	2.00	0.46
9:A:716:A:H2'	9:A:717:A:O4'	2.16	0.46
9:A:1269:G:P	13:E:143:PRO:HG3	2.56	0.46
9:A:1320:G:O5'	9:A:1320:G:H8	1.99	0.46
9:A:1632:U:O2'	9:A:1633:A:H5'	2.15	0.46
9:A:1704:A:O2'	9:A:1710:G:N7	2.38	0.46
17:I:73:CYS:SG	17:I:134:PHE:HB3	2.57	0.46
27:S:124:PHE:CE1	27:S:165:GLY:HA3	2.50	0.46
27:S:230:TYR:CG	27:S:231:PRO:HD2	2.51	0.46
31:W:30:A:H2'	31:W:31:U:O4'	2.16	0.46
9:A:701:U:H2'	9:A:702:C:O4'	2.16	0.45
9:A:1309:U:O2'	9:A:1683:G:N2	2.48	0.45
9:A:2112:U:H2'	9:A:2113:G:O4'	2.16	0.45
13:E:51:GLU:HB3	13:E:69:PHE:CD1	2.51	0.45
14:F:54:ILE:HG23	14:F:58:LYS:HZ2	1.81	0.45
29:U:109:LEU:HD21	29:U:141:ARG:HB3	1.98	0.45
5:4:156:ASN:OD1	5:4:158:LYS:HD3	2.16	0.45
9:A:1211:G:OP1	21:M:109:SER:OG	2.22	0.45
9:A:1246:G:OP1	27:S:194:LYS:NZ	2.38	0.45
11:C:97:LYS:O	11:C:98:ARG:HD3	2.17	0.45
11:C:133:LEU:HD21	11:C:163:LYS:HE2	1.97	0.45
15:G:115:MET:HE2	15:G:115:MET:HB3	1.80	0.45
17:I:96:LEU:HD12	17:I:102:LEU:HD22	1.98	0.45
26:R:116:ILE:HA	26:R:119:GLU:HG2	1.99	0.45
28:T:145:TYR:HD2	28:T:172:LEU:HD23	1.82	0.45
9:A:794:A:C5	9:A:796:G:H1'	2.51	0.45
9:A:1502:A:O5'	9:A:1502:A:H8	2.00	0.45
9:A:2007:U:H5''	12:D:223:THR:OG1	2.16	0.45
9:A:2260:U:H2'	9:A:2261:U:C6	2.51	0.45
9:A:2449:A:H1'	35:z:75:C:O2'	2.16	0.45
9:A:2709:C:H2'	9:A:2710:A:H8	1.81	0.45
21:M:140:ILE:HG23	21:M:141:PRO:HD2	1.99	0.45
5:4:112:ARG:HD2	21:M:140:ILE:HD13	1.97	0.45
7:6:131:TRP:O	7:6:132:PRO:C	2.57	0.45
9:A:116:A:N3	9:A:163:G:H1'	2.32	0.45
9:A:807:C:H2'	9:A:808:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1088:U:N1	9:A:1090:U:H5'	2.31	0.45
9:A:1511:U:H6	9:A:1511:U:O5'	1.98	0.45
21:M:143:LEU:HA	21:M:143:LEU:HD23	1.72	0.45
31:W:5:A:H3'	31:W:6:A:C8	2.51	0.45
9:A:457:C:O2'	9:A:458:G:H5'	2.17	0.45
9:A:1074:A:C2	17:I:109:LEU:HA	2.51	0.45
9:A:1559:A:H5'	9:A:1560:C:OP2	2.17	0.45
9:A:1801:A:OP1	11:C:207:LYS:HG3	2.16	0.45
14:F:83:LYS:O	14:F:211:THR:HG23	2.16	0.45
14:F:155:ARG:O	14:F:159:LEU:HB3	2.17	0.45
16:H:69:VAL:HG12	16:H:70:ARG:O	2.17	0.45
17:I:86:VAL:HA	17:I:89:PHE:HB2	1.99	0.45
20:L:50:THR:HG23	20:L:51:PRO:HD2	1.97	0.45
1:0:70:VAL:HG11	1:0:73:TRP:HB3	1.98	0.45
3:2:8:ARG:NH1	9:A:2302:C:OP2	2.49	0.45
22:N:17:MET:HE3	22:N:96:VAL:HG13	1.97	0.45
25:Q:148:ILE:HD13	25:Q:168:ILE:HG13	1.98	0.45
34:Z:79:GLU:HB3	34:Z:115:MET:HE1	1.97	0.45
8:7:60:MET:HB3	8:7:60:MET:HE2	1.83	0.45
9:A:739:G:O2'	9:A:741:U:H5''	2.16	0.45
9:A:2410:U:H2'	9:A:2411:C:C6	2.51	0.45
11:C:254:ARG:CZ	11:C:269:ARG:HH12	2.29	0.45
12:D:232:LEU:HA	12:D:232:LEU:HD12	1.70	0.45
19:K:225:LYS:HB2	19:K:225:LYS:HE3	1.55	0.45
21:M:163:ARG:O	21:M:167:VAL:HG23	2.17	0.45
22:N:11:LYS:HD3	22:N:87:LYS:HB3	1.99	0.45
1:0:50:LYS:HE3	1:0:58:VAL:HG22	1.99	0.45
9:A:1559:A:H3'	9:A:1560:C:H6	1.80	0.45
20:L:28:SER:HB2	20:L:29:ASN:H	1.62	0.45
22:N:54:MET:HE1	22:N:104:TYR:HB3	1.98	0.45
23:O:32:ARG:O	23:O:36:THR:HG23	2.17	0.45
28:T:91:LYS:HB3	28:T:93:PHE:HE1	1.82	0.45
31:W:36:A:O2'	31:W:37:C:OP1	2.34	0.45
9:A:33:A:O2'	9:A:466:A:N3	2.50	0.45
9:A:133:A:O2'	9:A:134:A:N7	2.40	0.45
9:A:876:A:H2'	9:A:876:A:N3	2.30	0.45
10:B:40:A:O2'	10:B:47:A:N1	2.49	0.45
14:F:164:THR:HG22	14:F:165:ARG:N	2.32	0.45
14:F:187:GLU:HG2	14:F:202:ALA:HB1	1.99	0.45
17:I:96:LEU:HD13	17:I:102:LEU:HB2	1.98	0.45
28:T:63:MET:HA	28:T:66:GLU:CD	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:94:ALA:HB1	4:3:98:LEU:HD12	1.98	0.45
9:A:674:C:H5''	21:M:96:LYS:HG3	1.98	0.45
9:A:1548:A:HO2'	9:A:1549:A:P	2.40	0.45
9:A:2792:C:H2'	9:A:2793:A:O4'	2.16	0.45
10:B:48:C:OP2	24:P:49:ARG:NH2	2.50	0.45
19:K:83:TRP:CG	19:K:84:MET:H	2.34	0.45
21:M:130:GLU:O	21:M:132:GLY:N	2.50	0.45
27:S:83:PRO:HB2	28:T:145:TYR:HE1	1.82	0.45
9:A:372:G:H2'	9:A:373:C:C6	2.53	0.44
9:A:506:G:O2'	28:T:90:ASN:ND2	2.51	0.44
9:A:591:C:H2'	9:A:592:G:C8	2.51	0.44
9:A:815:A:H2'	9:A:817:C:C4	2.52	0.44
9:A:984:G:P	22:N:87:LYS:HG3	2.57	0.44
9:A:1917:G:OP1	11:C:236:PRO:HB2	2.16	0.44
9:A:2108:G:N2	9:A:2210:C:H1'	2.33	0.44
13:E:88:LEU:HD22	21:M:85:LEU:HD12	1.98	0.44
33:Y:144:ASP:O	33:Y:148:GLU:HG3	2.18	0.44
9:A:1385:G:N2	9:A:1388:A:OP2	2.40	0.44
17:I:100:THR:HG21	17:I:143:ALA:HB2	1.99	0.44
27:S:204:LYS:HD3	27:S:204:LYS:HA	1.42	0.44
9:A:490:A:H1'	30:V:108:LYS:NZ	2.33	0.44
9:A:491:A:N3	9:A:493:G:H5''	2.32	0.44
9:A:1603:A:H2'	9:A:1604:A:C8	2.52	0.44
9:A:2284:A:H5''	9:A:2285:A:H5'	1.98	0.44
11:C:75:VAL:HG12	11:C:89:LEU:O	2.18	0.44
15:G:206:ASP:OD1	15:G:206:ASP:N	2.49	0.44
19:K:57:CYS:HG	19:K:61:TRP:CD1	2.35	0.44
1:O:79:PHE:O	1:O:80:TYR:CD2	2.69	0.44
9:A:1921:G:N2	9:A:1938:C:H1'	2.33	0.44
9:A:2116:C:C2	9:A:2201:G:N2	2.86	0.44
12:D:86:VAL:HG11	12:D:174:VAL:HG22	2.00	0.44
14:F:73:PHE:CE2	14:F:221:LYS:HD2	2.51	0.44
23:O:96:ARG:HD3	23:O:97:TYR:CE2	2.52	0.44
24:P:67:THR:HB	24:P:68:PRO:HD2	1.99	0.44
26:R:31:LEU:O	26:R:35:ILE:HG13	2.17	0.44
29:U:124:ALA:HB2	29:U:135:LEU:HD12	1.98	0.44
9:A:1055:A:C2	9:A:2505:A:H5'	2.52	0.44
9:A:1075:G:N2	9:A:1138:G:O2'	2.48	0.44
10:B:88:G:N2	10:B:90:G:H3'	2.32	0.44
11:C:76:THR:OG1	11:C:77:ILE:N	2.51	0.44
12:D:98:GLY:C	25:Q:123:MET:HE1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:204:LYS:HA	13:E:225:THR:HB	2.00	0.44
14:F:188:GLN:OE1	14:F:188:GLN:HA	2.16	0.44
15:G:76:TYR:HE1	15:G:108:PHE:HB3	1.82	0.44
19:K:48:ARG:HH22	31:W:1:A:H3'	1.82	0.44
24:P:105:ILE:HD13	24:P:123:ILE:HG12	1.99	0.44
25:Q:117:VAL:HG11	25:Q:125:ILE:HD12	2.00	0.44
25:Q:180:THR:HG23	25:Q:195:VAL:HG13	1.99	0.44
31:W:34:U:O3'	31:W:35:U:H4'	2.18	0.44
32:X:71:ASP:CG	32:X:72:SER:H	2.25	0.44
4:3:96:LEU:HD23	4:3:96:LEU:HA	1.78	0.44
9:A:1532:G:N1	11:C:94:ASP:OD1	2.51	0.44
9:A:2252:G:H2'	9:A:2253:U:O4'	2.18	0.44
12:D:261:ILE:HD12	12:D:283:PRO:HD3	1.99	0.44
18:J:183:LYS:HD3	18:J:199:ILE:HD11	2.00	0.44
20:L:75:MET:HE2	20:L:75:MET:HB3	1.74	0.44
25:Q:155:VAL:HA	25:Q:156:PRO:HD3	1.86	0.44
26:R:69:ILE:HD11	26:R:81:PHE:CD2	2.53	0.44
9:A:843:C:H2'	9:A:844:G:H8	1.82	0.44
9:A:1111:G:N2	9:A:1113:A:H3'	2.32	0.44
9:A:2237:A:H2'	9:A:2238:A:H8	1.83	0.44
9:A:2798:G:OP2	19:K:219:ASN:ND2	2.47	0.44
27:S:191:LEU:HD23	27:S:215:PRO:HA	1.99	0.44
34:Z:115:MET:HE2	34:Z:115:MET:HB3	1.88	0.44
9:A:411:U:H1'	16:H:42:GLN:NE2	2.31	0.44
9:A:1074:A:C6	17:I:63:VAL:HG21	2.53	0.44
9:A:1076:A:H62	9:A:1138:G:H21	1.64	0.44
9:A:1849:A:H5'	9:A:1850:G:OP2	2.18	0.44
9:A:2381:C:H2'	9:A:2382:G:O4'	2.18	0.44
15:G:195:GLU:HB2	15:G:196:PRO:HD2	2.00	0.44
26:R:58:ARG:HH12	26:R:94:ARG:NH1	2.15	0.44
27:S:137:ILE:HG13	27:S:140:ARG:HG3	1.99	0.44
34:Z:132:LEU:HA	34:Z:132:LEU:HD23	1.78	0.44
9:A:197:G:H2'	9:A:198:A:C8	2.52	0.44
9:A:2154:C:H42	9:A:2165:G:H22	1.65	0.44
13:E:210:MET:HE3	13:E:251:THR:HA	1.99	0.44
14:F:111:ALA:O	14:F:115:GLY:N	2.50	0.44
23:O:40:LYS:HB2	23:O:85:ILE:HD13	2.00	0.44
26:R:97:LEU:HD23	26:R:97:LEU:HA	1.75	0.44
29:U:119:ILE:HD12	29:U:135:LEU:HD13	1.99	0.44
9:A:16:G:H2'	9:A:17:C:C6	2.53	0.43
9:A:349:A:H2'	9:A:350:G:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:879:G:H4'	22:N:8:ARG:HH21	1.83	0.43
9:A:888:C:H3'	9:A:889:G:C8	2.38	0.43
9:A:1733:G:H4'	9:A:1992:A:H5''	1.99	0.43
9:A:2298:C:O2'	9:A:2299:G:H5'	2.18	0.43
11:C:90:ILE:HD11	11:C:92:TYR:CZ	2.53	0.43
14:F:113:ILE:O	14:F:155:ARG:NH2	2.50	0.43
14:F:117:ARG:HA	14:F:118:PRO:HD3	1.72	0.43
22:N:4:PRO:HG2	22:N:93:TRP:CZ3	2.53	0.43
24:P:82:LEU:HD12	24:P:82:LEU:HA	1.89	0.43
25:Q:118:LYS:HB2	25:Q:121:ASP:OD2	2.18	0.43
9:A:495:A:OP1	30:V:113:LYS:NZ	2.41	0.43
9:A:2769:G:C4	15:G:42:ARG:HD3	2.53	0.43
9:A:2770:C:H2'	9:A:2771:A:O4'	2.18	0.43
12:D:107:GLY:HA3	25:Q:202:ASN:ND2	2.33	0.43
22:N:1:MET:HG2	22:N:44:SER:HB2	2.00	0.43
30:V:137:LEU:HD23	30:V:137:LEU:HA	1.80	0.43
9:A:14:A:H5'	9:A:15:G:OP2	2.18	0.43
9:A:530:U:H2'	9:A:531:A:C8	2.53	0.43
9:A:1092:C:H4'	18:J:161:LYS:HG2	2.01	0.43
9:A:1142:G:O2'	9:A:1143:C:H5'	2.18	0.43
9:A:2245:U:H2'	9:A:2246:U:C6	2.53	0.43
12:D:223:THR:O	12:D:225:GLY:N	2.52	0.43
13:E:144:LYS:HA	13:E:144:LYS:HD3	1.73	0.43
21:M:81:ARG:H	21:M:84:ASN:ND2	2.17	0.43
21:M:187:ILE:O	21:M:189:PRO:HD3	2.18	0.43
22:N:29:PHE:CD2	22:N:67:ARG:HD3	2.53	0.43
3:2:8:ARG:NH1	3:2:38:ASN:HB2	2.34	0.43
9:A:254:U:C5	9:A:272:U:C4	3.07	0.43
9:A:640:G:H2'	9:A:641:C:C6	2.53	0.43
9:A:1087:G:H1'	18:J:198:ILE:HG23	2.00	0.43
10:B:81:U:H2'	10:B:82:G:C8	2.54	0.43
7:6:115:ARG:HA	7:6:118:ARG:HD2	2.00	0.43
9:A:1523:A:HO2'	9:A:1546:C:HO2'	1.63	0.43
9:A:1620:U:O2'	9:A:1621:C:H4'	2.19	0.43
9:A:1635:C:OP1	29:U:144:LYS:HB2	2.17	0.43
9:A:2201:G:N2	9:A:2202:C:N3	2.66	0.43
9:A:2373:C:H2'	9:A:2374:C:O4'	2.19	0.43
9:A:2410:U:H2'	9:A:2411:C:H6	1.84	0.43
15:G:147:LEU:HA	15:G:147:LEU:HD23	1.76	0.43
15:G:184:PHE:O	15:G:188:ILE:HG12	2.19	0.43
17:I:141:PRO:HB3	17:I:182:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:1:MET:HE3	20:L:32:TYR:CE2	2.53	0.43
1:0:38:LYS:HD2	1:0:41:ILE:HD13	2.00	0.43
9:A:556:C:H4'	9:A:557:C:OP1	2.15	0.43
11:C:257:LYS:HB2	11:C:260:LYS:HG3	1.99	0.43
13:E:202:ALA:O	13:E:225:THR:HG21	2.18	0.43
17:I:110:VAL:HG21	17:I:132:TRP:HE1	1.84	0.43
19:K:48:ARG:N	31:W:95:A:OP1	2.51	0.43
25:Q:154:GLU:HA	25:Q:162:LEU:HD22	2.01	0.43
26:R:26:GLY:O	26:R:30:ARG:NH1	2.52	0.43
27:S:100:THR:O	27:S:103:TYR:HB3	2.19	0.43
27:S:128:VAL:HG22	27:S:133:GLN:HG2	2.01	0.43
28:T:117:ARG:HA	28:T:117:ARG:HD2	1.38	0.43
32:X:93:ILE:C	32:X:94:ILE:HG13	2.44	0.43
7:6:121:ARG:HH12	9:A:1549:A:H5'	1.84	0.43
9:A:598:U:H2'	9:A:599:C:C6	2.53	0.43
9:A:888:C:H5	9:A:908:A:H2	1.66	0.43
9:A:2257:C:O2'	9:A:2258:A:H5'	2.19	0.43
10:B:37:U:OP1	10:B:37:U:H6	2.01	0.43
11:C:100:ILE:HD12	11:C:101:LEU:O	2.17	0.43
12:D:90:ILE:HD13	12:D:173:LEU:HD21	2.00	0.43
12:D:181:PRO:O	12:D:182:SER:HB3	2.19	0.43
24:P:70:ARG:HH11	24:P:138:LYS:HE3	1.84	0.43
25:Q:225:LYS:HB3	25:Q:229:LEU:HD12	2.00	0.43
27:S:116:PRO:HA	27:S:117:PRO:HD3	1.89	0.43
5:4:132:LEU:HD23	5:4:132:LEU:HA	1.84	0.43
9:A:169:C:H2'	9:A:170:U:H6	1.83	0.43
9:A:1857:A:O2'	9:A:1858:A:H8	2.02	0.43
9:A:1926:A:H62	9:A:1931:U:H3	1.67	0.43
9:A:2722:C:H2'	9:A:2723:A:O4'	2.19	0.43
11:C:161:ILE:HG13	11:C:162:ALA:N	2.33	0.43
14:F:204:GLY:C	14:F:205:MET:HG2	2.43	0.43
17:I:76:LEU:HD22	17:I:134:PHE:CD1	2.53	0.43
19:K:99:THR:HA	26:R:99:GLN:HE22	1.83	0.43
27:S:137:ILE:CG1	27:S:140:ARG:HG3	2.49	0.43
31:W:1:A:H2'	31:W:2:G:H8	1.83	0.43
34:Z:74:GLU:H	34:Z:74:GLU:HG3	1.44	0.43
34:Z:85:GLY:O	34:Z:88:PHE:HB3	2.19	0.43
13:E:203:GLU:O	13:E:204:LYS:HB2	2.19	0.43
14:F:221:LYS:O	14:F:225:LEU:HG	2.19	0.43
15:G:92:VAL:HG21	15:G:109:ARG:HB2	2.01	0.43
29:U:101:LYS:HG2	29:U:102:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:85:GLN:O	32:X:122:LEU:HA	2.18	0.43
2:1:35:ALA:HB2	28:T:67:LEU:HD12	2.00	0.43
7:6:115:ARG:NH1	9:A:1491:G:OP1	2.52	0.43
9:A:211:A:H2'	9:A:212:A:C8	2.54	0.43
9:A:891:G:C2	9:A:906:C:C2	3.07	0.43
12:D:120:GLY:HA3	12:D:141:TYR:O	2.19	0.43
20:L:63:VAL:HG23	20:L:64:ARG:HG3	2.00	0.43
32:X:87:ALA:O	32:X:120:ASP:HA	2.18	0.43
34:Z:92:LEU:HD23	34:Z:92:LEU:HA	1.86	0.43
1:0:76:ASN:O	1:0:76:ASN:ND2	2.52	0.42
4:3:138:LEU:HD23	4:3:138:LEU:HA	1.77	0.42
7:6:137:LYS:HE2	7:6:137:LYS:HB3	1.66	0.42
9:A:844:G:H2'	9:A:845:C:C6	2.54	0.42
9:A:1448:A:H4'	9:A:1449:C:O4'	2.19	0.42
9:A:2430:G:H2'	9:A:2431:G:O4'	2.18	0.42
10:B:41:U:H3'	10:B:42:C:C5'	2.48	0.42
12:D:90:ILE:HD11	12:D:137:VAL:HG11	2.01	0.42
13:E:109:ARG:HG2	13:E:110:GLY:N	2.33	0.42
19:K:144:THR:HG22	19:K:146:SER:H	1.84	0.42
21:M:161:ASN:HA	21:M:201:LEU:O	2.18	0.42
28:T:152:LEU:HD22	28:T:156:LYS:HB3	2.01	0.42
34:Z:76:LEU:HD22	34:Z:115:MET:CE	2.49	0.42
9:A:636:C:O2'	9:A:668:U:H5''	2.18	0.42
9:A:1689:C:H3'	23:O:12:LYS:HG2	2.00	0.42
9:A:2039:C:H2'	9:A:2040:U:O4'	2.18	0.42
9:A:2066:G:N3	12:D:243:HIS:HA	2.34	0.42
9:A:2139:A:O2'	9:A:2187:A:N6	2.52	0.42
11:C:193:ASN:OD1	11:C:196:VAL:HG23	2.19	0.42
14:F:65:MET:HE1	14:F:225:LEU:HB3	2.01	0.42
17:I:154:ARG:HG2	17:I:157:GLU:OE1	2.20	0.42
29:U:114:ILE:HG13	29:U:115:LEU:HG	2.00	0.42
9:A:213:A:N1	9:A:429:C:O2'	2.47	0.42
9:A:295:C:N4	9:A:296:G:O6	2.52	0.42
9:A:583:G:N1	9:A:2045:A:OP1	2.32	0.42
9:A:1840:C:OP1	11:C:200:ARG:NH2	2.52	0.42
9:A:1887:G:H2'	9:A:1888:G:H8	1.84	0.42
12:D:166:ARG:HG2	12:D:167:HIS:NE2	2.35	0.42
14:F:60:ASN:ND2	14:F:64:LYS:HD2	2.34	0.42
15:G:74:ILE:HG12	15:G:115:MET:SD	2.59	0.42
9:A:1559:A:H3'	9:A:1560:C:C6	2.54	0.42
9:A:1703:G:N2	9:A:2006:G:OP2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2204:A:H3'	9:A:2205:G:C8	2.54	0.42
