



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 07:50 AM UTC

PDB ID : 1Z58 / pdb_00001z58
Title : Crystal structure of a complex of the ribosome large subunit with rapamycin
Authors : Amit, M.; Berisio, R.; Baram, D.; Harms, J.; Bashan, A.; Yonath, A.
Deposited on : 2005-03-17
Resolution : 3.80 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

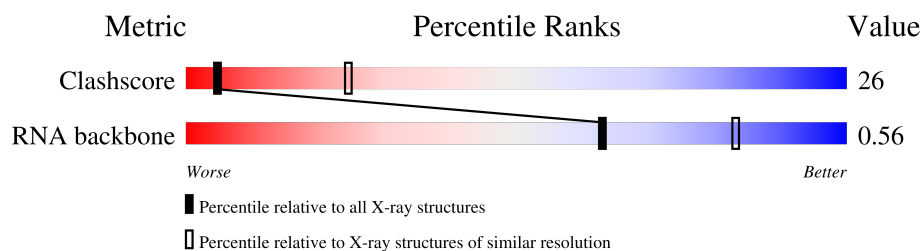
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	190562	1012 (3.94-3.66)
RNA backbone	3983	1007 (4.50-3.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	2	2880	 24% 56% 15% .

2 Entry composition [i](#)

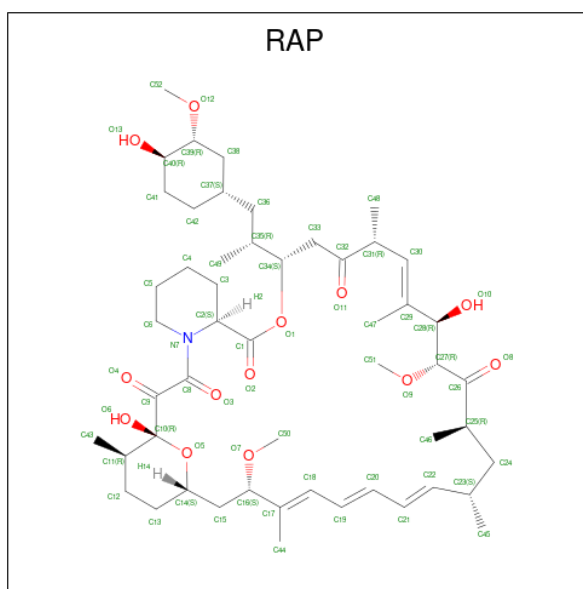
There are 2 unique types of molecules in this entry. The entry contains 59424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is RAPAMYCIN IMMUNOSUPPRESSANT DRUG (CCD ID: RAP) (formula: $C_{51}H_{79}NO_{13}$).



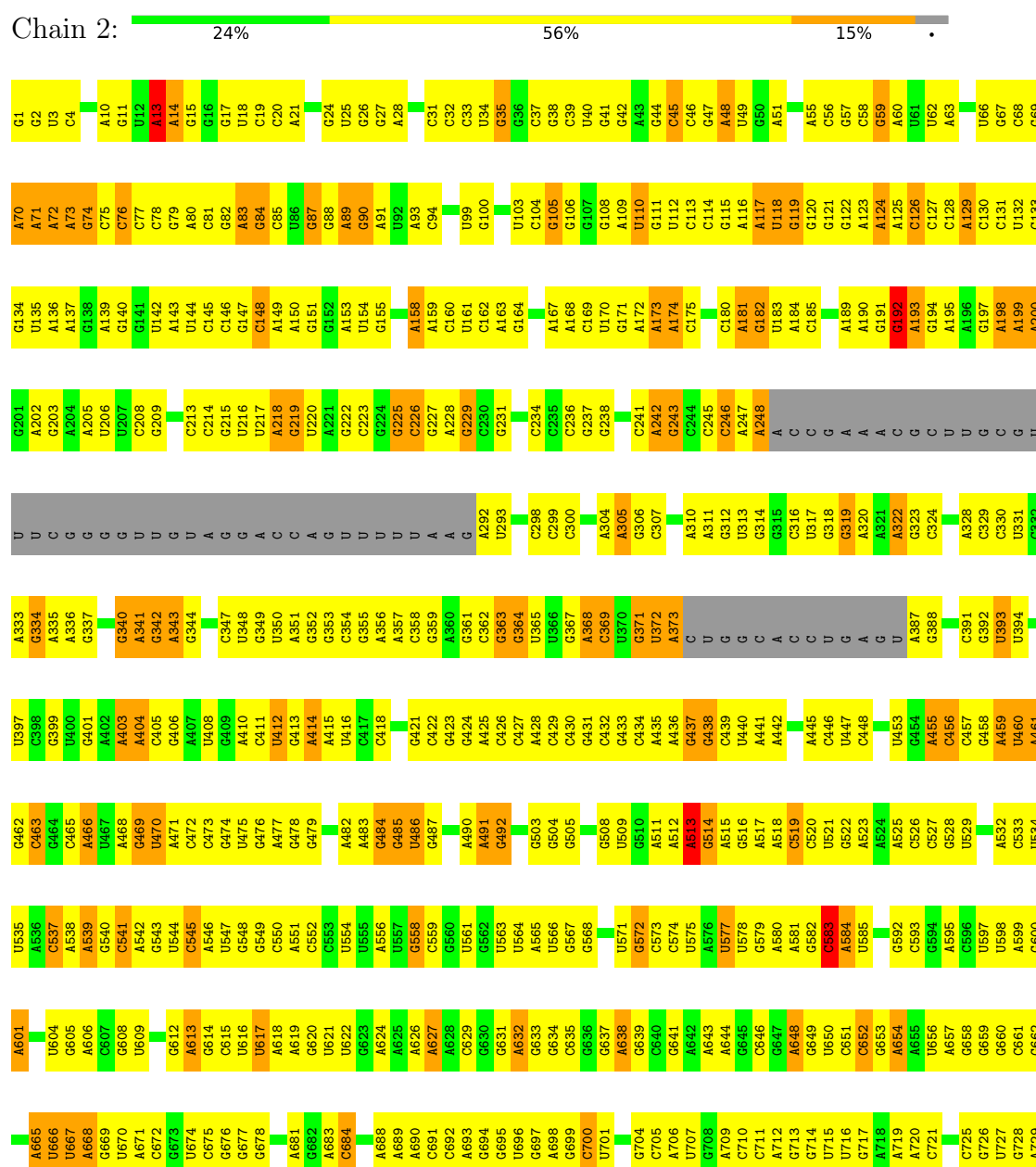
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	2	1	65	51	1	13	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA





