



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 08:48 pm GMT

PDB ID : 8RRU  
EMDB ID : EMD-19465  
Title : Structure of RyR1 reconstituted into lipid liposomes in primed state in complex with FKBP and Nb9657.  
Authors : Li, C.; Efremov, R.G.  
Deposited on : 2024-01-23  
Resolution : 4.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

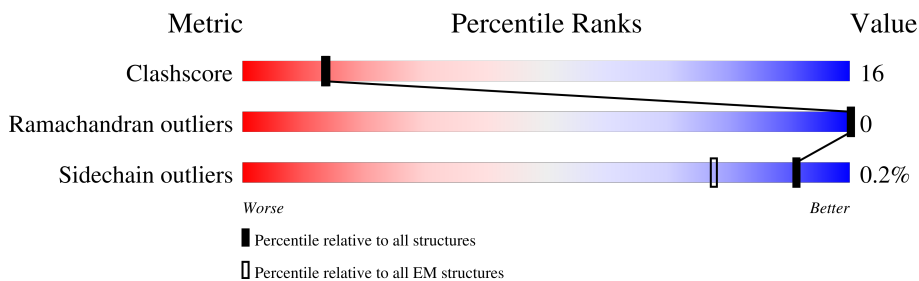
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.70 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.






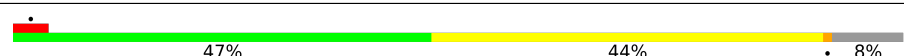
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	107	72% 28%
1	D	107	70% 30%
1	H	107	72% 28%
1	I	107	70% 30%
2	B	5027	57% 29% 14%
2	E	5027	57% 29% 14%
2	G	5027	57% 29% 14%
2	J	5027	57% 29% 14%

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Mol	Chain	Length	Quality of chain
3	C	137	 48% 43% 8%
3	F	137	 46% 45% 8%
3	K	137	 47% 44% 8%
3	M	137	 47% 44% 8%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 143907 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	107	818	516	144	154	4	0	0
1	D	107	818	516	144	154	4	0	0
1	H	107	818	516	144	154	4	0	0
1	I	107	818	516	144	154	4	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	GLY	conflict	UNP Q8HYX6
D	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	4319	34143	21748	5888	6283	224	1	0
2	E	4319	34143	21748	5888	6283	224	1	0
2	G	4319	34150	21752	5888	6285	225	1	0
2	J	4319	34143	21748	5888	6283	224	1	0

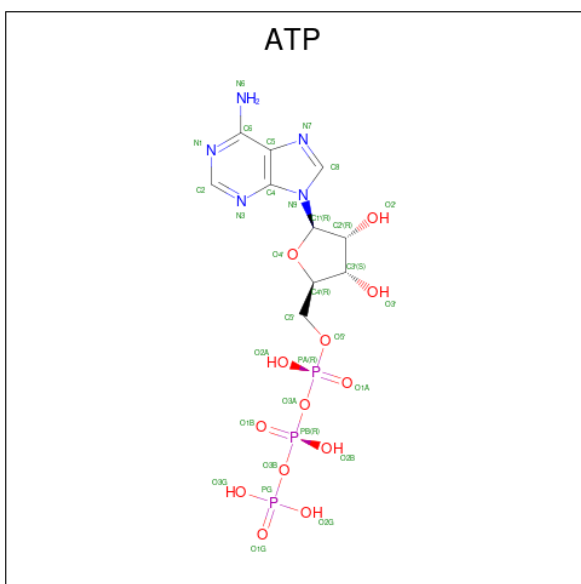
- Molecule 3 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	F	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	M	126	Total	C	N	O	S	0	0
			967	597	170	195	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	
4	J	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



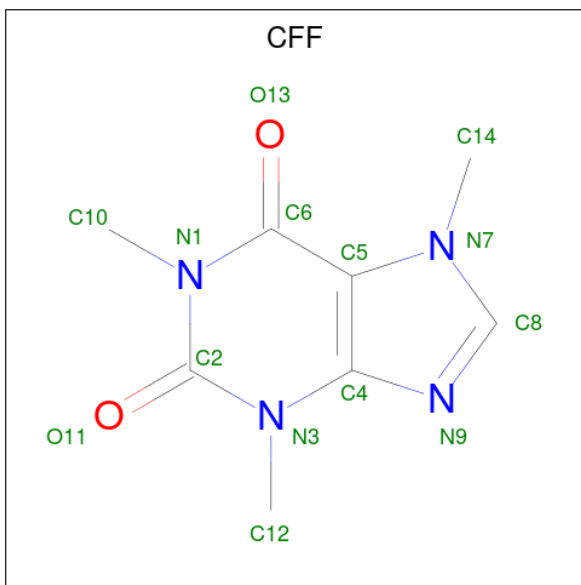
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
5	E	1	Total 31	C 10	N 5	O 13	P 3	0
5	G	1	Total 31	C 10	N 5	O 13	P 3	0
5	J	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula:  $C_8H_{10}N_4O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	Total 14	C 8	N 4	O 2	0
6	E	1	Total 14	C 8	N 4	O 2	0
6	G	1	Total 14	C 8	N 4	O 2	0
6	J	1	Total 14	C 8	N 4	O 2	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
7	B	1	Total 1	Ca 1	0

