



Full wwPDB EM Validation Report ⓘ

Feb 23, 2022 – 01:01 pm GMT

PDB ID : 7OIF
EMDB ID : EMD-12928
Title : CspA-27 cotranslational folding intermediate 2
Authors : Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.;
Novacek, J.; Valle, M.; Rodnina, M.V.
Deposited on : 2021-05-11
Resolution : 3.00 Å(reported)
Based on initial model : 6ORE

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

EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

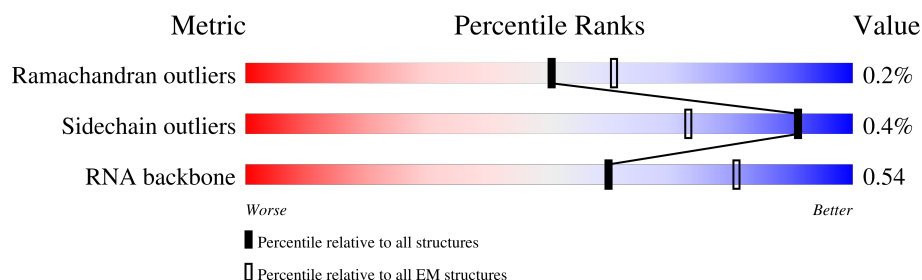
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



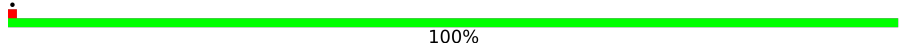
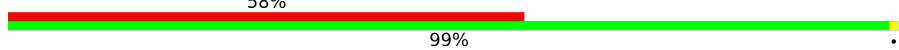
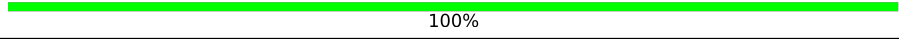
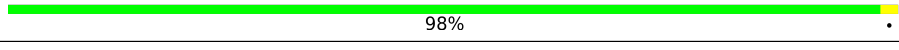
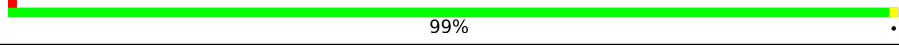
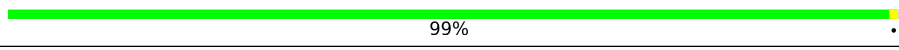
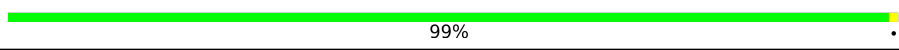
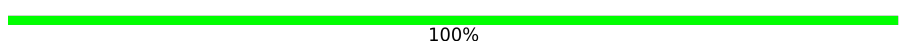
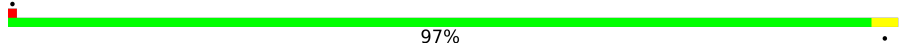
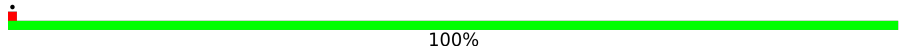
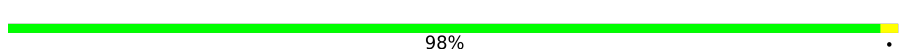
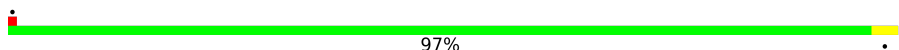
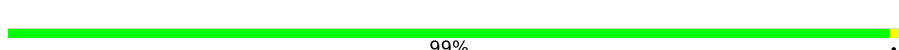
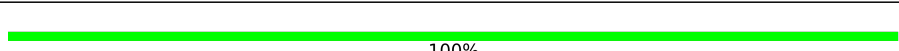
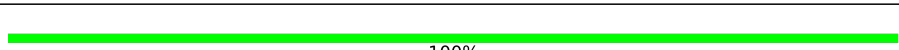
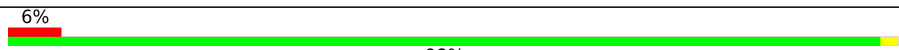
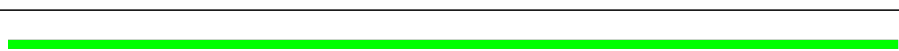
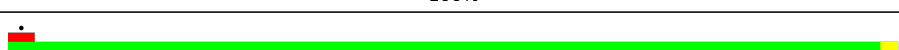
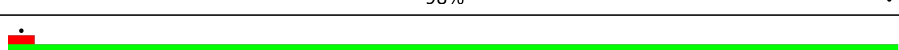
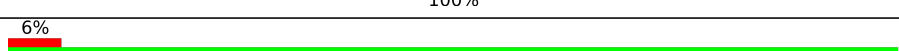
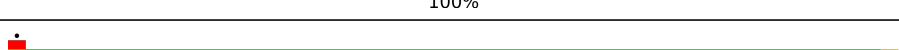
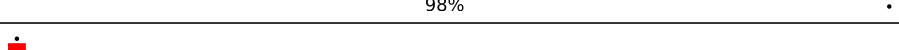
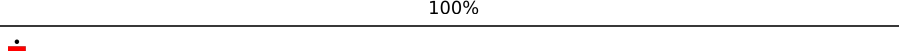
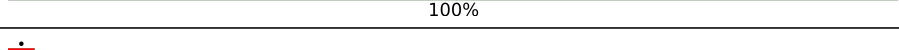
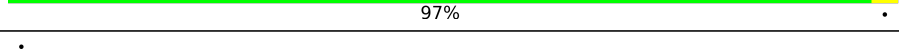
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1	2903	
2	2	1534	
3	3	120	
4	4	6	
5	C	271	
6	D	209	
7	E	201	
8	F	177	















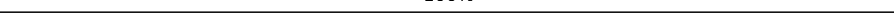
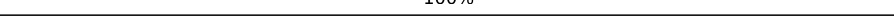
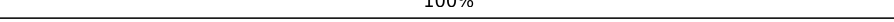
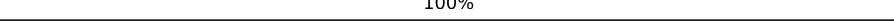
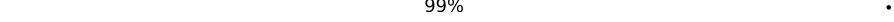
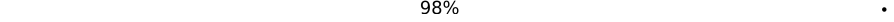
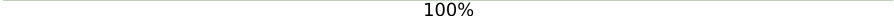

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Mol	Chain	Length	Quality of chain
9	G	175	
10	H	149	
11	I	142	
12	J	123	
13	K	144	
14	L	136	
15	M	119	
16	N	116	
17	O	114	
18	P	117	
19	Q	103	
20	R	110	
21	S	94	
22	T	103	
23	U	94	
24	V	80	
25	W	77	
26	X	62	
27	Y	58	
28	Z	66	
29	a	56	
30	b	52	
31	c	46	
32	d	64	
33	e	38	

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Mol	Chain	Length	Quality of chain
34	f	225	 100%
35	g	208	 100%
36	h	205	 100%
37	i	156	 97%
38	j	104	 99%
39	k	151	 100%
40	l	129	 100%
41	m	127	 99%
42	n	99	 98%
43	o	117	 99%
44	p	123	 100%
45	q	116	 100%
46	r	100	 100%
47	s	88	 100%
48	t	82	 100%
49	u	80	 100%
50	v	66	 100%
51	w	83	 99%
52	x	86	 98%
53	y	70	 7% 100%
54	z	88	 56% 35% 9%
55	B	27	 19% 89% 11%

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 145152 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	6	Total	C	N	O	P	0	0
			126	56	20	44	6		

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	103	Total	C	N	O		0	0
			788	498	148	142			

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	80	Total	C	N	O	S	0	0
			601	370	121	109	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	b	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 39 is a protein called 30S ribosomal protein S7.

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

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 43 is a protein called 30S ribosomal protein S11.

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

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

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

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

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

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 51 is a protein called 30S ribosomal protein S19.

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

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 54 is a RNA chain called tRNA-Ser.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	88	Total	C	N	O	P	0	0
			1891	841	341	621	88		

- Molecule 55 is a protein called CspA transcriptional activator.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B	27	Total	C	N	O	S	0	0
			205	132	32	39	2		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	1	276	Total 276	Mg 276	0
56	2	119	Total 119	Mg 119	0
56	3	8	Total 8	Mg 8	0
56	4	1	Total 1	Mg 1	0
56	C	1	Total 1	Mg 1	0
56	D	2	Total 2	Mg 2	0
56	P	1	Total 1	Mg 1	0
56	T	1	Total 1	Mg 1	0
56	a	2	Total 2	Mg 2	0
56	h	1	Total 1	Mg 1	0
56	q	1	Total 1	Mg 1	0
56	r	1	Total 1	Mg 1	0
56	z	2	Total 2	Mg 2	0

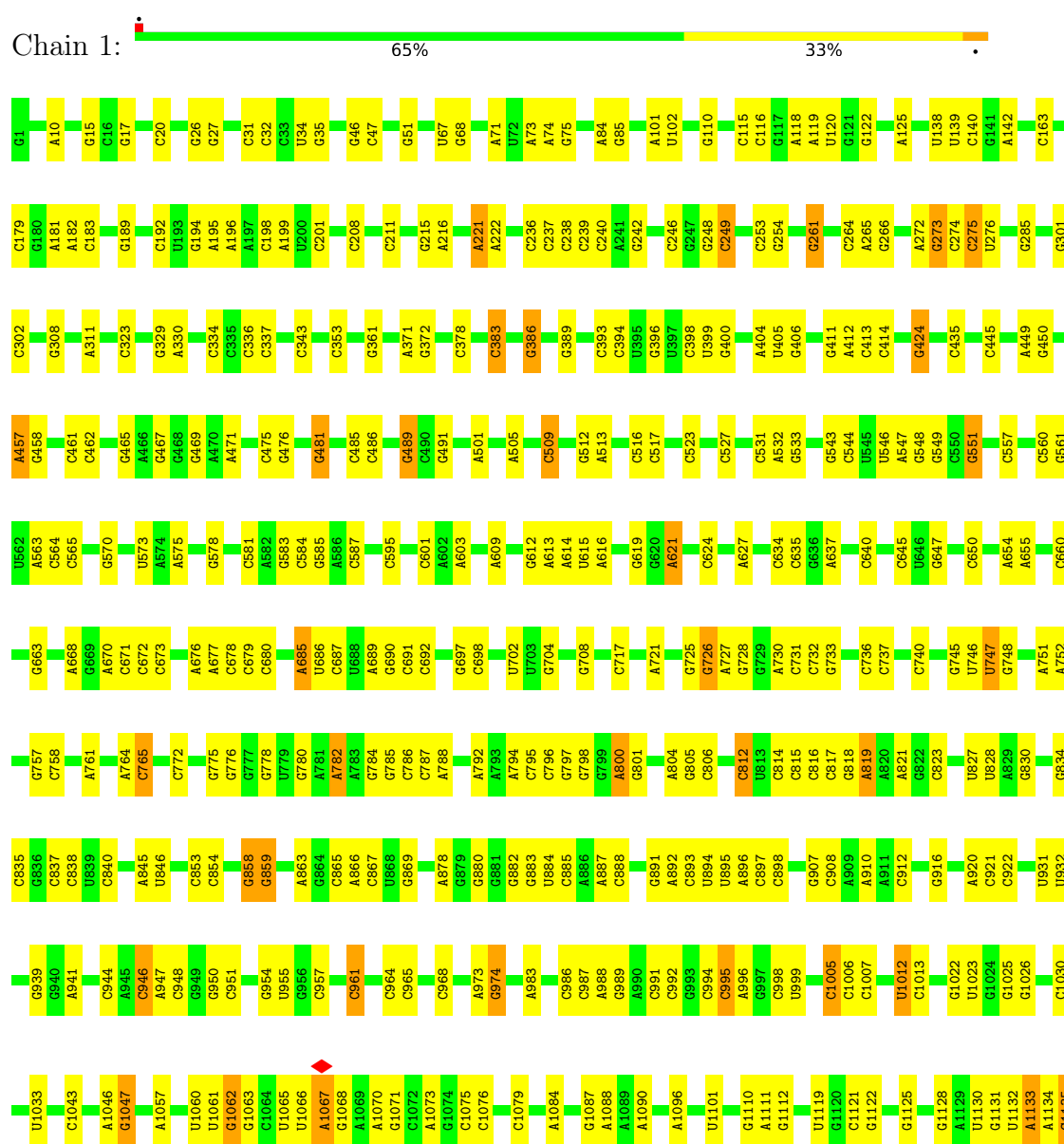
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	Z	1	Total 1	Zn 1	0
57	e	1	Total 1	Zn 1	0

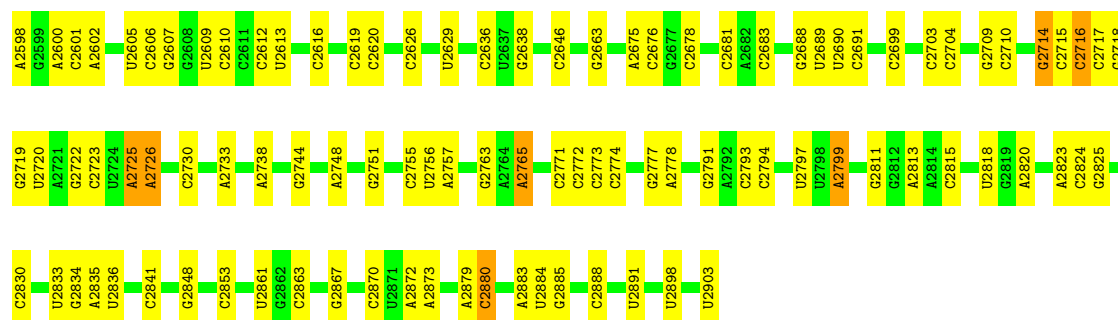
3 Residue-property plots

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

• Molecule 1: 23S rRNA

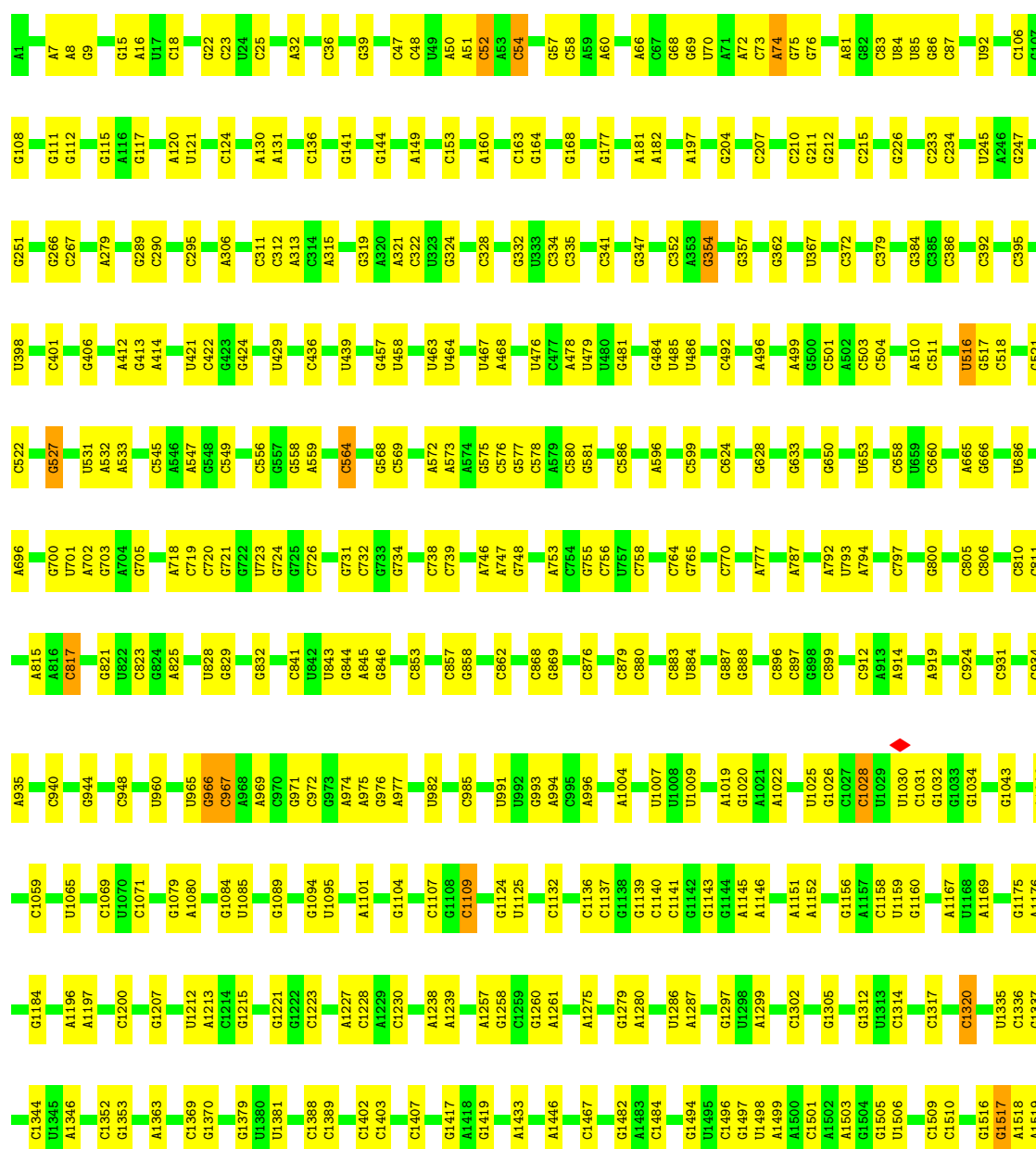


C2512	A2434	A3227	G2125	G1950	C1843	C1760	G1613	A1494	A1353	G1250	G1136
A2513	A2435	C2332	A2126	G1955	C1844	C1761	A1614	A1503	A1354	C1251	G1139
C2515	C2440	A2333	G2127	U1955	C1845	G2127	A1615	A1504	C1357	G1252	C1140
A2516	U2441	A2334	G2046	C1957	A1847	C1764	A1616	A1508	G1358	U1141	U1141
C2517	C2442	A2335	G2047	C1958	A1848	U1769	A1617	A1509	C1362	G1256	A1142
A2518	C2443	A2336	U2131	C1961	A1853	U1770	G1618	G1510	C1363	C1257	A1143
U2519	G2444	A2337	U2132	C1962	A1857	C1771	G1619	A1514	C1364	C1261	A1144
C2520	G2445	A2338	U2133	C1967	A1858	A1773	C1625	A1515	A1365	G1264	C1145
C2521	G2446	A2339	A2134	U1970	G1862	C1774	G1631	G1524	G1368	A1264	C1146
G2526	A2447	A2340	U2137	U1971	U1865	U1782	A1634	G1529	G1369	A1265	C1152
C2527	A2448	A2341	G2138	U1972	C1868	A1783	C1638	G1530	C1370	A1266	C1153
U2528	G2449	A2342	G2139	U1973	G1869	U1788	C1639	A1531	G1371	G1270	G1154
C2529	C2450	A2343	A2140	C1974	C1870	C1789	C1646	A1532	C1376	A1272	A1155
G2535	G2451	G2357	A2141	U1977	A1871	C1790	U1647	U1532	C1377	C1278	C1161
C2538	C2452	U2449	A2142	A1977	C1872	A1791	U1648	A1535	U1379	A1169	A1169
C2539	A2453	G2358	G2143	C1977	A1872	G1792	G1649	G1536	U1380	C1170	C1170
C2540	U2454	G2359	C2144	C1985	G1873	C1793	A1650	G1537	G1381	G1171	G1171
C2541	A2455	G2360	A2145	C1986	C1879	A1794	G1651	C1550	G1382	C1289	C1172
A2542	G2456	G2361	C2146	U1988	C1879	C1795	A1652	U1559	A1383	C1290	U1173
C2547	C2457	C2362	A2147	G1989	C1888	C1795	G1653	U1554	A1384	C1291	U1174
C2548	A2458	G2363	G2158	C1990	G1888	C1800	C1656	G1555	A1385	C1297	A1175
C2549	C2459	C2364	G2159	U1991	C1888	C1800	U1657	G1556	C1386	C1298	U1176
G2550	G2460	G2365	A2160	U1992	C1889	A1802	C1658	C1557	A1418	G1299	C1177
U2552	C2461	C2366	C2161	U1993	C1893	A1803	C1659	C1558	A1419	G1300	C1178
C2553	A2462	C2367	C2162	C1994	G1896	C1804	U1668	U1559	G1426	A1301	G1179
U2554	G2463	G2368	C2163	U1995	G1897	A1805	A1669	U1564	A1427	C1314	
C2558	C2464	C2369	U2166	C1996	C1902	A1806	C1670	C1564	C1428	C1319	
C2559	A2465	G2370	U2167	C1997	C1905	C1807	C1674	C1565	C1437	C1320	G1192
A2564	C2466	C2371	G2168	U1998	C1906	A1808	C1675	A1566	G1452	A1321	C1200
C2565	U2467	C2372	A2169	C2000	G1907	A1809	C1675	G1567	G1452	C1323	G1206
U2567	G2468	G2373	A2170	C2001	C1907	A1810	A1678	A1568	G1456	U1329	G1207
C2568	C2469	U2374	C2171	G2002	U1911	G1811	C1691	A1570	G1459	C1330	C1208
C2569	A2470	C2375	U2172	C2002	U1912	C1812	C1694	A1571	U1460	C1335	G1212
C2572	U2471	G2376	U2173	C2006	A1913	A1815	C1694	C1577	U1468	G1339	G1215
A2573	C2472	C2377	C2174	U2007	C1914	C1816	C1694	U1578	G1471	U1340	G1218
G2574	U2473	C2378	C2175	C2008	3TD1915	A1819	C1708	A1579	G1476	C1345	G1236
C2575	A2474	C2379	U2180	A2009	A1916	C1822	C1715	A1580	U1476	C1348	U1237
C2579	G2475	U2380	U2181	G2012	U1917	G1823	G1728	A1583	C1604	C1349	G1238
U2580	A2476	C2381	A2013	A2013	U1923	C1828	C1728	U1583	C1605	C1350	C1243
G2583	C2477	C2382	U2182	A2014	C1924	A1829	C1730	G1587	C1606	C1351	A1247
C2586	U2478	G2383	A2183	U2022	G1930	C1830	G1731	U1588	G1482	U1352	
A2587	A2479	C2384	U2184	C2023	C1934	G1831	C1732	G1589	C1490		
G2588	C2480	U2385	G2189	G2024	G1935	C1832	C1732	U1590	C1493		
A2589	U2481	C2386	C2190	C2025	C1936	C1833	C1738	C1604			
C2590	G2482	G2387	A2191	A2030	A1937	U1834	C1738	C1605			
U2591	A2483	A2287	U2192	A2031	A1938	G1835	C1752	C1606			
C2594	C2484	A2288	U2193	A2032	A1939	C1836	C1753	C1607			
C2597	U2485	C2289	U2194	A2033	U1939	C1837	A1754	A1608			
	A2486	C2290	U2195	C2036	C1947	C1838	G1756	C1612			
	G2487	C2291	A2196			G1839					
	C2488	C2292	U2197								
	U2489	C2293	U2198								
	A2490	C2294	U2199								
	C2491	C2295	U2200								
	U2492	C2296	U2201								
	A2493	C2297	U2202								
	C2494	C2298	U2203								
	U2495	C2299	U2204								
	A2496	C2300	U2205								
	C2497	C2301	U2206								
	U2498	C2302	U2207								
	A2499	C2303	U2208								
	C2500	C2304	U2209								
	U2501	C2305	U2210								
	C2502	C2306	U2211								
	A2503	C2307	U2212								
	U2504	C2308	U2213								
	A2505	C2309	U2214								
	C2506	A2314	C2115								
	U2507	A2315	C2116								
	C2508	A2316	C2117								
	A2509	A2317	U2118								
	C2510	A2318	A2119								
	U2511	A2319	U2120								
	C2512	A2320	U2121								
	A2513	C2321	U2122								
	U2514	A2322	U2123								
	C2515	C2323	U2124								
	A2516	C2324	U2125								
	U2517	A2325	U2126								
	C2518	C2326	U2127								
	A2519	C2327	U2128								
	U2520	A2328	U2129								
	C2521	C2329	U2130								
	A2522	A2330	U2131								
	U2523	C2331	U2132								
	C2524	A2332	U2133								
	A2525	C2333	U2134								
	U2526	A2334	U2135								
	C2527	C2335	U2136								
	A2528	A2336	U2137								
	U2529	C2337	U2138								
	C2530	A2338	U2139								
	A2531	C2339	U2140								
	U2532	A2340	U2141								
	C2533	C2341	U2142								
	A2534	A2342	U2143								
	U2535	C2343	U2144								
	C2536	A2344	U2145								
	A2537	C2345	U2146								
	U2538	A2346	U2147								
	C2539	C2347	U2148								
	A2540	A2348	U2149								
	U2541	C2349	U2150								
	C2542	A2350	U2151								
	A2543	C2351	U2152								
	U2544	A2352	U2153								
	C2545	C2353	U2154								
	A2546	A2354	U2155								
	U2547	C2355	U2156								
	C2548	A2356	U2157								
	A2549	C2357	U2158								
	U2550	A2358	U2159								
	C2551	C2359	U2160								
	A2552	A2360	U2161								
	U2553	C2361	U2162								
	C2554	A2362	U2163								
	A2555	C2363	U2164								
	U2556	A2364	U2165								
	C2557	C2365	U2166								
	A2558	A2366	U2167								
	U2559	C2367	U2168								
	C2560	A2368	U2169								
	A2561	C2369	U2170								
	U2562	A2370	U2171								
	C2563	C2371	U2172								
	A2564	A2372	U2173								
	U2565	C2373	U2174								
	C2566	A2374	U2175								
	A2567	C2375	U2176								
	U2568	A2376	U2177								
	C2569	C2377	U2178								
	A2570	A2378	U2179								
	U2571	C2379	U2180								
	C2572	A2380	U2181								
	A2573	C2381	U2182								
	U2574	A2382	U2183								
	C2575	C2383	U2184								
	A2576	A2384	U2185								
	U2577	C2385	U2186								
	C2578	A2386	U2187								
	A2579	C2387	U2188								
	U2580	A2388	U2189								
	C2581	C2389	U2190								
	A2582	A2390	U2191								
	U2583	C2391	U2192								
	C2584	A2392	U2193								
	A2585	C2393	U2194								
	U2586	A2394	U2195	</							



