



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 5VZM
BMRB ID : 30300
Title : Solution NMR structure of human Rev1 (932-1039) in complex with ubiquitin
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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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

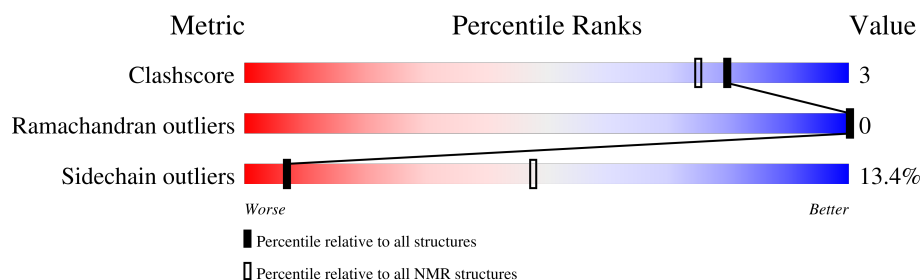
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	A	76	 79% 16% 5%
2	B	111	 15% 82%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:72, B:1015-B:1034 (92)	0.15	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 19
2	4, 17
Single-model clusters	20

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2898 atoms, of which 1455 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	

- Molecule 2 is a protein called DNA repair protein REV1.

Mol	Chain	Residues	Atoms						Trace
2	B	111	Total	C	H	N	O	S	0
			1667	522	826	145	171	3	

There are 3 discrepancies between the modelled and reference sequences:

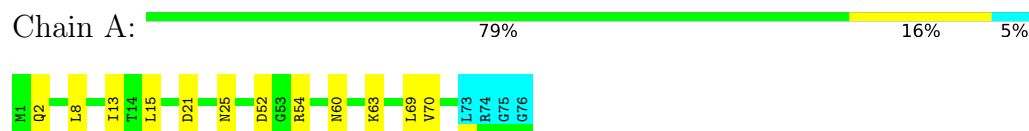
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q9UBZ9
B	-2	HIS	-	expression tag	UNP Q9UBZ9
B	-1	MET	-	expression tag	UNP Q9UBZ9

4 Residue-property plots

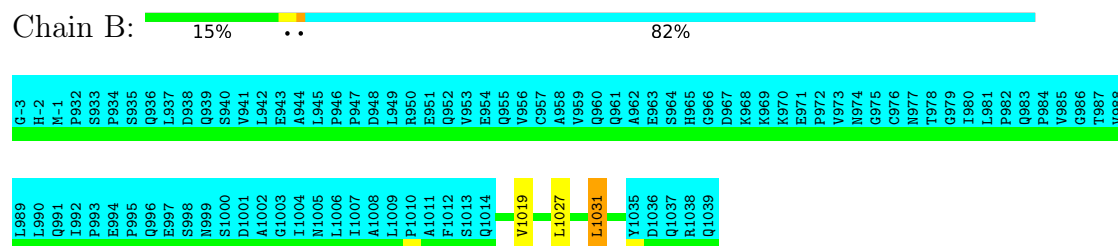
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Ubiquitin



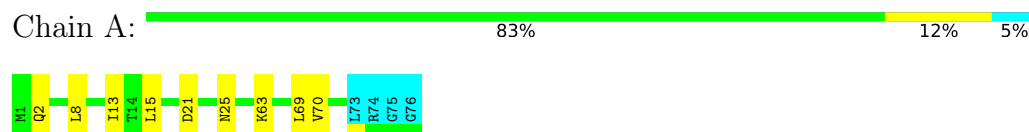
- Molecule 2: DNA repair protein REV1



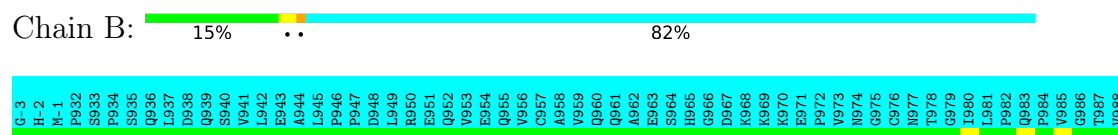
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Ubiquitin



