



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:52 AM GMT

PDB ID : 2OGN
Title : The crystal structure of the large ribosomal subunit from *Deinococcus radiodurans* complexed with the pleuromutilin derivative SB-280080
Authors : Davidovich, C.; Bashan, A.; Auerbach-Nevo, T.; Yonath, A.
Deposited on : 2007-01-07
Resolution : 3.56 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

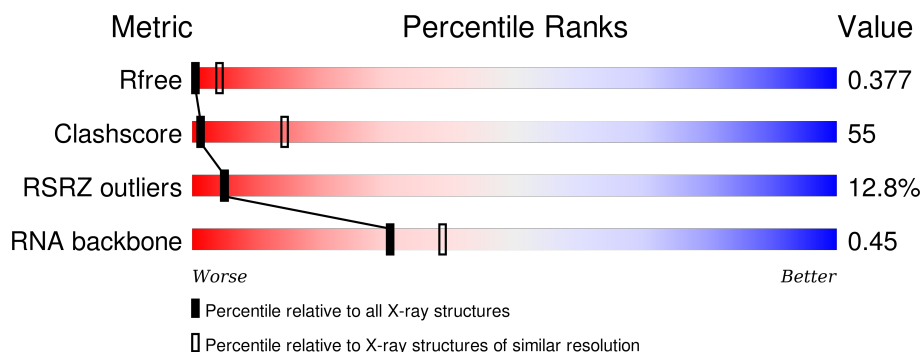
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.56 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}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)
RNA backbone	2183	1057 (4.30-2.80)

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.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	B	211	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 59597 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.

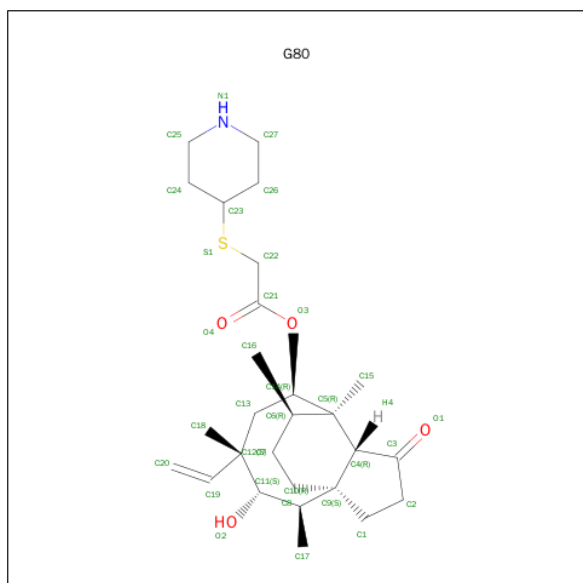
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	205	Total	C	0	0	205
			205	205			

- Molecule 3 is (3AS,4R,5S,6S,8R,9R,9AR,10R)-5-HYDROXY-4,6,9,10-TETRAMETHYL-1-OXO-6-VINYLDECAHYDRO-3A,9-PROPANOCYCLOPENTA[8]ANNULEN-8-YL (PIPERIDIN-4-YLTHIO)ACETATE (three-letter code: G80) (formula: C₂₇H₄₃NO₄S).

