



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2018 – 05:26 pm GMT

PDB ID : 1J5A
Title : STRUCTURAL BASIS FOR THE INTERACTION OF ANTIBIOTICS
WITH THE PEPTIDYL TRANSFERASE CENTER IN EUBACTERIA
Authors : Schlutzen, F.; Zarivach, R.; Harms, J.; Bashan, A.; Tocilj, A.; Albrecht, R.;
Yonath, A.; Franceschi, F.
Deposited on : 2002-03-06
Resolution : 3.50 Å(reported)

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A user guide is available at

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

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:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

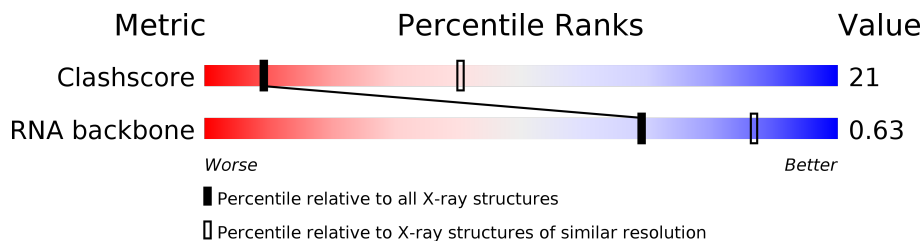
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

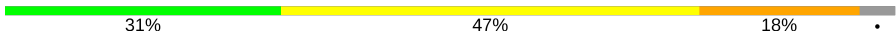

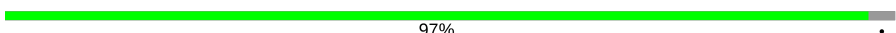

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122078	1485 (3.60-3.40)
RNA backbone	2633	1052 (4.10-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	
2	K	205	
3	L	134	
4	M	60	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CTY	A	2881	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59971 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2774	Total	C	N	O	P	0	0	0
			59532	26556	10982	19221	2773			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1526	U	Y	SEE REMARK 999	GB 15805042

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	K	197	Total	C	0	0	197
			197	197			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	L	130	Total	C	0	0	130
			130	130			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	M	58	Total	C	0	0	58
			58	58			

- Molecule 5 is CLARITHROMYCIN (three-letter code: CTY) (formula: C₃₈H₆₉NO₁₃).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mg 2 2	0	0