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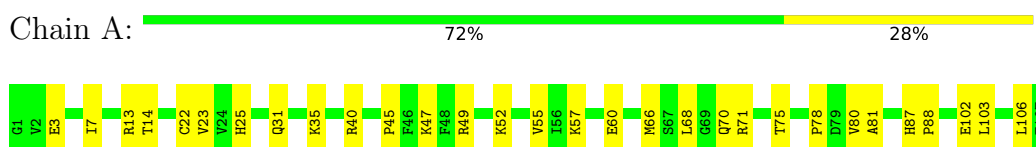
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
7	E	1	Total 1	Ca 1	0
7	G	1	Total 1	Ca 1	0
7	J	1	Total 1	Ca 1	0

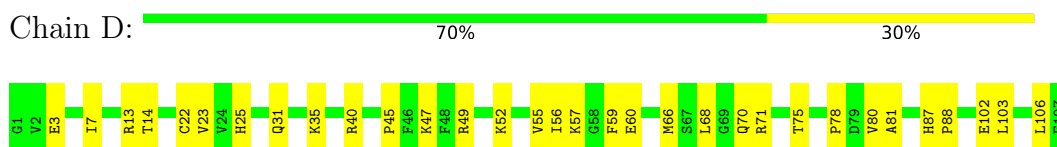
### 3 Residue-property plots [i](#)

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

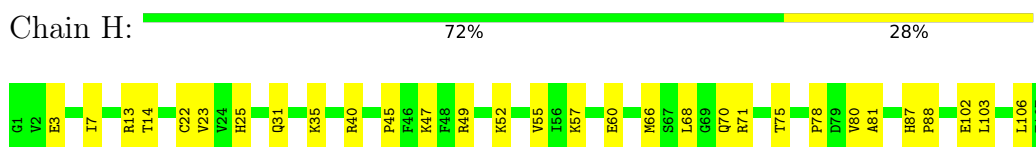
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



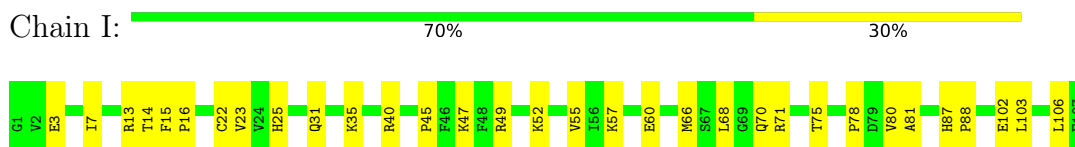
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



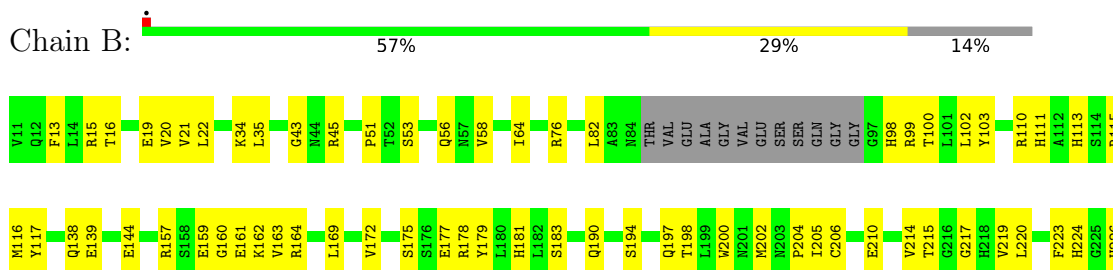
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1