- Molecule 2: DNA repair protein REV1



L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040	L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	L2077	L2078	L2079	L2080	L2081	L2082	L2083	L2084	L2085	L2086	L2087	L2088	L2089	L2090	L2091	L2092	L2093	L2094	L2095	L2096	L2097	L2098	L2099	L2100	L2101	L2102	L2103	L2104	L2105	L2106	L2107	L2108	L2109	L2110	L2111	L2112	L2113	L2114	L2115	L2116	L2117	L2118	L2119	L2120	L2121	L2122	L2123	L2124	L2125	L2126	L2127	L2128	L2129	L2130	L2131	L2132	L2133	L2134	L2135	L2136	L2137	L2138	L2139	L2140	L2141	L2142	L2143	L2144	L2145	L2146	L2147	L2148	L2149	L2150	L2151	L2152	L2153	L2154	L2155	L2156	L2157	L2158	L2159	L2160	L2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	L2261	L2262	L2263	L2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281	L2282	L2283	L2284	L2285	L2286	L2287	L2288	L2289	L2290	L2291	L2292	L2293	L2294	L2295	L2296	L2297	L2298	L2299	L2300	L2301	L2302	L2303	L2304	L2305	L2306	L2307	L2308	L2309	L2310	L2311	L2312	L2313	L2314	L2315	L2316	L2317	L2318	L2319	L2320	L2321	L2322	L2323	L2324	L2325	L2326	L2327	L2328	L2329	L2330	L2331	L2332	L2333	L2334	L2335	L2336	L2337	L2338	L2339	L2340	L2341	L2342	L2343	L2344	L2345	L2346	L2347	L2348	L2349	L2350	L2351	L2352	L2353	L2354	L2355	L2356	L2357	L2358	L2359	L2360	L2361	L2362	L2363	L2364	L2365	L2366	L2367	L2368	L2369	L2370	L2371	L2372	L2373	L2374	L2375	L2376	L2377	L2378	L2379	L2380	L2381	L2382	L2383	L2384	L2385	L2386	L2387	L2388	L2389	L2390	L2391	L2392	L2393	L2394	L2395	L2396	L2397	L2398	L2399	L2400	L2401	L2402	L2403	L2404	L2405	L2406	L2407	L2408	L2409	L2410	L2411	L2412	L2413	L2414	L2415	L2416	L2417	L2418	L2419	L2420	L2421	L2422	L2423	L2424	L2425	L2426	L2427	L2428	L2429	L2430	L2431	L2432	L2433	L2434	L2435	L2436	L2437	L2438	L2439	L2440	L2441	L2442	L2443	L2444	L2445	L2446	L2447	L2448	L2449	L2450	L2451	L2452	L2453	L2454	L2455	L2456	L2457	L2458	L2459	L2460	L2461	L2462	L2463	L2464	L2465	L2466	L2467	L2468	L2469	L2470	L2471	L2472	L2473	L2474	L2475	L2476	L2477	L2478	L2479	L2480	L2481	L2482	L2483	L2484	L2485	L2486	L2487	L2488	L2489	L2490	L2491	L2492	L2493	L2494	L2495	L2496	L2497	L2498	L2499	L2500	L2501	L2502	L2503	L2504	L2505	L2506	L2507	L2508	L2509	L2510	L2511	L2512	L2513	L2514	L2515	L2516	L2517	L2518	L2519	L2520	L2521	L2522	L2523	L2524	L2525	L2526	L2527	L2528	L2529	L2530	L2531	L2532	L2533	L2534	L2535	L2536	L2537	L2538	L2539	L2540	L2541	L2542	L2543	L2544	L2545	L2546	L2547	L2548	L2549	L2550	L2551	L2552	L2553	L2554	L2555	L2556	L2557	L2558	L2559	L2560	L2561	L2562	L2563	L2564	L2565	L2566	L2567	L2568	L2569	L2570	L2571	L2572	L2573	L2574	L2575	L2576	L2577	L2578	L2579	L2580	L2581	L2582	L2583	L2584	L2585	L2586	L2587	L2588	L2589	L2590	L2591	L2592	L2593	L2594	L2595	L2596	L2597	L2598	L2599	L2600	L2601	L2602	L2603	L2604	L2605	L2606	L2607	L2608	L2609	L2610	L2611	L2612	L2613	L2614	L2615	L2616	L2617	L2618	L2619	L2620	L2621	L2622	L2623	L2624	L2625	L2626	L2627	L2628	L2629	L2630	L2631	L2632	L2633	L2634	L2635	L2636	L2637	L2638	L2639	L2640	L2641	L2642	L2643	L2644	L2645	L2646	L2647	L2648	L2649	L2650	L2651	L2652	L2653	L2654	L2655	L2656	L2657	L2658	L2659	L2660	L2661	L2662	L2663	L2664	L2665	L2666	L2667	L2668	L2669	L2670	L2671	L2672	L2673	L2674	L2675	L2676	L2677	L2678	L2679	L2680	L2681	L2682	L2683	L2684	L2685	L2686	L2687	L2688	L2689	L2690	L2691	L2692	L2693	L2694	L2695	L2696	L2697	L2698	L2699	L2700	L2701	L2702	L2703	L2704	L2705	L2706	L2707	L2708	L2709	L2710	L2711	L2712	L2713	L2714	L2715	L2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	L2749	L2750	L2751	L2752	L2753	L2754	L2755	L2756	L2757	L2758	L2759	L2760	L2761	L2762	L2763	L2764	L2765	L2766	L2767	L2768	L2769	L2770	L2771	L2772	L2773	L2774	L2775	L2776	L2777	L2778	L2779	L2780	L2781	L2782	L2783	L2784	L2785	L2786	L2787	L2788	L2789	L2790	L2791	L2792	L2793	L2794	L2795	L2796	L2797	L2798	L2799	L2800	L2801	L2802	L2803	L2804	L2805	L2806	L2807	L2808	L2809	L2810	L2811	L2812	L2813	L2814	L2815	L2816	L2817	L2818	L2819	L2820	L2821	L2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5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	
Amber	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2268
Number of shifts mapped to atoms	2268
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality