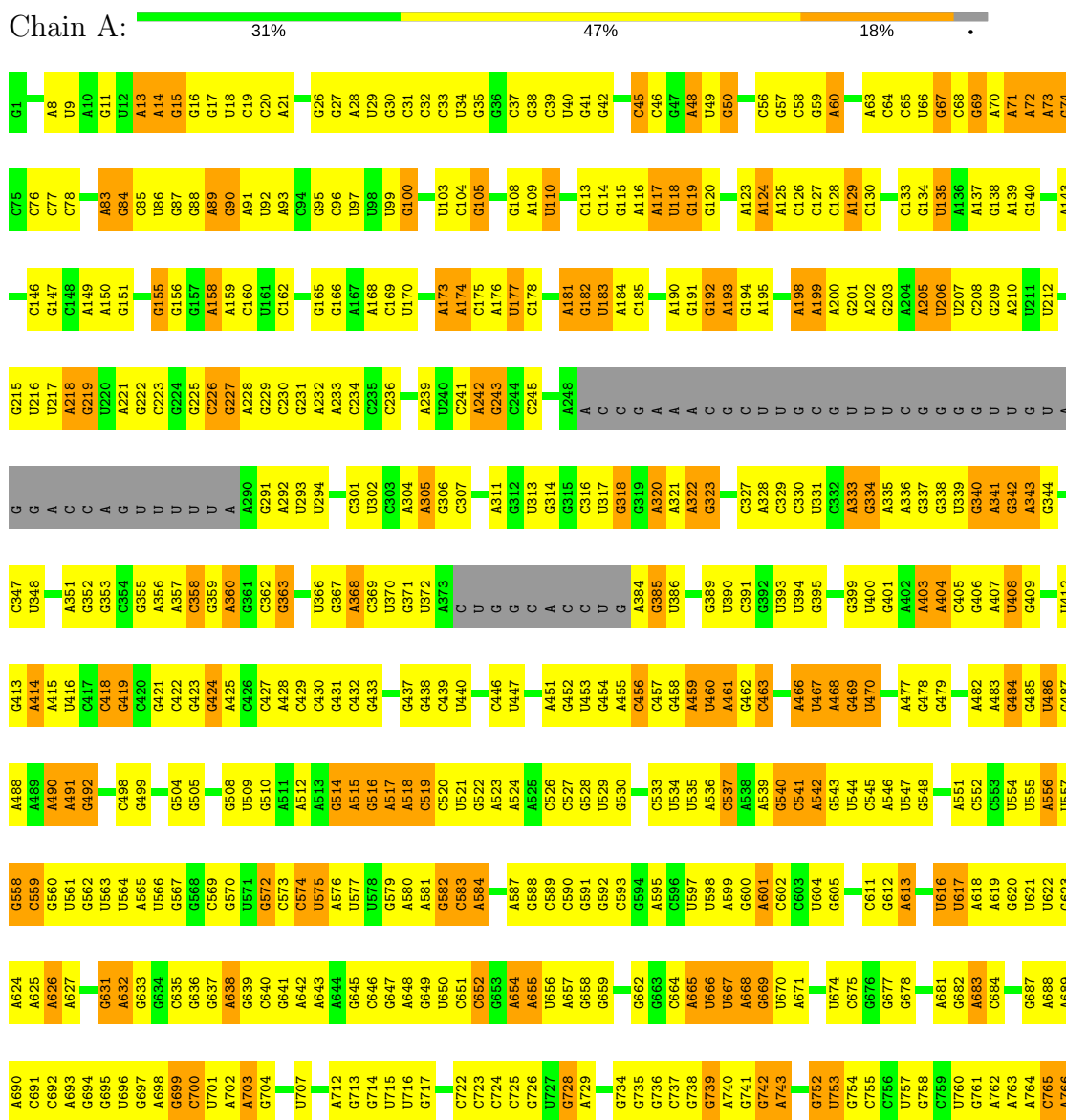
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3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: 23S rRNA