• Molecule 2: 16S rRNA

Chain 2: 74% 25%





- Molecule 3: 5S rRNA

Chain 3: 82% 18%



- Molecule 4: mRNA

Chain 4: 83% 17%



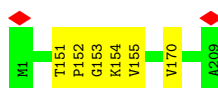
- Molecule 5: 50S ribosomal protein L2

Chain C: 99%



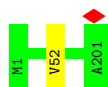
- Molecule 6: 50S ribosomal protein L3

Chain D: 97%



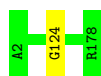
- Molecule 7: 50S ribosomal protein L4

Chain E: 100%



- Molecule 8: 50S ribosomal protein L5

Chain F: 99%



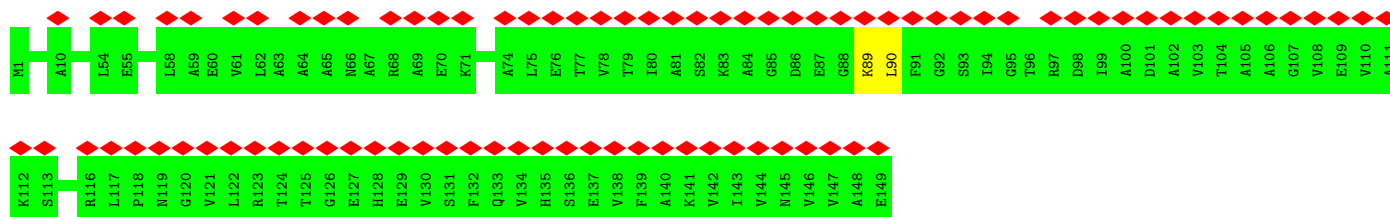
- Molecule 9: 50S ribosomal protein L6

Chain G: 100%



- Molecule 10: 50S ribosomal protein L9

Chain H: 58% 99%



- Molecule 11: 50S ribosomal protein L13

Chain I: 100%

There are no outlier residues recorded for this chain.

- Molecule 12: 50S ribosomal protein L14

Chain J: 98%



- Molecule 13: 50S ribosomal protein L15

Chain K: 99%



- Molecule 14: 50S ribosomal protein L16

Chain L: 99%



- Molecule 15: 50S ribosomal protein L17

Chain M: 99%



- Molecule 16: 50S ribosomal protein L18

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L19

Chain O:  97%



- Molecule 18: 50S ribosomal protein L20

Chain P:  100%



- Molecule 19: 50S ribosomal protein L21

Chain Q:  98%



- Molecule 20: 50S ribosomal protein L22

Chain R:  97%



- Molecule 21: 50S ribosomal protein L23

Chain S:  99%



- Molecule 22: 50S ribosomal protein L24

Chain T:  100%

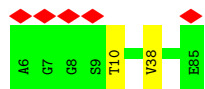
There are no outlier residues recorded for this chain.

- Molecule 23: 50S ribosomal protein L25

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L27

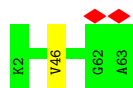


- Molecule 25: 50S ribosomal protein L28



There are no outlier residues recorded for this chain.

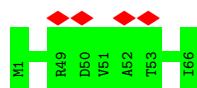
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33





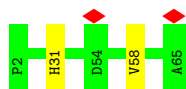
- Molecule 31: 50S ribosomal protein L34

Chain c:  100%



- Molecule 32: 50S ribosomal protein L35

Chain d:  97%



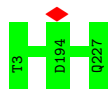
- Molecule 33: 50S ribosomal protein L36

Chain e:  100%



- Molecule 34: 30S ribosomal protein S2

Chain f:  100%



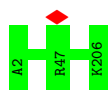
- Molecule 35: 30S ribosomal protein S3

Chain g:  100%



- Molecule 36: 30S ribosomal protein S4

Chain h:  100%



- Molecule 37: 30S ribosomal protein S5

Chain i:  97% .



- Molecule 38: 30S ribosomal protein S6

Chain j:  99% .



- Molecule 39: 30S ribosomal protein S7

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 30S ribosomal protein S8

Chain l:  100%

There are no outlier residues recorded for this chain.

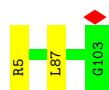
- Molecule 41: 30S ribosomal protein S9

Chain m:  99% .



- Molecule 42: 30S ribosomal protein S10

Chain n:  98% .



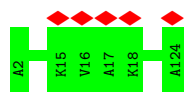
- Molecule 43: 30S ribosomal protein S11

Chain o:  99% .



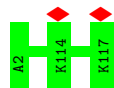
- Molecule 44: 30S ribosomal protein S12

Chain p:  100%



- Molecule 45: 30S ribosomal protein S13

Chain q:  100%



- Molecule 46: 30S ribosomal protein S14

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 30S ribosomal protein S15

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S16

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 30S ribosomal protein S17

Chain u:  100%



- Molecule 50: 30S ribosomal protein S18

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 51: 30S ribosomal protein S19

Chain w:  99%



- Molecule 52: 30S ribosomal protein S20

Chain x:  98% .



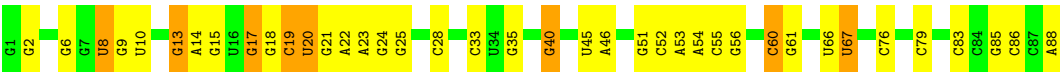
• Molecule 53: 30S ribosomal protein S21

Chain y:  7% 100%




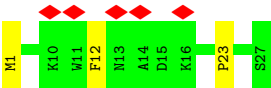
• Molecule 54: tRNA-Ser

Chain z:  56% 35% 9%



• Molecule 55: CspA transcriptional activator

Chain B:  19% 89% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44182	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.042	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FME, OMG, MG, G7M, 6MZ, UR3, 2MA, MA6, 5MC, OMU, OMC, 2MG, 0TD, 1MG, 3TD, PSU, 5MU, 4OC, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	1.78	464/69286 (0.7%)	1.30	284/108087 (0.3%)
2	2	1.57	104/36590 (0.3%)	1.23	64/57074 (0.1%)
3	3	1.52	4/2872 (0.1%)	1.21	4/4478 (0.1%)
4	4	1.38	1/139 (0.7%)	1.12	0/214
5	C	1.18	4/2121 (0.2%)	0.73	0/2852
6	D	1.18	2/1586 (0.1%)	0.72	0/2134
7	E	1.06	1/1571 (0.1%)	0.68	0/2113
8	F	0.80	0/1434	0.67	0/1926
9	G	0.77	0/1333	0.66	0/1805
10	H	0.57	0/1122	0.77	0/1515
11	I	1.14	0/1152	0.70	0/1551
12	J	1.12	1/955 (0.1%)	0.73	0/1279
13	K	1.11	1/1062 (0.1%)	0.77	0/1413
14	L	1.10	0/1093	0.69	0/1460
15	M	1.12	0/964	0.72	0/1289
16	N	0.95	0/902	0.70	0/1209
17	O	1.15	2/929 (0.2%)	0.68	1/1242 (0.1%)
18	P	1.27	0/960	0.73	0/1278
19	Q	1.13	0/829	0.69	0/1107
20	R	1.15	3/864 (0.3%)	0.71	0/1156
21	S	1.07	0/752	0.68	0/1005
22	T	0.90	0/796	0.62	0/1062
23	U	0.96	0/766	0.68	0/1025
24	V	1.13	1/608 (0.2%)	0.71	0/804
25	W	1.08	0/635	0.69	0/848
26	X	0.86	1/502 (0.2%)	0.70	0/667
27	Y	1.02	0/452	0.69	0/605
28	Z	0.66	0/531	0.63	0/709
29	a	1.09	1/450 (0.2%)	0.72	0/599
30	b	0.95	0/433	0.65	0/576
31	c	1.20	0/380	0.74	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	1.15	1/513 (0.2%)	0.71	0/676
33	e	1.15	0/303	0.69	0/397
34	f	0.69	0/1791	0.64	0/2413
35	g	0.90	0/1663	0.66	0/2241
36	h	0.88	0/1665	0.65	0/2227
37	i	1.03	2/1165 (0.2%)	0.74	0/1568
38	j	0.82	0/867	0.66	0/1171
39	k	0.75	0/1195	0.66	0/1602
40	l	0.98	0/989	0.67	0/1326
41	m	0.86	0/1034	0.73	0/1375
42	n	0.76	0/800	0.70	0/1082
43	o	0.86	0/893	0.67	0/1205
44	p	1.05	0/960	0.74	0/1286
45	q	0.82	0/909	0.68	0/1215
46	r	0.88	0/817	0.68	0/1088
47	s	0.86	0/722	0.67	0/964
48	t	0.96	0/659	0.68	0/884
49	u	0.87	0/657	0.67	0/881
50	v	0.86	0/553	0.71	0/743
51	w	0.78	0/680	0.67	0/915
52	x	0.84	0/675	0.71	0/895
53	y	0.73	0/597	0.62	0/792
54	z	1.50	13/2062 (0.6%)	1.53	27/3208 (0.8%)
55	B	0.56	0/200	0.86	0/267
All	All	1.53	606/156438 (0.4%)	1.16	380/234001 (0.2%)

