



wwPDB X-ray Structure Validation Summary Report

Aug 16, 2023 – 05:15 PM EDT

PDB ID : 2AAR
Title : Structure of trigger factor binding domain in biologically homologous complex with eubacterial ribosome.
Authors : Baram, D.; Pyetan, E.; Sittner, A.; Auerbach-Nevo, T.; Bashan, A.; Yonath, A.
Deposited on : 2005-07-14
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

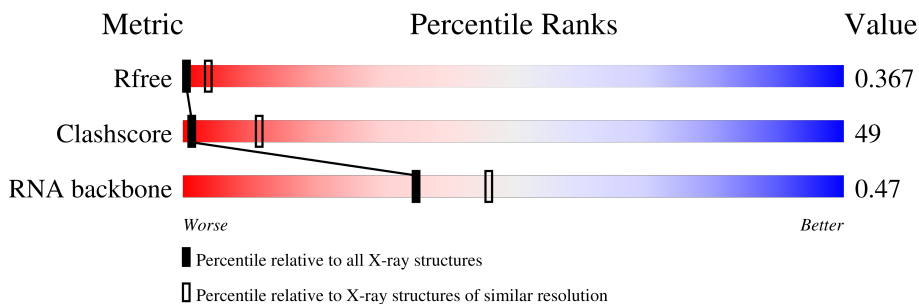
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	2880	12% (green), 59% (yellow), 21% (orange), . (red), . (grey)
2	R	95	98% (green), . (grey)
3	W	67	97% (green), . (grey)
4	7	113	100% (green)

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 59630 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
2	R	93	93	93	0	0	93

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
3	W	65	65	65	0	0	65

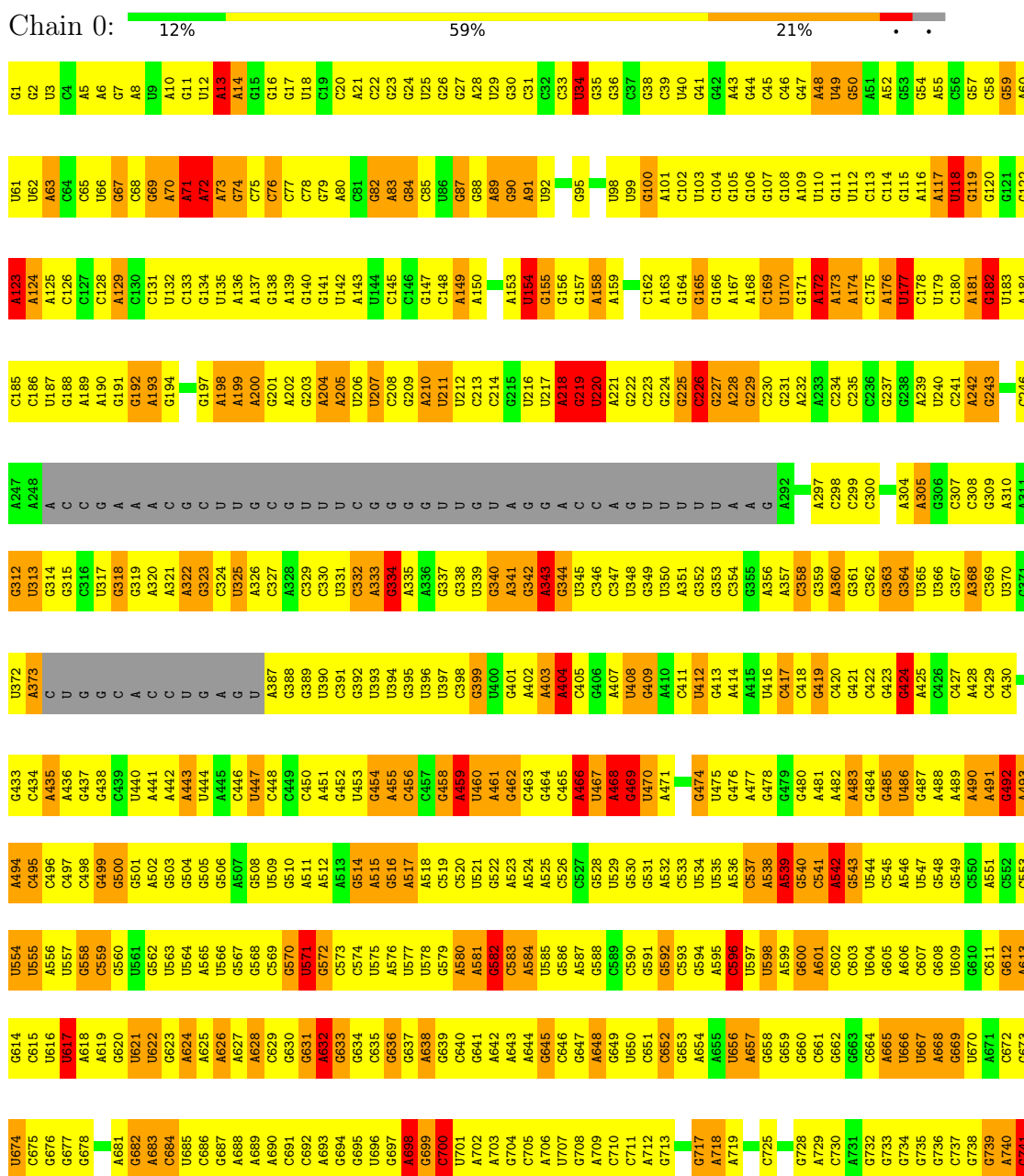
- Molecule 4 is a protein called Trigger Factor.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
4	7	113	113	113	0	0	113

