



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 09:28 PM UTC

PDB ID : 8VK0 / pdb_00008vk0
EMDB ID : EMD-43294
Title : Structure of Mycobacterium smegmatis 50S ribosomal subunit bound to HflX:50S-HflX-A
Authors : Majumdar, S.; Koripella, R.K.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K.
Deposited on : 2024-01-08
Resolution : 3.14 Å (reported)
Based on initial models : 5O61, 6DZI

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

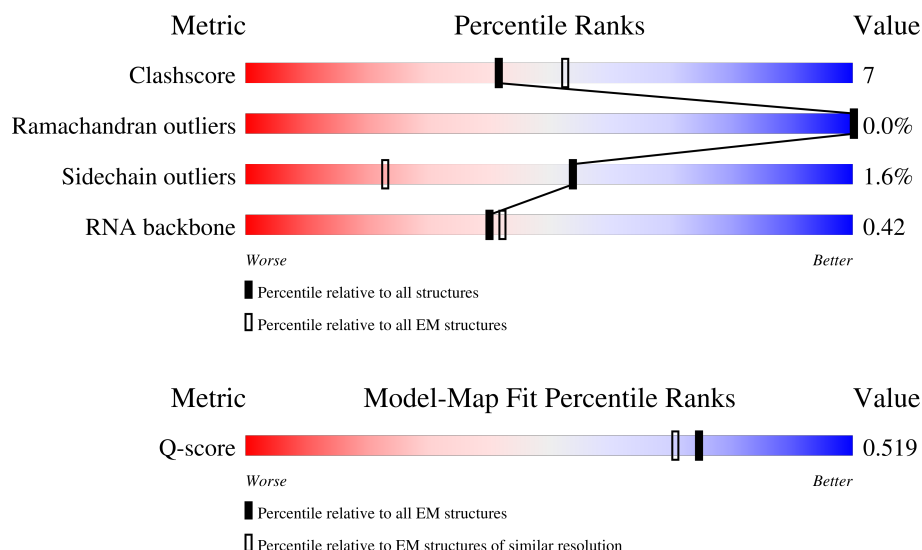
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.14 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	14483 (2.64 - 3.64)

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	2	61	
2	3	24	

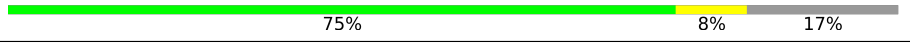
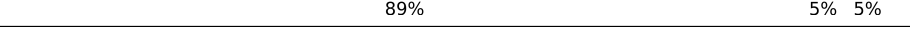
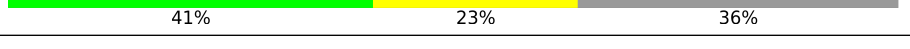
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Mol	Chain	Length	Quality of chain
3	4	470	
4	A	3120	
5	B	118	
6	C	278	
7	D	217	
8	E	215	
9	F	187	
10	G	179	
11	H	151	
12	I	175	
13	J	142	
14	K	147	
15	L	122	
16	M	147	
17	N	138	
18	O	199	
19	P	127	
20	Q	113	
21	R	129	
22	S	103	
23	T	153	
24	U	100	
25	V	105	
26	W	215	
27	X	88	

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Mol	Chain	Length	Quality of chain
28	Y	64	
29	Z	77	
30	b	57	
31	c	55	
32	d	47	
33	e	64	
34	f	37	
35	g	75	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	GCP	4	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 100928 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 L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 2 is a protein called 50S Ribosomal Protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 3 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	426	Total	C	N	O	S	0	0
			3228	1997	599	625	7		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	3119	Total	C	N	O	P	0	0
			66981	29854	12313	21695	3119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 8 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 9 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 14 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 19 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	126	Total	C	N	O	S	0	0
			956	586	199	171			

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 21 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	R	124	Total	C	N	O	0	0
			988	613	203	172		

- Molecule 22 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 23 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 24 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	X	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 28 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 31 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	e	63	Total	C	N	O	0	0
			502	302	115	85		

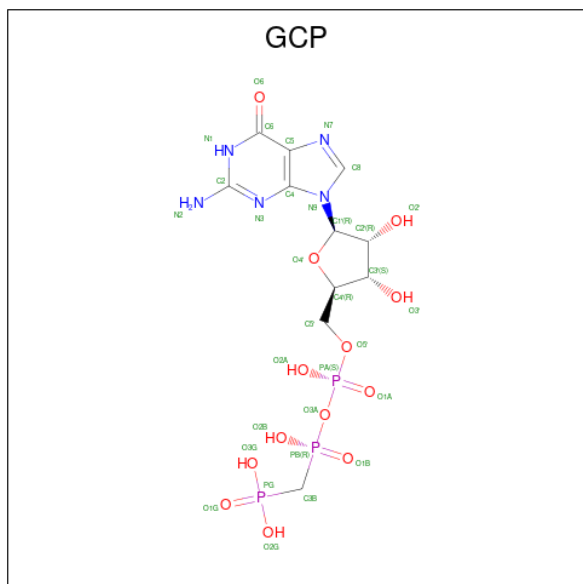
- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 35 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

- Molecule 36 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

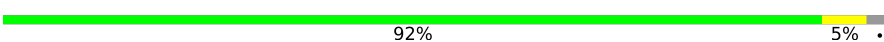


Mol	Chain	Residues	Atoms					AltConf
36	4	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

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

- Molecule 1: 50S ribosomal protein L30

Chain 2: 

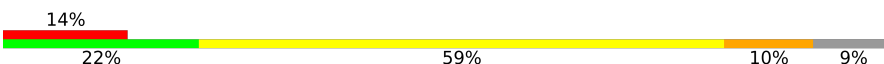


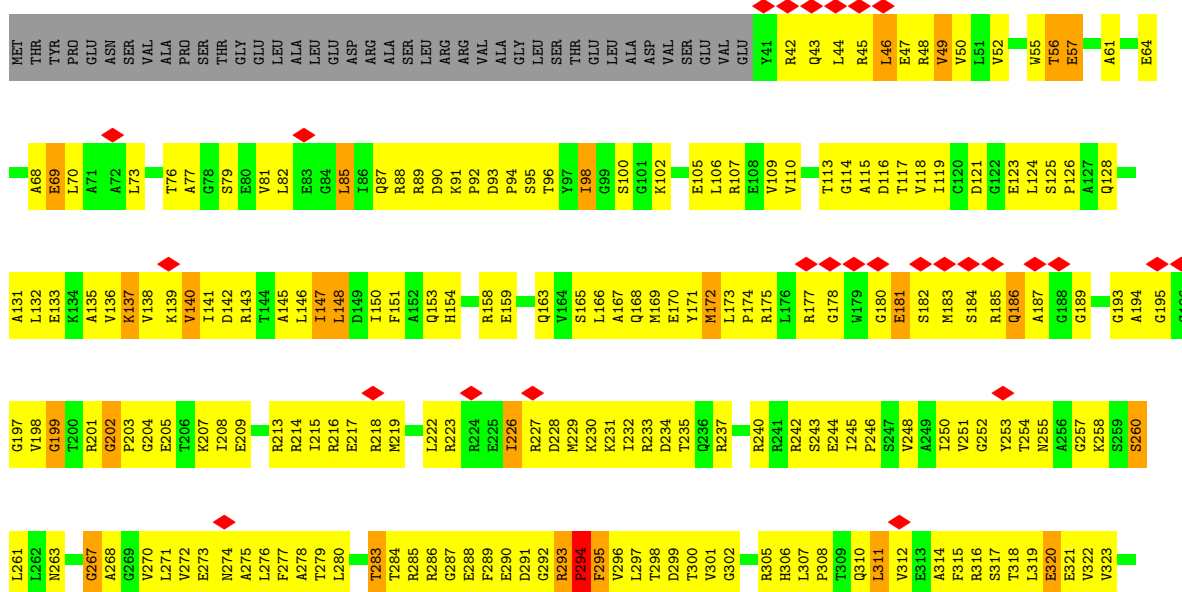
- Molecule 2: 50S Ribosomal Protein L37

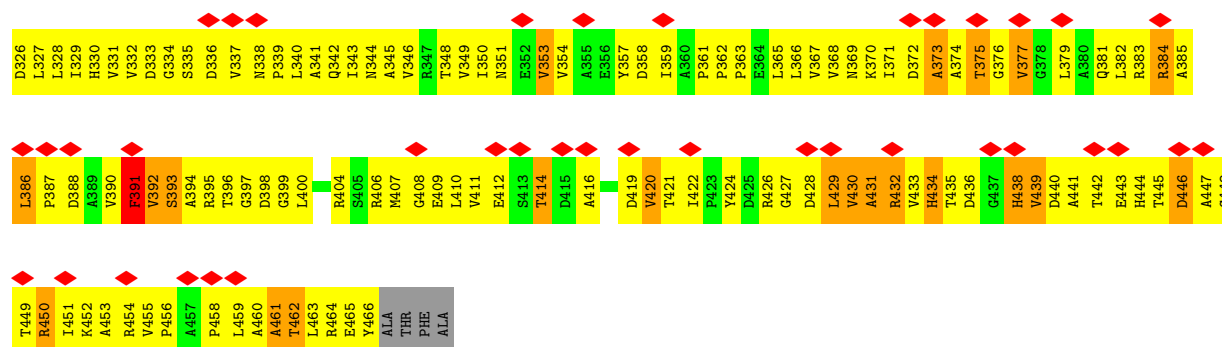
Chain 3: 



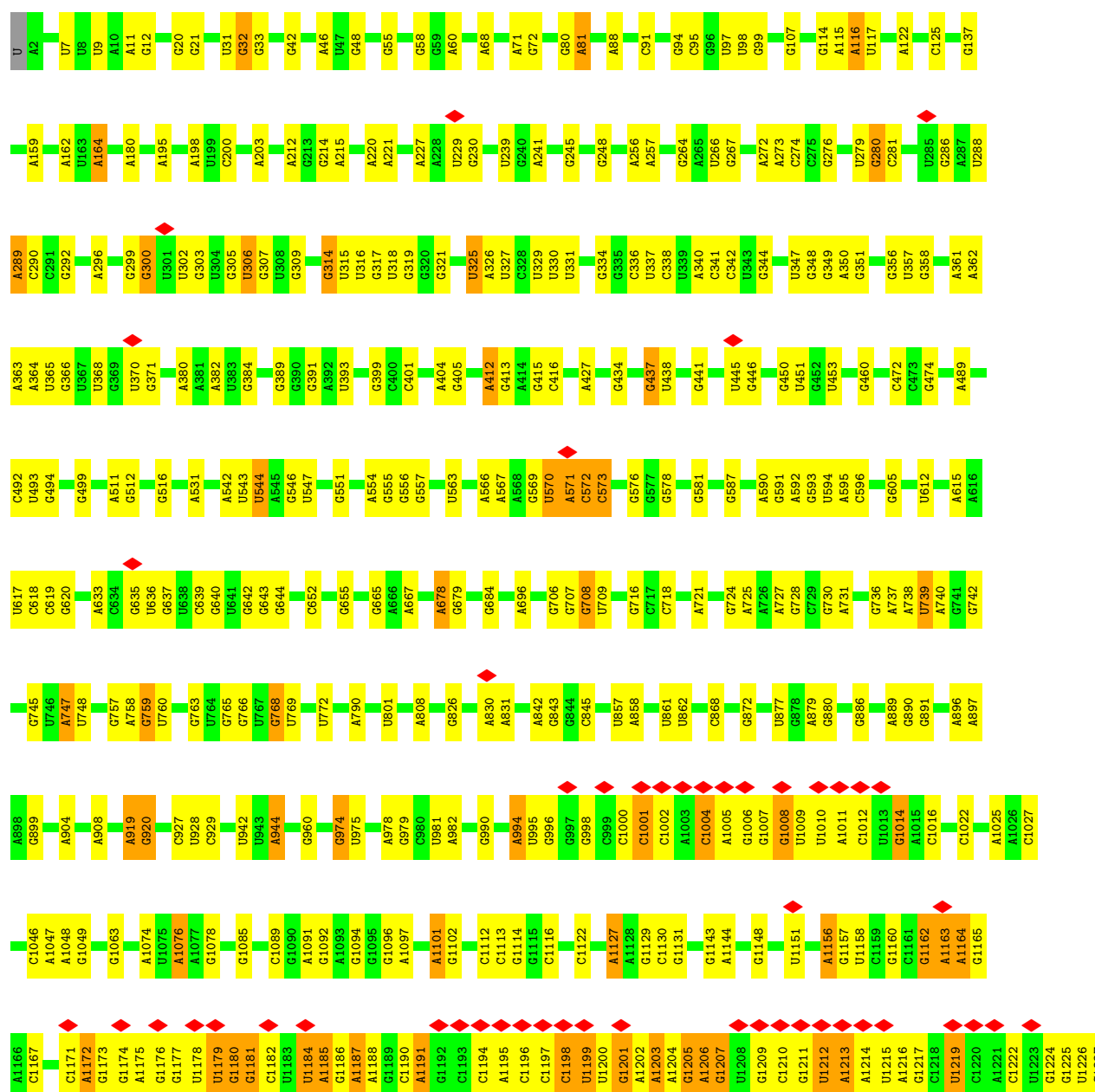
- Molecule 3: GTPase HflX

Chain 4: 

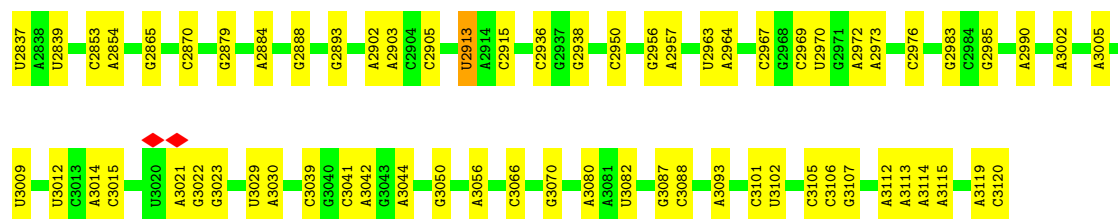




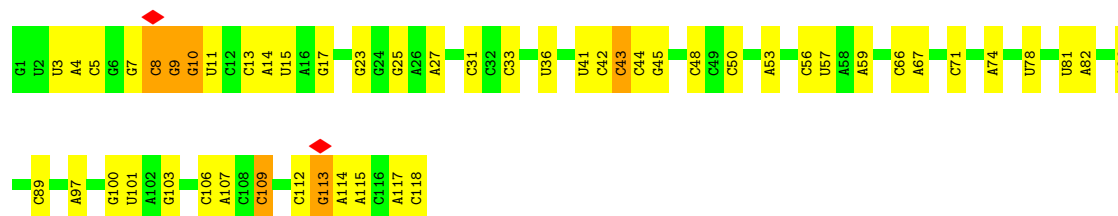
• Molecule 4: 23S ribosomal RNA



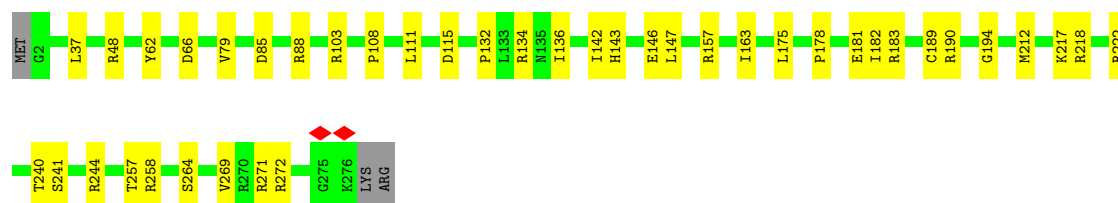
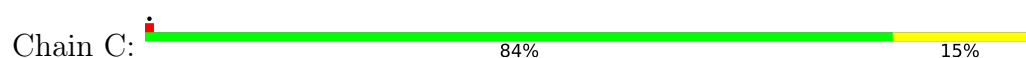
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A2699	A2700	A2559	A2434	C2360	A2142	U2015	U1847	G1707	G1607	U1540	G1379	A1229
A2701	A2702	U2567	G2446	U2361	C2143	G2016	U1848	U1709	U1608	G1230	A1380	G1231
U2703	U2704	U2568	U2449	C2362	C2145	C2017	G1851	A1710	G1609	U1231	G1386	U1232
U2705	U2706	U2569	A2449	A2363	A2146	G2018	A1862	U1713	C1610	G1233	A1387	A1233
U2707	U2708	A2570	G2462	C2364	U2147	C2025	G1863	A1716	A1546	U1234	U1388	U1235
U2709	U2710	A2571	G2463	A2365	A2151	A2026	U1864	U1717	C1548	U1236	G1389	G1237
U2711	U2712	U2572	U2467	C2366	A2152	U2033	U1865	C1718	G1550	U1238	G1398	U1239
U2713	U2714	U2573	U2467	G2367	G2153	U2034	A1866	U1723	C1618	A1400	A1399	G1240
U2715	U2716	C2574	A2470	C2368	G2154	U2035	G1866	U1728	U1619	A1401	A1400	C1239
U2717	U2718	A2582	G2474	C2369	A2160	C2043	A1871	U1729	U1620	A1402	A1402	G1240
U2719	U2720	C2583	G2475	A2370	A2161	U2044	A1872	A1729	C1621	A1246	A1247	A1247
U2721	U2722	U2584	G2476	G2371	A2162	G2045	A1873	U1730	G1622	A1248	U1248	U1248
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U2725	U2726	U2586	G2477	G2373	A2176	A2070	G1885	G1736	G1625	A1416	U1250	U1250
U2727	U2728	U2587	G2483	U2374	U2179	A2071	G1892	A1737	A1628	C1436	A1251	A1251
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U2737	U2738	A2602	G2503	G2379	A2194	U2087	U1916	G1756	A1636	C1465	C1270	C1270
U2739	U2740	G2607	G2506	G2380	U2195	U2088	A1931	U1757	A1637	U1467	G1271	G1271
U2741	U2742	A2608	G2507	A2381	G2196	C2089	U1940	G1758	G1638	A1468	C1272	C1272
U2743	U2744	U2609	C2508	U2382	G2197	U2090	A1941	A1759	G1639	A1469	G1273	G1273
U2745	U2746	G2620	C2509	U2383	U2200	U2091	A1942	U1760	A1640	U1470	A1274	A1274
U2747	U2748	U2621	A2510	U2384	U2201	U2092	A1943	A1761	A1641	C1478	A1275	A1275
U2749	U2750	U2622	U2511	U2385	U2202	U2093	G1944	G1762	C1668	U1292	U1292	U1292
U2751	U2752	U2623	U2512	U2386	U2203	U2094	U1945	A1575	G1669	G1293	G1293	G1293
U2753	U2754	U2624	U2513	U2387	U2204	U2095	U1946	C1576	G1670	G1302	G1302	G1302
U2755	U2756	U2625	U2514	U2388	U2205	U2096	U1947	C1577	U1671	U1303	U1303	U1303
U2757	U2758	U2626	U2515	U2389	U2206	U2097	A1948	C1581	G1672	C1314	C1314	C1314
U2759	U2760	U2627	U2516	U2390	U2207	U2098	C1949	U1583	U1673	G1332	G1332	G1332
U2761	U2762	U2628	U2517	U2391	U2208	U2099	A1955	U1584	U1674	G1337	G1337	G1337
U2763	U2764	U2629	U2518	U2392	U2209	U2100	A1961	U1585	G1675	U1508	A1508	A1508
U2765	U2766	U2630	U2519	U2393	U2210	U2101	G1972	U1586	U1676	U1509	U1509	U1509
U2767	U2768	U2631	U2520	U2394	U2211	U2102	C1973	G1587	U1677	A1518	A1518	A1518
U2769	U2770	U2632	U2521	U2395	U2212	U2103	A1974	U1588	U1678	G1522	G1522	G1522
U2771	U2772	U2633	U2522	U2396	U2213	U2104	U1975	G1589	U1679	G1343	G1343	G1343
U2773	U2774	U2634	U2523	U2397	U2214	U2105	A1976	G1590	U1680	A1344	A1344	A1344
U2775	U2776	U2635	U2524	U2398	U2215	U2106	C1977	G1591	U1681	G1353	G1353	G1353
U2777	U2778	U2636	U2525	U2399	U2216	U2107	U1978	U1592	U1682	A1362	A1362	A1362
U2779	U2780	U2637	U2526	U2400	U2217	U2108	G1979	G1593	U1683	G1363	G1363	G1363
U2781	U2782	U2638	U2527	U2401	U2218	U2109	A1981	G1594	U1684	U1364	U1364	U1364
U2783	U2784	U2639	U2528	U2402	U2219	U2110	U1982	G1595	U1685	G1365	G1365	G1365
U2785	U2786	U2640	U2529	U2403	U2220	U2111	A1990	G1596	U1686	G1371	G1371	G1371
U2787	U2788	U2641	U2530	U2404	U2221	U2112	U1991	U1704	U1687	A1377	A1377	A1377
U2789	U2790	U2642	U2531	U2405	U2222	U2113	U1992	G1703	U1688	G1530	G1530	G1530
U2791	U2792	U2643	U2532	U2406	U2223	U2114	U1993	U1704	U1689	G1531	G1531	G1531
U2793	U2794	U2644	U2533	U2407	U2224	U2115	U1994	G1705	U1690	G1532	G1532	G1532
U2795	U2796	U2645	U2534	U2408	U2225	U2116	U1995	G1706	U1691	U1533	U1533	U1533
U2797	U2798	U2646	U2535	U2409	U2226	U2117	U1996	G1707	U1692	C1534	C1534	C1534
U2799	U2800	U2647	U2536	U2410	U2227	U2118	U1997	G1708	U1693	C1535	C1535	C1535
U2801	U2802	U2648	U2537	U2411	U2228	U2119	U1998	G1709	U1694	A1536	A1536	A1536
U2803	U2804	U2649	U2538	U2412	U2229	U2120	U1999	G1710	U1695	U1537	U1537	U1537
U2805	U2806	U2650	U2539	U2413	U2230	U2121	U2000	G1711	U1696	G1538	G1538	G1538
U2807	U2808	U2651	U2540	U2414	U2231	U2122	U2001	G1712	U1697			
U2809	U2810	U2652	U2541	U2415	U2232	U2123	U2002	G1713	U1698			
U2811	U2812	U2653	U2542	U2416	U2233	U2124	U2003	G1714	U1699			
U2813	U2814	U2654	U2543	U2417	U2234	U2125	U2004	G1715	U1700			
U2815	U2816	U2655	U2544	U2418	U2235	U2126	U2005	G1716	U1701			
U2817	U2818	U2656	U2545	U2419	U2236	U2127	U2006	G1717	U1702			
U2819	U2820	U2657	U2546	U2420	U2237	U2128	U2007	G1718	U1703			
U2821	U2822	U2658	U2547	U2421	U2238	U2129	U2008	G1719	U1704			
U2823	U2824	U2659	U2548	U2422	U2239	U2130	U2009	G1720	U1705			
U2825	U2826	U2660	U2549	U2423	U2240	U2131	U2010	G1721	U1706			
U2827	U2828	U2661	U2550	U2424	U2241	U2132	U2011	G1722	U1707			
U2829	U2830	U2662	U2551	U2425	U2242	U2133	U2012	G1723	U1708			
U2831	U2832	U2663	U2552	U2426	U2243	U2134	U2013	G1724	U1709			
U2833	U2834	U2664	U2553	U2427	U2244	U2135	U2014	G1725	U1710			
U2835	U2836	U2665	U2554	U2428	U2245	U2136	U2015	G1726	U1711			
U2837	U2838	U2666	U2555	U2429	U2246	U2137	U2016	G1727	U1712			
U2839	U2840	U2667	U2556	U2430	U2247	U2138	U2017	G1728	U1713			
U2841	U2842	U2668	U2557	U2431	U2248	U2139	U2018	G1729	U1714			
U2843	U2844	U2669	U2558	U2432	U2249	U2140	U2019	G1730	U1715			
U2845	U2846	U2670	U2559	U2433	U2250	U2141	U2020	G1731	U1716			
U2847	U2848	U2671	U2560	U2434	U2251	U2142	U2021	G1732	U1717			
U2849	U2850	U2672	U2561	U2435	U2252	U2143	U2022	G1733	U1718			
U2851	U2852	U2673	U2562	U2436	U2253	U2144	U2023	G1734	U1719			
U2853	U2854	U2674	U2563	U2437	U2254	U2145	U2024	G1735	U1720			
U2855	U2856	U2675	U2564	U2438	U2255	U2146	U2025	G1736	U1721			
U2857	U2858	U2676	U2565	U2439	U2256	U2147	U2026	G1737	U1722			
U2859	U2860	U2677	U2566	U2440	U2257	U2148	U2027	G1738	U1723			
U2861	U2862	U2678	U2567	U2441	U2258	U2149	U2028	G1739	U1724			
U2863	U2864	U2679	U2568	U2442	U2259	U2150	U2029	G1740	U1725			
U2865	U2866	U2680	U2569	U2443	U2260	U2151	U2030	G1741	U1726			
U2867	U2868	U2681	U2570	U2444	U2261	U2152	U2031	G1742	U1727			
U2869	U2870	U2682	U2571	U2445	U2262	U2153	U2032	G1743	U1728			
U2871	U2872	U2683	U2572	U2446	U2263	U2154	U2033	G1744	U1729			
U2873	U2874	U2684	U2573	U2447	U2264	U2155	U2034	G1745	U1730			
U2875	U2876	U2685	U2574	U2448	U2265	U2156	U2035	G1746	U1731			
U2877	U2878	U2686	U2575	U2449	U2266	U2157	U2036	G1747	U1732			
U2879	U2880	U2687	U2576	U2450	U2267	U2158	U2037	G1748	U1733			
U2881	U2882	U2688	U2577	U2451	U2268	U2159	U2038	G1749	U1734			
U2883	U2884	U2689	U2578	U2452	U2269	U2160	U2039	G1750	U1735			
U2885	U2886	U2690	U2579	U2453	U2270	U2161	U2040	G1751	U1736			
U2887	U2888	U2691	U2580	U2454	U2271	U2162	U2041	G1752	U1737			
U2889	U2890	U2692	U2581	U2455	U2272	U2163	U2042	G1753	U1738			
U2891	U2892	U2693	U2582	U2456	U2273	U2164	U2043	G1754	U1739			
U2893	U2894	U2694	U2583	U2457	U2274	U2165	U2044	G1755	U1740			
U2895	U2896	U2695	U2584	U2458	U2275	U2166	U2045	G1756	U1741			
U2897	U											