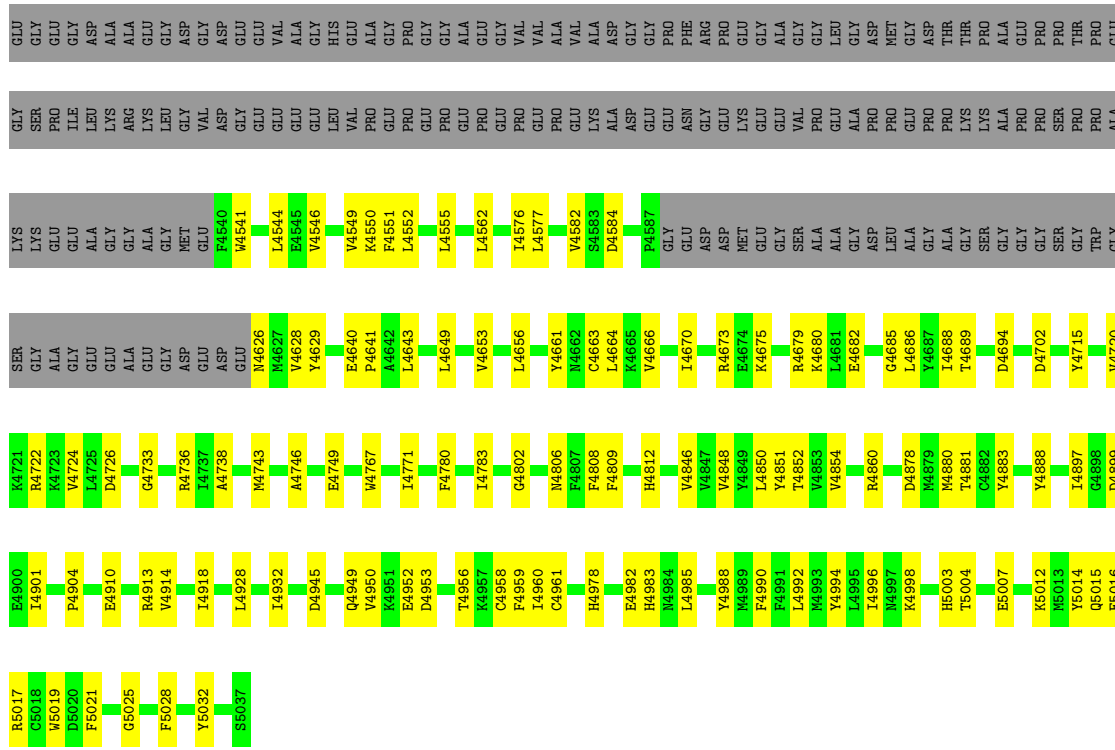




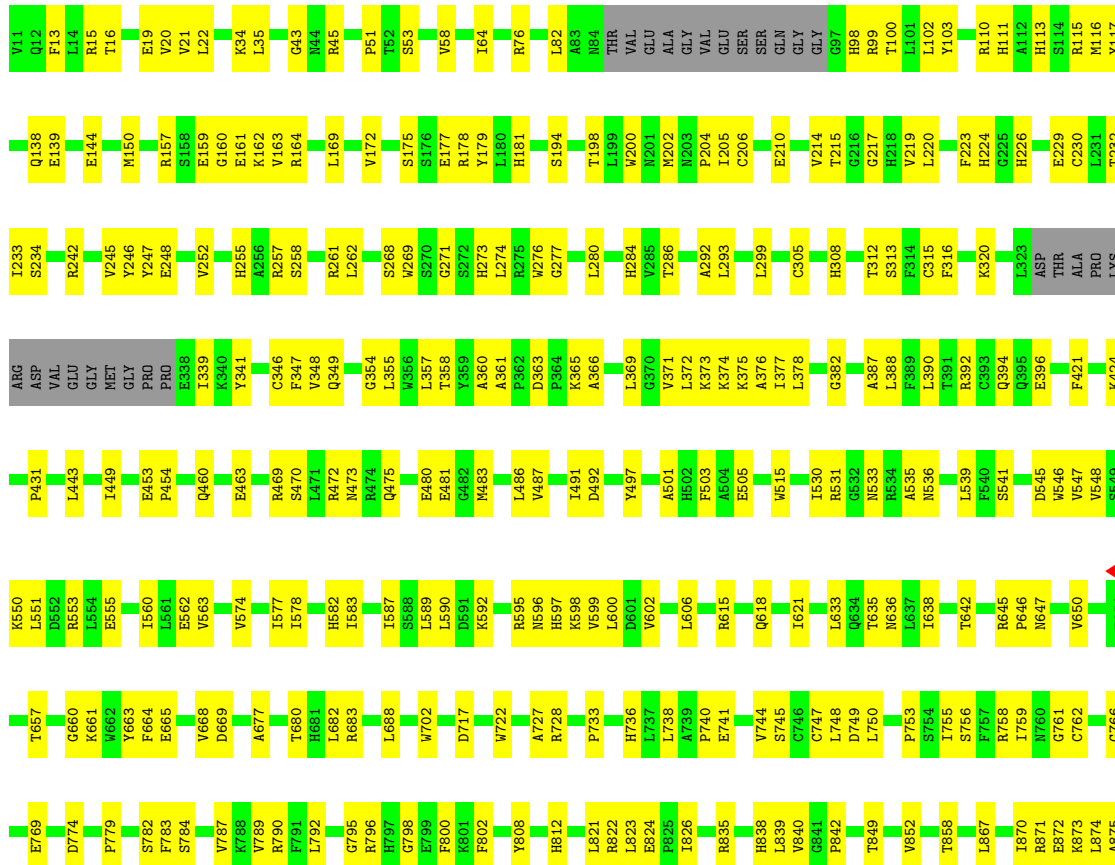
L1595	W1496	THR	ALA	L1272	I1161	M1065	R976	R871	G761	W546	E396
L1599	G1497	PRO	GLU	A1273	F1162	Q1066	L977	E872	C762	V547	E96
M1599	G1498	ALA	GLY	H1274	T1163	S1067	T978	K873	G766	V548	F421
P1609	D1499	LEU	GLY	L1287	L1164	R1068	T979	L874	G766	S549	L231
F1612	F1500	PRO	LYS	F1288	V1168	W1069	P979	A875	E769	K550	K424
V1615	S1502	LEU	GLY	L1288	V1171	R1070	Q981	E876	M877	L551	T232
V1616	P1503	PRO	THR	R1290	S1171	V1072	Q981	M877	D774	D552	S234
T1617	G1504	HIS	ALA	L1291	S1175	R1073	L984	I878	P779	R553	R242
R1618	GLN	ASP	ASP	L1292	E1176	F1075	Y985	G886	F778	L554	R242
R1619	VAL	VAL	GLY	L1293	T1177	R1076	H993	R886	W780	E555	V245
A1620	R1508	PRO	THR	P1294	A1178	A1077	H993	I887	V781	F664	Y246
G1621	L1514	ALA	PRO	F1297	F1179	E1078	R1000	W891	S782	E665	Y247
G1622	GLN	GLY	GLY	H1298	F1180	Y1081	W1005	T892	F783	V666	E248
R1623	E1616	THR	THR	Q1299	E1181	S1082	W1006	R893	S783	M667	V252
L1624	T1617	PRO	ALA	R1302	T1182	V1083	S1006	G894	W787	V668	K340
G1625	G1508	PRO	GLN	C1303	F1188	G1086	Y1007	R897	V789	D669	Y341
W1626	P1509	LEU	ALA	T1304	R1189	R1087	S1008	K901	R790	A677	H255
A1627	M1527	VAL	VAL	ALA	G1190	R1087	I1013	R902	L792	I577	A256
M1637	M1536	ALA	ALA	THR	C1191	F1092	R1016	L903	G795	I578	R257
L1639	K1547	PRO	PRO	PRO	P1196	V1095	R1017	H904	G795	H582	S288
H1640	L1548	VAL	VAL	ALA	V1199	M1100	R1018	P905	H797	I587	R261
I1641	L1549	ARG	ALA	GLY	G1200	R1101	R1018	G966	G798	S888	L262
P1642	F1549	GLU	GLY	THR	C1192	F1092	R1018	L907	F799	L589	S288
