



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 20, 2016 – 07:59 AM EST

PDB ID : 5MLC
EMDB ID: : EMD-3525
Title : Cryo-EM structure of the spinach chloroplast ribosome reveals the location of plastid-specific ribosomal proteins and extensions
Authors : Graf, M.; Arenz, S.; Huter, P.; Doenhoefer, A.; Novacek, J.; Wilson, D.N.
Deposited on : 2016-12-06
Resolution : 3.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

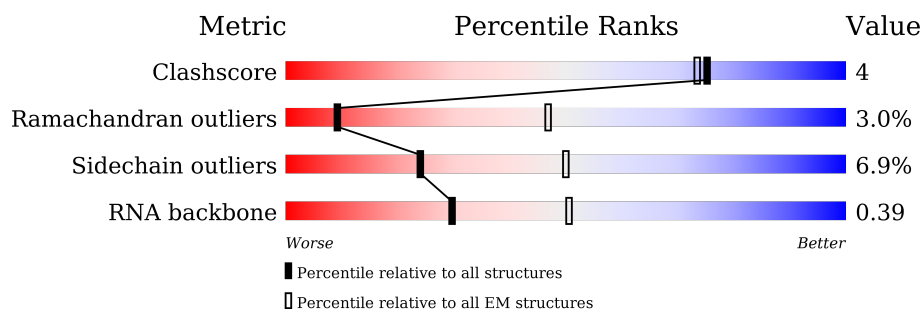
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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
















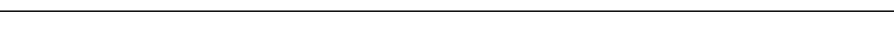
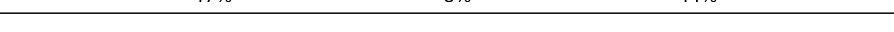
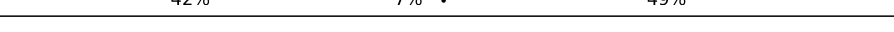
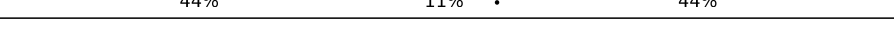
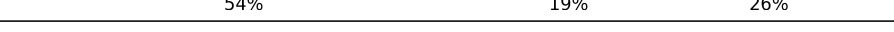



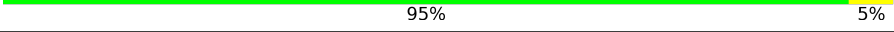


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	2811	59% 33% 6% .
2	B	121	73% 23% . .
3	C	103	53% 31% 6% 10%
4	D	272	74% 14% . 10%
5	E	305	62% 9% 28%
6	F	293	59% 10% . 30%
7	G	220	73% 9% 19%
8	H	220	70% 10% 19%

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Mol	Chain	Length	Quality of chain
9	I	196	
10	L	250	
11	M	121	
12	N	271	
13	O	135	
14	P	126	
15	Q	166	
16	R	233	
17	S	128	
18	T	256	
19	U	199	
20	V	198	
21	W	191	
22	X	194	
23	Y	148	
24	Z	168	
25	2	57	
26	3	66	
27	4	152	
28	5	159	
29	6	37	
30	9	271	
31	7	142	
32	8	116	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2750	Total	C	N	O	P	0	0
			59074	26351	10944	19029	2750		

- Molecule 2 is a RNA chain called 5S ribosomal RNA, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2564	1145	464	835	120		

- Molecule 3 is a RNA chain called 4.8S ribosomal RNA, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	93	Total	C	N	O	P	0	0
			2001	893	374	641	93		

- Molecule 4 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	246	Total	C	N	O	S	0	0
			1895	1175	388	326	6		

- Molecule 5 is a protein called 50S ribosomal protein L3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	219	Total	C	N	O	S	0	0
			1669	1056	304	298	11		

- Molecule 6 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	205	Total	C	N	O	S	0	0
			1617	1024	303	287	3		

- Molecule 7 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	179	Total	C	N	O	S	0	0
			1387	883	241	255	8		

- Molecule 8 is a protein called 50S ribosomal protein L6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	178	Total	C	N	O	S	0	0
			1386	874	255	253	4		

- Molecule 9 is a protein called 50S ribosomal protein L9, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	45	Total	C	N	O	0	0
			359	237	65	57		

- Molecule 10 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	196	Total	C	N	O	S	0	0
			1489	942	280	264	3		

- Molecule 11 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	120	Total	C	N	O	S	0	0
			934	582	178	169	5		

- Molecule 12 is a protein called 50S ribosomal protein L15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	182	Total	C	N	O	S	0	0
			1385	864	273	242	6		

- Molecule 13 is a protein called 50S ribosomal protein L16, chloroplastic.

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

- Molecule 14 is a protein called 50S ribosomal protein L17, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	116	Total	C	N	O	S	0	0
			945	592	193	156	4		

- Molecule 15 is a protein called 50S ribosomal protein L18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	118	Total	C	N	O	S	0	0
			931	579	179	168	5		

- Molecule 16 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	114	Total	C	N	O	S	0	0
			915	586	178	150	1		

- Molecule 17 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	116	Total	C	N	O	S	0	0
			1003	637	209	155	2		

- Molecule 18 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	T	134	Total	C	N	O	0	0
			1017	653	183	181		

- Molecule 19 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	152	Total	C	N	O	S	0	0
			1165	738	212	208	7		

- Molecule 20 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	91	Total	C	N	O	S	0	0
			734	474	127	131	2		

- Molecule 21 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	129	Total	C	N	O	S	0	0
			1018	641	193	182	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	108	Total	C	N	O	S	0	0
			866	545	172	149			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	75	Total	C	N	O	S	0	0
			616	391	125	99	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	94	Total	C	N	O	S	0	0
			788	492	156	137	3		

- Molecule 25 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	2	42	Total	C	N	O	0	0
			341	223	65	53		

- Molecule 26 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	60	Total	C	N	O	S	0	0
			489	304	98	83	4		

- Molecule 27 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	61	Total	C	N	O	S	0	0
			471	284	108	76	3		

- Molecule 28 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	70	Total	C	N	O	S	0	0
			575	362	121	91	1		

- Molecule 29 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	37	Total	C	N	O	S	0	0
			305	186	70	45	4		

- Molecule 30 is a protein called Ribosome-recycling factor, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	9	107	Total	C	N	O	S	0	0
			881	545	158	175	3		

- Molecule 31 is a protein called PSRP5alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	46	Total	C	N	O	S	0	0
			378	241	77	56	4		

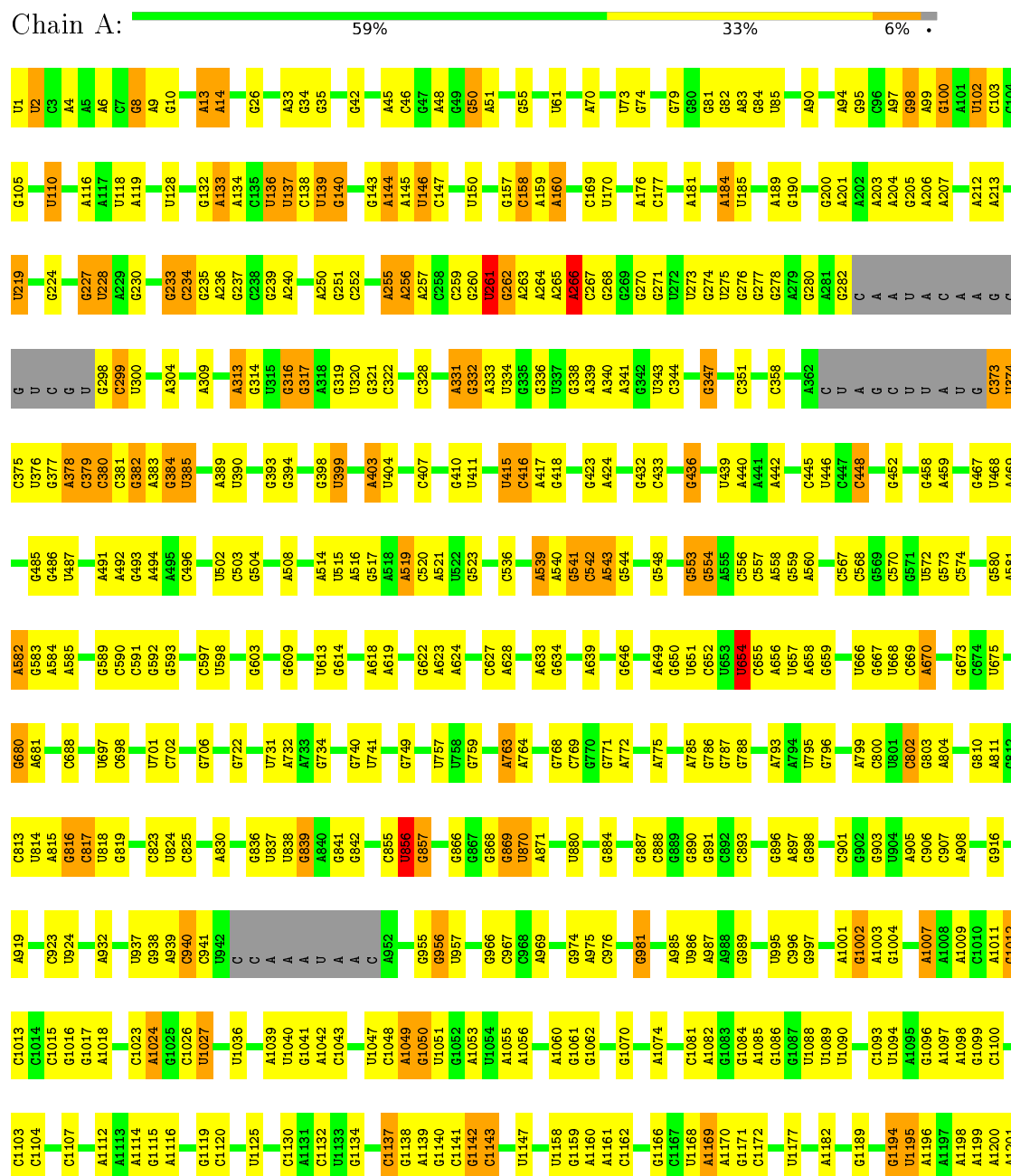
- Molecule 32 is a protein called PSRP6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	47	Total	C	N	O	S	0	0
			374	240	72	61	1		


3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal RNA, chloroplastic

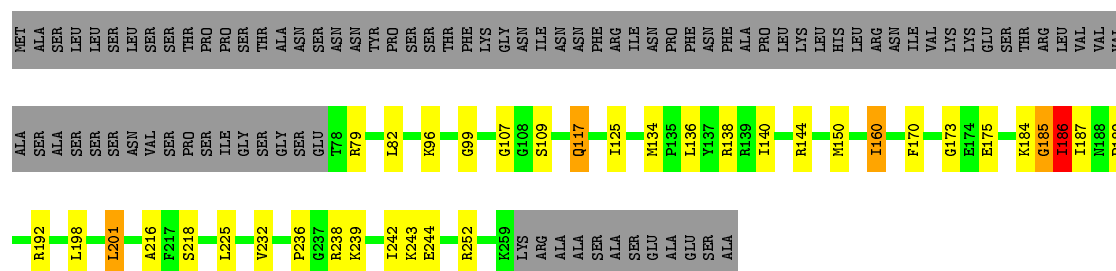


G2752	G2657	C2534	G2424	A2326	U2216	U2118	G2018	G1913	G1786	C1682	G1572	A	A1399	G1281	A1202
C2753	A2658	C2535	G2432	G2327	U2217	G2124	G2018	A1914	A1790	C1683	G1572	C	U1400	C1282	C1203
G2754	G2659	G2543	C2433	G2327	G2218	C2125	G2026	A1915	C1791	C1684	G1574	C	G1402	U1209	
G2762	A2661	C2544	U2436	U2329	U2219	G2126	U2030	C1919	C1792		G1580	U	A1403	A1289	G1213
A2766	C2662	G2545		C2335	G2220	C2127		G1920	A1796	G1687		U	C1404	G1292	
	C2663	G2546		U2336	U2221	A128		G1921	C1797		G1589	U	A1405	C1293	G1218
C2770	U2664		C2439	U2336	C2222	C2129	A2033	G1924	A1690	A1690	G1590	U	G1410	U1219	
A2771	U2665	U2552	U2440	C2337	A2223	C2130	C2034	U1925	C1798	U1693	C1591	U	U1411	A1294	
	U2666		C2441	G2338	G2224	U131	A2035	U1926		C1694	A1592	U	C1412	A1295	
U2774	A2559	G2560	A2442	A2339	G2225	U132	U2036	A	A1801	U1695	U1593	C		A1296	
U2775	G2672			G2340	A2226	A2133	G2037	A	U1806	C1696	A1594	A			
A2776	U2673	U2564	G2446	U2341	C2227			C	C1807	U1697	C1595	G	A1416	G1310	U1224
			A2447	G2342	C2228	U2136	G2043	U		C1698			U1417	G1225	G1226
A2782	G2678			C2343	U2229	G2141	A2044	A	C1810		A1600	G	U1418	U1227	
A2783	G2685	U2571	A2452	A2344	A2230	G2142	A2045	U	A1811	A1701	A1606	G	C1419	A1228	
G2784				A2345		G2143	G2046	A	A1812	G1702	G1602	U	C1420	G1229	
C2785	A2578	U2579	U2458	A2346	A2242	G2144	U2048	C1933		G1710	A1603	A		G1230	
C2786	A2688			G2347			G2049	C1934	A1819			G	U1426	G1231	
C2787	A2689		G2462	G2348	U2248	A2145		G1935	A1820		A1604				
C2788	G2690	A2583	G2463	C2349	G2252	G2147	A2053	C1939	A1821	A1713	A1605		C1429	A1322	A1232
C2791	G2691	G2584	A2464	A2350	U2253	G2147	A2056	G1943	A1822		G1607		U1432	U1327	G1233
C2792	A2692		A2465	G2351	A2254	A2148	C2057	G1944		G1730	A1608		U1433	G1332	A1236
				G2347	A2255			U1945	A1825	G1731	U1609		G1434	C1237	
A2796	A2696			G2348	U2256	C2153	A2057	G1944	U1826	G1732	C1610		U1435	G1238	
U2797	C2698		G2472	G2355	U2260	C2159	U2065	A1950	G1827	G1733	G1611		U1436	C1239	
G2798	U2699		C2473	G2356	U2261	G2160	G2066	A1951	U1828	G1734	A1612		G1437	G1240	
A2799	C2700		U2474	G2357	U2262	C2161	C2069	A1952	A1829	G1735	A1613		U1438	U1241	
	U2701	U2602	G2475	G2362	C2263	U2169	A2070	U1953	U1830	G1736	C1614		U1439	C1242	
C2808	G2702	C2603	A2476		U2264	C2169		U1954	C1843	U1742	A1615		C1440	C1243	
A2809	G2703			C2367		C2170	A2074	C1955		G1743	A1616		C1441	G1344	
A2810	U2704		C2481	C2374	G2267	G2171	G2075	C1956	G1866	C1744	C1617		C1442	G1345	C1250
	G2705	A2619	C2484	C2378	G2268	A2176	A2076	U1957	A1867		A1618		G1443	U1346	C1251
	A2707	U2620			G2269	U2177		U1958		C1748	U1619		G1444		C1252
C2708	C2708	U2621	U2490	C2378		A2178	U2080	G1959	U1870	U1749	C1620		G1445	G1253	U1254
		U2622	U2491	G2387	G2272	C2178					C1621				
C2721	C2721		C2492	G2388		U2181	G2083	U1965	G1875	C1750	A1622		A1448	G1359	
A2723	A2723	G2625	A2493	G2389	A2285		A2084	G1542	A1751	G1752	A1623		C1449	A1258	
C2724	C2724	U2626	G2494			G2184	G2085	U1969	A1753	A1471	C1624			C1362	
		C2628	A2495	G2396	G2296	A2185	G2086	C1975	A1880	A1472			A1472	A1363	C1259
A2729	A2629		G2501	U2397	G2299	A2186	C2092		U1882	A1754	A1628		A1473	G1364	G1260
A2730	U2630	G2631	G2502	G2399	U2300	A2187	U2093	C1979	G1883	A1755	G1629		A1474	U1365	A1261
G2731	C2731		G2503	G2400	A2303	C2188	G2094	A1980	A1884	G1756	G1630		U1475	C1366	A1262
G2732				C2401	A2304		G2101	U1981		G1759			G1476	A1367	G1263
		G2642	G2511	C2402	A2305	C2193	G2102	A1982	A1886	G1760	C1634		U1478	G1368	G1264
U2738	C2643	G2644	C2516	G2408	G2306	A2197		A1983	G1887				G1477		G1265
A2739	G2645		U2517	A2409	U2308		U2106	G1986	G1889	G1763	A1643		U1479	C1371	A1268
G2740	C2741		C2518	U2410	G2309	U2203	G2107		A1896	U1767	A1644		U1552	G1372	G1269
C2742	A2647		G2519	C2411	U2309	A2204	C2108	G1999	C1897	G1768	A1645		A1480	A1373	C1270
A2743	G2648		A2520	C2412	U2310	G2205	C2109	G2000	A1898	G1774	A1646			A1374	
A2744	A2649		U2521		A2206	A2206	U2110	G2001	A1899					A1375	
			G2522	G2419	C2314	A2207	U2111			G1766	A1662				G1389
G2747	U2653		U2523	C2420	G2315	U2208	U2112	U2005	G1778	U1767	G1663				
	U2654			C2421	G2321	U2209	G2113	G2006		G1768			U1558	A1272	U1278
G2750	G2655		U2530	G2422	G2321	U2209	G2114	U2007	A1783		A1671		C1494	G1385	C1279
A2751		A2656		A2423	A2322	A2212		U2007					C1495	A1386	