• Molecule 5: 5S ribosomal RNA



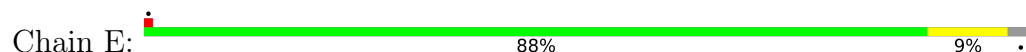
• Molecule 6: 50S ribosomal protein L2



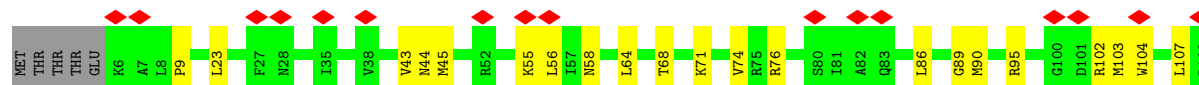
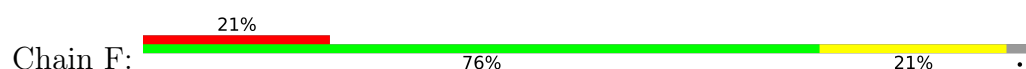
• Molecule 7: 50S ribosomal protein L3

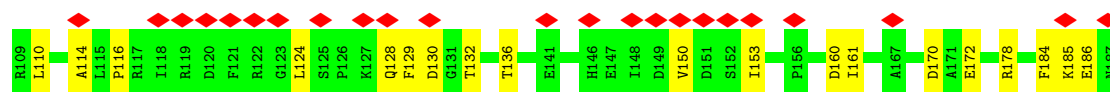


• Molecule 8: 50S Ribosomal Protein L4

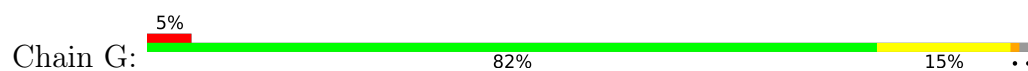


• Molecule 9: 50S Ribosomal Protein L5

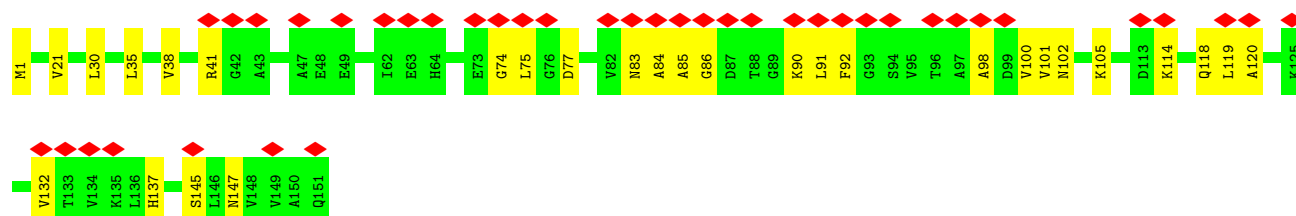
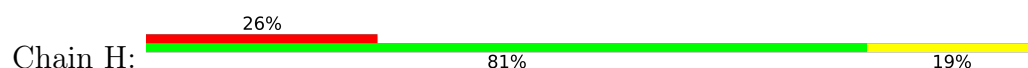




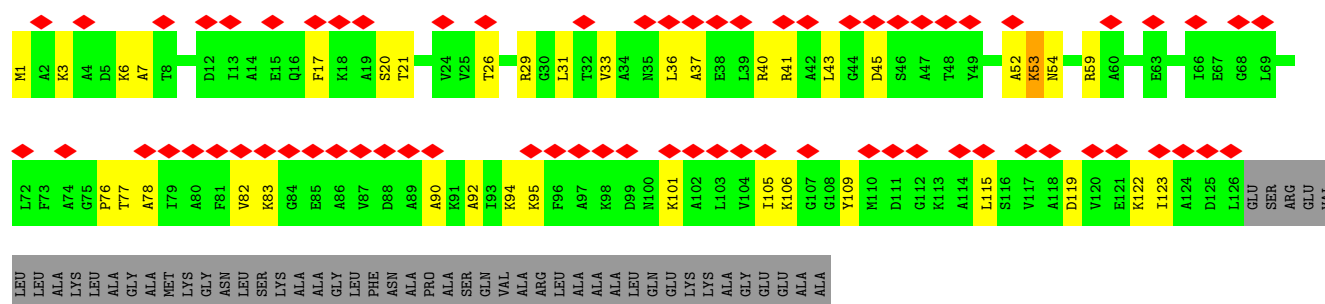
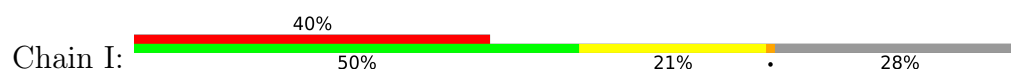
- Molecule 10: 50S ribosomal protein L6



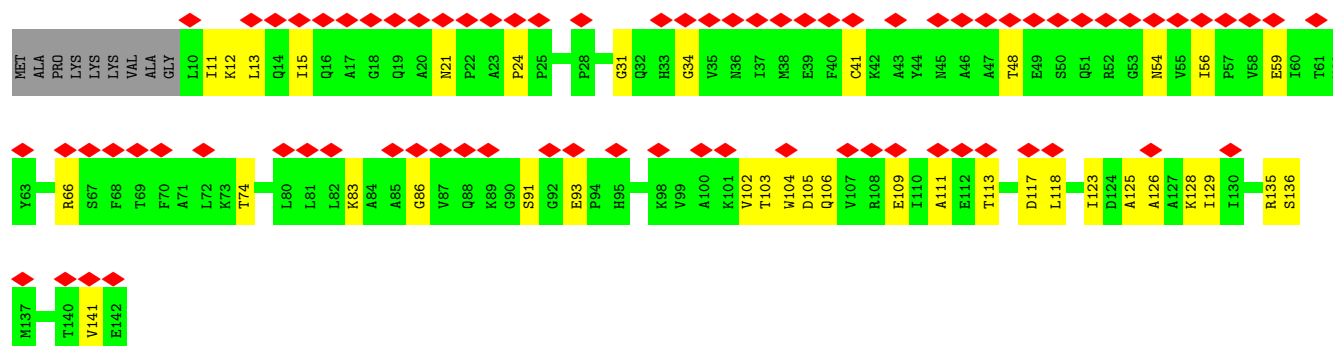
- Molecule 11: 50S ribosomal protein L9

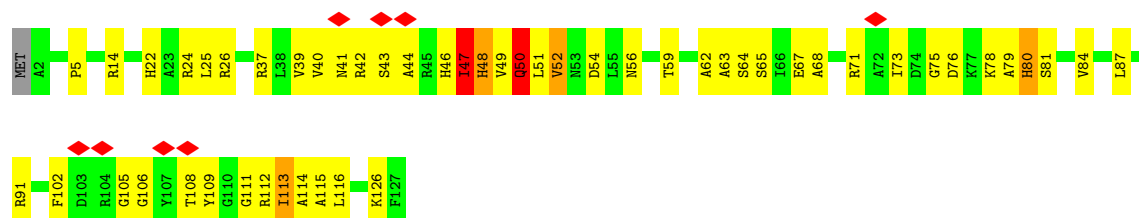
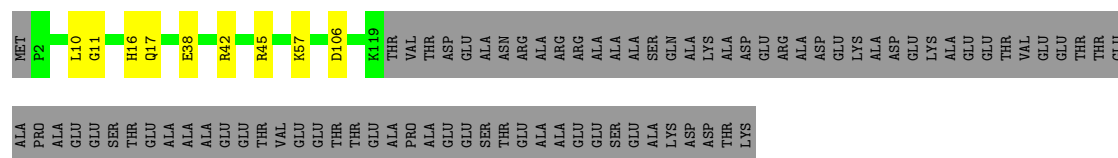
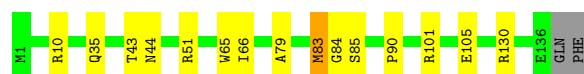
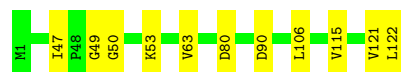
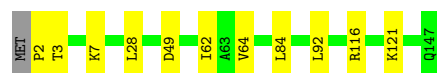


- Molecule 12: 50S ribosomal protein L10

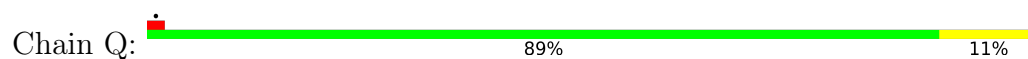


- Molecule 13: 50S ribosomal protein L11





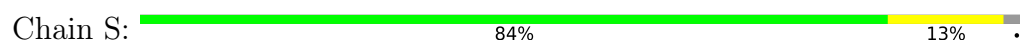
- Molecule 20: 50S ribosomal protein L19



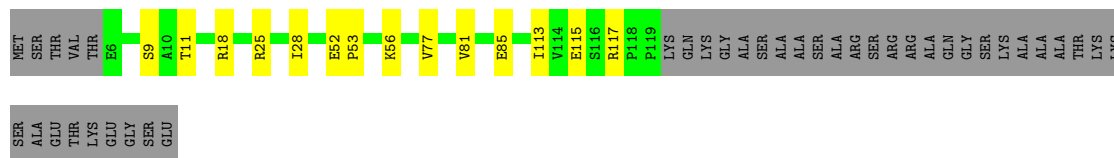
- Molecule 21: 50S Ribosomal Protein L20



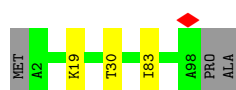
- Molecule 22: 50S Ribosomal Protein L21



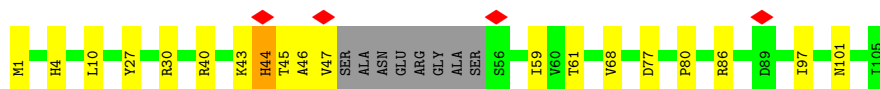
- Molecule 23: 50S Ribosomal Protein L22



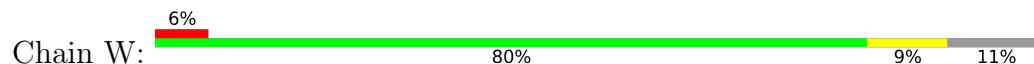
- Molecule 24: 50S Ribosomal Protein L23

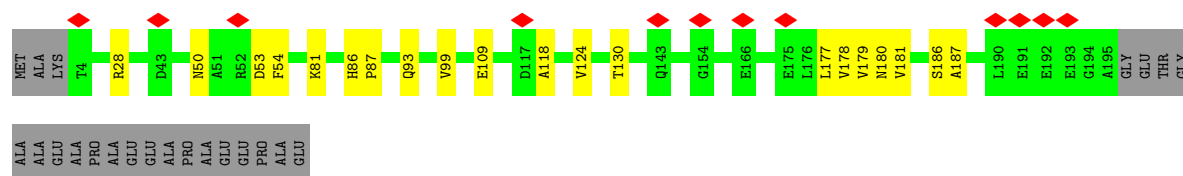


- Molecule 25: 50S ribosomal protein L24

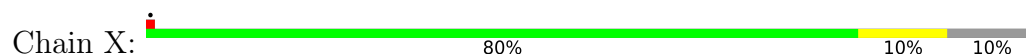


- Molecule 26: 50S ribosomal protein L25

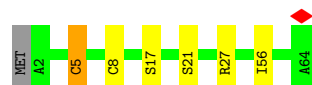




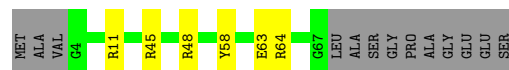
- Molecule 27: 50S ribosomal protein L27



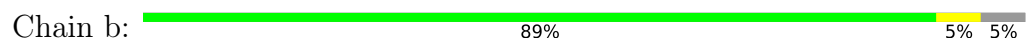
- Molecule 28: 50S Ribosomal Protein L28



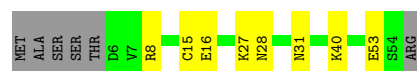
- Molecule 29: 50S ribosomal protein L29



- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 50S Ribosomal Protein L33



- Molecule 32: 50S ribosomal protein L34



- Molecule 33: 50S ribosomal protein L35

Chain e:

91%

8%

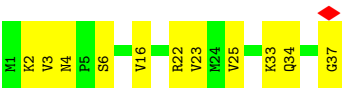


• Molecule 34: 50S ribosomal protein L36

Chain f:

70%

30%



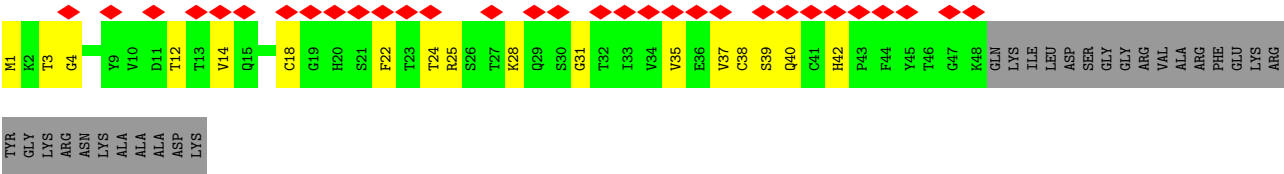
• Molecule 35: 50S Ribosomal Protein L31

Chain g:

41%

23%

36%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57434	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 ($e^-/\text{\AA}^2$)	51.22	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.771	Depositor
Minimum map value	-0.951	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	433.19998, 433.19998, 433.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2	0.45	0/477	0.52	0/640
2	3	0.38	0/191	0.56	0/247
3	4	0.83	0/3268	1.09	27/4428 (0.6%)
4	A	0.44	0/75001	0.47	2/117027 (0.0%)
5	B	0.36	0/2821	0.51	0/4396
6	C	0.45	0/2153	0.57	0/2895
7	D	0.46	0/1609	0.61	0/2165
8	E	0.42	0/1592	0.60	2/2153 (0.1%)
9	F	0.27	0/1467	0.66	0/1973
10	G	0.30	0/1369	0.62	0/1848
11	H	0.28	0/1027	0.71	0/1398
12	I	0.24	0/925	0.63	0/1246
13	J	0.29	0/1006	0.75	2/1364 (0.1%)
14	K	0.43	0/1157	0.50	0/1567
15	L	0.42	0/946	0.55	0/1268
16	M	0.40	0/1091	0.53	0/1457
17	N	0.42	0/1118	0.59	1/1506 (0.1%)
18	O	0.48	0/945	0.58	0/1267
19	P	0.45	1/966 (0.1%)	0.94	3/1298 (0.2%)
20	Q	0.43	0/921	0.60	0/1236
21	R	0.50	0/1000	0.56	0/1341
22	S	0.40	0/764	0.47	0/1030
23	T	0.45	0/887	0.56	0/1204
24	U	0.43	0/766	0.52	0/1030
25	V	0.38	0/738	0.64	0/987
26	W	0.27	0/1443	0.55	0/1970
27	X	0.41	0/595	0.61	0/798
28	Y	0.42	0/478	0.53	0/641
29	Z	0.39	0/534	0.52	0/713
30	b	0.45	0/427	0.61	0/572
31	c	0.36	0/413	0.49	0/553
32	d	0.47	0/380	0.56	0/500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.42	0/507	0.52	0/672
34	f	0.39	0/303	0.53	0/401
35	g	0.23	0/372	0.58	0/503
All	All	0.44	1/109657 (0.0%)	0.53	37/164294 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	F	0	1
10	G	0	2
11	H	0	1
12	I	0	2
13	J	0	1
18	O	0	1
19	P	0	4
26	W	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	50	GLN	N-CA	5.72	1.53	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	373	ALA	N-CA-C	-11.96	98.92	113.15
3	4	375	THR	N-CA-C	-9.38	100.44	113.20
3	4	260	SER	N-CA-C	-8.79	102.47	113.55
3	4	393	SER	N-CA-C	-8.47	103.53	114.04
3	4	432	ARG	N-CA-C	-7.50	102.05	113.89
3	4	267	GLY	N-CA-C	-7.30	100.51	110.80
3	4	294	PRO	N-CA-C	7.08	127.06	112.47
3	4	199	GLY	N-CA-C	-7.06	96.44	113.18
19	P	113	ILE	N-CA-C	-6.72	107.33	113.71
17	N	79	ALA	N-CA-C	6.67	120.75	110.20
19	P	48	HIS	N-CA-C	6.59	121.01	107.37
3	4	181	GLU	N-CA-C	-6.39	103.57	112.45
8	E	121	ASN	CA-C-N	6.35	131.41	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	121	ASN	C-N-CA	6.35	131.41	122.46
3	4	446	ASP	N-CA-C	-6.19	105.86	113.41
3	4	69	GLU	N-CA-C	-6.14	103.90	111.33
3	4	420	VAL	N-CA-C	5.98	116.78	108.23
3	4	434	HIS	N-CA-C	-5.94	105.69	113.12
3	4	202	GLY	CA-C-N	-5.84	112.54	119.84
3	4	202	GLY	C-N-CA	-5.84	112.54	119.84
3	4	461	ALA	CB-CA-C	-5.75	109.96	116.63
4	A	2320	C	C2'-C3'-O3'	5.74	118.10	109.50
3	4	462	THR	N-CA-C	-5.70	106.38	113.38
3	4	414	THR	N-CA-C	-5.67	102.52	110.35
3	4	77	ALA	N-CA-C	-5.66	106.42	113.38
3	4	293	ARG	N-CA-C	-5.65	101.68	109.71
3	4	392	VAL	N-CA-C	-5.56	101.62	109.63
3	4	377	VAL	N-CA-C	-5.42	106.57	112.80
3	4	320	GLU	N-CA-C	-5.39	105.51	111.71
13	J	86	GLY	N-CA-C	5.33	119.25	110.77
3	4	391	PHE	N-CA-C	-5.32	102.46	110.70
19	P	47	ILE	N-CA-C	5.28	120.31	109.34
3	4	399	GLY	N-CA-C	-5.18	107.54	115.00
3	4	49	VAL	N-CA-C	5.15	115.54	108.12
4	A	974	G	P-O3'-C3'	5.11	127.87	120.20
3	4	294	PRO	CB-CA-C	-5.08	103.17	111.56
13	J	24	PRO	N-CA-C	5.04	116.85	110.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	68	THR	Peptide
10	G	46	ALA	Peptide
10	G	52	VAL	Peptide
11	H	137	HIS	Peptide
12	I	52	ALA	Peptide
12	I	53	LYS	Peptide
13	J	54	ASN	Peptide
18	O	57	LYS	Peptide
19	P	102	PHE	Peptide
19	P	25	LEU	Peptide
19	P	5	PRO	Peptide
19	P	80	HIS	Peptide
26	W	118	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	2	474	0	500	2	0
2	3	189	0	205	3	0
3	4	3228	0	3284	534	0
4	A	66981	0	33700	316	0
5	B	2522	0	1285	21	0
6	C	2110	0	2165	28	0
7	D	1587	0	1630	12	0
8	E	1569	0	1607	14	0
9	F	1445	0	1476	25	0
10	G	1348	0	1399	20	0
11	H	1018	0	988	18	0
12	I	918	0	959	29	0
13	J	990	0	1021	26	0
14	K	1130	0	1167	8	0
15	L	938	0	1000	7	0
16	M	1078	0	1151	9	0
17	N	1092	0	1128	8	0
18	O	928	0	972	5	0
19	P	956	0	991	43	0
20	Q	907	0	938	8	0
21	R	988	0	1038	10	0
22	S	754	0	802	7	0
23	T	873	0	909	8	0
24	U	756	0	802	2	0
25	V	732	0	782	15	0
26	W	1428	0	1443	11	0
27	X	586	0	601	7	0
28	Y	470	0	482	4	0
29	Z	531	0	541	3	0
30	b	423	0	463	3	0
31	c	405	0	411	6	0
32	d	377	0	411	3	0
33	e	502	0	541	5	0
34	f	299	0	324	6	0
35	g	364	0	352	11	0
36	4	32	0	14	15	0
All	All	100928	0	67482	1104	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 7.