3 Residue-property plots

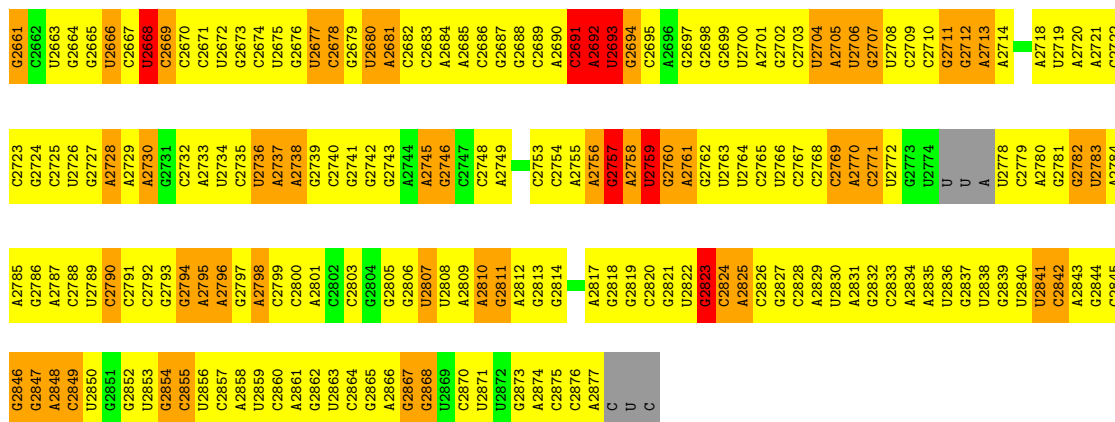
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: 23S ribosomal RNA