- Chain F: 
- | Position | Residue | Category |
|----------|---------|----------|
| 1 | Met | Grey |
| 2 | Ala | Grey |
| 3 | Thr | Green |
| 4 | Ser | Green |
| 5 | Thr | Green |
| 6 | Ser | Green |
| 7 | Ser | Green |
| 8 | Leu | Green |
| 9 | Ser | Green |
| 10 | Leu | Green |
| 11 | Ser | Green |
| 12 | Phe | Green |
| 13 | Phe | Green |
| 14 | Ser | Green |
| 15 | Ser | Green |
| 16 | Ser | Green |
| 17 | Leu | Green |
| 18 | Phe | Green |
| 19 | Ser | Green |
| 20 | Ser | Green |
| 21 | Lys | Green |
| 22 | Ser | Green |
| 23 | Arg | Green |
| 24 | Asn | Green |
| 25 | Phe | Green |
| 26 | Ser | Green |
| 27 | Ser | Green |
| 28 | Lys | Green |
| 29 | Pro | Green |
| 30 | Pro | Green |
| 31 | Ile | Green |
| 32 | Leu | Green |
| 33 | Lys | Green |
| 34 | Ser | Green |
| 35 | Ser | Green |
| 36 | Ser | Green |
| 37 | His | Green |
| 38 | Ser | Green |
| 39 | Gln | Green |
| 40 | Thr | Green |
| 41 | Ser | Green |
| 42 | Leu | Green |
| 43 | Ser | Green |
| 44 | Ser | Green |
| 45 | Ser | Green |
| 46 | Ile | Green |
| 47 | Lys | Green |
| 48 | Ser | Green |
| 49 | Val | Green |
| 50 | Leu | Green |
| 51 | Ile | Green |
| 52 | Pro | Green |
| 53 | Leu | Green |
| 54 | Thr | Green |
| 55 | Pro | Green |
| 56 | Leu | Green |
| 57 | Val | Green |
| 58 | Asp | Green |
| 59 | Val | Green |
| 60 | Asp | Green |
| 61 | Val | Green |
| 62 | Gly | Green |
| 63 | Asp | Green |
| 64 | Gly | Green |
| 65 | Thr | Green |
| 66 | Pro | Green |
| 67 | Glu | Green |
| 68 | Pro | Green |
| 69 | Ala | Green |
| 70 | Glu | Green |
| 71 | Arg | Green |
| 72 | Asn | Green |
| 73 | Phe | Green |
| 74 | Ser | Green |
| 75 | Ser | Green |
| 76 | Ser | Green |
| 77 | Ser | Green |
| 78 | Ser | Green |
| 79 | Ser | Green |
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| 93 | Ser | Green |
| 94 | Ser | Green |
| 95 | Ser | Green |
| 96 | Ser | Green |
| 97 | Ser | Green |
| 98 | Ser | Green |
| 99 | Ser | Green |
| 100 | Ser | Green |

- Molecule 12: 50S ribosomal protein L15, chloroplastic

Chain N: 



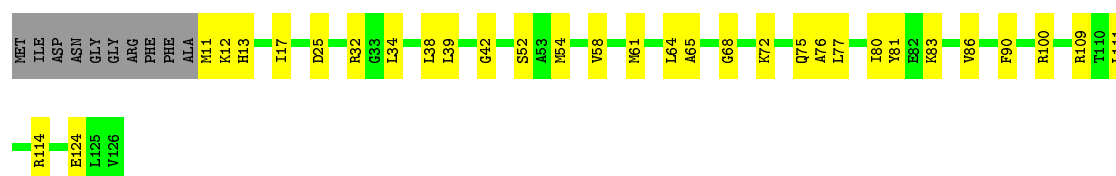
- Molecule 13: 50S ribosomal protein L16, chloroplastic

Chain O: 



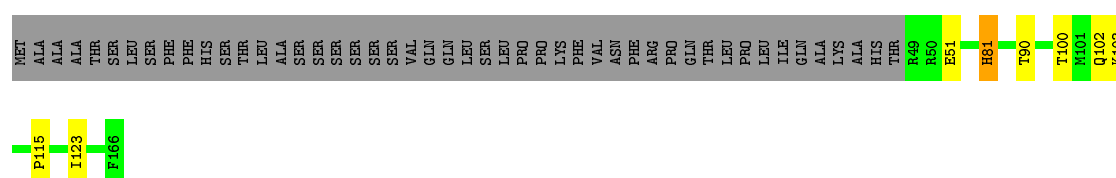
- Molecule 14: 50S ribosomal protein L17, chloroplastic

Chain P: 




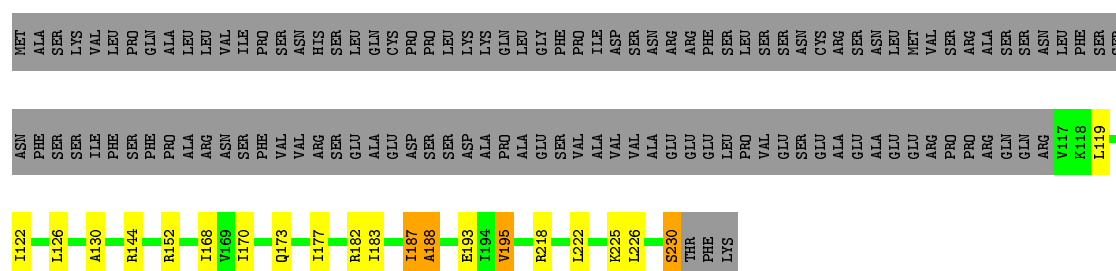
- Molecule 15: 50S ribosomal protein L18, chloroplastic

Chain Q: 



- Molecule 16: 50S ribosomal protein L19, chloroplastic

Chain R: 

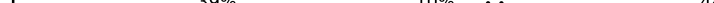


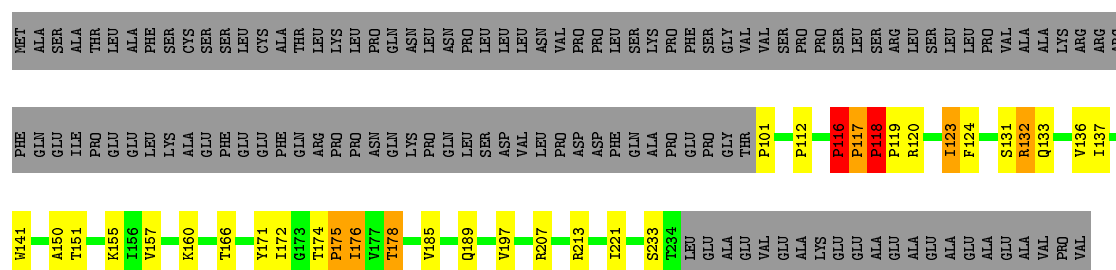
- Molecule 17: 50S ribosomal protein L20, chloroplastic

Chain S:  73% 18% 9%



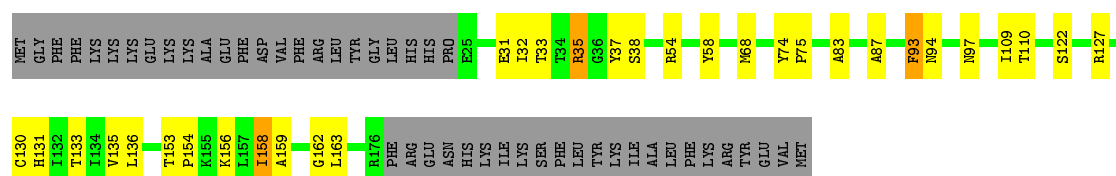
- Molecule 18: 50S ribosomal protein L21, chloroplastic

Chain T:  39% 10% 2% 49%

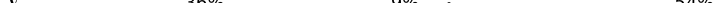


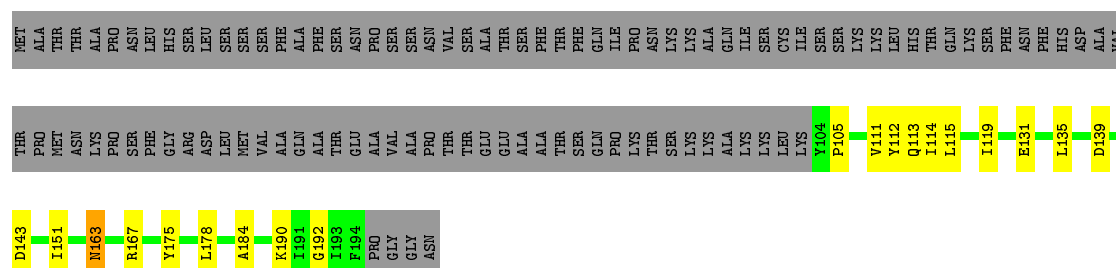
- Molecule 19: 50S ribosomal protein L22, chloroplastic

Chain U: 60% 15% 1% 24%



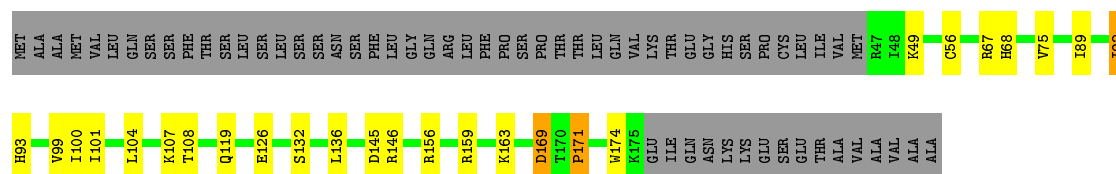
- Molecule 20: 50S ribosomal protein L23, chloroplastic

Chain V:  36% 9% . 54%

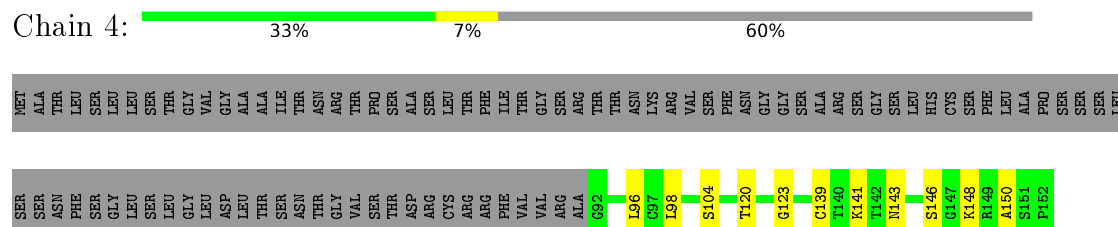


- Molecule 21: 50S ribosomal protein L24, chloroplastic

Chain W:  54% 12% 2% 32%

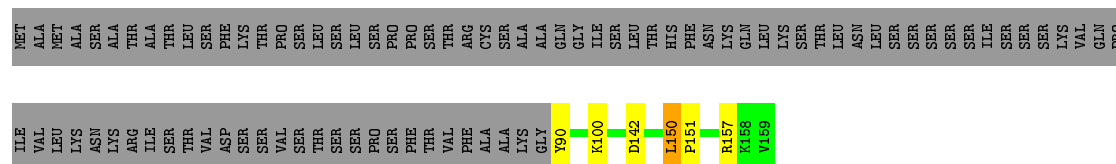


- Molecule 22: 50S ribosomal protein L27, chloroplastic



- Molecule 28: 50S ribosomal protein L35, chloroplactic

Chain 5:  40% 56%



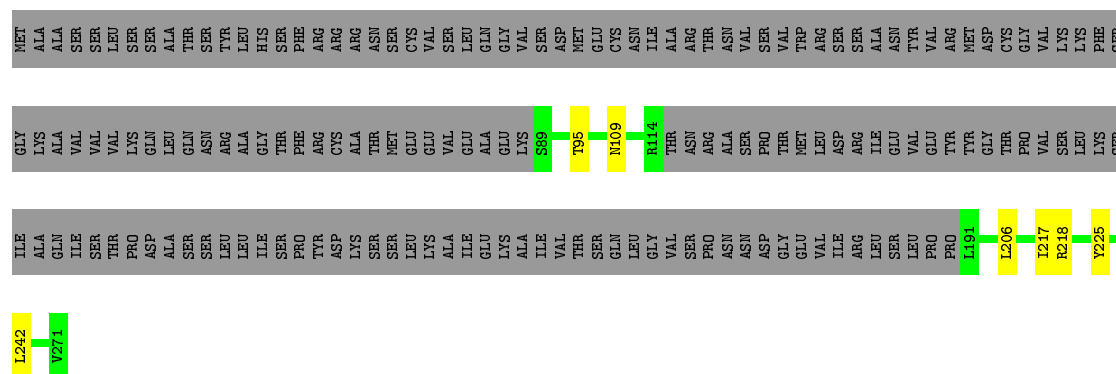
- Molecule 29: 50S ribosomal protein L36, chloroplactic