All (1104) 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)
3:4:445:THR:CG2	3:4:450:ARG:HB2	1.86	1.06
3:4:202:GLY:HA3	4:A:2676:C:C4'	1.86	1.05
3:4:354:VAL:HG11	3:4:361:PRO:HG3	1.38	1.04
3:4:426:ARG:HG3	3:4:429:LEU:HB2	1.38	1.04
3:4:85:LEU:HD11	3:4:106:LEU:HD21	1.40	1.02
3:4:261:LEU:HD11	3:4:392:VAL:HG11	1.40	1.00
3:4:202:GLY:HA3	4:A:2676:C:H4'	1.40	0.99
3:4:102:LYS:HG2	4:A:2132:U:H5'	1.43	0.98
3:4:85:LEU:CD1	3:4:106:LEU:HD21	1.95	0.97
3:4:395:ARG:HH21	36:4:501:GCP:C2	1.79	0.96
3:4:288:GLU:HG3	3:4:292:GLY:HA2	1.46	0.94
3:4:288:GLU:CG	3:4:292:GLY:HA2	1.97	0.94
3:4:177:ARG:HA	3:4:183:MET:SD	2.08	0.94
3:4:48:ARG:HB3	3:4:115:ALA:HA	1.50	0.93
3:4:250:ILE:CD1	3:4:258:LYS:HA	1.98	0.93
3:4:373:ALA:CB	36:4:501:GCP:HN1	1.82	0.92
4:A:1209:G:H1	4:A:1219:U:H3	1.18	0.91
3:4:42:ARG:HH12	3:4:44:LEU:HB2	1.35	0.91
3:4:181:GLU:HA	3:4:184:SER:CB	2.00	0.90
3:4:445:THR:HG23	3:4:450:ARG:HB2	1.50	0.90
4:A:2329:G:H1	4:A:2406:U:H3	1.17	0.90
3:4:173:LEU:HD13	3:4:215:ILE:HG21	1.52	0.90
3:4:379:LEU:HG	3:4:383:ARG:HD2	1.55	0.88
3:4:187:ALA:HA	4:A:2826:A:C5	2.08	0.88
3:4:354:VAL:HG13	3:4:359:ILE:HG13	1.56	0.87
3:4:181:GLU:HA	3:4:184:SER:HB2	1.53	0.87
3:4:186:GLN:HB3	3:4:207:LYS:HZ3	1.37	0.87
3:4:384:ARG:HG2	3:4:385:ALA:N	1.90	0.87
3:4:227:ARG:NE	3:4:227:ARG:HA	1.90	0.85
3:4:286:ARG:HB2	4:A:2697:U:O2'	1.76	0.85
3:4:434:HIS:HB3	4:A:1185:A:H1'	1.59	0.85
3:4:426:ARG:HA	3:4:429:LEU:HD23	1.56	0.85
3:4:383:ARG:HH21	3:4:391:PHE:HE1	1.24	0.85
19:P:50:GLN:HA	19:P:63:ALA:HB3	1.59	0.84
3:4:82:LEU:HD13	3:4:113:THR:HB	1.59	0.84
3:4:294:PRO:O	3:4:295:PHE:C	2.19	0.83
3:4:327:LEU:C	3:4:328:LEU:HD12	2.04	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:371:ILE:HA	3:4:374:ALA:HB2	1.60	0.83
3:4:271:LEU:HD22	3:4:278:ALA:HB1	1.61	0.83
3:4:350:ILE:O	3:4:353:VAL:HG22	1.79	0.82
3:4:373:ALA:HB3	36:4:501:GCP:HN1	1.39	0.82
3:4:432:ARG:HB3	3:4:436:ASP:HB2	1.61	0.82
3:4:85:LEU:HD21	3:4:106:LEU:CD1	2.09	0.82
3:4:228:ASP:O	3:4:231:LYS:HG2	1.80	0.82
3:4:372:ASP:C	3:4:374:ALA:H	1.86	0.82
3:4:46:LEU:HD12	3:4:117:THR:CG2	2.09	0.82
3:4:294:PRO:HB3	3:4:296:VAL:HG23	1.62	0.81
3:4:445:THR:HG21	3:4:450:ARG:HB2	1.61	0.81
3:4:250:ILE:HD11	3:4:258:LYS:HA	1.64	0.80
3:4:326:ASP:HB3	3:4:412:GLU:OE1	1.81	0.80
3:4:461:ALA:HB3	3:4:463:LEU:HD13	1.62	0.80
3:4:187:ALA:HA	4:A:2826:A:C4	2.16	0.80
3:4:253:TYR:HE1	3:4:332:VAL:HG12	1.45	0.80
3:4:227:ARG:HA	3:4:227:ARG:HE	1.46	0.79
3:4:250:ILE:HD13	3:4:258:LYS:HA	1.63	0.79
3:4:251:VAL:HG22	3:4:252:GLY:H	1.47	0.79
4:A:2140:A:H5'	4:A:2141:U:C5	2.18	0.79
4:A:2367:G:N2	4:A:2370:A:C5	2.50	0.79
3:4:49:VAL:HG12	3:4:117:THR:OG1	1.83	0.79
3:4:293:ARG:HH22	3:4:414:THR:HA	1.47	0.78
3:4:395:ARG:NH2	36:4:501:GCP:N3	2.30	0.78
3:4:420:VAL:HA	3:4:466:TYR:HD1	1.47	0.78
3:4:426:ARG:HE	3:4:430:VAL:HG13	1.48	0.77
4:A:1566:A:H61	4:A:1606:G:N2	1.83	0.77
3:4:271:LEU:CD2	3:4:278:ALA:HB1	2.15	0.76
4:A:2367:G:C2	4:A:2370:A:N7	2.53	0.76
3:4:42:ARG:NH1	3:4:44:LEU:HB2	1.99	0.76
3:4:107:ARG:O	3:4:110:VAL:HG12	1.84	0.76
3:4:381:GLN:O	3:4:384:ARG:HD3	1.86	0.76
3:4:420:VAL:HG22	3:4:421:THR:N	2.02	0.75
3:4:456:PRO:HB2	3:4:459:LEU:HD23	1.69	0.75
3:4:199:GLY:C	3:4:201:ARG:H	1.94	0.75
3:4:382:LEU:HB3	3:4:386:LEU:HD12	1.68	0.75
12:I:37:ALA:O	12:I:41:ARG:HB3	1.87	0.74
3:4:371:ILE:HG22	3:4:372:ASP:H	1.52	0.74
3:4:45:ARG:C	3:4:46:LEU:HD22	2.11	0.74
3:4:344:ASN:O	3:4:348:THR:HG23	1.86	0.74
3:4:250:ILE:HG22	3:4:298:THR:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:426:ARG:C	3:4:428:ASP:H	1.93	0.74
3:4:257:GLY:O	36:4:501:GCP:O3A	2.05	0.74
3:4:443:GLU:HG2	3:4:452:LYS:HD3	1.69	0.73
3:4:366:LEU:HD11	3:4:387:PRO:HD2	1.69	0.73
3:4:430:VAL:O	3:4:431:ALA:C	2.31	0.73
3:4:173:LEU:HD13	3:4:215:ILE:CG2	2.19	0.73
3:4:379:LEU:O	3:4:383:ARG:HG3	1.88	0.72
3:4:223:ARG:HA	3:4:226:ILE:HD11	1.71	0.72
3:4:420:VAL:HG22	3:4:421:THR:H	1.52	0.72
3:4:443:GLU:HG2	3:4:452:LYS:CD	2.18	0.72
3:4:300:THR:HB	3:4:318:THR:HG23	1.70	0.72
3:4:395:ARG:HG2	3:4:396:THR:H	1.54	0.72
3:4:45:ARG:O	3:4:46:LEU:HD13	1.88	0.72
3:4:288:GLU:CB	3:4:292:GLY:HA2	2.19	0.72
3:4:383:ARG:HB3	3:4:383:ARG:NH1	2.03	0.72
3:4:339:PRO:HG2	3:4:382:LEU:HD21	1.72	0.72
3:4:147:ILE:HD11	3:4:151:PHE:CE2	2.24	0.72
3:4:422:ILE:HG23	3:4:429:LEU:HG	1.71	0.72
19:P:42:ARG:HH11	19:P:109:TYR:H	1.38	0.72
3:4:153:GLN:HG3	3:4:154:HIS:HD2	1.56	0.71
3:4:424:TYR:CZ	3:4:447:ALA:HA	2.24	0.71
3:4:87:GLN:HG3	4:A:2133:G:H5''	1.71	0.71
3:4:213:ARG:O	3:4:217:GLU:HG3	1.90	0.71
3:4:288:GLU:HG3	3:4:292:GLY:CA	2.20	0.71
3:4:366:LEU:HD23	3:4:366:LEU:H	1.56	0.71
3:4:87:GLN:NE2	4:A:2133:G:H8	1.89	0.70
3:4:102:LYS:O	3:4:106:LEU:HD23	1.90	0.70
3:4:181:GLU:HA	3:4:184:SER:HB3	1.73	0.70
4:A:1566:A:N6	4:A:1606:G:H21	1.89	0.70
4:A:1158:U:H3	4:A:1232:G:H1	1.37	0.70
19:P:73:ILE:HG13	19:P:75:GLY:H	1.56	0.70
3:4:102:LYS:HD3	4:A:2133:G:O5'	1.91	0.70
3:4:50:VAL:CG2	3:4:118:VAL:HG22	2.22	0.69
3:4:251:VAL:HG22	3:4:252:GLY:N	2.04	0.69
3:4:373:ALA:HB3	36:4:501:GCP:N1	2.08	0.69
3:4:263:ASN:HD21	3:4:270:VAL:H	1.41	0.69
3:4:147:ILE:HG21	3:4:308:PRO:HG3	1.74	0.69
7:D:63:ILE:HG22	7:D:65:PRO:HD2	1.73	0.69
3:4:199:GLY:CA	3:4:201:ARG:HD2	2.23	0.69
3:4:340:LEU:H	3:4:340:LEU:HD22	1.58	0.68
4:A:2413:G:H2'	4:A:2414:G:H8	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:202:GLY:O	3:4:203:PRO:C	2.35	0.68
5:B:112:C:H3'	5:B:113:G:H4'	1.73	0.68
4:A:365:U:H3	4:A:437:G:H1	1.41	0.68
3:4:260:SER:OG	3:4:394:ALA:HB1	1.94	0.68
3:4:311:LEU:HD23	3:4:312:VAL:H	1.58	0.68
3:4:327:LEU:HD23	3:4:328:LEU:N	2.09	0.68
3:4:46:LEU:HD12	3:4:117:THR:HG21	1.76	0.67
3:4:349:VAL:O	3:4:353:VAL:HG13	1.94	0.67
3:4:371:ILE:HB	3:4:391:PHE:HA	1.75	0.67
3:4:199:GLY:HA2	3:4:201:ARG:CZ	2.24	0.67
3:4:374:ALA:C	3:4:376:GLY:H	2.00	0.67
3:4:436:ASP:HB3	3:4:439:VAL:HG13	1.76	0.67
3:4:271:LEU:HD23	3:4:273:GLU:H	1.57	0.67
3:4:432:ARG:HA	3:4:435:THR:HG23	1.75	0.67
9:F:124:LEU:HB2	9:F:185:LYS:HG2	1.74	0.67
3:4:432:ARG:HB3	3:4:436:ASP:CB	2.24	0.67
25:V:43:LYS:HB3	25:V:59:ILE:HA	1.77	0.67
4:A:2140:A:H5'	4:A:2141:U:H5	1.59	0.67
3:4:202:GLY:N	3:4:203:PRO:HD2	2.10	0.66
3:4:288:GLU:HB2	3:4:292:GLY:HA2	1.78	0.66
3:4:455:VAL:HB	3:4:460:ALA:HB3	1.75	0.66
3:4:422:ILE:HG21	3:4:426:ARG:NH1	2.10	0.66
3:4:370:LYS:O	3:4:374:ALA:HA	1.96	0.66
4:A:2367:G:C2	4:A:2370:A:C5	2.84	0.66
3:4:307:LEU:HD13	3:4:312:VAL:HG21	1.76	0.66
3:4:372:ASP:C	3:4:374:ALA:N	2.49	0.66
3:4:271:LEU:HD21	3:4:273:GLU:HB2	1.78	0.66
4:A:1209:G:N1	4:A:1219:U:N3	2.39	0.66
11:H:84:ALA:HA	11:H:91:LEU:HA	1.78	0.66
4:A:2474:G:H5''	4:A:2474:G:N3	2.11	0.65
3:4:461:ALA:HB3	3:4:463:LEU:CD1	2.26	0.65
3:4:445:THR:HG21	3:4:450:ARG:CB	2.27	0.65
4:A:1636:A:H62	4:A:1802:G:H21	1.45	0.65
3:4:85:LEU:HD21	3:4:106:LEU:HD13	1.77	0.65
3:4:199:GLY:C	3:4:201:ARG:N	2.55	0.65
3:4:371:ILE:HG22	3:4:372:ASP:N	2.11	0.65
3:4:148:LEU:HD12	3:4:148:LEU:O	1.96	0.65
3:4:432:ARG:HH21	3:4:459:LEU:HA	1.62	0.65
4:A:2134:G:N2	4:A:2146:A:O2'	2.29	0.65
4:A:2335:G:N7	4:A:2392:A:N6	2.45	0.65
3:4:379:LEU:CG	3:4:383:ARG:HD2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:186:GLN:HB3	3:4:207:LYS:NZ	2.10	0.64
3:4:237:ARG:O	3:4:237:ARG:HG3	1.97	0.64
3:4:199:GLY:HA3	3:4:201:ARG:HD2	1.79	0.64
4:A:347:U:H2'	4:A:348:G:H8	1.63	0.64
4:A:2034:G:OP1	6:C:88:ARG:NH2	2.30	0.64
3:4:445:THR:HG21	3:4:450:ARG:HG3	1.80	0.63
3:4:243:SER:O	3:4:244:GLU:C	2.40	0.63
11:H:118:GLN:HG3	11:H:120:ALA:H	1.63	0.63
3:4:426:ARG:NE	3:4:430:VAL:HG13	2.14	0.63
4:A:2136:A:N6	4:A:2139:U:C4	2.67	0.63
3:4:443:GLU:CG	3:4:452:LYS:HD3	2.28	0.63
13:J:135:ARG:NH1	13:J:136:SER:OG	2.32	0.63
3:4:424:TYR:OH	3:4:447:ALA:HA	1.97	0.63
6:C:212:MET:HE3	6:C:217:LYS:HD3	1.80	0.63
9:F:150:VAL:HA	9:F:153:ILE:HD12	1.81	0.62
4:A:2137:A:H4'	4:A:2142:A:N1	2.13	0.62
4:A:2754:G:N7	10:G:173:LYS:NZ	2.47	0.62
3:4:323:VAL:HG21	3:4:357:TYR:CD1	2.34	0.62
3:4:46:LEU:O	3:4:47:GLU:HB2	1.99	0.62
3:4:263:ASN:OD1	3:4:270:VAL:HG22	1.99	0.62
4:A:747:A:N6	4:A:768:G:O2'	2.33	0.62
3:4:424:TYR:HB3	13:J:31:GLY:O	2.00	0.62
4:A:2363:A:H61	4:A:2374:U:H3	1.47	0.62
3:4:165:SER:HA	3:4:168:GLN:HG3	1.82	0.61
3:4:171:TYR:HB2	3:4:310:GLN:OE1	1.99	0.61
3:4:242:ARG:O	3:4:243:SER:C	2.43	0.61
4:A:572:C:H2'	25:V:46:ALA:HA	1.82	0.61
3:4:123:GLU:C	3:4:124:LEU:HD12	2.24	0.61
3:4:442:THR:HG23	3:4:442:THR:O	2.00	0.61
12:I:1:MET:SD	12:I:6:LYS:NZ	2.73	0.61
19:P:39:VAL:O	19:P:49:VAL:HG13	2.00	0.61
4:A:2137:A:O3'	4:A:2138:C:H4'	2.00	0.61
3:4:85:LEU:HD21	3:4:106:LEU:HD11	1.82	0.61
3:4:408:GLY:O	3:4:411:VAL:HG22	2.00	0.61
4:A:1273:G:OP2	21:R:58:ARG:NH1	2.33	0.61
4:A:1599:U:H5''	4:A:1600:G:H8	1.66	0.61
4:A:1825:C:N4	4:A:1840:G:OP2	2.32	0.61
3:4:76:THR:CG2	3:4:150:ILE:HD11	2.31	0.61
3:4:319:LEU:O	3:4:322:VAL:HG12	2.01	0.61
3:4:438:HIS:O	3:4:439:VAL:C	2.42	0.61
19:P:42:ARG:NH1	19:P:109:TYR:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:245:ILE:CG2	3:4:294:PRO:HG2	2.30	0.61
3:4:444:HIS:CD2	3:4:445:THR:H	2.18	0.61
3:4:148:LEU:HA	3:4:311:LEU:HD13	1.83	0.61
6:C:136:ILE:HG21	6:C:142:ILE:HD11	1.82	0.61
3:4:147:ILE:O	3:4:150:ILE:HG22	2.01	0.61
4:A:570:U:O4'	25:V:44:HIS:NE2	2.34	0.61
3:4:383:ARG:HB3	3:4:383:ARG:HH11	1.64	0.60
4:A:325:U:O2	4:A:450:G:C2	2.54	0.60
18:O:10:LEU:HB2	18:O:17:GLN:HG3	1.84	0.60
3:4:50:VAL:HG23	3:4:118:VAL:HG22	1.83	0.60
3:4:117:THR:HA	3:4:139:LYS:HB2	1.82	0.60
4:A:1187:A:O2'	4:A:1191:A:N1	2.33	0.60
4:A:1611:A:H2	6:C:134:ARG:HH21	1.47	0.60
3:4:371:ILE:HD12	3:4:390:VAL:O	2.00	0.60
3:4:443:GLU:HG2	3:4:452:LYS:CG	2.31	0.60
4:A:1863:G:H5''	4:A:1864:U:H5'	1.83	0.60
3:4:340:LEU:HD22	3:4:340:LEU:N	2.16	0.60
3:4:393:SER:C	3:4:395:ARG:H	2.10	0.60
3:4:354:VAL:HG13	3:4:359:ILE:CG1	2.29	0.60
3:4:426:ARG:C	3:4:428:ASP:N	2.59	0.60
4:A:2160:A:H61	4:A:2187:U:H3	1.48	0.60
26:W:28:ARG:NH1	26:W:93:GLN:O	2.34	0.60
4:A:2245:C:OP1	21:R:25:ARG:NH1	2.35	0.60
28:Y:17:SER:HB3	28:Y:27:ARG:HD2	1.83	0.60
3:4:353:VAL:CG2	3:4:354:VAL:N	2.65	0.60
3:4:366:LEU:HD21	3:4:387:PRO:HB2	1.82	0.60
19:P:43:SER:HB2	19:P:47:ILE:HG22	1.84	0.60
19:P:84:VAL:HG13	19:P:116:LEU:HD13	1.83	0.60
4:A:1156:A:H2'	4:A:1157:G:C8	2.37	0.60
18:O:11:GLY:O	18:O:16:HIS:ND1	2.34	0.60
4:A:587:G:N1	4:A:590:A:OP2	2.35	0.59
3:4:167:ALA:O	3:4:170:GLU:HG2	2.03	0.59
7:D:7:LEU:H	7:D:34:ASN:HD21	1.50	0.59
10:G:51:ILE:HD11	10:G:73:ILE:HD12	1.84	0.59
3:4:294:PRO:O	3:4:296:VAL:N	2.35	0.59
3:4:180:GLY:O	3:4:184:SER:HB2	2.01	0.59
15:L:115:VAL:HG13	15:L:121:VAL:HG21	1.84	0.59
4:A:1001:C:N4	4:A:1004:C:OP2	2.34	0.59
3:4:291:ASP:OD2	3:4:438:HIS:HB3	2.01	0.59
3:4:392:VAL:HG13	3:4:400:LEU:CD2	2.32	0.59
3:4:426:ARG:HA	3:4:429:LEU:CD2	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:861:U:O4	7:D:142:GLN:NE2	2.35	0.59
5:B:9:G:H5'	5:B:10:G:H2'	1.84	0.59
12:I:20:SER:OG	12:I:21:THR:N	2.36	0.59
3:4:153:GLN:HG3	3:4:154:HIS:CD2	2.37	0.59
3:4:219:MET:O	3:4:223:ARG:HG3	2.03	0.59
6:C:163:ILE:HG22	6:C:178:PRO:HD3	1.82	0.59
2:3:22:PRO:HB3	4:A:1102:G:H2'	1.84	0.59
3:4:436:ASP:HB3	3:4:439:VAL:HG22	1.85	0.59
4:A:896:A:OP1	6:C:218:ARG:NH2	2.35	0.59
4:A:1582:C:N4	4:A:1589:G:O6	2.35	0.59
5:B:45:G:OP1	35:g:1:MET:N	2.36	0.59
5:B:50:C:H5''	19:P:78:LYS:HB3	1.84	0.59
3:4:46:LEU:HD12	3:4:117:THR:HG22	1.84	0.58
3:4:292:GLY:O	3:4:293:ARG:C	2.43	0.58
3:4:295:PHE:CG	3:4:295:PHE:O	2.55	0.58
4:A:1555:A:N6	4:A:1617:C:O2	2.36	0.58
4:A:2131:G:O6	4:A:2148:C:N4	2.36	0.58
3:4:148:LEU:HD12	3:4:148:LEU:C	2.27	0.58
4:A:1198:C:H41	4:A:1205:G:H5''	1.68	0.58
6:C:66:ASP:OD1	6:C:103:ARG:NH1	2.36	0.58
35:g:38:CYS:SG	35:g:39:SER:N	2.76	0.58
4:A:1209:G:O6	4:A:1219:U:C4	2.56	0.58
29:Z:45:ARG:HH12	29:Z:48:ARG:HH21	1.52	0.58
3:4:420:VAL:HG23	3:4:466:TYR:HA	1.84	0.58
4:A:325:U:O2	4:A:450:G:N2	2.36	0.58
3:4:202:GLY:HA3	4:A:2676:C:O4'	2.02	0.58
3:4:327:LEU:HA	3:4:363:PRO:O	2.03	0.58
4:A:2385:G:OP1	4:A:2396:A:N6	2.36	0.58
3:4:106:LEU:HA	3:4:109:VAL:HG22	1.85	0.58
3:4:150:ILE:HG23	3:4:151:PHE:HD2	1.69	0.58
3:4:293:ARG:NH2	3:4:414:THR:HA	2.19	0.58
4:A:1177:G:H21	13:J:113:THR:HB	1.68	0.58
13:J:13:LEU:HD13	13:J:15:ILE:HG22	1.86	0.58
3:4:311:LEU:HD23	3:4:312:VAL:N	2.19	0.57
3:4:329:ILE:O	3:4:329:ILE:HG22	2.04	0.57
3:4:432:ARG:HE	3:4:459:LEU:HD12	1.69	0.57
4:A:289:A:N6	4:A:300:G:O6	2.37	0.57
3:4:377:VAL:C	3:4:379:LEU:H	2.12	0.57
3:4:443:GLU:HG2	3:4:452:LYS:HG3	1.86	0.57
4:A:1094:G:HO2'	4:A:1274:A:HO2'	1.49	0.57
3:4:353:VAL:HG23	3:4:354:VAL:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2135:U:C5	4:A:2137:A:C8	2.92	0.57
4:A:2967:C:O2'	10:G:151:ARG:NH1	2.37	0.57
19:P:42:ARG:H	19:P:106:GLY:HA3	1.70	0.57
17:N:65:TRP:HB2	17:N:105:GLU:HB2	1.87	0.57
3:4:100:SER:OG	4:A:2131:G:H4'	2.05	0.57
3:4:283:THR:HG23	3:4:299:ASP:HB3	1.86	0.57
3:4:107:ARG:HD3	3:4:135:ALA:O	2.04	0.57
3:4:369:ASN:C	3:4:371:ILE:H	2.13	0.57
3:4:367:VAL:CG1	3:4:392:VAL:HG21	2.35	0.57
4:A:730:G:H2'	16:M:113:LEU:HD13	1.87	0.57
4:A:2286:A:H2	4:A:2727:A:H62	1.52	0.57
4:A:2390:U:O2	4:A:2392:A:N6	2.38	0.57
4:A:2532:G:H3'	4:A:2533:C:H2'	1.85	0.57
9:F:55:LYS:HA	9:F:58:ASN:HD22	1.70	0.57
13:J:74:THR:HG23	13:J:83:LYS:HD3	1.86	0.57
4:A:759:G:H1	27:X:64:PRO:HB3	1.69	0.57
6:C:108:PRO:HD2	6:C:111:LEU:HD22	1.87	0.57
29:Z:11:ARG:NH1	29:Z:63:GLU:OE1	2.38	0.57
4:A:1272:C:OP1	21:R:92:ARG:NH2	2.37	0.56
9:F:129:PHE:HE1	9:F:136:THR:H	1.54	0.56
3:4:267:GLY:O	3:4:268:ALA:HB3	2.05	0.56
3:4:371:ILE:O	3:4:372:ASP:HB2	2.04	0.56
3:4:379:LEU:HD21	3:4:391:PHE:CE2	2.39	0.56
4:A:1541:G:OP2	4:A:1629:G:N2	2.39	0.56
4:A:2335:G:OP2	4:A:2338:G:N1	2.37	0.56
17:N:35:GLN:OE1	17:N:130:ARG:NH2	2.39	0.56
3:4:47:GLU:HA	3:4:79:SER:CA	2.35	0.56
3:4:443:GLU:O	3:4:451:ILE:HD13	2.05	0.56
4:A:1172:A:N3	12:I:29:ARG:NH1	2.53	0.56
4:A:1398:G:N2	4:A:1401:A:OP2	2.37	0.56
3:4:263:ASN:ND2	3:4:270:VAL:H	2.02	0.56
4:A:2015:U:OP2	6:C:272:ARG:NH2	2.38	0.56
4:A:2509:C:OP2	31:c:8:ARG:NH1	2.38	0.56
4:A:2802:G:H21	7:D:135:GLN:HE21	1.54	0.56
5:B:7:G:O2'	19:P:37:ARG:NH2	2.39	0.56
3:4:436:ASP:HB3	3:4:439:VAL:CG1	2.35	0.56
3:4:61:ALA:HA	3:4:64:GLU:OE2	2.05	0.56
4:A:2476:G:H2'	4:A:2477:G:H8	1.70	0.56
4:A:2587:U:OP2	33:e:43:ARG:NH2	2.39	0.56
5:B:43:C:H5'	9:F:71:LYS:HD2	1.86	0.56
3:4:132:LEU:O	3:4:136:VAL:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:393:SER:O	36:4:501:GCP:N7	2.39	0.56
4:A:1556:A:H2	4:A:1615:G:H22	1.52	0.56
13:J:34:GLY:O	13:J:66:ARG:NH1	2.39	0.56
4:A:2043:C:O2'	4:A:2195:U:OP2	2.24	0.56
3:4:47:GLU:HA	3:4:79:SER:HA	1.88	0.56
4:A:1112:C:O2	22:S:12:LYS:NZ	2.37	0.56
4:A:2367:G:N3	4:A:2370:A:N7	2.54	0.56
19:P:46:HIS:NE2	19:P:65:SER:O	2.39	0.56
3:4:47:GLU:HA	3:4:79:SER:HB3	1.87	0.56
3:4:327:LEU:HD21	3:4:329:ILE:CD1	2.35	0.56
4:A:2035:U:OP2	6:C:157:ARG:NH1	2.39	0.56
3:4:43:GLN:HA	3:4:43:GLN:NE2	2.20	0.55
3:4:183:MET:HA	3:4:186:GLN:HB2	1.86	0.55
4:A:365:U:O2	4:A:437:G:N2	2.37	0.55
4:A:1224:G:O2'	12:I:54:ASN:ND2	2.40	0.55
5:B:112:C:N4	5:B:113:G:N3	2.54	0.55
19:P:50:GLN:HA	19:P:63:ALA:CB	2.34	0.55
3:4:420:VAL:CG2	3:4:466:TYR:HA	2.36	0.55
35:g:18:CYS:SG	35:g:40:GLN:NE2	2.80	0.55
3:4:76:THR:HG21	3:4:150:ILE:HD11	1.88	0.55
15:L:50:GLY:O	15:L:53:LYS:NZ	2.39	0.55
3:4:178:GLY:C	3:4:180:GLY:H	2.14	0.55
4:A:573:C:H41	25:V:47:VAL:HB	1.72	0.55
4:A:652:C:O2'	21:R:48:ARG:NH1	2.40	0.55
10:G:29:PRO:HD3	10:G:80:VAL:HA	1.89	0.55
4:A:1209:G:O6	4:A:1219:U:O4	2.24	0.55
4:A:1540:U:O2	4:A:1632:G:O6	2.25	0.55
3:4:202:GLY:O	3:4:204:GLY:N	2.40	0.55
3:4:246:PRO:CD	3:4:293:ARG:HB3	2.37	0.55
4:A:2136:A:N3	4:A:2136:A:H2'	2.22	0.55
3:4:167:ALA:HB2	3:4:311:LEU:HA	1.89	0.55
3:4:187:ALA:CA	4:A:2826:A:C5	2.86	0.55
3:4:333:ASP:OD2	3:4:336:ASP:HB2	2.07	0.55
3:4:432:ARG:HA	3:4:435:THR:O	2.07	0.55
4:A:1181:G:N2	13:J:136:SER:O	2.39	0.55
4:A:1455:U:OP1	24:U:19:LYS:NZ	2.39	0.55
4:A:2510:A:OP1	31:c:31:ASN:ND2	2.40	0.55
4:A:2584:A:OP1	33:e:24:ARG:NH2	2.40	0.55
4:A:3102:U:O2	18:O:45:ARG:NH2	2.39	0.55
15:L:63:VAL:HG12	15:L:106:LEU:HD11	1.89	0.55
3:4:370:LYS:HE3	36:4:501:GCP:HI'	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:615:A:OP2	14:K:116:ARG:NH1	2.40	0.55
3:4:441:ALA:H	3:4:453:ALA:CB	2.20	0.55
32:d:37:ARG:NH1	32:d:44:ALA:O	2.40	0.55
3:4:193:GLY:O	3:4:194:ALA:C	2.49	0.55
3:4:294:PRO:C	3:4:296:VAL:N	2.62	0.55
3:4:422:ILE:O	3:4:448:GLY:HA3	2.07	0.55
3:4:444:HIS:CG	3:4:445:THR:H	2.25	0.55
4:A:1710:A:N6	4:A:1716:A:N7	2.54	0.55
3:4:253:TYR:CD1	3:4:342:GLN:HB3	2.42	0.54
4:A:889:A:OP1	6:C:48:ARG:NH1	2.40	0.54
4:A:3066:C:H5''	20:Q:52:GLY:HA3	1.89	0.54
4:A:1122:C:H2'	4:A:1129:G:H2'	1.89	0.54
4:A:2538:A:OP1	9:F:95:ARG:NH2	2.40	0.54
3:4:340:LEU:H	3:4:340:LEU:CD2	2.20	0.54
3:4:445:THR:HG21	3:4:450:ARG:CG	2.37	0.54
4:A:1562:C:H2'	4:A:1563:A:C8	2.41	0.54
3:4:444:HIS:CG	3:4:445:THR:N	2.74	0.54
4:A:2137:A:H3'	4:A:2137:A:N3	2.21	0.54
12:I:3:LYS:O	12:I:7:ALA:HB3	2.08	0.54
3:4:271:LEU:CD2	3:4:273:GLU:H	2.21	0.54
4:A:2323:G:O6	4:A:2412:U:C4	2.61	0.54
4:A:3070:G:O2'	4:A:3087:G:N2	2.41	0.54
19:P:22:HIS:HA	19:P:105:GLY:HA2	1.88	0.54
3:4:159:GLU:HG3	3:4:229:MET:SD	2.47	0.54
3:4:430:VAL:O	3:4:432:ARG:N	2.40	0.54
19:P:40:VAL:HG23	19:P:106:GLY:H	1.73	0.54
20:Q:48:ARG:HD2	20:Q:50:GLN:HB2	1.88	0.54
16:M:91:GLY:H	16:M:122:VAL:HG23	1.73	0.54
23:T:25:ARG:HA	23:T:28:ILE:HG12	1.89	0.54
3:4:251:VAL:CG2	3:4:252:GLY:H	2.20	0.54
4:A:1552:A:O2'	4:A:1618:C:N4	2.40	0.54
3:4:294:PRO:CB	3:4:296:VAL:HG23	2.34	0.54
3:4:323:VAL:HG21	3:4:357:TYR:CE1	2.43	0.54
3:4:432:ARG:O	3:4:433:VAL:C	2.51	0.54
4:A:1181:G:O2'	13:J:91:SER:O	2.26	0.54
4:A:1199:U:OP1	4:A:1201:G:N2	2.41	0.54
3:4:436:ASP:CB	3:4:439:VAL:HG13	2.37	0.54
4:A:544:U:O2	4:A:547:U:O2'	2.26	0.54
4:A:1560:U:O2	6:C:134:ARG:NH2	2.41	0.54
5:B:78:U:OP1	26:W:28:ARG:NH2	2.41	0.54
3:4:136:VAL:O	3:4:137:LYS:HB2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:163:GLN:HB3	3:4:314:ALA:HB3	1.90	0.53
3:4:181:GLU:C	3:4:184:SER:H	2.16	0.53
15:L:90:ASP:OD2	15:L:90:ASP:N	2.40	0.53
3:4:158:ARG:HD2	3:4:158:ARG:C	2.32	0.53
3:4:339:PRO:CG	3:4:382:LEU:HD21	2.38	0.53
3:4:374:ALA:C	3:4:376:GLY:N	2.62	0.53
3:4:420:VAL:HG23	3:4:466:TYR:CA	2.38	0.53
3:4:463:LEU:HD12	3:4:463:LEU:H	1.73	0.53
4:A:708:G:N2	8:E:187:ASP:OD1	2.41	0.53
3:4:246:PRO:HD3	3:4:293:ARG:HB3	1.90	0.53
3:4:463:LEU:CD1	3:4:463:LEU:H	2.22	0.53
4:A:2219:U:OP1	7:D:133:ARG:NH2	2.42	0.53
20:Q:62:LYS:HE2	20:Q:64:SER:HB3	1.90	0.53
31:c:15:CYS:SG	31:c:16:GLU:N	2.81	0.53
3:4:173:LEU:HB3	3:4:174:PRO:HD3	1.90	0.53
3:4:187:ALA:C	3:4:189:GLY:H	2.15	0.53
27:X:11:ARG:O	27:X:14:ARG:NH1	2.38	0.53
3:4:263:ASN:HD21	3:4:270:VAL:N	2.04	0.53
4:A:571:A:OP1	4:A:572:C:N4	2.34	0.53
4:A:1535:C:H3'	4:A:1536:A:H8	1.73	0.53
11:H:98:ALA:O	11:H:102:ASN:ND2	2.41	0.53
3:4:214:ARG:O	3:4:218:ARG:HD3	2.09	0.53
5:B:48:C:OP2	19:P:14:ARG:NH1	2.42	0.53
8:E:119:ALA:HB2	8:E:124:ILE:HD12	1.90	0.53
9:F:103:MET:HG3	9:F:107:LEU:HD12	1.91	0.53
19:P:50:GLN:CA	19:P:63:ALA:HB3	2.37	0.53
3:4:87:GLN:HE21	4:A:2133:G:H8	1.55	0.53
3:4:185:ARG:C	3:4:187:ALA:H	2.17	0.53
3:4:397:GLY:O	3:4:398:ASP:C	2.50	0.53
4:A:1436:C:O2'	23:T:18:ARG:NH2	2.42	0.53
4:A:2536:U:O2	9:F:44:ASN:ND2	2.42	0.53
3:4:280:LEU:HD12	3:4:315:PHE:CZ	2.44	0.53
3:4:368:VAL:HB	3:4:371:ILE:HD11	1.91	0.53
3:4:136:VAL:HG23	3:4:138:VAL:H	1.73	0.52
3:4:202:GLY:N	3:4:203:PRO:CD	2.72	0.52
4:A:2380:G:N2	4:A:2382:G:OP2	2.43	0.52
4:A:1113:C:O2	14:K:3:THR:OG1	2.25	0.52
11:H:77:ASP:HB2	11:H:147:ASN:HB2	1.90	0.52
4:A:1337:G:OP2	22:S:91:ARG:NH1	2.42	0.52
3:4:213:ARG:HB3	3:4:214:ARG:HH21	1.74	0.52
3:4:365:LEU:HD11	3:4:388:ASP:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:416:ALA:O	3:4:454:ARG:HB2	2.08	0.52
4:A:2519:C:OP2	19:P:24:ARG:NH2	2.43	0.52
15:L:47:ILE:HG22	15:L:49:GLY:H	1.74	0.52
3:4:73:LEU:HG	3:4:146:LEU:CD2	2.40	0.52
3:4:73:LEU:HG	3:4:146:LEU:HG	1.91	0.52
3:4:426:ARG:HG2	3:4:427:GLY:N	2.24	0.52
19:P:41:ASN:ND2	19:P:48:HIS:O	2.43	0.52
9:F:116:PRO:HB3	35:g:42:HIS:HB2	1.91	0.52
13:J:125:ALA:O	13:J:129:ILE:HB	2.09	0.52
3:4:215:ILE:O	3:4:219:MET:HG3	2.10	0.52
3:4:85:LEU:HD13	3:4:106:LEU:HD21	1.89	0.52
3:4:330:HIS:NE2	3:4:346:VAL:HB	2.25	0.52
3:4:348:THR:O	3:4:351:ASN:HB2	2.10	0.52
4:A:349:G:H2'	4:A:350:A:H8	1.75	0.52
3:4:124:LEU:HD12	3:4:124:LEU:N	2.25	0.52
3:4:180:GLY:HA2	3:4:183:MET:HG2	1.91	0.52
3:4:328:LEU:HD12	3:4:328:LEU:N	2.24	0.52
3:4:432:ARG:NE	3:4:459:LEU:HD12	2.24	0.52
4:A:306:U:OP2	11:H:41:ARG:NH1	2.43	0.52
4:A:724:G:N2	4:A:727:A:OP2	2.36	0.52
35:g:14:VAL:HB	35:g:22:PHE:HB3	1.92	0.52
3:4:132:LEU:HG	3:4:140:VAL:HG11	1.91	0.52
7:D:144:VAL:HA	7:D:147:ARG:HG3	1.92	0.52
13:J:111:ALA:HB2	13:J:126:ALA:HB2	1.91	0.52
3:4:102:LYS:HD3	4:A:2133:G:P	2.50	0.51
3:4:227:ARG:HE	3:4:227:ARG:CA	2.20	0.51
13:J:21:ASN:ND2	13:J:41:CYS:SG	2.82	0.51
26:W:178:VAL:HG12	26:W:179:VAL:HG23	1.91	0.51
26:W:186:SER:OG	26:W:187:ALA:N	2.41	0.51
3:4:82:LEU:HD12	3:4:115:ALA:HB2	1.92	0.51
3:4:222:LEU:CD2	3:4:226:ILE:HG23	2.40	0.51
3:4:248:VAL:HG21	3:4:295:PHE:CD1	2.45	0.51
4:A:1379:G:OP1	30:b:16:ARG:NH2	2.35	0.51
4:A:2726:G:H5''	4:A:2727:A:H5''	1.91	0.51
6:C:146:GLU:HB2	6:C:189:CYS:HB3	1.93	0.51
3:4:151:PHE:CE1	3:4:315:PHE:CE2	2.99	0.51
12:I:76:PRO:O	12:I:106:LYS:NZ	2.33	0.51
16:M:94:GLY:N	16:M:97:GLU:OE1	2.43	0.51
3:4:106:LEU:O	3:4:109:VAL:HG22	2.11	0.51
3:4:280:LEU:HD12	3:4:315:PHE:HZ	1.74	0.51
3:4:456:PRO:HB2	3:4:458:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:55:TRP:CG	3:4:55:TRP:O	2.64	0.51
3:4:119:ILE:N	3:4:119:ILE:HD12	2.24	0.51
4:A:2142:A:H2'	4:A:2143:A:O4'	2.10	0.51
25:V:10:LEU:HD13	25:V:80:PRO:HG3	1.92	0.51
3:4:48:ARG:HB2	3:4:116:ASP:OD1	2.11	0.51
3:4:335:SER:HB3	3:4:375:THR:OG1	2.11	0.51
3:4:420:VAL:HA	3:4:466:TYR:CD1	2.36	0.51
3:4:47:GLU:HA	3:4:79:SER:CB	2.40	0.51
3:4:49:VAL:HG22	3:4:81:VAL:HA	1.91	0.51
3:4:223:ARG:HA	3:4:226:ILE:CD1	2.41	0.51
4:A:1212:U:H4'	4:A:1215:U:H5	1.76	0.51
4:A:1546:A:N6	4:A:1625:G:O6	2.44	0.51
4:A:2983:G:N2	10:G:140:GLN:OE1	2.43	0.51
12:I:3:LYS:O	12:I:7:ALA:CB	2.59	0.51
3:4:180:GLY:CA	3:4:183:MET:HG2	2.40	0.51
4:A:2138:C:H4'	4:A:2142:A:C2	2.46	0.51
3:4:76:THR:O	3:4:76:THR:HG22	2.10	0.51
3:4:261:LEU:HD11	3:4:392:VAL:CG1	2.29	0.51
4:A:2476:G:H2'	4:A:2477:G:C8	2.45	0.51
3:4:70:LEU:HD22	3:4:121:ASP:HB3	1.92	0.50
3:4:392:VAL:HG13	3:4:400:LEU:HD23	1.92	0.50
4:A:1566:A:N6	4:A:1606:G:N2	2.47	0.50
3:4:430:VAL:HG12	3:4:434:HIS:HD2	1.75	0.50
3:4:456:PRO:HD2	3:4:459:LEU:HB2	1.94	0.50
3:4:148:LEU:HD11	3:4:168:GLN:HB3	1.92	0.50
3:4:436:ASP:HB3	3:4:439:VAL:CG2	2.41	0.50
3:4:458:PRO:HG2	3:4:459:LEU:HD22	1.93	0.50
13:J:48:THR:HB	13:J:56:ILE:HD13	1.94	0.50
4:A:380:A:N3	4:A:401:C:O2'	2.41	0.50
33:e:29:ARG:NH1	33:e:44:LEU:O	2.38	0.50
4:A:2176:A:N3	4:A:2784:C:O2'	2.39	0.50
5:B:101:U:O3'	26:W:81:LYS:NZ	2.45	0.50
12:I:33:VAL:O	12:I:37:ALA:N	2.39	0.50
19:P:49:VAL:HG12	19:P:50:GLN:N	2.26	0.50
3:4:456:PRO:CB	3:4:459:LEU:HD23	2.38	0.50
4:A:2323:G:O6	4:A:2412:U:O4	2.30	0.50
4:A:2528:G:N2	9:F:160:ASP:OD2	2.45	0.50
25:V:1:MET:HE2	25:V:68:VAL:HG21	1.92	0.50
3:4:46:LEU:HD22	3:4:46:LEU:N	2.26	0.50
3:4:95:SER:O	3:4:131:ALA:HB3	2.11	0.50
3:4:371:ILE:CA	3:4:374:ALA:HB2	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:420:VAL:CG2	3:4:421:THR:N	2.72	0.50
3:4:452:LYS:NZ	3:4:452:LYS:HB3	2.26	0.50
32:d:13:ARG:HH21	32:d:17:ARG:HH21	1.58	0.50
3:4:419:ASP:HA	3:4:452:LYS:HA	1.93	0.50
3:4:424:TYR:CE2	3:4:447:ALA:HA	2.47	0.50
34:f:22:ARG:NH1	34:f:37:GLY:O	2.45	0.50
4:A:1209:G:N2	4:A:1219:U:O2	2.40	0.50
4:A:2086:U:H3	4:A:2096:G:H1	1.59	0.50
16:M:84:ASN:HB2	16:M:118:LEU:HD12	1.94	0.50
3:4:89:ARG:HD3	3:4:91:LYS:O	2.11	0.49
3:4:284:THR:O	3:4:285:ARG:HD3	2.12	0.49
25:V:86:ARG:HB2	25:V:97:ILE:HD12	1.94	0.49
3:4:331:VAL:HA	3:4:367:VAL:O	2.12	0.49
3:4:392:VAL:HG13	3:4:400:LEU:HD21	1.94	0.49
7:D:14:THR:OG1	7:D:15:GLN:N	2.44	0.49
10:G:36:ASP:OD1	10:G:36:ASP:N	2.46	0.49
3:4:173:LEU:N	3:4:174:PRO:CD	2.75	0.49
4:A:2086:U:O4	4:A:2096:G:O6	2.30	0.49
3:4:201:ARG:NH2	4:A:2286:A:N7	2.60	0.49
3:4:110:VAL:HG21	3:4:138:VAL:HG21	1.94	0.49
3:4:199:GLY:C	3:4:201:ARG:HD2	2.37	0.49
3:4:222:LEU:HD23	3:4:226:ILE:HG23	1.95	0.49
3:4:382:LEU:O	3:4:386:LEU:HB2	2.13	0.49
8:E:184:ASN:OD1	8:E:184:ASN:N	2.45	0.49
12:I:77:THR:OG1	12:I:106:LYS:NZ	2.45	0.49
34:f:16:VAL:HG12	34:f:25:VAL:HG22	1.93	0.49
3:4:230:LYS:HD3	3:4:233:ARG:HH21	1.77	0.49
4:A:1209:G:N1	4:A:1219:U:C2	2.77	0.49
4:A:1548:C:H42	4:A:1621:C:H5	1.60	0.49
4:A:2400:C:H3'	4:A:2401:U:H4'	1.95	0.49
10:G:35:LEU:HD22	10:G:76:LEU:HD22	1.95	0.49
3:4:250:ILE:HD13	3:4:258:LYS:CA	2.40	0.49
3:4:350:ILE:O	3:4:354:VAL:HG23	2.12	0.49
19:P:43:SER:CB	19:P:47:ILE:HG22	2.41	0.49
34:f:2:LYS:HG3	34:f:34:GLN:HG2	1.95	0.49
3:4:166:LEU:HD22	3:4:226:ILE:CD1	2.43	0.49
4:A:920:G:N2	4:A:944:A:OP1	2.44	0.49
4:A:1076:A:N6	17:N:83:MET:HE1	2.27	0.49
7:D:7:LEU:HB2	7:D:34:ASN:HD21	1.78	0.49
14:K:49:ASP:OD1	14:K:121:LYS:NZ	2.44	0.49
3:4:87:GLN:HG2	3:4:88:ARG:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:88:ARG:HG2	4:A:2137:A:N6	2.28	0.49