11:C:102:HIS:HA	11:C:103:PRO:HD3	1.89	0.42
14:F:56:ARG:O	14:F:60:ASN:HB3	2.19	0.42
17:I:140:ILE:O	17:I:144:ILE:HG12	2.20	0.42
19:K:101:TYR:HA	19:K:102:PRO:HD3	1.91	0.42
21:M:257:PHE:CD1	21:M:257:PHE:N	2.86	0.42
25:Q:119:LEU:O	25:Q:122:ILE:HB	2.19	0.42
30:V:175:TRP:CZ3	30:V:176:LYS:HG3	2.54	0.42
2:1:26:TRP:O	2:1:30:LYS:HG2	2.19	0.42
4:3:113:GLY:HA2	4:3:141:LYS:O	2.20	0.42
9:A:1116:A:N6	18:J:205:ASN:HB2	2.35	0.42
9:A:1192:A:H2'	9:A:1193:U:C6	2.54	0.42
10:B:4:U:H2'	10:B:5:C:C6	2.55	0.42
13:E:51:GLU:HG3	13:E:53:ILE:H	1.85	0.42
19:K:144:THR:HA	19:K:145:PRO:HD3	1.84	0.42
25:Q:185:ARG:HG3	25:Q:187:ILE:HG13	2.01	0.42
26:R:28:HIS:O	26:R:35:ILE:HG12	2.20	0.42
1:0:53:CYS:SG	1:0:73:TRP:NE1	2.92	0.42
2:1:11:TYR:CD1	2:1:11:TYR:C	2.98	0.42
9:A:262:G:C2	9:A:264:A:H5''	2.54	0.42
9:A:331:A:OP2	13:E:222:ASN:HB2	2.20	0.42
9:A:712:G:N2	9:A:743:C:C2	2.88	0.42
9:A:1009:A:N1	9:A:2041:G:O2'	2.44	0.42
9:A:1543:G:H5'	9:A:1544:A:OP2	2.20	0.42
12:D:90:ILE:HD13	12:D:90:ILE:HA	1.65	0.42
2:1:43:SER:OG	31:W:89:A:H1'	2.19	0.42
7:6:96:LEU:O	7:6:100:LEU:HG	2.20	0.42
9:A:483:A:H2'	9:A:484:G:C8	2.54	0.42
9:A:1088:U:C2	9:A:1090:U:H5'	2.54	0.42
9:A:1114:A:H4'	9:A:1131:A:C2	2.54	0.42
9:A:1337:U:H2'	9:A:1338:C:H6	1.85	0.42
9:A:1364:G:N2	9:A:1426:U:C2	2.88	0.42
9:A:1632:U:C2'	9:A:1633:A:H5'	2.50	0.42
13:E:175:VAL:HG12	13:E:177:GLU:H	1.83	0.42
14:F:159:LEU:HD21	14:F:192:PRO:CG	2.49	0.42
15:G:53:ASN:HB3	15:G:68:PRO:HG3	2.01	0.42
22:N:32:TYR:HB2	22:N:106:ILE:HG23	2.02	0.42
22:N:65:TRP:HB2	22:N:105:GLU:HB2	2.02	0.42
23:O:62:ILE:HG21	23:O:104:TYR:CD2	2.55	0.42
25:Q:152:ARG:HG2	25:Q:164:VAL:HG22	2.02	0.42
28:T:173:LEU:HD23	28:T:173:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:98:SER:O	30:V:98:SER:OG	2.35	0.42
4:3:114:PHE:CZ	4:3:118:MET:HE3	2.55	0.42
9:A:844:G:C6	9:A:845:C:N4	2.88	0.42
9:A:1317:C:H2'	9:A:1318:C:H6	1.85	0.42
9:A:2255:G:N3	9:A:2255:G:H2'	2.34	0.42
11:C:237:ILE:HD13	11:C:237:ILE:HG21	1.85	0.42
22:N:77:ARG:HH21	22:N:86:GLY:C	2.26	0.42
25:Q:185:ARG:NH2	25:Q:233:LYS:HD3	2.34	0.42
26:R:88:ARG:HE	26:R:118:LYS:HG3	1.85	0.42
33:Y:110:TRP:CE3	33:Y:113:GLY:HA3	2.55	0.42
1:0:77:HIS:HD2	1:0:79:PHE:CD1	2.38	0.42
3:2:36:GLN:HE21	9:A:2302:C:N4	2.17	0.42
9:A:1196:A:H61	9:A:1201:A:H61	1.67	0.42
9:A:1289:A:C2	9:A:2027:A:C4	3.07	0.42
9:A:2142:G:H21	9:A:2187:A:H4'	1.84	0.42
9:A:2167:G:H2'	9:A:2168:C:O4'	2.20	0.42
9:A:2464:G:H8	9:A:2464:G:H5''	1.84	0.42
17:I:148:ARG:HD2	17:I:180:GLU:OE2	2.19	0.42
23:O:92:GLU:O	23:O:95:GLU:HB3	2.20	0.42
31:W:17:A:H1'	31:W:23:G:C2	2.55	0.42
1:0:46:ARG:NH1	1:0:66:LYS:HB2	2.35	0.42
9:A:166:A:H2'	9:A:167:A:C8	2.55	0.42
9:A:1882:U:OP2	21:M:260:LYS:NZ	2.43	0.42
9:A:1913:G:N3	9:A:1913:G:H2'	2.34	0.42
13:E:123:ARG:O	13:E:124:ALA:HB2	2.20	0.42
14:F:54:ILE:H	14:F:54:ILE:HG13	1.57	0.42
19:K:120:THR:HA	19:K:160:LYS:HB2	2.02	0.42
24:P:80:LYS:O	24:P:111:TYR:OH	2.30	0.42
29:U:125:ILE:O	29:U:128:ILE:HB	2.20	0.42
32:X:131:ASP:OD1	32:X:132:LYS:N	2.51	0.42
7:6:131:TRP:HA	7:6:131:TRP:CE3	2.55	0.41
9:A:115:G:C6	9:A:117:A:N6	2.88	0.41
9:A:628:A:H2'	9:A:629:C:O4'	2.19	0.41
9:A:754:A:O2'	9:A:1695:U:OP1	2.34	0.41
9:A:1082:A:H4'	17:I:83:GLY:CA	2.47	0.41
9:A:2303:A:H4'	9:A:2304:A:O4'	2.20	0.41
9:A:2589:A:OP1	9:A:2591:G:H4'	2.20	0.41
9:A:2595:G:N7	12:D:234:SER:HB2	2.35	0.41
10:B:53:U:C4	10:B:54:G:C2	3.09	0.41
11:C:226:HIS:HA	11:C:227:PRO:HD3	1.82	0.41
12:D:203:THR:HG22	12:D:204:ILE:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:212:LEU:HD23	13:E:212:LEU:HA	1.91	0.41
15:G:160:GLU:OE2	15:G:176:ARG:HG3	2.20	0.41
17:I:126:MET:HA	17:I:130:ASN:ND2	2.35	0.41
27:S:102:GLU:H	27:S:102:GLU:HG3	1.66	0.41
29:U:188:ALA:HB1	29:U:193:ILE:O	2.20	0.41
32:X:71:ASP:OD1	32:X:72:SER:N	2.50	0.41
4:3:114:PHE:HA	4:3:139:CYS:SG	2.60	0.41
9:A:1837:U:H2'	9:A:1838:G:O4'	2.19	0.41
10:B:51:G:OP1	24:P:116:THR:HG23	2.19	0.41
27:S:146:ARG:HA	27:S:217:THR:OG1	2.20	0.41
27:S:161:VAL:O	27:S:177:VAL:HG23	2.20	0.41
28:T:126:LYS:O	28:T:128:PRO:HD3	2.20	0.41
30:V:175:TRP:CH2	30:V:176:LYS:HG3	2.55	0.41
34:Z:81:LEU:HD11	34:Z:144:ILE:HD12	2.02	0.41
4:3:146:SER:HA	4:3:150:ALA:HB2	2.01	0.41
5:4:95:HIS:NE2	9:A:236:A:OP1	2.48	0.41
7:6:130:ALA:HB1	7:6:136:MET:CG	2.51	0.41
9:A:585:A:H2'	9:A:586:U:H6	1.85	0.41
9:A:1518:U:C5	9:A:1519:A:H2	2.38	0.41
9:A:1678:G:H2'	9:A:1679:G:O4'	2.20	0.41
9:A:2086:G:H2'	9:A:2087:C:O4'	2.21	0.41
9:A:2093:U:H2'	9:A:2094:G:O4'	2.20	0.41
9:A:2374:C:H2'	9:A:2376:C:OP2	2.20	0.41
13:E:79:THR:O	13:E:83:VAL:HG23	2.20	0.41
24:P:76:PHE:HE2	24:P:78:SER:HB3	1.86	0.41
27:S:121:GLU:HB3	27:S:123:ILE:HG22	2.02	0.41
28:T:30:ASP:HB3	28:T:137:ARG:HG3	2.02	0.41
28:T:68:MET:HA	28:T:69:PRO:HD3	1.89	0.41
30:V:139:SER:HB2	30:V:162:LEU:CD1	2.50	0.41
31:W:32:C:H5'	31:W:33:A:OP2	2.20	0.41
2:1:4:PRO:HG2	9:A:2030:U:O2	2.21	0.41
9:A:1928:C:H2'	9:A:1929:U:C6	2.56	0.41
9:A:2595:G:H4'	9:A:2595:G:OP2	2.20	0.41
12:D:90:ILE:HD12	12:D:90:ILE:HG23	1.84	0.41
23:O:91:ALA:O	23:O:94:PRO:HD2	2.21	0.41
2:1:18:ASN:ND2	9:A:14:A:O3'	2.54	0.41
3:2:8:ARG:NH2	9:A:2302:C:C5	2.89	0.41
9:A:1099:G:O2'	9:A:1117:G:OP2	2.38	0.41
9:A:1141:C:H2'	9:A:1142:G:H8	1.85	0.41
9:A:1883:G:C2	21:M:257:PHE:CE1	3.09	0.41
9:A:2078:C:O2	9:A:2464:G:N2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2653:U:O2'	12:D:134:TYR:OH	2.28	0.41
12:D:185:LEU:O	12:D:186:LEU:HD23	2.20	0.41
13:E:161:LEU:HA	13:E:161:LEU:HD23	1.71	0.41
17:I:56:ARG:HA	17:I:59:LYS:HE2	2.02	0.41
21:M:191:GLY:O	21:M:194:ARG:HB2	2.21	0.41
9:A:236:A:H8	9:A:236:A:O5'	2.04	0.41
9:A:368:U:H4'	9:A:368:U:OP1	2.20	0.41
9:A:988:A:H5''	9:A:989:G:OP1	2.20	0.41
9:A:2213:A:OP1	33:Y:107:ARG:NH2	2.54	0.41
9:A:2267:G:H8	9:A:2268:G:H5''	1.86	0.41
9:A:2339:A:C6	9:A:2350:A:N6	2.89	0.41
11:C:221:MET:H	11:C:221:MET:HG3	1.63	0.41
12:D:186:LEU:HB2	12:D:189:GLU:HG3	2.02	0.41
19:K:208:LEU:HA	19:K:208:LEU:HD23	1.70	0.41
21:M:181:LEU:HB3	21:M:187:ILE:HD12	2.02	0.41
23:O:117:ASN:O	23:O:117:ASN:CG	2.63	0.41
27:S:108:ASN:ND2	27:S:113:LYS:HE3	2.35	0.41
8:7:54:LYS:HE2	9:A:2473:C:O3'	2.21	0.41
9:A:842:G:C6	9:A:843:C:C4	3.08	0.41
9:A:2074:A:H4'	9:A:2075:G:OP1	2.20	0.41
9:A:2354:G:H2'	9:A:2354:G:N3	2.36	0.41
15:G:166:GLU:C	15:G:168:ASN:H	2.28	0.41
21:M:137:TYR:CD1	21:M:137:TYR:C	2.98	0.41
24:P:146:TYR:HA	24:P:147:PRO:HD3	1.97	0.41
27:S:166:THR:HG22	27:S:168:ALA:H	1.85	0.41
27:S:234:THR:HB	27:S:236:GLU:HG3	2.03	0.41
30:V:62:LEU:HD23	30:V:62:LEU:HA	1.84	0.41
30:V:177:GLU:HG2	30:V:181:LYS:HE3	2.02	0.41
2:1:3:VAL:HG12	9:A:2029:A:N3	2.35	0.41
2:1:34:LEU:HD12	2:1:34:LEU:HA	1.87	0.41
3:2:52:CYS:HA	3:2:53:PRO:HD3	1.87	0.41
9:A:311:U:OP2	30:V:147:ARG:NH2	2.54	0.41
9:A:644:A:H2'	9:A:645:A:C8	2.55	0.41
9:A:722:G:C2	9:A:732:A:C6	3.09	0.41
9:A:1672:U:H2'	9:A:1673:A:C8	2.55	0.41
9:A:1702:G:O3'	20:L:6:THR:HG23	2.20	0.41
9:A:2751:A:H1'	12:D:298:VAL:HG13	2.03	0.41
19:K:100:TRP:CE3	26:R:102:ILE:HD13	2.55	0.41
27:S:127:VAL:HG12	27:S:161:VAL:HG22	2.02	0.41
28:T:145:TYR:O	28:T:149:LEU:HG	2.20	0.41
9:A:116:A:OP2	9:A:117:A:H2'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:531:A:H2'	9:A:532:A:H8	1.83	0.41
9:A:1075:G:H8	9:A:1075:G:OP2	2.04	0.41
9:A:1142:G:C6	9:A:1143:C:N4	2.88	0.41
9:A:2045:A:C6	9:A:2515:C:H1'	2.56	0.41
9:A:2136:U:OP1	9:A:2182:G:N2	2.53	0.41
9:A:2699:U:H2'	9:A:2700:C:C6	2.56	0.41
11:C:131:MET:HA	11:C:132:PRO:HD3	1.81	0.41
12:D:166:ARG:HH12	31:W:26:G:P	2.43	0.41
13:E:105:ARG:HA	13:E:138:GLY:HA3	2.02	0.41
14:F:148:LEU:HD12	14:F:148:LEU:HA	1.84	0.41
14:F:159:LEU:HD21	14:F:192:PRO:HG3	2.02	0.41
15:G:63:LEU:HD11	15:G:84:LYS:NZ	2.36	0.41
18:J:146:ALA:HB3	18:J:202:THR:HG21	2.01	0.41
19:K:48:ARG:NH2	31:W:1:A:H3'	2.34	0.41
19:K:83:TRP:CG	19:K:84:MET:N	2.89	0.41
21:M:109:SER:O	21:M:110:CYS:HB2	2.20	0.41
23:O:89:LEU:HD22	23:O:93:VAL:CG2	2.50	0.41
30:V:68:MET:SD	30:V:93:ILE:HD11	2.60	0.41
5:4:136:ILE:HD13	5:4:136:ILE:HA	1.85	0.41
9:A:295:C:N4	9:A:296:G:C6	2.89	0.41
9:A:767:A:H2'	9:A:768:G:O4'	2.21	0.41
9:A:1146:U:H2'	9:A:1147:U:C6	2.55	0.41
9:A:1570:C:H5''	9:A:1571:G:OP1	2.20	0.41
9:A:1717:A:N3	9:A:1772:A:H2'	2.36	0.41
9:A:2075:G:H5''	9:A:2520:A:OP1	2.21	0.41
12:D:101:SER:HB3	25:Q:178:HIS:HD2	1.86	0.41
15:G:104:MET:O	15:G:107:LEU:HB3	2.21	0.41
15:G:214:GLY:O	15:G:215:LYS:HB2	2.20	0.41
22:N:23:ARG:HG3	22:N:23:ARG:HH11	1.86	0.41
25:Q:140:VAL:HA	25:Q:141:PRO:HD3	1.79	0.41
32:X:146:ASN:HB2	32:X:149:SER:OG	2.21	0.41
2:1:6:LYS:HD3	2:1:6:LYS:HA	1.82	0.40
9:A:424:A:N6	9:A:2429:A:O4'	2.54	0.40
9:A:643:A:O2'	21:M:145:GLY:HA3	2.20	0.40
9:A:887:G:O2'	9:A:909:A:N6	2.54	0.40
12:D:166:ARG:HG2	12:D:167:HIS:CD2	2.56	0.40
23:O:69:SER:OG	23:O:72:LYS:HG2	2.20	0.40
32:X:119:ILE:HG22	32:X:120:ASP:O	2.21	0.40
9:A:1378:U:H2'	9:A:1379:C:O4'	2.21	0.40
9:A:1493:C:H5'	9:A:1494:G:OP2	2.21	0.40
9:A:2073:A:O2'	9:A:2074:A:P	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2570:G:H2'	9:A:2571:U:O4'	2.22	0.40
14:F:116:GLN:NE2	14:F:117:ARG:O	2.54	0.40
17:I:138:GLU:HG3	17:I:139:GLU:H	1.86	0.40
18:J:111:LYS:HA	18:J:111:LYS:HD2	1.85	0.40
19:K:50:SER:HA	31:W:1:A:N7	2.35	0.40
22:N:41:TRP:HZ2	22:N:72:LYS:HE2	1.84	0.40
25:Q:184:ARG:NH2	25:Q:193:GLU:OE1	2.54	0.40
29:U:105:PRO:HD2	34:Z:142:ARG:HG2	2.03	0.40
31:W:76:G:H5''	31:W:77:A:OP1	2.22	0.40
9:A:311:U:H3	9:A:325:A:H61	1.68	0.40
9:A:758:U:H4'	28:T:121:ARG:HH21	1.87	0.40
9:A:2101:G:C3'	9:A:2102:G:H5''	2.52	0.40
9:A:2208:U:H2'	9:A:2209:U:O4'	2.22	0.40
9:A:2806:U:O2'	31:W:5:A:N3	2.52	0.40
10:B:29:C:C2	10:B:30:A:C8	3.09	0.40
10:B:77:A:H2'	10:B:78:U:C6	2.57	0.40
11:C:140:ILE:HB	11:C:150:LEU:HB2	2.02	0.40
12:D:282:VAL:HB	12:D:283:PRO:HD2	2.03	0.40
18:J:152:LYS:HE3	18:J:152:LYS:HB2	1.94	0.40
19:K:56:LYS:O	19:K:60:GLU:HG3	2.21	0.40
19:K:100:TRP:N	26:R:99:GLN:HE22	2.16	0.40
19:K:239:LEU:HD12	19:K:239:LEU:HA	1.95	0.40
24:P:122:LYS:HD2	24:P:122:LYS:HA	1.79	0.40
27:S:93:PHE:CG	28:T:163:LEU:HD22	2.55	0.40
7:6:138:LYS:HB3	7:6:138:LYS:HE2	1.82	0.40
9:A:1063:U:OP1	15:G:99:ARG:NH2	2.54	0.40
10:B:17:G:N2	10:B:70:G:H1'	2.36	0.40
10:B:54:G:H8	10:B:54:G:O5'	2.05	0.40
10:B:103:A:H2'	10:B:104:A:O4'	2.22	0.40
12:D:288:ASN:ND2	12:D:289:LEU:H	2.19	0.40
26:R:112:TYR:OH	26:R:116:ILE:HD11	2.21	0.40
5:4:125:ASN:OD1	5:4:127:LYS:HB3	2.22	0.40
9:A:1800:C:H5''	9:A:1801:A:OP1	2.21	0.40
9:A:2628:C:H3'	9:A:2629:A:C8	2.56	0.40
10:B:38:C:OP2	10:B:39:C:H5	2.04	0.40
11:C:49:HIS:CD2	11:C:215:VAL:HG22	2.57	0.40
14:F:113:ILE:HG22	14:F:152:PHE:HE1	1.86	0.40
21:M:136:LEU:HG	21:M:140:ILE:HD12	2.03	0.40
28:T:33:THR:HG23	28:T:135:VAL:HG22	2.03	0.40
28:T:164:MET:HE2	28:T:164:MET:HB3	1.93	0.40
31:W:35:U:H6	31:W:35:U:H2'	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:W:54:A:H2'	31:W:55:A:C8	2.57	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	42/130 (32%)	39 (93%)	3 (7%)	0	100	100
2	1	46/57 (81%)	44 (96%)	2 (4%)	0	100	100
3	2	58/66 (88%)	53 (91%)	5 (9%)	0	100	100
4	3	58/152 (38%)	54 (93%)	4 (7%)	0	100	100
5	4	70/159 (44%)	66 (94%)	4 (6%)	0	100	100
6	5	35/37 (95%)	35 (100%)	0	0	100	100
7	6	47/142 (33%)	46 (98%)	0	1 (2%)	5	31
8	7	44/116 (38%)	40 (91%)	3 (7%)	1 (2%)	5	29
11	C	251/272 (92%)	238 (95%)	12 (5%)	1 (0%)	30	62
12	D	219/305 (72%)	205 (94%)	13 (6%)	1 (0%)	24	59
13	E	210/293 (72%)	193 (92%)	17 (8%)	0	100	100
14	F	191/258 (74%)	178 (93%)	13 (7%)	0	100	100
15	G	176/220 (80%)	167 (95%)	9 (5%)	0	100	100
16	H	46/196 (24%)	43 (94%)	3 (6%)	0	100	100
17	I	135/232 (58%)	132 (98%)	3 (2%)	0	100	100
18	J	131/224 (58%)	126 (96%)	5 (4%)	0	100	100
19	K	201/250 (80%)	194 (96%)	7 (4%)	0	100	100
20	L	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
21	M	183/271 (68%)	169 (92%)	12 (7%)	2 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	N	133/135 (98%)	122 (92%)	11 (8%)	0	100	100
23	O	114/126 (90%)	110 (96%)	4 (4%)	0	100	100
24	P	120/166 (72%)	114 (95%)	6 (5%)	0	100	100
25	Q	116/233 (50%)	114 (98%)	2 (2%)	0	100	100
26	R	117/128 (91%)	110 (94%)	7 (6%)	0	100	100
27	S	168/256 (66%)	157 (94%)	9 (5%)	2 (1%)	10	42
28	T	170/199 (85%)	161 (95%)	8 (5%)	1 (1%)	21	56
29	U	94/198 (48%)	89 (95%)	5 (5%)	0	100	100
30	V	132/192 (69%)	121 (92%)	10 (8%)	1 (1%)	16	50
32	X	107/194 (55%)	95 (89%)	12 (11%)	0	100	100
33	Y	75/148 (51%)	74 (99%)	1 (1%)	0	100	100
34	Z	99/168 (59%)	95 (96%)	3 (3%)	1 (1%)	12	45
All	All	3707/5644 (66%)	3499 (94%)	197 (5%)	11 (0%)	37	68