Chain 6:  95% 5%



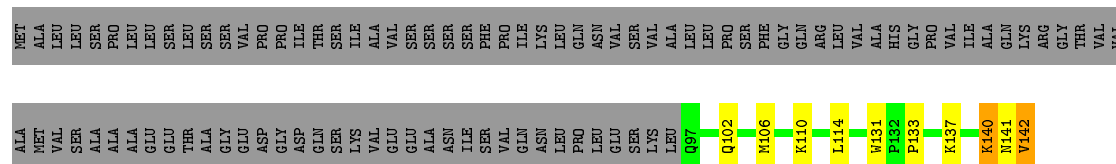
- Molecule 30: Ribosome-recycling factor, chloroplactic

Chain 9:  37% 61%



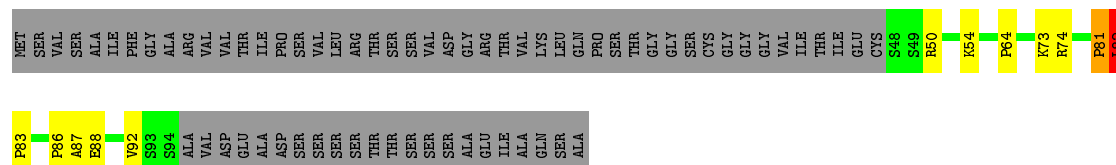
- Molecule 31: PSRP5alpha, chloroplactic