C1824	U1752	G1683	U1612	G1542	G1480	G1338	G1269	G1193	U1124	A1055	G977	C908	U840	G773
C1825	A1753	G1684	G1613	G1543	G1481	U1339	U1269	U1194	G1125	U1056	U978	C910	G841	G774
U1826	G1754	A1695	C1614	A1544	U1481	C1340	C1270	U1195	A1126	A1057	A979	A911	A842	A775
G1827	G1755	A1696	C1615	U1482	U1482	G1341	C1271	U1196	G1127	G1058	G980	A912	G843	G776
C1828	G1756	C1687	G1616	U1548	G1483	U1342	C1272	U1197	G1128	A1059	C981	C913	G844	A777
C1829	C1757	U1688	G1617	C1549	G1484	C1343	C1273	U1198	A1129	C1060	C982	C914	U845	G778
C1830	C1758	U1689	U1618	C1550	U1485	C1344	U1274	U1199	U1130	A1061	G983	C915	A846	
C1831		U1690	A1619	U1551	A1486	G1345	A1275	U1200	C1134	A1065	A984	A918	C850	U784
	C1762	C1691		C1552	C1416	G1346	U1276	G1201	C1135	U1066	G985	U919	C851	U785
C1834	G1763	C1692	C1623	G1553	G1488	C1347	A1278	U1202	G1136	G1067			U852	U786
C1835	A1764	A1693	A1624	G1554	A1420	C1348	A1279	U1203	G1137	A1068	A994	A922	U857	A787
C1836	C1765	A1694	A1625	A1555	U1490	A1349	U1280	G1204	A1137	G1069	A995	A923	U858	G788
	U1766		A1626	A1556		G1350	A1281	G1205	A1138	G1070	C996	C924	U859	G789
A1840	G1767	U1697	C1627	G1557	U1493	G1351	A1282		A1139		C997	U925	U860	G790
A1851	U1768	C1698		C1558	G1494	G1352	C1283	G1209	U1140	U1071	C998	U926	U861	
	U1769	A1699	C1631	G1559	G1495	G1353	C1284	C1210	U1141	U1072	A999	C927	U862	
G1854	G1770	A1632	A1632	G1496	G1427	A1354	A1285	G1211	G1142	G1073	A1001	G928	C863	A794
G1855	A1771	C1633	G1633	A1561	C1497	A1355	U1286	U1212	A1143	G1074	C1002	A929	C864	A795
U1856	C1772	G1634	A1634	G1498	A1429	G1356	A1287	U1213	U1144	C1075	C1003	A930	C865	A796
C1857	G1773	U1635	G1635	U1563	A1499	U1357	A1288	G1214	G1145		G1004	A931	C866	A797
U1857	A1774	U1564		U1564	U1500	C1358	A1289	C1215	C1146	U1079	G931	A932	C867	A798
A1867	U1775	G1571	C1640	G1572	C1501	G1359	A1290	U1216	G1149	A1080	U1005	G932	U868	U800
	A1776	C1572	G1641	C1573	G1502		G1291	G1217	U1150	C1082	A1007	G933	C869	A801
U1871	U1777	G1573	U1709	A1574	G1503	U1365	A1292	C1218	U1151	C1083	C1008	G934	C870	A802
	U1778	U1575	U1645		U1505	A1367	A1293	C1219	C1152	A1084		C937	U871	C803
	A1782	C1576		G1576	U1506	G1368	G1298	C1221	A1153	G1095	A1012	G938	U872	C804
C1876	U1787	G1577	C1648		A1507	A1437	U1299	G1222	U1154	C1096	G1013	C939	U873	C805
C1877	A1714	C1579	U1651	G1579	C1508	G1369	A1300	G1223	G1155	C1087	G1014	G940	U874	A806
C1878	A1715	U1580	G1652	C1580	A1509	U1370	A1301	A1224	U1015	C1088	U1015	U941	C875	A807
C1879	G1716	C1581	U1653	C1581	A1510	G1371	C1302	G1225	C1160	C1089	C1016	U942	C876	C808
U1881	U1717	C1582	C1653	C1582	A1511	A1372	U1306	A1226	U1161	C1090	U1019	U943	C877	C809
U1882	C1791	A1583	U1654	A1583	U1512	G1373	U1307	A1227	A1162	C1091	A1020	G945	C878	U810
A1883	C1792	G1584	C1655	U1584	U1513	G1374	C1308	A1233	C1163	U1093	A1021	G946	C879	U811
A1884	A1793	U1656	U1514	U1446	U1514		G1309	C1234	G1165	U1093	A1022	C948	C880	
C1885	A1794	U1657	U1515	U1447	U1515	G1377	C1310		A1166	A1096	U1023	G949	A886	A813
									A1167	A1097	G1024	G950	U887	G812
C1888	G1798	U1660	G1660	A1588	G1519	C1380	C1311	G1240	G1167	A1098		G951	A888	G814
G1889	A1799	C1661	C1661	G1589	U1520	G1381	U1312	G1241	G1168	G1099	U1030	G952	C889	A815
G1890	C1728	C1590	G1662	C1590	U1521	G1382	U1313		G1169	A1099	G1031	U953	U890	U816
C1891	C1729	U1591	C1663	U1591	C1522	C1383	A1314	U1244	U1170	G1100	A1032	U954	C891	A817
	A1802	G1730	U1592	U1592	A1523	G1384	A1315	G1245	A1171	U1101	U1034	G955	U891	C818
U1894	G1803	C1593	C1665	C1593	C1524	C1385	G1316		U1172	G1102	G1033	A956	C892	C819
A1895		U1594	G1666	U1594	A1525	A1386	U1325	G1249	G1173	C1103	U1034	U957	G	U820