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	C	232	GLU
21	M	131	GLY
27	S	78	PRO
34	Z	151	SER
7	6	131	TRP
8	7	88	GLU
21	M	208	THR
27	S	79	PRO
28	T	146	ASP
30	V	117	GLU
12	D	212	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	39/117 (33%)	36 (92%)	3 (8%)	12	41
2	1	41/50 (82%)	36 (88%)	5 (12%)	5	22
3	2	56/60 (93%)	49 (88%)	7 (12%)	4	21
4	3	50/125 (40%)	42 (84%)	8 (16%)	2	13
5	4	62/140 (44%)	56 (90%)	6 (10%)	8	32
6	5	34/34 (100%)	29 (85%)	5 (15%)	3	16
7	6	46/124 (37%)	43 (94%)	3 (6%)	15	47
8	7	40/96 (42%)	35 (88%)	5 (12%)	4	21
11	C	201/217 (93%)	179 (89%)	22 (11%)	6	26
12	D	182/259 (70%)	165 (91%)	17 (9%)	8	33
13	E	179/255 (70%)	160 (89%)	19 (11%)	6	27
14	F	152/214 (71%)	137 (90%)	15 (10%)	7	31
15	G	151/190 (80%)	140 (93%)	11 (7%)	13	43
16	H	42/170 (25%)	35 (83%)	7 (17%)	2	11
17	I	119/204 (58%)	112 (94%)	7 (6%)	18	50
18	J	106/189 (56%)	102 (96%)	4 (4%)	29	62
19	K	176/213 (83%)	166 (94%)	10 (6%)	18	51
20	L	101/101 (100%)	92 (91%)	9 (9%)	9	34
21	M	141/215 (66%)	125 (89%)	16 (11%)	5	24
22	N	108/108 (100%)	97 (90%)	11 (10%)	7	29
23	O	96/103 (93%)	84 (88%)	12 (12%)	4	21
24	P	100/139 (72%)	92 (92%)	8 (8%)	11	40
25	Q	104/207 (50%)	93 (89%)	11 (11%)	6	27
26	R	106/115 (92%)	97 (92%)	9 (8%)	10	37
27	S	137/223 (61%)	131 (96%)	6 (4%)	25	59
28	T	152/176 (86%)	138 (91%)	14 (9%)	8	33
29	U	85/171 (50%)	76 (89%)	9 (11%)	6	27
30	V	121/169 (72%)	114 (94%)	7 (6%)	18	51
32	X	92/163 (56%)	78 (85%)	14 (15%)	3	14
33	Y	67/130 (52%)	61 (91%)	6 (9%)	9	34
34	Z	93/153 (61%)	85 (91%)	8 (9%)	10	36
All	All	3179/4830 (66%)	2885 (91%)	294 (9%)	11	33