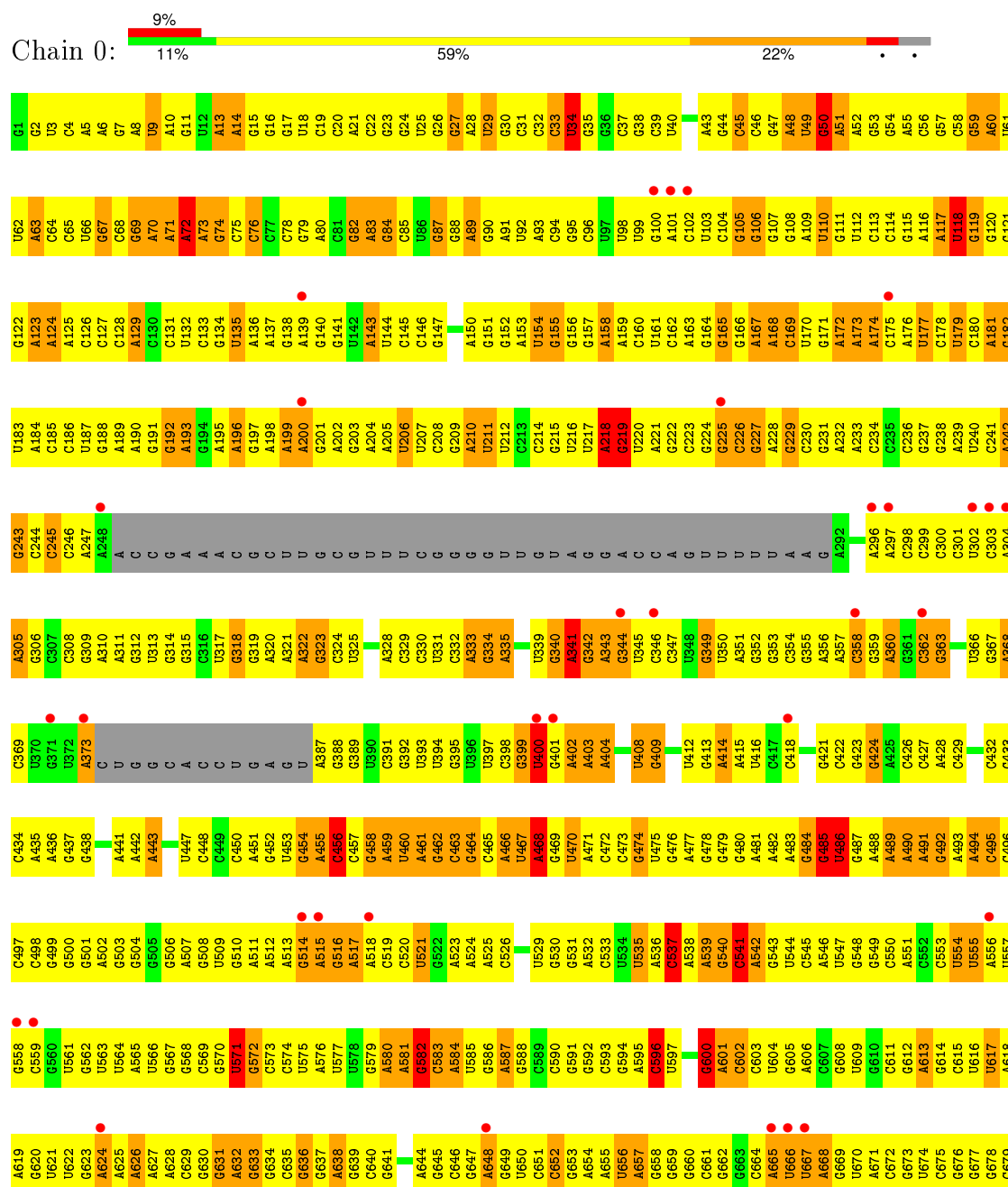


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	0	1	Total	C	N	O	S	0	0
			33	27	1	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 ($\text{RSRZ} > 2$). 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.