E1643	P1550	LEU	GLY	PRO	C1192	F1092	R1018	H911	F800	L590	W269
E1644	A1551	ASN	ASN	LEU	P1196	V1095	R1018	H911	F800	D591	L357
H1645	V1552	GLU	GLN	GLN	S1210	A1105	L1026	L913	F802	M482	G277
R1646	F1553	LYS	PRO	PRO	F1223	G1116	K1032	E917	Y808	L486	L260
C1647	L1554	ASP	PRO	PRO	A1227	G1116	K1032	L922	H812	V487	H284
M1648	P1556	THR	ALA	ALA	V1234	V1123	R1036	L929	L821	I491	V285
E1652	Q1559	GLU	GLY	GLU	W1237	M1125	R1036	K930	R822	K598	T286
L1653	W1560	LYS	LYS	ALA	Q1244	G1129	Q1041	T931	L823	H502	L371
R1656	V1561	ASN	ASN	ALA	F1245	Q1130	A1042	L932	E824	F503	L286
Q1660	I1562	LYS	ARG	ALA	F1246	Q1131	R1044	L933	I826	A594	A292
R1661	E1565	ARG	ALA	ALA	P1247	R1131	L1046	A934	R835	E505	L293
F1662	K1568	PHE	PHE	ASP	P1247	W1132	G1048	C937	W744	W515	L299
H1663	Q1569	LEU	PHE	PRO	V1248	H1133	Y1049	H938	S745	A376	C305
S1664	M1570	LEU	LEU	ASP	P1249	G1133	G1050	V939	C746	I377	H308
Y1670	M1571	LYS	LYS	TYR	H1252	P1138	Y1051	G940	G747	I530	T312
A1672	I1572	ALA	ALA	ASN	H1252	H1138	Y1052	E947	L748	G531	S313
V1673	M1573	LYS	LYS	LEU	E1256	D1147	E1054	L950	D749	G532	C315
L1676	P1574	ALA	ALA	ARG	V1257	M1152	F1054	K951	L750	M533	F316
L1677	A1578	ALA	ALA	ARG	V1257	I1152	F1056	K951	T849	M533	F316
L1678	M1579	ALA	ALA	ARG	M1260	D1154	ASP	P753	S754	M536	F316
L1680	M1579	ALA	ALA	SER	D1261	L1155	GLN	Y859	V852	L638	F316
H1683	F1580	THR	GLY	GLY	P1268	T1156	GLU	T858	T858	T642	F316
L1694	R1584	PRO	GLN	GLY	C1269	E1157	PRO	P969	F757	F580	K320
		PRO	PRO	TRP	L1270	M1158	SER	L970	R758	S541	Q393
		ALA	ALA	GLU	R1271	I1160	VAL	D971	I759	P646	Q393
				GLU			GLU	L972	I870	N647	L323