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	51	VAL
1	0	57	LEU
1	0	59	MET
2	1	6	LYS
2	1	7	ARG
2	1	11	TYR
2	1	13	LYS
2	1	14	ARG
3	2	19	VAL
3	2	28	ARG
3	2	34	ILE
3	2	42	THR
3	2	45	ARG
3	2	59	THR
3	2	60	ILE
4	3	96	LEU
4	3	97	CYS
4	3	98	LEU
4	3	118	MET
4	3	126	LEU
4	3	127	LEU
4	3	129	ARG
4	3	142	THR
5	4	104	VAL
5	4	110	ILE
5	4	118	GLN
5	4	119	HIS
5	4	125	ASN
5	4	147	ILE
6	5	3	ILE
6	5	4	ARG
6	5	24	ILE
6	5	29	ASN
6	5	36	GLN
7	6	118	ARG
7	6	137	LYS
7	6	138	LYS
8	7	50	ARG
8	7	54	LYS
8	7	66	LYS
8	7	74	ARG
8	7	88	GLU

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Mol	Chain	Res	Type
11	C	19	GLN
11	C	20	VAL
11	C	44	ILE
11	C	54	HIS
11	C	71	TYR
11	C	90	ILE
11	C	96	GLU
11	C	126	LEU
11	C	142	ILE
11	C	152	ARG
11	C	170	LEU
11	C	178	ARG
11	C	179	LEU
11	C	196	VAL
11	C	203	ARG
11	C	223	PRO
11	C	224	VAL
11	C	228	HIS
11	C	240	LYS
11	C	255	SER
11	C	260	LYS
11	C	270	ARG
12	D	109	VAL
12	D	137	VAL
12	D	139	VAL
12	D	146	ASP
12	D	174	VAL
12	D	178	ASP
12	D	193	GLU
12	D	206	LYS
12	D	219	ARG
12	D	221	LEU
12	D	244	VAL
12	D	260	LYS
12	D	262	ARG
12	D	273	LEU
12	D	288	ASN
12	D	292	LEU
12	D	298	VAL
13	E	52	LEU
13	E	61	SER
13	E	68	THR

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Mol	Chain	Res	Type
13	E	74	THR
13	E	97	ARG
13	E	113	ARG
13	E	114	LYS
13	E	120	LYS
13	E	157	ARG
13	E	161	LEU
13	E	174	VAL
13	E	209	LEU
13	E	213	VAL
13	E	223	ILE
13	E	230	THR
13	E	238	ASP
13	E	245	LEU
13	E	251	THR
13	E	261	VAL
14	F	53	THR
14	F	56	ARG
14	F	57	LEU
14	F	59	THR
14	F	84	VAL
14	F	88	VAL
14	F	110	LEU
14	F	119	VAL
14	F	122	LYS
14	F	125	THR
14	F	127	ILE
14	F	155	ARG
14	F	188	GLN
14	F	190	VAL
14	F	205	MET
15	G	40	GLU
15	G	50	VAL
15	G	63	LEU
15	G	74	ILE
15	G	84	LYS
15	G	100	ARG
15	G	109	ARG
15	G	127	LEU
15	G	129	LEU
15	G	169	THR
15	G	213	GLU

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Mol	Chain	Res	Type
16	H	47	LYS
16	H	52	ILE
16	H	57	ILE
16	H	75	ARG
16	H	79	LEU
16	H	85	GLU
16	H	87	VAL
17	I	75	LEU
17	I	79	ILE
17	I	89	PHE
17	I	101	THR
17	I	114	VAL
17	I	117	THR
17	I	119	TRP
18	J	90	THR
18	J	95	VAL
18	J	129	ILE
18	J	171	ILE
19	K	48	ARG
19	K	62	ARG
19	K	64	LEU
19	K	79	LEU
19	K	116	VAL
19	K	147	VAL
19	K	156	VAL
19	K	191	LEU
19	K	195	ILE
19	K	199	ILE
20	L	2	ILE
20	L	10	VAL
20	L	23	ARG
20	L	25	ILE
20	L	28	SER
20	L	34	ARG
20	L	42	VAL
20	L	102	ILE
20	L	105	GLU
21	M	83	ASP
21	M	84	ASN
21	M	92	ARG
21	M	93	LYS
21	M	106	GLN

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Mol	Chain	Res	Type
21	M	125	ILE
21	M	138	ARG
21	M	154	LEU
21	M	164	ASP
21	M	186	ILE
21	M	208	THR
21	M	212	ILE
21	M	215	ARG
21	M	220	SER
21	M	246	VAL
21	M	257	PHE
22	N	5	LYS
22	N	9	PHE
22	N	27	ILE
22	N	28	CYS
22	N	44	SER
22	N	48	GLU
22	N	52	ARG
22	N	56	ARG
22	N	94	VAL
22	N	109	VAL
22	N	118	VAL
23	O	11	MET
23	O	22	ARG
23	O	27	ARG
23	O	28	ARG
23	O	73	ARG
23	O	74	ARG
23	O	86	VAL
23	O	89	LEU
23	O	105	THR
23	O	111	LEU
23	O	123	ILE
23	O	126	VAL
24	P	49	ARG
24	P	52	ASP
24	P	59	ARG
24	P	87	ILE
24	P	127	ILE
24	P	143	ARG
24	P	151	ARG
24	P	161	GLU