Chain 7:  25% 6%



- Molecule 32: PSRP6, chloroplactic

Chain 8:  30% 9%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	37636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 2	RMSZ	# Z > 2
1	A	0.40	19/66169 (0.0%)	0.73	32/103225 (0.0%)
10	L	0.47	1/1521 (0.1%)	0.72	2/2062 (0.1%)
11	M	0.41	0/943	0.69	0/1271
12	N	0.44	0/1405	0.78	0/1864
13	O	0.43	0/1097	0.76	0/1471
14	P	0.47	0/960	0.82	0/1280
15	Q	0.43	0/946	0.69	0/1268
16	R	0.48	1/928 (0.1%)	0.71	0/1248
17	S	0.46	0/1020	0.82	0/1361
18	T	0.81	1/1034 (0.1%)	0.82	5/1405 (0.4%)
19	U	0.86	1/1184 (0.1%)	0.73	0/1593
2	B	0.29	0/2868	0.71	0/4469
20	V	0.50	1/744 (0.1%)	0.67	0/1000
21	W	0.55	1/1030 (0.1%)	0.71	1/1374 (0.1%)
22	X	0.41	0/882	0.64	1/1172 (0.1%)
23	Y	0.45	0/626	0.76	0/833
24	Z	0.42	0/796	0.77	0/1056
25	2	0.59	0/348	0.74	0/462
26	3	0.42	0/497	0.75	0/664
27	4	0.45	0/474	0.92	0/624
28	5	0.39	0/581	0.81	0/768
29	6	0.39	0/307	0.80	0/403
3	C	0.28	0/2241	0.69	0/3492
30	9	0.41	0/883	0.57	0/1169
31	7	0.45	0/381	0.75	0/498
32	8	0.45	0/388	0.73	0/528
4	D	0.43	0/1928	0.74	0/2588
5	E	0.41	0/1696	0.71	0/2269
6	F	0.56	2/1648 (0.1%)	0.72	0/2215
7	G	0.46	0/1408	0.58	0/1896
8	H	0.57	2/1407 (0.1%)	0.61	0/1892
9	I	0.47	0/362	0.69	0/480
All	All	0.43	29/98702 (0.0%)	0.73	41/147900 (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
18	T	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1554	C	O3'-P	-23.08	1.33	1.61
19	U	158	ILE	C-N	22.12	1.84	1.34
18	T	118	PRO	C-N	19.55	1.71	1.34
1	A	1435	U	O3'-P	-13.97	1.44	1.61
8	H	71	GLU	CD-OE2	12.96	1.40	1.25
6	F	180	GLU	CD-OE2	11.81	1.38	1.25
21	W	169	ASP	C-N	10.59	1.58	1.34
1	A	1618	C	O3'-P	-10.03	1.49	1.61
1	A	1264	C	N1-C6	9.51	1.42	1.37
1	A	1264	C	C4-C5	9.37	1.50	1.43
1	A	1239	C	C3'-O3'	7.75	1.52	1.42
1	A	1264	C	N1-C2	7.68	1.47	1.40
1	A	2530	U	N1-C2	7.65	1.45	1.38
1	A	1239	C	O3'-P	7.59	1.70	1.61
8	H	71	GLU	CD-OE1	7.48	1.33	1.25
1	A	2530	U	C4-C5	7.38	1.50	1.43
16	R	230	SER	C-O	7.17	1.36	1.23
1	A	2530	U	N1-C6	7.14	1.44	1.38
1	A	1608	C	O3'-P	-6.96	1.52	1.61
1	A	1264	C	N3-C4	6.65	1.38	1.33
6	F	211	ASP	CB-CG	6.41	1.65	1.51
1	A	1698	C	N1-C6	6.18	1.40	1.37
1	A	2530	U	N3-C4	5.82	1.43	1.38
1	A	1698	C	C4-C5	5.77	1.47	1.43
20	V	131	GLU	CD-OE1	5.66	1.31	1.25
10	L	84	MET	C-N	5.58	1.46	1.34
1	A	1015	C	N1-C6	5.44	1.40	1.37
1	A	261	U	O3'-P	5.20	1.67	1.61
1	A	399	U	N1-C2	5.06	1.43	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	U	N1-C1'-C2'	-11.30	99.31	114.00
1	A	1618	C	P-O3'-C3'	-10.44	107.17	119.70
1	A	763	A	C2'-C3'-O3'	8.73	128.71	109.50
1	A	50	G	C2'-C3'-O3'	7.76	126.57	109.50
1	A	261	U	C2'-C3'-O3'	7.38	125.74	109.50
1	A	1411	U	C2'-C3'-O3'	7.28	125.52	109.50
1	A	1618	C	OP2-P-O3'	6.89	120.36	105.20
1	A	1239	C	OP1-P-O3'	6.88	120.33	105.20
1	A	313	A	C2'-C3'-O3'	6.83	124.63	113.70
1	A	1264	C	C6-N1-C2	6.66	122.97	120.30
1	A	1435	U	OP2-P-O3'	6.39	119.25	105.20
1	A	1435	U	O3'-P-O5'	-6.34	91.95	104.00
18	T	118	PRO	N-CA-CB	6.28	110.83	103.30
1	A	266	A	O4'-C1'-N9	6.27	113.22	108.20
1	A	2628	C	C2'-C3'-O3'	6.27	123.72	113.70
1	A	2254	A	C4'-C3'-O3'	6.22	125.44	113.00
1	A	1264	C	N3-C4-C5	6.15	124.36	121.90
1	A	1239	C	C4'-C3'-O3'	6.12	125.25	113.00
1	A	1493	C	C2'-C3'-O3'	6.04	123.36	113.70
1	A	2216	U	C2'-C3'-O3'	6.03	123.34	113.70
1	A	1536	A	C2'-C3'-O3'	6.01	123.32	113.70
21	W	171	PRO	N-CA-CB	6.01	110.52	103.30
1	A	1608	C	O3'-P-O5'	6.01	115.42	104.00
18	T	116	PRO	N-CA-CB	6.00	110.50	103.30
1	A	1439	U	C2'-C3'-O3'	5.99	123.29	113.70
18	T	101	PRO	N-CA-CB	5.99	110.49	103.30
10	L	78	PRO	N-CA-CB	5.97	110.47	103.30
18	T	117	PRO	N-CA-CB	5.97	110.47	103.30
1	A	1260	G	C4'-C3'-O3'	5.69	124.38	113.00
1	A	261	U	C4'-C3'-C2'	-5.61	96.99	102.60
1	A	2408	G	C4'-C3'-O3'	5.58	124.15	113.00
1	A	1399	A	C4'-C3'-O3'	5.57	124.13	113.00
1	A	261	U	C4'-C3'-O3'	5.51	124.03	113.00
18	T	118	PRO	O-C-N	5.46	131.47	121.10
1	A	654	U	C2'-C3'-O3'	5.41	122.35	113.70
1	A	856	U	C2'-C3'-O3'	5.39	122.33	113.70
10	L	75	PRO	N-CA-CB	5.36	109.73	103.30
1	A	1050	G	C2'-C3'-O3'	5.28	122.15	113.70
22	X	76	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	1002	G	N9-C1'-C2'	5.19	120.75	114.00
1	A	1610	C	C2'-C3'-O3'	5.19	122.00	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	T	116	PRO	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	A	59074	0	29746	385	0
2	B	2564	0	1295	7	0
3	C	2001	0	1008	11	0
4	D	1895	0	1977	18	0
5	E	1669	0	1753	11	0
6	F	1617	0	1677	10	0
7	G	1387	0	1443	7	0
8	H	1386	0	1448	12	0
9	I	359	0	415	3	0
10	L	1489	0	1434	8	0
11	M	934	0	985	10	0
12	N	1385	0	1464	13	0
13	O	1075	0	1134	13	0
14	P	945	0	1004	11	0
15	Q	931	0	952	3	0
16	R	915	0	1008	8	0
17	S	1003	0	1069	6	0
18	T	1017	0	1017	15	0
19	U	1165	0	1175	11	0
20	V	734	0	780	9	0
21	W	1018	0	1072	7	0
22	X	866	0	909	7	0
23	Y	616	0	665	7	0
24	Z	788	0	849	23	0
25	2	341	0	379	5	0
26	3	489	0	511	5	0
27	4	471	0	529	2	0
28	5	575	0	642	3	0
29	6	305	0	344	0	0
30	9	881	0	932	4	0
31	7	378	0	445	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	8	374	0	391	5	0
All	All	90647	0	60452	576	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (576) 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)
1:A:133:A:C6	24:Z:131:ARG:NH1	1.78	1.50
1:A:133:A:C2	24:Z:131:ARG:NH2	1.80	1.45
18:T:118:PRO:C	18:T:119:PRO:N	1.71	1.42
1:A:133:A:C5	24:Z:131:ARG:NH1	1.78	1.36
19:U:158:ILE:C	19:U:159:ALA:N	1.84	1.27
1:A:137:U:N3	1:A:160:A:N1	1.85	1.24
1:A:81:G:N2	1:A:102:U:O4	1.71	1.21
1:A:1049:A:N1	1:A:1168:U:O4	1.71	1.20
1:A:133:A:C6	24:Z:131:ARG:CZ	2.33	1.11
1:A:137:U:O2	1:A:160:A:H2	1.32	1.11
1:A:133:A:N1	24:Z:131:ARG:CZ	2.21	1.03
1:A:219:U:H3	1:A:442:A:N6	1.58	1.02
1:A:1524:G:N3	31:7:102:GLN:NE2	2.06	1.02
1:A:1239:C:H2'	1:A:1240:G:H5''	1.37	1.00
1:A:262:G:C8	1:A:262:G:H5''	1.99	0.98
1:A:2666:U:N3	1:A:2688:A:C2	2.31	0.98
1:A:2227:C:O2	1:A:2230:A:N6	1.97	0.97
1:A:1242:G:H8	1:A:1242:G:H5'	1.26	0.97
1:A:1529:A:N1	1:A:1537:U:N3	2.14	0.95
1:A:133:A:C2	24:Z:131:ARG:CZ	2.51	0.93
1:A:1524:G:C2	31:7:102:GLN:NE2	2.38	0.92
1:A:2666:U:O4	1:A:2688:A:N1	2.03	0.91
1:A:137:U:O2	1:A:160:A:C2	2.23	0.90
1:A:2517:U:O2	1:A:2521:U:O4	1.90	0.90
1:A:940:C:O2	1:A:956:G:N2	2.06	0.88
1:A:219:U:O2	1:A:219:U:H2'	1.75	0.86
1:A:1239:C:C5	1:A:1240:G:N2	2.44	0.85
1:A:2666:U:H3	1:A:2688:A:H2	0.86	0.85
1:A:2666:U:N3	1:A:2688:A:H2	1.67	0.85
1:A:110:U:OP2	24:Z:130:LYS:NZ	2.11	0.84
1:A:1239:C:C2'	1:A:1240:G:H5''	2.05	0.84
1:A:133:A:N1	24:Z:131:ARG:NH2	2.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1242:G:C8	1:A:1242:G:H5'	2.14	0.83
1:A:1535:A:O2'	4:D:97:LYS:NZ	2.12	0.83
1:A:137:U:C2	1:A:160:A:C2	2.67	0.82
1:A:2321:G:H22	1:A:2329:U:H3	1.24	0.82
19:U:33:THR:HG22	19:U:135:VAL:HG22	1.58	0.82
1:A:1047:U:N3	1:A:1169:A:N6	2.29	0.81
1:A:227:G:O2'	1:A:228:U:OP2	1.99	0.81
1:A:137:U:N3	1:A:160:A:C2	2.46	0.80
1:A:98:G:N2	1:A:100:G:H22	1.78	0.80
1:A:2663:C:C4	1:A:2750:G:C2	2.71	0.78
1:A:2663:C:C5	1:A:2750:G:C2	2.71	0.78
14:P:61:MET:HE1	14:P:80:ILE:HD11	1.66	0.78
4:D:142:ILE:HD11	4:D:150:LEU:HD21	1.65	0.78
1:A:1434:G:O6	1:A:1623:A:N6	2.16	0.78
1:A:137:U:C2	1:A:160:A:H2	2.01	0.77
1:A:219:U:H3	1:A:442:A:H61	0.80	0.77
1:A:2666:U:C4	1:A:2688:A:N1	2.53	0.77
11:M:102:ILE:HD11	11:M:117:ALA:HB2	1.67	0.77
5:E:199:ILE:HD11	5:E:278:ILE:HD13	1.67	0.75
1:A:1438:G:C2'	1:A:1623:A:HO2'	1.98	0.74
1:A:941:C:O2	1:A:955:G:N2	2.18	0.74
1:A:98:G:C2	1:A:100:G:N2	2.56	0.74
1:A:541:G:O6	1:A:2037:G:OP1	2.06	0.73
1:A:1749:U:O4	1:A:1755:A:N1	2.20	0.73
1:A:98:G:N2	1:A:100:G:N2	2.36	0.73
1:A:1242:G:H8	1:A:1242:G:C5'	2.03	0.72
1:A:158:C:N4	24:Z:129:GLY:O	2.23	0.71
1:A:1950:A:N1	1:A:1957:U:O4	2.24	0.71
16:R:130:ALA:HB1	16:R:177:ILE:HD12	1.73	0.71
1:A:1530:G:H22	1:A:1536:A:H2	1.37	0.71
18:T:118:PRO:C	18:T:119:PRO:CA	2.59	0.70
1:A:2663:C:C5	1:A:2750:G:N2	2.58	0.70
1:A:1049:A:N1	1:A:1168:U:C4	2.58	0.70
1:A:2521:U:H2'	1:A:2521:U:O2	1.92	0.69
1:A:2128:A:C6	1:A:2131:U:C4	2.79	0.69
1:A:1004:G:O6	1:A:1016:G:N2	2.26	0.69
20:V:178:LEU:HD12	20:V:184:ALA:HB2	1.75	0.68
1:A:1438:G:O2'	1:A:1623:A:O2'	1.69	0.68
1:A:2329:U:H2'	1:A:2329:U:O2	1.92	0.68
1:A:2665:U:H2'	1:A:2666:U:C6	2.29	0.68
1:A:1663:G:N7	31:7:142:VAL:HB	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:U:O2	1:A:219:U:C2'	2.43	0.67
1:A:2328:A:O2'	1:A:2329:U:H6	1.78	0.66
1:A:1524:G:N2	31:7:102:GLN:NE2	2.44	0.66
13:O:68:ILE:HD13	13:O:103:LEU:HD23	1.78	0.66
1:A:133:A:C4	24:Z:131:ARG:NH1	2.44	0.66
1:A:2328:A:HO2'	1:A:2329:U:H6	1.44	0.65
18:T:123:ILE:HG22	18:T:166:THR:HB	1.78	0.65
1:A:1227:U:N3	1:A:1261:A:N6	2.43	0.65
1:A:234:C:O2	28:5:100:LYS:NZ	2.30	0.65
1:A:2128:A:C6	1:A:2131:U:O4	2.50	0.65
15:Q:100:THR:HG23	15:Q:123:ILE:HD11	1.78	0.65
1:A:102:U:C5	1:A:103:C:C5	2.86	0.64
1:A:446:U:O2	1:A:448:C:C4	2.49	0.64
30:9:225:TYR:CE1	30:9:242:LEU:HD13	2.33	0.64
1:A:2224:G:O6	1:A:2228:C:N4	2.31	0.64
1:A:2663:C:C4	1:A:2750:G:N2	2.66	0.64
1:A:2128:A:N6	1:A:2131:U:C4	2.66	0.64
5:E:90:ILE:HD11	5:E:179:PHE:CE1	2.33	0.63
1:A:1439:U:H2'	1:A:1440:C:O4'	1.98	0.63
1:A:609:G:C2	1:A:670:A:C2	2.87	0.63
1:A:1047:U:C4	1:A:1169:A:N6	2.67	0.63
1:A:1530:G:N2	1:A:1536:A:H2	1.97	0.63
20:V:119:ILE:HD12	20:V:135:LEU:HG	1.81	0.63
1:A:1049:A:C2	1:A:1168:U:O4	2.51	0.62
1:A:1476:G:O6	1:A:2721:C:N3	2.32	0.62
10:L:119:ALA:HA	10:L:122:LEU:HD12	1.80	0.61
14:P:38:LEU:HD23	14:P:58:VAL:HG21	1.82	0.61
18:T:160:LYS:HD2	18:T:176:ILE:HD11	1.81	0.61
1:A:133:A:N6	24:Z:131:ARG:NH1	2.44	0.61
16:R:119:LEU:HD23	16:R:122:ILE:HD12	1.83	0.61
2:B:66:C:C5	2:B:110:C:C4	2.89	0.60
1:A:446:U:C2	1:A:448:C:N4	2.69	0.60
1:A:26:G:C2	1:A:523:G:N3	2.69	0.60
1:A:932:A:O2'	22:X:85:GLN:NE2	2.27	0.60
13:O:118:VAL:HG21	13:O:131:PHE:CD1	2.37	0.60
5:E:237:ALA:HB3	5:E:241:PRO:HG3	1.82	0.60
1:A:261:U:H3	1:A:266:A:H2	1.47	0.59
1:A:2784:G:H2'	1:A:2784:G:N3	2.17	0.59
1:A:1880:G:N7	12:N:252:ARG:NH1	2.49	0.59
18:T:118:PRO:CA	18:T:119:PRO:N	2.62	0.59
1:A:1475:U:O2'	1:A:1476:G:N2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:A:O2'	1:A:1229:G:O5'	2.18	0.59
1:A:2339:A:H2'	1:A:2340:G:O4'	2.03	0.59
1:A:651:U:H2'	1:A:652:C:C6	2.38	0.58
1:A:966:G:OP1	28:5:157:ARG:NH2	2.37	0.58
1:A:2472:G:H2'	1:A:2473:C:H6	1.68	0.58
1:A:1870:U:H3	1:A:1896:G:H1	1.51	0.58
1:A:1227:U:N3	1:A:1261:A:C6	2.70	0.58
1:A:2218:G:C2	1:A:2220:G:C5	2.92	0.58
1:A:6:A:C2	3:C:98:U:C2	2.92	0.57
27:4:120:THR:HG23	27:4:123:GLY:HA3	1.86	0.57
1:A:227:G:HO2'	1:A:228:U:P	2.22	0.57
24:Z:68:LEU:O	24:Z:122:ARG:NH2	2.36	0.57
1:A:2344:A:H2'	1:A:2345:A:C8	2.40	0.57
1:A:956:G:C6	1:A:957:U:O4	2.57	0.57
6:F:212:LEU:HD11	6:F:228:LEU:HD23	1.87	0.57
1:A:1047:U:C2	1:A:1171:G:N2	2.73	0.57
5:E:167:HIS:CG	5:E:289:LEU:HD11	2.40	0.57
1:A:1239:C:C6	1:A:1240:G:N2	2.72	0.57
1:A:26:G:N2	1:A:523:G:H1'	2.21	0.56
12:N:160:ILE:HD11	12:N:198:LEU:HD13	1.88	0.56
1:A:255:A:O2'	1:A:256:A:O4'	2.22	0.56
1:A:2472:G:H2'	1:A:2473:C:C6	2.40	0.56
4:D:129:THR:HG22	4:D:182:LYS:HD2	1.87	0.56
1:A:379:C:H2'	1:A:380:C:H6	1.71	0.56
1:A:446:U:O2	1:A:448:C:N4	2.38	0.56
5:E:97:LEU:HD11	16:R:119:LEU:HD22	1.88	0.56
14:P:77:LEU:HD13	14:P:86:VAL:HG11	1.87	0.56
1:A:1:U:H2'	1:A:2:U:C5	2.40	0.56
1:A:389:A:C6	1:A:390:U:C4	2.94	0.56
1:A:378:A:C8	1:A:379:C:C5	2.94	0.56
1:A:839:G:H4'	1:A:842:G:N1	2.21	0.56
1:A:298:G:C2	1:A:299:C:C6	2.94	0.55
1:A:981:G:OP2	13:O:16:ARG:NH1	2.38	0.55
32:8:82:LEU:HD23	32:8:83:PRO:HD2	1.88	0.55
1:A:2328:A:C2'	1:A:2329:U:H6	2.19	0.55
1:A:2703:G:H2'	1:A:2704:U:O4'	2.07	0.55
1:A:2688:A:H2'	1:A:2689:A:C8	2.41	0.55
18:T:136:VAL:HG23	18:T:221:ILE:HG13	1.86	0.55
26:3:15:CYS:HB3	26:3:17:GLY:O	2.07	0.55
12:N:225:LEU:HD13	12:N:232:VAL:HG21	1.89	0.55
1:A:2655:G:HO2'	1:A:2656:A:H8	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2108:G:H1	1:A:2209:U:H3	1.55	0.55
1:A:1238:G:N2	1:A:1253:G:H22	2.05	0.55
1:A:262:G:C5'	1:A:262:G:C8	2.85	0.55
1:A:856:U:O2'	1:A:857:G:OP1	2.16	0.55
1:A:1238:G:N2	1:A:1253:G:N2	2.55	0.54
1:A:446:U:O2	1:A:448:C:C5	2.60	0.54
3:C:85:C:O4'	3:C:85:C:O2	2.23	0.54
10:L:122:LEU:O	10:L:162:ALA:HB3	2.07	0.54
1:A:494:A:O2'	1:A:508:A:N1	2.36	0.54
1:A:769:C:H2'	1:A:769:C:O2	2.07	0.54
11:M:24:ILE:HD12	11:M:33:ALA:HB2	1.88	0.54
1:A:102:U:C4	1:A:103:C:C5	2.95	0.54
15:Q:100:THR:CG2	15:Q:123:ILE:HD11	2.37	0.54
1:A:1056:A:N3	1:A:2503:G:O2'	2.33	0.54
1:A:1547:C:OP1	31:7:106:MET:HE1	2.08	0.54
31:7:110:LYS:HG2	31:7:114:LEU:HD12	1.90	0.54
26:3:18:CYS:HG	26:3:55:CYS:HG	1.50	0.54
1:A:1047:U:N3	1:A:1169:A:C6	2.72	0.54
12:N:99:GLY:HA2	12:N:107:GLY:HA2	1.90	0.53
1:A:1500:U:O2	1:A:1500:U:H2'	2.07	0.53
30:9:109:ASN:HB3	30:9:206:LEU:HD22	1.90	0.53
1:A:2362:G:N3	1:A:2398:C:H2'	2.24	0.53
25:2:34:LEU:O	25:2:34:LEU:HD13	2.09	0.53
1:A:1559:A:H2'	1:A:1559:A:N3	2.23	0.53
1:A:2345:A:H2'	1:A:2346:A:C8	2.43	0.53
1:A:2472:G:C4	1:A:2473:C:C5	2.97	0.53
21:W:75:VAL:HG21	21:W:89:ILE:HD11	1.91	0.53
1:A:13:A:H2'	1:A:14:A:C8	2.43	0.53
21:W:101:ILE:HG21	21:W:104:LEU:HD22	1.90	0.53
1:A:2644:G:O2'	1:A:2799:A:N1	2.32	0.53
1:A:975:A:O2'	1:A:1012:G:N2	2.39	0.52
1:A:2328:A:O2'	1:A:2329:U:C6	2.55	0.52
1:A:1612:A:H2'	1:A:1613:A:O4'	2.10	0.52
1:A:1004:G:C6	1:A:1016:G:N2	2.78	0.52
1:A:1693:U:H2'	1:A:1694:C:H6	1.75	0.52
1:A:2701:U:OP2	16:R:173:GLN:NE2	2.42	0.52
14:P:65:ALA:HA	14:P:90:PHE:CE1	2.44	0.52
1:A:1438:G:C2'	1:A:1623:A:O2'	2.54	0.52
1:A:2227:C:C2	1:A:2230:A:N6	2.76	0.52
1:A:2517:U:O2	1:A:2521:U:C4	2.61	0.52
24:Z:93:GLN:N	24:Z:93:GLN:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2303:A:H4'	1:A:2304:A:O4'	2.09	0.52
1:A:2329:U:O2	7:G:52:ASN:ND2	2.43	0.52
1:A:403:A:C4	1:A:404:U:C6	2.98	0.52
2:B:13:C:O2	2:B:13:C:O4'	2.25	0.52
1:A:415:U:O2'	1:A:416:C:O2	2.24	0.52
24:Z:130:LYS:NZ	24:Z:130:LYS:CB	2.73	0.52
1:A:138:C:H2'	1:A:138:C:O2	2.09	0.51
1:A:204:A:H2	1:A:219:U:O2	1.93	0.51
1:A:956:G:C4	1:A:957:U:C5	2.99	0.51
1:A:1410:G:N2	1:A:1420:C:C2	2.79	0.51
1:A:133:A:C4	24:Z:131:ARG:NH2	2.73	0.51
1:A:1227:U:H2'	1:A:1228:A:O5'	2.10	0.51
1:A:2033:A:N7	25:2:6:LYS:NZ	2.52	0.51
1:A:333:A:N6	1:A:347:G:O2'	2.43	0.51
1:A:1024:A:OP1	18:T:132:ARG:HD2	2.10	0.51
1:A:138:C:C2'	1:A:138:C:O2	2.58	0.51
1:A:2329:U:O2	1:A:2329:U:C2'	2.58	0.51
16:R:187:ILE:HG23	16:R:188:ALA:N	2.24	0.51
1:A:2535:C:H2'	1:A:2535:C:O2	2.11	0.51
1:A:1213:G:OP2	12:N:96:LYS:NZ	2.44	0.51
13:O:21:SER:HB2	13:O:98:LYS:HB2	1.93	0.51
17:S:14:ARG:HD2	17:S:32:THR:HG23	1.93	0.51
1:A:1242:G:C8	1:A:1242:G:C5'	2.87	0.51
1:A:771:G:H2'	1:A:772:A:O4'	2.11	0.51
1:A:1819:A:H2'	1:A:1820:A:C8	2.45	0.50
1:A:133:A:N3	24:Z:131:ARG:NH2	2.17	0.50
1:A:384:G:O2'	1:A:385:U:OP2	2.29	0.50
1:A:1693:U:H2'	1:A:1694:C:C6	2.46	0.50
12:N:185:GLY:C	12:N:186:ILE:HD12	2.31	0.50
1:A:2307:G:H2'	1:A:2308:U:C6	2.46	0.50
1:A:740:G:OP2	4:D:203:ARG:NH2	2.45	0.50
19:U:130:CYS:SG	19:U:131:HIS:N	2.85	0.50
1:A:416:C:O4'	1:A:416:C:O2	2.29	0.50
18:T:175:PRO:HG2	32:8:82:LEU:HD21	1.94	0.50
1:A:2784:G:C2	1:A:2785:C:C6	3.00	0.50
1:A:2521:U:O2	1:A:2521:U:C2'	2.60	0.50
1:A:956:G:C6	1:A:957:U:C4	2.99	0.49
1:A:570:C:O2'	17:S:52:ARG:NH2	2.41	0.49
1:A:1114:A:H2'	1:A:1114:A:N3	2.26	0.49
1:A:1495:C:C2	1:A:1548:A:N6	2.80	0.49
1:A:1950:A:N1	1:A:1957:U:C4	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:G:H2'	1:A:2044:A:N7	2.27	0.49
1:A:8:G:O2'	3:C:96:A:N6	2.46	0.49
8:H:50:VAL:HG13	8:H:54:VAL:HG11	1.94	0.49
16:R:170:ILE:HD11	16:R:182:ARG:HD3	1.94	0.49
1:A:1228:A:O2'	1:A:1229:G:H8	1.94	0.49
1:A:2707:A:O2'	1:A:2708:C:O5'	2.30	0.49
1:A:1806:U:H2'	1:A:1807:C:H6	1.77	0.49
1:A:818:U:C2	1:A:819:G:C8	3.01	0.49
1:A:2707:A:O2'	1:A:2708:C:P	2.70	0.49
8:H:138:VAL:HG21	8:H:165:VAL:HG21	1.95	0.49