- Molecule 1: 23S ribosomal RNA





A2405	C2343	G2283	U2222	C2162	C1917	G1853	C1791	G1730	A1610
C2406	G2344	U2284	U2223	U2163	G1918	G1854	C1792	C1731	U1611
C2407	A2345	U2285	U2224	A2164	A1919	G1855	A1792	U1732	U1612
G2408	G2346	G2286	A2225	A2041	A1920	G1856	A1793	U1733	G1613
A2409	C2347	G2287	A2226	U2105	A1921	G1857	A1794	C1734	C1614
U2410	A2348	A2288	C2227	G2106	U1922	G1858	G1797	G1735	C1615
A2411	G2349	A2289	U2228	G2107	U1923	A1859	G1798	C1736	C1616
A2412	G2350	A2290	G2229	A2108	U1924	A1860	G1799	U1737	C1617
A2413	G2351	U2291	G2230	A2109	C1925	G1861	A1800	U1738	C1618
U2417	A2352	C2292	G2232	G2110	U1926	G1862	C1801	U1739	U1619
A2418	G2353	G2293	C2233	C	U1927	U1863	A1802	U1680	C1620
A2419	G2354	U2294	C2234	C	G2049	G1864	G1803	G1742	G1621
G2420	A2355	G2295	G2235	U	U1928	G1865	U1804	C1743	G1622
U2421	A2356	U2296	U2236	G	C1930	G1866	G1805	G1744	C1623
A2422	A2357	C2297	C2237	U2051	U1990	A1867	G1806	C1745	A1624
G2423	C2358	U2298	G2238	G2052	C1991	U1868	A1807	A1746	A1685
G2424	U2359	A2299	C2239	G2053	G1992	A1869	C1808	G1747	A1686
G2425	C2360	G2300	C2240	U1994	U1993	U1870	G1809	U1748	C1627
U2426	G2361	A2301	U2241	G1995	A1935	G1871	U1810	G1749	C1628
G2427	G2362	C2302	C2242	U1996	A1936	A1872	U1811	A1750	U1689
A2428	C2363	C2303	C2243	U1997	G1937	U1873	U1812	A1751	G1630
U2429	G2364	G2304	C2244	A1998	U1938	U1874	A1813	U1752	G1631
A2430	U2365	C2305	A2245	U1999	U1939	G1878	G1814	A1753	A1632
A2431	A2366	A2306	A2246	G2000	C1940	G1879	G1815	G1754	A1693
G2432	A2367	A2307	A2247	A2002	C1941	G1880	G1816	G1755	A1694
U2433	G2368	A2308	A2248	A2003	G1942	U1881	U1817	C1756	U1695
G2434	U2369	G2309	U2249	A2004	A1943	G1882	G1818	C1757	C1636
A2435	C2370	G2310	G2250	U2005	C1944	U1883	U1819	G1758	U1697
U2436	A2371	U2311	U2251	U2006	U1945	G1886	A1820	G1759	C1698
G2437	A2372	A2312	A2252	G2067	G2006	U1887	G1821	G1760	U1699
A2438	C2373	G2313	A2253	C2068	G2007	G1888	C1822	G1761	C1700
U2439	G2374	A2314	C2254	U2069	C2008	U1889	G1823	C1762	C1641
G2440	C2375	A2315	G2255	G2070	U2009	G1890	C1824	G1763	C1642
U2441	U2376	G2316	A2256	C2072	G2010	G1891	C1825	A1764	A1643
C2442	U2377	U2317	G2257	A2073	U2011	C1892	U1826	G1765	G1644
U2443	U2378	U2318	G2258	G2074	A2012	A1952	G1827	U1766	U1705
U2444	A2381	G2319	G2259	U2075	A2013	G1893	G1828	G1767	G1646
G2445	C2382	G2320	C2260	G2076	A2014	U1894	G1829	U1768	U1647
A2446	G2383	C2321	G2261	G2077	A2015	A1954	C1830	U1769	C1648
U2447	G2384	U2322	G2262	G2078	G2016	G1956	G1831	U1770	A1649
G2448	U2385	G2323	C2263	A2079	U2017	C1957	G1832	U1771	U1709
A2450	G2386	G2324	C2264	U2080	G2018	U1958	U1833	C1772	U1710
U2451	U2387	A2325	A2265	U2081	C2019	U1959	C1835	G1773	U1651
C2454	G2388	C2326	A2266	C2082	G2020	A1960	C1836	A1774	C1652
A2455	A2389	U2327	A2267	A	G2021	A1961	G1837	A1775	C1653
U2456	A2390	C2328	G2268	G2084	C2022	C1962	G1838	A1776	C1654
G2457	A2391	G2329	C2269	U2086	C2023	G1963	A1839	A1777	C1655
U2458	G2392	G2330	U2270	U2086	U2024	A1964	U1840	U1778	U1656
C2459	G2393	A2331	C2271	U2090	A2025	G1904	A1841	C1779	A1657
G2460	C2394	G2332	C2272	C2091	C2026	U1906	G1842	G1780	G1658
U2461	A2395	A2333	C2273	A	G2029	U1907	U1843	C1781	G1659
G2462	C2396	G2334	C2274	U2092	U2030	G1968	C1844	C1782	G1660
G2463	A2397	U2335	U2275	C2093	U2031	G1969	A1845	G1783	G1661
U2464	U2398	G2336	C2276	U2094	A2031	U1970	A1846	C1784	G1662
G2465	C2399	A2337	A2277	G2095	G2032	C1971	G1847	A1785	C1663
U2466	G2400	C2338	A2278	U2096	C2033	U1912	U1848	G1786	G1664
A2401	A2401	A2339	A2279	A2097	A2034	C1973	G1849	U1787	C1665
U2402	U2402	C2340	G	G	G2035	U1974	G1850	U1788	G1666
G2403	C2403	G2341	A2220	A2097	G2036	U1975	A1851	U1789	A1667
A2404	A2404	U2342	A	A	A2037	U1976	G1916	G1790	A1669