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C1897	C1808	G1735	G1668	A1596	G1527		G1322	G1251	A1175	U1105	G1036	C958	G	G822
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U1900	A1811	U1738	A1671	U1599	U1530	G1393	U1326		C1178	U1108	A1039		C	C825
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	A1813	G1742	C1673	U1601	A1532		C1327	A1259	C1183	G1110	G1041		A	C827
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C1907	U1676	U1676	A1604	C1535	G1535	C1399	G1330	U1262	G1186	C1113	G1045	A970	C	C830
U1908	U1817	C1677	G1677	G1536	G1470	G1401	G1333	G1263	A1187	G1118	U1046	A971	A	C831
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U1911	G1820	U1680	U1680	U1539	A1474	G1403	A1335	G1266	C1190	A1122	C1049	U974	U	
A1912	A1821	A1750	C1540	U1540	U1475	U1404	G1336	A1267	G1191			C975	U	A838
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A2861	G2866	G2793	C2709	C2630	C2558	G2492	C2420	C2348	C2263	A2190	C2124	A2060	C1989	A1915
G2862	G2867	G2794	C2710	A2633	U2559	C2493	C2421	A2348	C2264	A2191	C2125	C2061	U1994	G1916
G2865	A2866	A2795	G2711	G2634	G2560	C2494	C2422	G2349	A2265	U2192	U	U2062	G1995	C1917
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G2893	G2894	G2822	G2742	U2672	C2595	G2524	A2455	U2380	U2299	A2226	C2157	G2093	U2024	C1950
G2894	G2895	G2823	G2743	C2673	C2596	U2525	U2456	A2381	C2300	C2227	C2158	C2094	A2025	G1951
G2895	G2896	G2824	A2744	G2674	U2597	U2526	A2457	C2382	U2228	A2159	A2159	G2095	C2026	A1952
G2896	G2897	G2825	A2745	U2675	A2600	G2527	U2458		G2229		C2160	U2096	C2026	A1953
G2897	G2898	G2826		C2676	C2601	G2528	C2459	U2385	A2306	G2234	C2162	A2097	G2032	A1954
G2898	G2899	G2827	A2756	U2677	C2602	G2529	G2460	A2390	A2307	G2235	C2162	G	C2033	G1956
G2899	G2900	G2828	G2757	C2678	G2603	U2530	G2461	A2391	A2308	U2236	U2163	A	A2034	G1956
G2900	G2901	G2829	A2758	G2679	G2604	C2531	G2463	C2392		U2237	C2166	U	G2035	
G2901	G2902	G2830	G2759	U2680	C2605	U2532	G2464	C2393	A2312	G2238	A2167	A	C2038	A1964
G2902	G2903	G2831	G2760	A2681	G2606	U2533	G2465	G2394	G2313	C2239	G2168	U	G2039	C1966
G2903	G2904	G2832	A2761		C2607	U2534	C2466	C2395	A2314	C2240	G2103	A2040	A2040	
G2904	G2905	G2833			A2608	U2535	A2467	C2396	A2315	U2241	G2104	A2041	A2041	G1970
G2905	G2906	G2834	U2766	C2686	G2609	C2536	G2468	C2397	G2316	C2242	C2170	A2042	A2042	C1971
G2906	G2907	G2835	C2767	G2687	G2610	A2540	C2469	A2397	G2317	C2243	U2171	G2106	A2043	G1972
G2907	G2908	G2836	G2768	C2688	G2611	U2541	U2470	U2398	U2318	C2244	U2172		A2044	G1973
G2908	G2909	G2837	G2769	C2689	A2613	A2543	U2471	C2399	G2319	C2245	A2109		G2044	C1974
G2909	G2910	G2838	A2770	C2690	C2614	A2544			G2320	A2246	G2110		A2045	U1974
G2910	G2911	G2839	G2771	A2692	U2615	A2545	C2475	C2403	C2321	A2247	C		A2045	G1975
G2911	G2912	G2840	U2772	G2693	U2616	G2546	A2476	A2404	U2322	A2248	U	C	C2048	U1976
G2912	G2913	G2841	G2773	G2694	C2547	C2547	C2477	A2405	U2323		U	U	C2049	C1977
G2913	G2914	G2842	U2774	C2695	G2548	G2548		C2406	G2324	U2180	G	C	G2050	U1978
G2914	G2915	G2843	U	G2696	G2621	G2549	C2480	G2407	A2325	U2251	U	C	U2051	C1979
G2915	G2916	G2844	U	A2697	C2622	C2550	G2481	C2408	C2326	A2252	A2181	C	G2052	A1980
G2916	G2917	G2845	A	G2698	A2623	A2551	A2482	A2409	U2327	A2253	A2182	A2117	G2053	
G2917	G2918	G2846	G2775	G2699	C2552	C2552	U2483	U2410	G2328	C2254	A2183	A2118	A2054	A1984
G2918	G2919	G2847	U2776	G2700	G2625	G2553	G2484	U2416	C2329	G2255	C2184	A2119	G2055	G1985
G2919	G2920	G2848	A2780	A2705	U2626	C2554	U2485		G2330	G2256	U2185	C2120	C2056	G1986
G2920	G2921	G2849	G2781	U2706	G2627	G2555	C2486	U2417	G2331		G2186	U2121	U2057	G1987
G2921	G2922	G2850	C2782	C2628	C2628	G2556	C2487	U2418	A2327	C2261		U2122	U2058	A1989