L2894	H2902	L2905	V2906	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	R2920	Q2924	K2928	F2929	Y2935	R2939	GLY	LEU	LYS	PRO	ARG	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	V2855	N2856	F2857	Q2858	F2859	P2860	S2863	Q2864	L2867	S2868	R2869	E2870	L2871	L2878	A2879	E2880	N2881	I2869	S2970	Q2971	E2972	F2973	I2974	A2975	H2976																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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D2752	S2753	F2754	I2755	K2756	K2757	F2758	A2759	W2766	D2684	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	W2774	W2775	S2776	Y2777	G2778	E2779	N2780	W2781	D2782	E2783	K2786	T2787	H2788	P2789	W2790	L2791	R2792	F2793	Y2794	K2795	I2796	F2797	S2798	E2799	K2800	R2801	K2802	E2803	R2806	I2809	K2810	L2813	K2814	A2815	W2819	E2820	W2821																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
L2672	R2676	K2677	L2678	F2679	W2680	G2681	D2684	S2685	H2688	Y2691	E2694	L2695	Y2696	M2698	A2699	M2700	P2701	C2702	L2706	A2709	L2710	P2711	Y2714	W2715	E2724	K2725	LYS	THR	VAL	ASP	ALA	GLU	GLY	N2734	P2737	R2738	P2739	V2740	W2745	L2746	P2748	E2749	K2750	L2751																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
L2453	R2454	A2455	I2456	L2457	R2458	S2459	L2460	G2468	I2469	L2470	S2471	L2472	P2473	L2474	P2477	T2478	L2479	D2482	L2485	K2489	A2492	S2493	F2494	V2495	P2496	D2497	H2498	K2499	S2501	M2502	R2508	V2509	Y2510	G2511	L2512	L2518	L2522	G2525	F2526	L2527	T2528	R2531	L2536	D2537	T2538	F2541																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
S2542	F2543	T2544	E2545	M2546	L2550	L2554	C2555	L2559	T2563	I2577	M2578	M2582	T2585	R2588	G2592	L2595	Q2599	R2600	L2603	E2604	C2611	L2619	Q2620	H2621	L2623	R2624	L2625	L2626	V2627	M2639	P2640	L2641	K2642	L2643	T2645	R2650	Y2655	S2668	E2669																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
A2367	L2368	G2374	S2375	L2376	L2377	I2380	E2381	L2382	A2383	L2384	R2385	F2395	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	L2307	L2313	L2314	THR	LYS	GLU	I2223	T2230	R2234	Y2238	I2242	Q2245	N2246	Q2247	F2251	L2254	S2255	Y2256	L2258	L2259	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	K2297	V2298	V2299	V2212	R2213	R2214	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