All (606) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	20	U	C2-N3	15.39	1.48	1.37
54	z	20	U	C5-C6	14.07	1.46	1.34
54	z	9	G	OP3-P	-11.48	1.47	1.61
54	z	20	U	N1-C2	10.20	1.47	1.38
1	1	565	C	N1-C6	-8.15	1.32	1.37
54	z	67	U	OP3-P	-8.11	1.51	1.61
1	1	1376	C	N1-C6	-8.10	1.32	1.37
1	1	2499	C	N1-C6	-8.01	1.32	1.37
54	z	20	U	OP3-P	-8.00	1.51	1.61
1	1	2512	C	N1-C6	-7.88	1.32	1.37
1	1	673	C	N1-C6	-7.71	1.32	1.37
1	1	2681	C	N1-C6	-7.67	1.32	1.37
1	1	815	C	N1-C6	-7.65	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1571	A	N9-C4	-7.62	1.33	1.37
1	1	1832	C	N1-C6	-7.59	1.32	1.37
1	1	2065	C	N1-C6	-7.59	1.32	1.37
54	z	20	U	N3-C4	7.51	1.45	1.38
1	1	678	C	N1-C6	-7.48	1.32	1.37
1	1	672	C	N1-C6	-7.38	1.32	1.37
1	1	1790	C	N1-C6	-7.36	1.32	1.37
1	1	786	C	N1-C6	-7.33	1.32	1.37
1	1	2551	C	N1-C6	-7.32	1.32	1.37
1	1	564	C	N1-C6	-7.30	1.32	1.37
1	1	1986	C	N1-C6	-7.29	1.32	1.37
54	z	8	U	OP3-P	-7.26	1.52	1.61
1	1	1298	C	N1-C6	-7.24	1.32	1.37
1	1	2050	C	N1-C6	-7.15	1.32	1.37
1	1	2612	C	N1-C6	-7.15	1.32	1.37
1	1	2064	C	N1-C6	-7.14	1.32	1.37
1	1	732	C	N1-C6	-7.11	1.32	1.37
1	1	796	C	N1-C6	-7.09	1.32	1.37
1	1	2066	C	N1-C6	-7.08	1.32	1.37
1	1	787	C	N1-C6	-7.05	1.32	1.37
2	2	880	C	N1-C6	-7.05	1.32	1.37
1	1	679	C	N1-C6	-7.04	1.32	1.37
1	1	581	C	N1-C6	-7.04	1.32	1.37
1	1	2540	C	N1-C6	-7.03	1.32	1.37
1	1	986	C	N1-C6	-7.03	1.32	1.37
1	1	1934	C	N1-C6	-7.00	1.32	1.37
1	1	2091	C	N1-C6	-6.99	1.32	1.37
1	1	2591	C	N1-C6	-6.94	1.32	1.37
1	1	2264	C	N1-C6	-6.92	1.32	1.37
1	1	987	C	N1-C6	-6.92	1.33	1.37
2	2	1501	C	N1-C6	-6.88	1.33	1.37
2	2	758	C	N1-C6	-6.88	1.33	1.37
1	1	1261	C	N1-C6	-6.87	1.33	1.37
1	1	1999	C	N1-C6	-6.86	1.33	1.37
1	1	1658	C	N1-C6	-6.85	1.33	1.37
1	1	964	C	N1-C6	-6.82	1.33	1.37
1	1	2594	C	N1-C6	-6.81	1.33	1.37
1	1	2443	C	N1-C6	-6.79	1.33	1.37
1	1	691	C	N1-C6	-6.79	1.33	1.37
1	1	1363	C	N1-C6	-6.78	1.33	1.37
1	1	1612	C	N1-C6	-6.78	1.33	1.37
1	1	671	C	N1-C6	-6.77	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2008	C	N1-C6	-6.77	1.33	1.37
2	2	879	C	N1-C6	-6.77	1.33	1.37
2	2	1230	C	N1-C6	-6.77	1.33	1.37
2	2	810	C	N1-C6	-6.73	1.33	1.37
1	1	2000	C	N1-C6	-6.73	1.33	1.37
1	1	398	C	N1-C6	-6.72	1.33	1.37
1	1	944	C	N1-C6	-6.71	1.33	1.37
1	1	1152	C	N1-C6	-6.71	1.33	1.37
1	1	1006	C	N1-C6	-6.69	1.33	1.37
1	1	1291	C	N1-C6	-6.69	1.33	1.37
1	1	1822	C	N1-C6	-6.69	1.33	1.37
1	1	946	C	N1-C6	-6.66	1.33	1.37
1	1	1905	C	N1-C6	-6.65	1.33	1.37
1	1	2260	C	N1-C6	-6.64	1.33	1.37
1	1	2006	C	N1-C6	-6.62	1.33	1.37
1	1	1795	C	N1-C6	-6.62	1.33	1.37
1	1	2496	C	N1-C6	-6.62	1.33	1.37
1	1	2717	C	N1-C6	-6.61	1.33	1.37
1	1	698	C	N1-C6	-6.59	1.33	1.37
1	1	239	C	N1-C6	-6.59	1.33	1.37
1	1	584	C	N1-C6	-6.59	1.33	1.37
1	1	635	C	N1-C6	-6.58	1.33	1.37
2	2	16	A	N9-C4	-6.56	1.33	1.37
1	1	2426	A	N9-C4	-6.56	1.33	1.37
1	1	1639	C	N1-C6	-6.54	1.33	1.37
1	1	1974	C	N1-C6	-6.53	1.33	1.37
1	1	2456	C	N1-C6	-6.53	1.33	1.37
2	2	719	C	N1-C6	-6.53	1.33	1.37
4	4	5	C	N1-C6	-6.52	1.33	1.37
1	1	1958	C	N1-C6	-6.52	1.33	1.37
1	1	1947	C	N1-C6	-6.51	1.33	1.37
1	1	968	C	N1-C6	-6.51	1.33	1.37
1	1	634	C	N1-C6	-6.50	1.33	1.37
1	1	1351	C	N1-C6	-6.50	1.33	1.37
1	1	817	C	N1-C6	-6.47	1.33	1.37
1	1	1638	C	N1-C6	-6.47	1.33	1.37
1	1	1793	C	N1-C6	-6.47	1.33	1.37
1	1	692	C	N1-C6	-6.46	1.33	1.37
1	1	782	A	N9-C4	-6.46	1.33	1.37
1	1	1007	C	N1-C6	-6.44	1.33	1.37
1	1	823	C	N1-C6	-6.41	1.33	1.37
1	1	2045	C	N1-C6	-6.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	840	C	N1-C6	-6.40	1.33	1.37
1	1	1604	C	N1-C6	-6.40	1.33	1.37
1	1	523	C	N1-C6	-6.38	1.33	1.37
1	1	2515	C	N1-C6	-6.37	1.33	1.37
1	1	2730	C	N1-C6	-6.37	1.33	1.37
2	2	811	C	N1-C6	-6.36	1.33	1.37
1	1	1370	C	N1-C6	-6.36	1.33	1.37
1	1	806	C	N1-C6	-6.35	1.33	1.37
1	1	1161	C	N1-C6	-6.34	1.33	1.37
1	1	2442	C	N1-C6	-6.34	1.33	1.37
1	1	238	C	N1-C6	-6.32	1.33	1.37
1	1	601	C	N1-C6	-6.32	1.33	1.37
1	1	414	C	N1-C6	-6.31	1.33	1.37
1	1	1257	C	N1-C6	-6.29	1.33	1.37
1	1	2715	C	N1-C6	-6.29	1.33	1.37
1	1	516	C	N1-C6	-6.29	1.33	1.37
1	1	2716	C	N1-C6	-6.28	1.33	1.37
1	1	772	C	N1-C6	-6.25	1.33	1.37
1	1	2704	C	N1-C6	-6.24	1.33	1.37
1	1	951	C	N1-C6	-6.24	1.33	1.37
1	1	814	C	N1-C6	-6.23	1.33	1.37
1	1	2063	C	N1-C6	-6.22	1.33	1.37
1	1	2521	C	N1-C6	-6.22	1.33	1.37
1	1	32	C	N1-C6	-6.21	1.33	1.37
1	1	2738	A	N9-C4	-6.21	1.34	1.37
1	1	2841	C	N1-C6	-6.21	1.33	1.37
2	2	23	C	N1-C6	-6.21	1.33	1.37
1	1	2350	C	N1-C6	-6.21	1.33	1.37
1	1	2501	C	N1-C6	-6.21	1.33	1.37
1	1	2427	C	N1-C6	-6.19	1.33	1.37
1	1	2055	C	N1-C6	-6.19	1.33	1.37
1	1	1270	C	N1-C6	-6.17	1.33	1.37
1	1	731	C	N1-C6	-6.17	1.33	1.37
1	1	2368	C	N1-C6	-6.16	1.33	1.37
2	2	1389	C	N1-C6	-6.16	1.33	1.37
20	R	50	VAL	CB-CG1	-6.16	1.40	1.52
1	1	1564	C	N1-C6	-6.16	1.33	1.37
54	z	20	U	C4-O4	-6.15	1.18	1.23
1	1	1153	C	N1-C6	-6.14	1.33	1.37
1	1	2510	C	N1-C6	-6.13	1.33	1.37
2	2	919	A	N9-C4	-6.13	1.34	1.37
1	1	2347	C	N1-C6	-6.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2285	C	N1-C6	-6.11	1.33	1.37
2	2	1520	C	N1-C6	-6.11	1.33	1.37
1	1	1646	C	N1-C6	-6.09	1.33	1.37
1	1	2044	C	N1-C6	-6.09	1.33	1.37
1	1	531	C	N1-C6	-6.09	1.33	1.37
1	1	31	C	N1-C6	-6.08	1.33	1.37
1	1	246	C	N1-C6	-6.08	1.33	1.37
1	1	1606	C	N1-C6	-6.08	1.33	1.37
1	1	1675	C	N1-C6	-6.08	1.33	1.37
1	1	378	C	N1-C6	-6.07	1.33	1.37
1	1	1789	A	N9-C4	-6.07	1.34	1.37
1	1	2683	C	N1-C6	-6.07	1.33	1.37
1	1	2042	A	N9-C4	-6.07	1.34	1.37
2	2	311	C	N1-C6	-6.07	1.33	1.37
1	1	462	C	N1-C6	-6.06	1.33	1.37
1	1	2710	C	N1-C6	-6.06	1.33	1.37
1	1	527	C	N1-C6	-6.05	1.33	1.37
1	1	1985	C	N1-C6	-6.05	1.33	1.37
1	1	486	C	N1-C6	-6.03	1.33	1.37
2	2	1071	C	N1-C6	-6.03	1.33	1.37
2	2	868	C	N1-C6	-6.02	1.33	1.37
1	1	1354	A	N9-C4	-6.01	1.34	1.37
1	1	253	C	N1-C6	-6.00	1.33	1.37
1	1	2001	C	N1-C6	-6.00	1.33	1.37
1	1	758	C	N1-C6	-6.00	1.33	1.37
2	2	1496	C	N1-C6	-5.99	1.33	1.37
1	1	1760	C	N1-C6	-5.99	1.33	1.37
2	2	1509	C	N1-C6	-5.99	1.33	1.37
1	1	394	C	N1-C6	-5.99	1.33	1.37
1	1	992	C	N1-C6	-5.98	1.33	1.37
1	1	1656	C	N1-C6	-5.98	1.33	1.37
1	1	237	C	N1-C6	-5.98	1.33	1.37
1	1	2078	C	N1-C6	-5.98	1.33	1.37
1	1	2374	C	N1-C6	-5.98	1.33	1.37
2	2	924	C	N1-C6	-5.97	1.33	1.37
1	1	1305	C	N1-C6	-5.97	1.33	1.37
1	1	1957	C	N1-C6	-5.97	1.33	1.37
1	1	991	C	N1-C6	-5.97	1.33	1.37
1	1	1967	C	N1-C6	-5.96	1.33	1.37
1	1	2606	C	N1-C6	-5.96	1.33	1.37
1	1	1783	A	N9-C4	-5.95	1.34	1.37
1	1	2261	C	N1-C6	-5.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	660	C	N1-C6	-5.95	1.33	1.37
1	1	737	C	N1-C6	-5.95	1.33	1.37
1	1	676	A	N9-C4	-5.94	1.34	1.37
1	1	211	C	N1-C6	-5.93	1.33	1.37
1	1	804	A	N9-C4	-5.93	1.34	1.37
1	1	947	A	N9-C4	-5.93	1.34	1.37
6	D	155	VAL	CB-CG2	-5.93	1.40	1.52
1	1	795	C	N1-C6	-5.93	1.33	1.37
1	1	2118	U	O3'-P	-5.93	1.54	1.61
1	1	595	C	N1-C6	-5.93	1.33	1.37
1	1	1187	G	N9-C4	-5.93	1.33	1.38
1	1	1140	C	N1-C6	-5.92	1.33	1.37
1	1	583	G	N9-C8	-5.92	1.33	1.37
1	1	740	C	N1-C6	-5.92	1.33	1.37
1	1	461	C	N1-C6	-5.92	1.33	1.37
1	1	1833	C	N1-C6	-5.91	1.33	1.37
1	1	1802	A	N9-C4	-5.91	1.34	1.37
1	1	2678	C	N1-C6	-5.91	1.33	1.37
1	1	2601	C	N1-C6	-5.91	1.33	1.37
2	2	756	C	N1-C6	-5.90	1.33	1.37
1	1	1264	A	N9-C4	-5.90	1.34	1.37
1	1	2723	C	N1-C6	-5.90	1.33	1.37
1	1	2539	C	N1-C6	-5.89	1.33	1.37
2	2	18	C	N1-C6	-5.89	1.33	1.37
1	1	1208	C	N1-C6	-5.89	1.33	1.37
1	1	2263	C	N1-C6	-5.89	1.33	1.37
1	1	865	C	N1-C6	-5.88	1.33	1.37
1	1	2626	C	N1-C6	-5.88	1.33	1.37
2	2	401	C	N1-C6	-5.88	1.33	1.37
2	2	1433	A	N9-C4	-5.88	1.34	1.37
1	1	2248	C	N1-C6	-5.87	1.33	1.37
2	2	720	C	N1-C6	-5.85	1.33	1.37
1	1	1837	C	N1-C6	-5.85	1.33	1.37
1	1	624	C	N1-C6	-5.83	1.33	1.37
1	1	249	C	N1-C6	-5.83	1.33	1.37
1	1	445	C	N1-C6	-5.83	1.33	1.37
1	1	1670	C	N1-C6	-5.83	1.33	1.37
1	1	2520	C	N1-C6	-5.83	1.33	1.37
1	1	821	A	N9-C4	-5.83	1.34	1.37
1	1	912	C	N1-C6	-5.83	1.33	1.37
1	1	867	C	N1-C6	-5.82	1.33	1.37
1	1	2359	C	N1-C6	-5.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1278	C	N1-C6	-5.82	1.33	1.37
2	2	912	C	N1-C6	-5.82	1.33	1.37
2	2	290	C	N1-C6	-5.81	1.33	1.37
2	2	25	C	N1-C6	-5.81	1.33	1.37
1	1	2619	C	N1-C6	-5.81	1.33	1.37
2	2	549	C	N1-C6	-5.81	1.33	1.37
1	1	672	C	C4-C5	-5.80	1.38	1.43
1	1	1768	C	N1-C6	-5.80	1.33	1.37
1	1	2853	C	N1-C6	-5.80	1.33	1.37
1	1	800	A	N9-C4	-5.80	1.34	1.37
1	1	1752	C	N1-C6	-5.80	1.33	1.37
1	1	1990	C	N1-C6	-5.80	1.33	1.37
2	2	931	C	N1-C6	-5.80	1.33	1.37
2	2	1344	C	N1-C6	-5.79	1.33	1.37
1	1	2497	A	N9-C4	-5.79	1.34	1.37
1	1	2014	A	N9-C4	-5.78	1.34	1.37
2	2	295	C	N1-C6	-5.78	1.33	1.37
1	1	801	G	N9-C4	-5.78	1.33	1.38
1	1	1556	C	N1-C6	-5.78	1.33	1.37
1	1	838	C	N1-C6	-5.77	1.33	1.37
1	1	1121	C	N1-C6	-5.77	1.33	1.37
1	1	2538	C	N1-C6	-5.77	1.33	1.37
1	1	1617	C	N1-C6	-5.77	1.33	1.37
1	1	1652	A	N9-C4	-5.76	1.34	1.37
1	1	1357	C	N1-C6	-5.75	1.33	1.37
1	1	994	C	N1-C6	-5.75	1.33	1.37
1	1	1794	A	N9-C4	-5.75	1.34	1.37
1	1	2824	C	N1-C6	-5.75	1.33	1.37
1	1	922	C	N1-C6	-5.75	1.33	1.37
1	1	1805	A	N9-C4	-5.74	1.34	1.37
2	2	1510	C	N1-C6	-5.74	1.33	1.37
1	1	650	C	N1-C6	-5.73	1.33	1.37
1	1	1668	A	N9-C4	-5.73	1.34	1.37
1	1	2051	A	N9-C4	-5.73	1.34	1.37
1	1	727	A	N9-C4	-5.72	1.34	1.37
1	1	1200	C	N1-C6	-5.72	1.33	1.37
1	1	2676	C	N1-C6	-5.72	1.33	1.37
2	2	1200	C	N1-C6	-5.72	1.33	1.37
1	1	2517	C	N1-C6	-5.72	1.33	1.37
1	1	2226	C	N1-C6	-5.72	1.33	1.37
1	1	2364	C	N1-C6	-5.72	1.33	1.37
1	1	1994	C	N1-C6	-5.72	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	73	A	N9-C4	-5.71	1.34	1.37
1	1	192	C	N1-C6	-5.71	1.33	1.37
1	1	1362	C	N1-C6	-5.71	1.33	1.37
2	2	586	C	N1-C6	-5.71	1.33	1.37
1	1	1902	C	N1-C6	-5.71	1.33	1.37
1	1	2616	C	N1-C6	-5.70	1.33	1.37
1	1	581	C	C4-C5	-5.70	1.38	1.43
1	1	457	A	N9-C4	-5.70	1.34	1.37
1	1	920	A	N9-C4	-5.70	1.34	1.37
1	1	1265	A	N9-C4	-5.70	1.34	1.37
1	1	2073	C	N1-C6	-5.69	1.33	1.37
2	2	1059	C	N1-C6	-5.68	1.33	1.37
2	2	335	C	N1-C6	-5.67	1.33	1.37
5	C	221	ARG	CB-CG	-5.67	1.37	1.52
1	1	509	C	N1-C6	-5.67	1.33	1.37
1	1	1251	C	N1-C6	-5.67	1.33	1.37
1	1	2699	C	N1-C6	-5.67	1.33	1.37
1	1	837	C	N1-C6	-5.67	1.33	1.37
1	1	1936	A	N9-C4	-5.67	1.34	1.37
1	1	1350	C	N1-C6	-5.67	1.33	1.37
1	1	2065	C	C4-C5	-5.67	1.38	1.43
54	z	33	C	N1-C6	-5.66	1.33	1.37
1	1	816	C	N1-C6	-5.65	1.33	1.37
1	1	2830	C	N1-C6	-5.65	1.33	1.37
1	1	2025	C	N1-C6	-5.65	1.33	1.37
1	1	765	C	N1-C6	-5.65	1.33	1.37
1	1	2072	C	N1-C6	-5.65	1.33	1.37
1	1	1838	C	N1-C6	-5.65	1.33	1.37
1	1	413	C	N1-C6	-5.64	1.33	1.37
1	1	2009	A	N9-C4	-5.64	1.34	1.37
1	1	1815	A	N9-C4	-5.64	1.34	1.37
1	1	2598	A	N9-C4	-5.64	1.34	1.37
20	R	47	VAL	CB-CG1	-5.64	1.41	1.52
1	1	1568	G	N9-C4	-5.63	1.33	1.38
1	1	1806	C	N1-C6	-5.63	1.33	1.37
1	1	195	A	N9-C4	-5.63	1.34	1.37
1	1	393	C	N1-C6	-5.63	1.33	1.37
2	2	1223	C	N1-C6	-5.63	1.33	1.37
1	1	1961	C	N1-C6	-5.63	1.33	1.37
1	1	2053	G	N9-C8	-5.63	1.33	1.37
1	1	2502	G	N9-C4	-5.63	1.33	1.38
1	1	587	C	N1-C6	-5.62	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	334	C	N1-C6	-5.62	1.33	1.37
1	1	1977	A	N9-C4	-5.62	1.34	1.37
1	1	1823	G	N9-C8	-5.62	1.33	1.37
2	2	313	A	N9-C4	-5.61	1.34	1.37
1	1	2815	C	N1-C6	-5.61	1.33	1.37
1	1	998	C	N1-C6	-5.61	1.33	1.37
1	1	2254	C	N1-C6	-5.61	1.33	1.37
2	2	726	C	N1-C6	-5.60	1.33	1.37
2	2	522	C	N1-C6	-5.60	1.33	1.37
1	1	1836	C	N1-C6	-5.60	1.33	1.37
32	d	58	VAL	CB-CG2	-5.60	1.41	1.52
1	1	1843	C	N1-C6	-5.60	1.33	1.37
2	2	797	C	N1-C6	-5.60	1.33	1.37
1	1	334	C	N1-C6	-5.59	1.33	1.37
1	1	201	C	N1-C6	-5.59	1.33	1.37
1	1	2036	C	N1-C6	-5.59	1.33	1.37
1	1	2452	C	N1-C6	-5.58	1.33	1.37
1	1	948	C	N1-C6	-5.58	1.33	1.37
1	1	2465	C	N1-C6	-5.58	1.33	1.37
2	2	312	C	N1-C6	-5.58	1.33	1.37
1	1	2023	C	N1-C6	-5.58	1.33	1.37
1	1	2006	C	C4-C5	-5.58	1.38	1.43
2	2	1069	C	N1-C6	-5.58	1.33	1.37
1	1	236	C	N1-C6	-5.57	1.33	1.37
1	1	689	A	N9-C4	-5.57	1.34	1.37
1	1	1819	A	N9-C4	-5.57	1.34	1.37
24	V	38	VAL	CB-CG1	-5.56	1.41	1.52
1	1	2772	C	N1-C6	-5.55	1.33	1.37
2	2	823	C	N1-C6	-5.55	1.33	1.37
1	1	2089	C	N1-C6	-5.55	1.33	1.37
1	1	517	C	N1-C6	-5.55	1.33	1.37
2	2	897	C	N1-C6	-5.55	1.33	1.37
1	1	2232	C	N1-C6	-5.54	1.33	1.37
1	1	863	A	N9-C4	-5.54	1.34	1.37
1	1	1146	C	N1-C6	-5.54	1.33	1.37
1	1	2499	C	C5-C6	-5.54	1.29	1.34
1	1	1577	C	N1-C6	-5.53	1.33	1.37
54	z	20	U	C4-C5	5.52	1.48	1.43
1	1	2564	A	N9-C4	-5.52	1.34	1.37
1	1	2880	C	N1-C6	-5.52	1.33	1.37
1	1	680	C	N1-C6	-5.52	1.33	1.37
1	1	2047	C	N1-C6	-5.52	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2486	C	N1-C6	-5.52	1.33	1.37
1	1	2579	C	N1-C6	-5.51	1.33	1.37
1	1	2620	C	N1-C6	-5.50	1.33	1.37
1	1	1804	C	N1-C6	-5.50	1.33	1.37
1	1	2358	A	N9-C4	-5.50	1.34	1.37
1	1	908	C	N1-C6	-5.50	1.33	1.37
1	1	2480	C	N1-C6	-5.50	1.33	1.37
1	1	1625	C	N1-C6	-5.50	1.33	1.37
1	1	198	C	C4-C5	-5.50	1.38	1.43
1	1	2440	C	N1-C6	-5.50	1.33	1.37
1	1	557	C	N1-C6	-5.50	1.33	1.37
1	1	1830	C	C4-C5	-5.50	1.38	1.43
1	1	2466	C	N1-C6	-5.50	1.33	1.37
1	1	1650	A	N9-C4	-5.49	1.34	1.37
1	1	751	A	N9-C4	-5.49	1.34	1.37
1	1	383	C	N1-C6	-5.49	1.33	1.37
2	2	738	C	N1-C6	-5.49	1.33	1.37
1	1	988	A	N9-C4	-5.48	1.34	1.37
1	1	475	C	N1-C6	-5.48	1.33	1.37
1	1	794	A	N9-C4	-5.48	1.34	1.37
2	2	1314	C	N1-C6	-5.47	1.33	1.37
1	1	1557	C	N1-C6	-5.47	1.33	1.37
2	2	341	C	N1-C6	-5.47	1.33	1.37
1	1	1810	A	N9-C4	-5.47	1.34	1.37
1	1	1708	C	N1-C6	-5.46	1.33	1.37
1	1	501	A	N9-C4	-5.46	1.34	1.37
1	1	687	C	N1-C6	-5.46	1.33	1.37
2	2	545	C	N1-C6	-5.46	1.33	1.37
1	1	337	C	N1-C6	-5.46	1.33	1.37
1	1	1565	C	N3-C4	-5.45	1.30	1.33
1	1	1005	C	N1-C6	-5.45	1.33	1.37
1	1	116	C	N1-C6	-5.44	1.33	1.37
5	C	162	VAL	CB-CG1	-5.44	1.41	1.52
1	1	1678	A	N9-C4	-5.44	1.34	1.37
1	1	1615	C	N1-C6	-5.44	1.33	1.37
1	1	1997	C	N1-C6	-5.44	1.33	1.37
1	1	2475	C	N1-C6	-5.44	1.33	1.37
1	1	1243	C	N1-C6	-5.43	1.33	1.37
2	2	770	C	N1-C6	-5.43	1.33	1.37
1	1	2230	G	N9-C8	-5.43	1.34	1.37
1	1	208	C	N1-C6	-5.43	1.33	1.37
1	1	780	G	N9-C4	-5.42	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1694	C	N1-C6	-5.42	1.33	1.37
2	2	940	C	N1-C6	-5.42	1.33	1.37
1	1	2417	C	N1-C6	-5.42	1.33	1.37
1	1	2591	C	C4-C5	-5.40	1.38	1.43
7	E	52	VAL	CB-CG2	-5.40	1.41	1.52
1	1	583	G	N9-C4	-5.40	1.33	1.38
1	1	1319	C	N1-C6	-5.40	1.33	1.37
1	1	1348	C	N1-C6	-5.39	1.33	1.37
1	1	2468	A	N9-C4	-5.39	1.34	1.37
2	2	556	C	N1-C6	-5.39	1.33	1.37
2	2	1388	C	N1-C6	-5.39	1.33	1.37
1	1	194	G	N9-C8	-5.39	1.34	1.37
2	2	1080	A	N9-C4	-5.39	1.34	1.37
1	1	757	G	N9-C4	-5.39	1.33	1.38
3	3	97	C	N1-C6	-5.39	1.33	1.37
1	1	240	C	N1-C6	-5.38	1.33	1.37
1	1	2774	C	N1-C6	-5.38	1.33	1.37
2	2	985	C	N1-C6	-5.38	1.33	1.37
1	1	1427	A	N9-C4	-5.37	1.34	1.37
2	2	899	C	N1-C6	-5.37	1.33	1.37
2	2	1484	C	N1-C6	-5.37	1.33	1.37
1	1	1670	C	C4-C5	-5.37	1.38	1.43
1	1	1879	C	N1-C6	-5.36	1.33	1.37
2	2	732	C	N1-C6	-5.35	1.33	1.37
1	1	2675	A	N9-C4	-5.35	1.34	1.37
2	2	501	C	N1-C6	-5.34	1.33	1.37
3	3	90	C	N1-C6	-5.34	1.33	1.37
1	1	2771	C	N1-C6	-5.34	1.33	1.37
1	1	26	G	N9-C4	-5.34	1.33	1.38
1	1	1570	A	N9-C4	-5.34	1.34	1.37
1	1	806	C	C4-C5	-5.34	1.38	1.43
2	2	1109	C	N1-C6	-5.34	1.33	1.37
1	1	2332	C	N1-C6	-5.33	1.33	1.37
2	2	106	C	N1-C6	-5.33	1.33	1.37
1	1	1691	C	N1-C6	-5.32	1.33	1.37
3	3	91	C	N1-C6	-5.32	1.33	1.37
1	1	2559	C	N1-C6	-5.32	1.33	1.37
1	1	1550	C	N1-C6	-5.32	1.33	1.37
1	1	2274	A	N9-C4	-5.31	1.34	1.37
1	1	2500	U	N1-C6	-5.31	1.33	1.38
1	1	183	C	N1-C6	-5.30	1.33	1.37
1	1	2507	C	N1-C6	-5.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	883	C	N1-C6	-5.30	1.33	1.37
1	1	1143	A	C5-C6	-5.30	1.36	1.41
1	1	778	G	N9-C8	-5.30	1.34	1.37
1	1	1364	G	N9-C8	-5.30	1.34	1.37
1	1	2013	A	C6-N1	-5.30	1.31	1.35
2	2	580	C	N1-C6	-5.30	1.33	1.37
1	1	921	C	N1-C6	-5.29	1.33	1.37
1	1	2043	C	N1-C6	-5.29	1.33	1.37
1	1	1135	C	N1-C6	-5.29	1.33	1.37
1	1	1774	C	C4-C5	-5.28	1.38	1.43
1	1	2773	C	N1-C6	-5.28	1.33	1.37
17	O	61	VAL	CB-CG1	-5.28	1.41	1.52
2	2	599	C	N1-C6	-5.27	1.33	1.37
1	1	1614	A	N9-C4	-5.27	1.34	1.37
1	1	560	C	N1-C6	-5.26	1.33	1.37
1	1	1297	C	N1-C6	-5.26	1.33	1.37
2	2	36	C	N1-C6	-5.26	1.33	1.37
1	1	2575	C	N1-C6	-5.26	1.33	1.37
2	2	857	C	N1-C6	-5.26	1.33	1.37
1	1	1192	G	N9-C4	-5.25	1.33	1.38
2	2	379	C	N1-C6	-5.25	1.33	1.37
2	2	862	C	N1-C6	-5.25	1.33	1.37
1	1	621	A	N9-C4	-5.25	1.34	1.37
2	2	825	A	N9-C4	-5.25	1.34	1.37
1	1	835	C	N1-C6	-5.25	1.34	1.37
1	1	1323	C	N1-C6	-5.25	1.34	1.37
1	1	2715	C	C4-C5	-5.25	1.38	1.43
1	1	2813	A	N9-C4	-5.25	1.34	1.37
1	1	640	C	N1-C6	-5.24	1.34	1.37
1	1	1754	A	N9-C4	-5.24	1.34	1.37
1	1	788	A	N9-C4	-5.24	1.34	1.37
1	1	2722	G	N3-C4	-5.24	1.31	1.35
1	1	20	C	N1-C6	-5.23	1.34	1.37
1	1	668	A	N9-C4	-5.23	1.34	1.37
1	1	1386	C	N1-C6	-5.23	1.34	1.37
1	1	1893	C	N1-C6	-5.23	1.34	1.37
1	1	2719	G	N1-C2	-5.23	1.33	1.37
1	1	965	C	N1-C6	-5.22	1.34	1.37
2	2	564	C	N1-C6	-5.22	1.34	1.37
1	1	115	C	N1-C6	-5.22	1.34	1.37
1	1	1330	C	N1-C6	-5.22	1.34	1.37
54	z	35	G	N9-C4	-5.22	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	471	A	N9-C4	-5.22	1.34	1.37
1	1	2266	A	N9-C4	-5.21	1.34	1.37
37	i	137	VAL	CB-CG1	-5.21	1.42	1.52
2	2	696	A	N9-C4	-5.21	1.34	1.37
1	1	585	G	N9-C8	-5.20	1.34	1.37
2	2	1521	C	N1-C6	-5.20	1.34	1.37
1	1	1030	C	N1-C6	-5.20	1.34	1.37
2	2	817	C	N1-C6	-5.20	1.34	1.37
2	2	52	C	N1-C6	-5.20	1.34	1.37
54	z	83	C	N1-C6	-5.20	1.34	1.37
1	1	1771	C	N1-C6	-5.20	1.34	1.37
1	1	1853	A	N9-C4	-5.19	1.34	1.37
1	1	485	C	N1-C6	-5.19	1.34	1.37
2	2	853	C	N1-C6	-5.19	1.34	1.37
2	2	58	C	N1-C6	-5.19	1.34	1.37
2	2	503	C	N1-C6	-5.19	1.34	1.37
1	1	2459	A	N9-C4	-5.19	1.34	1.37
1	1	2590	A	N9-C4	-5.18	1.34	1.37
1	1	2863	C	N1-C6	-5.18	1.34	1.37
1	1	2636	C	N1-C6	-5.18	1.34	1.37
1	1	954	G	N9-C8	-5.18	1.34	1.37
1	1	1670	C	C4-N4	-5.18	1.29	1.33
29	a	3	VAL	CB-CG1	-5.17	1.42	1.52
1	1	2283	C	N1-C6	-5.17	1.34	1.37
1	1	1253	A	N9-C4	-5.17	1.34	1.37
1	1	449	A	N9-C4	-5.17	1.34	1.37
1	1	1306	C	N1-C6	-5.17	1.34	1.37
1	1	854	C	N1-C6	-5.17	1.34	1.37
1	1	2691	C	N1-C6	-5.17	1.34	1.37
1	1	853	C	N1-C6	-5.16	1.34	1.37
1	1	1996	C	N1-C6	-5.16	1.34	1.37
1	1	991	C	C4-C5	-5.16	1.38	1.43
1	1	2579	C	C4-C5	-5.16	1.38	1.43
1	1	1788	C	N1-C6	-5.16	1.34	1.37
2	2	896	C	N1-C6	-5.16	1.34	1.37
2	2	948	C	N1-C6	-5.16	1.34	1.37
1	1	995	C	N1-C6	-5.16	1.34	1.37
2	2	624	C	N1-C6	-5.16	1.34	1.37
1	1	2870	C	N1-C6	-5.15	1.34	1.37
13	K	60	ARG	C-N	-5.15	1.22	1.34
1	1	179	C	N1-C6	-5.15	1.34	1.37
2	2	504	C	N1-C6	-5.15	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	170	VAL	CB-CG2	-5.15	1.42	1.52
1	1	1790	C	C4-C5	-5.14	1.38	1.43
1	1	2600	A	N9-C4	-5.14	1.34	1.37
1	1	242	G	N9-C4	-5.14	1.33	1.38
1	1	1145	C	N1-C6	-5.14	1.34	1.37
5	C	228	VAL	CB-CG1	-5.14	1.42	1.52
1	1	2550	G	N9-C8	-5.14	1.34	1.37
1	1	2258	C	N1-C6	-5.13	1.34	1.37
1	1	2362	C	N1-C6	-5.13	1.34	1.37
1	1	677	A	N9-C4	-5.13	1.34	1.37
1	1	2565	A	N9-C4	-5.13	1.34	1.37
2	2	806	C	N1-C6	-5.13	1.34	1.37
2	2	1352	C	N1-C6	-5.13	1.34	1.37
1	1	469	G	C6-N1	-5.13	1.35	1.39
1	1	740	C	C4-C5	-5.13	1.38	1.43
1	1	939	G	N9-C8	-5.13	1.34	1.37
17	O	47	VAL	CB-CG2	-5.12	1.42	1.52
1	1	806	C	N3-C4	-5.12	1.30	1.33
20	R	98	LYS	CA-CB	-5.12	1.42	1.53
1	1	1335	C	N1-C6	-5.12	1.34	1.37
2	2	578	C	N1-C6	-5.12	1.34	1.37
1	1	182	A	N9-C4	-5.12	1.34	1.37
2	2	233	C	N1-C6	-5.12	1.34	1.37
2	2	876	C	N1-C6	-5.12	1.34	1.37
1	1	812	C	N1-C6	-5.11	1.34	1.37
1	1	469	G	N1-C2	-5.11	1.33	1.37
1	1	47	C	N1-C6	-5.11	1.34	1.37
1	1	1385	A	N9-C4	-5.11	1.34	1.37
1	1	2036	C	C4-C5	-5.11	1.38	1.43
2	2	54	C	N1-C6	-5.11	1.34	1.37
2	2	234	C	N1-C6	-5.11	1.34	1.37
1	1	2448	A	N9-C4	-5.10	1.34	1.37
2	2	764	C	N1-C6	-5.10	1.34	1.37
2	2	1524	C	N1-C6	-5.10	1.34	1.37
26	X	46	VAL	CB-CG1	-5.10	1.42	1.52
1	1	1196	C	N1-C6	-5.09	1.34	1.37
1	1	2451	A	N9-C4	-5.09	1.34	1.37
1	1	761	A	N9-C4	-5.09	1.34	1.37
1	1	834	G	N9-C4	-5.09	1.33	1.38
2	2	315	A	N9-C4	-5.09	1.34	1.37
2	2	765	G	N9-C4	-5.09	1.33	1.38
1	1	2434	A	N9-C4	-5.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1803	A	N9-C4	-5.08	1.34	1.37
2	2	395	C	N1-C6	-5.08	1.34	1.37
3	3	93	C	N1-C6	-5.08	1.34	1.37
37	i	94	VAL	CB-CG1	-5.08	1.42	1.52
5	C	195	VAL	CB-CG2	-5.08	1.42	1.52
1	1	2281	A	N9-C4	-5.07	1.34	1.37
1	1	2339	C	N1-C6	-5.07	1.34	1.37
1	1	2443	C	C4-C5	-5.07	1.38	1.43
2	2	739	C	N1-C6	-5.07	1.34	1.37
1	1	2490	G	N9-C4	-5.06	1.33	1.38
2	2	658	C	N1-C6	-5.06	1.34	1.37
1	1	797	G	N9-C8	-5.06	1.34	1.37
1	1	2719	G	N9-C4	-5.06	1.33	1.38
2	2	115	G	N9-C4	-5.06	1.33	1.38
1	1	2462	C	N1-C6	-5.05	1.34	1.37
1	1	2688	G	N9-C4	-5.05	1.33	1.38
2	2	386	C	N1-C6	-5.05	1.34	1.37
2	2	136	C	N1-C6	-5.05	1.34	1.37
1	1	998	C	C4-C5	-5.05	1.39	1.43
1	1	2558	C	N1-C6	-5.05	1.34	1.37
1	1	2527	C	N1-C6	-5.05	1.34	1.37
2	2	805	C	N1-C6	-5.05	1.34	1.37
1	1	1143	A	N9-C4	-5.04	1.34	1.37
1	1	1187	G	N3-C4	-5.04	1.31	1.35
1	1	1314	C	C4-C5	-5.04	1.39	1.43
2	2	124	C	N1-C6	-5.04	1.34	1.37
1	1	690	G	N9-C8	-5.04	1.34	1.37
2	2	569	C	N1-C6	-5.03	1.34	1.37
1	1	782	A	N3-C4	-5.03	1.31	1.34
1	1	2526	G	N9-C4	-5.03	1.33	1.38
1	1	1605	C	N1-C6	-5.03	1.34	1.37
1	1	1844	C	N1-C6	-5.03	1.34	1.37
1	1	2456	C	C4-C5	-5.03	1.39	1.43
1	1	1371	G	N9-C4	-5.02	1.33	1.38
1	1	2725	A	N9-C4	-5.02	1.34	1.37
1	1	1133	A	N9-C4	-5.02	1.34	1.37
1	1	2542	A	N9-C4	-5.02	1.34	1.37
1	1	2589	A	N9-C4	-5.02	1.34	1.37
12	J	92	GLU	C-N	-5.02	1.22	1.34
1	1	863	A	C6-N6	-5.01	1.29	1.33
1	1	2380	C	N1-C6	-5.01	1.34	1.37
1	1	1339	G	N9-C4	-5.01	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1369	C	N1-C6	-5.01	1.34	1.37
1	1	336	C	N1-C6	-5.01	1.34	1.37
1	1	302	C	N1-C6	-5.00	1.34	1.37
1	1	736	C	C4-C5	-5.00	1.39	1.43
2	2	1467	C	N1-C6	-5.00	1.34	1.37