• Molecule 2: RIBOSOMAL PROTEIN L4

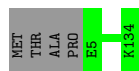
Chain K:

96%

MET	A2	E198	GLU	ALA	GLY	GLU	GLN	GLN
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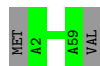
- Molecule 3: RIBOSOMAL PROTEIN L22

Chain L:  97% .



- Molecule 4: RIBOSOMAL PROTEIN L32

Chain M:  97% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 412.70Å 697.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.273 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59971	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	A	0.23	0/66661	0.66	2/103976 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1746	A	C2'-C3'-O3'	5.89	123.12	113.70
1	A	777	A	C2'-C3'-O3'	5.52	122.53	113.70

There are no chirality outliers.

There are no planarity outliers.

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	A	59532	0	30004	1877	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	52	0	69	32	0
6	A	2	0	0	0	0
All	All	59971	0	30073	1896	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 21.

The worst 5 of 1896 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2042:A:C2	5:A:2881:CTY:H383	1.63	1.30
1:A:2042:A:N3	5:A:2881:CTY:H383	1.62	1.14
1:A:1747:G:H4'	1:A:1749:G:H1'	1.29	1.12
1:A:940:G:H3'	1:A:941:U:H5''	1.34	1.09
1:A:1199:U:H3'	1:A:1200:G:H5''	1.35	1.08

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	A	2765/2880 (96%)	555 (20%)	142 (5%)

5 of 555 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	45	C
1	A	48	A

5 of 142 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1278	A
1	A	1563	U
1	A	2633	A
1	A	1285	A
1	A	1354	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	CTY	A	2881	-	54,54,54	1.61	10 (18%)	83,83,83	3.04	42 (50%)

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
5	CTY	A	2881	-	-	1/75/110/110	1/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	CTY	O2-C13	-3.19	1.40	1.46
5	A	2881	CTY	C19-C16	-2.20	1.47	1.52
5	A	2881	CTY	C2-C1	2.04	1.56	1.51
5	A	2881	CTY	C12-C13	2.06	1.58	1.54
5	A	2881	CTY	C15-C16	2.16	1.57	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	CTY	O5-C16-C19	-7.44	98.20	110.95
5	A	2881	CTY	O5-C16-C15	-5.20	104.43	112.95
5	A	2881	CTY	C7-C6-C5	-5.19	103.81	110.22
5	A	2881	CTY	C15-C16-C17	-5.10	98.23	107.65
5	A	2881	CTY	C27-C26-C25	-5.09	105.25	113.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C20-O5-C16-C17

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C14-C15-C16-C17-C18-O4

1 monomer is involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	CTY	32	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.