● Molecule 2: Ryanodine receptor 1



V2214	H2125	V1841	M1730	G1621	R1508	ASP	LYS	R1290	D1070	L984	E876
L2215	R2126	L1849	L1731	E1622	L1514	VAL	GLY	L1291	R1071	V985	M877
G2216	Q2127	V1850	S1732	R1623	L1514	VAL	GLY	S1292	V1072	L878	H879
GLY	Y2128	L1850	E1733	L1624	C1518	PRO	THR	L1293	R1073	H993	H879
GLY	GLY	M1851	Y1734	G1625	C1518	ALA	PRO	P1294	F1074	W996	R886
THR	L2134	G1852	I1735	W1626	L1519	ASP	GLY	F1297	F1075	R1000	I887
LYS	L2136	I1853	P1740	A1627	L1522	M1420	THR	H1298	R1076	R1000	W891
ARG	R2136	F1854	R1743	M1637	A1523	R1421	PRO	Q1299	Al077	W1005	T892
LEU	A2137	D1858	R1743	A1638	A1523	D1422	PRO	H1299	Al078	W1006	Y893
ARG	L2138	L1862	P1749	L1639	M1527	D1423	GLN	T1304	Y1081	Y1007	Y893
SER	P2139	I1862	P1749	L1639	M1527	E1425	PRO	T1304	T1082	S1008	G894
LEU	R2140	M1865	R1758	H1640	K1547	I1426	VAL	ALA	M1083		
LEU	R2144	I1866	R1759	I1641	L1548		GLY	ALA			
THR	V2149	F1871	F1549	E1644	L1548	T1431	ALA	THR	I1013		
VAL	V2149	F1871	F1550	M1645	P1550	T1432	GLN	ALA	G1086	K901	R902
LEU	T2152	F1945	A1551	R1646	V1552	T1433	ALA	PRO	R1016	R903	L903
VAL	Q2245	F1946	V1552	C1647	F1553	Y1434	VAL	ALA	R1017	H904	H904
LYS	R2246	E1874	F1554	M1648	V1554	Y1435	ARG	PRO	M1018	P905	P905
LYS	Q2247	E1874	L1555	E1652	V1556		ALA	GLY	L1021	C906	C906
GLY	R2251	E1877	P1556	L1653	P1556	V1439	ASN	LEU	P1022	L907	L907
GLY	V2168	H1776	H1776	R1656	Q1559	Q1443	GLY	GLN	P1023	H911	H911
PRO	Q2173	V1783	V1783	R1661	Q1559	C1447	LYS	PRO	L1026	S912	S912
GLY	E2174	L1786	L1786	F1662	V1561	V1448	ALA	PRO	L1027	L913	L913
GLY	E2175	ALA	ALA	H1663	I1562	V1449	THR	ALA	K1032	E917	E917
LEU	S2176	GLY	GLY	S1664	E1565	W1450	THR	ASP	R1036	L929	L929
PRO	N2176	VAL	VAL	H1665	Q1568	W1452	LYS	ALA		K930	K930
ALA	L2177	GLY	VAL	Y1670	Q1568	T1484	LYS	ALA	Q1041	T931	T931
GLY	M2179	GLY	ALA	R1671	L1570	P1485	LYS	ALA	Al042	L932	L932
GLY	L2179	GLY	E1793	R1672	I1572	M1462	ARG	GLY	V1043	L932	L932
GLY	Q2180	GLY	M1571	V1673	I1572		GLY	PRO	R1044	A934	A934
S2181	L2182	ASP	M1573	L1676	P1574	M1476	PHE	ASP	Q1130	C937	C937
ALA	M2185	GLY	M1574	L1676	L1575	G1477	LYS	TYR	L1046	H938	H938
GLY	M2186	GLY	L1575	R1680	L1575	D1478	LYS	GLY	L1047	V939	V939
GLY	K2189	GLY	A1578	L1694	A1578	M1482	ALA	GLY	G1048	G940	G940
Y2182	M2196	GLY	M1579	L1694	F1580	V1483	LYS	LEU	Y1049	Y1051	Y1051
M2196	L2197	GLY	F1580	L1698	R1584	H1484	LYS	LEU	N1052	E947	E947
L2198	R2199	GLY	R1584	L1703	R1584	S1485	ALA	ARG	L1053	L950	L950
A2200	L2201	GLY	R1594	P1704	R1594	C1489	MET	SER	E1054	K951	K951
L2201	G2202	ASP	R1594	Y1711	L1596	M1494	MET	GLY	P1056	Y959	Y959
G2202	H2203	ALA	L1815	D1713	L1596	M1495	THR	GLY	P1056	P969	P969
H2204	M2208	GLY	G1816	L1714	Q1598	W1496	PRO	GLY	ASP	L970	L970
M2208	Q2291	GLY	R1827	L1715	P1609	W1496	ALA	GLY	GLN	D971	D971
V2298	E2292	GLY	D1828	F1612	F1612	G1497	ALA	GLY	GLN	L972	L972
V2299	Q2293	GLY	V1830	E1616	F1612	G1498	ALA	GLY	VAL	R976	R976
A2303	R2297	GLY	E1835	E1616	E1616	V1501	LEU	LYS	GLU	L977	L977
	V2298	GLY	Q1837	F1616	E1616	S1502	PRO	ARG	M1065	T978	T978
	V2299	GLY	Q1837	F1616	E1616	P1504	ARG	GLY	Q1066	P979	P979
	A2303	PRO	F1838	R1618	T1617	G1504	LEU	GLY	S1068	A980	A980
		ALA	V1839	R1618	T1617	GLN	PRO	THR	L1068	Q981	Q981
		ALA	P1840	R1727	A1620	GLY	ALA	ALA	W1069		