All (380) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	67	U	O5'-P-OP1	-26.51	78.89	110.70
54	z	8	U	O5'-P-OP1	-19.49	87.31	110.70
54	z	20	U	C2-N3-C4	-14.79	118.13	127.00
54	z	20	U	C5-C4-O4	-12.55	118.37	125.90
54	z	20	U	N3-C4-C5	9.82	120.49	114.60
1	1	1871	A	O4'-C1'-N9	9.71	115.97	108.20
54	z	20	U	N1-C2-N3	9.16	120.40	114.90
54	z	19	C	OP2-P-O3'	-9.04	85.32	105.20
1	1	1509	A	O4'-C1'-N9	8.77	115.22	108.20
1	1	1923	U	O4'-C1'-N1	8.69	115.15	108.20
1	1	2193	G	C4-N9-C1'	8.67	137.77	126.50
54	z	67	U	O5'-P-OP2	8.47	120.86	110.70
1	1	1670	C	N3-C4-C5	8.44	125.28	121.90
1	1	1313	U	C2-N1-C1'	8.39	127.77	117.70
1	1	2719	G	C2-N3-C4	-8.30	107.75	111.90
2	2	74	A	O4'-C1'-N9	8.28	114.82	108.20
1	1	221	A	O4'-C1'-N9	8.22	114.78	108.20
1	1	1062	G	N3-C4-N9	8.21	130.93	126.00
1	1	1670	C	C5-C4-N4	-8.03	114.58	120.20
1	1	1067	A	O4'-C1'-N9	-7.97	101.82	108.20
1	1	2193	G	C8-N9-C1'	-7.74	116.94	127.00
1	1	1062	G	C8-N9-C1'	-7.72	116.96	127.00
1	1	752	A	N1-C6-N6	7.71	123.22	118.60
1	1	1062	G	C4-N9-C1'	7.70	136.50	126.50
1	1	2193	G	C6-C5-N7	-7.66	125.81	130.40
54	z	40	G	N1-C2-N2	-7.56	109.40	116.20
1	1	1761	C	C5-C4-N4	-7.39	115.02	120.20
54	z	9	G	C2-N3-C4	-7.38	108.21	111.90
1	1	565	C	C6-N1-C2	7.35	123.24	120.30
1	1	481	G	O4'-C1'-N9	7.34	114.07	108.20
54	z	20	U	OP1-P-OP2	7.31	130.57	119.60
1	1	801	G	C2-N3-C4	-7.21	108.30	111.90
1	1	1790	C	C5-C4-N4	-7.18	115.18	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2512	C	C5'-C4'-C3'	7.14	127.43	116.00
54	z	19	C	OP1-P-O3'	-7.09	89.61	105.20
2	2	800	G	C2-N3-C4	-7.03	108.38	111.90
1	1	1125	G	C2-N3-C4	-7.02	108.39	111.90
2	2	1200	C	C5-C4-N4	-7.00	115.30	120.20
54	z	20	U	C5-C6-N1	-6.91	119.25	122.70
1	1	1313	U	C6-N1-C1'	-6.87	111.58	121.20
1	1	2755	C	C5-C4-N4	-6.85	115.40	120.20
1	1	1171	G	C8-N9-C1'	-6.85	118.10	127.00
2	2	1403	C	C5-C4-N4	-6.79	115.44	120.20
2	2	575	G	N3-C4-N9	-6.78	121.93	126.00
1	1	801	G	N3-C4-C5	6.78	131.99	128.60
1	1	974	G	O4'-C1'-N9	6.74	113.59	108.20
1	1	1075	C	N1-C2-O2	6.74	122.94	118.90
54	z	8	U	O5'-P-OP2	6.71	118.75	110.70
1	1	1143	A	N1-C6-N6	6.68	122.61	118.60
54	z	40	G	C2-N3-C4	-6.66	108.57	111.90
1	1	2799	A	N9-C4-C5	-6.66	103.14	105.80
1	1	1062	G	C6-C5-N7	-6.65	126.41	130.40
1	1	1143	A	C5-C6-N6	-6.64	118.39	123.70
2	2	686	U	O4'-C1'-N1	6.62	113.50	108.20
2	2	792	A	O4'-C1'-N9	6.62	113.50	108.20
2	2	117	G	C2-N3-C4	-6.60	108.60	111.90
2	2	354	G	C2-N3-C4	-6.58	108.61	111.90
1	1	916	G	C2-N3-C4	-6.57	108.61	111.90
1	1	2688	G	C2-N3-C4	-6.57	108.61	111.90
2	2	15	G	C2-N3-C4	-6.54	108.63	111.90
1	1	450	G	C2-N3-C4	-6.54	108.63	111.90
1	1	2314	A	O4'-C1'-N9	6.54	113.43	108.20
1	1	728	G	N3-C2-N2	-6.54	115.33	119.90
1	1	818	G	C2-N3-C4	-6.47	108.66	111.90
1	1	733	G	C2-N3-C4	-6.44	108.68	111.90
1	1	2351	G	C2-N3-C4	-6.42	108.69	111.90
1	1	1062	G	N9-C4-C5	-6.41	102.83	105.40
1	1	1350	C	N3-C4-C5	6.41	124.46	121.90
1	1	2610	C	N3-C4-C5	6.41	124.46	121.90
1	1	2195	U	O4'-C1'-N1	6.41	113.33	108.20
54	z	35	G	N3-C4-C5	6.41	131.80	128.60
54	z	60	C	C5-C4-N4	-6.39	115.73	120.20
1	1	476	G	C2-N3-C4	-6.38	108.71	111.90
1	1	275	C	C2-N1-C1'	-6.37	111.80	118.80
1	1	1075	C	N3-C2-O2	-6.37	117.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	323	C	C2-N1-C1'	6.35	125.79	118.80
1	1	27	G	C2-N3-C4	-6.33	108.73	111.90
1	1	1187	G	N3-C4-C5	6.31	131.76	128.60
1	1	2607	G	C2-N3-C4	-6.29	108.75	111.90
1	1	1076	C	N3-C2-O2	-6.26	117.52	121.90
1	1	2765	A	O4'-C1'-N9	6.25	113.20	108.20
1	1	1261	C	C6-N1-C2	6.21	122.78	120.30
1	1	801	G	N3-C4-N9	-6.19	122.28	126.00
1	1	1870	C	O5'-P-OP1	6.19	118.13	110.70
1	1	2248	C	C2-N1-C1'	6.18	125.60	118.80
1	1	2715	C	C2-N1-C1'	6.16	125.58	118.80
1	1	806	C	N1-C2-O2	6.14	122.58	118.90
1	1	512	G	O4'-C1'-N9	6.13	113.11	108.20
2	2	1221	G	N3-C4-C5	6.13	131.66	128.60
1	1	2499	C	C5-C4-N4	-6.12	115.92	120.20
1	1	2799	A	C4-C5-N7	6.10	113.75	110.70
1	1	1814	G	C2-N3-C4	-6.09	108.86	111.90
2	2	1337	G	N3-C4-C5	6.08	131.64	128.60
1	1	2365	G	C2-N3-C4	-6.07	108.86	111.90
1	1	469	G	C2-N3-C4	-6.04	108.88	111.90
1	1	748	G	O4'-C1'-N9	6.04	113.03	108.20
1	1	2499	C	C6-N1-C2	6.03	122.71	120.30
1	1	1171	G	N9-C4-C5	-6.03	102.99	105.40
2	2	324	G	N3-C4-C5	6.02	131.61	128.60
2	2	1482	G	C2-N3-C4	-6.02	108.89	111.90
1	1	2709	G	C2-N3-C4	-6.01	108.89	111.90
1	1	198	C	N1-C2-O2	6.01	122.51	118.90
1	1	254	G	C2-N3-C4	-6.01	108.90	111.90
1	1	561	G	C2-N3-C4	-6.01	108.90	111.90
1	1	2597	G	C2-N3-C4	-6.00	108.90	111.90
1	1	2720	U	N3-C4-O4	5.99	123.59	119.40
1	1	2715	C	C6-N1-C1'	-5.99	113.62	120.80
2	2	324	G	C2-N3-C4	-5.98	108.91	111.90
1	1	1187	G	C2-N3-C4	-5.97	108.92	111.90
54	z	40	G	N1-C2-N3	5.95	127.47	123.90
1	1	242	G	N3-C4-N9	-5.93	122.44	126.00
1	1	1996	C	C5-C4-N4	-5.93	116.05	120.20
1	1	1670	C	C6-N1-C2	5.93	122.67	120.30
2	2	362	G	C2-N3-C4	-5.92	108.94	111.90
1	1	2332	C	C6-N1-C2	5.92	122.67	120.30
54	z	13	G	C2-N3-C4	-5.91	108.94	111.90
1	1	704	G	O4'-C1'-N9	5.91	112.93	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2499	C	N3-C4-C5	5.91	124.26	121.90
1	1	1283	G	N3-C4-N9	-5.91	122.45	126.00
1	1	1171	G	C4-N9-C1'	5.90	134.17	126.50
1	1	189	G	C2-N3-C4	-5.90	108.95	111.90
17	O	51	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	1	1568	G	N3-C4-C5	5.90	131.55	128.60
1	1	1568	G	N3-C4-N9	-5.89	122.46	126.00
1	1	1350	C	C6-N1-C2	5.89	122.66	120.30
1	1	1792	G	C2-N3-C4	-5.89	108.96	111.90
1	1	323	C	C6-N1-C1'	-5.88	113.74	120.80
1	1	619	G	C2-N3-C4	-5.87	108.96	111.90
1	1	961	C	C5-C4-N4	-5.87	116.09	120.20
1	1	1358	G	C2-N3-C4	-5.84	108.98	111.90
1	1	242	G	N3-C4-C5	5.83	131.51	128.60
2	2	1156	G	N3-C4-C5	5.83	131.51	128.60
1	1	2248	C	C6-N1-C1'	-5.83	113.81	120.80
1	1	476	G	N3-C4-C5	5.81	131.50	128.60
1	1	998	C	N1-C2-O2	5.79	122.38	118.90
1	1	1653	G	C2-N3-C4	-5.78	109.01	111.90
1	1	2638	G	C2-N3-C4	-5.78	109.01	111.90
1	1	1382	G	C5-C6-O6	5.78	132.06	128.60
2	2	991	U	O4'-C1'-N1	5.77	112.81	108.20
1	1	458	G	O4'-C1'-N9	5.76	112.81	108.20
1	1	1567	G	C2-N3-C4	-5.76	109.02	111.90
1	1	2193	G	C4-C5-N7	5.76	113.10	110.80
1	1	2499	C	C6-N1-C1'	-5.75	113.89	120.80
1	1	663	G	C2-N3-C4	-5.75	109.02	111.90
1	1	2244	U	N3-C4-O4	5.75	123.43	119.40
1	1	565	C	N3-C4-C5	5.74	124.20	121.90
1	1	2286	G	C2-N3-C4	-5.74	109.03	111.90
1	1	2100	G	C4-C5-N7	5.74	113.10	110.80
1	1	386	G	N3-C4-N9	-5.74	122.56	126.00
1	1	1615	C	C5-C4-N4	-5.74	116.19	120.20
1	1	1172	C	C6-N1-C2	5.73	122.59	120.30
2	2	1337	G	N3-C4-N9	-5.72	122.57	126.00
1	1	1299	G	C2-N3-C4	-5.72	109.04	111.90
2	2	1007	U	O4'-C1'-N1	5.71	112.77	108.20
1	1	2591	C	C2-N1-C1'	5.71	125.08	118.80
1	1	2715	C	N1-C2-O2	5.71	122.33	118.90
1	1	274	C	N1-C2-O2	5.70	122.32	118.90
1	1	1154	G	C2-N3-C4	-5.68	109.06	111.90
1	1	67	U	N3-C4-O4	5.68	123.37	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1790	C	C6-N1-C2	5.68	122.57	120.30
2	2	1320	C	C6-N1-C2	5.67	122.57	120.30
1	1	1371	G	C2-N3-C4	-5.67	109.06	111.90
1	1	697	G	C2-N3-C4	-5.67	109.06	111.90
1	1	1377	G	C2-N3-C4	-5.67	109.07	111.90
1	1	1857	G	O4'-C1'-N9	5.66	112.72	108.20
1	1	2591	C	C6-N1-C1'	-5.65	114.02	120.80
1	1	726	G	N3-C4-N9	-5.64	122.61	126.00
1	1	1728	C	C2-N1-C1'	-5.64	112.59	118.80
1	1	400	G	C2-N3-C4	-5.64	109.08	111.90
1	1	672	C	C2-N1-C1'	5.63	125.00	118.80
1	1	1349	C	N3-C2-O2	-5.63	117.96	121.90
1	1	2726	A	C5-C6-N6	-5.63	119.20	123.70
1	1	957	C	C5-C4-N4	-5.62	116.26	120.20
3	3	76	G	C2-N3-C4	-5.62	109.09	111.90
1	1	708	G	O3'-P-O5'	-5.62	93.32	104.00
1	1	786	C	C6-N1-C2	5.62	122.55	120.30
2	2	1200	C	N3-C4-N4	5.62	121.93	118.00
1	1	585	G	C2-N3-C4	-5.62	109.09	111.90
1	1	2704	C	C2-N1-C1'	5.61	124.97	118.80
1	1	1283	G	N3-C4-C5	5.61	131.41	128.60
1	1	1771	C	N1-C2-O2	5.61	122.26	118.90
1	1	1075	C	C6-N1-C1'	-5.60	114.08	120.80
1	1	1471	G	C2-N3-C4	-5.60	109.10	111.90
1	1	2100	G	N1-C6-O6	5.60	123.26	119.90
1	1	1670	C	C2-N3-C4	-5.60	117.10	119.90
1	1	1830	C	N1-C2-O2	5.60	122.26	118.90
2	2	558	G	C2-N3-C4	-5.57	109.11	111.90
3	3	75	G	C2-N3-C4	-5.57	109.11	111.90
2	2	215	C	C2-N1-C1'	5.56	124.92	118.80
1	1	1770	G	C2-N3-C4	-5.55	109.12	111.90
1	1	672	C	N1-C2-O2	5.55	122.23	118.90
1	1	2799	A	C6-C5-N7	-5.55	128.42	132.30
1	1	386	G	C2-N3-C4	-5.54	109.13	111.90
2	2	746	A	N9-C4-C5	-5.54	103.58	105.80
1	1	1950	G	C2-N3-C4	-5.54	109.13	111.90
1	1	2430	A	N1-C6-N6	5.54	121.92	118.60
2	2	858	G	C2-N3-C4	-5.54	109.13	111.90
1	1	640	C	C2-N1-C1'	5.52	124.87	118.80
1	1	581	C	C5-C4-N4	-5.51	116.34	120.20
1	1	1631	G	C2-N3-C4	-5.51	109.15	111.90
2	2	1337	G	C4-N9-C1'	-5.50	119.35	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2714	G	C2-N3-C4	-5.50	109.15	111.90
2	2	111	G	C2-N3-C4	-5.50	109.15	111.90
1	1	2704	C	C6-N1-C1'	-5.49	114.21	120.80
1	1	275	C	C6-N1-C1'	5.49	127.39	120.80
1	1	2502	G	N3-C4-N9	-5.49	122.71	126.00
2	2	549	C	C6-N1-C2	5.49	122.50	120.30
1	1	1062	G	C4-C5-N7	5.47	112.99	110.80
1	1	2424	C	N3-C4-C5	5.46	124.09	121.90
1	1	2722	G	C2-N3-C4	-5.46	109.17	111.90
1	1	2237	G	C2-N3-C4	-5.45	109.17	111.90
1	1	1426	G	C2-N3-C4	-5.45	109.17	111.90
1	1	757	G	N3-C4-C5	5.45	131.32	128.60
1	1	1530	G	C4-C5-N7	5.45	112.98	110.80
1	1	1930	G	C2-N3-C4	-5.45	109.17	111.90
54	z	35	G	C2-N3-C4	-5.44	109.18	111.90
1	1	858	G	C2-N3-C4	-5.44	109.18	111.90
1	1	578	G	C2-N3-C4	-5.44	109.18	111.90
1	1	551	G	C8-N9-C1'	-5.44	119.93	127.00
1	1	2601	C	C6-N1-C2	5.44	122.47	120.30
2	2	581	G	C2-N3-C4	-5.44	109.18	111.90
1	1	883	G	N3-C4-N9	-5.43	122.74	126.00
2	2	362	G	N3-C4-C5	5.43	131.31	128.60
1	1	640	C	C6-N1-C2	-5.42	118.13	120.30
1	1	386	G	N3-C4-C5	5.42	131.31	128.60
1	1	1989	G	C2-N3-C4	-5.42	109.19	111.90
2	2	1505	G	N3-C4-C5	5.42	131.31	128.60
1	1	2282	G	O4'-C1'-N9	5.39	112.51	108.20
54	z	28	C	C2-N1-C1'	5.39	124.73	118.80
1	1	583	G	C2-N3-C4	-5.38	109.21	111.90
1	1	725	G	C2-N3-C4	-5.38	109.21	111.90
2	2	869	G	C2-N3-C4	-5.38	109.21	111.90
1	1	2415	G	C2-N3-C4	-5.37	109.21	111.90
2	2	168	G	C4-C5-N7	5.37	112.95	110.80
1	1	2834	G	C2-N3-C4	-5.37	109.21	111.90
1	1	2454	G	C2-N3-C4	-5.37	109.22	111.90
1	1	570	G	C2-N3-C4	-5.36	109.22	111.90
1	1	1514	G	C2-N3-C4	-5.36	109.22	111.90
1	1	2447	G	C2-N3-C4	-5.36	109.22	111.90
1	1	748	G	N3-C4-N9	-5.35	122.79	126.00
1	1	2193	G	N3-C4-N9	5.34	129.21	126.00
2	2	1467	C	N3-C4-C5	5.33	124.03	121.90
1	1	685	A	O4'-C1'-N9	5.33	112.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1459	G	N3-C4-C5	5.33	131.27	128.60
1	1	1564	C	N1-C2-O2	5.33	122.10	118.90
1	1	1936	A	N1-C6-N6	5.32	121.79	118.60
1	1	2127	G	N3-C4-N9	-5.32	122.81	126.00
1	1	1790	C	N3-C4-C5	5.31	124.03	121.90
1	1	830	G	C2-N3-C4	-5.31	109.24	111.90
1	1	1313	U	C5-C6-N1	5.31	125.36	122.70
1	1	1459	G	N3-C4-N9	-5.30	122.82	126.00
1	1	261	G	N3-C4-C5	5.30	131.25	128.60
1	1	1047	G	O4'-C1'-N9	5.30	112.44	108.20
1	1	465	G	C2-N3-C4	-5.29	109.25	111.90
1	1	424	G	N3-C4-C5	5.29	131.24	128.60
1	1	1675	C	C5-C4-N4	-5.28	116.50	120.20
1	1	1063	G	N1-C2-N2	-5.28	111.45	116.20
2	2	1028	C	O4'-C1'-N1	-5.27	103.99	108.20
2	2	168	G	C6-C5-N7	-5.26	127.24	130.40
1	1	1187	G	N3-C4-N9	-5.26	122.84	126.00
54	z	25	G	N3-C4-C5	5.26	131.23	128.60
1	1	1079	C	C2-N1-C1'	5.25	124.58	118.80
1	1	2258	C	N1-C2-O2	5.25	122.05	118.90
54	z	83	C	C6-N1-C2	5.25	122.40	120.30
2	2	108	G	C4-C5-N7	5.25	112.90	110.80
2	2	60	A	C8-N9-C4	-5.25	103.70	105.80
1	1	2100	G	N9-C4-C5	-5.24	103.30	105.40
1	1	2848	G	O4'-C1'-N9	5.24	112.39	108.20
1	1	2012	G	C2-N3-C4	-5.24	109.28	111.90
1	1	581	C	C6-N1-C1'	-5.24	114.52	120.80
1	1	2583	G	C2-N3-C4	-5.24	109.28	111.90
1	1	2405	G	C2-N3-C4	-5.23	109.28	111.90
1	1	273	G	N9-C4-C5	-5.23	103.31	105.40
1	1	1800	C	C5-C4-N4	-5.23	116.54	120.20
2	2	153	C	C6-N1-C1'	-5.23	114.53	120.80
1	1	26	G	C2-N3-C4	-5.22	109.29	111.90
1	1	1888	G	C2-N3-C4	-5.22	109.29	111.90
1	1	1935	G	C2-N3-C4	-5.22	109.29	111.90
54	z	6	G	N3-C4-N9	-5.22	122.87	126.00
1	1	2382	G	C2-N3-C4	-5.22	109.29	111.90
2	2	1417	G	C2-N3-C4	-5.22	109.29	111.90
2	2	1521	C	N1-C2-O2	5.22	122.03	118.90
1	1	389	G	C2-N3-C4	-5.22	109.29	111.90
1	1	1761	C	N3-C4-N4	5.22	121.65	118.00
1	1	587	C	C5-C4-N4	-5.21	116.55	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1339	G	C2-N3-C4	-5.21	109.29	111.90
1	1	1961	C	N3-C4-C5	5.21	123.98	121.90
1	1	2481	G	C2-N3-C4	-5.20	109.30	111.90
1	1	2490	G	N3-C4-C5	5.20	131.20	128.60
1	1	1897	G	N3-C4-C5	5.20	131.20	128.60
1	1	2502	G	C2-N3-C4	-5.20	109.30	111.90
1	1	2703	C	C6-N1-C1'	-5.20	114.56	120.80
2	2	549	C	N3-C4-C5	5.20	123.98	121.90
1	1	1838	C	C5-C4-N4	-5.19	116.56	120.20
1	1	27	G	N3-C4-C5	5.19	131.20	128.60
1	1	2193	G	N7-C8-N9	5.19	115.70	113.10
2	2	1079	G	C2-N3-C4	-5.19	109.31	111.90
1	1	721	A	N9-C4-C5	-5.18	103.73	105.80
2	2	944	G	C2-N3-C4	-5.18	109.31	111.90
2	2	586	C	C6-N1-C2	5.18	122.37	120.30
1	1	672	C	C6-N1-C1'	-5.17	114.59	120.80
2	2	1107	C	N3-C4-C5	5.17	123.97	121.90
1	1	752	A	C5-N7-C8	-5.17	101.32	103.90
1	1	1012	U	N3-C4-O4	5.17	123.02	119.40
1	1	1828	G	C2-N3-C4	-5.17	109.32	111.90
2	2	628	G	N3-C4-C5	5.17	131.18	128.60
1	1	859	G	N3-C4-N9	-5.16	122.91	126.00
1	1	950	G	C2-N3-C4	-5.16	109.32	111.90
2	2	168	G	N9-C4-C5	-5.15	103.34	105.40
1	1	1075	C	C2-N1-C1'	5.15	124.47	118.80
1	1	2763	G	C2-N3-C4	-5.15	109.32	111.90
1	1	726	G	N3-C4-C5	5.15	131.17	128.60
1	1	301	G	N3-C4-C5	5.15	131.17	128.60
1	1	2719	G	N1-C2-N3	5.15	126.99	123.90
1	1	2006	C	C5-C4-N4	-5.15	116.60	120.20
1	1	2063	C	C2-N3-C4	-5.14	117.33	119.90
1	1	1289	C	N1-C2-O2	5.14	121.99	118.90
1	1	1530	G	N1-C6-O6	5.14	122.98	119.90
1	1	752	A	C5-C6-N6	-5.14	119.59	123.70
2	2	357	G	C2-N3-C4	-5.14	109.33	111.90
2	2	1221	G	N3-C4-N9	-5.13	122.92	126.00
1	1	1349	C	C2-N1-C1'	5.13	124.44	118.80
1	1	2100	G	C6-C5-N7	-5.12	127.33	130.40
1	1	2214	C	N3-C4-C5	5.11	123.95	121.90
1	1	2452	C	N3-C4-C5	5.11	123.95	121.90
2	2	1221	G	C2-N3-C4	-5.11	109.34	111.90
1	1	1171	G	C6-C5-N7	-5.11	127.33	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1186	G	C2-N3-C4	-5.11	109.35	111.90
2	2	112	G	C2-N3-C4	-5.11	109.35	111.90
1	1	67	U	C5-C4-O4	-5.10	122.84	125.90
1	1	489	G	C2-N3-C4	-5.10	109.35	111.90
2	2	1505	G	C2-N3-C4	-5.10	109.35	111.90
1	1	551	G	C4-N9-C1'	5.10	133.12	126.50
2	2	322	C	C5-C4-N4	-5.10	116.63	120.20
1	1	1215	G	C2-N3-C4	-5.09	109.36	111.90
1	1	1839	G	C2-N3-C4	-5.09	109.36	111.90
3	3	96	G	N3-C4-N9	-5.09	122.95	126.00
1	1	780	G	C2-N3-C4	-5.09	109.36	111.90
1	1	2688	G	N3-C4-C5	5.08	131.14	128.60
2	2	666	G	N3-C4-N9	-5.08	122.95	126.00
1	1	2722	G	N1-C2-N3	5.08	126.95	123.90
2	2	705	G	C2-N3-C4	-5.08	109.36	111.90
1	1	1771	C	C2-N1-C1'	5.08	124.38	118.80
2	2	492	C	C6-N1-C1'	-5.08	114.71	120.80
1	1	1313	U	O4'-C1'-N1	5.07	112.26	108.20
1	1	2214	C	C5-C4-N4	-5.07	116.65	120.20
1	1	1350	C	C6-N1-C1'	-5.07	114.72	120.80
1	1	704	G	N3-C4-C5	5.07	131.13	128.60
54	z	60	C	N3-C4-C5	5.07	123.93	121.90
1	1	1788	C	C2-N1-C1'	5.06	124.37	118.80
1	1	2307	G	N3-C4-N9	-5.06	122.96	126.00
1	1	2888	C	N1-C2-O2	5.06	121.94	118.90
1	1	1278	C	C6-N1-C2	5.06	122.32	120.30
2	2	1517	G	C2-N3-C4	-5.06	109.37	111.90
1	1	527	C	O4'-C1'-N1	5.05	112.24	108.20
2	2	888	G	C2-N3-C4	-5.04	109.38	111.90
3	3	117	G	N3-C4-C5	5.04	131.12	128.60
1	1	728	G	C2-N3-C4	-5.04	109.38	111.90
54	z	9	G	OP1-P-OP2	5.04	127.16	119.60
1	1	17	G	C2-N3-C4	-5.04	109.38	111.90
1	1	819	A	N1-C6-N6	5.04	121.62	118.60
1	1	308	G	C2-N3-C4	-5.04	109.38	111.90
1	1	68	G	C2-N3-C4	-5.04	109.38	111.90
1	1	469	G	N1-C2-N2	-5.03	111.67	116.20
1	1	560	C	N1-C2-O2	5.03	121.92	118.90
1	1	2588	G	C2-N3-C4	-5.03	109.38	111.90
54	z	35	G	N3-C4-N9	-5.03	122.98	126.00
1	1	798	G	N3-C4-C5	5.03	131.12	128.60
1	1	2100	G	C5-C6-O6	-5.03	125.58	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2189	U	O4'-C1'-N1	5.03	112.22	108.20
1	1	1452	G	N3-C4-C5	5.02	131.11	128.60
1	1	2505	G	C2-N3-C4	-5.02	109.39	111.90
2	2	1084	G	N3-C4-C5	5.02	131.11	128.60
2	2	207	C	C2-N1-C1'	-5.02	113.28	118.80
2	2	869	G	N3-C4-C5	5.02	131.11	128.60
2	2	57	G	N3-C4-C5	5.02	131.11	128.60
1	1	1456	G	N3-C4-C5	5.01	131.11	128.60
1	1	1171	G	N3-C4-N9	5.01	129.01	126.00
1	1	2719	G	N3-C4-C5	5.01	131.11	128.60
1	1	1905	C	N3-C4-C5	5.00	123.90	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
5	C	269/271 (99%)	256 (95%)	13 (5%)	0	100	100
6	D	207/209 (99%)	200 (97%)	4 (2%)	3 (1%)	11	43
7	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
8	F	175/177 (99%)	163 (93%)	11 (6%)	1 (1%)	25	64
9	G	173/175 (99%)	161 (93%)	12 (7%)	0	100	100
10	H	147/149 (99%)	137 (93%)	8 (5%)	2 (1%)	11	43
11	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	J	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
13	K	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	L	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
15	M	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
16	N	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
17	O	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
18	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
19	Q	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	7	34
20	R	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
21	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	T	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
23	U	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
24	V	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
25	W	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
26	X	60/62 (97%)	60 (100%)	0	0	100	100
27	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
28	Z	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
29	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	b	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
31	c	44/46 (96%)	44 (100%)	0	0	100	100
32	d	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
33	e	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	f	223/225 (99%)	209 (94%)	14 (6%)	0	100	100
35	g	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
36	h	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
37	i	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
38	j	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
39	k	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
40	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
41	m	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
42	n	97/99 (98%)	92 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	o	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
44	p	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
45	q	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
46	r	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
47	s	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
48	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
49	u	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
50	v	64/66 (97%)	64 (100%)	0	0	100	100
51	w	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
52	x	84/86 (98%)	84 (100%)	0	0	100	100
53	y	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
55	B	25/27 (93%)	19 (76%)	5 (20%)	1 (4%)	3	17
All	All	5637/5738 (98%)	5420 (96%)	208 (4%)	9 (0%)	50	82