	A2684	A2685	A2686	A2687	A2688	A2689	A2690	A2691	A2692	A2693	A2694	A2695	A2696	A2697	A2698	A2699	A2700	A2701	A2702	A2703	A2704	A2705	A2706	A2707	A2708	A2709	A2710	A2711	A2712	A2713	A2714	A2715	A2716	A2717	A2718	A2719	A2720	A2721	A2722	A2723	A2724	A2725	A2726	A2727	A2728	A2729	A2730	A2731	A2732	A2733	A2734	A2735	A2736	A2737	A2738	A2739	A2740	A2741	A2744								
G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	A2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681						
U2485	C2486	G2487	A2488	C2489	G2490	C2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	C2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2552
G2553	C2554	G2555	A2556	G2557	G2558	G2559	G2560	G2561	G2562	G2563	G2564	G2565	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	G2579	G2580	G2581	G2582	G2583	G2584	G2585	G2586	G2587	G2588	G2589	G2590	G2591	G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601	G2602	G2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612								
U2485	C2486	G2487	A2488	C2489	G2490	C2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	C2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2552
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A2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	A2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	A2438	A2439	A2440	A2441	A2442	A2443	A2444	A2445	A2446	A2447	A2448	A2449	A2450	A2451	A2452	A2453	A2454	A2455	A2456	A2457	A2458	A2459	A2460	A2461	A2462	A2463	A2464	A2465	A2466	A2467	A2468	A2469	A2470	A2471	A2472	A2473	A2474	A2475	A2476	A2477	A2478	A2479	A2480	A2481	A2482	A2483	A2484	
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U1946	G1947	C1948	A1949	C1950	G1951	A1952	A1953	A1954	G1955	G1956	C1957	C1962	G1963	A1964	U1965	C1966	U1967	G1968	G1969	G1970	C1971	G1972	C1973	U1974	G1975	U1976	C1977	U1978	C1979	A1980	A1981	G1982	G1983	C1984	G1985	G1986	G1987	A1988	C1991	G1992	G1993	U1994	G1995	A1996	A1997	G2001	A2002	U2003	U2004	U2005	G2006	C2007	C2008	U2009	G2010	U2011											
A2012	A2013	A2014	G2015	U2016	U2017	G2018	C2019	G2020	G2021	C2022	G2023	A2024	A2025	C2026	G2029	A2030	A2031	C2032	G2033	A2034	G2035	G2036	A2037	C2038	G2039	A2042	A2043	G2044	A2045	C2046	C2047	C2048	C2049	G2050	U2051	C2052	G2053	A2054	G2055	C2056	U2057	U2058	U2059	A2060	C2061	U2062	A2063	U2064	A2065	G2066	U2067	C2068	U2069	G2070	C2071	G2072	A2073										
U2074	U2075	G2076	G2077	U2080	U2081	C2082	A2083	A2084	G2085	U2086	U2087	U2088	C2089	U2090	U2091	G2092	G2093	C2094	U2095	A2096	A2097	G	A	U	A	G2103	G2104	U2105	G2106	A2109	C2110	C	U	U	G	C	G2117	A2118	G2122	G2123	C2124	C2125	U	U	U	G	G2132	G2133	U2134	G2135	C2136	G2137															
U2138	G2139	G2140	A	G	G	C	A	A	C	G	U	G	A	A	U	A	A	C2157	C2158	A2159	C2162	A2185	G2166	A2167	A2168	C2169	C2170	U2171	U2172	G2173	G2174	A2175	U2176	U2177	U2178	C2179	U2180	A2181	A2182	C2183	C2184	U2185	A2189	A2190	A2191	U2192	C2193	A2194	C2195	U2198	C2199	G2200	G2201	G2202													
G2203	A2204	C2205	G2206	U2207	U2208	G2209	C2210	U2211	U2212	G2213	G2214	C2215	G2216	G2217	A2218	U2219	A2220	G2221	U2224	G2225	A2226	C2227	U2228	G2229	G2230	A2231	G2232	G2233	G2235	U2236	G2237	G2238	C2239	U2240	U2241	C2242	A2245	A2246	A2247	A2248	U2249	G2250	A2251	A2252	A2253	C2254	G2255	G2258	G2261	C2262	C2263	C2264	A2265	A2266	A2267	G2268											
G2269	U2270	C2271	C2272	C2273	C2274	C2275	A2280	C2281	G2282	G2283	U2284	U2285	G2286	G2287	A2288	A2289	A2290	U2291	C2292	G2293	U2294	G2295	G2296	U2297																																											