● Molecule 2: Ryanodine receptor 1

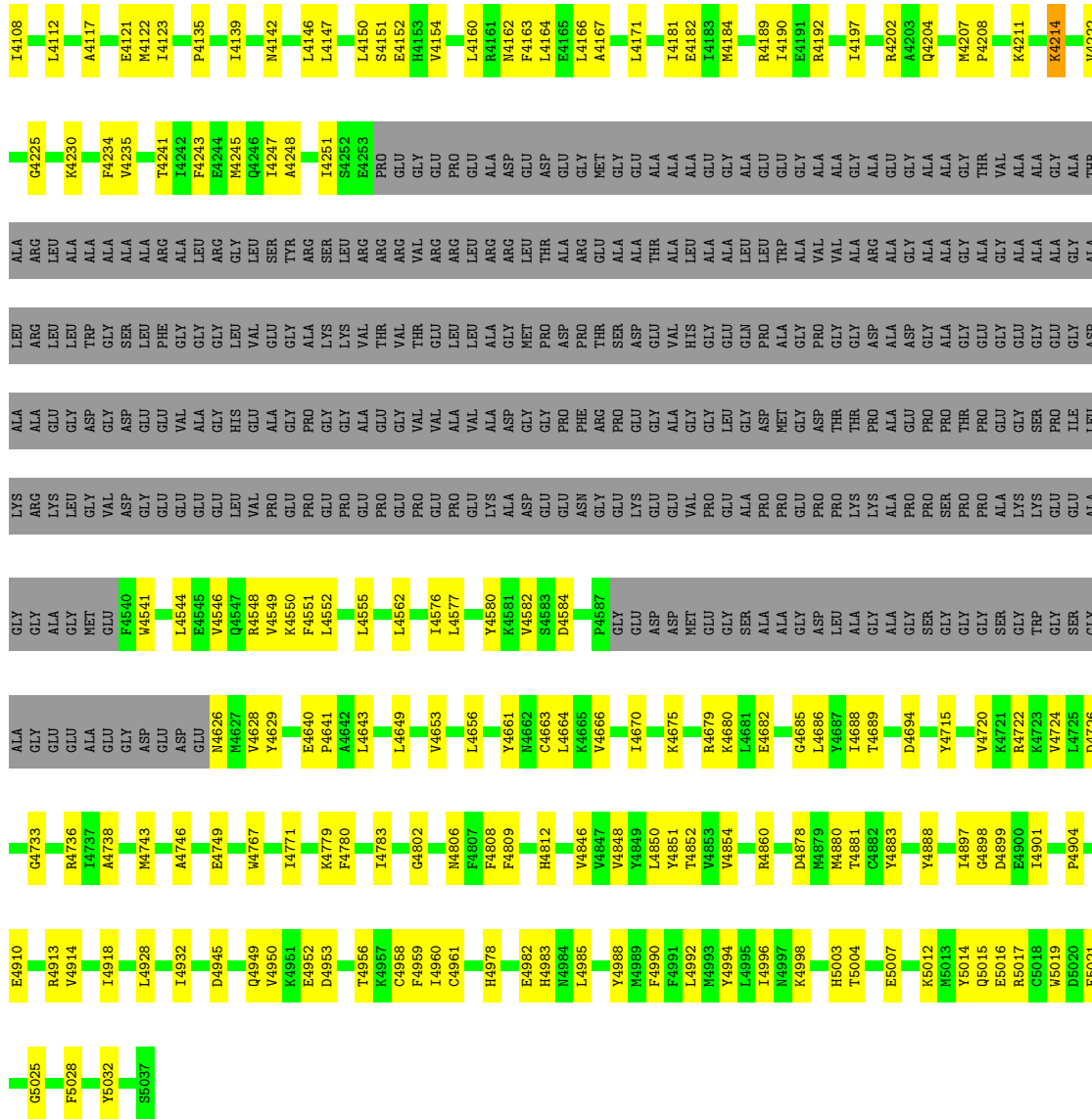


Table listing amino acid residues for Chain G, including residue numbers, amino acid abbreviations, and their corresponding colors (green, yellow, grey).