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.47Å 412.74Å 696.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.56 29.95 – 3.56	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.96-3.56) 90.6 (29.95-3.56)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.338 0.360 , 0.377	Depositor DCC
R_{free} test set	13101 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 79.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 263343 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	59597	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: G80

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	0.62	9/66467 (0.0%)	0.83	95/103673 (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	158

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	788	G	N9-C4	8.60	1.44	1.38
1	0	700	C	N1-C2	8.52	1.48	1.40
1	0	788	G	C5-C6	6.89	1.49	1.42
1	0	824	U	N1-C2	6.74	1.44	1.38
1	0	788	G	C2-N3	5.96	1.37	1.32

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1342	U	N1-C1'-C2'	10.68	127.89	114.00
1	0	985	G	N9-C1'-C2'	10.52	127.68	114.00
1	0	2497	A	N9-C1'-C2'	10.09	127.12	114.00
1	0	1975	G	N9-C1'-C2'	9.37	126.19	114.00
1	0	2660	C	N1-C1'-C2'	9.30	126.09	114.00

There are no chirality outliers.

5 of 158 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	154	U	Sidechain
1	0	29	U	Sidechain
1	0	50	G	Sidechain
1	0	67	G	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	4825	0
2	B	205	0	0	2	0
3	0	33	0	43	7	0
All	All	59597	0	29960	4828	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 55.

The worst 5 of 4828 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)
1:0:2040:A:H2'	1:0:2041:A:C8	1.52	1.42
1:0:2040:A:C2'	1:0:2041:A:H8	1.48	1.27
1:0:2564:U:O2'	1:0:2565:C:H5'	1.34	1.26
1:0:2418:A:H1'	1:0:2565:C:O2'	1.31	1.24
1:0:2810:A:C6	1:0:2854:G:C8	2.27	1.22

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%)	664 (24%)	167 (6%)

5 of 664 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	9	U
1	0	13	A
1	0	14	A
1	0	27	G
1	0	33	C

5 of 167 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1326	U
1	0	1634	A
1	0	2660	C
1	0	1337	G
1	0	1407	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	G80	0	2881	-	30,36,36	2.66	12 (40%)	29,56,56	2.05	8 (27%)

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
3	G80	0	2881	-	-	0/10/81/81	0/2/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	2881	G80	C24-C25	2.03	1.60	1.52
3	0	2881	G80	C27-N1	2.12	1.55	1.47
3	0	2881	G80	C9-C4	2.45	1.66	1.54
3	0	2881	G80	C10-C11	2.53	1.63	1.57
3	0	2881	G80	C8-C9	3.08	1.63	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	2881	G80	C16-C6-C7	-4.59	103.04	110.44
3	0	2881	G80	C13-C12-C19	-2.96	103.81	109.77
3	0	2881	G80	C27-N1-C25	-2.54	101.89	110.33
3	0	2881	G80	C15-C5-C4	2.17	115.87	110.65
3	0	2881	G80	C14-O3-C21	2.41	123.18	118.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	0	2881	G80	7	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	0	2766/2880 (96%)	0.43	246 (8%)	12 10	12, 79, 200, 200	0
2	B	205/211 (97%)	3.03	133 (64%)	0 0	3, 58, 141, 202	0
All	All	2971/3091 (96%)	0.61	379 (12%)	5 5	3, 77, 200, 202	0

The worst 5 of 379 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	146	THR	16.3
1	0	558	G	13.0
2	B	128	SER	11.1
2	B	144	ARG	10.8
1	0	730	C	10.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	G80	0	2881	33/33	0.91	0.25	0.73	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.