A2745	G2746	C2747	C2748	A2749	G2750	C2751	C2752	C2753	C2754	A2755	A2756	G2757	A2758	U2759	G2760	A2761	G2762		C2765	U2766	C2767	C2768	C2769	A2770	C2771	U2772	G2773	U2774	U	U	A	U2778	C2779	A2780	G2781	G2782	U2783	A2784	A2785	G2786	A2787	C2788	U2789	C2790	C2791	C2792	G2793	G2794	A2795	A2796	G2797		C2800	A2801		G2805	G2806	U2807	U2808
A2809	A2810	G2811	A2812	G2813		A2817	G2818	G2819	C2820	G2821	U2822	G2823	C2824	A2825	C2826	G2827	C2828	A2829	U2830	A2831		U2836	G2837	U2838	G2839	U2840	U2841	C2842	A2843	G2844	C2845	G2846	G2847	A2848	C2849		G2854		A2858	U2859	C2860	A2861	G2862	U2863	C2864	G2865	A2866	G2867	G2868	U2869	C2870		A2874	C2875	C2876	A2877	C	U	C

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	168.50 Å 404.00 Å 689.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.80)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.368	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59424	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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: RAP

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	2	0.25	0/66467	0.53	13/103673 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	2018	G	C2'-C3'-O3'	6.88	119.82	109.50
1	2	513	A	C2'-C3'-O3'	6.50	123.44	113.70
1	2	192	G	C2'-C3'-O3'	5.40	117.60	109.50
1	2	2245	A	C2'-C3'-O3'	5.39	117.58	109.50
1	2	1154	A	C2'-C3'-O3'	5.38	117.56	109.50

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	2	59359	0	29917	2270	0
2	2	65	0	79	20	0
All	All	59424	0	29996	2270	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 26.

The worst 5 of 2270 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)
1:2:1773:C:H41	2:2:2881:RAP:C15	1.42	1.32
1:2:1773:C:N4	2:2:2881:RAP:H151	1.54	1.20
1:2:700:C:H42	1:2:800:U:H4'	1.11	1.15
1:2:1663:C:H5'	1:2:1664:G:H5''	1.32	1.08
1:2:940:G:H3'	1:2:941:U:H5''	1.36	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	2757/2880 (95%)	529 (19%)	66 (2%)

5 of 529 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	14	A
1	2	35	G
1	2	45	C
1	2	48	A
1	2	49	U

5 of 66 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	2437	G
1	2	2560	G

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Mol	Chain	Res	Type
1	2	2867	G
1	2	1249	G
1	2	1231	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 oligosaccharides 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$
2	RAP	2	2881	-	65,68,68	1.89	14 (21%)	77,96,96	1.47	8 (10%)

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
2	RAP	2	2881	-	-	3/81/124/124	0/3/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2881	RAP	C8-C9	-8.41	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2881	RAP	C40-C39	4.54	1.60	1.52
2	2	2881	RAP	O1-C1	3.94	1.43	1.34
2	2	2881	RAP	O1-C34	-3.37	1.40	1.46
2	2	2881	RAP	C44-C17	3.03	1.56	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2881	RAP	O1-C1-C2	5.29	121.78	110.80
2	2	2881	RAP	C34-O1-C1	4.46	124.60	117.85
2	2	2881	RAP	C9-C8-N7	3.91	123.72	119.25
2	2	2881	RAP	O1-C1-O2	-3.16	118.24	123.95
2	2	2881	RAP	C3-C2-N7	-3.04	106.49	110.55

There are no chirality outliers.