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	152	PRO
6	D	153	GLY
6	D	154	LYS
10	H	90	LEU
19	Q	52	PRO
19	Q	53	PHE
10	H	89	LYS
8	F	124	GLY
55	B	23	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	216/216 (100%)	216 (100%)	0	100	100
6	D	164/164 (100%)	163 (99%)	1 (1%)	86	95
7	E	165/165 (100%)	165 (100%)	0	100	100
8	F	148/148 (100%)	148 (100%)	0	100	100
9	G	136/136 (100%)	136 (100%)	0	100	100
10	H	114/114 (100%)	114 (100%)	0	100	100
11	I	116/116 (100%)	116 (100%)	0	100	100
12	J	104/104 (100%)	103 (99%)	1 (1%)	76	91
13	K	103/103 (100%)	102 (99%)	1 (1%)	76	91
14	L	109/109 (100%)	108 (99%)	1 (1%)	78	92
15	M	99/99 (100%)	98 (99%)	1 (1%)	76	91
16	N	86/86 (100%)	86 (100%)	0	100	100
17	O	99/99 (100%)	99 (100%)	0	100	100
18	P	89/89 (100%)	89 (100%)	0	100	100
19	Q	84/84 (100%)	84 (100%)	0	100	100
20	R	93/93 (100%)	93 (100%)	0	100	100
21	S	81/81 (100%)	80 (99%)	1 (1%)	71	90
22	T	84/84 (100%)	84 (100%)	0	100	100
23	U	78/78 (100%)	78 (100%)	0	100	100
24	V	59/59 (100%)	58 (98%)	1 (2%)	60	85
25	W	67/67 (100%)	67 (100%)	0	100	100
26	X	54/54 (100%)	54 (100%)	0	100	100
27	Y	48/48 (100%)	48 (100%)	0	100	100
28	Z	59/59 (100%)	59 (100%)	0	100	100
29	a	47/47 (100%)	47 (100%)	0	100	100
30	b	47/47 (100%)	47 (100%)	0	100	100
31	c	38/38 (100%)	38 (100%)	0	100	100
32	d	51/51 (100%)	50 (98%)	1 (2%)	55	83
33	e	34/34 (100%)	34 (100%)	0	100	100
34	f	187/187 (100%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	g	171/171 (100%)	170 (99%)	1 (1%)	86	95
36	h	172/172 (100%)	172 (100%)	0	100	100
37	i	119/119 (100%)	117 (98%)	2 (2%)	60	85
38	j	91/91 (100%)	90 (99%)	1 (1%)	73	90
39	k	124/124 (100%)	124 (100%)	0	100	100
40	l	104/104 (100%)	104 (100%)	0	100	100
41	m	105/105 (100%)	104 (99%)	1 (1%)	76	91
42	n	86/86 (100%)	84 (98%)	2 (2%)	50	80
43	o	90/90 (100%)	89 (99%)	1 (1%)	73	90
44	p	102/102 (100%)	102 (100%)	0	100	100
45	q	94/94 (100%)	94 (100%)	0	100	100
46	r	83/83 (100%)	83 (100%)	0	100	100
47	s	76/76 (100%)	76 (100%)	0	100	100
48	t	65/65 (100%)	65 (100%)	0	100	100
49	u	74/74 (100%)	74 (100%)	0	100	100
50	v	57/57 (100%)	57 (100%)	0	100	100
51	w	72/72 (100%)	71 (99%)	1 (1%)	67	88
52	x	65/65 (100%)	63 (97%)	2 (3%)	40	75
53	y	60/60 (100%)	60 (100%)	0	100	100
55	B	20/20 (100%)	19 (95%)	1 (5%)	24	60
All	All	4689/4689 (100%)	4669 (100%)	20 (0%)	91	97

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	151	THR
12	J	17	ARG
13	K	48	ARG
14	L	59	ARG
15	M	80	PHE
21	S	72	GLN
24	V	10	THR
32	d	31	HIS
35	g	164	ARG
37	i	29	ARG

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Mol	Chain	Res	Type
37	i	93	ARG
38	j	72	ASP
41	m	106	ARG
42	n	5	ARG
42	n	87	LEU
43	o	56	ARG
51	w	78	ARG
52	x	57	ILE
52	x	85	LYS
55	B	12	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
32	d	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	498 (17%)	14 (0%)
2	2	1529/1534 (99%)	249 (16%)	4 (0%)
3	3	119/120 (99%)	15 (12%)	0
4	4	5/6 (83%)	0	0
54	z	87/88 (98%)	31 (35%)	0
All	All	4638/4651 (99%)	793 (17%)	18 (0%)

All (793) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	51	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	84	A
1	1	85	G

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Mol	Chain	Res	Type
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G
1	1	125	A
1	1	138	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	221	A
1	1	222	A
1	1	248	G
1	1	249	C
1	1	261	G
1	1	264	C
1	1	265	A
1	1	266	G
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	285	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	343	C
1	1	353	C
1	1	361	G
1	1	371	A
1	1	372	G
1	1	383	C
1	1	386	G
1	1	396	G

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Mol	Chain	Res	Type
1	1	399	U
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	435	C
1	1	457	A
1	1	467	G
1	1	481	G
1	1	489	G
1	1	491	G
1	1	505	A
1	1	509	C
1	1	513	A
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	603	A
1	1	609	A
1	1	612	G
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	655	A
1	1	670	A

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Mol	Chain	Res	Type
1	1	685	A
1	1	686	U
1	1	702	U
1	1	717	C
1	1	726	G
1	1	730	A
1	1	747	5MU
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	792	A
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	866	A
1	1	869	G
1	1	878	A
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	898	C
1	1	907	G

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Mol	Chain	Res	Type
1	1	910	A
1	1	931	U
1	1	932	U
1	1	941	A
1	1	946	C
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1096	A
1	1	1101	U
1	1	1110	G

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Mol	Chain	Res	Type
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1128	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1139	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1206	G
1	1	1212	G
1	1	1218	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1300	G
1	1	1301	A
1	1	1321	A

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Mol	Chain	Res	Type
1	1	1329	U
1	1	1341	G
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1408	G
1	1	1411	U
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1460	U
1	1	1468	U
1	1	1476	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1503	A
1	1	1504	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1532	A
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U

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Mol	Chain	Res	Type
1	1	1580	A
1	1	1583	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1608	A
1	1	1619	G
1	1	1634	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1756	G
1	1	1764	C
1	1	1773	A
1	1	1782	U
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1862	G
1	1	1865	U
1	1	1868	C
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1896	G

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Mol	Chain	Res	Type
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1914	C
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1938	A
1	1	1955	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2093	G
1	1	2095	A
1	1	2100	G
1	1	2102	G
1	1	2104	C
1	1	2107	G
1	1	2110	G
1	1	2112	G
1	1	2113	U

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Mol	Chain	Res	Type
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2121	G
1	1	2122	U
1	1	2125	G
1	1	2127	G
1	1	2128	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2140	G
1	1	2142	A
1	1	2143	C
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2168	G
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2178	C
1	1	2183	A
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2211	A
1	1	2225	A

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Mol	Chain	Res	Type
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2278	A
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2309	A
1	1	2319	G
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G
1	1	2476	A

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Mol	Chain	Res	Type
1	1	2478	A
1	1	2480	C
1	1	2491	U
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2586	U
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2629	U
1	1	2646	C
1	1	2663	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2725	A
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2757	A
1	1	2765	A
1	1	2777	G
1	1	2778	A

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Mol	Chain	Res	Type
1	1	2791	G
1	1	2793	C
1	1	2794	C
1	1	2797	U
1	1	2799	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2833	U
1	1	2835	A
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2898	U
1	1	2903	U
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	66	A
2	2	68	G
2	2	69	G
2	2	70	U
2	2	72	A

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Mol	Chain	Res	Type
2	2	73	C
2	2	74	A
2	2	75	G
2	2	76	G
2	2	81	A
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	92	U
2	2	120	A
2	2	121	U
2	2	130	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	163	C
2	2	164	G
2	2	177	G
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	210	C
2	2	211	G
2	2	212	G
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	289	G
2	2	306	A
2	2	319	G
2	2	321	A
2	2	328	C
2	2	332	G

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Mol	Chain	Res	Type
2	2	347	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C
2	2	384	G
2	2	392	C
2	2	398	U
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	496	A
2	2	499	A
2	2	510	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	521	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A