3:4:173:LEU:CD1	3:4:215:ILE:HG21	2.34	0.49
4:A:347:U:H2'	4:A:348:G:C8	2.47	0.49
4:A:380:A:N1	4:A:404:A:O2'	2.41	0.49
4:A:2137:A:H4'	4:A:2142:A:C2	2.47	0.49
4:A:2224:C:O2'	4:A:2913:U:OP2	2.30	0.49
27:X:53:ARG:NH1	27:X:57:ASP:OD1	2.46	0.49
3:4:125:SER:OG	3:4:128:GLN:HG3	2.13	0.49
3:4:233:ARG:O	3:4:237:ARG:HG2	2.13	0.49
4:A:2329:G:O6	4:A:2406:U:O4	2.30	0.49
35:g:24:THR:OG1	35:g:25:ARG:N	2.45	0.49
3:4:288:GLU:HG2	3:4:289:PHE:O	2.13	0.48
3:4:295:PHE:O	3:4:295:PHE:CD1	2.66	0.48
4:A:1184:U:O5'	4:A:1187:A:N6	2.45	0.48
4:A:2161:A:O2'	4:A:2163:U:OP2	2.24	0.48
23:T:77:VAL:HG21	23:T:117:ARG:HD2	1.95	0.48
3:4:45:ARG:CZ	3:4:45:ARG:HB3	2.43	0.48
3:4:251:VAL:CG2	3:4:252:GLY:N	2.74	0.48
3:4:393:SER:C	3:4:395:ARG:N	2.71	0.48
4:A:2141:U:O2'	4:A:2142:A:H5''	2.12	0.48
6:C:143:HIS:ND1	6:C:194:GLY:O	2.30	0.48
12:I:53:LYS:O	12:I:54:ASN:ND2	2.45	0.48
23:T:9:SER:HB3	23:T:115:GLU:HG2	1.94	0.48
3:4:199:GLY:O	3:4:201:ARG:N	2.47	0.48
3:4:213:ARG:CB	3:4:214:ARG:HH21	2.26	0.48
11:H:101:VAL:HG22	11:H:114:LYS:HB2	1.96	0.48
12:I:115:LEU:HD11	12:I:119:ASP:HB3	1.94	0.48
3:4:187:ALA:CB	4:A:2826:A:C5	2.97	0.48
3:4:223:ARG:O	3:4:226:ILE:HG12	2.13	0.48
3:4:395:ARG:HG2	3:4:396:THR:N	2.26	0.48
3:4:463:LEU:HD12	3:4:463:LEU:N	2.29	0.48
4:A:1163:A:OP1	4:A:1229:A:N6	2.46	0.48
4:A:2530:C:H3'	4:A:2531:G:H2'	1.94	0.48
4:A:2690:C:H5''	34:f:6:SER:HB2	1.94	0.48
22:S:27:LEU:HB2	22:S:95:THR:HG21	1.95	0.48
3:4:142:ASP:OD1	3:4:142:ASP:N	2.46	0.48
3:4:287:GLY:O	3:4:294:PRO:O	2.32	0.48
3:4:432:ARG:HB3	3:4:436:ASP:CG	2.38	0.48
4:A:2014:G:O2'	6:C:257:THR:OG1	2.27	0.48
6:C:182:ILE:HB	6:C:269:VAL:HB	1.95	0.48
11:H:118:GLN:HE21	11:H:120:ALA:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:119:ASP:HA	12:I:122:LYS:HD2	1.95	0.48
19:P:79:ALA:HB3	19:P:115:ALA:HB3	1.95	0.48
4:A:1157:G:N2	4:A:1234:U:O2	2.47	0.48
4:A:1160:G:H1	4:A:1230:G:H22	1.61	0.48
11:H:85:ALA:N	11:H:90:LYS:O	2.46	0.48
35:g:14:VAL:N	35:g:22:PHE:O	2.45	0.48
3:4:228:ASP:C	3:4:230:LYS:N	2.70	0.48
3:4:443:GLU:CD	3:4:452:LYS:HD3	2.39	0.48
4:A:356:G:H21	4:A:362:A:H62	1.62	0.48
4:A:1548:C:C2	4:A:1622:G:H1'	2.49	0.48
5:B:44:C:O3'	9:F:102:ARG:NH2	2.46	0.48
9:F:45:MET:HG3	9:F:64:LEU:HD22	1.95	0.48
3:4:102:LYS:CG	4:A:2132:U:H5'	2.31	0.48
3:4:151:PHE:HE2	3:4:277:PHE:CG	2.31	0.48
3:4:329:ILE:HA	3:4:365:LEU:O	2.14	0.48
3:4:395:ARG:NH2	36:4:501:GCP:C2	2.62	0.48
4:A:2463:G:OP1	6:C:244:ARG:NH2	2.43	0.48
15:L:122:LEU:HD13	20:Q:69:VAL:HG11	1.95	0.48
3:4:49:VAL:CG2	3:4:81:VAL:HA	2.43	0.48
3:4:90:ASP:HB3	4:A:2137:A:C2	2.48	0.48
3:4:147:ILE:CD1	3:4:151:PHE:CE2	2.95	0.48
4:A:81:A:OP1	25:V:4:HIS:NE2	2.47	0.48
4:A:1564:A:N7	4:A:1607:C:O2'	2.46	0.48
19:P:64:SER:OG	19:P:65:SER:N	2.47	0.48
3:4:76:THR:HG22	3:4:150:ILE:HD11	1.96	0.48
11:H:1:MET:N	11:H:21:VAL:O	2.44	0.48
11:H:100:VAL:HG23	11:H:114:LYS:HG3	1.96	0.48
26:W:50:ASN:ND2	26:W:53:ASP:OD1	2.41	0.48
4:A:1537:U:H2'	4:A:1538:G:H8	1.78	0.47
4:A:1542:A:N1	4:A:1628:A:O2'	2.41	0.47
10:G:17:VAL:HG12	10:G:26:VAL:HG22	1.96	0.47
10:G:27:LYS:NZ	10:G:28:GLY:O	2.47	0.47
11:H:75:LEU:O	11:H:145:SER:OG	2.31	0.47
4:A:1116:C:OP2	21:R:58:ARG:NH2	2.47	0.47
4:A:3014:A:H62	4:A:3113:A:H2	1.62	0.47
24:U:30:THR:HG23	24:U:83:ILE:HG12	1.96	0.47
12:I:45:ASP:OD2	12:I:45:ASP:N	2.46	0.47
20:Q:91:VAL:HG11	20:Q:96:LEU:HD21	1.95	0.47
3:4:305:ARG:HH22	3:4:341:ALA:C	2.22	0.47
3:4:436:ASP:CB	3:4:439:VAL:CG1	2.92	0.47
4:A:2735:U:O2'	7:D:148:PRO:O	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:43:THR:OG1	17:N:44:ASN:N	2.41	0.47
3:4:151:PHE:CE1	3:4:315:PHE:CZ	3.03	0.47
3:4:187:ALA:C	3:4:189:GLY:N	2.71	0.47
3:4:195:GLY:C	3:4:197:GLY:N	2.69	0.47
3:4:426:ARG:NH2	3:4:433:VAL:HG11	2.30	0.47
3:4:455:VAL:CB	3:4:460:ALA:HB3	2.44	0.47
4:A:164:A:OP2	11:H:118:GLN:NE2	2.47	0.47
4:A:2367:G:N2	4:A:2370:A:C4	2.83	0.47
6:C:181:GLU:HG2	6:C:271:ARG:HA	1.96	0.47
13:J:12:LYS:HE2	13:J:59:GLU:HB2	1.97	0.47
21:R:26:GLY:O	21:R:30:ARG:NH1	2.48	0.47
3:4:231:LYS:O	3:4:235:THR:HG22	2.15	0.47
4:A:1198:C:H2'	13:J:128:LYS:HD2	1.96	0.47
3:4:258:LYS:HD3	36:4:501:GCP:O1B	2.15	0.47
3:4:432:ARG:HG2	3:4:459:LEU:HD12	1.95	0.47
4:A:551:G:N2	4:A:554:A:OP2	2.42	0.47
4:A:808:A:O2'	4:A:1468:A:N3	2.42	0.47
4:A:2764:C:O2'	4:A:2964:A:N3	2.42	0.47
22:S:21:VAL:HG22	22:S:98:LYS:HG3	1.96	0.47
3:4:102:LYS:N	4:A:2132:U:OP1	2.41	0.47
4:A:994:A:N6	4:A:1014:G:O2'	2.46	0.47
4:A:1127:A:N3	4:A:1272:C:O2'	2.47	0.47
4:A:2340:A:O2'	4:A:2342:A:OP1	2.32	0.47
9:F:124:LEU:HG	9:F:184:PHE:HA	1.96	0.47
10:G:99:LEU:HG	10:G:101:GLY:H	1.80	0.47
3:4:118:VAL:C	3:4:119:ILE:HD12	2.39	0.47
9:F:86:LEU:HD12	9:F:90:MET:HE2	1.97	0.47
3:4:449:THR:OG1	3:4:451:ILE:HG12	2.15	0.47
4:A:1198:C:N4	4:A:1206:A:OP2	2.48	0.47
4:A:1365:G:O6	16:M:21:ARG:NH2	2.46	0.46
3:4:208:ILE:HG23	3:4:209:GLU:N	2.30	0.46
3:4:395:ARG:CG	3:4:396:THR:H	2.23	0.46
4:A:678:A:H5'	8:E:90:VAL:HG13	1.95	0.46
4:A:2367:G:C2	4:A:2370:A:C8	3.03	0.46
31:c:27:LYS:NZ	31:c:53:GLU:OE1	2.43	0.46
3:4:433:VAL:O	3:4:439:VAL:HB	2.15	0.46
4:A:32:G:H1'	4:A:542:A:C4	2.50	0.46
4:A:1162:G:OP2	4:A:1164:A:N6	2.40	0.46
4:A:2136:A:N6	4:A:2139:U:O4	2.48	0.46
4:A:2385:G:H5''	4:A:2396:A:H61	1.80	0.46
10:G:51:ILE:HD12	10:G:70:ARG:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:52:GLU:HG2	23:T:53:PRO:HD3	1.97	0.46
25:V:43:LYS:O	25:V:43:LYS:NZ	2.36	0.46
3:4:46:LEU:HA	3:4:116:ASP:OD2	2.15	0.46
4:A:256:A:H2'	4:A:257:A:H8	1.80	0.46
19:P:49:VAL:O	19:P:50:GLN:HB3	2.15	0.46
19:P:49:VAL:O	19:P:64:SER:HA	2.16	0.46
19:P:68:ALA:O	19:P:71:ARG:NH1	2.49	0.46
3:4:253:TYR:CE1	3:4:332:VAL:HG12	2.37	0.46
4:A:1364:U:C4	16:M:21:ARG:HD3	2.51	0.46
13:J:103:THR:OG1	13:J:104:TRP:N	2.46	0.46
19:P:52:VAL:HG13	19:P:59:THR:HG22	1.97	0.46
3:4:226:ILE:HA	3:4:229:MET:HE2	1.98	0.46
3:4:357:TYR:O	3:4:358:ASP:C	2.59	0.46
4:A:1269:C:O2'	21:R:121:VAL:O	2.29	0.46
4:A:1562:C:H2'	4:A:1563:A:H8	1.80	0.46
20:Q:48:ARG:HB2	20:Q:95:LYS:HD3	1.97	0.46
21:R:73:ASP:O	21:R:114:ARG:NH2	2.49	0.46
25:V:27:TYR:HB2	25:V:30:ARG:HB2	1.98	0.46
27:X:76:LYS:HB3	27:X:76:LYS:HE3	1.72	0.46
28:Y:21:SER:O	28:Y:21:SER:OG	2.33	0.46
3:4:163:GLN:HB3	3:4:314:ALA:CB	2.45	0.46
3:4:232:ILE:HA	3:4:235:THR:HG22	1.97	0.46
3:4:275:ALA:C	3:4:276:LEU:HD12	2.40	0.46
3:4:438:HIS:CE1	3:4:456:PRO:HG3	2.51	0.46
4:A:1577:C:H2'	4:A:1578:G:H8	1.81	0.46
4:A:2527:G:O2'	9:F:128:GLN:O	2.33	0.46
7:D:10:LYS:HB3	7:D:198:ILE:HD11	1.98	0.46
10:G:19:ILE:HG12	10:G:24:LEU:HD13	1.97	0.46
19:P:62:ALA:HB3	19:P:91:ARG:HH12	1.81	0.46
3:4:147:ILE:O	3:4:147:ILE:HD12	2.15	0.46
3:4:240:ARG:HG2	4:A:2697:U:O2	2.16	0.46
3:4:393:SER:O	36:4:501:GCP:O6	2.34	0.46
4:A:1696:G:O2'	4:A:1736:G:O6	2.32	0.46
11:H:74:GLY:HA3	11:H:105:LYS:HE3	1.96	0.46
3:4:172:MET:O	3:4:172:MET:SD	2.74	0.46
9:F:132:THR:HG22	9:F:170:ASP:HA	1.98	0.46
3:4:361:PRO:HA	3:4:362:PRO:HD3	1.84	0.46
3:4:430:VAL:HG12	3:4:434:HIS:CD2	2.51	0.46
3:4:445:THR:OG1	3:4:449:THR:HA	2.16	0.46
4:A:556:G:OP2	32:d:40:LYS:NZ	2.46	0.46
4:A:790:A:OP1	8:E:64:LYS:NZ	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:106:ASP:OD2	18:O:106:ASP:N	2.48	0.46
4:A:531:A:H2'	8:E:46:ARG:HH12	1.81	0.45
4:A:2008:A:N6	4:A:2045:G:O2'	2.42	0.45
5:B:15:U:OP2	5:B:71:C:O2'	2.34	0.45
13:J:106:GLN:HB3	13:J:109:GLU:HB3	1.97	0.45
25:V:44:HIS:H	25:V:59:ILE:HG12	1.80	0.45
3:4:171:TYR:CD1	3:4:171:TYR:C	2.95	0.45
3:4:289:PHE:HD1	3:4:290:GLU:H	1.64	0.45
3:4:332:VAL:HG11	3:4:343:ILE:HG12	1.97	0.45
3:4:334:GLY:C	3:4:336:ASP:H	2.24	0.45
4:A:1209:G:C6	4:A:1219:U:N3	2.84	0.45
5:B:9:G:O6	5:B:109:C:N4	2.49	0.45
12:I:20:SER:HA	12:I:83:LYS:HD3	1.99	0.45
19:P:67:GLU:OE2	19:P:91:ARG:NH1	2.49	0.45
2:3:16:ALA:O	4:A:1096:G:N2	2.37	0.45
3:4:201:ARG:HG3	4:A:2675:A:H2	1.80	0.45
3:4:426:ARG:HG3	3:4:429:LEU:CB	2.28	0.45
4:A:1705:C:H2'	4:A:1706:A:H8	1.80	0.45
4:A:2190:A:N3	4:A:2816:G:O2'	2.47	0.45
12:I:82:VAL:HG11	12:I:90:ALA:HB2	1.97	0.45
19:P:39:VAL:O	19:P:49:VAL:CG1	2.64	0.45
3:4:89:ARG:HG2	3:4:91:LYS:H	1.81	0.45
3:4:369:ASN:C	3:4:371:ILE:N	2.73	0.45
3:4:370:LYS:HD3	36:4:501:GCP:C4	2.45	0.45
3:4:460:ALA:O	3:4:463:LEU:HD13	2.16	0.45
14:K:28:LEU:HD22	14:K:62:ILE:HD11	1.98	0.45
3:4:48:ARG:HD2	3:4:82:LEU:HD11	1.98	0.45
3:4:102:LYS:HG2	4:A:2132:U:OP1	2.16	0.45
3:4:290:GLU:CD	3:4:291:ASP:N	2.75	0.45
3:4:301:VAL:HG12	3:4:302:GLY:N	2.32	0.45
3:4:406:ARG:HA	3:4:409:GLU:CD	2.42	0.45
2:3:7:LYS:NZ	4:A:1252:G:OP2	2.40	0.45
3:4:125:SER:HB2	3:4:126:PRO:CD	2.47	0.45
3:4:305:ARG:HG2	3:4:306:HIS:CD2	2.52	0.45
3:4:430:VAL:O	3:4:433:VAL:N	2.50	0.45
22:S:8:LYS:HG2	22:S:13:GLN:HG2	1.99	0.45
3:4:462:THR:O	3:4:463:LEU:C	2.60	0.45
4:A:2137:A:O4'	4:A:2143:A:N6	2.50	0.45
4:A:2323:G:C6	4:A:2412:U:N3	2.84	0.45
19:P:47:ILE:HG21	19:P:112:ARG:HD3	1.99	0.45
3:4:151:PHE:CD1	3:4:311:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:327:LEU:HD21	3:4:329:ILE:HD13	1.98	0.45
3:4:391:PHE:CD1	3:4:391:PHE:N	2.83	0.45
6:C:240:THR:OG1	6:C:241:SER:N	2.50	0.45
3:4:178:GLY:C	3:4:180:GLY:N	2.73	0.45
3:4:271:LEU:HD23	3:4:271:LEU:C	2.42	0.45
3:4:317:SER:O	3:4:321:GLU:HG2	2.16	0.45
4:A:368:U:H3	4:A:434:G:H1	1.64	0.45
4:A:1194:C:C2	13:J:93:GLU:HG2	2.52	0.45
4:A:1198:C:C2	13:J:128:LYS:HE3	2.52	0.45
4:A:1582:C:N4	4:A:1583:U:O2	2.50	0.45
4:A:2321:U:O4	4:A:2414:G:O6	2.35	0.45
9:F:76:ARG:HD3	9:F:89:GLY:HA2	1.99	0.45
19:P:26:ARG:NH2	19:P:54:ASP:OD2	2.38	0.45
21:R:68:ALA:O	21:R:72:ASN:ND2	2.48	0.45
35:g:28:LYS:HD2	35:g:28:LYS:HA	1.82	0.45
3:4:89:ARG:CD	3:4:92:PRO:HA	2.47	0.45
3:4:93:ASP:OD2	3:4:94:PRO:HD2	2.17	0.45
3:4:416:ALA:HB1	3:4:455:VAL:N	2.32	0.45
3:4:459:LEU:O	3:4:460:ALA:C	2.58	0.45
4:A:1089:C:O2'	4:A:1101:A:N3	2.46	0.45
9:F:110:LEU:HA	9:F:114:ALA:HB3	1.99	0.45
13:J:102:VAL:HB	13:J:141:VAL:HG13	1.99	0.45
25:V:45:THR:OG1	25:V:46:ALA:N	2.49	0.45
3:4:323:VAL:HG11	3:4:357:TYR:HD1	1.82	0.44
4:A:2270:G:H5'	30:b:16:ARG:HG3	1.99	0.44
4:A:2348:G:N2	4:A:2394:A:OP2	2.49	0.44
4:A:3012:U:O2'	4:A:3030:A:N3	2.42	0.44
13:J:105:ASP:OD1	13:J:105:ASP:N	2.45	0.44
3:4:167:ALA:HA	3:4:170:GLU:OE2	2.18	0.44
3:4:271:LEU:HD21	3:4:273:GLU:CB	2.45	0.44
4:A:858:A:O2'	4:A:1877:U:OP1	2.35	0.44
4:A:1022:C:O2'	17:N:101:ARG:NH2	2.49	0.44
5:B:112:C:C4	5:B:113:G:H1'	2.53	0.44
8:E:47:GLN:HE21	8:E:47:GLN:HB3	1.61	0.44
25:V:77:ASP:OD1	25:V:101:ASN:ND2	2.50	0.44
27:X:72:LYS:HD3	27:X:72:LYS:HA	1.70	0.44
3:4:254:THR:OG1	36:4:501:GCP:O1G	2.27	0.44
4:A:1179:U:C2	13:J:11:ILE:HD11	2.53	0.44
4:A:1478:C:O2'	4:A:2026:A:N3	2.50	0.44
12:I:40:ARG:HD2	13:J:123:ILE:HD13	1.99	0.44
3:4:185:ARG:C	3:4:187:ALA:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:326:ASP:CB	3:4:412:GLU:OE1	2.57	0.44
4:A:576:G:O2'	23:T:56:LYS:NZ	2.34	0.44
4:A:718:C:O2'	4:A:772:U:OP1	2.31	0.44
10:G:27:LYS:HA	10:G:32:THR:HG22	1.98	0.44
11:H:30:LEU:HD13	11:H:35:LEU:HB2	1.98	0.44
12:I:3:LYS:HG3	12:I:7:ALA:HB2	1.98	0.44
13:J:128:LYS:HD2	13:J:128:LYS:HA	1.71	0.44
22:S:69:LYS:HD2	22:S:91:ARG:HG2	2.00	0.44
3:4:186:GLN:HG3	3:4:207:LYS:HZ1	1.83	0.44
3:4:383:ARG:NE	3:4:391:PHE:CZ	2.85	0.44
4:A:279:U:H2'	4:A:280:G:H8	1.83	0.44
4:A:499:G:OP2	4:A:2630:A:O2'	2.33	0.44
6:C:85:ASP:OD2	6:C:88:ARG:NH1	2.47	0.44
12:I:6:LYS:HE2	12:I:6:LYS:HB3	1.82	0.44
3:4:383:ARG:HH11	3:4:383:ARG:CB	2.31	0.44
3:4:441:ALA:H	3:4:453:ALA:HB2	1.82	0.44
4:A:886:G:O2'	4:A:1470:G:O2'	2.30	0.44
4:A:1249:G:H4'	14:K:84:LEU:HD22	1.99	0.44
4:A:1314:C:H1'	21:R:4:VAL:HG12	1.99	0.44
5:B:8:C:H2'	5:B:9:G:H4'	1.98	0.44
10:G:20:ASN:OD1	10:G:20:ASN:N	2.50	0.44
19:P:126:LYS:HE2	19:P:126:LYS:HB3	1.80	0.44
3:4:305:ARG:NH1	3:4:345:ALA:HB2	2.32	0.44
3:4:393:SER:O	3:4:394:ALA:HB3	2.17	0.44
4:A:1210:C:H3'	4:A:1211:G:C8	2.52	0.44
10:G:28:GLY:HA2	10:G:80:VAL:HG22	1.99	0.44
3:4:96:THR:O	3:4:98:ILE:N	2.49	0.44
3:4:165:SER:HA	3:4:168:GLN:CG	2.48	0.44
3:4:193:GLY:CA	4:A:2809:U:H1'	2.48	0.44
3:4:367:VAL:HG22	3:4:388:ASP:OD2	2.18	0.44
3:4:369:ASN:CG	3:4:370:LYS:N	2.74	0.44
12:I:43:LEU:HB3	12:I:92:ALA:HB1	1.99	0.44
19:P:49:VAL:O	19:P:64:SER:CA	2.66	0.44
35:g:3:THR:OG1	35:g:4:GLY:N	2.50	0.44
3:4:243:SER:O	3:4:245:ILE:HG23	2.18	0.44
3:4:248:VAL:HG23	3:4:297:LEU:HD13	2.00	0.44
3:4:371:ILE:O	3:4:373:ALA:N	2.51	0.44
4:A:998:G:H1	4:A:1009:U:H3	1.66	0.44
4:A:1708:A:H1'	4:A:1709:U:H5'	2.00	0.44
17:N:10:ARG:HG2	17:N:90:PRO:HG2	2.00	0.44
3:4:50:VAL:HG23	3:4:50:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:204:GLY:O	3:4:205:GLU:HG3	2.17	0.43
3:4:456:PRO:HG2	3:4:459:LEU:HD23	1.98	0.43
4:A:1185:A:OP1	4:A:1187:A:N6	2.50	0.43
4:A:1537:U:H2'	4:A:1538:G:C8	2.53	0.43
9:F:178:ARG:NH2	9:F:186:GLU:OE2	2.48	0.43
3:4:300:THR:CB	3:4:318:THR:HG23	2.44	0.43
3:4:369:ASN:OD1	3:4:370:LYS:HG2	2.17	0.43
4:A:1302:G:N2	4:A:1303:U:O4	2.48	0.43
4:A:2143:A:N6	4:A:2144:C:N4	2.66	0.43
4:A:2249:G:H2'	4:A:2250:A:C8	2.54	0.43
11:H:83:ASN:HB3	11:H:92:PHE:HB2	2.01	0.43
19:P:37:ARG:NE	19:P:54:ASP:OD2	2.51	0.43
23:T:11:THR:HG22	23:T:113:ILE:HG12	2.01	0.43
3:4:230:LYS:HE2	3:4:234:ASP:OD1	2.18	0.43
3:4:272:VAL:CG2	36:4:501:GCP:H5'2	2.48	0.43
3:4:327:LEU:HD12	3:4:410:LEU:HB2	2.00	0.43
3:4:381:GLN:HG2	3:4:384:ARG:HD3	2.00	0.43
3:4:426:ARG:O	3:4:428:ASP:N	2.51	0.43
3:4:440:ASP:O	3:4:441:ALA:HB3	2.17	0.43
4:A:1210:C:H3'	4:A:1211:G:H8	1.84	0.43
4:A:2070:A:H2'	4:A:2071:A:C8	2.53	0.43
5:B:9:G:N1	5:B:109:C:N3	2.66	0.43
6:C:37:LEU:HG	6:C:62:TYR:HB2	1.98	0.43
9:F:9:PRO:HG3	9:F:104:TRP:HA	2.00	0.43
12:I:31:LEU:HD13	12:I:36:LEU:HD21	1.98	0.43
12:I:94:LYS:HE2	12:I:105:ILE:HD13	1.99	0.43
12:I:95:LYS:HA	12:I:95:LYS:HD3	1.82	0.43
15:L:80:ASP:OD2	20:Q:103:ARG:NH1	2.51	0.43
3:4:167:ALA:HA	3:4:170:GLU:HG2	2.00	0.43
3:4:328:LEU:CD1	3:4:362:PRO:HB2	2.48	0.43
3:4:373:ALA:O	3:4:374:ALA:C	2.62	0.43
30:b:43:LEU:HD23	30:b:52:VAL:HG11	2.00	0.43
3:4:272:VAL:O	3:4:272:VAL:HG22	2.18	0.43
4:A:114:G:OP2	4:A:116:A:O2'	2.29	0.43
4:A:738:A:H4'	4:A:739:U:H5	1.82	0.43
4:A:1207:G:N7	13:J:118:LEU:HG	2.33	0.43
4:A:2143:A:C6	4:A:2144:C:C4	3.06	0.43
17:N:51:ARG:HD3	17:N:66:ILE:HD11	2.00	0.43
17:N:84:GLY:O	17:N:85:SER:OG	2.28	0.43
3:4:87:GLN:NE2	4:A:2133:G:C8	2.77	0.43
3:4:110:VAL:HG21	3:4:138:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:348:THR:HA	3:4:351:ASN:ND2	2.33	0.43
3:4:393:SER:O	3:4:395:ARG:N	2.44	0.43
4:A:325:U:C2	4:A:450:G:N1	2.86	0.43
4:A:1558:C:H2'	4:A:1559:A:C8	2.53	0.43
11:H:86:GLY:HA3	11:H:90:LYS:HB3	2.00	0.43
3:4:182:SER:O	3:4:186:GLN:CD	2.62	0.43
3:4:357:TYR:N	3:4:357:TYR:CD2	2.86	0.43
3:4:371:ILE:CG2	3:4:372:ASP:N	2.80	0.43
3:4:436:ASP:CB	3:4:439:VAL:HG22	2.49	0.43
3:4:441:ALA:H	3:4:453:ALA:HB1	1.83	0.43
26:W:124:VAL:HG22	26:W:181:VAL:HG22	2.00	0.43
3:4:68:ALA:O	3:4:69:GLU:C	2.58	0.43
3:4:105:GLU:OE1	3:4:105:GLU:HA	2.18	0.43
3:4:420:VAL:CG2	3:4:421:THR:H	2.25	0.43
4:A:245:G:O2'	4:A:472:C:O2	2.35	0.43
4:A:314:G:O2'	4:A:321:G:O2'	2.36	0.43
4:A:546:G:O2'	4:A:557:G:O6	2.32	0.43
4:A:2017:C:OP2	6:C:183:ARG:NH2	2.40	0.43
8:E:13:LYS:HB3	8:E:13:LYS:HE3	1.88	0.43
10:G:164:ARG:HG3	10:G:165:TYR:H	1.84	0.43
12:I:17:PHE:O	12:I:109:TYR:OH	2.33	0.43
26:W:50:ASN:O	26:W:54:PHE:HB2	2.19	0.43
3:4:254:THR:O	3:4:255:ASN:HB2	2.19	0.43
3:4:289:PHE:CD2	3:4:404:ARG:HG2	2.54	0.43
4:A:1172:A:H62	4:A:1203:A:N6	2.17	0.43
4:A:2138:C:N4	4:A:2141:U:O4	2.52	0.43
8:E:183:LEU:HD23	8:E:183:LEU:HA	1.87	0.43
19:P:76:ASP:HB3	19:P:80:HIS:HA	2.01	0.43
3:4:85:LEU:HD21	3:4:106:LEU:CD2	2.49	0.43
3:4:316:ARG:O	3:4:320:GLU:HG3	2.18	0.43
3:4:426:ARG:CG	3:4:427:GLY:N	2.81	0.43
5:B:81:U:H2'	5:B:82:A:C8	2.53	0.43
10:G:46:ALA:HB3	10:G:50:ALA:HB3	2.00	0.43
19:P:41:ASN:N	19:P:49:VAL:HG22	2.34	0.43
3:4:46:LEU:O	3:4:47:GLU:CB	2.65	0.42
3:4:295:PHE:CE1	3:4:407:MET:SD	3.13	0.42
4:A:21:G:O2'	23:T:85:GLU:O	2.31	0.42
4:A:1668:C:O2'	4:A:1764:A:N3	2.42	0.42
12:I:115:LEU:HD21	12:I:123:ILE:HD12	2.01	0.42
3:4:431:ALA:C	3:4:432:ARG:HD3	2.44	0.42
3:4:435:THR:HG23	3:4:435:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2552:A:H2'	4:A:2553:G:C8	2.54	0.42
4:A:2970:U:H4'	10:G:139:LYS:HB2	2.02	0.42
3:4:82:LEU:CD1	3:4:113:THR:HB	2.40	0.42
4:A:759:G:N1	27:X:64:PRO:HB3	2.34	0.42
4:A:2083:A:N6	4:A:2099:G:O2'	2.51	0.42
4:A:2135:U:C5	4:A:2137:A:H8	2.37	0.42
4:A:2204:G:O2'	4:A:2206:C:OP2	2.37	0.42
4:A:2323:G:N1	4:A:2412:U:N3	2.68	0.42
4:A:2340:A:N6	4:A:2388:G:O6	2.44	0.42
4:A:2515:U:H2'	4:A:2516:U:C6	2.53	0.42
4:A:2967:C:OP1	34:f:33:LYS:NZ	2.52	0.42
8:E:2:THR:OG1	8:E:20:LEU:O	2.37	0.42
22:S:80:ASN:OD1	22:S:80:ASN:N	2.51	0.42
27:X:50:ASN:HD22	27:X:50:ASN:HA	1.67	0.42
3:4:357:TYR:N	3:4:357:TYR:HD2	2.17	0.42
3:4:426:ARG:HE	3:4:430:VAL:CG1	2.25	0.42
3:4:434:HIS:CB	4:A:1185:A:H1'	2.37	0.42
4:A:745:G:H5'	33:e:19:THR:HG23	2.00	0.42
4:A:2116:C:H2'	4:A:2117:C:H6	1.84	0.42
4:A:2529:A:H2'	4:A:2530:C:C6	2.54	0.42
4:A:2879:G:O2'	4:A:2888:G:O6	2.37	0.42
3:4:133:GLU:O	3:4:137:LYS:HA	2.19	0.42
3:4:199:GLY:CA	3:4:201:ARG:CZ	2.97	0.42
4:A:2973:A:H4'	10:G:63:ARG:HG2	2.01	0.42
9:F:56:LEU:HD13	9:F:56:LEU:HA	1.88	0.42
11:H:100:VAL:HG12	11:H:119:LEU:HD12	2.01	0.42
19:P:44:ALA:O	19:P:112:ARG:NH1	2.52	0.42
19:P:79:ALA:O	19:P:81:SER:N	2.53	0.42
35:g:12:THR:HG22	35:g:31:GLY:HA2	2.01	0.42
3:4:124:LEU:HD13	3:4:142:ASP:HB3	2.00	0.42
3:4:321:GLU:O	3:4:322:VAL:C	2.61	0.42
3:4:443:GLU:CB	3:4:452:LYS:HB2	2.50	0.42
4:A:1690:A:H2'	4:A:1691:A:C8	2.54	0.42
4:A:2527:G:H2'	4:A:2528:G:C8	2.55	0.42
4:A:2753:G:H5''	4:A:2754:G:H5''	2.02	0.42
9:F:23:LEU:HD21	9:F:172:GLU:HG3	2.01	0.42
3:4:116:ASP:C	3:4:117:THR:HG23	2.44	0.42
3:4:245:ILE:HG21	3:4:294:PRO:HG2	1.99	0.42
3:4:250:ILE:HG23	3:4:250:ILE:O	2.19	0.42
3:4:463:LEU:O	3:4:464:ARG:C	2.62	0.42
4:A:1212:U:H2'	4:A:1213:A:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1479:G:H4'	4:A:2025:C:H5	1.85	0.42
18:O:38:GLU:OE1	18:O:42:ARG:NH2	2.47	0.42
3:4:55:TRP:O	3:4:55:TRP:CD1	2.73	0.42
3:4:327:LEU:C	3:4:327:LEU:HD23	2.45	0.42
3:4:390:VAL:C	3:4:392:VAL:H	2.28	0.42
4:A:928:U:H2'	4:A:929:C:C6	2.54	0.42
4:A:1621:C:H2'	4:A:1622:G:H4'	2.01	0.42
4:A:1728:U:H4'	4:A:1729:A:H5'	2.02	0.42
19:P:111:GLY:H	19:P:114:ALA:HB3	1.85	0.42
3:4:143:ARG:NH2	3:4:305:ARG:O	2.51	0.42
4:A:1179:U:H2'	13:J:13:LEU:HA	2.01	0.42
4:A:1619:U:H2'	4:A:1620:U:C2	2.55	0.42
16:M:104:VAL:HG11	16:M:110:VAL:HG13	2.02	0.42
31:c:40:LYS:HB3	31:c:40:LYS:HE3	1.82	0.42
3:4:93:ASP:HA	3:4:94:PRO:HD3	1.91	0.42
3:4:246:PRO:HA	3:4:326:ASP:OD2	2.20	0.42
3:4:283:THR:CG2	3:4:299:ASP:HB3	2.49	0.42
3:4:291:ASP:OD2	3:4:293:ARG:HG3	2.20	0.42
4:A:389:G:H21	4:A:412:A:H61	1.65	0.42
4:A:857:U:H2'	4:A:858:A:C8	2.54	0.42
4:A:960:G:OP2	4:A:960:G:N2	2.47	0.42
6:C:222:ARG:HE	6:C:222:ARG:HB2	1.67	0.42
6:C:258:ARG:NH2	6:C:264:SER:OG	2.53	0.42
12:I:33:VAL:HG21	13:J:117:ASP:HB2	2.02	0.42
3:4:445:THR:HG23	3:4:450:ARG:H	1.84	0.41
6:C:163:ILE:HD12	6:C:175:LEU:HB3	2.01	0.41
11:H:119:LEU:HA	11:H:132:VAL:HG21	2.01	0.41
12:I:101:LYS:HD2	12:I:101:LYS:HA	1.78	0.41
26:W:86:HIS:CD2	26:W:87:PRO:HD2	2.55	0.41
3:4:410:LEU:HD12	3:4:410:LEU:N	2.34	0.41
4:A:919:A:OP1	16:M:44:LYS:NZ	2.40	0.41
4:A:1000:C:O2	4:A:1008:G:N1	2.53	0.41
5:B:9:G:H2'	5:B:10:G:C4	2.54	0.41
3:4:56:THR:HG23	3:4:57:GLU:OE2	2.21	0.41
3:4:319:LEU:HD12	3:4:319:LEU:N	2.35	0.41
3:4:424:TYR:CD1	3:4:424:TYR:N	2.88	0.41
4:A:570:U:O2'	25:V:47:VAL:O	2.34	0.41
4:A:1008:G:H2'	4:A:1009:U:C6	2.55	0.41
5:B:9:G:H5'	5:B:10:G:C8	2.56	0.41
6:C:132:PRO:HA	6:C:190:ARG:HA	2.01	0.41
6:C:147:LEU:HD23	6:C:147:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:2:PRO:HB2	14:K:3:THR:H	1.60	0.41
19:P:56:ASN:OD1	19:P:56:ASN:N	2.51	0.41
25:V:40:ARG:HD3	25:V:61:THR:HG22	2.02	0.41
26:W:177:LEU:HD23	26:W:180:ASN:HB3	2.02	0.41
29:Z:11:ARG:O	29:Z:64:ARG:NH2	2.53	0.41
34:f:4:ASN:OD1	34:f:4:ASN:N	2.51	0.41
1:2:40:ASN:OD1	1:2:40:ASN:N	2.52	0.41
3:4:287:GLY:C	3:4:295:PHE:CD2	2.98	0.41
4:A:239:U:O2'	4:A:716:G:O2'	2.31	0.41
4:A:264:G:H4'	4:A:516:G:H22	1.85	0.41
8:E:9:THR:HG22	8:E:128:THR:HG21	2.02	0.41
8:E:152:LYS:HG3	8:E:153:LYS:HG2	2.02	0.41
12:I:26:THR:H	12:I:78:ALA:HB3	1.86	0.41
19:P:50:GLN:HA	19:P:63:ALA:C	2.45	0.41
19:P:87:LEU:HD23	19:P:87:LEU:HA	1.86	0.41
3:4:106:LEU:C	3:4:109:VAL:HG22	2.46	0.41
3:4:187:ALA:HB2	4:A:2826:A:N7	2.35	0.41
3:4:327:LEU:HD21	3:4:329:ILE:HD11	2.02	0.41
3:4:372:ASP:N	3:4:374:ALA:H	2.18	0.41
3:4:386:LEU:HD23	3:4:386:LEU:HA	1.76	0.41
3:4:116:ASP:C	3:4:117:THR:CG2	2.94	0.41
3:4:169:MET:HE3	3:4:219:MET:HG2	2.03	0.41
3:4:386:LEU:HA	3:4:387:PRO:HD3	1.89	0.41
3:4:429:LEU:HD13	3:4:429:LEU:HA	1.70	0.41
5:B:9:G:H2'	5:B:10:G:N9	2.36	0.41
6:C:79:VAL:HG22	6:C:115:ASP:H	1.86	0.41
7:D:125:GLY:O	7:D:129:ARG:HB3	2.20	0.41
3:4:173:LEU:C	3:4:175:ARG:H	2.29	0.41
3:4:284:THR:HG22	3:4:298:THR:HG23	2.02	0.41
3:4:308:PRO:HG2	3:4:311:LEU:HD21	2.01	0.41
4:A:1548:C:O2'	4:A:1549:G:O4'	2.36	0.41
5:B:27:A:N3	5:B:115:A:O2'	2.53	0.41
8:E:42:LEU:HD23	8:E:42:LEU:HA	1.94	0.41
9:F:110:LEU:HD23	9:F:114:ALA:HB3	2.03	0.41
12:I:3:LYS:HE3	12:I:59:ARG:HH11	1.85	0.41
3:4:184:SER:O	3:4:185:ARG:HB2	2.20	0.41
3:4:186:GLN:CB	3:4:207:LYS:NZ	2.83	0.41
3:4:198:VAL:O	4:A:2286:A:N6	2.54	0.41
3:4:257:GLY:HA2	36:4:501:GCP:O5'	2.21	0.41
4:A:1758:G:O2'	4:A:1759:A:O4'	2.36	0.41
10:G:33:LEU:HB3	10:G:76:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:35:VAL:HG13	35:g:37:VAL:H	1.85	0.41
1:2:47:ILE:O	1:2:51:HIS:HB3	2.21	0.41
3:4:47:GLU:CA	3:4:79:SER:HB3	2.51	0.41
3:4:202:GLY:CA	4:A:2676:C:O4'	2.67	0.41
3:4:237:ARG:HE	3:4:240:ARG:NH2	2.19	0.41
4:A:1180:G:O6	4:A:1206:A:O2'	2.37	0.41
4:A:2902:A:H2'	4:A:2903:A:C8	2.56	0.41
3:4:43:GLN:HA	3:4:43:GLN:HE21	1.85	0.41
3:4:148:LEU:HA	3:4:311:LEU:CD1	2.49	0.41
3:4:199:GLY:CA	3:4:201:ARG:CD	2.98	0.41
3:4:337:VAL:HG23	3:4:338:ASN:H	1.86	0.41
4:A:368:U:O2	4:A:434:G:N2	2.44	0.41
4:A:745:G:OP1	33:e:19:THR:OG1	2.37	0.41
3:4:141:ILE:HG22	3:4:145:ALA:HB3	2.04	0.40
3:4:440:ASP:HB3	3:4:453:ALA:HA	2.03	0.40
4:A:159:A:N3	4:A:2431:C:O2'	2.42	0.40
4:A:1885:G:O2'	4:A:2215:U:O4	2.34	0.40
4:A:2314:U:H4'	28:Y:56:ILE:HD11	2.03	0.40
8:E:101:ARG:HH11	8:E:101:ARG:HD3	1.76	0.40
14:K:92:LEU:HA	14:K:92:LEU:HD23	1.89	0.40
20:Q:3:THR:HG23	20:Q:4:LEU:HG	2.02	0.40
3:4:250:ILE:CG2	3:4:299:ASP:HA	2.51	0.40
3:4:261:LEU:HD13	3:4:261:LEU:HA	1.93	0.40
3:4:371:ILE:CG2	3:4:391:PHE:CD2	3.03	0.40
4:A:2905:C:OP2	7:D:119:LYS:NZ	2.52	0.40
28:Y:5:CYS:SG	28:Y:8:CYS:N	2.75	0.40
31:c:28:ASN:HB3	31:c:31:ASN:HB2	2.02	0.40
3:4:42:ARG:NH1	3:4:44:LEU:CB	2.79	0.40
3:4:52:VAL:HG12	3:4:106:LEU:HD11	2.03	0.40
3:4:215:ILE:HG23	3:4:216:ARG:N	2.35	0.40
3:4:288:GLU:HA	3:4:295:PHE:HD2	1.87	0.40
4:A:2526:U:O2'	9:F:130:ASP:O	2.40	0.40
16:M:137:ILE:HG21	16:M:144:ALA:HB2	2.03	0.40
26:W:109:GLU:HG2	26:W:130:THR:HB	2.04	0.40
3:4:114:GLY:O	3:4:115:ALA:C	2.64	0.40
3:4:371:ILE:CG2	3:4:372:ASP:H	2.28	0.40
4:A:978:A:H2'	4:A:979:G:H8	1.86	0.40
4:A:1007:G:N1	4:A:1008:G:N3	2.70	0.40
4:A:2599:G:N2	4:A:2601:A:O2'	2.55	0.40
9:F:43:VAL:HG13	9:F:161:ILE:HG22	2.02	0.40
14:K:7:LYS:HD3	14:K:7:LYS:HA	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:50:GLN:HB2	19:P:63:ALA:N	2.36	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	2	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
2	3	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
3	4	424/470 (90%)	343 (81%)	79 (19%)	2 (0%)	24	54
6	C	273/278 (98%)	258 (94%)	15 (6%)	0	100	100
7	D	212/217 (98%)	196 (92%)	16 (8%)	0	100	100
8	E	207/215 (96%)	192 (93%)	15 (7%)	0	100	100
9	F	180/187 (96%)	146 (81%)	34 (19%)	0	100	100
10	G	174/179 (97%)	151 (87%)	23 (13%)	0	100	100
11	H	149/151 (99%)	110 (74%)	39 (26%)	0	100	100
12	I	124/175 (71%)	108 (87%)	16 (13%)	0	100	100
13	J	131/142 (92%)	100 (76%)	31 (24%)	0	100	100
14	K	144/147 (98%)	137 (95%)	7 (5%)	0	100	100
15	L	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
16	M	143/147 (97%)	130 (91%)	13 (9%)	0	100	100
17	N	134/138 (97%)	124 (92%)	10 (8%)	0	100	100
18	O	116/199 (58%)	107 (92%)	9 (8%)	0	100	100
19	P	124/127 (98%)	88 (71%)	36 (29%)	0	100	100
20	Q	111/113 (98%)	95 (86%)	16 (14%)	0	100	100
21	R	122/129 (95%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	S	98/103 (95%)	92 (94%)	6 (6%)	0	100	100
23	T	112/153 (73%)	110 (98%)	2 (2%)	0	100	100
24	U	95/100 (95%)	90 (95%)	5 (5%)	0	100	100
25	V	93/105 (89%)	82 (88%)	11 (12%)	0	100	100
26	W	190/215 (88%)	170 (90%)	20 (10%)	0	100	100
27	X	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
28	Y	61/64 (95%)	55 (90%)	6 (10%)	0	100	100
29	Z	62/77 (80%)	62 (100%)	0	0	100	100
30	b	52/57 (91%)	52 (100%)	0	0	100	100
31	c	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
32	d	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
33	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
34	f	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	g	46/75 (61%)	41 (89%)	5 (11%)	0	100	100
All	All	4039/4461 (90%)	3594 (89%)	443 (11%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	294	PRO
3	4	431	ALA