6.1 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 (average) 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	0.57±0.00	0±0/581 (0.0± 0.0%)	1.03±0.02	1±0/784 (0.1± 0.1%)
2	B	0.61±0.01	0±0/155 (0.0± 0.0%)	1.00±0.03	0±0/212 (0.0± 0.1%)
All	All	0.58	0/14720 (0.0%)	1.03	13/19920 (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	Planarity
1	A	0.0±0.0	0.1±0.4
All	All	0	3

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ARG	NE-CZ-NH1	-6.48	117.06	120.30	15	4
1	A	54	ARG	NE-CZ-NH2	-6.39	117.10	120.30	11	8
2	B	1031	LEU	CB-CA-C	5.08	119.85	110.20	1	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	42	ARG	Sidechain	3

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	574	599	599	4±1
2	B	152	155	155	2±1
All	All	14520	15080	15080	79

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 3.

5 of 9 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:1023:LEU:HD22	2:B:1024:PRO:HD2	0.71	1.62	16	3
2:B:1023:LEU:HD21	2:B:1027:LEU:HD12	0.56	1.76	16	2
1:A:8:LEU:HD11	2:B:1031:LEU:HD21	0.55	1.77	8	18
1:A:70:VAL:HG21	2:B:1027:LEU:CD1	0.51	2.35	16	16
1:A:8:LEU:HD21	1:A:70:VAL:HG22	0.48	1.86	9	13

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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	
1	A	71/76 (93%)	68±0 (96±0%)	3±0 (4±0%)	0±0 (0±0%)	100	100
2	B	20/111 (18%)	20±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1820/3740 (49%)	1760 (97%)	60 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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 NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/68 (97%)	57±1 (87±2%)	9±1 (13±2%)	7	48
2	B	15/94 (16%)	13±1 (86±4%)	2±1 (14±4%)	6	46
All	All	1620/3240 (50%)	1403 (87%)	217 (13%)	7	48

5 of 24 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	2	GLN	20
1	A	13	ILE	20
1	A	15	LEU	20
1	A	69	LEU	20
2	B	1019	VAL	20

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Ub-Rev1_Complex_31.str*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2268
Number of shifts mapped to atoms	2268
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	183	-0.27 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	172	0.25 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	176	-0.29 ± 0.11	None needed (< 0.5 ppm)
^{15}N	165	-0.11 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1205 atoms were assigned a chemical shift out of a possible 1290. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	443/454 (98%)	180/183 (98%)	179/184 (97%)	84/87 (97%)
Sidechain	722/790 (91%)	491/512 (96%)	221/249 (89%)	10/29 (34%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	40/46 (87%)	20/23 (87%)	20/22 (91%)	0/1 (0%)
Overall	1205/1290 (93%)	691/718 (96%)	420/455 (92%)	94/117 (80%)

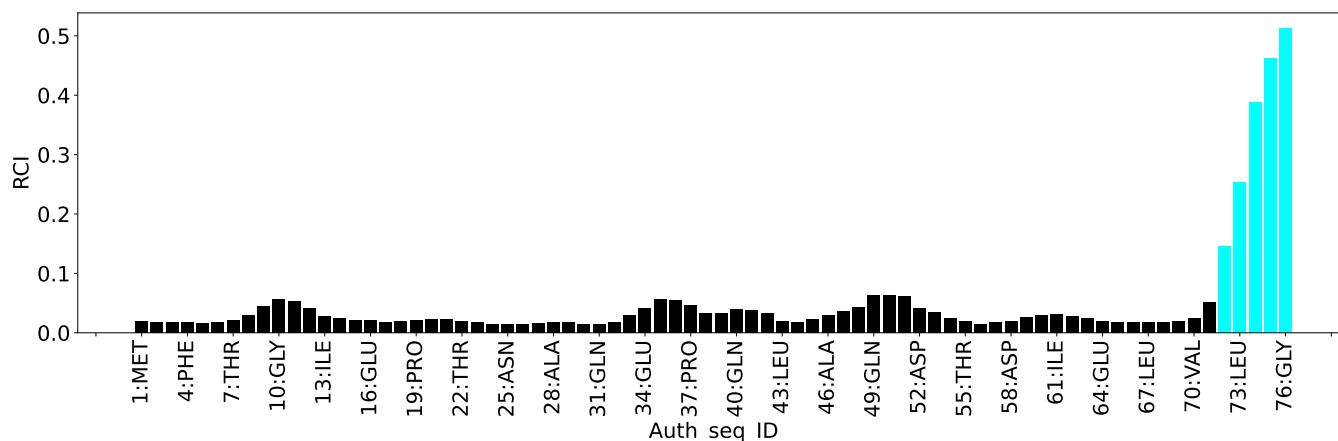
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