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Mol	Chain	Res	Type
2	2	547	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	633	G
2	2	650	G
2	2	653	U
2	2	660	C
2	2	665	A
2	2	700	G
2	2	701	U
2	2	702	A
2	2	703	G
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	753	A
2	2	755	G
2	2	777	A
2	2	787	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	821	G
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	843	U
2	2	844	G
2	2	845	A

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Mol	Chain	Res	Type
2	2	846	G
2	2	884	U
2	2	887	G
2	2	914	A
2	2	934	C
2	2	935	A
2	2	960	U
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	971	G
2	2	972	C
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1004	A
2	2	1009	U
2	2	1019	A
2	2	1020	G
2	2	1022	A
2	2	1025	U
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1034	G
2	2	1043	G
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1089	G
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1104	G

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Mol	Chain	Res	Type
2	2	1124	G
2	2	1125	U
2	2	1132	C
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1169	A
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1212	U
2	2	1213	A
2	2	1215	G
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G
2	2	1299	A
2	2	1302	C
2	2	1305	G

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Mol	Chain	Res	Type
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1335	U
2	2	1336	C
2	2	1346	A
2	2	1353	G
2	2	1363	A
2	2	1370	G
2	2	1379	G
2	2	1381	U
2	2	1419	G
2	2	1446	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	24	G
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
54	z	2	G
54	z	8	U
54	z	10	U
54	z	13	G
54	z	14	A

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Mol	Chain	Res	Type
54	z	15	G
54	z	17	OMG
54	z	18	G
54	z	19	C
54	z	20	U
54	z	21	G
54	z	22	A
54	z	23	A
54	z	24	G
54	z	40	G
54	z	45	U
54	z	46	A
54	z	51	G
54	z	52	C
54	z	53	A
54	z	54	A
54	z	55	C
54	z	56	G
54	z	60	C
54	z	61	G
54	z	67	U
54	z	76	C
54	z	79	C
54	z	85	G
54	z	86	C
54	z	88	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	613	A
1	1	784	G
1	1	887	A
1	1	891	G
1	1	894	U
1	1	1175	A
1	1	1379	U
1	1	2116	G
1	1	2118	U
1	1	2127	G
1	1	2146	C

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Mol	Chain	Res	Type
1	1	2189	U
1	1	2756	U
2	2	516	PSU
2	2	966	2MG
2	2	1109	C
2	2	1145	A

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

37 non-standard protein/DNA/RNA residues are 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$
1	PSU	1	2605	1	17,21,22	1.56	3 (17%)	20,30,33	3.43	7 (35%)
2	MA6	2	1519	2	19,26,27	1.43	2 (10%)	18,38,41	3.51	2 (11%)
2	2MG	2	1207	2	19,26,27	3.84	7 (36%)	21,38,41	2.03	7 (33%)
1	3TD	1	1915	1	17,22,23	3.04	8 (47%)	19,32,35	1.52	3 (15%)
1	6MZ	1	1618	1	18,25,26	1.89	4 (22%)	16,36,39	3.32	3 (18%)
1	OMU	1	2552	1	14,22,23	2.97	5 (35%)	14,31,34	1.14	1 (7%)
1	PSU	1	1911	1	17,21,22	1.39	3 (17%)	20,30,33	2.97	7 (35%)
54	OMG	z	17	54	22,27,27	4.27	7 (31%)	27,41,41	2.64	10 (37%)
1	PSU	1	746	1,56	17,21,22	1.19	2 (11%)	20,30,33	3.27	7 (35%)
1	G7M	1	2069	1	20,26,27	2.94	7 (35%)	20,39,42	2.15	6 (30%)
2	2MG	2	966	2	19,26,27	3.92	7 (36%)	21,38,41	1.97	7 (33%)
2	MA6	2	1518	2	19,26,27	1.44	1 (5%)	18,38,41	3.79	2 (11%)
2	PSU	2	516	2,56	17,21,22	1.47	3 (17%)	20,30,33	3.24	7 (35%)
2	5MC	2	967	2	15,22,23	2.80	5 (33%)	19,32,35	1.11	1 (5%)
1	OMG	1	2251	1,54	18,26,27	2.88	8 (44%)	20,38,41	1.57	5 (25%)
2	UR3	2	1498	2,56	14,22,23	2.52	4 (28%)	15,32,35	0.57	0
2	G7M	2	527	2	20,26,27	3.14	8 (40%)	20,39,42	2.44	5 (25%)
1	PSU	1	2580	1,56	17,21,22	1.45	3 (17%)	20,30,33	3.44	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2MG	2	1516	2	19,26,27	3.67	8 (42%)	21,38,41	2.39	7 (33%)
1	5MU	1	1939	1,56	15,22,23	2.68	3 (20%)	16,32,35	2.91	3 (18%)
2	5MC	2	1407	2	15,22,23	2.48	5 (33%)	19,32,35	1.23	1 (5%)
54	5MU	z	66	54	15,22,23	2.63	3 (20%)	16,32,35	2.74	2 (12%)
1	5MC	1	1962	1	15,22,23	2.64	5 (33%)	19,32,35	1.15	2 (10%)
44	0TD	p	89	44	4,9,10	1.51	0	3,11,13	0.72	0
1	PSU	1	955	1,56	17,21,22	1.59	4 (23%)	20,30,33	3.12	6 (30%)
1	PSU	1	1917	1	17,21,22	1.36	3 (17%)	20,30,33	2.99	6 (30%)
2	4OC	2	1402	2	16,23,24	2.72	6 (37%)	17,32,35	2.13	1 (5%)
55	FME	B	1	55	8,9,10	0.50	0	7,9,11	1.12	1 (14%)
1	2MA	1	2503	1,56	17,25,26	3.29	6 (35%)	19,37,40	2.03	5 (26%)
1	2MG	1	2445	1	19,26,27	3.48	9 (47%)	21,38,41	1.96	7 (33%)
1	PSU	1	2504	1	17,21,22	1.42	4 (23%)	20,30,33	3.01	6 (30%)
1	PSU	1	2457	1	17,21,22	1.55	3 (17%)	20,30,33	2.91	7 (35%)
1	2MG	1	1835	1	19,26,27	3.54	8 (42%)	21,38,41	1.95	8 (38%)
1	OMC	1	2498	1,56	15,22,23	2.53	5 (33%)	17,31,34	1.33	2 (11%)
1	5MU	1	747	1	15,22,23	2.69	3 (20%)	16,32,35	2.73	2 (12%)
1	1MG	1	745	1	18,26,27	3.31	6 (33%)	19,39,42	2.85	3 (15%)
1	6MZ	1	2030	1	18,25,26	1.96	5 (27%)	16,36,39	3.17	3 (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
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	2/7/29/30	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
1	3TD	1	1915	1	-	2/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	4/5/27/28	0/3/3/3
1	OMU	1	2552	1	-	0/7/27/28	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
54	OMG	z	17	54	-	3/8/28/28	0/3/3/3
1	PSU	1	746	1,56	-	3/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	1/3/25/26	0/3/3/3
2	2MG	2	966	2	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
2	PSU	2	516	2,56	-	2/7/25/26	0/2/2/2
2	5MC	2	967	2	-	2/5/25/26	0/2/2/2
1	OMG	1	2251	1,54	-	0/5/27/28	0/3/3/3
2	UR3	2	1498	2,56	-	0/5/25/26	0/2/2/2
2	G7M	2	527	2	-	3/3/25/26	0/3/3/3
1	PSU	1	2580	1,56	-	1/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	5MU	1	1939	1,56	-	0/5/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/5/25/26	0/2/2/2
54	5MU	z	66	54	-	2/5/25/26	0/2/2/2
1	5MC	1	1962	1	-	2/5/25/26	0/2/2/2
44	0TD	p	89	44	-	1/3/12/14	-
1	PSU	1	955	1,56	-	0/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
55	FME	B	1	55	-	4/7/9/11	-
1	2MA	1	2503	1,56	-	2/3/25/26	0/3/3/3
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
1	OMC	1	2498	1,56	-	1/7/27/28	0/2/2/2
1	5MU	1	747	1	-	0/5/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
1	6MZ	1	2030	1	-	4/5/27/28	0/3/3/3

All (173) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	17	OMG	C4-N3	11.94	1.54	1.35
2	2	966	2MG	C2-N2	10.96	1.43	1.34
2	2	1207	2MG	C2-N2	10.93	1.43	1.34
2	2	1516	2MG	C2-N2	9.86	1.42	1.34
1	1	2445	2MG	C2-N2	9.82	1.42	1.34
1	1	1835	2MG	C2-N2	9.57	1.42	1.34
54	z	17	OMG	C2-N1	8.24	1.50	1.35
54	z	66	5MU	C5-C4	8.18	1.59	1.41
1	1	747	5MU	C5-C4	8.13	1.58	1.41
2	2	527	G7M	C4-N3	8.05	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	17	OMG	O6-C6	-8.03	1.04	1.24
1	1	1939	5MU	C5-C4	8.01	1.58	1.41
2	2	966	2MG	C4-N3	7.96	1.48	1.35
2	2	1207	2MG	C4-N3	7.81	1.47	1.35
1	1	2503	2MA	C4-N3	7.76	1.47	1.35
1	1	1835	2MG	C4-N3	7.29	1.47	1.35
1	1	745	1MG	C4-N3	7.25	1.47	1.35
2	2	1516	2MG	C4-N3	7.20	1.46	1.35
54	z	17	OMG	C5-C6	7.18	1.53	1.41
1	1	2251	OMG	C4-N3	6.93	1.46	1.35
1	1	745	1MG	C2-N2	6.90	1.47	1.33
1	1	2503	2MA	C5-C6	6.89	1.52	1.41
1	1	2552	OMU	C4-N3	6.77	1.44	1.33
1	1	2445	2MG	C4-N3	6.75	1.46	1.35
2	2	1516	2MG	C5-C6	6.70	1.52	1.41
1	1	1962	5MC	C4-N3	6.68	1.44	1.35
2	2	966	2MG	C5-C6	6.66	1.52	1.41
1	1	2069	G7M	C4-N3	6.62	1.46	1.35
1	1	1915	3TD	C6-C5	6.57	1.48	1.38
2	2	967	5MC	C4-N3	6.56	1.44	1.35
1	1	745	1MG	C5-C6	6.49	1.51	1.41
2	2	1207	2MG	C5-C6	6.43	1.52	1.41
54	z	17	OMG	C6-N1	6.24	1.43	1.33
1	1	1835	2MG	C5-C6	6.18	1.52	1.41
2	2	1402	4OC	C6-N1	5.92	1.43	1.35
2	2	527	G7M	C5-C6	5.83	1.51	1.41
2	2	1498	UR3	C6-N1	5.82	1.43	1.35
1	1	2251	OMG	C5-C6	5.77	1.51	1.41
1	1	2503	2MA	C2-N3	5.76	1.44	1.34
2	2	1407	5MC	C4-N3	5.72	1.43	1.35
1	1	2069	G7M	C5-C6	5.46	1.50	1.41
1	1	2445	2MG	C5-C6	5.44	1.50	1.41
1	1	2030	6MZ	C6-N6	5.43	1.43	1.35
2	2	527	G7M	C2-N2	5.23	1.44	1.33
1	1	747	5MU	C4-N3	-5.21	1.23	1.33
1	1	2552	OMU	C2-N3	5.21	1.48	1.38
1	1	1618	6MZ	C6-N6	5.20	1.43	1.35
1	1	1939	5MU	C4-N3	-5.18	1.24	1.33
1	1	2498	OMC	C6-N1	5.14	1.42	1.35
2	2	1516	2MG	C6-N1	5.13	1.42	1.33
2	2	966	2MG	C6-N1	5.13	1.42	1.33
1	1	1915	3TD	C2-N1	5.08	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-N1	5.04	1.45	1.34
1	1	745	1MG	C2-N3	4.99	1.42	1.34
1	1	2552	OMU	C6-N1	4.92	1.41	1.35
1	1	2251	OMG	C6-N1	4.89	1.41	1.33
1	1	2069	G7M	C6-N1	4.88	1.41	1.33
2	2	1207	2MG	C6-N1	4.83	1.41	1.33
2	2	1498	UR3	C6-C5	4.83	1.48	1.38
2	2	967	5MC	C2-N3	4.82	1.47	1.38
2	2	527	G7M	C6-N1	4.78	1.41	1.33
1	1	1962	5MC	C2-N3	4.76	1.47	1.38
54	z	66	5MU	C4-N3	-4.67	1.24	1.33
1	1	2069	G7M	C5-C4	-4.62	1.33	1.39
1	1	1835	2MG	C6-N1	4.60	1.41	1.33
2	2	1402	4OC	C2-N3	4.57	1.47	1.38
1	1	2503	2MA	C2-N1	4.55	1.42	1.34
2	2	1402	4OC	C4-N3	4.51	1.43	1.34
2	2	967	5MC	C5-C4	4.48	1.48	1.41
1	1	2069	G7M	C2-N2	4.35	1.42	1.33
2	2	1407	5MC	C2-N3	4.30	1.46	1.38
1	1	2498	OMC	C2-N3	4.29	1.46	1.38
1	1	1915	3TD	C4-N3	4.29	1.44	1.38
2	2	527	G7M	C2-N1	4.26	1.43	1.35
1	1	2498	OMC	C4-N3	4.22	1.42	1.35
1	1	2445	2MG	C6-N1	4.19	1.40	1.33
2	2	967	5MC	C4-N4	4.18	1.44	1.34
54	z	17	OMG	C2-N2	4.15	1.42	1.33
1	1	2605	PSU	C5-C1'	-4.12	1.48	1.52
1	1	1915	3TD	C5-C4	4.12	1.50	1.41
2	2	1402	4OC	C6-C5	4.10	1.47	1.38
1	1	745	1MG	O6-C6	-4.01	1.14	1.24
1	1	955	PSU	C5-C1'	-3.98	1.48	1.52
1	1	2498	OMC	C6-C5	3.97	1.46	1.38
1	1	1962	5MC	C4-N4	3.92	1.44	1.34
54	z	17	OMG	C2-N3	3.85	1.52	1.34
2	2	1407	5MC	C4-N4	3.82	1.43	1.34
1	1	2069	G7M	C2-N1	3.73	1.42	1.35
2	2	1407	5MC	C5-C4	3.71	1.47	1.41
1	1	1962	5MC	C5-C4	3.69	1.47	1.41
2	2	1498	UR3	C4-N3	3.68	1.43	1.38
1	1	2552	OMU	C6-C5	3.67	1.46	1.38
2	2	1519	MA6	C5-C4	-3.66	1.31	1.40
2	2	1518	MA6	C5-C4	-3.59	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	966	2MG	C2-N3	3.57	1.45	1.34
2	2	516	PSU	C5-C1'	-3.51	1.49	1.52
1	1	2457	PSU	C5-C1'	-3.50	1.49	1.52
1	1	2504	PSU	C5-C1'	-3.47	1.49	1.52
1	1	2503	2MA	C6-N1	3.46	1.41	1.35
2	2	527	G7M	C5-C4	-3.45	1.34	1.39
1	1	2251	OMG	C2-N1	3.43	1.41	1.35
2	2	1207	2MG	C2-N3	3.41	1.45	1.34
1	1	2030	6MZ	C5-C4	-3.37	1.32	1.40
1	1	1618	6MZ	C5-C4	-3.35	1.32	1.40
1	1	1911	PSU	C5-C1'	-3.31	1.49	1.52
1	1	1835	2MG	C2-N3	3.29	1.44	1.34
1	1	1917	PSU	C5-C1'	-3.27	1.49	1.52
2	2	1402	4OC	C4-N4	3.23	1.43	1.36
2	2	1516	2MG	C2-N3	3.17	1.44	1.34
1	1	1915	3TD	C5-C1'	-3.15	1.49	1.52
1	1	2251	OMG	C2-N2	3.08	1.40	1.33
1	1	2445	2MG	C2-N3	3.06	1.44	1.34
2	2	1498	UR3	C3U-N3	-3.06	1.40	1.47
1	1	747	5MU	O4-C4	-3.04	1.16	1.24
2	2	1402	4OC	C5-C4	3.00	1.46	1.39
1	1	2580	PSU	C5-C1'	-2.94	1.49	1.52
1	1	1939	5MU	O4-C4	-2.88	1.17	1.24
54	z	66	5MU	O4-C4	-2.84	1.17	1.24
1	1	2251	OMG	O6-C6	-2.75	1.17	1.24
2	2	967	5MC	C6-C5	2.74	1.47	1.40
1	1	2445	2MG	O6-C6	-2.70	1.17	1.24
1	1	2069	G7M	O6-C6	-2.67	1.17	1.24
2	2	966	2MG	C2-N1	2.66	1.42	1.34
2	2	1516	2MG	C2-N1	2.65	1.42	1.34
1	1	2030	6MZ	C6-N1	-2.65	1.30	1.34
1	1	1915	3TD	O4-C4	-2.64	1.18	1.24
1	1	1835	2MG	O6-C6	-2.62	1.18	1.24
2	2	1407	5MC	C6-C5	2.62	1.47	1.40
1	1	2445	2MG	C2'-C1'	-2.52	1.49	1.53
1	1	2498	OMC	C4-N4	2.52	1.42	1.35
2	2	516	PSU	C4-N3	2.51	1.37	1.33
1	1	746	PSU	C4-N3	2.48	1.37	1.33
2	2	1207	2MG	C2-N1	2.46	1.42	1.34
2	2	516	PSU	C2'-C1'	-2.46	1.51	1.54
1	1	1911	PSU	C4-N3	2.45	1.37	1.33
1	1	2503	2MA	C5-C4	-2.44	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	527	G7M	O6-C6	-2.44	1.18	1.24
1	1	1618	6MZ	C6-N1	-2.43	1.30	1.34
1	1	2457	PSU	O4'-C1'	-2.43	1.41	1.44
2	2	1516	2MG	O6-C6	-2.42	1.18	1.24
2	2	1207	2MG	O6-C6	-2.42	1.18	1.24
1	1	2445	2MG	C5-C4	-2.40	1.34	1.40
1	1	2552	OMU	O4-C4	-2.37	1.18	1.24
1	1	1915	3TD	O4'-C1'	-2.36	1.41	1.44
1	1	955	PSU	C2'-C1'	-2.33	1.51	1.54
1	1	745	1MG	C2'-C1'	-2.33	1.50	1.53
2	2	527	G7M	C2-N3	2.32	1.45	1.34
1	1	1962	5MC	C6-C5	2.31	1.46	1.40
1	1	1917	PSU	C4-N3	2.30	1.37	1.33
1	1	955	PSU	O4'-C1'	-2.29	1.41	1.44
2	2	1519	MA6	C4-N3	-2.28	1.32	1.35
1	1	746	PSU	O4'-C1'	-2.28	1.41	1.44
1	1	2580	PSU	O4'-C1'	-2.28	1.41	1.44
1	1	2504	PSU	O4'-C1'	-2.27	1.41	1.44
1	1	1835	2MG	C2-N1	2.27	1.41	1.34
1	1	2251	OMG	C5-C4	-2.26	1.35	1.40
1	1	1911	PSU	O4'-C1'	-2.25	1.41	1.44
1	1	2445	2MG	C2-N1	2.25	1.41	1.34
2	2	966	2MG	O6-C6	-2.24	1.18	1.24
1	1	2030	6MZ	C5-N7	-2.23	1.31	1.39
1	1	2457	PSU	C2'-C1'	-2.15	1.51	1.54
2	2	1516	2MG	C5-C4	-2.12	1.35	1.40
1	1	1917	PSU	O4'-C1'	-2.10	1.41	1.44
1	1	2605	PSU	C4-N3	2.08	1.36	1.33
1	1	955	PSU	C4-N3	2.07	1.36	1.33
1	1	1835	2MG	C5-C4	-2.06	1.35	1.40
1	1	2580	PSU	C4-N3	2.06	1.36	1.33
1	1	2504	PSU	C4-N3	2.04	1.36	1.33
1	1	1618	6MZ	C5-N7	-2.04	1.32	1.39
1	1	2605	PSU	O4'-C1'	-2.02	1.41	1.44
1	1	2030	6MZ	C2'-C1'	-2.01	1.50	1.53
1	1	2251	OMG	C2-N3	2.00	1.44	1.34
1	1	2504	PSU	C5-C4	-2.00	1.37	1.41