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	2	52/54 (96%)	52 (100%)	0	100	100
2	3	18/19 (95%)	18 (100%)	0	100	100
3	4	337/372 (91%)	309 (92%)	28 (8%)	10	32
6	C	215/218 (99%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	160/163 (98%)	158 (99%)	2 (1%)	61	73
8	E	169/173 (98%)	169 (100%)	0	100	100
9	F	151/156 (97%)	150 (99%)	1 (1%)	76	79
10	G	148/150 (99%)	147 (99%)	1 (1%)	76	79
11	H	90/116 (78%)	89 (99%)	1 (1%)	65	75
12	I	89/120 (74%)	89 (100%)	0	100	100
13	J	102/108 (94%)	102 (100%)	0	100	100
14	K	119/120 (99%)	118 (99%)	1 (1%)	73	78
15	L	100/100 (100%)	100 (100%)	0	100	100
16	M	112/114 (98%)	112 (100%)	0	100	100
17	N	114/116 (98%)	113 (99%)	1 (1%)	70	77
18	O	97/158 (61%)	97 (100%)	0	100	100
19	P	93/94 (99%)	87 (94%)	6 (6%)	15	40
20	Q	100/100 (100%)	100 (100%)	0	100	100
21	R	97/99 (98%)	96 (99%)	1 (1%)	68	76
22	S	81/83 (98%)	78 (96%)	3 (4%)	30	57
23	T	90/117 (77%)	89 (99%)	1 (1%)	65	75
24	U	83/85 (98%)	83 (100%)	0	100	100
25	V	81/86 (94%)	80 (99%)	1 (1%)	63	74
26	W	155/168 (92%)	154 (99%)	1 (1%)	78	80
27	X	58/63 (92%)	57 (98%)	1 (2%)	53	70
28	Y	50/51 (98%)	49 (98%)	1 (2%)	48	68
29	Z	58/66 (88%)	57 (98%)	1 (2%)	53	70
30	b	43/46 (94%)	43 (100%)	0	100	100
31	c	47/52 (90%)	47 (100%)	0	100	100
32	d	35/36 (97%)	35 (100%)	0	100	100
33	e	53/54 (98%)	53 (100%)	0	100	100
34	f	35/35 (100%)	33 (94%)	2 (6%)	18	45
35	g	43/63 (68%)	43 (100%)	0	100	100
All	All	3275/3555 (92%)	3222 (98%)	53 (2%)	54	71