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Mol	Chain	Res	Type
25	Q	117	VAL
25	Q	125	ILE
25	Q	138	ARG
25	Q	149	VAL
25	Q	172	ARG
25	Q	185	ARG
25	Q	198	LEU
25	Q	200	SER
25	Q	203	ILE
25	Q	206	ILE
25	Q	215	ARG
26	R	23	SER
26	R	31	LEU
26	R	33	ARG
26	R	76	TYR
26	R	85	LEU
26	R	90	LEU
26	R	96	ILE
26	R	108	ILE
26	R	115	ILE
27	S	87	ASP
27	S	102	GLU
27	S	195	VAL
27	S	204	LYS
27	S	208	ARG
27	S	216	ILE
28	T	38	SER
28	T	43	VAL
28	T	53	ILE
28	T	62	LEU
28	T	100	ILE
28	T	109	ILE
28	T	117	ARG
28	T	134	ILE
28	T	139	ILE
28	T	153	THR
28	T	160	LEU
28	T	163	LEU
28	T	174	CYS
28	T	183	ILE
29	U	102	LEU
29	U	103	LYS

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Mol	Chain	Res	Type
29	U	111	VAL
29	U	119	ILE
29	U	138	VAL
29	U	143	ASP
29	U	171	THR
29	U	172	LYS
29	U	178	LEU
30	V	48	ARG
30	V	93	ILE
30	V	113	LYS
30	V	130	ILE
30	V	136	MET
30	V	146	SER
30	V	173	ASP
32	X	73	LYS
32	X	81	ILE
32	X	85	GLN
32	X	86	VAL
32	X	97	ARG
32	X	105	LYS
32	X	107	VAL
32	X	109	ILE
32	X	111	LYS
32	X	120	ASP
32	X	123	VAL
32	X	135	VAL
32	X	142	ILE
32	X	155	ARG
33	Y	83	ASN
33	Y	92	ASN
33	Y	98	LEU
33	Y	126	LEU
33	Y	135	ASP
33	Y	144	ASP
34	Z	59	VAL
34	Z	65	LEU
34	Z	76	LEU
34	Z	87	LEU
34	Z	107	ARG
34	Z	130	LYS
34	Z	132	LEU
34	Z	146	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	42	HIS
1	0	65	GLN
1	0	77	HIS
3	2	36	GLN
4	3	112	HIS
4	3	143	ASN
11	C	23	ASN
12	D	121	ASN
12	D	216	ASN
12	D	288	ASN
13	E	118	GLN
13	E	171	ASN
14	F	60	ASN
14	F	99	ASN
15	G	102	ASN
15	G	103	GLN
16	H	42	GLN
17	I	90	GLN
17	I	99	ASN
17	I	130	ASN
17	I	151	GLN
18	J	114	ASN
18	J	205	ASN
19	K	97	ASN
20	L	92	ASN
21	M	84	ASN
21	M	133	GLN
21	M	161	ASN
22	N	13	HIS
23	O	18	HIS
23	O	71	HIS
23	O	75	GLN
23	O	84	GLN
23	O	87	HIS
24	P	81	HIS
24	P	85	GLN
24	P	93	HIS
24	P	108	ASN
24	P	162	HIS
25	Q	178	HIS
26	R	28	HIS

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Mol	Chain	Res	Type
26	R	37	GLN
26	R	53	GLN
26	R	83	HIS
26	R	99	GLN
26	R	113	ASN
27	S	108	ASN
28	T	90	ASN
28	T	97	ASN
29	U	127	ASN
29	U	153	ASN
30	V	142	GLN
30	V	179	GLN
30	V	180	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	120/121 (99%)	19 (15%)	0
31	W	105/106 (99%)	38 (36%)	0
35	z	1/2 (50%)	1 (100%)	0
9	A	2794/2810 (99%)	642 (22%)	8 (0%)
All	All	3020/3039 (99%)	700 (23%)	8 (0%)

All (700) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	9	A
9	A	10	G
9	A	12	A
9	A	13	A
9	A	14	A
9	A	31	C
9	A	33	A
9	A	34	G
9	A	39	C
9	A	45	A
9	A	46	C
9	A	54	G
9	A	57	G
9	A	66	G
9	A	70	A

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Mol	Chain	Res	Type
9	A	73	U
9	A	74	G
9	A	82	G
9	A	84	G
9	A	90	A
9	A	94	A
9	A	97	A
9	A	98	G
9	A	99	A
9	A	100	G
9	A	116	A
9	A	117	A
9	A	118	U
9	A	123	C
9	A	130	U
9	A	131	C
9	A	143	G
9	A	144	A
9	A	149	A
9	A	158	C
9	A	159	A
9	A	160	A
9	A	181	A
9	A	184	A
9	A	200	G
9	A	201	A
9	A	206	A
9	A	207	A
9	A	208	A
9	A	216	C
9	A	218	A
9	A	224	G
9	A	226	A
9	A	233	G
9	A	249	C
9	A	250	A
9	A	251	G
9	A	252	C
9	A	266	A
9	A	267	C
9	A	275	U
9	A	276	G

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Mol	Chain	Res	Type
9	A	282	G
9	A	284	A
9	A	286	U
9	A	287	A
9	A	288	C
9	A	289	A
9	A	294	U
9	A	297	U
9	A	298	G
9	A	299	C
9	A	304	A
9	A	311	U
9	A	316	G
9	A	317	G
9	A	320	U
9	A	326	A
9	A	332	G
9	A	333	A
9	A	338	G
9	A	339	A
9	A	340	A
9	A	344	C
9	A	362	A
9	A	363	C
9	A	364	U
9	A	368	U
9	A	370	A
9	A	377	G
9	A	379	C
9	A	383	A
9	A	384	G
9	A	398	G
9	A	400	G
9	A	415	U
9	A	416	C
9	A	417	A
9	A	418	G
9	A	423	G
9	A	424	A
9	A	436	G
9	A	437	G
9	A	448	C

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Mol	Chain	Res	Type
9	A	451	G
9	A	452	G
9	A	453	U
9	A	454	G
9	A	466	A
9	A	467	G
9	A	468	U
9	A	469	A
9	A	471	U
9	A	479	G
9	A	492	A
9	A	493	G
9	A	502	U
9	A	507	G
9	A	519	A
9	A	520	C
9	A	529	G
9	A	539	A
9	A	541	G
9	A	542	C
9	A	543	A
9	A	544	G
9	A	549	A
9	A	554	G
9	A	556	C
9	A	557	C
9	A	558	A
9	A	559	G
9	A	560	A
9	A	561	C
9	A	562	C
9	A	565	G
9	A	573	G
9	A	582	A
9	A	583	G
9	A	585	A
9	A	593	G
9	A	597	C
9	A	608	U
9	A	609	G
9	A	610	G
9	A	612	U

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Mol	Chain	Res	Type
9	A	613	U
9	A	614	G
9	A	623	A
9	A	630	C
9	A	632	G
9	A	633	A
9	A	635	C
9	A	639	A
9	A	643	A
9	A	645	A
9	A	649	A
9	A	657	U
9	A	658	A
9	A	665	U
9	A	667	G
9	A	680	G
9	A	681	A
9	A	696	A
9	A	697	U
9	A	701	U
9	A	705	U
9	A	712	G
9	A	713	A
9	A	724	G
9	A	727	A
9	A	728	A
9	A	729	A
9	A	730	C
9	A	731	U
9	A	734	G
9	A	740	G
9	A	741	U
9	A	749	G
9	A	758	U
9	A	759	G
9	A	760	A
9	A	768	G
9	A	775	A
9	A	776	G
9	A	782	G
9	A	786	G
9	A	787	G

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Mol	Chain	Res	Type
9	A	788	G
9	A	793	A
9	A	795	U
9	A	796	G
9	A	803	G
9	A	816	G
9	A	817	C
9	A	823	C
9	A	838	U
9	A	839	G
9	A	853	G
9	A	856	U
9	A	857	G
9	A	858	G
9	A	859	A
9	A	866	G
9	A	869	G
9	A	879	G
9	A	880	U
9	A	888	C
9	A	890	G
9	A	893	C
9	A	895	C
9	A	902	G
9	A	904	U
9	A	905	A
9	A	906	C
9	A	907	C
9	A	910	A
9	A	913	G
9	A	916	G
9	A	919	A
9	A	923	C
9	A	924	U
9	A	937	U
9	A	938	G
9	A	939	A
9	A	943	C
9	A	946	A
9	A	947	A
9	A	948	U
9	A	965	G

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Mol	Chain	Res	Type
9	A	974	G
9	A	981	G
9	A	989	G
9	A	1002	G
9	A	1007	A
9	A	1011	A
9	A	1017	G
9	A	1018	A
9	A	1024	A
9	A	1039	A
9	A	1040	U
9	A	1041	G
9	A	1045	G
9	A	1050	G
9	A	1051	U
9	A	1052	G
9	A	1053	A
9	A	1054	U
9	A	1055	A
9	A	1061	G
9	A	1062	G
9	A	1065	G
9	A	1071	C
9	A	1072	A
9	A	1075	G
9	A	1098	A
9	A	1099	G
9	A	1116	A
9	A	1118	U
9	A	1140	G
9	A	1143	C
9	A	1144	U
9	A	1147	U
9	A	1148	G
9	A	1155	A
9	A	1158	U
9	A	1160	A
9	A	1162	C
9	A	1163	G
9	A	1169	A
9	A	1170	A
9	A	1173	G

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Mol	Chain	Res	Type
9	A	1184	G
9	A	1190	G
9	A	1196	A
9	A	1197	A
9	A	1198	A
9	A	1199	A
9	A	1202	A
9	A	1226	U
9	A	1227	U
9	A	1231	G
9	A	1239	C
9	A	1241	U
9	A	1248	G
9	A	1253	G
9	A	1254	U
9	A	1255	U
9	A	1257	G
9	A	1259	C
9	A	1261	A
9	A	1274	A
9	A	1277	G
9	A	1289	A
9	A	1292	G
9	A	1293	C
9	A	1295	A
9	A	1296	A
9	A	1310	C
9	A	1315	G
9	A	1321	A
9	A	1322	A
9	A	1327	U
9	A	1333	U
9	A	1342	A
9	A	1353	A
9	A	1357	A
9	A	1359	G
9	A	1362	G
9	A	1366	C
9	A	1371	C
9	A	1380	A
9	A	1381	G
9	A	1386	A

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Mol	Chain	Res	Type
9	A	1400	U
9	A	1405	A
9	A	1416	A
9	A	1417	U
9	A	1420	C
9	A	1423	U
9	A	1431	C
9	A	1432	U
9	A	1433	U
9	A	1435	U
9	A	1436	U
9	A	1437	G
9	A	1438	G
9	A	1444	A
9	A	1446	G
9	A	1449	C
9	A	1450	G
9	A	1456	G
9	A	1458	C
9	A	1465	A
9	A	1472	A
9	A	1475	U
9	A	1476	G
9	A	1477	G
9	A	1480	A
9	A	1483	G
9	A	1484	G
9	A	1485	U
9	A	1493	C
9	A	1494	G
9	A	1497	A
9	A	1500	U
9	A	1501	G
9	A	1513	C
9	A	1519	A
9	A	1520	A
9	A	1521	G
9	A	1523	A
9	A	1524	G
9	A	1526	G
9	A	1527	G
9	A	1533	A

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Mol	Chain	Res	Type
9	A	1544	A
9	A	1554	C
9	A	1557	G
9	A	1558	U
9	A	1559	A
9	A	1563	G
9	A	1566	G
9	A	1567	C
9	A	1568	U
9	A	1570	C
9	A	1571	G
9	A	1588	U
9	A	1594	A
9	A	1600	A
9	A	1603	A
9	A	1612	A
9	A	1620	U
9	A	1621	C
9	A	1629	G
9	A	1630	G
9	A	1631	G
9	A	1632	U
9	A	1634	C
9	A	1635	C
9	A	1642	C
9	A	1643	G
9	A	1644	A
9	A	1645	A
9	A	1682	C
9	A	1683	G
9	A	1684	C
9	A	1710	G
9	A	1711	C
9	A	1734	A
9	A	1739	G
9	A	1746	C
9	A	1750	C
9	A	1760	G
9	A	1762	C
9	A	1766	G
9	A	1774	G
9	A	1778	G

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Mol	Chain	Res	Type
9	A	1783	A
9	A	1785	U
9	A	1791	C
9	A	1801	A
9	A	1810	C
9	A	1812	A
9	A	1818	U
9	A	1821	G
9	A	1826	U
9	A	1833	G
9	A	1839	A
9	A	1849	A
9	A	1850	G
9	A	1858	A
9	A	1866	G
9	A	1869	G
9	A	1870	U
9	A	1877	C
9	A	1882	U
9	A	1883	G
9	A	1884	A
9	A	1885	C
9	A	1888	G
9	A	1889	G
9	A	1914	A
9	A	1920	G
9	A	1923	C
9	A	1927	A
9	A	1928	C
9	A	1930	A
9	A	1931	U
9	A	1933	A
9	A	1934	C
9	A	1940	U
9	A	1943	G
9	A	1944	G
9	A	1951	A
9	A	1952	A
9	A	1953	U
9	A	1969	U
9	A	1975	C
9	A	1981	C