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1518	MA6	N1-C6-N6	-14.84	101.43	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1519	MA6	N1-C6-N6	-13.59	102.76	117.06
1	1	745	1MG	C1'-N9-C4	-11.65	106.17	126.64
1	1	2030	6MZ	C1'-N9-C4	-11.46	106.51	126.64
1	1	1618	6MZ	C1'-N9-C4	-11.32	106.75	126.64
2	2	516	PSU	N3-C2-N1	-11.10	119.61	128.43
1	1	746	PSU	N3-C2-N1	-10.62	119.99	128.43
1	1	2580	PSU	N3-C2-N1	-10.42	120.15	128.43
1	1	2605	PSU	N3-C2-N1	-10.18	120.33	128.43
1	1	1911	PSU	N3-C2-N1	-10.03	120.45	128.43
1	1	2504	PSU	N3-C2-N1	-9.89	120.57	128.43
1	1	955	PSU	N3-C2-N1	-9.78	120.66	128.43
1	1	1917	PSU	N3-C2-N1	-9.69	120.73	128.43
1	1	2457	PSU	N3-C2-N1	-9.14	121.16	128.43
54	z	66	5MU	C5-C6-N1	-8.90	112.60	122.19
1	1	747	5MU	C5-C6-N1	-8.44	113.10	122.19
2	2	1402	4OC	CM4-N4-C4	-8.29	115.84	122.97
1	1	1939	5MU	C5-C6-N1	-8.22	113.33	122.19
2	2	527	G7M	C1'-N9-C4	7.59	139.97	126.64
1	1	1939	5MU	C2-N3-C4	7.29	121.30	115.14
1	1	2580	PSU	O4'-C1'-C5	7.21	121.10	109.93
1	1	747	5MU	C2-N3-C4	6.27	120.44	115.14
54	z	66	5MU	C2-N3-C4	6.09	120.28	115.14
54	z	17	OMG	OP3-P-OP1	-6.06	86.95	110.68
1	1	2503	2MA	C1'-N9-C4	5.96	137.12	126.64
1	1	2605	PSU	O4'-C1'-C5	5.93	119.11	109.93
54	z	17	OMG	OP3-P-O5'	-5.83	91.21	106.73
2	2	1516	2MG	CM2-N2-C2	-5.75	116.66	123.59
1	1	746	PSU	O4'-C1'-C5	5.74	118.82	109.93
1	1	1835	2MG	CM2-N2-C2	-5.63	116.80	123.59
2	2	1518	MA6	N3-C2-N1	-5.46	120.14	128.68
1	1	2457	PSU	O4'-C1'-C5	5.32	118.17	109.93
54	z	17	OMG	OP3-P-OP2	-5.29	87.43	107.64
2	2	1519	MA6	N3-C2-N1	-5.18	120.59	128.68
2	2	1516	2MG	N2-C2-N1	5.09	121.85	116.96
1	1	2580	PSU	C2-N3-C4	5.08	119.43	115.14
1	1	2504	PSU	C2-N3-C4	4.96	119.33	115.14
1	1	2069	G7M	C1'-N9-C4	4.95	135.33	126.64
2	2	1516	2MG	C1'-N9-C4	-4.82	118.17	126.64
1	1	2605	PSU	C5-C1'-C2'	-4.80	106.75	115.32
54	z	17	OMG	OP2-P-OP1	4.80	129.47	110.68
1	1	1618	6MZ	N3-C2-N1	-4.80	121.18	128.68
54	z	17	OMG	C4-C5-C6	-4.71	116.30	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	955	PSU	O4'-C1'-C5	4.69	117.19	109.93
1	1	746	PSU	C2-N3-C4	4.64	119.06	115.14
2	2	1207	2MG	C1'-N9-C4	-4.64	118.49	126.64
2	2	527	G7M	N3-C2-N1	-4.57	121.12	127.22
1	1	1618	6MZ	C9-N6-C6	-4.49	119.00	122.87
1	1	1911	PSU	C2-N3-C4	4.49	118.93	115.14
1	1	2069	G7M	N3-C2-N1	-4.46	121.28	127.22
1	1	1917	PSU	C5-C4-N3	-4.45	119.63	125.36
1	1	1917	PSU	C2-N3-C4	4.44	118.89	115.14
1	1	2504	PSU	C5-C4-N3	-4.42	119.67	125.36
1	1	2580	PSU	C5-C4-N3	-4.41	119.68	125.36
1	1	955	PSU	C5-C4-N3	-4.36	119.74	125.36
1	1	2445	2MG	CM2-N2-C2	-4.34	118.35	123.59
1	1	2030	6MZ	N3-C2-N1	-4.31	121.95	128.68
1	1	955	PSU	C2-N3-C4	4.27	118.75	115.14
1	1	2605	PSU	C5-C6-N1	-4.22	119.25	124.44
1	1	2503	2MA	C2-N3-C4	4.18	118.92	115.52
2	2	516	PSU	C2-N3-C4	4.11	118.61	115.14
1	1	1911	PSU	C5-C4-N3	-4.03	120.17	125.36
1	1	2605	PSU	C5-C4-N3	-4.02	120.18	125.36
1	1	955	PSU	C5-C6-N1	-3.99	119.53	124.44
1	1	2445	2MG	C1'-N9-C4	-3.98	119.64	126.64
1	1	2605	PSU	C2-N3-C4	3.98	118.50	115.14
2	2	1207	2MG	CM2-N2-C2	-3.95	118.83	123.59
2	2	516	PSU	C5-C6-N1	-3.93	119.61	124.44
2	2	1407	5MC	C4-N3-C2	3.90	120.72	116.02
2	2	516	PSU	C6-N1-C2	3.78	121.59	115.36
1	1	1917	PSU	C5-C6-N1	-3.76	119.81	124.44
1	1	2457	PSU	C5-C4-N3	-3.76	120.52	125.36
1	1	2504	PSU	C5-C6-N1	-3.71	119.88	124.44
1	1	2251	OMG	N3-C2-N1	-3.65	122.36	127.22
1	1	2605	PSU	C6-N1-C2	3.55	121.22	115.36
2	2	966	2MG	N2-C2-N3	3.53	120.35	116.96
2	2	527	G7M	C5-C6-N1	-3.52	118.62	123.43
1	1	746	PSU	C5-C4-N3	-3.50	120.85	125.36
1	1	2498	OMC	C4-N3-C2	3.50	119.89	116.34
2	2	516	PSU	C5-C4-N3	-3.50	120.85	125.36
1	1	2457	PSU	C2-N3-C4	3.48	118.08	115.14
1	1	2069	G7M	C5-C6-N1	-3.46	118.70	123.43
1	1	1911	PSU	C5-C6-N1	-3.45	120.20	124.44
1	1	2445	2MG	C5-C6-N1	-3.44	118.72	123.43
1	1	1917	PSU	O4'-C1'-C5	3.42	115.23	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	966	2MG	CM2-N2-C2	-3.42	119.47	123.59
1	1	2457	PSU	C5-C6-N1	-3.42	120.24	124.44
1	1	1915	3TD	C5-C6-N1	-3.40	120.26	124.44
2	2	966	2MG	C1'-N9-C4	-3.40	120.67	126.64
1	1	746	PSU	C6-N1-C2	3.37	120.92	115.36
1	1	2552	OMU	CM2-O2'-C2'	-3.35	105.74	114.52
54	z	17	OMG	O5'-P-OP1	3.31	115.75	106.47
2	2	967	5MC	C4-N3-C2	3.30	120.00	116.02
1	1	2251	OMG	C5-C6-N1	-3.29	118.93	123.43
2	2	966	2MG	C5-C6-N1	-3.28	118.94	123.43
2	2	1207	2MG	N2-C2-N3	3.27	120.10	116.96
1	1	955	PSU	C6-N1-C2	3.26	120.73	115.36
1	1	1915	3TD	C6-N1-C2	3.25	120.72	115.36
1	1	2069	G7M	N2-C2-N1	3.24	122.29	117.25
1	1	2580	PSU	C6-N1-C2	3.13	120.53	115.36
1	1	746	PSU	C5-C1'-C2'	-3.13	109.73	115.32
2	2	1207	2MG	C5-C6-N1	-3.12	119.17	123.43
2	2	527	G7M	C2-N3-C4	3.11	118.91	115.36
1	1	1911	PSU	C6-N1-C2	3.09	120.46	115.36
1	1	1917	PSU	C6-N1-C2	3.09	120.45	115.36
1	1	2580	PSU	C5-C6-N1	-3.07	120.66	124.44
2	2	1516	2MG	C2-N3-C4	3.04	118.72	115.28
1	1	1835	2MG	C5-C6-N1	-3.04	119.28	123.43
1	1	2069	G7M	C2-N3-C4	3.02	118.81	115.36
1	1	1835	2MG	C2-N3-C4	3.02	118.71	115.28
1	1	2504	PSU	C6-N1-C2	3.02	120.34	115.36
1	1	2457	PSU	C6-N1-C2	2.98	120.28	115.36
2	2	1207	2MG	N3-C2-N1	-2.97	121.53	126.23
1	1	2498	OMC	CM2-O2'-C2'	-2.97	106.73	114.52
1	1	1962	5MC	N4-C4-N3	2.96	121.22	117.03
2	2	516	PSU	C5-C1'-C2'	-2.94	110.07	115.32
54	z	17	OMG	OP2-P-O5'	2.94	114.54	106.73
1	1	746	PSU	C5-C6-N1	-2.93	120.84	124.44
2	2	1516	2MG	C5-C6-N1	-2.90	119.46	123.43
1	1	2503	2MA	N3-C2-N1	-2.87	120.45	125.72
2	2	966	2MG	C2-N3-C4	2.86	118.53	115.28
2	2	966	2MG	N3-C2-N1	-2.84	121.73	126.23
1	1	745	1MG	N2-C2-N3	2.79	121.92	117.40
1	1	2251	OMG	CM2-O2'-C2'	-2.77	107.26	114.52
1	1	1915	3TD	C5-C1'-C2'	-2.75	110.42	115.32
1	1	1962	5MC	C4-N3-C2	2.74	119.33	116.02
2	2	1516	2MG	N3-C2-N1	-2.74	121.90	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1835	2MG	N3-C2-N1	-2.74	121.90	126.23
1	1	2445	2MG	N3-C2-N1	-2.72	121.93	126.23
2	2	1207	2MG	C2-N3-C4	2.72	118.36	115.28
54	z	17	OMG	N3-C2-N1	-2.70	123.62	127.22
2	2	1207	2MG	C2-N1-C6	2.58	119.81	115.18
1	1	2445	2MG	C2-N1-C6	2.51	119.68	115.18
2	2	966	2MG	C2-N1-C6	2.43	119.53	115.18
1	1	2445	2MG	N2-C2-N3	2.42	119.29	116.96
55	B	1	FME	O-C-CA	-2.42	118.44	124.78
1	1	1939	5MU	C5M-C5-C4	2.41	125.70	121.37
2	2	527	G7M	C2-N1-C6	2.40	119.75	115.93
1	1	745	1MG	C2-N3-C4	2.39	118.08	115.36
1	1	2503	2MA	CM2-C2-N1	2.37	120.85	117.15
1	1	2503	2MA	C5-C6-N1	-2.37	120.58	123.06
1	1	1835	2MG	C2-N1-C6	2.27	119.24	115.18
1	1	2445	2MG	C2-N3-C4	2.23	117.81	115.28
1	1	2251	OMG	C2-N3-C4	2.22	117.90	115.36
1	1	1911	PSU	C5-C1'-C2'	-2.21	111.37	115.32
1	1	1835	2MG	N2-C2-N3	2.21	119.08	116.96
1	1	2504	PSU	C5-C1'-C2'	-2.20	111.39	115.32
1	1	2069	G7M	C2-N1-C6	2.20	119.42	115.93
2	2	516	PSU	O4'-C1'-C2'	2.19	108.22	104.66
1	1	2580	PSU	O4'-C1'-C2'	2.19	108.22	104.66
54	z	17	OMG	C5-C6-N1	2.19	126.43	123.43
1	1	1911	PSU	O4'-C1'-C5	2.18	113.31	109.93
54	z	17	OMG	C1'-N9-C4	2.17	130.45	126.64
1	1	2030	6MZ	C9-N6-C6	-2.14	121.03	122.87
1	1	1835	2MG	N2-C2-N1	2.14	119.02	116.96
1	1	2457	PSU	O4'-C1'-C2'	2.12	108.09	104.66
2	2	1516	2MG	C2-N1-C6	2.06	118.87	115.18
1	1	1835	2MG	C1'-N9-C4	-2.03	123.07	126.64
1	1	2251	OMG	C2-N1-C6	2.03	119.16	115.93

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	516	PSU	O4'-C1'-C5-C4
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
44	p	89	0TD	CG-CB-SB-CSB
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1962	5MC	O4'-C1'-N1-C6
1	1	1962	5MC	C2'-C1'-N1-C6
1	1	2030	6MZ	N1-C6-N6-C9
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2498	OMC	O4'-C1'-N1-C6
1	1	2504	PSU	O4'-C4'-C5'-O5'
54	z	17	OMG	C5'-O5'-P-OP3
2	2	1519	MA6	C3'-C4'-C5'-O5'
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
55	B	1	FME	CA-CB-CG-SD
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
55	B	1	FME	N-CA-CB-CG
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
54	z	66	5MU	O4'-C4'-C5'-O5'
54	z	17	OMG	C5'-O5'-P-OP1
55	B	1	FME	O1-CN-N-CA
55	B	1	FME	CB-CG-SD-CE
54	z	66	5MU	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C1'-C5-C6
1	1	746	PSU	O4'-C1'-C5-C6
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	1618	6MZ	C5-C6-N6-C9
1	1	2030	6MZ	C5-C6-N6-C9
2	2	1402	4OC	C3'-C4'-C5'-O5'
2	2	527	G7M	C4'-C5'-O5'-P
1	1	2503	2MA	C3'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
1	1	746	PSU	O4'-C1'-C5-C4
2	2	966	2MG	O4'-C4'-C5'-O5'
1	1	746	PSU	C2'-C1'-C5-C6
1	1	2580	PSU	C2'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
1	1	2069	G7M	O4'-C4'-C5'-O5'
54	z	17	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 418 ligands modelled in this entry, 418 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

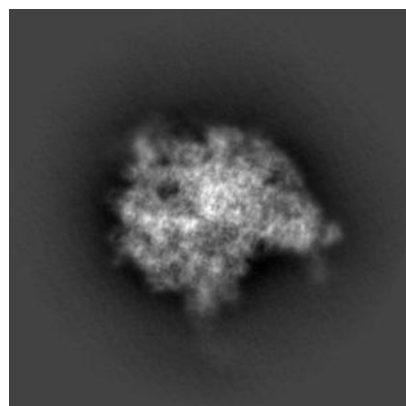
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12928. These allow visual inspection of the internal detail of the map and identification of artifacts.

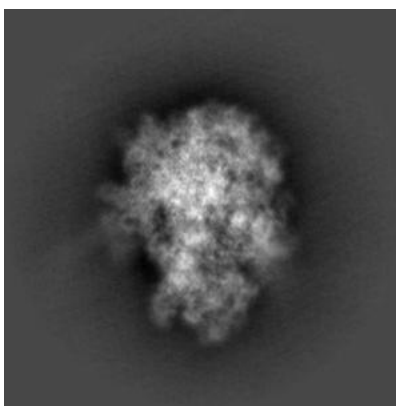
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

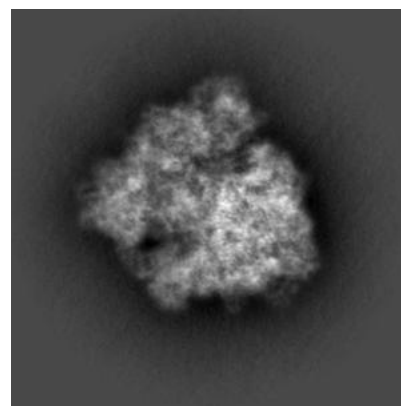
6.1.1 Primary map



X

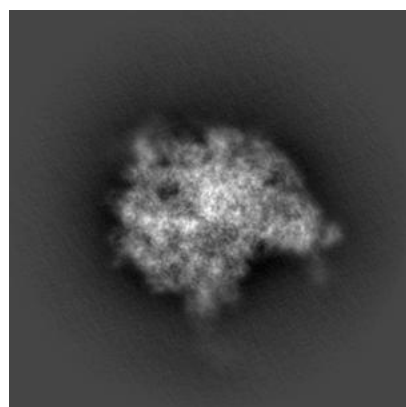


Y

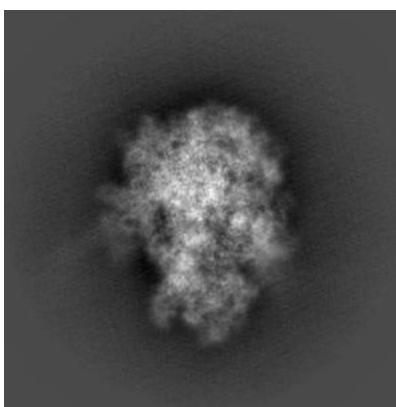


Z

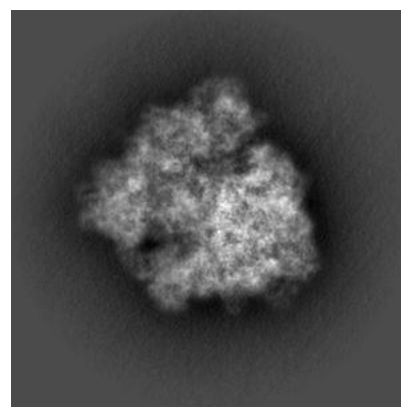
6.1.2 Raw map



X



Y

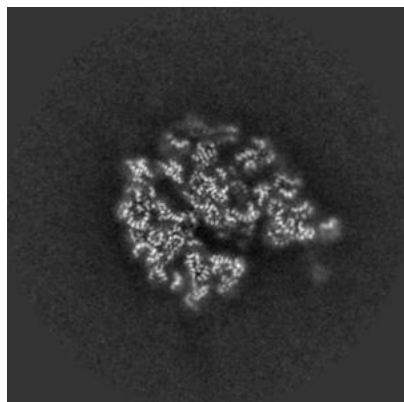


Z

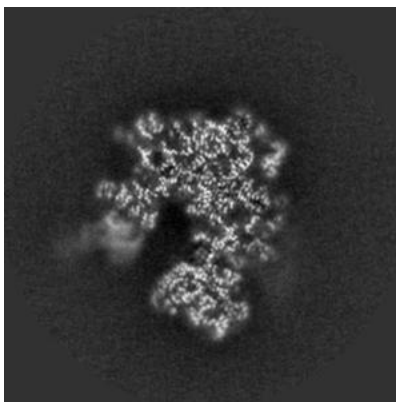
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

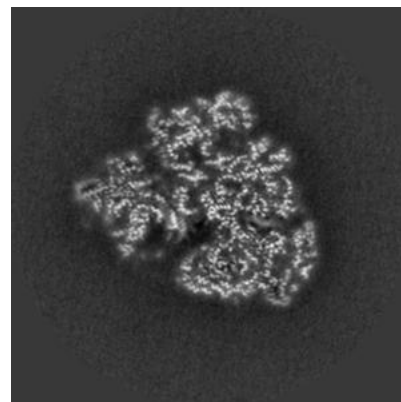
6.2.1 Primary map



X Index: 200

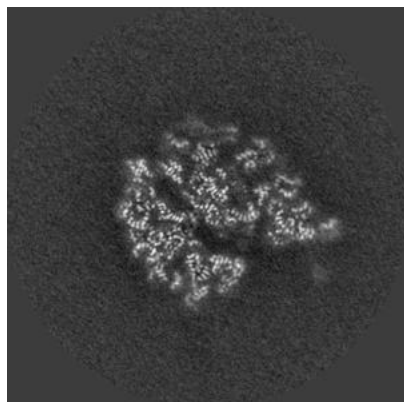


Y Index: 200

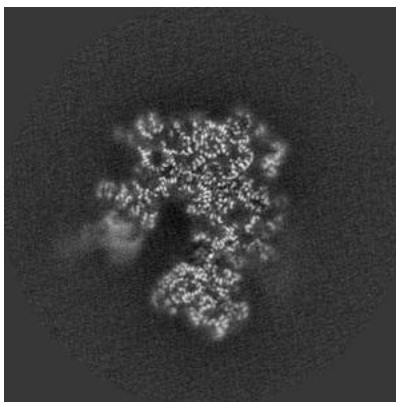


Z Index: 200

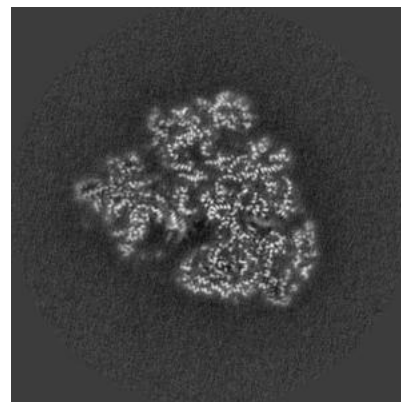
6.2.2 Raw map



X Index: 200



Y Index: 200

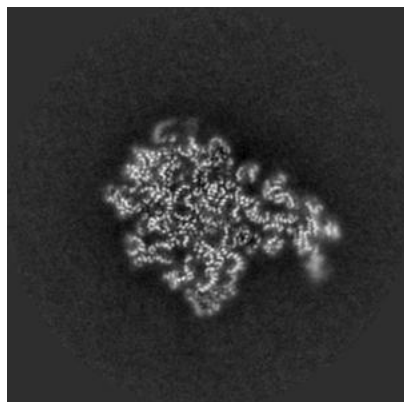


Z Index: 200

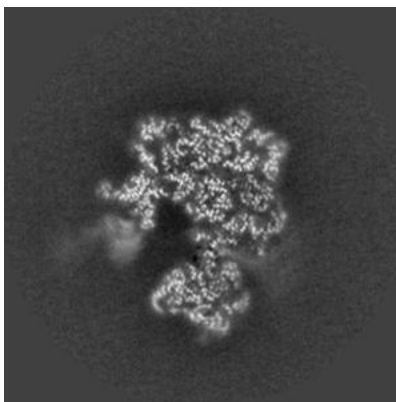
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

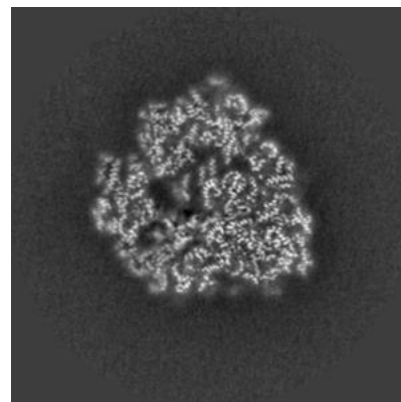
6.3.1 Primary map



X Index: 216

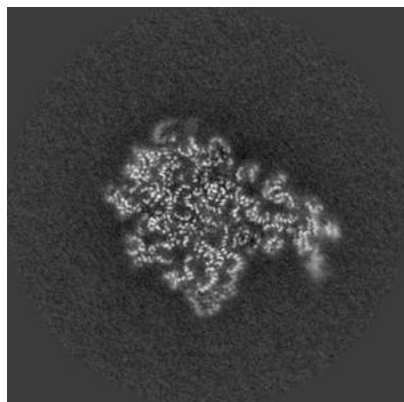


Y Index: 205

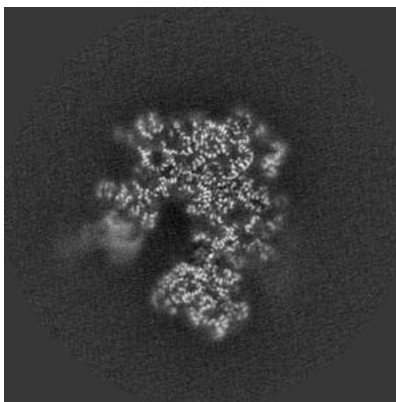


Z Index: 187

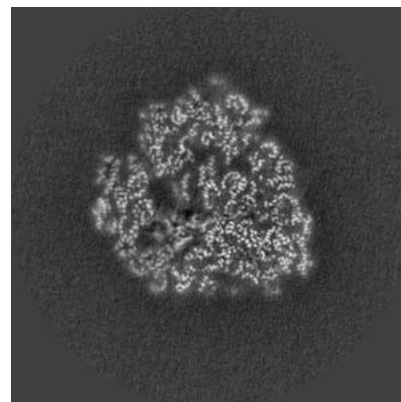
6.3.2 Raw map



X Index: 216



Y Index: 200

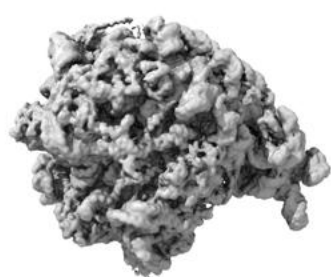


Z Index: 188

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

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.