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	46	LEU
3	4	56	THR
3	4	57	GLU
3	4	85	LEU
3	4	98	ILE
3	4	137	LYS
3	4	140	VAL
3	4	147	ILE
3	4	148	LEU
3	4	172	MET
3	4	186	GLN
3	4	226	ILE
3	4	274	ASN
3	4	279	THR
3	4	283	THR
3	4	295	PHE
3	4	311	LEU
3	4	353	VAL
3	4	384	ARG
3	4	386	LEU
3	4	391	PHE
3	4	429	LEU
3	4	430	VAL
3	4	438	HIS
3	4	439	VAL
3	4	446	ASP
3	4	450	ARG
3	4	465	GLU
7	D	26	VAL
7	D	156	THR
9	F	74	VAL
10	G	36	ASP
11	H	38	VAL
14	K	64	VAL
17	N	83	MET
19	P	47	ILE
19	P	50	GLN
19	P	51	LEU
19	P	52	VAL
19	P	108	THR
19	P	113	ILE
21	R	4	VAL
22	S	60	VAL

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Mol	Chain	Res	Type
22	S	64	VAL
22	S	73	ILE
23	T	81	VAL
25	V	44	HIS
26	W	99	VAL
27	X	67	VAL
28	Y	5	CYS
29	Z	58	TYR
34	f	3	VAL
34	f	23	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	33	GLN
2	3	13	HIS
3	4	43	GLN
3	4	87	GLN
3	4	128	GLN
3	4	154	HIS
3	4	434	HIS
3	4	444	HIS
6	C	91	ASN
6	C	261	ASN
7	D	34	ASN
7	D	76	ASN
7	D	80	HIS
7	D	189	ASN
8	E	100	GLN
9	F	58	ASN
9	F	62	ASN
10	G	86	GLN
10	G	169	GLN
11	H	102	ASN
11	H	118	GLN
12	I	54	ASN
13	J	21	ASN
13	J	36	ASN
13	J	88	GLN
14	K	77	HIS
14	K	119	GLN
14	K	144	GLN

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Mol	Chain	Res	Type
15	L	91	ASN
16	M	69	ASN
16	M	76	GLN
16	M	84	ASN
16	M	127	ASN
17	N	55	ASN
18	O	77	HIS
19	P	16	ASN
19	P	53	ASN
21	R	27	GLN
21	R	39	GLN
22	S	76	HIS
22	S	90	HIS
23	T	67	ASN
23	T	109	HIS
24	U	41	GLN
26	W	14	ASN
26	W	46	HIS
26	W	126	GLN
27	X	44	HIS
27	X	50	ASN
35	g	40	GLN
35	g	42	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	3118/3120 (99%)	760 (24%)	22 (0%)
5	B	117/118 (99%)	37 (31%)	2 (1%)
All	All	3235/3238 (99%)	797 (24%)	24 (0%)

All (797) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	7	U
4	A	9	U
4	A	11	A
4	A	12	G
4	A	20	G
4	A	31	U
4	A	32	G

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Mol	Chain	Res	Type
4	A	33	G
4	A	42	G
4	A	46	A
4	A	48	G
4	A	55	G
4	A	58	G
4	A	60	A
4	A	68	A
4	A	71	A
4	A	72	G
4	A	80	G
4	A	81	A
4	A	88	A
4	A	91	C
4	A	94	G
4	A	95	C
4	A	98	U
4	A	99	G
4	A	107	G
4	A	115	A
4	A	116	A
4	A	117	U
4	A	122	A
4	A	125	C
4	A	137	G
4	A	162	A
4	A	164	A
4	A	180	A
4	A	195	A
4	A	198	A
4	A	200	C
4	A	203	A
4	A	212	A
4	A	214	G
4	A	215	A
4	A	220	A
4	A	221	A
4	A	227	A
4	A	229	U
4	A	230	G
4	A	241	A
4	A	248	G

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Mol	Chain	Res	Type
4	A	266	U
4	A	267	G
4	A	273	A
4	A	274	C
4	A	276	G
4	A	280	G
4	A	281	C
4	A	286	G
4	A	288	U
4	A	289	A
4	A	290	C
4	A	292	G
4	A	296	A
4	A	299	G
4	A	300	G
4	A	302	U
4	A	303	G
4	A	305	G
4	A	306	U
4	A	307	G
4	A	309	G
4	A	314	G
4	A	315	U
4	A	316	U
4	A	317	G
4	A	318	U
4	A	319	G
4	A	325	U
4	A	326	A
4	A	327	U
4	A	329	U
4	A	330	U
4	A	331	U
4	A	334	G
4	A	337	U
4	A	338	C
4	A	340	A
4	A	341	C
4	A	342	C
4	A	344	G
4	A	351	G
4	A	357	U

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Mol	Chain	Res	Type
4	A	358	G
4	A	361	A
4	A	363	A
4	A	364	A
4	A	366	G
4	A	370	U
4	A	371	G
4	A	382	A
4	A	384	G
4	A	391	G
4	A	393	U
4	A	399	G
4	A	405	G
4	A	412	A
4	A	413	G
4	A	415	G
4	A	416	C
4	A	427	A
4	A	437	G
4	A	438	U
4	A	441	G
4	A	445	U
4	A	446	G
4	A	451	U
4	A	453	U
4	A	460	G
4	A	474	G
4	A	489	A
4	A	492	C
4	A	493	U
4	A	494	G
4	A	511	A
4	A	512	G
4	A	543	U
4	A	544	U
4	A	555	G
4	A	563	U
4	A	566	A
4	A	567	A
4	A	569	G
4	A	570	U
4	A	571	A

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Mol	Chain	Res	Type
4	A	572	C
4	A	573	C
4	A	578	G
4	A	581	G
4	A	591	G
4	A	592	A
4	A	593	G
4	A	594	U
4	A	595	A
4	A	596	C
4	A	605	G
4	A	612	U
4	A	617	U
4	A	618	C
4	A	619	C
4	A	620	G
4	A	633	A
4	A	635	G
4	A	636	U
4	A	637	G
4	A	639	C
4	A	640	G
4	A	642	G
4	A	644	G
4	A	655	G
4	A	665	G
4	A	667	A
4	A	678	A
4	A	679	G
4	A	684	G
4	A	696	A
4	A	706	G
4	A	707	G
4	A	708	G
4	A	709	U
4	A	721	A
4	A	725	A
4	A	728	G
4	A	731	A
4	A	736	G
4	A	737	A
4	A	739	U

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Mol	Chain	Res	Type
4	A	740	A
4	A	742	G
4	A	747	A
4	A	748	U
4	A	757	G
4	A	758	A
4	A	759	G
4	A	760	U
4	A	763	G
4	A	765	G
4	A	766	G
4	A	768	G
4	A	769	U
4	A	801	U
4	A	826	G
4	A	830	A
4	A	831	A
4	A	842	A
4	A	843	G
4	A	845	C
4	A	862	U
4	A	868	C
4	A	872	G
4	A	877	U
4	A	879	A
4	A	880	G
4	A	890	G
4	A	891	G
4	A	897	A
4	A	899	G
4	A	904	A
4	A	908	A
4	A	919	A
4	A	920	G
4	A	927	C
4	A	942	U
4	A	944	A
4	A	974	G
4	A	975	U
4	A	981	U
4	A	982	A
4	A	990	G

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Mol	Chain	Res	Type
4	A	994	A
4	A	995	U
4	A	996	G
4	A	1001	C
4	A	1002	C
4	A	1004	C
4	A	1005	A
4	A	1006	G
4	A	1008	G
4	A	1010	U
4	A	1011	A
4	A	1012	C
4	A	1014	G
4	A	1016	C
4	A	1025	A
4	A	1027	C
4	A	1046	C
4	A	1047	A
4	A	1048	A
4	A	1049	G
4	A	1063	G
4	A	1074	A
4	A	1076	A
4	A	1078	G
4	A	1085	G
4	A	1091	A
4	A	1092	G
4	A	1097	A
4	A	1101	A
4	A	1114	G
4	A	1127	A
4	A	1130	C
4	A	1131	G
4	A	1143	G
4	A	1144	A
4	A	1148	G
4	A	1151	U
4	A	1156	A
4	A	1162	G
4	A	1163	A
4	A	1164	A
4	A	1165	G

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Mol	Chain	Res	Type
4	A	1167	C
4	A	1171	C
4	A	1172	A
4	A	1173	G
4	A	1174	G
4	A	1175	A
4	A	1176	G
4	A	1178	U
4	A	1179	U
4	A	1180	G
4	A	1181	G
4	A	1182	C
4	A	1184	U
4	A	1185	A
4	A	1186	G
4	A	1187	A
4	A	1188	A
4	A	1190	C
4	A	1191	A
4	A	1195	A
4	A	1196	C
4	A	1197	C
4	A	1198	C
4	A	1199	U
4	A	1200	U
4	A	1201	G
4	A	1202	A
4	A	1203	A
4	A	1204	A
4	A	1205	G
4	A	1206	A
4	A	1207	G
4	A	1212	U
4	A	1213	A
4	A	1214	A
4	A	1216	A
4	A	1217	G
4	A	1219	U
4	A	1222	C
4	A	1225	G
4	A	1226	U
4	A	1227	C

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Mol	Chain	Res	Type
4	A	1228	A
4	A	1229	A
4	A	1230	G
4	A	1231	U
4	A	1236	G
4	A	1237	U
4	A	1238	G
4	A	1239	C
4	A	1240	G
4	A	1246	A
4	A	1248	U
4	A	1251	A
4	A	1253	C
4	A	1254	G
4	A	1260	C
4	A	1261	A
4	A	1270	G
4	A	1275	A
4	A	1292	U
4	A	1293	G
4	A	1332	G
4	A	1343	G
4	A	1344	A
4	A	1353	G
4	A	1362	A
4	A	1365	G
4	A	1371	G
4	A	1377	A
4	A	1380	A
4	A	1386	G
4	A	1387	A
4	A	1389	U
4	A	1399	A
4	A	1401	A
4	A	1402	A
4	A	1404	C
4	A	1415	A
4	A	1416	A
4	A	1436	C
4	A	1444	U
4	A	1456	G
4	A	1465	C

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Mol	Chain	Res	Type
4	A	1467	U
4	A	1480	A
4	A	1493	A
4	A	1494	U
4	A	1499	A
4	A	1508	A
4	A	1510	A
4	A	1518	A
4	A	1522	G
4	A	1530	G
4	A	1531	C
4	A	1532	G
4	A	1533	U
4	A	1535	C
4	A	1536	A
4	A	1538	G
4	A	1542	A
4	A	1546	A
4	A	1548	C
4	A	1549	G
4	A	1550	G
4	A	1551	U
4	A	1553	C
4	A	1556	A
4	A	1564	A
4	A	1566	A
4	A	1567	C
4	A	1573	U
4	A	1574	G
4	A	1575	A
4	A	1577	C
4	A	1578	G
4	A	1580	A
4	A	1582	C
4	A	1583	U
4	A	1584	U
4	A	1585	U
4	A	1586	C
4	A	1587	G
4	A	1588	G
4	A	1589	G
4	A	1592	G

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Mol	Chain	Res	Type
4	A	1593	U
4	A	1597	G
4	A	1598	U
4	A	1599	U
4	A	1600	G
4	A	1601	G
4	A	1603	G
4	A	1608	U
4	A	1609	G
4	A	1610	C
4	A	1616	A
4	A	1617	C
4	A	1618	C
4	A	1619	U
4	A	1621	C
4	A	1622	G
4	A	1623	U
4	A	1624	U
4	A	1625	G
4	A	1628	A
4	A	1629	G
4	A	1630	U
4	A	1632	G
4	A	1636	A
4	A	1638	C
4	A	1640	A
4	A	1648	A
4	A	1649	C
4	A	1670	G
4	A	1671	U
4	A	1673	A
4	A	1674	G
4	A	1676	G
4	A	1678	U
4	A	1679	A
4	A	1681	U
4	A	1688	G
4	A	1703	G
4	A	1708	A
4	A	1709	U
4	A	1710	A
4	A	1713	U

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Mol	Chain	Res	Type
4	A	1716	A
4	A	1717	U
4	A	1718	C
4	A	1723	U
4	A	1728	U
4	A	1730	U
4	A	1731	A
4	A	1737	A
4	A	1744	A
4	A	1746	G
4	A	1754	G
4	A	1756	G
4	A	1757	U
4	A	1759	A
4	A	1767	U
4	A	1768	C
4	A	1769	G
4	A	1777	U
4	A	1778	A
4	A	1786	G
4	A	1787	A
4	A	1789	A
4	A	1798	U
4	A	1803	A
4	A	1813	C
4	A	1825	C
4	A	1826	A
4	A	1835	C
4	A	1844	A
4	A	1847	U
4	A	1848	A
4	A	1851	G
4	A	1852	A
4	A	1864	U
4	A	1866	C
4	A	1871	G
4	A	1872	A
4	A	1892	G
4	A	1893	C
4	A	1904	C
4	A	1911	U
4	A	1912	C

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Mol	Chain	Res	Type
4	A	1916	A
4	A	1931	A
4	A	1940	A
4	A	1941	A
4	A	1942	G
4	A	1943	C
4	A	1945	U
4	A	1946	U
4	A	1947	U
4	A	1948	A
4	A	1949	C
4	A	1955	A
4	A	1961	G
4	A	1972	A
4	A	1973	C
4	A	1975	A
4	A	1981	U
4	A	1990	A
4	A	1999	U
4	A	2017	C
4	A	2018	G
4	A	2026	A
4	A	2033	U
4	A	2046	A
4	A	2075	G
4	A	2083	A
4	A	2085	C
4	A	2086	U
4	A	2089	C
4	A	2092	U
4	A	2093	G
4	A	2094	G
4	A	2095	G
4	A	2107	G
4	A	2113	A
4	A	2128	G
4	A	2130	G
4	A	2131	G
4	A	2132	U
4	A	2133	G
4	A	2134	G
4	A	2135	U

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Mol	Chain	Res	Type
4	A	2136	A
4	A	2137	A
4	A	2138	C
4	A	2139	U
4	A	2140	A
4	A	2141	U
4	A	2142	A
4	A	2145	C
4	A	2146	A
4	A	2147	U
4	A	2148	C
4	A	2151	A
4	A	2152	A
4	A	2153	G
4	A	2154	G
4	A	2160	A
4	A	2161	A
4	A	2162	A
4	A	2163	U
4	A	2179	U
4	A	2187	U
4	A	2190	A
4	A	2191	C
4	A	2194	A
4	A	2195	U
4	A	2196	G
4	A	2215	U
4	A	2216	G
4	A	2217	U
4	A	2221	A
4	A	2227	A
4	A	2246	U
4	A	2247	A
4	A	2251	G
4	A	2254	A
4	A	2255	A
4	A	2256	G
4	A	2257	A
4	A	2263	G
4	A	2267	C
4	A	2276	G
4	A	2279	C

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Mol	Chain	Res	Type
4	A	2280	G
4	A	2284	A
4	A	2285	G
4	A	2286	A
4	A	2310	G
4	A	2316	G
4	A	2320	C
4	A	2321	U
4	A	2323	G
4	A	2326	A
4	A	2327	C
4	A	2329	G
4	A	2330	U
4	A	2332	U
4	A	2333	G
4	A	2334	U
4	A	2335	G
4	A	2336	U
4	A	2339	G
4	A	2340	A
4	A	2341	U
4	A	2342	A
4	A	2343	G
4	A	2345	U
4	A	2346	G
4	A	2348	G
4	A	2350	G
4	A	2351	A
4	A	2353	U
4	A	2354	G
4	A	2355	U
4	A	2356	G
4	A	2357	A
4	A	2358	A
4	A	2362	C
4	A	2363	A
4	A	2365	A
4	A	2366	C
4	A	2367	G
4	A	2368	C
4	A	2369	C
4	A	2371	G