6:F:102:THR:HB	6:F:139:VAL:HG11	1.95	0.49
6:F:116:TYR:HB2	6:F:117:PRO:HD2	1.95	0.49
22:X:119:ILE:HG23	22:X:120:ASP:O	2.13	0.49
1:A:542:C:O2'	17:S:41:ARG:NH2	2.42	0.48
4:D:131:MET:SD	4:D:137:ILE:HG21	2.53	0.48
14:P:38:LEU:CD2	14:P:58:VAL:HG21	2.42	0.48
4:D:200:ARG:O	4:D:202:GLY:N	2.46	0.48
1:A:1499:G:H2'	1:A:1500:U:C6	2.48	0.48
6:F:94:ASN:ND2	6:F:149:THR:HG23	2.28	0.48
1:A:1194:G:O2'	1:A:1195:U:O5'	2.31	0.48
23:Y:88:VAL:HG13	23:Y:92:ASN:HA	1.95	0.48
1:A:1007:A:H4'	32:8:64:PRO:HG3	1.94	0.48
1:A:2642:G:H2'	1:A:2643:C:O4'	2.13	0.48
1:A:403:A:C5	1:A:404:U:C5	3.01	0.48
24:Z:130:LYS:HZ3	24:Z:130:LYS:HB3	1.78	0.48
1:A:1551:G:C2	1:A:1552:U:C5	3.01	0.48
1:A:85:U:H3	1:A:95:G:H1	1.62	0.48
5:E:122:ILE:HD12	5:E:165:MET:CE	2.44	0.48
1:A:2738:U:C2	1:A:2739:A:C8	3.02	0.47
9:I:53:LEU:HD13	9:I:65:GLN:HB2	1.96	0.47
1:A:2809:U:O2	1:A:2809:U:O4'	2.30	0.47
1:A:394:G:H22	1:A:404:U:H3	1.62	0.47
1:A:382:G:C6	1:A:436:G:N7	2.82	0.47
6:F:208:PHE:CE1	6:F:234:LEU:HD13	2.50	0.47
1:A:1224:U:O4	1:A:1225:G:C2	2.68	0.47
21:W:145:ASP:CG	21:W:146:ARG:N	2.68	0.47
27:4:146:SER:O	27:4:150:ALA:HB2	2.14	0.47
1:A:2328:A:C2'	1:A:2329:U:C6	2.97	0.47
1:A:373:C:H2'	1:A:374:U:C6	2.50	0.47
4:D:84:ASN:ND2	4:D:196:VAL:HG11	2.29	0.47
1:A:1220:U:H2'	1:A:1221:C:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2663:C:C5	1:A:2750:G:N3	2.82	0.47
1:A:816:G:O4'	12:N:117:GLN:HG3	2.14	0.47
1:A:378:A:H2'	1:A:378:A:N3	2.29	0.47
1:A:589:G:H2'	1:A:590:C:C6	2.49	0.47
19:U:32:ILE:HG21	19:U:87:ALA:HB2	1.95	0.47
1:A:445:C:H2'	1:A:446:U:C6	2.49	0.47
1:A:955:G:C6	1:A:956:G:C8	3.02	0.47
1:A:2263:C:H2'	1:A:2264:U:C6	2.50	0.47
14:P:64:LEU:HD23	14:P:76:ALA:HB2	1.96	0.47
1:A:2310:U:H3	1:A:2356:G:H1	1.63	0.47
1:A:2707:A:C8	1:A:2708:C:C6	3.03	0.47
1:A:1:U:H2'	1:A:2:U:C6	2.49	0.47
3:C:100:G:H2'	3:C:101:A:C8	2.49	0.47
4:D:29:ILE:O	4:D:29:ILE:HG23	2.14	0.47
1:A:138:C:N3	1:A:139:U:C5	2.82	0.47
1:A:1419:C:O2	1:A:1419:C:H2'	2.14	0.47
1:A:261:U:O4	1:A:266:A:N1	2.48	0.47
1:A:880:U:OP1	13:O:6:ARG:NH1	2.48	0.47
8:H:183:GLN:O	8:H:187:THR:HG23	2.14	0.47
18:T:124:PHE:CB	18:T:137:ILE:HG22	2.44	0.47
1:A:328:C:N3	1:A:332:G:O6	2.47	0.46
1:A:553:G:O2'	1:A:554:G:O5'	2.33	0.46
1:A:932:A:C2'	22:X:85:GLN:HE22	2.27	0.46
1:A:176:A:H2'	1:A:177:C:C6	2.49	0.46
1:A:2658:A:OP2	10:L:175:ARG:NH2	2.49	0.46
11:M:58:ILE:HD13	11:M:86:ILE:HG23	1.98	0.46
12:N:201:LEU:HD23	12:N:218:SER:HB3	1.98	0.46
1:A:1950:A:C2	1:A:1957:U:N3	2.83	0.46
1:A:2707:A:HO2'	1:A:2708:C:H6	1.61	0.46
1:A:824:U:H2'	1:A:825:C:C6	2.50	0.46
12:N:160:ILE:HD11	12:N:198:LEU:CD1	2.45	0.46
20:V:112:TYR:CE1	24:Z:146:VAL:HG23	2.51	0.46
22:X:141:GLU:HB3	22:X:142:ILE:HD12	1.96	0.46
1:A:133:A:C4	24:Z:131:ARG:CZ	2.98	0.46
1:A:1321:A:C2	1:A:1662:A:N6	2.84	0.46
14:P:77:LEU:HD11	14:P:83:LYS:HG2	1.97	0.46
1:A:137:U:C4	1:A:160:A:N1	2.76	0.46
5:E:197:VAL:CG2	5:E:266:ILE:HD11	2.46	0.46
11:M:98:ILE:HD13	11:M:113:ILE:HG23	1.98	0.46
18:T:176:ILE:HD13	32:8:86:PRO:HD2	1.98	0.46
1:A:384:G:O2'	1:A:385:U:P	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:192:GLY:HA3	24:Z:93:GLN:HE21	1.81	0.46
23:Y:104:GLN:O	23:Y:120:ARG:HA	2.16	0.46
1:A:379:C:H2'	1:A:380:C:C6	2.51	0.46
20:V:135:LEU:HD13	20:V:175:TYR:CD1	2.51	0.46
23:Y:88:VAL:HG12	23:Y:89:SER:O	2.16	0.46
8:H:194:PRO:CG	8:H:209:VAL:HG21	2.45	0.46
8:H:194:PRO:HB2	8:H:209:VAL:HG11	1.97	0.46
13:O:53:ALA:HB1	13:O:120:ILE:CG2	2.46	0.46
1:A:138:C:C2	1:A:139:U:C5	3.04	0.46
1:A:1558:U:H2'	1:A:1559:A:O4'	2.16	0.46
1:A:2043:G:N1	1:A:2047:A:OP2	2.43	0.46
1:A:299:C:H2'	1:A:300:U:C6	2.51	0.46
3:C:25:U:O2	3:C:80:C:C4	2.69	0.46
1:A:227:G:C2'	1:A:228:U:OP2	2.64	0.45
1:A:2354:G:H2'	1:A:2354:G:N3	2.31	0.45
1:A:1239:C:C4	1:A:1240:G:N2	2.84	0.45
1:A:119:A:C8	1:A:132:G:C5	3.05	0.45
6:F:93:GLN:HE21	6:F:93:GLN:HB3	1.64	0.45
1:A:79:G:N2	1:A:105:G:C4	2.84	0.45
1:A:2663:C:C6	1:A:2750:G:N2	2.85	0.45
1:A:2653:U:O2'	5:E:134:TYR:OH	2.32	0.45
1:A:869:G:O2'	1:A:870:U:P	2.75	0.45
1:A:2722:C:O2'	3:C:53:G:OP1	2.27	0.45
4:D:137:ILE:HG22	4:D:188:VAL:HA	1.97	0.45
1:A:1957:U:N3	1:A:1959:G:O4'	2.49	0.45
1:A:2092:C:H2'	1:A:2093:U:O4'	2.16	0.45
2:B:44:C:O2	7:G:107:ARG:NH1	2.49	0.45
11:M:35:ILE:HD12	11:M:69:LEU:HD23	1.98	0.45
1:A:144:A:C2	1:A:2224:G:N2	2.85	0.45
1:A:2304:A:O2'	1:A:2305:A:H2'	2.17	0.45
1:A:2663:C:N4	1:A:2750:G:C2	2.85	0.45
20:V:163:ASN:OD1	20:V:163:ASN:N	2.49	0.45
7:G:119:ILE:HD13	7:G:189:GLY:O	2.17	0.45
23:Y:72:ARG:CD	23:Y:74:ILE:HD12	2.46	0.45
1:A:2128:A:N1	1:A:2131:U:O4	2.50	0.45
13:O:53:ALA:HB1	13:O:120:ILE:HG22	1.99	0.45
1:A:603:G:H1	1:A:675:U:H3	1.63	0.45
3:C:36:A:C2	3:C:80:C:C6	3.05	0.45
1:A:1201:A:H2'	1:A:1202:A:C8	2.50	0.45
1:A:1500:U:H3	1:A:1545:G:H1	1.65	0.45
1:A:869:G:HO2'	1:A:870:U:P	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:75:VAL:HG21	4:D:91:HIS:ND1	2.32	0.45
11:M:81:ASP:OD2	11:M:83:ALA:HB2	2.17	0.45
1:A:1694:C:C2	1:A:1695:U:C5	3.05	0.44
1:A:2218:G:C2	1:A:2220:G:N7	2.85	0.44
1:A:2102:G:H1	1:A:2248:U:H3	1.66	0.44
26:3:15:CYS:SG	26:3:61:HIS:CE1	3.11	0.44
1:A:1701:A:H2'	1:A:1702:G:O4'	2.17	0.44
1:A:1749:U:C4	1:A:1755:A:N1	2.84	0.44
1:A:701:U:H2'	1:A:702:C:O4'	2.17	0.44
1:A:2770:C:OP2	8:H:43:ILE:HD11	2.18	0.44
19:U:74:TYR:HB3	19:U:75:PRO:HD3	1.99	0.44
1:A:404:U:H2'	1:A:404:U:O2	2.16	0.44
1:A:650:G:H2'	1:A:651:U:C6	2.52	0.44
21:W:92:ILE:HG23	21:W:92:ILE:O	2.18	0.44
1:A:1629:G:H2'	1:A:1630:G:O4'	2.17	0.44
1:A:2421:C:H2'	1:A:2422:G:O4'	2.18	0.44
10:L:243:ASP:HB3	10:L:246:ILE:HB	1.99	0.44
14:P:61:MET:CE	14:P:80:ILE:HD11	2.42	0.44
1:A:1605:A:H2'	1:A:1606:A:C8	2.53	0.44
3:C:96:A:N3	3:C:96:A:H2'	2.32	0.44
7:G:78:GLN:NE2	7:G:105:THR:O	2.51	0.44
1:A:1001:A:O4'	1:A:1209:U:C6	2.71	0.44
1:A:1296:A:N6	1:A:1317:C:H4'	2.33	0.44
1:A:1763:G:C2	1:A:1766:G:C2	3.05	0.44
1:A:966:G:C6	1:A:967:C:C4	3.06	0.44
1:A:2707:A:O2'	1:A:2708:C:H6	2.01	0.44
1:A:2791:C:N3	1:A:2792:C:C5	2.86	0.44
7:G:119:ILE:HG21	7:G:189:GLY:O	2.18	0.44
10:L:242:ARG:O	10:L:243:ASP:HB2	2.18	0.44
1:A:1250:C:H2'	1:A:1251:G:C8	2.53	0.44
1:A:1261:A:C5	1:A:1262:A:C8	3.06	0.44
1:A:1559:A:C2	1:A:1560:C:C2	3.05	0.44
1:A:2387:G:C6	1:A:2388:G:C6	3.05	0.44
1:A:680:G:H2'	1:A:680:G:N3	2.32	0.44
17:S:47:HIS:CE1	18:T:197:VAL:HG13	2.53	0.44
22:X:146:ASN:HD22	22:X:148:ASN:HB2	1.83	0.44
1:A:2474:U:H2'	1:A:2475:G:O4'	2.18	0.43
1:A:316:G:H1'	1:A:317:G:OP2	2.18	0.43
1:A:856:U:C2'	1:A:857:G:OP1	2.66	0.43
2:B:91:G:C2'	2:B:92:U:OP2	2.66	0.43
7:G:94:VAL:HG23	7:G:95:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1731:G:N2	1:A:1732:G:C8	2.85	0.43
1:A:2085:A:H2'	1:A:2086:G:H8	1.84	0.43
1:A:410:G:C6	1:A:411:U:C4	3.06	0.43
1:A:519:A:N6	19:U:38:SER:OG	2.50	0.43
1:A:824:U:H2'	1:A:825:C:H6	1.83	0.43
8:H:163:VAL:HG22	8:H:173:VAL:HG13	2.00	0.43
8:H:56:ILE:HG21	8:H:84:LYS:HD3	2.00	0.43
14:P:42:GLY:O	14:P:124:GLU:HB2	2.18	0.43
1:A:1261:A:H3'	1:A:1261:A:C8	2.54	0.43
2:B:66:C:C6	2:B:110:C:N4	2.87	0.43
1:A:1798:C:C5'	4:D:220:VAL:HG21	2.48	0.43
14:P:64:LEU:HD12	14:P:72:LYS:HD2	2.01	0.43
1:A:1042:A:C6	1:A:1043:C:N4	2.86	0.43
1:A:1344:G:O6	1:A:1345:G:C6	2.72	0.43
1:A:2303:A:C2	26:3:48:LEU:HD11	2.53	0.43
1:A:389:A:C5	1:A:390:U:C5	3.06	0.43
1:A:572:U:C2	1:A:582:A:C8	3.06	0.43
1:A:869:G:O2'	1:A:870:U:OP2	2.34	0.43
13:O:12:GLN:HE21	13:O:73:PRO:HD2	1.82	0.43
1:A:2085:A:H2'	1:A:2086:G:C8	2.54	0.43
1:A:2663:C:N4	1:A:2750:G:N1	2.66	0.43
4:D:256:ARG:O	4:D:257:LYS:C	2.56	0.43
16:R:168:ILE:O	16:R:183:ILE:HA	2.19	0.43
1:A:1230:G:O2'	1:A:1258:A:N1	2.35	0.43
1:A:591:C:H2'	1:A:592:G:C8	2.54	0.43
2:B:66:C:C6	2:B:110:C:C4	3.07	0.43
3:C:63:G:H2'	3:C:64:U:O4'	2.19	0.43
19:U:87:ALA:HB1	19:U:93:PHE:HE2	1.83	0.43
4:D:138:HIS:ND1	4:D:189:GLY:O	2.51	0.43
1:A:1610:C:H6	1:A:1610:C:H5''	1.83	0.43
1:A:2111:U:O2'	1:A:2112:U:C6	2.59	0.43
1:A:2411:C:H2'	1:A:2412:C:O4'	2.19	0.43
1:A:503:C:H2'	1:A:504:G:O4'	2.18	0.43
32:8:81:PRO:O	32:8:82:LEU:HB2	2.19	0.43
1:A:1084:G:N2	1:A:1130:C:C5	2.87	0.43
1:A:1440:C:H2'	1:A:1441:C:O4'	2.19	0.43
1:A:298:G:H2'	1:A:298:G:N3	2.34	0.43
1:A:618:A:H2'	1:A:619:A:O4'	2.19	0.43
1:A:799:A:OP1	1:A:802:C:N4	2.48	0.43
6:F:207:PHE:CD1	6:F:226:LEU:HD11	2.54	0.43
1:A:2030:U:O2'	25:2:4:PRO:O	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:A:C3'	1:A:1261:A:C8	3.02	0.42
1:A:1363:A:O2'	1:A:1365:U:OP2	2.28	0.42
1:A:976:C:O2	1:A:1012:G:O2'	2.37	0.42
6:F:206:LEU:HD11	6:F:229:LEU:HD12	2.00	0.42
12:N:187:ILE:HG22	12:N:189:PRO:HD3	2.02	0.42
12:N:160:ILE:HD11	12:N:198:LEU:HD22	2.00	0.42
21:W:89:ILE:HD12	21:W:99:VAL:HG21	2.01	0.42
1:A:1026:C:H2'	1:A:1027:U:O4'	2.19	0.42
1:A:1142:G:C6	1:A:1143:C:C4	3.08	0.42
1:A:1171:G:H2'	1:A:1172:C:H6	1.84	0.42
1:A:2396:G:H2'	1:A:2397:U:C6	2.54	0.42
1:A:591:C:H2'	1:A:592:G:H8	1.84	0.42
18:T:150:ALA:HB3	18:T:189:GLN:HE22	1.84	0.42
1:A:1374:A:H2'	1:A:1375:A:C8	2.54	0.42
1:A:1806:U:H2'	1:A:1807:C:C6	2.54	0.42
1:A:373:C:H2'	1:A:374:U:H6	1.84	0.42
7:G:133:ASN:HD22	7:G:136:SER:HB2	1.84	0.42
21:W:68:HIS:O	21:W:159:ARG:NH2	2.53	0.42
26:3:52:CYS:SG	26:3:55:CYS:SG	3.14	0.42
1:A:668:U:H2'	1:A:669:C:C6	2.54	0.42
1:A:1743:G:C5	1:A:1744:C:C5	3.07	0.42
1:A:227:G:HO2'	1:A:239:G:H1	1.67	0.42
1:A:2791:C:C4	1:A:2792:C:C5	3.07	0.42
11:M:76:ILE:HG12	16:R:195:VAL:HG22	2.02	0.42
14:P:34:LEU:HB3	14:P:54:MET:SD	2.60	0.42
18:T:172:ILE:HD12	18:T:175:PRO:HA	2.01	0.42
18:T:155:LYS:HA	18:T:185:VAL:HA	2.01	0.42
21:W:93:HIS:CE1	21:W:100:ILE:HD11	2.55	0.42
1:A:1671:A:H2'	1:A:1672:U:O4'	2.20	0.42
1:A:176:A:H2'	1:A:177:C:H6	1.83	0.42
1:A:2743:A:O2'	1:A:2744:A:C8	2.73	0.42
1:A:559:G:O6	18:T:141:TRP:CD1	2.73	0.42
1:A:654:U:O2	1:A:654:U:O4'	2.36	0.42
1:A:836:G:H2'	1:A:837:U:O4'	2.20	0.42
11:M:63:VAL:HG12	11:M:106:LEU:HD21	2.02	0.42
22:X:107:VAL:CG2	22:X:137:VAL:HG23	2.49	0.42
1:A:2543:G:C5	1:A:2544:C:C5	3.08	0.42
5:E:167:HIS:CD2	5:E:289:LEU:HD11	2.55	0.42
19:U:83:ALA:HB1	19:U:136:LEU:HD11	2.02	0.42
1:A:1202:A:H2'	1:A:1203:C:C6	2.54	0.42
1:A:2607:A:H5''	4:D:234:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:G:C5	1:A:411:U:C5	3.08	0.42
1:A:539:A:C2	1:A:2056:A:H2'	2.55	0.42
1:A:815:A:H2'	1:A:817:C:C4	2.55	0.42
12:N:136:LEU:HD22	12:N:140:ILE:CD1	2.49	0.42
13:O:43:THR:HG22	13:O:92:TYR:CD2	2.54	0.42
10:L:95:ILE:O	17:S:99:GLN:NE2	2.53	0.42
20:V:115:LEU:HD21	20:V:151:ILE:CG1	2.50	0.42
1:A:1530:G:H1	1:A:1536:A:H2	1.64	0.41
1:A:1634:C:H2'	1:A:1634:C:O2	2.20	0.41
1:A:2472:G:C5	1:A:2473:C:C5	3.08	0.41
1:A:2484:C:O2	13:O:124:LYS:NZ	2.52	0.41
4:D:91:HIS:CD2	4:D:97:LYS:HD3	2.55	0.41
6:F:207:PHE:CE1	6:F:246:VAL:HG11	2.55	0.41
1:A:102:U:C4	1:A:103:C:C6	3.08	0.41
1:A:1261:A:H8	1:A:1261:A:C5'	2.33	0.41
1:A:1530:G:C2	1:A:1536:A:H2	2.39	0.41
1:A:2307:G:H2'	1:A:2308:U:O4'	2.20	0.41
1:A:309:A:N1	1:A:331:A:O2'	2.39	0.41
5:E:151:MET:N	5:E:152:PRO:HD2	2.36	0.41
13:O:2:LEU:N	13:O:44:SER:OG	2.53	0.41
1:A:1137:C:N3	1:A:1138:G:C2	2.88	0.41
1:A:136:U:C4	1:A:137:U:O4	2.74	0.41
1:A:1500:U:O2	1:A:1500:U:C2'	2.68	0.41
1:A:1956:C:O2'	30:9:218:ARG:NH2	2.54	0.41
1:A:1982:G:O2'	1:A:1983:A:O4'	2.37	0.41
1:A:548:G:N2	1:A:567:C:N4	2.69	0.41
19:U:153:THR:HB	19:U:154:PRO:HD3	2.02	0.41
24:Z:80:ILE:HG22	24:Z:84:LYS:HD2	2.01	0.41
1:A:2207:A:H2'	1:A:2208:U:O4'	2.21	0.41
1:A:233:G:H5'	1:A:235:G:N7	2.35	0.41
1:A:393:G:H2'	1:A:394:G:O4'	2.20	0.41
4:D:117:GLU:O	4:D:118:VAL:O	2.39	0.41
8:H:194:PRO:HG3	8:H:209:VAL:HG21	2.02	0.41
24:Z:112:VAL:HG12	24:Z:116:LEU:HD12	2.02	0.41
1:A:2205:G:H2'	1:A:2206:A:O4'	2.21	0.41
1:A:26:G:C4	1:A:523:G:C2	3.08	0.41
8:H:138:VAL:HG22	8:H:143:LEU:HD23	2.01	0.41
1:A:1362:G:N3	20:V:163:ASN:ND2	2.69	0.41
1:A:14:A:N3	25:2:15:ILE:HD12	2.35	0.41
1:A:169:C:H2'	1:A:170:U:C6	2.55	0.41
1:A:567:C:O2'	10:L:146:SER:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:130:LYS:HA	24:Z:133:SER:OG	2.20	0.41
28:5:150:LEU:HA	28:5:151:PRO:HD3	1.87	0.41
1:A:1169:A:H8	1:A:1169:A:O5'	2.03	0.41
1:A:1601:G:OP1	4:D:56:ARG:NH2	2.53	0.41
1:A:2691:G:H2'	1:A:2692:A:C8	2.56	0.41
1:A:205:G:C6	1:A:439:U:C5	3.08	0.41
4:D:237:ILE:HD11	4:D:242:PRO:HA	2.03	0.41
13:O:30:GLY:HA2	13:O:107:SER:HB2	2.03	0.41
17:S:8:TYR:CZ	17:S:12:ARG:HD3	2.56	0.41
20:V:115:LEU:HD21	20:V:151:ILE:HG12	2.01	0.41
1:A:1168:U:H4'	1:A:1169:A:O5'	2.21	0.41
1:A:1278:U:H2'	1:A:1279:C:C6	2.55	0.41
1:A:139:U:O2	1:A:140:G:C8	2.74	0.41
1:A:1875:G:H2'	1:A:1889:G:N2	2.36	0.41
8:H:145:LEU:HD21	8:H:188:ILE:HG23	2.03	0.41
11:M:110:PHE:HB3	11:M:113:ILE:HD12	2.02	0.41
1:A:856:U:O4	22:X:162:ARG:NH1	2.54	0.41
9:I:55:GLU:HG3	9:I:56:ASP:N	2.36	0.41
25:2:8:THR:HG21	25:2:16:ARG:HH12	1.86	0.41
1:A:145:A:N6	1:A:146:U:O4	2.54	0.41
1:A:2446:G:OP2	1:A:2447:A:OP2	2.39	0.41
1:A:185:U:H5'	23:Y:93:HIS:ND1	2.36	0.41
1:A:1530:G:N1	1:A:1536:A:H2	2.18	0.40
1:A:184:A:H1'	23:Y:93:HIS:CE1	2.56	0.40
1:A:2660:G:H2'	1:A:2661:A:O4'	2.20	0.40
19:U:35:ARG:HB3	19:U:133:THR:HG23	2.02	0.40
1:A:2047:A:O2'	1:A:2049:G:OP2	2.34	0.40
1:A:2543:G:C6	1:A:2544:C:C4	3.09	0.40
1:A:618:A:H2'	1:A:619:A:C8	2.56	0.40
1:A:79:G:C6	1:A:105:G:C6	3.09	0.40
5:E:195:ASP:O	5:E:196:MET:HB2	2.21	0.40
10:L:120:THR:HG23	10:L:160:LYS:HB3	2.02	0.40
1:A:98:G:N3	1:A:100:G:N2	2.69	0.40
1:A:2260:U:H2'	1:A:2261:U:C6	2.57	0.40
3:C:70:G:H2'	3:C:71:C:C6	2.56	0.40
1:A:2432:G:H2'	1:A:2433:C:H6	1.86	0.40
1:A:2559:A:H4'	1:A:2560:G:C8	2.56	0.40
1:A:2578:A:C2	1:A:2579:U:H1'	2.56	0.40
1:A:2661:A:H2'	1:A:2662:C:H5''	2.03	0.40
3:C:50:G:N2	3:C:67:G:O2'	2.55	0.40
6:F:58:LEU:HD21	6:F:169:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:80:PRO:HB3	23:Y:109:TRP:CE2	2.57	0.40
11:M:33:ALA:HB1	11:M:37:ASP:HB2	2.03	0.40
12:N:136:LEU:HD22	12:N:140:ILE:HD12	2.04	0.40
13:O:62:GLY:HA3	13:O:109:VAL:HG13	2.03	0.40
30:9:95:THR:HG23	30:9:217:ILE:HG22	2.04	0.40
1:A:1169:A:O5'	1:A:1169:A:C8	2.74	0.40
1:A:1337:U:H2'	1:A:1338:C:C6	2.57	0.40
1:A:541:G:O2'	1:A:543:A:C8	2.66	0.40
8:H:107:LEU:O	8:H:111:LEU:N	2.54	0.40
2:B:28:C:OP1	15:Q:81:HIS:NE2	2.54	0.40
19:U:94:ASN:HB3	19:U:97:ASN:HD22	1.87	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	
4	D	244/272 (90%)	200 (82%)	34 (14%)	10 (4%)	3	36
5	E	217/305 (71%)	191 (88%)	24 (11%)	2 (1%)	21	65
6	F	203/293 (69%)	170 (84%)	28 (14%)	5 (2%)	7	48
7	G	177/220 (80%)	160 (90%)	15 (8%)	2 (1%)	17	63
8	H	176/220 (80%)	152 (86%)	23 (13%)	1 (1%)	30	73
9	I	43/196 (22%)	33 (77%)	7 (16%)	3 (7%)	1	23
10	L	194/250 (78%)	171 (88%)	19 (10%)	4 (2%)	9	51
11	M	118/121 (98%)	101 (86%)	15 (13%)	2 (2%)	11	55
12	N	180/271 (66%)	142 (79%)	26 (14%)	12 (7%)	1	25
13	O	133/135 (98%)	120 (90%)	10 (8%)	3 (2%)	8	50
14	P	114/126 (90%)	102 (90%)	10 (9%)	2 (2%)	11	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	Q	116/166 (70%)	103 (89%)	11 (10%)	2 (2%)	11	55
16	R	112/233 (48%)	95 (85%)	16 (14%)	1 (1%)	21	65
17	S	114/128 (89%)	105 (92%)	7 (6%)	2 (2%)	11	54
18	T	132/256 (52%)	99 (75%)	23 (17%)	10 (8%)	1	20
19	U	150/199 (75%)	119 (79%)	29 (19%)	2 (1%)	15	59
20	V	89/198 (45%)	77 (86%)	9 (10%)	3 (3%)	5	42
21	W	127/191 (66%)	102 (80%)	20 (16%)	5 (4%)	4	37
22	X	106/194 (55%)	99 (93%)	5 (5%)	2 (2%)	10	53
23	Y	73/148 (49%)	64 (88%)	6 (8%)	3 (4%)	3	36
24	Z	92/168 (55%)	73 (79%)	14 (15%)	5 (5%)	2	30
25	2	40/57 (70%)	36 (90%)	3 (8%)	1 (2%)	7	48
26	3	58/66 (88%)	43 (74%)	9 (16%)	6 (10%)	1	12
27	4	59/152 (39%)	55 (93%)	2 (3%)	2 (3%)	5	42
28	5	68/159 (43%)	60 (88%)	8 (12%)	0	100	100
29	6	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	6	45
30	9	103/271 (38%)	100 (97%)	3 (3%)	0	100	100
31	7	44/142 (31%)	39 (89%)	2 (4%)	3 (7%)	1	24
32	8	45/116 (39%)	32 (71%)	6 (13%)	7 (16%)	0	5
All	All	3362/5290 (64%)	2874 (86%)	387 (12%)	101 (3%)	9	44