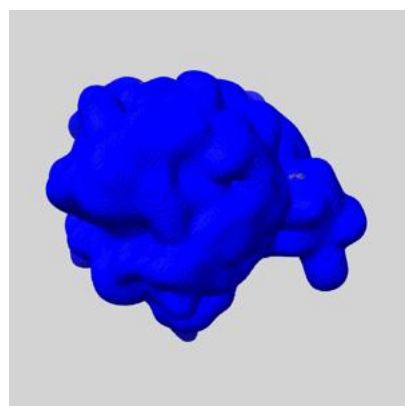
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

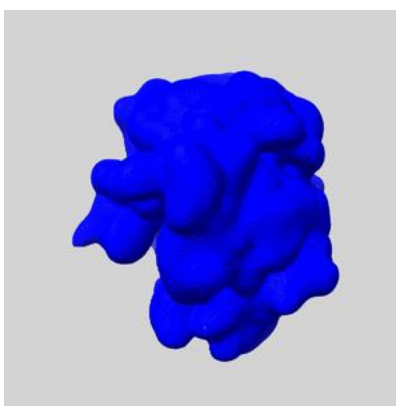
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

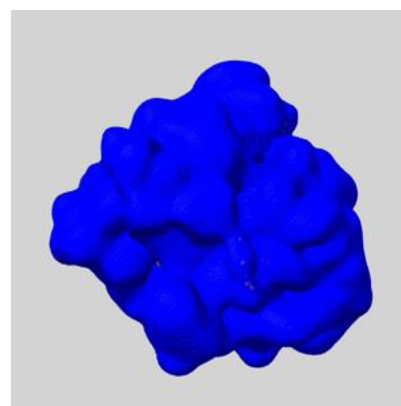
6.5.1 emd_12928_msk_1.map [i](#)



X



Y

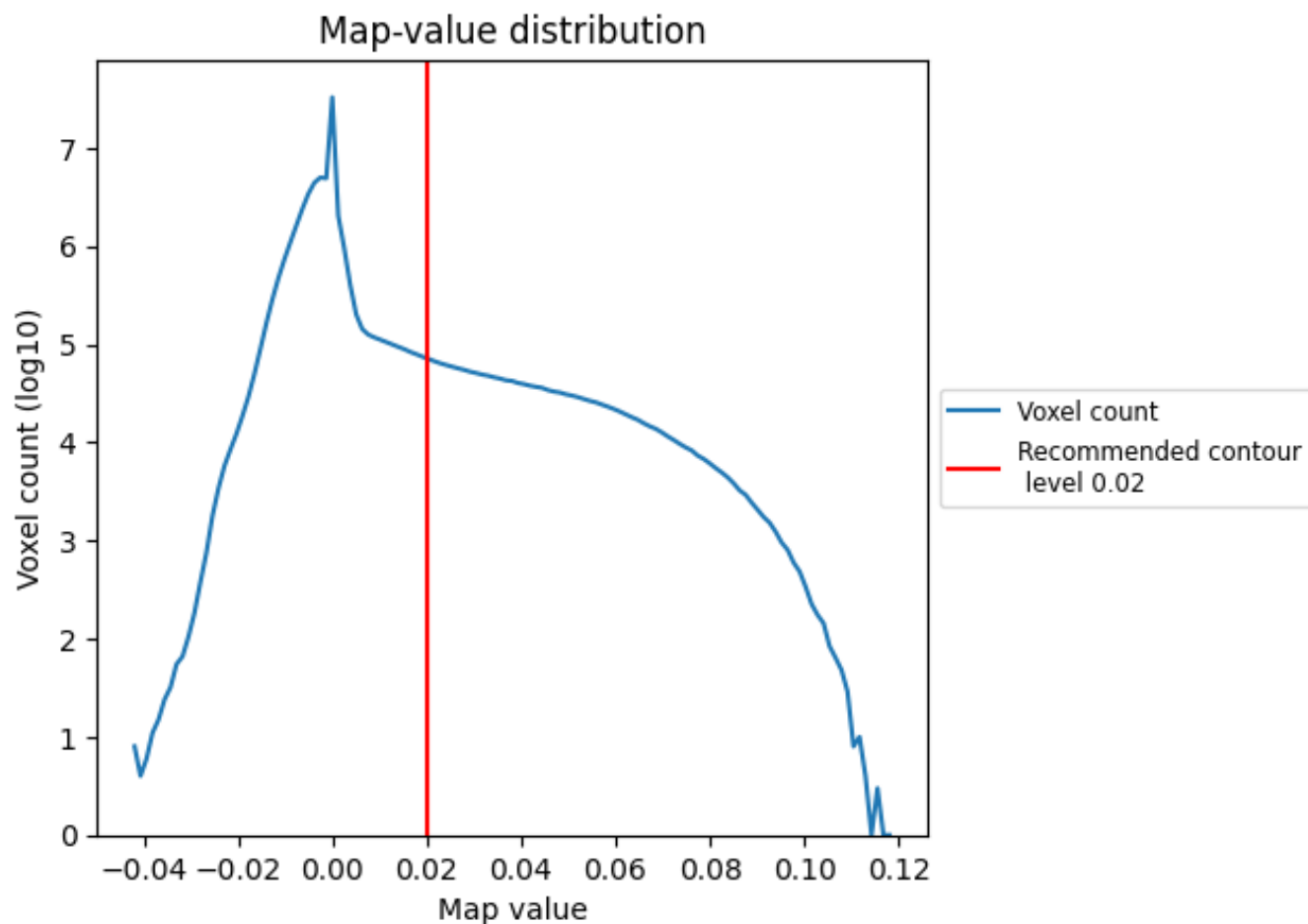


Z

7 Map analysis [i](#)

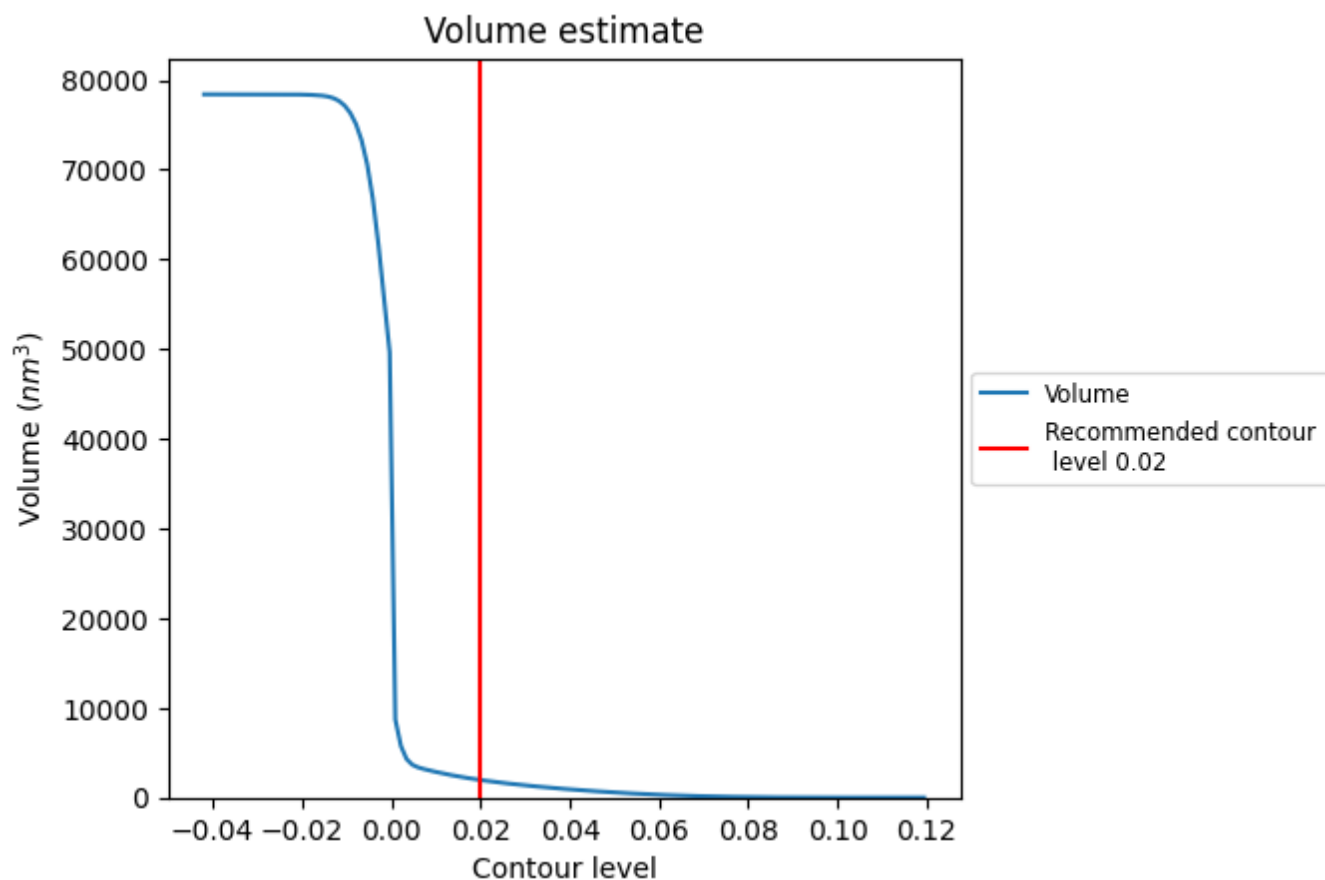
This section contains the results of statistical analysis of the map.

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.

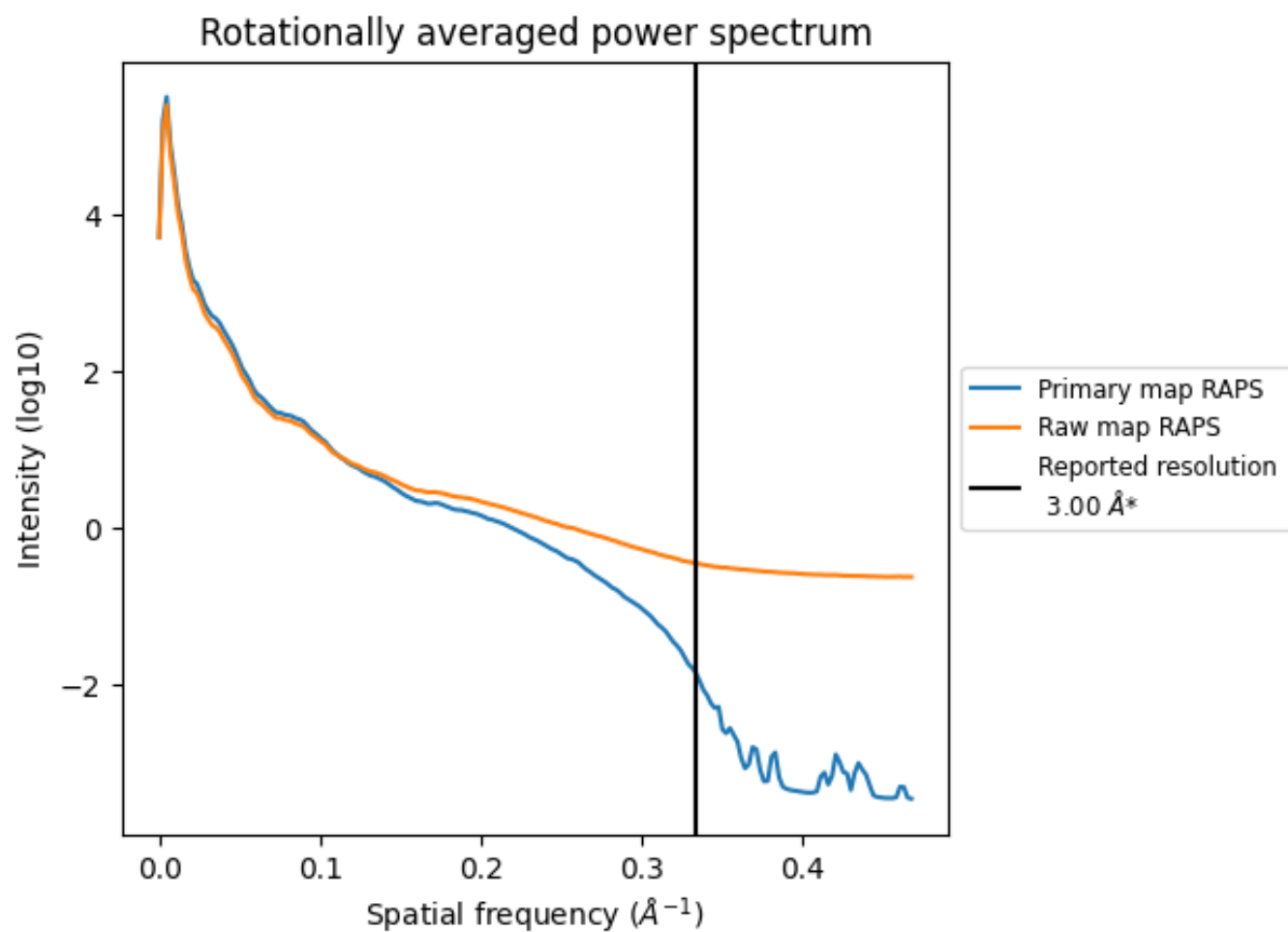
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1958 nm^3 ; this corresponds to an approximate mass of 1769 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 ⓘ

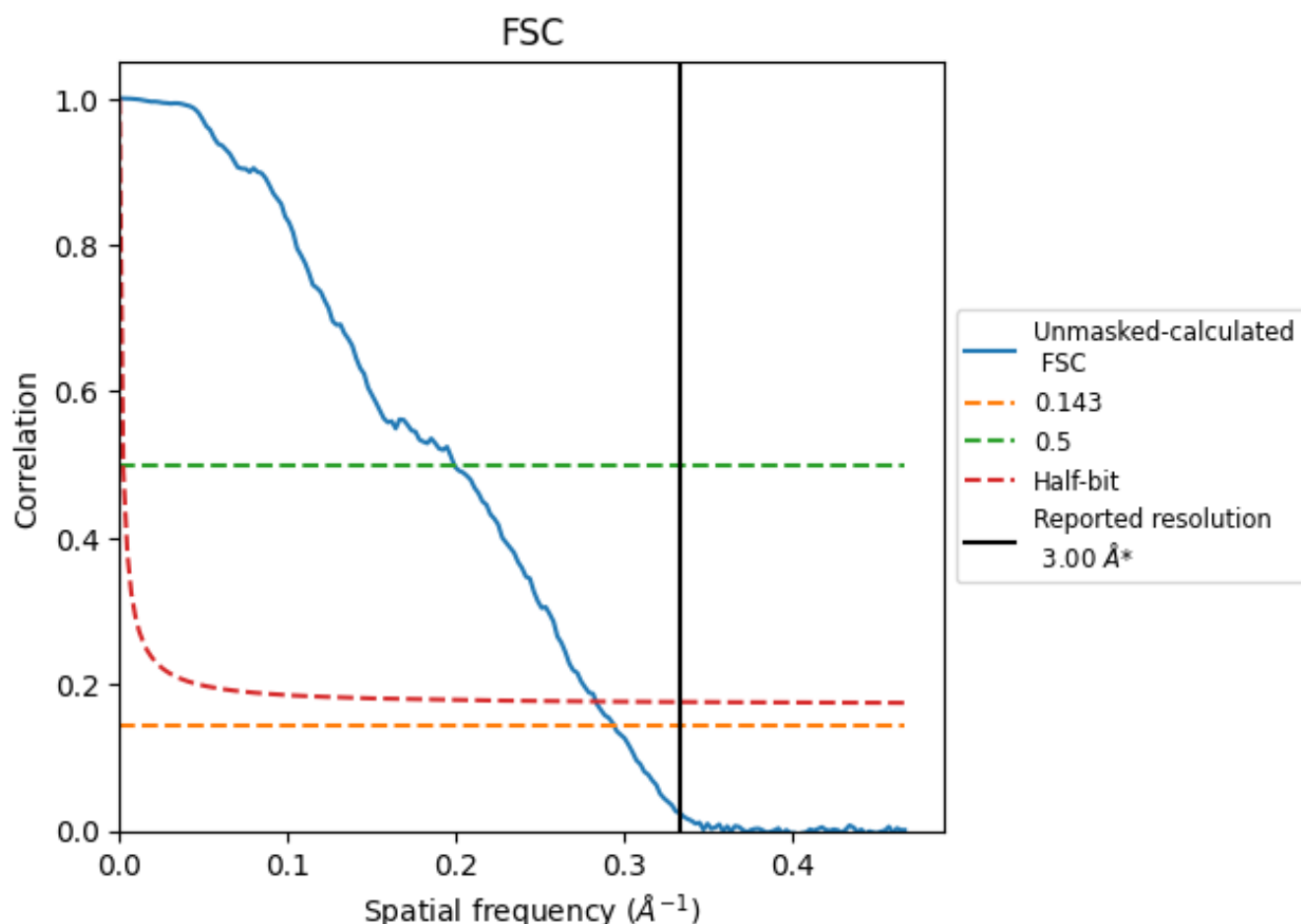


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

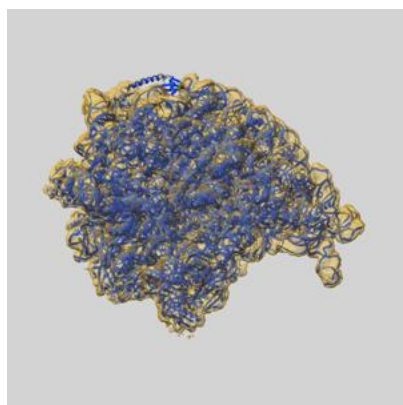
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	5.02	3.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 3.0 by more than 10 %

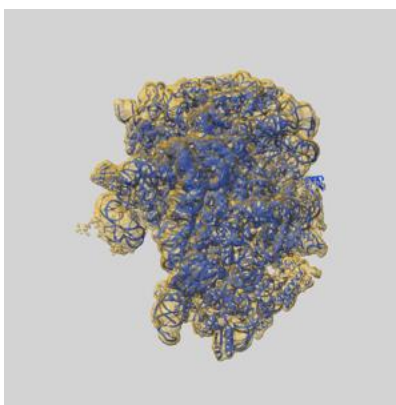
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12928 and PDB model 7OIF. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

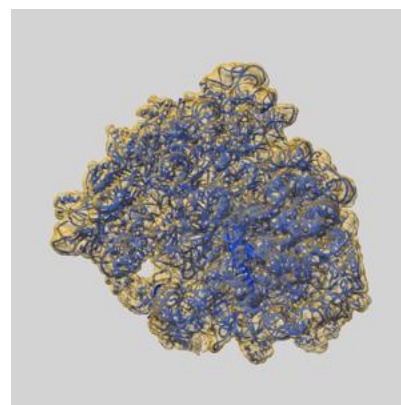
9.1 Map-model overlay [i](#)



X



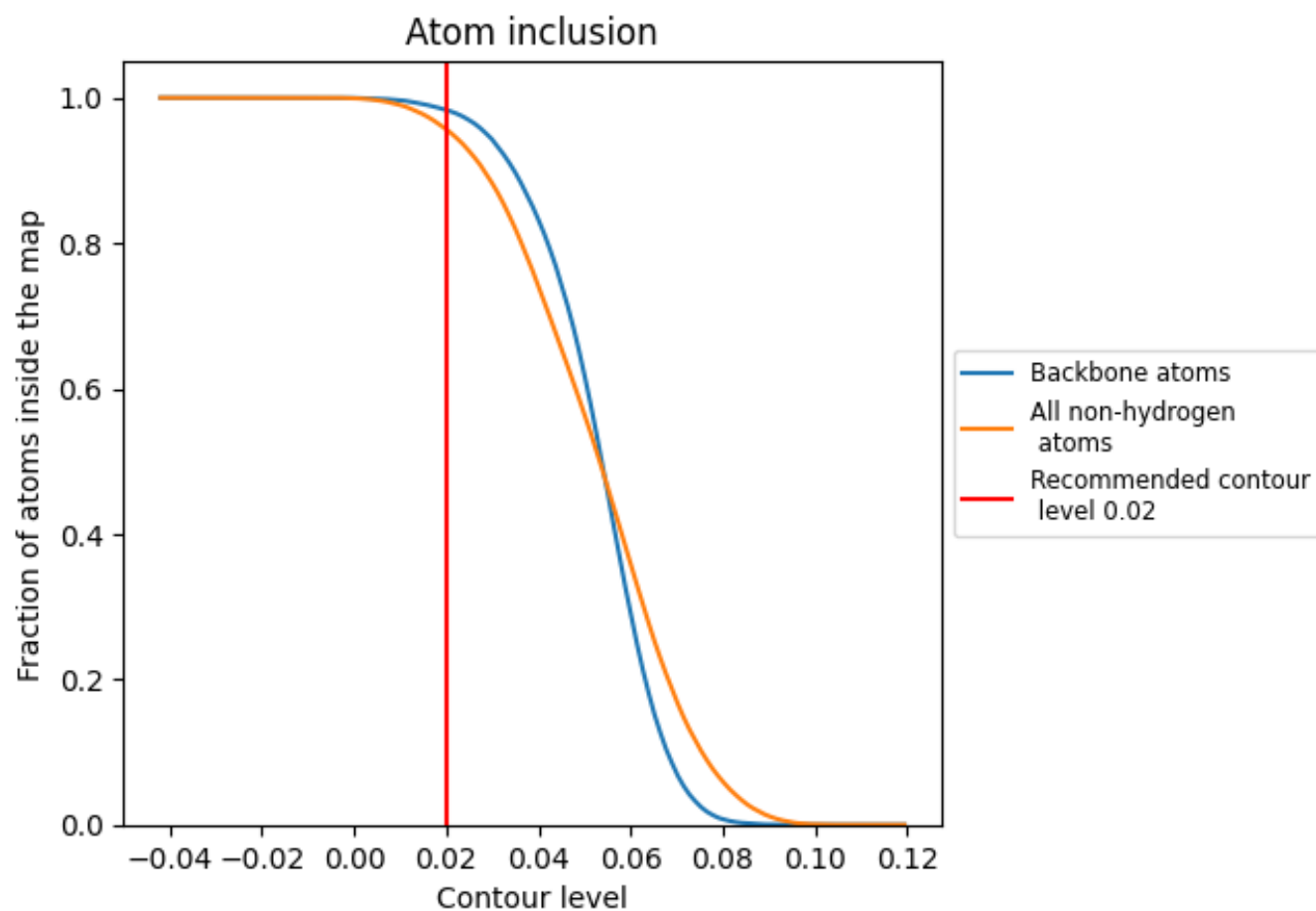
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.