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Mol	Chain	Res	Type
9	A	1984	A
9	A	1985	A
9	A	1986	G
9	A	2005	U
9	A	2006	G
9	A	2007	U
9	A	2011	G
9	A	2015	A
9	A	2016	G
9	A	2034	C
9	A	2037	G
9	A	2045	A
9	A	2046	G
9	A	2047	A
9	A	2053	A
9	A	2057	C
9	A	2065	U
9	A	2069	C
9	A	2073	A
9	A	2074	A
9	A	2075	G
9	A	2076	A
9	A	2077	C
9	A	2081	A
9	A	2082	U
9	A	2083	G
9	A	2102	G
9	A	2103	G
9	A	2107	G
9	A	2115	G
9	A	2116	C
9	A	2119	U
9	A	2125	C
9	A	2126	G
9	A	2127	C
9	A	2129	G
9	A	2130	C
9	A	2131	U
9	A	2132	U
9	A	2133	A
9	A	2137	G
9	A	2140	A

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Mol	Chain	Res	Type
9	A	2145	A
9	A	2146	A
9	A	2147	G
9	A	2148	A
9	A	2150	G
9	A	2151	G
9	A	2159	C
9	A	2160	C
9	A	2161	G
9	A	2162	G
9	A	2163	G
9	A	2173	G
9	A	2174	C
9	A	2175	C
9	A	2176	A
9	A	2177	U
9	A	2178	C
9	A	2179	A
9	A	2181	U
9	A	2182	G
9	A	2183	A
9	A	2184	G
9	A	2185	A
9	A	2186	U
9	A	2187	A
9	A	2191	C
9	A	2192	U
9	A	2193	C
9	A	2195	G
9	A	2199	G
9	A	2201	G
9	A	2202	C
9	A	2204	A
9	A	2205	G
9	A	2212	A
9	A	2213	A
9	A	2217	U
9	A	2219	U
9	A	2220	G
9	A	2223	A
9	A	2227	C
9	A	2229	U

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Mol	Chain	Res	Type
9	A	2230	A
9	A	2232	G
9	A	2242	A
9	A	2254	A
9	A	2255	G
9	A	2256	A
9	A	2266	U
9	A	2267	G
9	A	2269	G
9	A	2290	A
9	A	2296	G
9	A	2297	G
9	A	2300	U
9	A	2303	A
9	A	2304	A
9	A	2305	A
9	A	2315	G
9	A	2316	G
9	A	2322	A
9	A	2323	C
9	A	2325	G
9	A	2339	A
9	A	2341	U
9	A	2342	G
9	A	2343	C
9	A	2344	A
9	A	2349	C
9	A	2352	A
9	A	2362	G
9	A	2364	C
9	A	2367	C
9	A	2375	A
9	A	2378	C
9	A	2400	G
9	A	2402	C
9	A	2408	G
9	A	2417	G
9	A	2419	G
9	A	2423	A
9	A	2427	G
9	A	2428	A
9	A	2431	G

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Mol	Chain	Res	Type
9	A	2436	U
9	A	2442	A
9	A	2444	C
9	A	2446	G
9	A	2447	A
9	A	2448	U
9	A	2452	A
9	A	2458	U
9	A	2462	G
9	A	2464	G
9	A	2465	A
9	A	2466	U
9	A	2467	A
9	A	2481	C
9	A	2487	G
9	A	2493	A
9	A	2507	G
9	A	2508	U
9	A	2509	U
9	A	2518	C
9	A	2519	G
9	A	2521	U
9	A	2522	G
9	A	2523	U
9	A	2524	C
9	A	2526	G
9	A	2535	C
9	A	2546	G
9	A	2553	G
9	A	2569	U
9	A	2571	U
9	A	2583	A
9	A	2584	G
9	A	2589	A
9	A	2590	C
9	A	2591	G
9	A	2593	G
9	A	2594	A
9	A	2599	G
9	A	2601	U
9	A	2602	U
9	A	2603	C

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Mol	Chain	Res	Type
9	A	2619	A
9	A	2625	G
9	A	2626	U
9	A	2627	C
9	A	2630	U
9	A	2646	U
9	A	2649	A
9	A	2662	C
9	A	2671	A
9	A	2672	G
9	A	2680	G
9	A	2688	A
9	A	2689	A
9	A	2702	G
9	A	2706	U
9	A	2707	A
9	A	2709	C
9	A	2721	C
9	A	2729	A
9	A	2732	G
9	A	2740	G
9	A	2744	A
9	A	2751	A
9	A	2753	C
9	A	2754	G
9	A	2762	G
9	A	2766	A
9	A	2768	A
9	A	2769	G
9	A	2770	C
9	A	2774	U
9	A	2776	A
9	A	2778	U
9	A	2783	A
9	A	2784	G
9	A	2787	C
9	A	2796	A
9	A	2807	C
9	A	2809	U
10	B	2	A
10	B	10	G
10	B	15	A

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Mol	Chain	Res	Type
10	B	16	G
10	B	17	G
10	B	19	G
10	B	25	G
10	B	31	C
10	B	37	U
10	B	38	C
10	B	39	C
10	B	41	U
10	B	42	C
10	B	57	U
10	B	68	G
10	B	93	C
10	B	105	U
10	B	107	G
10	B	111	G
31	W	3	A
31	W	4	G
31	W	5	A
31	W	14	G
31	W	16	G
31	W	17	A
31	W	19	A
31	W	20	C
31	W	21	G
31	W	26	G
31	W	27	U
31	W	28	U
31	W	29	U
31	W	30	A
31	W	31	U
31	W	32	C
31	W	33	A
31	W	34	U
31	W	35	U
31	W	36	A
31	W	37	C
31	W	38	G
31	W	59	C
31	W	65	U
31	W	71	C
31	W	72	A

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Mol	Chain	Res	Type
31	W	77	A
31	W	79	G
31	W	83	C
31	W	84	C
31	W	85	U
31	W	86	A
31	W	90	G
31	W	95	A
31	W	96	C
31	W	97	A
31	W	99	A
31	W	103	G
35	z	76	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	548	G
9	A	556	C
9	A	680	G
9	A	795	U
9	A	1520	A
9	A	2447	A
9	A	2518	C
9	A	2753	C

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](#)

Of 503 ligands modelled in this entry, 503 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

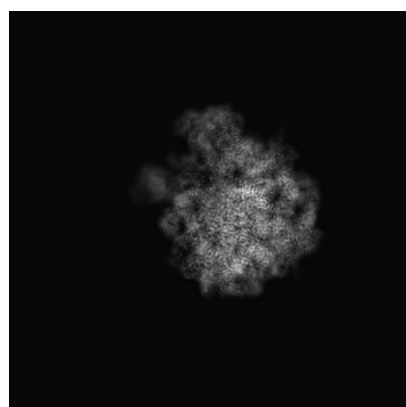
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3531. These allow visual inspection of the internal detail of the map and identification of artifacts.

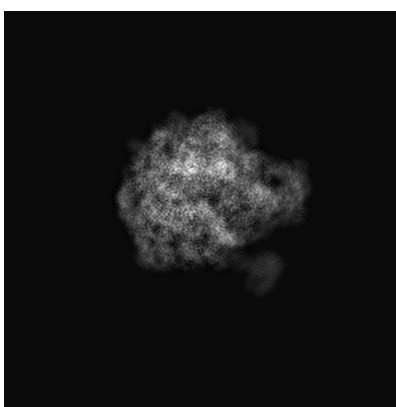
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

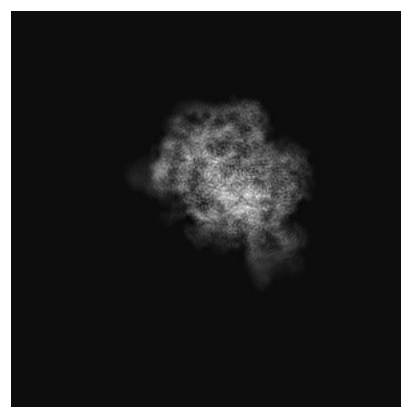
6.1.1 Primary map



X



Y

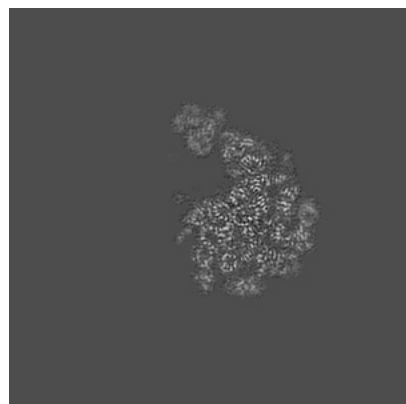


Z

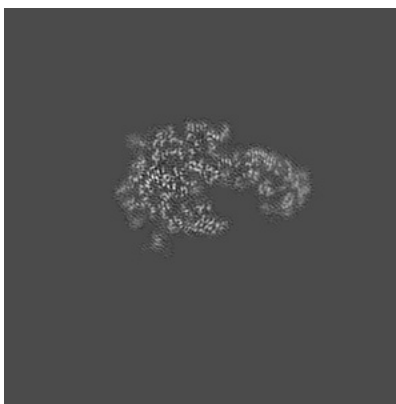
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

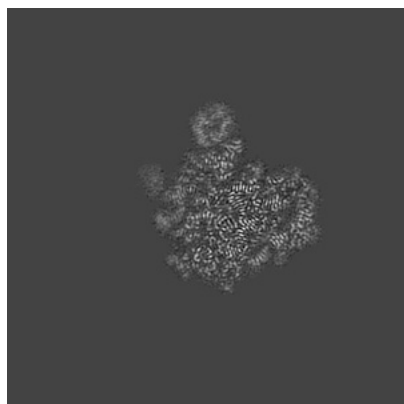


Z Index: 160

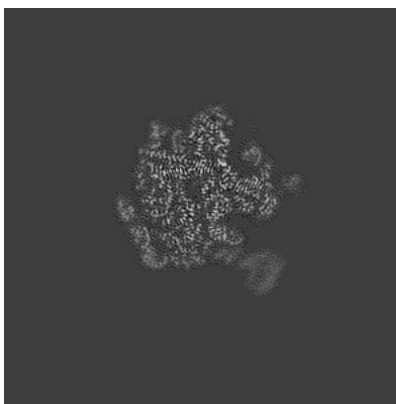
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

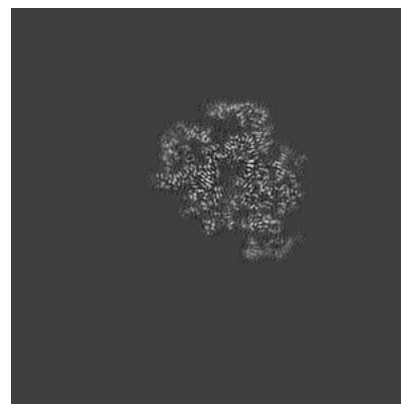
6.3.1 Primary map



X Index: 190



Y Index: 187

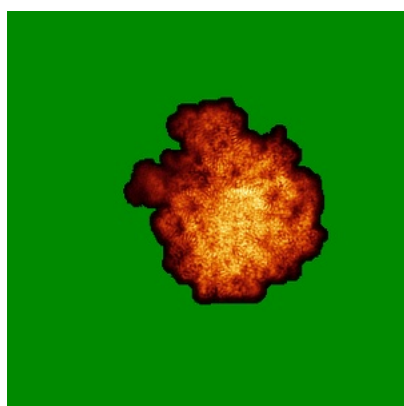


Z Index: 149

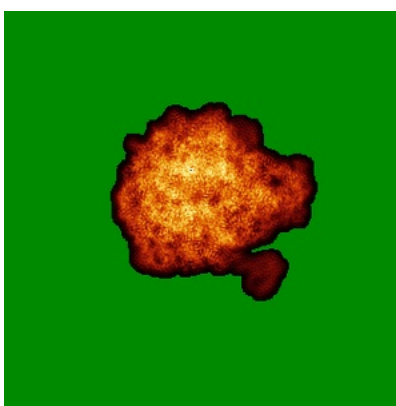
The images above show the largest variance slices of the map in three orthogonal directions.