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	118	VAL
4	D	201	LEU
4	D	253	ARG
4	D	257	LYS
12	N	201	LEU
12	N	216	ALA
12	N	236	PRO
12	N	243	LYS
14	P	111	LEU
18	T	118	PRO
18	T	175	PRO
18	T	176	ILE
19	U	163	LEU

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Mol	Chain	Res	Type
20	V	113	GLN
21	W	171	PRO
24	Z	72	THR
26	3	24	ASN
26	3	25	LYS
27	4	139	CYS
31	7	131	TRP
32	8	73	LYS
32	8	88	GLU
4	D	229	GLY
5	E	119	GLU
7	G	89	ILE
7	G	92	PHE
9	I	44	LYS
9	I	64	GLY
10	L	82	ARG
10	L	182	GLY
12	N	109	SER
12	N	144	ARG
12	N	175	GLU
12	N	185	GLY
14	P	68	GLY
16	R	188	ALA
17	S	7	GLY
17	S	72	ARG
18	T	117	PRO
18	T	178	THR
20	V	105	PRO
23	Y	134	LEU
24	Z	84	LYS
24	Z	95	SER
31	7	140	LYS
4	D	52	GLY
4	D	258	ARG
6	F	64	LYS
6	F	139	VAL
11	M	68	GLU
11	M	118	PRO
12	N	239	LYS
15	Q	115	PRO
18	T	120	ARG
21	W	49	LYS

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Mol	Chain	Res	Type
21	W	67	ARG
21	W	174	TRP
22	X	129	GLY
24	Z	91	ARG
26	3	29	GLY
26	3	30	VAL
32	8	74	ARG
32	8	81	PRO
32	8	87	ALA
6	F	200	ASP
8	H	150	SER
9	I	57	ILE
10	L	243	ASP
12	N	173	GLY
13	O	6	ARG
13	O	59	ARG
23	Y	142	GLY
25	2	40	THR
5	E	193	GLU
10	L	142	SER
12	N	150	MET
13	O	70	PRO
15	Q	81	HIS
18	T	233	SER
20	V	114	ILE
29	6	36	GLN
32	8	92	VAL
4	D	249	PRO
6	F	72	LEU
6	F	140	ILE
12	N	186	ILE
18	T	112	PRO
21	W	163	LYS
22	X	141	GLU
27	4	148	LYS
32	8	82	LEU
4	D	237	ILE
23	Y	113	GLY
26	3	26	GLY
19	U	162	GLY
24	Z	128	VAL
4	D	147	GLY