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Mol	Chain	Res	Type
4	A	2374	U
4	A	2376	G
4	A	2379	G
4	A	2380	G
4	A	2381	A
4	A	2382	G
4	A	2384	C
4	A	2385	G
4	A	2386	U
4	A	2387	U
4	A	2388	G
4	A	2389	U
4	A	2390	U
4	A	2391	G
4	A	2392	A
4	A	2393	A
4	A	2394	A
4	A	2395	U
4	A	2396	A
4	A	2398	C
4	A	2399	A
4	A	2400	C
4	A	2401	U
4	A	2402	C
4	A	2403	U
4	A	2405	A
4	A	2407	C
4	A	2410	A
4	A	2413	G
4	A	2421	A
4	A	2422	A
4	A	2434	A
4	A	2446	G
4	A	2449	A
4	A	2462	G
4	A	2463	G
4	A	2467	U
4	A	2470	A
4	A	2474	G
4	A	2475	G
4	A	2476	G
4	A	2483	G

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Mol	Chain	Res	Type
4	A	2490	A
4	A	2492	A
4	A	2503	G
4	A	2506	G
4	A	2507	C
4	A	2511	A
4	A	2516	U
4	A	2528	G
4	A	2529	A
4	A	2531	G
4	A	2532	G
4	A	2533	C
4	A	2534	A
4	A	2535	A
4	A	2536	U
4	A	2538	A
4	A	2544	U
4	A	2545	G
4	A	2549	G
4	A	2559	A
4	A	2567	U
4	A	2569	G
4	A	2571	C
4	A	2572	U
4	A	2574	C
4	A	2582	A
4	A	2585	U
4	A	2600	A
4	A	2601	A
4	A	2602	A
4	A	2607	G
4	A	2609	A
4	A	2620	G
4	A	2630	A
4	A	2631	G
4	A	2646	C
4	A	2647	U
4	A	2649	A
4	A	2653	G
4	A	2654	A
4	A	2655	U
4	A	2656	A

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Mol	Chain	Res	Type
4	A	2657	A
4	A	2659	A
4	A	2665	C
4	A	2672	A
4	A	2676	C
4	A	2683	A
4	A	2694	G
4	A	2698	C
4	A	2700	A
4	A	2702	A
4	A	2715	U
4	A	2718	G
4	A	2726	G
4	A	2728	U
4	A	2729	G
4	A	2742	A
4	A	2744	C
4	A	2749	G
4	A	2753	G
4	A	2759	G
4	A	2780	C
4	A	2786	U
4	A	2790	A
4	A	2791	G
4	A	2796	A
4	A	2797	C
4	A	2822	A
4	A	2823	G
4	A	2826	A
4	A	2827	G
4	A	2832	G
4	A	2833	U
4	A	2834	C
4	A	2837	U
4	A	2839	U
4	A	2853	C
4	A	2854	A
4	A	2865	G
4	A	2870	C
4	A	2884	A
4	A	2893	G
4	A	2913	U

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Mol	Chain	Res	Type
4	A	2915	C
4	A	2936	C
4	A	2938	G
4	A	2950	C
4	A	2956	G
4	A	2957	A
4	A	2963	U
4	A	2969	C
4	A	2972	A
4	A	2976	C
4	A	2985	G
4	A	2990	A
4	A	3002	A
4	A	3005	A
4	A	3009	U
4	A	3015	C
4	A	3021	A
4	A	3022	G
4	A	3023	G
4	A	3029	U
4	A	3039	C
4	A	3041	C
4	A	3042	A
4	A	3044	A
4	A	3050	G
4	A	3056	A
4	A	3080	A
4	A	3082	U
4	A	3088	C
4	A	3093	A
4	A	3101	C
4	A	3105	C
4	A	3106	C
4	A	3107	G
4	A	3112	A
4	A	3114	A
4	A	3115	A
4	A	3119	A
4	A	3120	C
5	B	3	U
5	B	4	A
5	B	5	C

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Mol	Chain	Res	Type
5	B	8	C
5	B	9	G
5	B	10	G
5	B	11	U
5	B	13	C
5	B	14	A
5	B	17	G
5	B	23	G
5	B	25	G
5	B	31	C
5	B	33	C
5	B	36	U
5	B	41	U
5	B	42	C
5	B	43	C
5	B	53	A
5	B	56	C
5	B	57	U
5	B	59	A
5	B	66	C
5	B	67	A
5	B	74	A
5	B	86	A
5	B	89	C
5	B	97	A
5	B	100	G
5	B	103	G
5	B	106	C
5	B	107	A
5	B	109	C
5	B	113	G
5	B	114	A
5	B	117	A
5	B	118	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	97	U
4	A	272	A
4	A	336	C
4	A	357	U

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Mol	Chain	Res	Type
4	A	643	G
4	A	842	A
4	A	974	G
4	A	981	U
4	A	1199	U
4	A	1206	A
4	A	1230	G
4	A	1292	U
4	A	1947	U
4	A	2094	G
4	A	2135	U
4	A	2141	U
4	A	2320	C
4	A	2328	G
4	A	2345	U
4	A	2397	C
4	A	2656	A
4	A	2779	U
5	B	10	G
5	B	113	G

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	GCP	4	501	-	32,34,34	1.38	6 (18%)	49,54,54	1.87	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GCP	4	501	-	-	5/19/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	4	501	GCP	PG-O2G	2.85	1.61	1.55
36	4	501	GCP	C5-C4	2.76	1.46	1.38
36	4	501	GCP	PG-O3G	2.61	1.60	1.55
36	4	501	GCP	C6-N1	-2.58	1.34	1.38
36	4	501	GCP	C5-N7	-2.15	1.34	1.39
36	4	501	GCP	C4-N9	-2.03	1.32	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	4	501	GCP	C5-C4-N3	-5.78	119.19	128.39
36	4	501	GCP	C2-N3-C4	4.88	120.70	112.30
36	4	501	GCP	PB-O3A-PA	-4.58	117.42	132.37
36	4	501	GCP	N9-C4-N3	4.18	134.31	125.95
36	4	501	GCP	C6-C5-N7	3.58	136.80	130.29
36	4	501	GCP	C4-C5-N7	-2.75	106.32	110.67
36	4	501	GCP	C3'-C2'-C1'	2.17	105.57	101.46
36	4	501	GCP	O6-C6-C5	-2.08	121.06	126.53
36	4	501	GCP	C8-N7-C5	2.02	107.86	104.26

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	4	501	GCP	PB-C3B-PG-O1G
36	4	501	GCP	PB-C3B-PG-O2G
36	4	501	GCP	PB-C3B-PG-O3G
36	4	501	GCP	C5'-O5'-PA-O1A

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Continued from previous page...

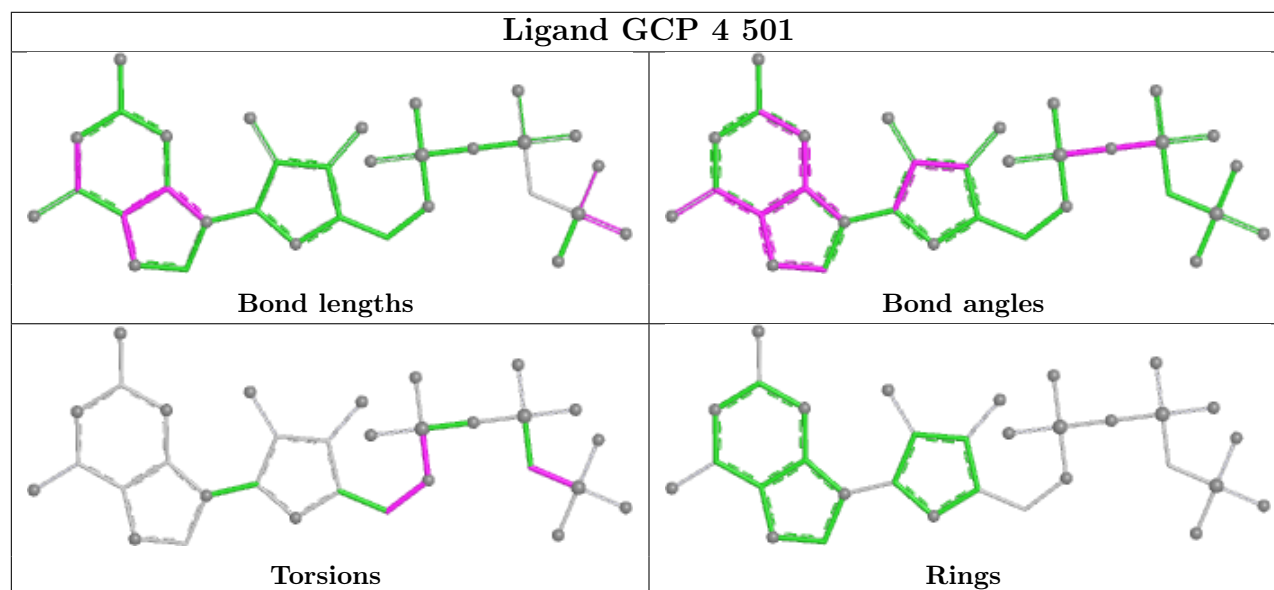
Mol	Chain	Res	Type	Atoms
36	4	501	GCP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	4	501	GCP	15	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

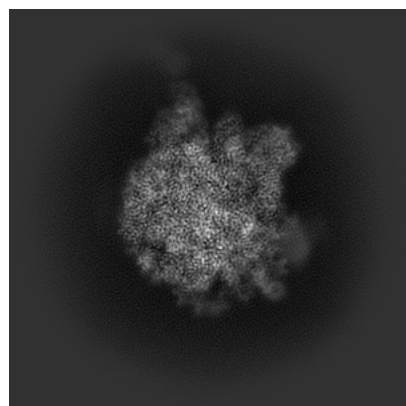
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43294. These allow visual inspection of the internal detail of the map and identification of artifacts.

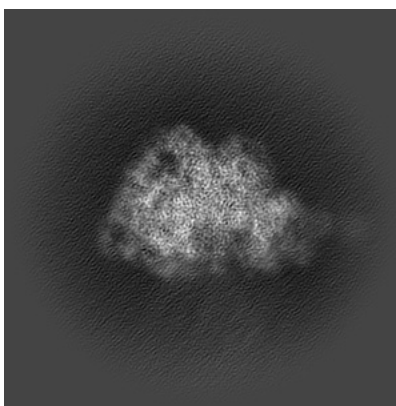
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

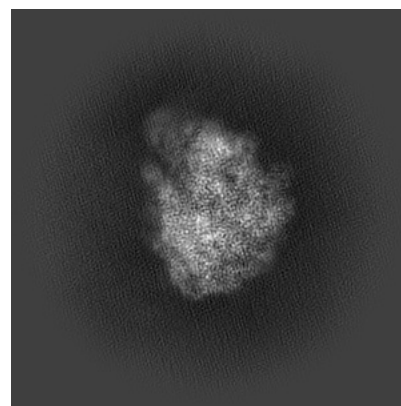
6.1.1 Primary map



X

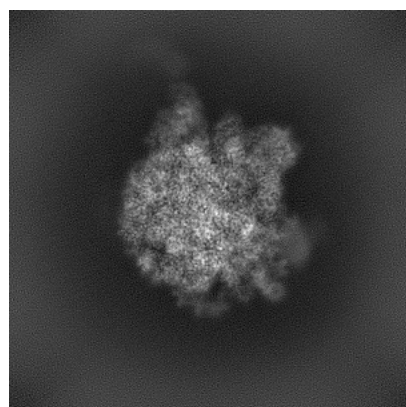


Y

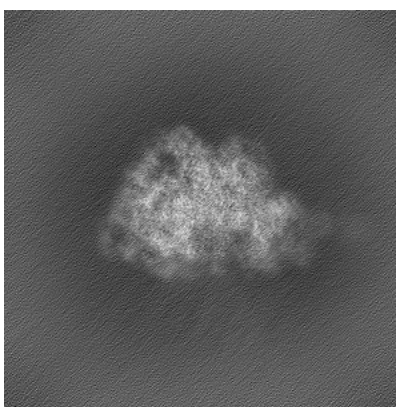


Z

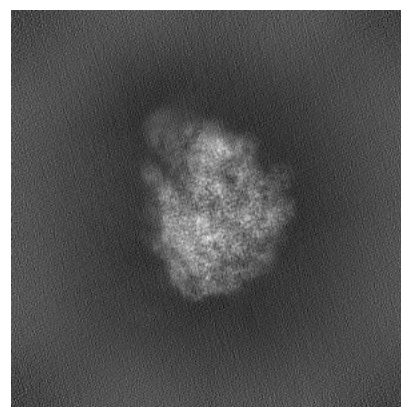
6.1.2 Raw map



X



Y

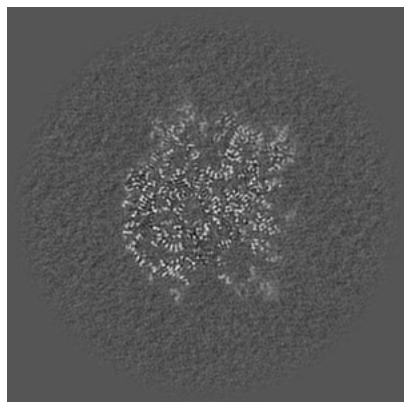


Z

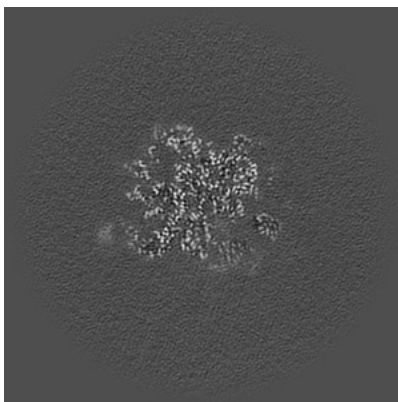
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

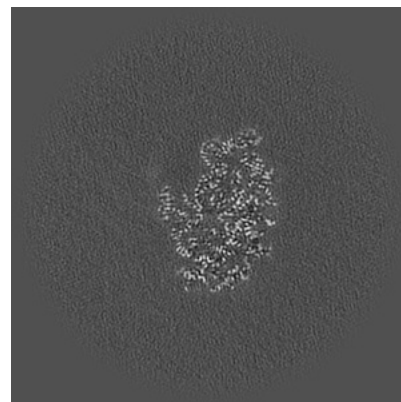
6.2.1 Primary map



X Index: 200

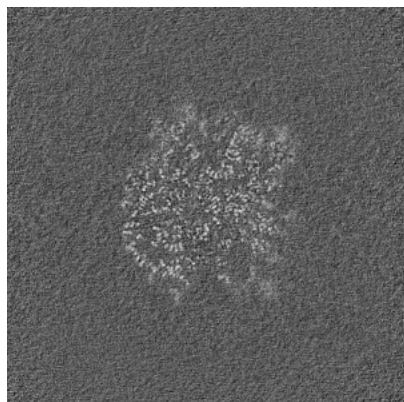


Y Index: 200

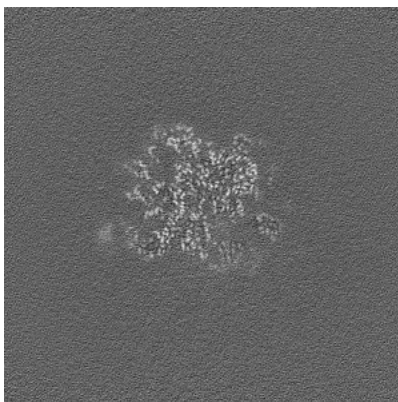


Z Index: 200

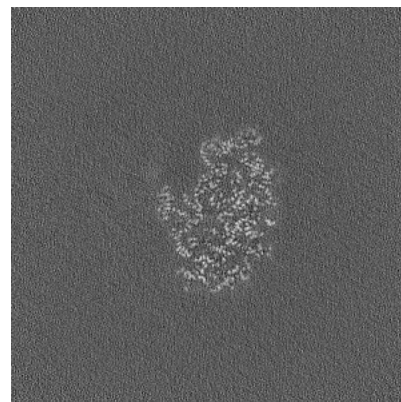
6.2.2 Raw map



X Index: 200



Y Index: 200

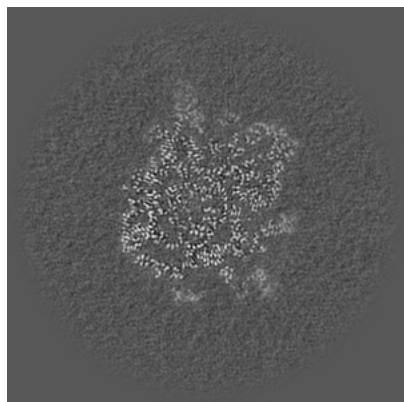


Z Index: 200

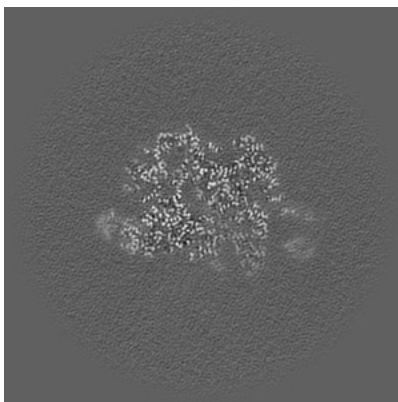
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

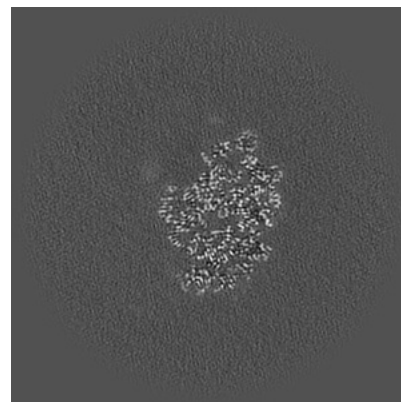
6.3.1 Primary map



X Index: 194

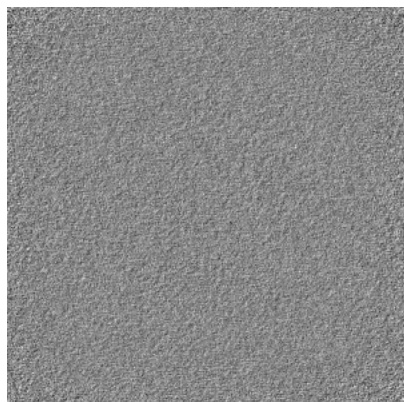


Y Index: 190

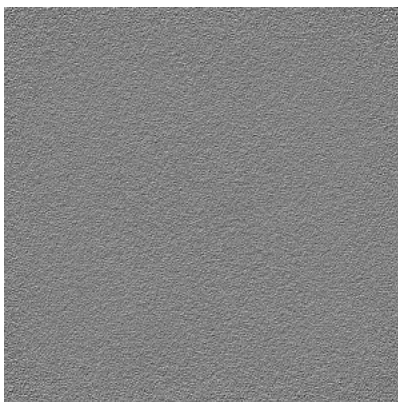


Z Index: 196

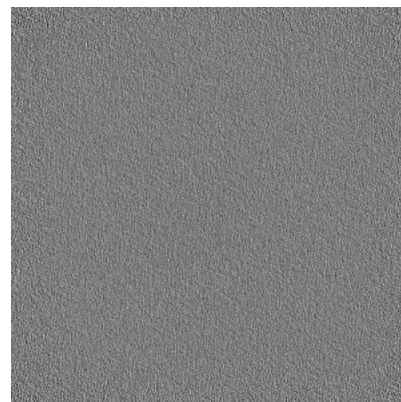
6.3.2 Raw map



X Index: 0



Y Index: 0

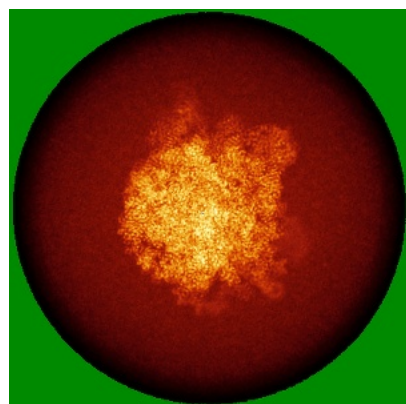


Z Index: 0

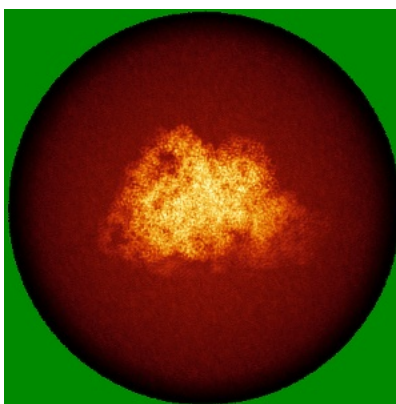
The images above show the largest variance slices of the map in three orthogonal directions.

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

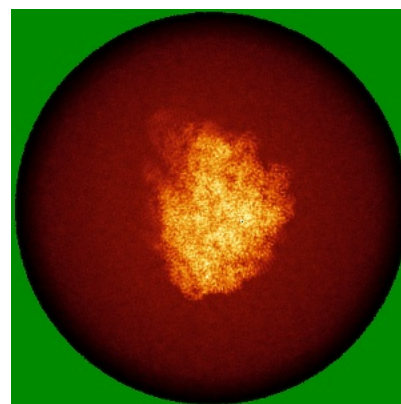
6.4.1 Primary map



X

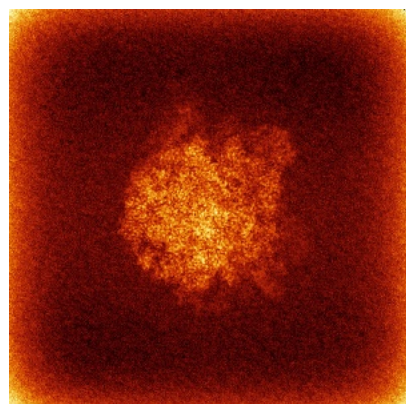


Y

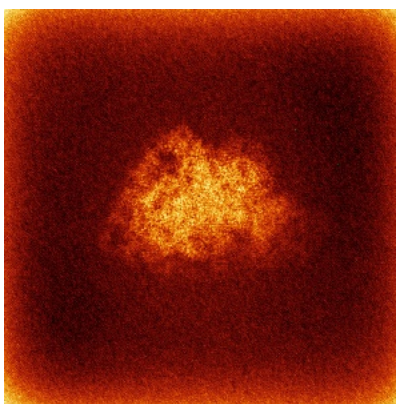


Z

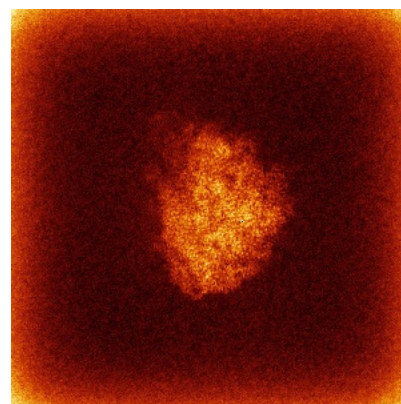
6.4.2 Raw map



X



Y

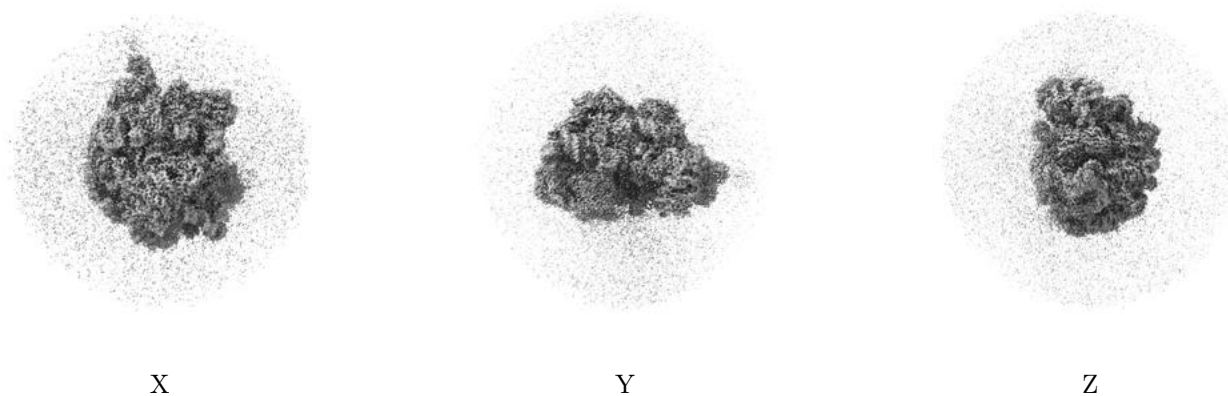


Z

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

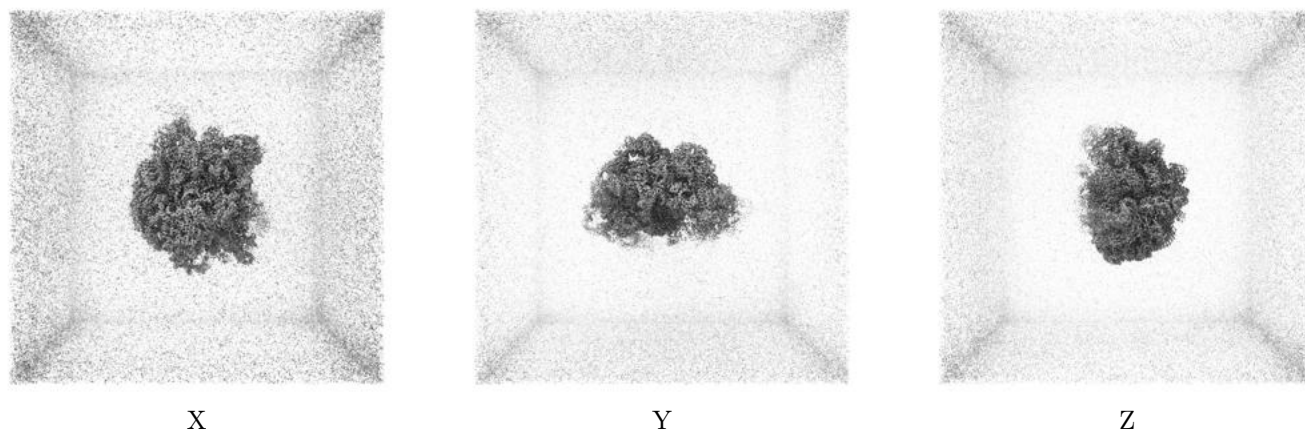
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