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

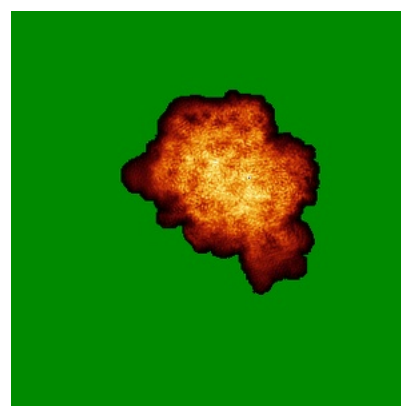
6.4.1 Primary map



X



Y

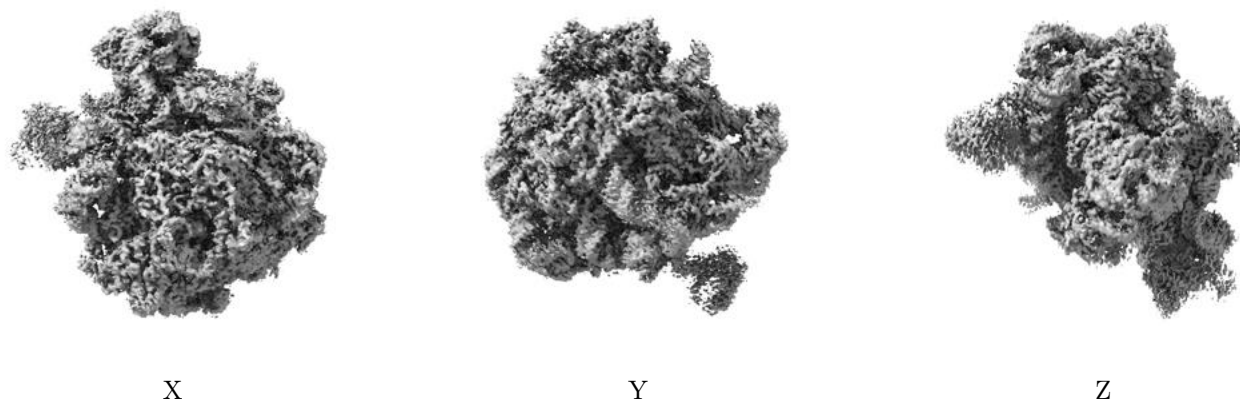


Z

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

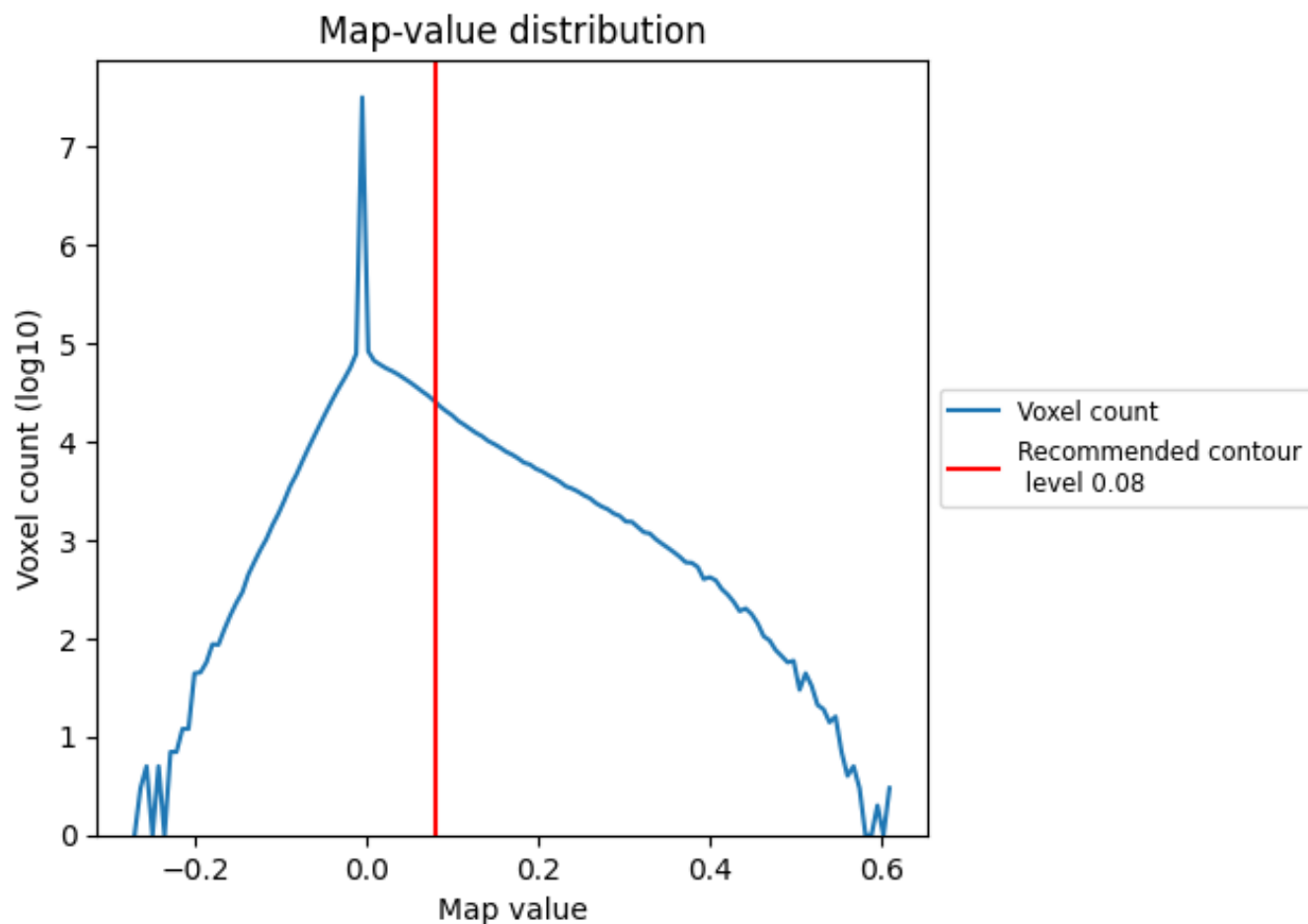
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

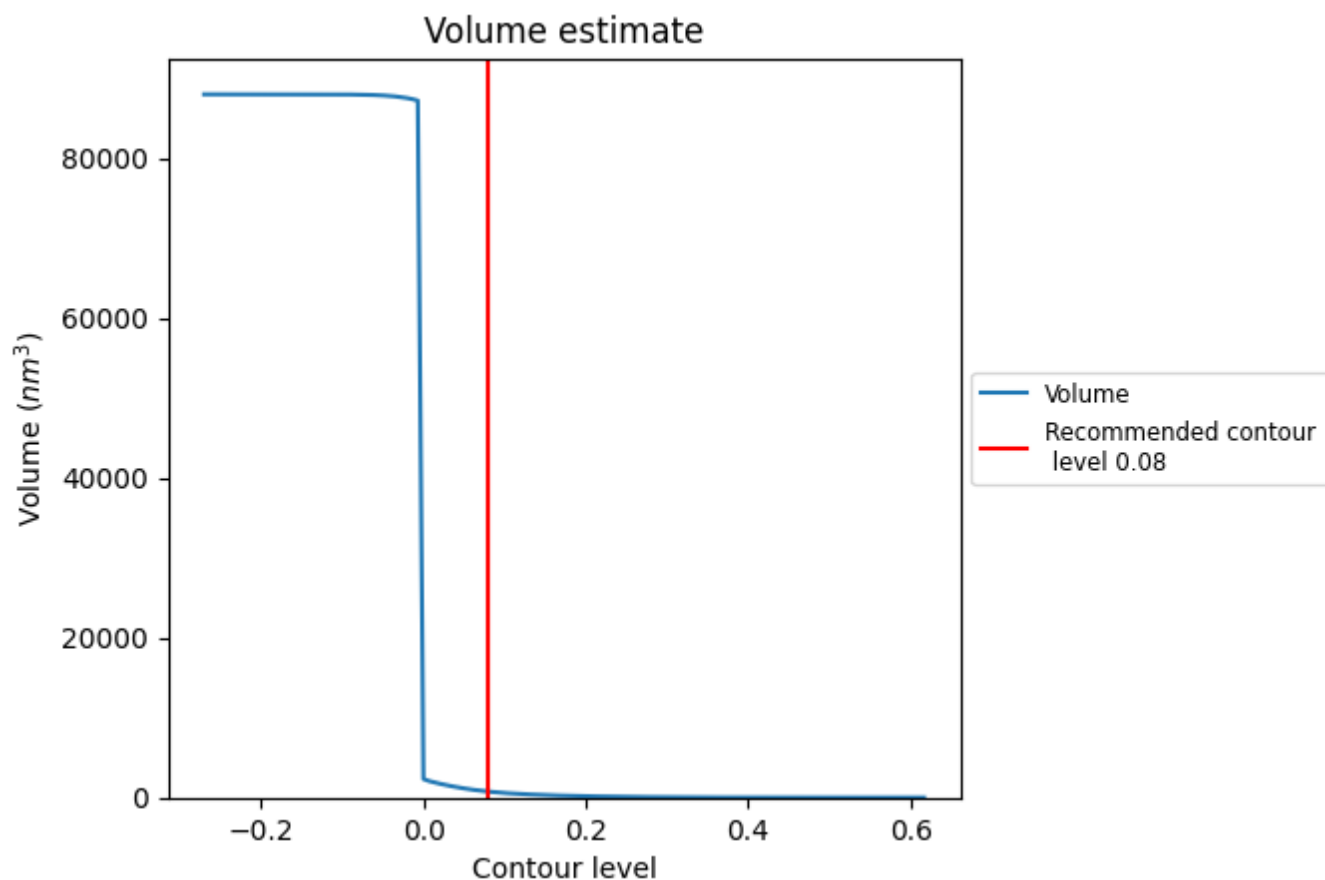
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

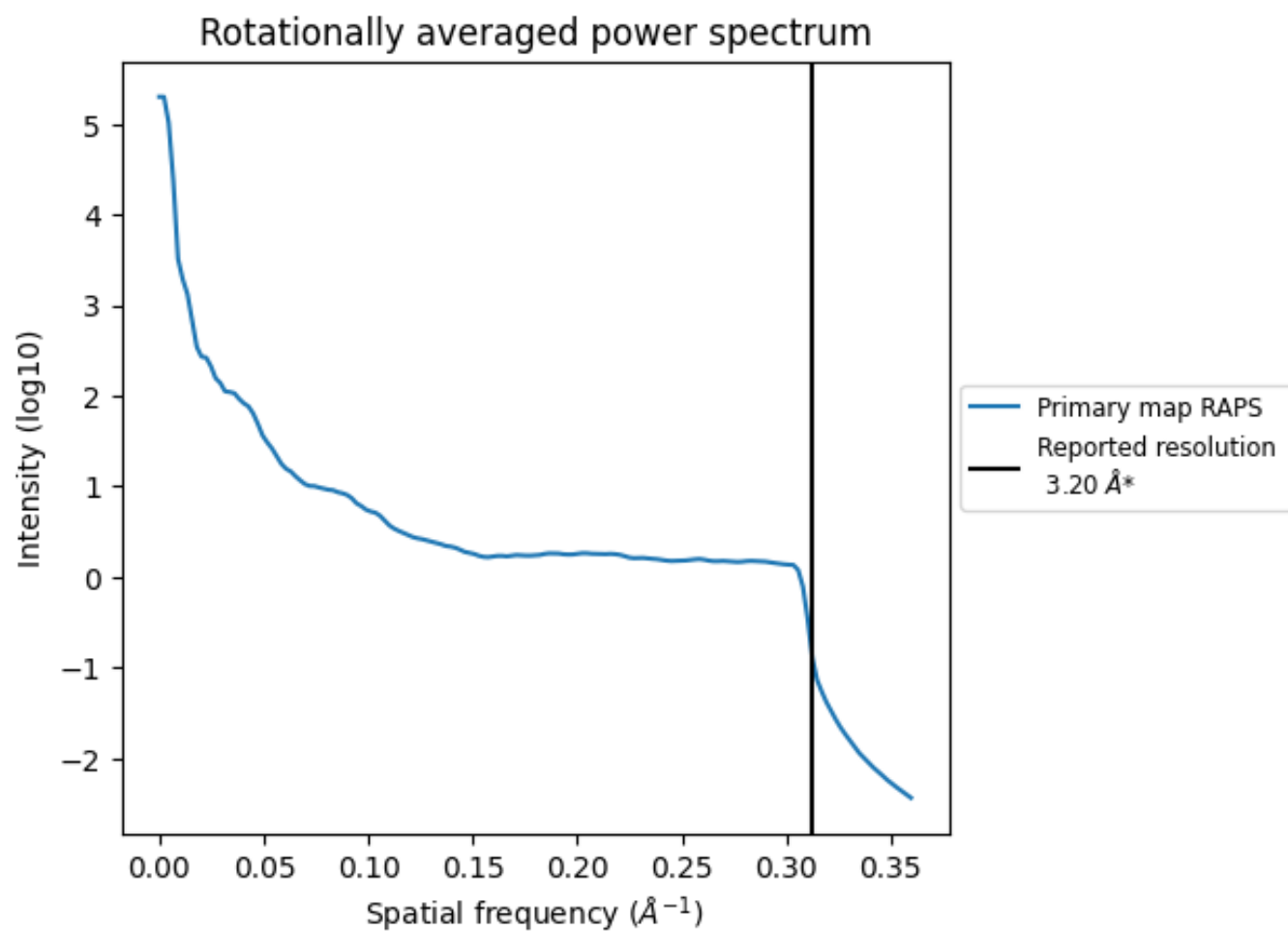
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 750 nm^3 ; this corresponds to an approximate mass of 678 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 ⓘ