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Mol	Chain	Res	Type
18	T	116	PRO
31	7	133	PRO
18	T	174	THR
26	3	64	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	194/217 (89%)	181 (93%)	13 (7%)	20	60
5	E	180/259 (70%)	170 (94%)	10 (6%)	26	65
6	F	171/254 (67%)	160 (94%)	11 (6%)	22	61
7	G	152/183 (83%)	145 (95%)	7 (5%)	33	70
8	H	150/190 (79%)	147 (98%)	3 (2%)	63	86
9	I	39/170 (23%)	35 (90%)	4 (10%)	9	40
10	L	142/213 (67%)	134 (94%)	8 (6%)	26	65
11	M	100/101 (99%)	94 (94%)	6 (6%)	24	63
12	N	139/215 (65%)	125 (90%)	14 (10%)	9	41
13	O	108/108 (100%)	100 (93%)	8 (7%)	17	56
14	P	96/103 (93%)	83 (86%)	13 (14%)	5	30
15	Q	97/139 (70%)	93 (96%)	4 (4%)	37	73
16	R	100/207 (48%)	89 (89%)	11 (11%)	8	38
17	S	103/115 (90%)	90 (87%)	13 (13%)	5	31
18	T	101/223 (45%)	91 (90%)	10 (10%)	10	42
19	U	119/176 (68%)	107 (90%)	12 (10%)	9	41
20	V	80/171 (47%)	74 (92%)	6 (8%)	17	56
21	W	111/171 (65%)	101 (91%)	10 (9%)	12	47
22	X	90/163 (55%)	86 (96%)	4 (4%)	35	71
23	Y	65/130 (50%)	62 (95%)	3 (5%)	33	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Z	87/153 (57%)	82 (94%)	5 (6%)	25	65
25	2	35/50 (70%)	31 (89%)	4 (11%)	7	36
26	3	56/60 (93%)	55 (98%)	1 (2%)	66	87
27	4	50/125 (40%)	45 (90%)	5 (10%)	9	42
28	5	61/140 (44%)	58 (95%)	3 (5%)	31	69
29	6	34/34 (100%)	33 (97%)	1 (3%)	50	79
30	9	101/244 (41%)	101 (100%)	0	100	100
31	7	41/121 (34%)	37 (90%)	4 (10%)	10	43
32	8	41/96 (43%)	38 (93%)	3 (7%)	17	57
All	All	2843/4531 (63%)	2647 (93%)	196 (7%)	24	59

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	28	LEU
4	D	84	ASN
4	D	97	LYS
4	D	121	LYS
4	D	200	ARG
4	D	209	TRP
4	D	213	ARG
4	D	241	SER
4	D	243	THR
4	D	259	ASN
4	D	262	SER
4	D	268	ARG
4	D	270	ARG
5	E	99	MET
5	E	113	THR
5	E	119	GLU
5	E	132	ASP
5	E	173	LEU
5	E	209	GLN
5	E	257	THR
5	E	282	VAL
5	E	292	LEU
5	E	300	LYS
6	F	63	GLU
6	F	65	VAL

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Mol	Chain	Res	Type
6	F	67	GLU
6	F	71	ASN
6	F	81	ARG
6	F	92	LEU
6	F	93	GLN
6	F	97	ARG
6	F	118	GLN
6	F	208	PHE
6	F	230	THR
7	G	22	ASN
7	G	126	THR
7	G	127	ARG
7	G	159	GLU
7	G	174	THR
7	G	177	THR
7	G	178	ASP
8	H	69	LEU
8	H	151	HIS
8	H	176	ARG
9	I	43	LYS
9	I	56	ASP
9	I	68	ASP
9	I	73	PHE
10	L	87	LEU
10	L	88	GLU
10	L	104	SER
10	L	121	ASP
10	L	160	LYS
10	L	175	ARG
10	L	205	ARG
10	L	238	ASP
11	M	5	GLN
11	M	23	ARG
11	M	32	TYR
11	M	105	GLU
11	M	108	GLN
11	M	114	VAL
12	N	79	ARG
12	N	82	LEU
12	N	117	GLN
12	N	125	ILE
12	N	134	MET

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Mol	Chain	Res	Type
12	N	138	ARG
12	N	160	ILE
12	N	170	PHE
12	N	184	LYS
12	N	186	ILE
12	N	192	ARG
12	N	238	ARG
12	N	242	ILE
12	N	244	GLU
13	O	14	ARG
13	O	44	SER
13	O	52	ARG
13	O	71	ASP
13	O	77	ARG
13	O	87	LYS
13	O	111	GLU
13	O	125	MET
14	P	11	MET
14	P	12	LYS
14	P	13	HIS
14	P	17	ILE
14	P	25	ASP
14	P	32	ARG
14	P	39	LEU
14	P	52	SER
14	P	75	GLN
14	P	81	TYR
14	P	100	ARG
14	P	109	ARG
14	P	114	ARG
15	Q	51	GLU
15	Q	90	THR
15	Q	102	GLN
15	Q	103	LYS
16	R	126	LEU
16	R	144	ARG
16	R	152	ARG
16	R	187	ILE
16	R	193	GLU
16	R	195	VAL
16	R	218	ARG
16	R	222	LEU

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Mol	Chain	Res	Type
16	R	225	LYS
16	R	226	LEU
16	R	230	SER
17	S	3	ARG
17	S	6	ARG
17	S	11	ARG
17	S	13	ARG
17	S	18	ARG
17	S	23	SER
17	S	56	ASP
17	S	59	ARG
17	S	83	HIS
17	S	90	LEU
17	S	97	LEU
17	S	107	CYS
17	S	113	ASN
18	T	123	ILE
18	T	131	SER
18	T	132	ARG
18	T	133	GLN
18	T	151	THR
18	T	157	VAL
18	T	171	TYR
18	T	178	THR
18	T	207	ARG
18	T	213	ARG
19	U	31	GLU
19	U	35	ARG
19	U	37	TYR
19	U	54	ARG
19	U	58	TYR
19	U	68	MET
19	U	93	PHE
19	U	109	ILE
19	U	110	THR
19	U	122	SER
19	U	127	ARG
19	U	156	LYS
20	V	111	VAL
20	V	139	ASP
20	V	143	ASP
20	V	163	ASN

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Mol	Chain	Res	Type
20	V	167	ARG
20	V	190	LYS
21	W	56	CYS
21	W	92	ILE
21	W	107	LYS
21	W	108	THR
21	W	119	GLN
21	W	126	GLU
21	W	132	SER
21	W	136	LEU
21	W	156	ARG
21	W	169	ASP
22	X	112	ASP
22	X	131	ASP
22	X	154	LYS
22	X	159	ARG
23	Y	104	GLN
23	Y	120	ARG
23	Y	121	LEU
24	Z	117	THR
24	Z	130	LYS
24	Z	137	ASP
24	Z	138	LYS
24	Z	145	VAL
25	2	5	LYS
25	2	9	SER
25	2	11	TYR
25	2	29	LEU
26	3	30	VAL
27	4	96	LEU
27	4	98	LEU
27	4	104	SER
27	4	141	LYS
27	4	143	ASN
28	5	90	TYR
28	5	142	ASP
28	5	150	LEU
29	6	7	VAL
31	7	137	LYS
31	7	140	LYS
31	7	141	ASN
31	7	142	VAL

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Mol	Chain	Res	Type
32	8	50	ARG
32	8	54	LYS
32	8	82	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	84	ASN
5	E	167	HIS
5	E	301	ASN
6	F	93	GLN
6	F	181	ASN
7	G	22	ASN
7	G	133	ASN
8	H	102	ASN
10	L	97	ASN
10	L	157	ASN
10	L	235	GLN
11	M	3	GLN
11	M	5	GLN
12	N	133	GLN
13	O	12	GLN
13	O	35	GLN
14	P	26	GLN
14	P	101	ASN
16	R	202	ASN
17	S	99	GLN
20	V	153	ASN
20	V	179	ASN
21	W	93	HIS
21	W	133	ASN
22	X	68	ASN
22	X	85	GLN
24	Z	75	GLN
26	3	61	HIS
27	4	143	ASN
28	5	95	HIS
28	5	118	GLN
29	6	36	GLN
30	9	97	GLN
30	9	109	ASN
30	9	216	ASN

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Mol	Chain	Res	Type
31	7	102	GLN
31	7	141	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2745/2811 (97%)	824 (30%)	128 (4%)
2	B	119/121 (98%)	29 (24%)	3 (2%)
3	C	92/103 (89%)	28 (30%)	2 (2%)
All	All	2956/3035 (97%)	881 (29%)	133 (4%)

All (881) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	4	A
1	A	8	G
1	A	9	A
1	A	10	G
1	A	13	A
1	A	14	A
1	A	33	A
1	A	34	G
1	A	35	G
1	A	42	G
1	A	45	A
1	A	46	C
1	A	48	A
1	A	50	G
1	A	51	A
1	A	55	G
1	A	61	U
1	A	70	A
1	A	73	U
1	A	74	G
1	A	82	G
1	A	83	A
1	A	84	G
1	A	90	A
1	A	94	A
1	A	97	A

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Mol	Chain	Res	Type
1	A	98	G
1	A	99	A
1	A	100	G
1	A	102	U
1	A	110	U
1	A	116	A
1	A	118	U
1	A	128	U
1	A	133	A
1	A	134	A
1	A	136	U
1	A	137	U
1	A	139	U
1	A	140	G
1	A	144	A
1	A	146	U
1	A	147	C
1	A	150	U
1	A	157	G
1	A	158	C
1	A	159	A
1	A	160	A
1	A	181	A
1	A	184	A
1	A	189	A
1	A	200	G
1	A	201	A
1	A	203	A
1	A	206	A
1	A	207	A
1	A	212	A
1	A	213	A
1	A	219	U
1	A	224	G
1	A	227	G
1	A	228	U
1	A	230	G
1	A	233	G
1	A	234	C
1	A	236	A
1	A	237	G
1	A	240	A

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Mol	Chain	Res	Type
1	A	250	A
1	A	251	G
1	A	252	C
1	A	255	A
1	A	256	A
1	A	257	A
1	A	259	C
1	A	260	G
1	A	261	U
1	A	262	G
1	A	264	A
1	A	265	A
1	A	266	A
1	A	267	C
1	A	268	G
1	A	270	G
1	A	271	G
1	A	273	U
1	A	274	G
1	A	275	U
1	A	276	G
1	A	277	G
1	A	278	G
1	A	280	G
1	A	282	G
1	A	299	C
1	A	304	A
1	A	313	A
1	A	314	G
1	A	316	G
1	A	317	G
1	A	319	G
1	A	320	U
1	A	321	G
1	A	322	C
1	A	331	A
1	A	332	G
1	A	334	U
1	A	336	G
1	A	338	G
1	A	339	A
1	A	340	A

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Mol	Chain	Res	Type
1	A	341	A
1	A	343	U
1	A	344	C
1	A	347	G
1	A	351	C
1	A	358	C
1	A	374	U
1	A	375	C
1	A	376	U
1	A	377	G
1	A	378	A
1	A	379	C
1	A	380	C
1	A	381	C
1	A	382	G
1	A	383	A
1	A	384	G
1	A	385	U
1	A	398	G
1	A	399	U
1	A	403	A
1	A	407	C
1	A	416	C
1	A	417	A
1	A	418	G
1	A	423	G
1	A	424	A
1	A	432	G
1	A	433	C
1	A	436	G
1	A	440	A
1	A	448	C
1	A	452	G
1	A	467	G
1	A	468	U
1	A	469	A
1	A	485	G
1	A	486	G
1	A	487	U
1	A	491	A
1	A	492	A
1	A	493	G

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Mol	Chain	Res	Type
1	A	496	C
1	A	502	U
1	A	514	A
1	A	515	U
1	A	516	A
1	A	517	G
1	A	519	A
1	A	520	C
1	A	521	A
1	A	536	C
1	A	539	A
1	A	540	A
1	A	541	G
1	A	542	C
1	A	543	A
1	A	544	G
1	A	553	G
1	A	554	G
1	A	556	C
1	A	557	C
1	A	558	A
1	A	560	A
1	A	568	C
1	A	573	G
1	A	574	C
1	A	582	A
1	A	583	G
1	A	584	A
1	A	585	A
1	A	593	G
1	A	597	C
1	A	598	U
1	A	613	U
1	A	614	G
1	A	622	G
1	A	623	A
1	A	624	A
1	A	628	A
1	A	633	A
1	A	634	G
1	A	639	A
1	A	646	G

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Mol	Chain	Res	Type
1	A	649	A
1	A	654	U
1	A	655	C
1	A	656	A
1	A	657	U
1	A	658	A
1	A	659	G
1	A	667	G
1	A	670	A
1	A	673	G
1	A	680	G
1	A	681	A
1	A	688	C
1	A	697	U
1	A	698	C
1	A	706	G
1	A	722	G
1	A	731	U
1	A	732	A
1	A	734	G
1	A	741	U
1	A	749	G
1	A	759	G
1	A	763	A
1	A	764	A
1	A	768	G
1	A	775	A
1	A	785	A
1	A	786	G
1	A	787	G
1	A	788	G
1	A	793	A
1	A	795	U
1	A	796	G
1	A	800	C
1	A	802	C
1	A	803	G
1	A	804	A
1	A	810	G
1	A	811	A
1	A	813	C
1	A	814	U

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Mol	Chain	Res	Type
1	A	816	G
1	A	817	C
1	A	823	C
1	A	830	A
1	A	838	U
1	A	839	G
1	A	841	G
1	A	855	C
1	A	856	U
1	A	857	G
1	A	866	G
1	A	869	G
1	A	870	U
1	A	871	A
1	A	884	G
1	A	887	G
1	A	888	C
1	A	890	G
1	A	891	G
1	A	893	C
1	A	896	G
1	A	897	A
1	A	898	G
1	A	901	C
1	A	903	G
1	A	905	A
1	A	906	C
1	A	907	C
1	A	908	A
1	A	916	G
1	A	919	A
1	A	923	C
1	A	924	U
1	A	937	U
1	A	938	G
1	A	939	A
1	A	940	C
1	A	956	G
1	A	969	A
1	A	974	G
1	A	981	G
1	A	985	A

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Mol	Chain	Res	Type
1	A	986	U
1	A	987	A
1	A	989	G
1	A	995	U
1	A	996	C
1	A	997	G
1	A	1002	G
1	A	1003	A
1	A	1007	A
1	A	1009	A
1	A	1011	A
1	A	1013	C
1	A	1017	G
1	A	1018	A
1	A	1023	C
1	A	1024	A
1	A	1027	U
1	A	1036	U
1	A	1040	U
1	A	1041	G
1	A	1048	C
1	A	1049	A
1	A	1050	G
1	A	1051	U
1	A	1053	A
1	A	1055	A
1	A	1060	A
1	A	1061	G
1	A	1062	G
1	A	1070	G
1	A	1074	A
1	A	1081	C
1	A	1082	A
1	A	1085	A
1	A	1086	G
1	A	1088	U
1	A	1089	U
1	A	1090	U
1	A	1093	C
1	A	1094	U
1	A	1096	G
1	A	1097	A