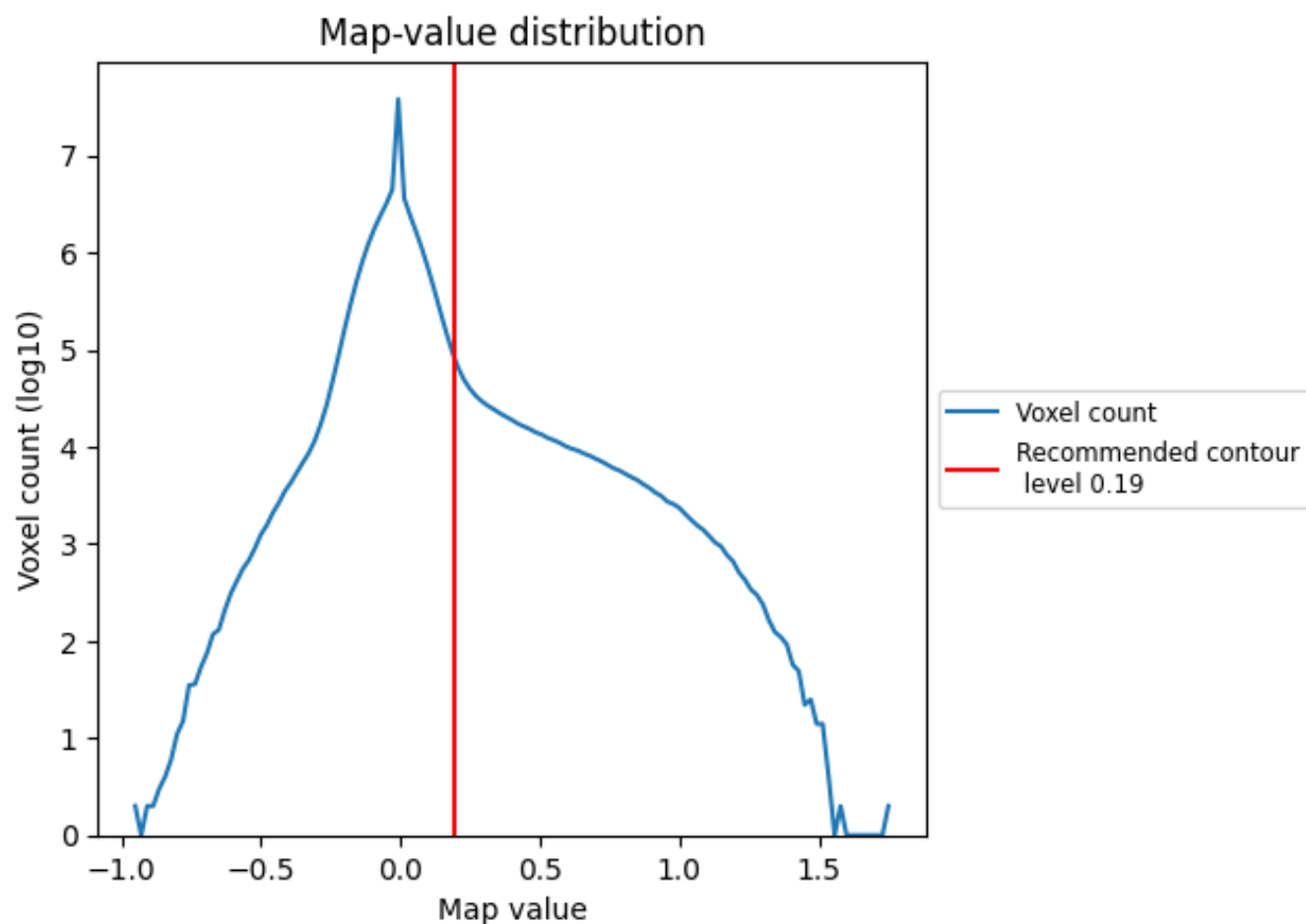
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

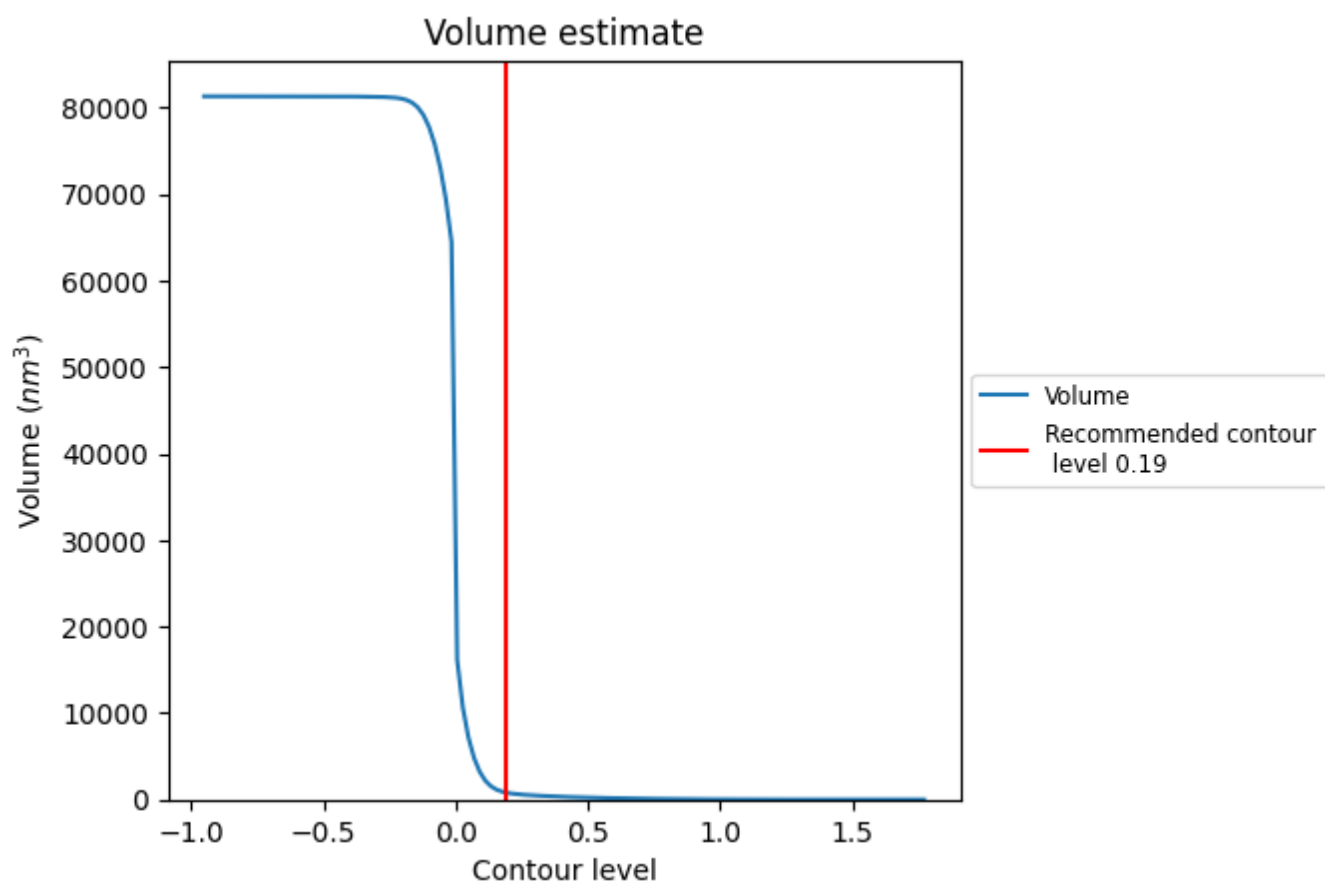
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

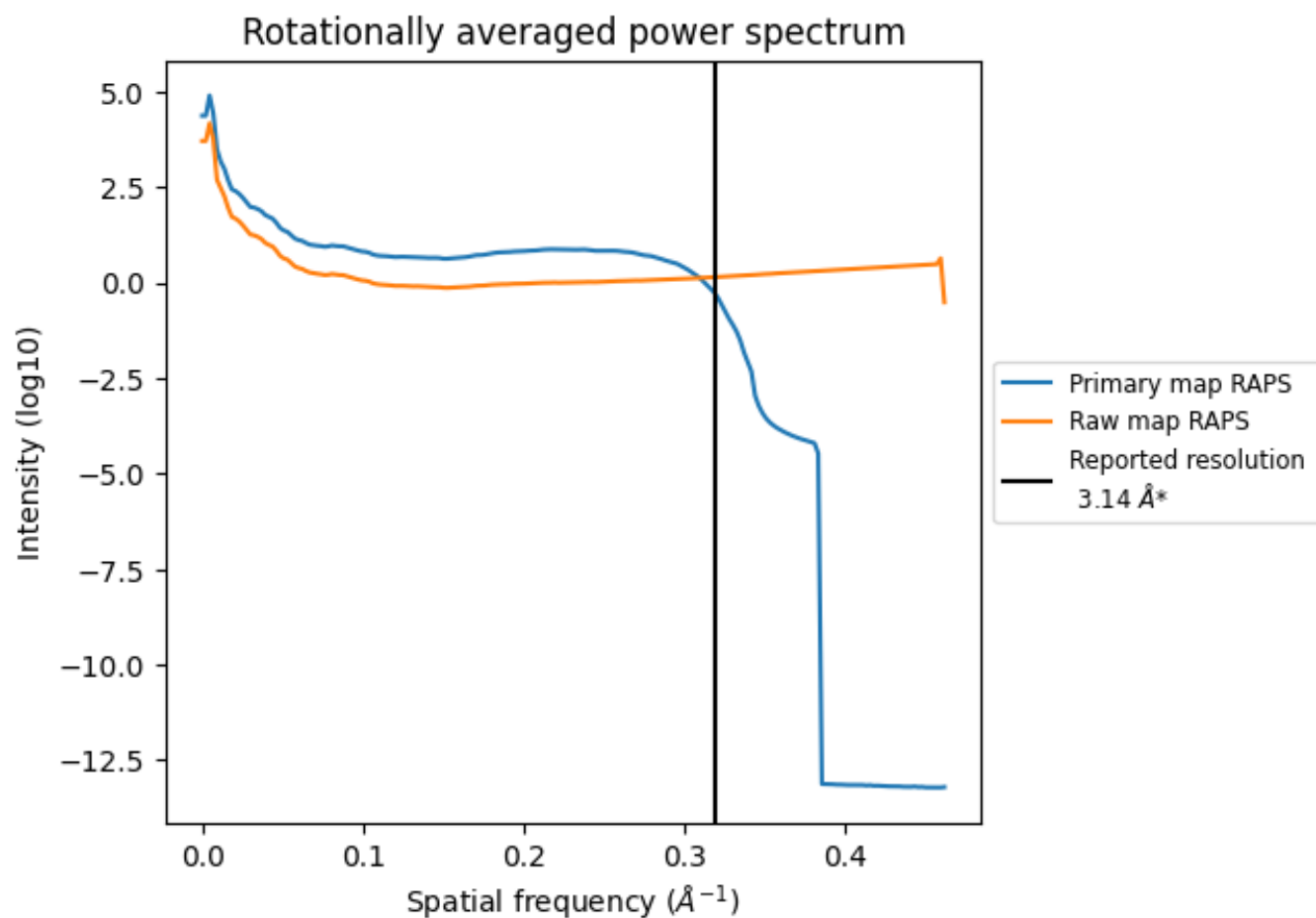
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 817 nm³; this corresponds to an approximate mass of 738 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 ⓘ

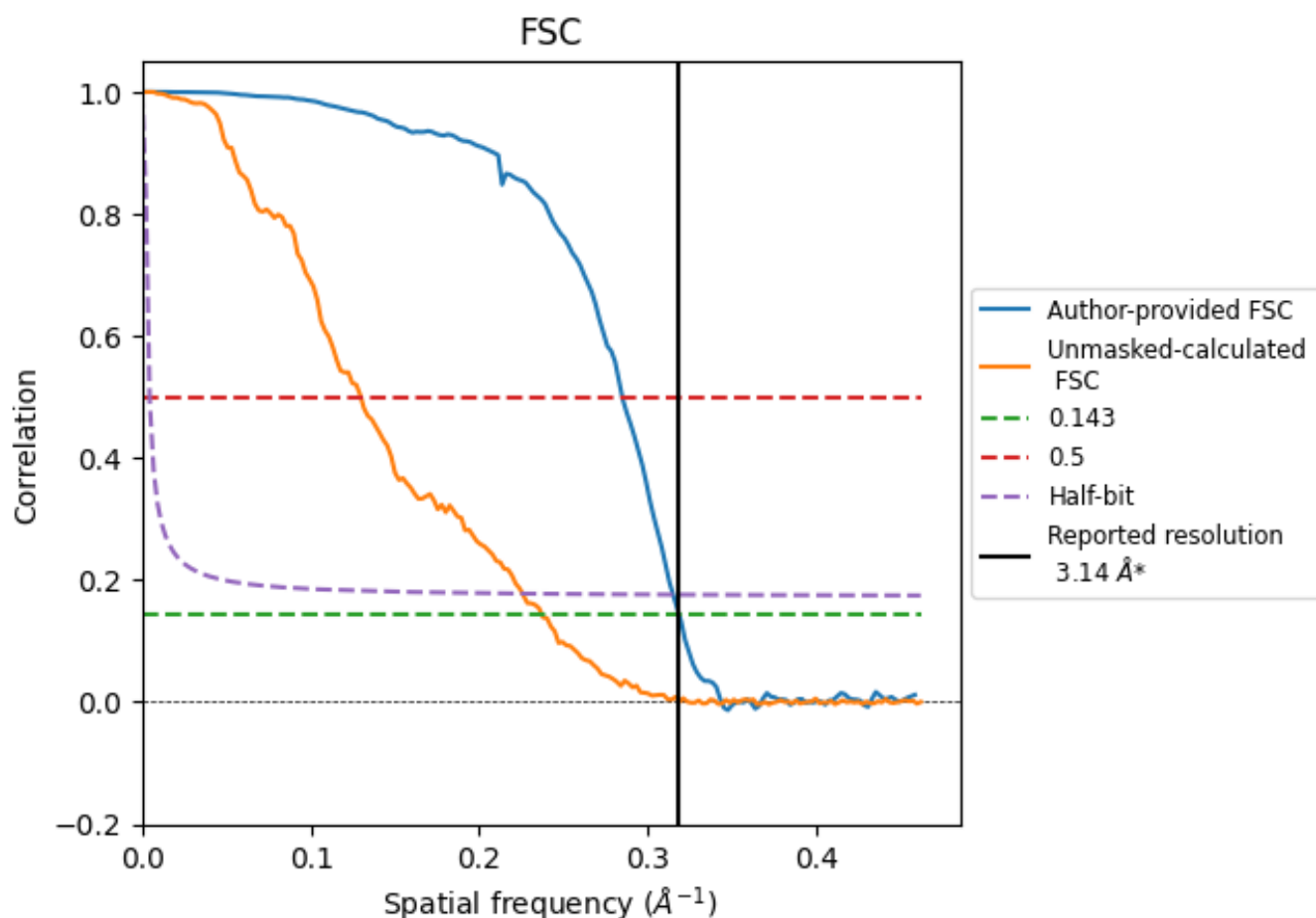


*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

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 0.318 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

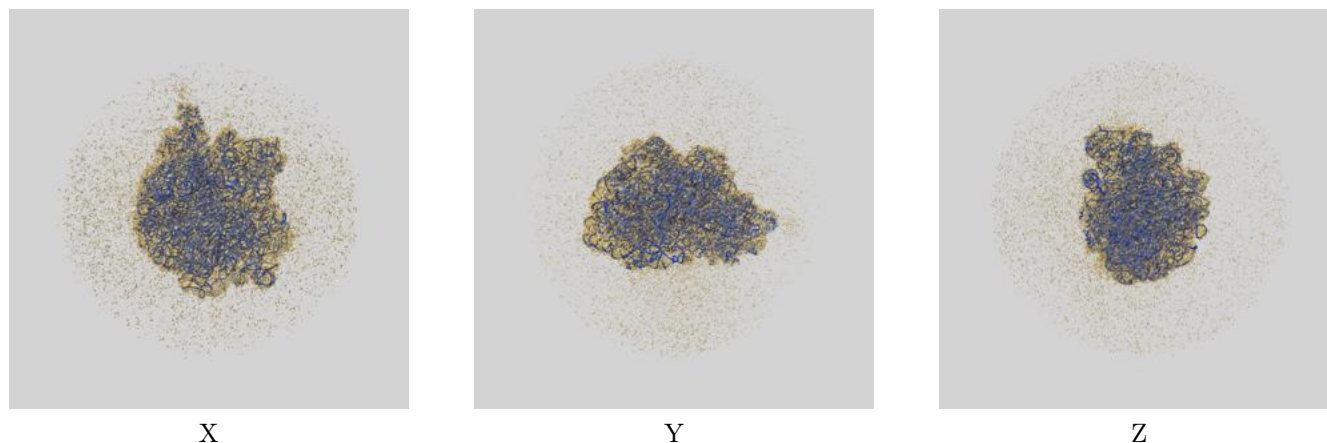
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.51	3.18
Unmasked-calculated*	4.22	7.72	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

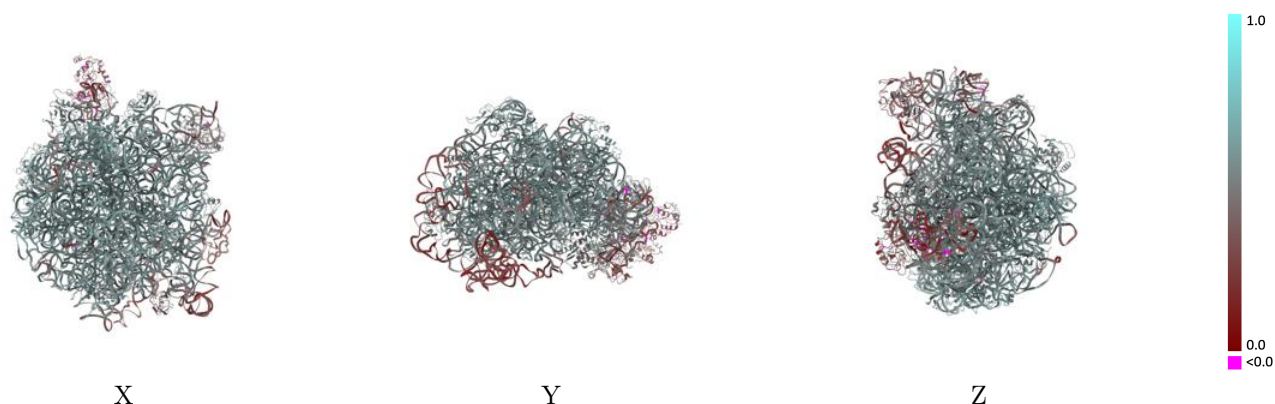
This section contains information regarding the fit between EMDB map EMD-43294 and PDB model 8VK0. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



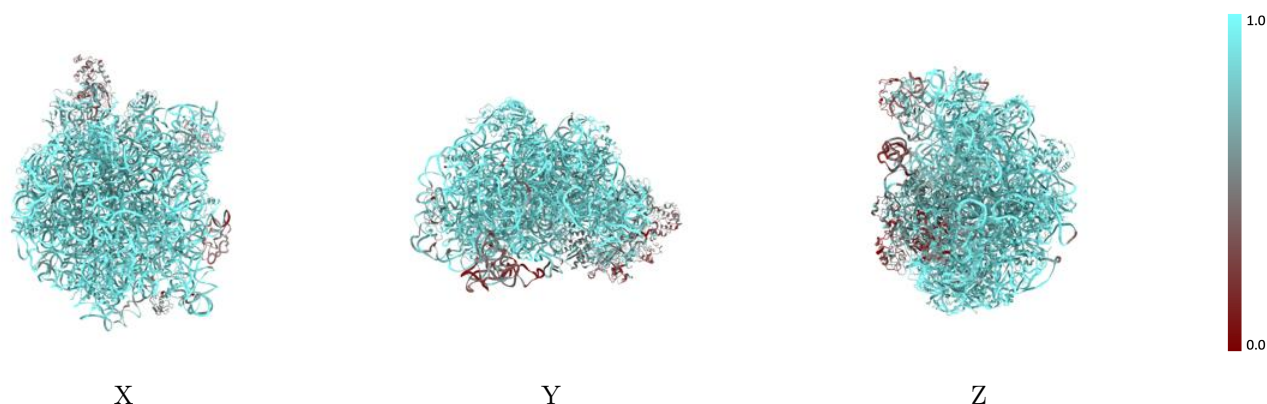
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



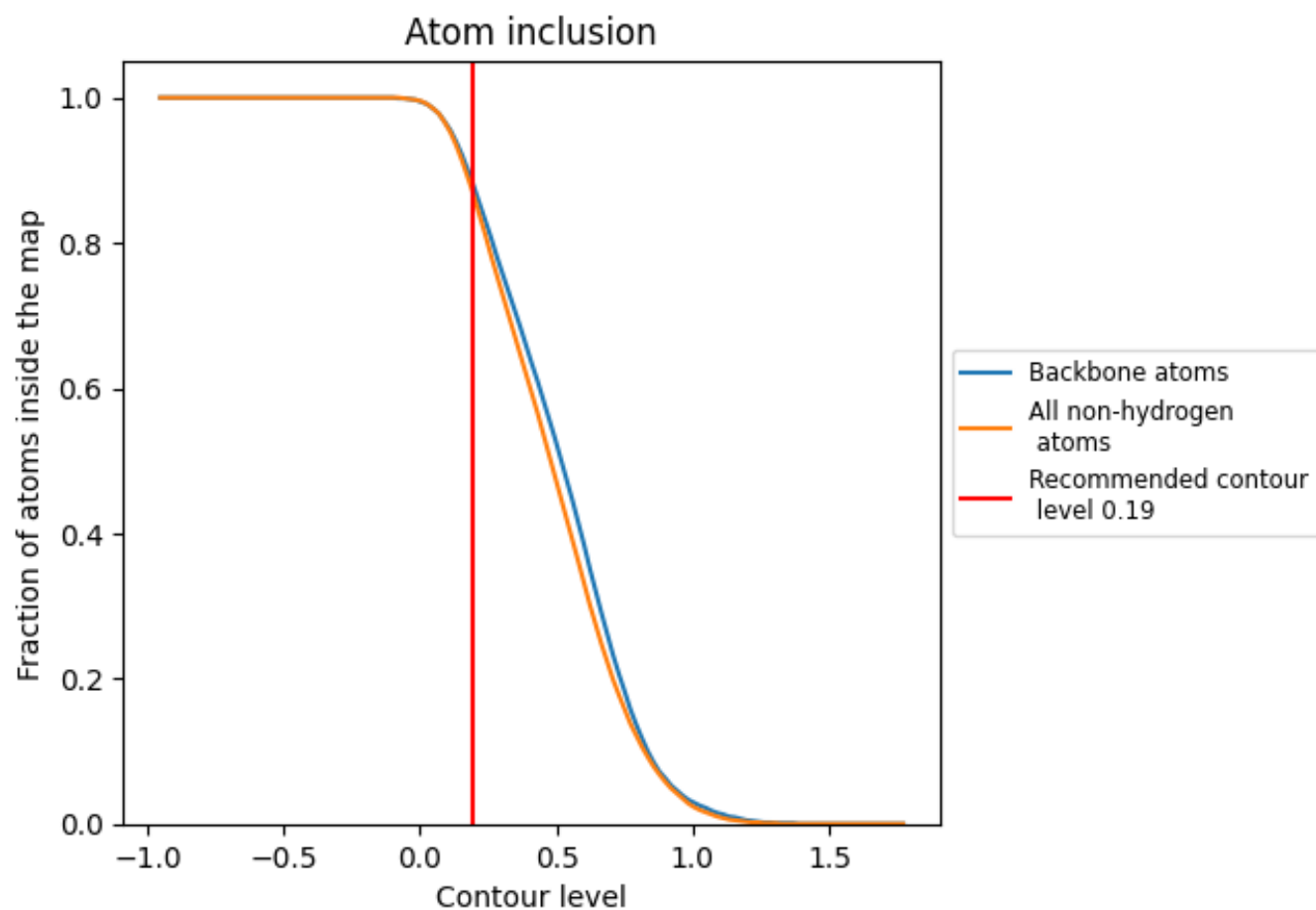
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5190
2	 0.9410	 0.5870
3	 0.8660	 0.5910
4	 0.6210	 0.4740
A	 0.9060	 0.5190
B	 0.9180	 0.4820
C	 0.9240	 0.5820
D	 0.9270	 0.5810
E	 0.9000	 0.5690
F	 0.6140	 0.3960
G	 0.7870	 0.4960
H	 0.5930	 0.4280
I	 0.3830	 0.2960
J	 0.3570	 0.2730
K	 0.9350	 0.5860
L	 0.8990	 0.5700
M	 0.9170	 0.5720
N	 0.8540	 0.5740
O	 0.9300	 0.5840
P	 0.7640	 0.4290
Q	 0.8660	 0.5520
R	 0.9370	 0.5890
S	 0.9310	 0.5870
T	 0.9240	 0.5810
U	 0.9120	 0.5700
V	 0.8560	 0.5250
W	 0.7330	 0.5330
X	 0.9190	 0.5790
Y	 0.9230	 0.5720
Z	 0.8900	 0.5520
b	 0.9030	 0.5800
c	 0.9090	 0.5780
d	 0.9230	 0.5910
e	 0.9190	 0.5970
f	 0.8570	 0.5790
g	 0.3360	 0.3560