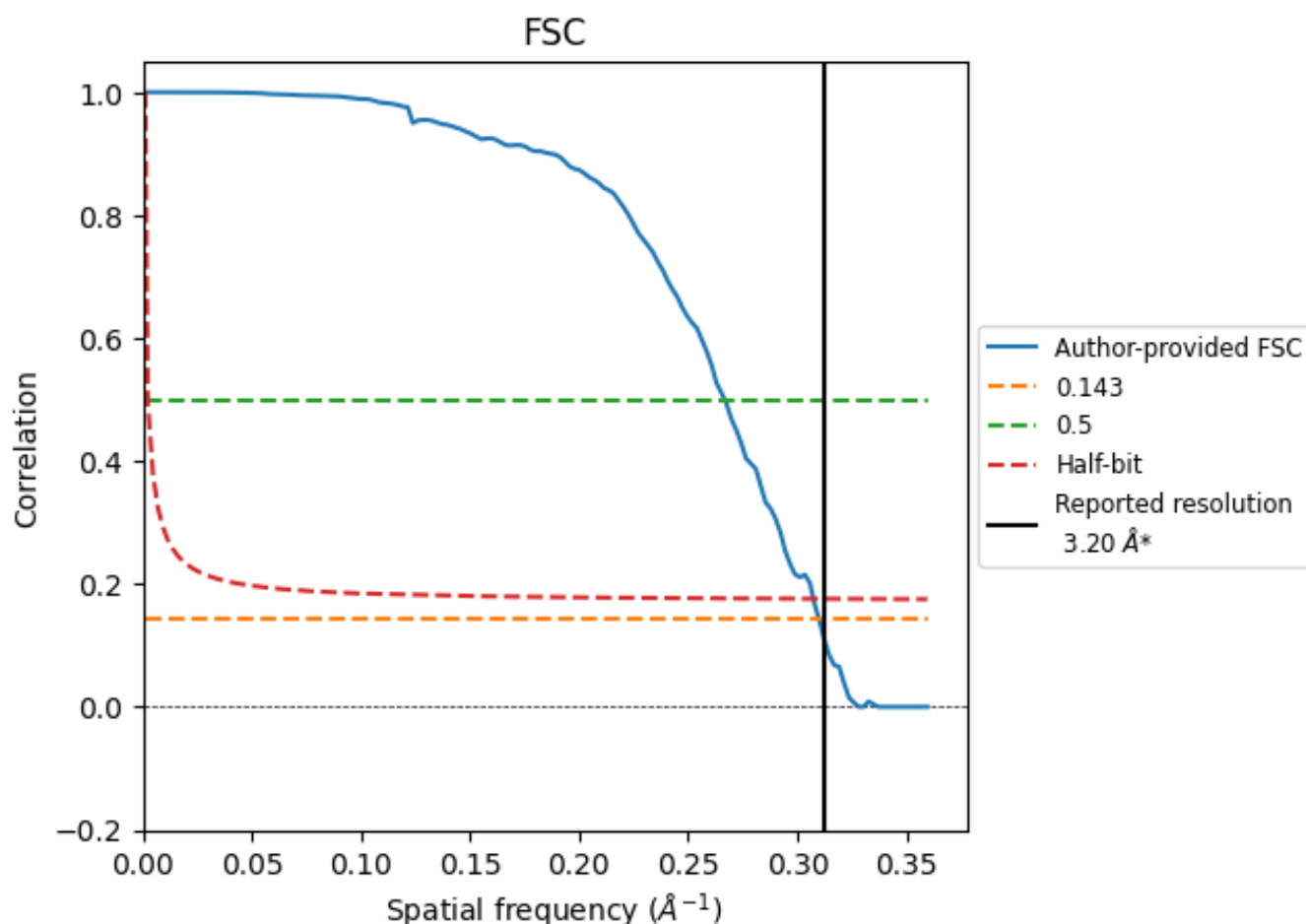


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

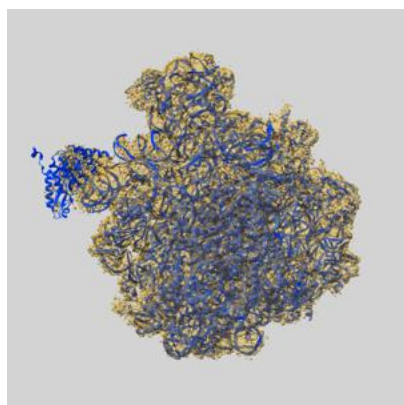
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.75	3.25
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

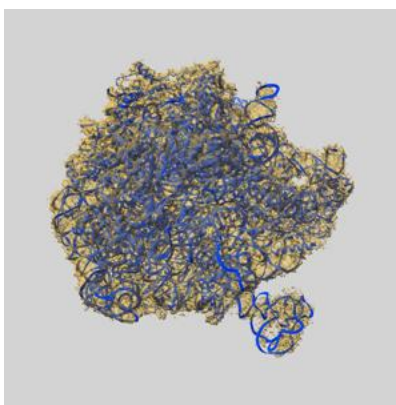
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3531 and PDB model 5MMI. Per-residue inclusion information can be found in section 3 on page 12.

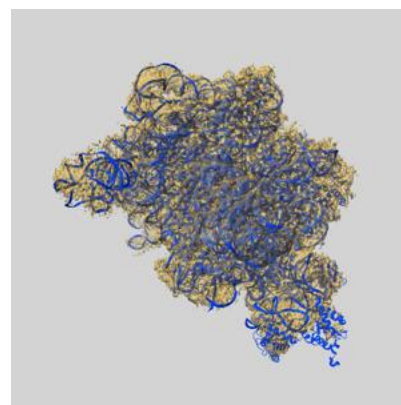
9.1 Map-model overlay [i](#)



X



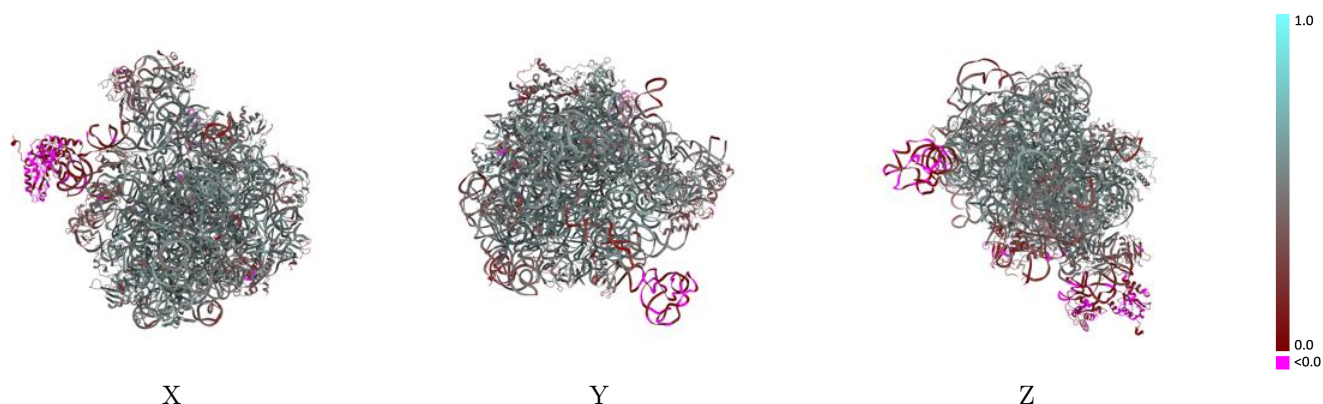
Y



Z

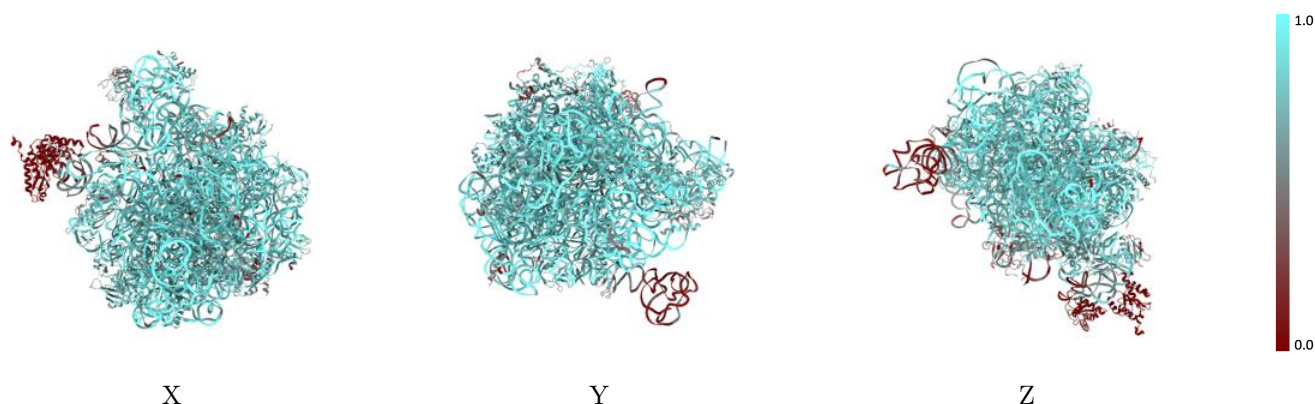
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



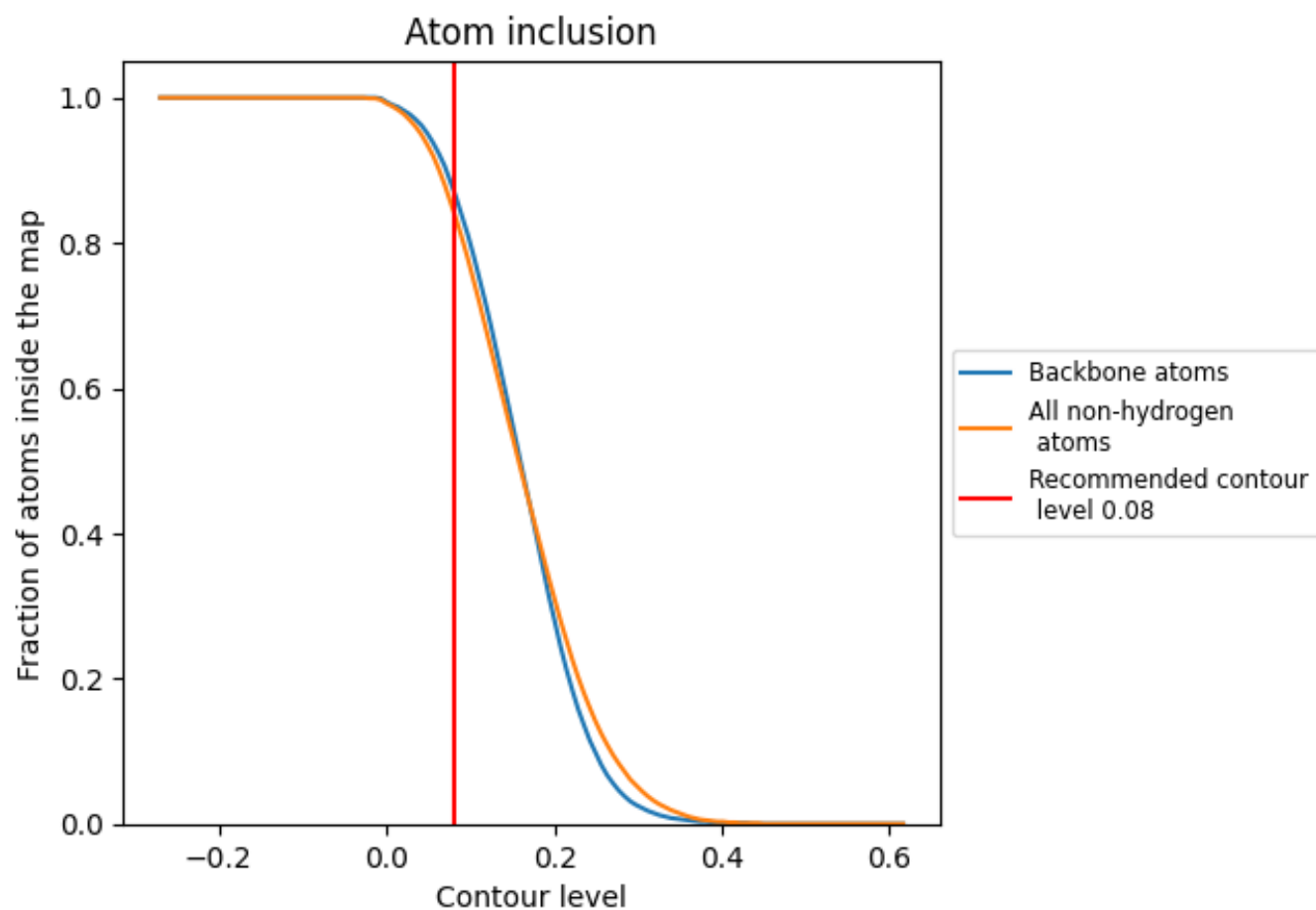
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.4690
0	 0.4420	 0.2120
1	 0.8360	 0.5280
2	 0.7610	 0.4720
3	 0.8600	 0.5580
4	 0.8310	 0.5360
5	 0.7550	 0.4690
6	 0.7270	 0.4260
7	 0.8270	 0.4900
A	 0.8990	 0.4880
B	 0.9400	 0.4510
C	 0.7870	 0.4900
D	 0.8460	 0.5130
E	 0.8080	 0.4880
F	 0.5710	 0.3020
G	 0.6580	 0.3450
H	 0.4830	 0.3860
I	 0.0380	 0.0170
J	 0.0700	 0.0320
K	 0.8320	 0.4980
L	 0.7310	 0.4880
M	 0.8290	 0.4810
N	 0.5410	 0.4030
O	 0.8500	 0.5190
P	 0.8050	 0.4350
Q	 0.7780	 0.4790
R	 0.8710	 0.5220
S	 0.7600	 0.4590
T	 0.7690	 0.4630
U	 0.7460	 0.4570
V	 0.7460	 0.4450
W	 0.9460	 0.5100
X	 0.8170	 0.4850
Y	 0.8070	 0.5030
Z	 0.7470	 0.4290
z	 0.4050	 0.4000