G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1679	G1680	G1681	G1682	G1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729					
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U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482										
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G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803							
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U9594	U2534	U2472	A2412	G2351	U2285	U2223	U2163	A	A2042	A1981	A1919	G1854	A1793	U1753
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G2611	G2548	G2486	G2426	U2365	A2301	G2237	U2177	G	G2056	G1995	G1933	A1869	A1807	C1746
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G2614	A2551	C2489	A2429	G2368	G2304	C2240	U2180	A2119	U2059	A1998	U1937	A1872	U1810	G1749
A2615	C2552	U2490	A2430	U2369	C2305	U2241	A2181	C2120	A2060	U1999	U1938	G1881	A1811	A1750
G2616	G2553	C2491	C2431	G2370	A2306	C2242	A2182	U2121	C2061	U2000	U1939	C1876	U1812	G1751
G2617	C2554	G2492	A2432	A2371	A2307	C2243	C2183	G2122	U2062	G2001	C1940	C1877	A1813	U1752
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G2621	C2558	C2496	U2436	G2375	U2311	A2247	A2187	U	G2066	G2005	C1946	U1881	U1817	C1756
G2622	U2559	G2497	G2437	G2376	A2312	A2248	A2188	U	U2067	G2006	U1946	U1882	G1818	G1757
G2623	G2560	U2498	A2438	G2377	G2313	A2249	A2189	U	C2068	G2007	C1947	A1883	U1819	U1758
G2624	C2561	C2499	U2439	G2378	A2314	U2251	A2190	U	U2069	C2008	G1948	A1884	G1820	A1759
G2625	G2562	G2500	C2440	U2380	A2252	A2252	A2191	C	G2070	U2009	A1949	C1885	A1821	G1760
G2626	U2563	U2501	U2441	A2381	A2253	A2253	U2192	G	C2071	G2010	C1950	C1886	C1822	G1761
G2627	U2564	G2502	C2442	C2382	G2317	C2254	C2193	G2132	C2072	U2011	G1951	C1887	G1823	C1762
G2628	C2565	U2503	C2443	C2383	G2320	G2255	A2194	U2133	A2073	A2012	A1952	C1888	C1824	G1763
G2629	U2566	G2504	G2444	G2384	C2321	G2256	C2195	G2134	U2074	A2013	A1953	C1889	C1825	A1764
G2630	G2567	G2505	C2445	U2385	A2257	A2257	U2196	C2135	G2075	G2014	A1954	C1890	U1826	C1765
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G2632	A2569	U2507	G2447	U2387	G2259	G2259	U2198	G2137	G2077	A2016	G1956	C1891	G1828	G1767
G2633	C2570	G2508	A2448	G2388	C2260	C2260	C2199	U2138	G2078	U2017	C1957	U1894	C1829	U1768
G2634	G2571	U2509	G2449	G2389	G2261	G2261	G2200	G2139	A2079	G2018	G1958	A1895	C1830	U1769
G2635	U2572	A2510	A2450	A2390	C2262	C2262	G2201	G2140	U2080	C2019	U1959	A1896	G1831	U1770
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G2637	G2574	A2512	U2452	G2392	C2264	C2264	G2203	G	C2082	G2021	A1961	U1898	G1833	C1772
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G2639	G2576	A2514	G2454	G2394	A2266	A2266	C2205	C	G2084	C2023	G1963	U1900	C1835	A1774
G2640	A2577	G2515	A2455	C2395	A2267	A2267	C2206	A	G2085	U2024	A1964	A1901	C1836	A1775
G2641	G2578	U2516	U2456	C2396	G2268	G2268	G2207	A	U2086	A2025	A1965	A1902	G1837	A1776
G2642	C2579	C2517	A2457	U2397	G2269	G2269	U2208	C	U2087	C2026	C1966	C1903	G1838	A1777
G2643	U2580	G2518	U2458	G2398	U2270	U2270	G2209	G	U2088	G2027	U1967	G1904	G1839	U1778
G2644	A2581	C2519	C2459	C2399	C2271	C2271	C2210	U	C2089	C2027	G1968	G1905	A1840	C1779
G2645	G2582	A2520	G2460	G2400	A2272	A2272	U2211	G	U2090	U2030	G1969	G1908	G1841	A1780
G2646	U2583	A2521	G2461	A2401	C2273	C2273	U2212	G	C2091	A2031	C1970	C1908	G1842	U1781
G2647	C2584	G2522	C2462	U2402	C2274	C2274	G2213	A	U2092	G2032	U1909	U1909	G1843	C1782
G2648	U2585	G2523	G2463	C2403	U2275	U2275	G2214	A	G2093	C2033	G1972	A1910	G1844	G1783
G2649	G2586	G2524	A2404	C2343	A2276	A2276	C2215	U	C2094	A2034	C1973	A1911	A1845	C1784
G2650	U2587	A2405	G2464	G2344	C2277	C2277	G2216	A	G2095	G2035	U1974	G1912	A1846	G1785
G2651	G2588	C2406	G2465	A2345	A2278	A2278	G2217	A	U2096	G2036	G1975	G1913	G1849	U1787
G2652	C2589	G2407	G2466	G2346	G2279	G2279	U2218	C2137	A2097	A2037	U1976	U1914	G1850	U1789
G2653	U2591	U2408	G2468	C2347	A2280	A2280	U2219	G	G	C2038	U1977	A1915	U1789	G1790
G2654	C2591	A2409	G2469	A2348	G	G	A2220	C2160	G	G2039	U1978	G1916	A1851	



- Molecule 2: 50S ribosomal protein L23

Chain R: 98%



- Molecule 3: 50S ribosomal protein L29

Chain W: 97%



- Molecule 4: Trigger Factor

Chain 7: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.39Å 407.06Å 692.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 19.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-3.50) 100.0 (19.99-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.52Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.320 0.336 , 0.367	Depositor DCC
R_{free} test set	13451 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	98.5	Xtrriage
Anisotropy	0.659	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	59630	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.65	7/66467 (0.0%)	0.84	119/103673 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	128

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	700	C	N1-C2	10.10	1.50	1.40
1	0	538	A	C5-C6	-5.66	1.35	1.41
1	0	788	G	N9-C4	5.49	1.42	1.38
1	0	2593	A	C5-C6	-5.46	1.36	1.41
1	0	774	A	C5-C6	-5.29	1.36	1.41

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1279	G	N9-C1'-C2'	10.85	128.10	114.00
1	0	1266	G	N9-C1'-C2'	10.62	127.81	114.00
1	0	765	C	O4'-C1'-N1	9.33	115.66	108.20
1	0	2237	C	N1-C1'-C2'	9.28	126.06	114.00
1	0	985	G	N9-C1'-C2'	9.24	126.01	114.00

There are no chirality outliers.

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	123	A	Sidechain
1	0	154	U	Sidechain
1	0	67	G	Sidechain
1	0	71	A	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59359	0	29917	4315	0
2	R	93	0	0	0	0
3	W	65	0	0	0	0
4	7	113	0	0	0	0
All	All	59630	0	29917	4315	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

The worst 5 of 4315 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:541:C:O2'	1:0:2018:G:N2	1.63	1.29
1:0:788:G:H22	1:0:801:A:P	1.58	1.26
1:0:1066:G:H3'	1:0:1067:G:H4'	1.23	1.20
1:0:2170:C:H2'	1:0:2171:U:H5'	1.23	1.17
1:0:1314:A:O2'	1:0:1315:A:H3'	1.42	1.15

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	657 (23%)	223 (8%)

5 of 657 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	14	A
1	0	34	U
1	0	45	C
1	0	48	A

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1338	G
1	0	2854	G
1	0	1715	A
1	0	2846	G
1	0	2521	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.