All (3) torsion outliers are listed below:

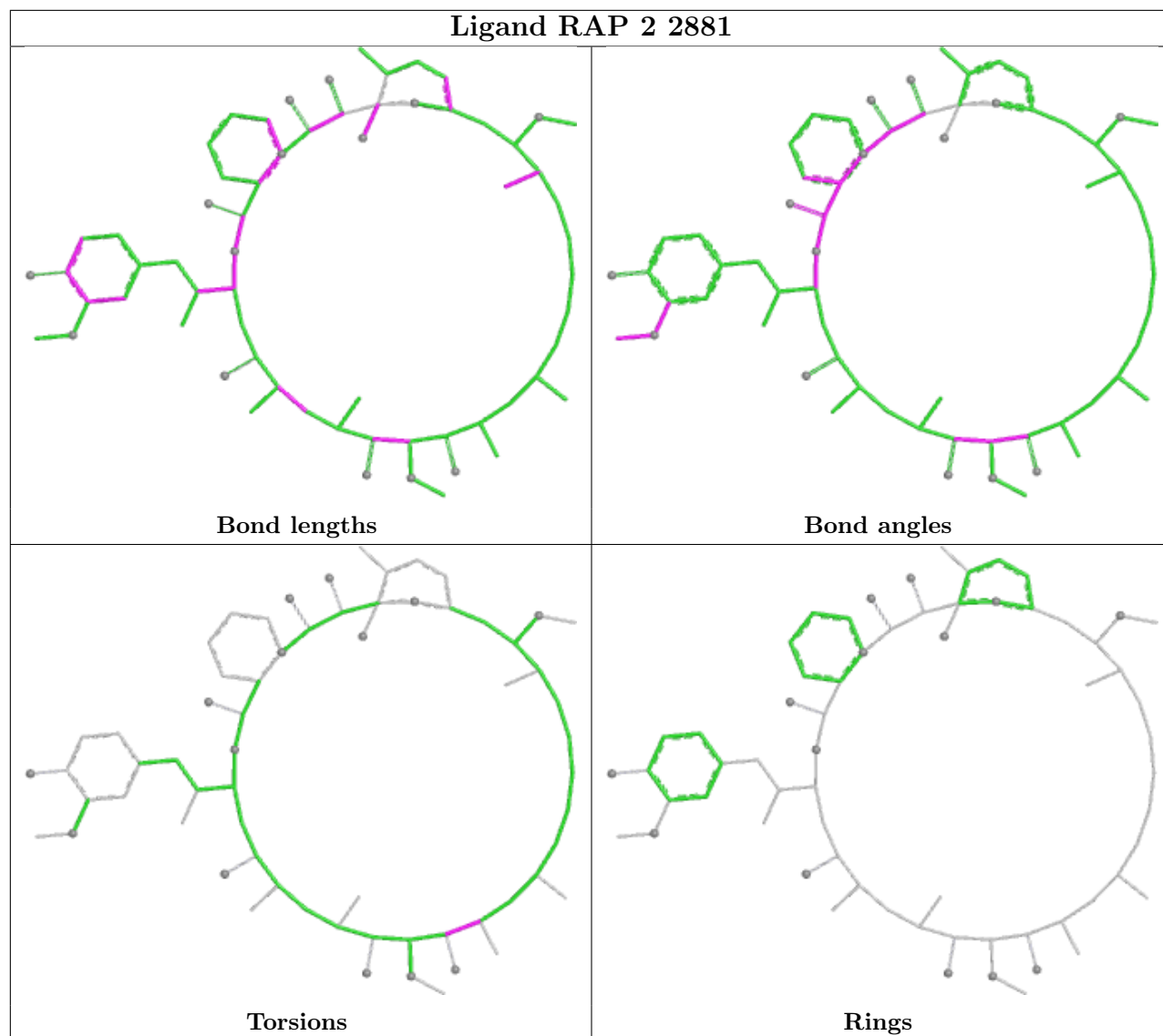
Mol	Chain	Res	Type	Atoms
2	2	2881	RAP	C46-C25-C26-O8
2	2	2881	RAP	C24-C25-C26-O8
2	2	2881	RAP	C24-C25-C26-C27

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	2881	RAP	20	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.