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Mol	Chain	Res	Type
1	A	1098	A
1	A	1099	G
1	A	1100	C
1	A	1103	C
1	A	1104	C
1	A	1107	C
1	A	1112	A
1	A	1115	G
1	A	1116	A
1	A	1119	G
1	A	1120	C
1	A	1125	U
1	A	1132	C
1	A	1134	G
1	A	1137	C
1	A	1139	A
1	A	1140	G
1	A	1141	C
1	A	1142	G
1	A	1143	C
1	A	1147	U
1	A	1158	U
1	A	1159	G
1	A	1160	A
1	A	1161	A
1	A	1162	C
1	A	1166	G
1	A	1169	A
1	A	1170	A
1	A	1177	U
1	A	1182	A
1	A	1189	G
1	A	1194	G
1	A	1195	U
1	A	1196	A
1	A	1199	A
1	A	1200	A
1	A	1202	A
1	A	1203	C
1	A	1218	G
1	A	1227	U
1	A	1229	G

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Mol	Chain	Res	Type
1	A	1232	A
1	A	1233	G
1	A	1236	A
1	A	1240	G
1	A	1241	U
1	A	1242	G
1	A	1243	C
1	A	1251	G
1	A	1253	G
1	A	1254	U
1	A	1258	A
1	A	1259	C
1	A	1260	G
1	A	1261	A
1	A	1262	A
1	A	1265	G
1	A	1268	A
1	A	1269	G
1	A	1270	C
1	A	1272	A
1	A	1273	G
1	A	1274	A
1	A	1277	G
1	A	1281	G
1	A	1283	U
1	A	1289	A
1	A	1292	G
1	A	1293	C
1	A	1294	A
1	A	1295	A
1	A	1296	A
1	A	1310	C
1	A	1315	G
1	A	1321	A
1	A	1322	A
1	A	1327	U
1	A	1339	C
1	A	1342	A
1	A	1346	U
1	A	1351	C
1	A	1359	G
1	A	1362	G

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Mol	Chain	Res	Type
1	A	1366	C
1	A	1368	G
1	A	1371	C
1	A	1373	U
1	A	1385	G
1	A	1386	A
1	A	1389	G
1	A	1395	G
1	A	1399	A
1	A	1400	U
1	A	1402	G
1	A	1404	C
1	A	1405	A
1	A	1412	G
1	A	1416	A
1	A	1417	U
1	A	1426	U
1	A	1429	C
1	A	1432	U
1	A	1434	G
1	A	1436	U
1	A	1437	G
1	A	1438	G
1	A	1439	U
1	A	1440	C
1	A	1441	C
1	A	1443	G
1	A	1445	G
1	A	1449	C
1	A	1472	A
1	A	1473	G
1	A	1474	A
1	A	1475	U
1	A	1476	G
1	A	1478	U
1	A	1479	U
1	A	1480	A
1	A	1494	G
1	A	1495	C
1	A	1496	A
1	A	1497	A
1	A	1498	G

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Mol	Chain	Res	Type
1	A	1500	U
1	A	1501	G
1	A	1524	G
1	A	1527	G
1	A	1528	U
1	A	1529	A
1	A	1530	G
1	A	1531	A
1	A	1532	G
1	A	1533	A
1	A	1534	A
1	A	1535	A
1	A	1536	A
1	A	1537	U
1	A	1540	C
1	A	1542	C
1	A	1543	G
1	A	1544	A
1	A	1545	G
1	A	1549	A
1	A	1550	U
1	A	1558	U
1	A	1559	A
1	A	1567	C
1	A	1568	U
1	A	1569	A
1	A	1570	C
1	A	1572	G
1	A	1573	C
1	A	1574	G
1	A	1580	G
1	A	1589	G
1	A	1591	C
1	A	1592	A
1	A	1593	U
1	A	1594	A
1	A	1595	C
1	A	1600	A
1	A	1603	A
1	A	1610	C
1	A	1611	G
1	A	1612	A

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Mol	Chain	Res	Type
1	A	1615	G
1	A	1616	A
1	A	1617	C
1	A	1618	C
1	A	1619	U
1	A	1620	U
1	A	1621	C
1	A	1622	A
1	A	1623	A
1	A	1624	C
1	A	1628	A
1	A	1630	G
1	A	1634	C
1	A	1643	G
1	A	1644	A
1	A	1645	A
1	A	1647	C
1	A	1653	C
1	A	1662	A
1	A	1663	G
1	A	1682	C
1	A	1683	G
1	A	1684	C
1	A	1687	G
1	A	1690	A
1	A	1696	C
1	A	1698	C
1	A	1710	G
1	A	1713	A
1	A	1730	C
1	A	1731	G
1	A	1734	A
1	A	1736	A
1	A	1742	U
1	A	1748	C
1	A	1749	U
1	A	1750	C
1	A	1751	A
1	A	1752	C
1	A	1753	A
1	A	1754	A
1	A	1755	A

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Mol	Chain	Res	Type
1	A	1756	G
1	A	1759	G
1	A	1760	G
1	A	1767	U
1	A	1768	G
1	A	1774	G
1	A	1783	A
1	A	1786	G
1	A	1790	A
1	A	1791	C
1	A	1792	C
1	A	1796	A
1	A	1801	A
1	A	1810	C
1	A	1811	A
1	A	1812	A
1	A	1821	G
1	A	1822	A
1	A	1825	A
1	A	1826	U
1	A	1828	U
1	A	1830	U
1	A	1843	C
1	A	1866	G
1	A	1867	A
1	A	1870	U
1	A	1876	A
1	A	1881	A
1	A	1882	U
1	A	1883	G
1	A	1884	A
1	A	1885	C
1	A	1886	A
1	A	1888	G
1	A	1898	G
1	A	1899	A
1	A	1910	G
1	A	1912	U
1	A	1914	A
1	A	1915	A
1	A	1919	C
1	A	1920	G

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Mol	Chain	Res	Type
1	A	1921	G
1	A	1924	G
1	A	1935	G
1	A	1939	C
1	A	1943	G
1	A	1944	G
1	A	1945	U
1	A	1950	A
1	A	1951	A
1	A	1952	A
1	A	1953	U
1	A	1954	U
1	A	1955	C
1	A	1965	U
1	A	1969	U
1	A	1975	C
1	A	1979	C
1	A	1981	C
1	A	1984	A
1	A	1985	A
1	A	1986	G
1	A	1999	G
1	A	2001	G
1	A	2005	U
1	A	2007	U
1	A	2018	G
1	A	2026	G
1	A	2034	C
1	A	2036	U
1	A	2037	G
1	A	2045	A
1	A	2046	G
1	A	2047	A
1	A	2053	A
1	A	2056	A
1	A	2057	C
1	A	2065	U
1	A	2066	G
1	A	2069	C
1	A	2070	A
1	A	2074	A
1	A	2075	G

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Mol	Chain	Res	Type
1	A	2076	A
1	A	2080	U
1	A	2083	G
1	A	2086	G
1	A	2094	G
1	A	2101	G
1	A	2107	G
1	A	2109	C
1	A	2110	U
1	A	2111	U
1	A	2112	U
1	A	2113	G
1	A	2114	G
1	A	2118	U
1	A	2124	G
1	A	2125	C
1	A	2126	G
1	A	2127	C
1	A	2129	G
1	A	2130	C
1	A	2132	U
1	A	2133	A
1	A	2136	U
1	A	2141	G
1	A	2143	C
1	A	2145	A
1	A	2146	A
1	A	2147	G
1	A	2148	A
1	A	2153	C
1	A	2154	C
1	A	2159	C
1	A	2161	G
1	A	2169	C
1	A	2171	G
1	A	2176	A
1	A	2178	C
1	A	2181	U
1	A	2184	G
1	A	2185	A
1	A	2186	U
1	A	2187	A

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Mol	Chain	Res	Type
1	A	2188	C
1	A	2193	C
1	A	2197	A
1	A	2203	U
1	A	2206	A
1	A	2212	A
1	A	2217	U
1	A	2219	U
1	A	2220	G
1	A	2221	U
1	A	2223	A
1	A	2224	G
1	A	2225	G
1	A	2226	A
1	A	2227	C
1	A	2228	C
1	A	2229	U
1	A	2230	A
1	A	2242	A
1	A	2252	G
1	A	2254	A
1	A	2255	G
1	A	2256	A
1	A	2260	U
1	A	2267	G
1	A	2269	G
1	A	2272	G
1	A	2285	A
1	A	2296	G
1	A	2300	U
1	A	2303	A
1	A	2304	A
1	A	2314	C
1	A	2315	G
1	A	2322	A
1	A	2326	A
1	A	2328	A
1	A	2329	U
1	A	2335	C
1	A	2336	U
1	A	2337	C
1	A	2339	A

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Mol	Chain	Res	Type
1	A	2342	G
1	A	2343	C
1	A	2344	A
1	A	2348	G
1	A	2350	A
1	A	2351	G
1	A	2352	A
1	A	2356	G
1	A	2362	G
1	A	2367	C
1	A	2374	C
1	A	2378	C
1	A	2389	G
1	A	2399	G
1	A	2400	G
1	A	2401	C
1	A	2402	C
1	A	2409	A
1	A	2419	G
1	A	2423	A
1	A	2424	G
1	A	2436	U
1	A	2439	C
1	A	2440	U
1	A	2441	C
1	A	2442	A
1	A	2446	G
1	A	2447	A
1	A	2452	A
1	A	2458	U
1	A	2462	G
1	A	2464	G
1	A	2465	A
1	A	2466	U
1	A	2467	A
1	A	2476	A
1	A	2481	C
1	A	2490	U
1	A	2491	U
1	A	2492	C
1	A	2493	A
1	A	2495	A

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Mol	Chain	Res	Type
1	A	2501	G
1	A	2511	G
1	A	2516	C
1	A	2517	U
1	A	2519	G
1	A	2520	A
1	A	2522	G
1	A	2523	U
1	A	2535	C
1	A	2546	G
1	A	2552	U
1	A	2564	U
1	A	2571	U
1	A	2579	U
1	A	2583	A
1	A	2584	G
1	A	2589	A
1	A	2590	C
1	A	2591	G
1	A	2595	G
1	A	2602	U
1	A	2603	C
1	A	2607	A
1	A	2619	A
1	A	2620	G
1	A	2622	U
1	A	2625	G
1	A	2626	U
1	A	2627	C
1	A	2628	C
1	A	2629	A
1	A	2630	U
1	A	2631	A
1	A	2646	U
1	A	2647	A
1	A	2649	A
1	A	2653	U
1	A	2654	U
1	A	2659	G
1	A	2662	C
1	A	2663	C
1	A	2664	U

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Mol	Chain	Res	Type
1	A	2666	U
1	A	2672	G
1	A	2673	U
1	A	2678	G
1	A	2685	G
1	A	2696	A
1	A	2699	U
1	A	2702	G
1	A	2706	U
1	A	2707	A
1	A	2708	C
1	A	2724	C
1	A	2729	A
1	A	2730	A
1	A	2731	C
1	A	2732	G
1	A	2740	G
1	A	2742	C
1	A	2743	A
1	A	2747	G
1	A	2750	G
1	A	2751	A
1	A	2752	G
1	A	2753	C
1	A	2754	G
1	A	2762	G
1	A	2766	A
1	A	2771	A
1	A	2775	A
1	A	2776	A
1	A	2782	A
1	A	2783	A
1	A	2784	G
1	A	2787	C
1	A	2796	A
1	A	2797	U
1	A	2798	G
1	A	2808	C
1	A	2809	U
1	A	2810	A
1	A	2811	U
2	B	4	U

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Mol	Chain	Res	Type
2	B	5	C
2	B	7	G
2	B	11	U
2	B	12	C
2	B	13	C
2	B	14	U
2	B	16	G
2	B	31	C
2	B	32	A
2	B	36	A
2	B	45	G
2	B	46	A
2	B	54	G
2	B	55	G
2	B	57	U
2	B	64	U
2	B	65	A
2	B	67	U
2	B	68	G
2	B	87	G
2	B	89	A
2	B	90	G
2	B	91	G
2	B	92	U
2	B	109	U
2	B	110	C
2	B	111	G
2	B	120	A
3	C	2	A
3	C	7	C
3	C	13	G
3	C	14	A
3	C	16	A
3	C	25	U
3	C	37	U
3	C	61	A
3	C	62	U
3	C	67	G
3	C	68	C
3	C	69	A
3	C	74	A
3	C	78	A

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Mol	Chain	Res	Type
3	C	80	C
3	C	81	C
3	C	85	C
3	C	87	G
3	C	88	A
3	C	91	C
3	C	92	A
3	C	93	C
3	C	94	A
3	C	95	G
3	C	96	A
3	C	99	U
3	C	101	A
3	C	103	C

All (133) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	45	A
1	A	50	G
1	A	73	U
1	A	98	G
1	A	133	A
1	A	143	G
1	A	190	G
1	A	212	A
1	A	227	G
1	A	234	C
1	A	255	A
1	A	261	U
1	A	262	G
1	A	263	A
1	A	265	A
1	A	274	G
1	A	313	A
1	A	316	G
1	A	317	G
1	A	332	G
1	A	373	C
1	A	374	U
1	A	379	C

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Mol	Chain	Res	Type
1	A	384	G
1	A	415	U
1	A	416	C
1	A	458	G
1	A	459	A
1	A	486	G
1	A	491	A
1	A	514	A
1	A	539	A
1	A	543	A
1	A	553	G
1	A	581	A
1	A	597	C
1	A	613	U
1	A	627	C
1	A	654	U
1	A	656	A
1	A	666	U
1	A	757	U
1	A	763	A
1	A	775	A
1	A	785	A
1	A	787	G
1	A	800	C
1	A	838	U
1	A	856	U
1	A	868	G
1	A	869	G
1	A	896	G
1	A	985	A
1	A	1012	G
1	A	1039	A
1	A	1048	C
1	A	1050	G
1	A	1098	A
1	A	1139	A
1	A	1158	U
1	A	1169	A
1	A	1194	G
1	A	1198	A
1	A	1228	A
1	A	1241	U

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Mol	Chain	Res	Type
1	A	1242	G
1	A	1257	G
1	A	1272	A
1	A	1332	G
1	A	1399	A
1	A	1411	U
1	A	1417	U
1	A	1437	G
1	A	1439	U
1	A	1448	A
1	A	1471	A
1	A	1472	A
1	A	1474	A
1	A	1480	A
1	A	1493	C
1	A	1495	C
1	A	1496	A
1	A	1529	A
1	A	1534	A
1	A	1536	A
1	A	1543	G
1	A	1569	A
1	A	1600	A
1	A	1617	C
1	A	1644	A
1	A	1662	A
1	A	1754	A
1	A	1755	A
1	A	1778	G
1	A	1796	A
1	A	1825	A
1	A	1882	U
1	A	1885	C
1	A	1898	G
1	A	1914	A
1	A	1944	G
1	A	1950	A
1	A	1953	U
1	A	1954	U
1	A	2106	U
1	A	2111	U
1	A	2113	G

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Mol	Chain	Res	Type
1	A	2216	U
1	A	2219	U
1	A	2229	U
1	A	2254	A
1	A	2299	G
1	A	2303	A
1	A	2343	C
1	A	2408	G
1	A	2439	C
1	A	2465	A
1	A	2475	G
1	A	2534	C
1	A	2583	A
1	A	2626	U
1	A	2628	C
1	A	2646	U
1	A	2662	C
1	A	2672	G
1	A	2698	C
1	A	2774	U
2	B	45	G
2	B	67	U
2	B	89	A
3	C	1	G
3	C	80	C

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
18	T	1
19	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	158:ILE	C	159:ALA	N	1.84
1	T	118:PRO	C	119:PRO	N	1.71
1	A	1554:C	O3'	1555:G	P	1.33