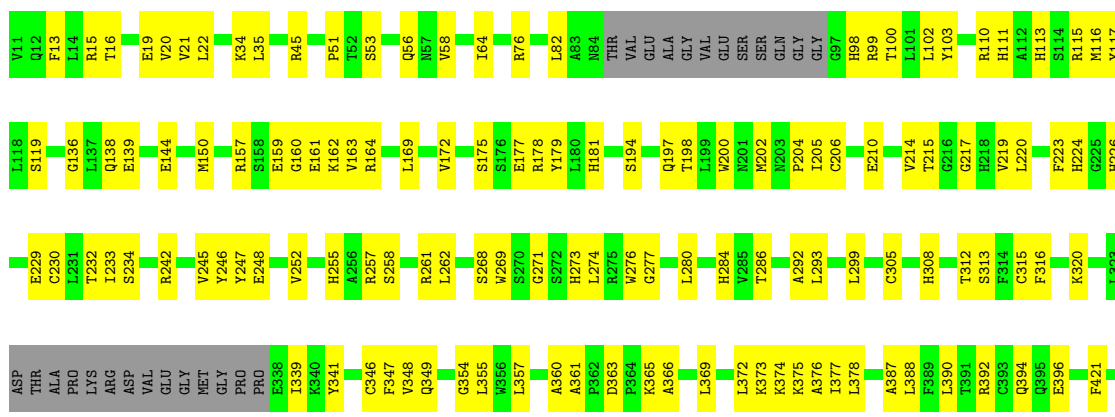


S2685	L2554	L2376	Y2192	Q2107	Q2036	GLU	K1810	L1703	M1599	F1500	ALA
H2688	C2555	L2377	Q2193	E2108	L2039	GLU	M1814	P1704	P1609	V1501	LEU
Y2691	L2559	I2380	N2196	D2109	A2040	GLU	L1815	R1708	F1612	S1502	PRO
E2694	L2469	E2381	L2197	Y2110	A2045	GLU	G1816	R1709	F1616	P1503	ARG
L2696	L2470	E2382	N2198	Q2112	LEU	LYS	R1827	Y1711	V1615	GLN	PRO
L2697	S2471	A2383	R2199	S2113	GLY	ASP	D1828	Y1712	E1616	GLY	HIS
L2698	L2472	A2384	A2200	S2114	ALA	ALA	P1829	D1713	T1617	GLY	ASP
A2699	P2473	R2385	G2202	E2115	GLU	GLU	L1830	L1714	R1618	VAL	VAL
F2700	P2395	P2395	M2202	E2116	GLU	LYS	V1830	L1715	R1619	PRO	PRO
C2702	G2477	VAL	H2204	V2117	GLU	GLU	E1835	I1718	A1620	ALA	ALA
I2706	ARG	ARG	M2208	F2121	PRO	PRO	F1836	H1719	G1621	ASP	ASP
A2709	ARG	ARG	M2211	S2122	GLU	GLU	Q1837	H1720	E1622	M1420	M1420
L2710	ASP	ASP	L2123	L2123	GLU	GLU	F1838	R1727	R1623	R1421	R1421
L2711	ARG	ARG	L2124	L2124	GLU	ALA	V1839	M1730	L1624	D1422	D1422
Y2714	ARG	ARG	H2125	H2125	GLU	PRO	G1840	M1731	G1625	D1423	D1423
V2715	ARG	ARG	N2213	R2126	THR	GLU	V1841	L1731	V1626	P1424	P1424
E2724	GLU	GLU	V2214	Q2127	SER	GLY	F1854	S1732	A1627	E1425	E1425
K2725	HIS	THR	L2215	Y2128	LEU	GLU	L1849	E1733	M1637	I1426	I1426
L2623	PHI	GLY	G2216	E2133	SER	LYS	Y1850	Y1734	A1638	V1431	V1431
L2624	GLY	GLY	L2307	L2133	ARG	ASP	M1851	I1735	L1639	T1432	T1432
R2625	GLU	GLU	L2313	R2135	LEU	GLU	I1852	P1740	G1640	Y1433	Y1433
R2626	GLU	THR	L2314	L2136	LEU	GLU	F1854	R1743	I1641	Y1434	Y1434
R2627	PRO	LYS	Y2318	A2137	SER	SER	L1862	E1643	P1642	Y1435	Y1435
R2628	PRO	GLU	L2321	L2138	LEU	LEU	D1868	Y1749	E1644	V1439	V1439
R2629	GLU	L2223	P2139	R2140	LEU	LEU	I1862	R1758	E1645	V1440	V1440
R2630	GLU	T2230	Q2234	T2144	THR	THR	M1865	R1759	C1647	Q1443	Q1443
R2631	GLU	R2234	L2144	V2149	VAL	VAL	I1866	P1763	M1648	C1447	C1447
R2632	GLU	Y2238	Y2149	V2152	ARG	ARG	E1874	E1652	E1652	V1448	V1448
R2633	GLU	L2242	T2152	T2152	VAL	VAL	GLU	L1771	M1653	Y1449	Y1449
R2634	GLU	Q2245	L2156	L2156	LYS	LYS	GLU	R1772	M1656	G1451	G1451
R2635	GLU	Q2246	E2157	E2157	GLU	GLU	GLU	P1773	R1666	M1452	M1452
R2636	GLU	Q2247	R2163	R2163	GLU	GLU	GLU	H1776	F1662	Y1453	Y1453
R2637	GLU	F2251	V2168	V2168	PRO	PRO	GLU	V1783	F1662	T1454	T1454
R2638	GLU	L2254	Q2173	Q2173	GLU	GLU	GLU	L1786	S1664	M1462	M1462
R2639	GLU	S2255	E2174	E2174	LEU	LEU	GLU	P1787	H1665	Q1569	Q1569
R2640	GLU	Y2256	M2175	M2175	PRO	PRO	GLU	ALA	T1666	M1570	M1570
R2641	GLU	L2257	N2176	N2176	ALA	ALA	GLU	ALA	Y1670	G1477	G1477
R2642	GLU	L2258	M2177	M2177	GLU	GLU	GLU	GLY	R1671	D1478	D1478
R2643	GLU	L2259	M2178	M2178	GLU	GLU	GLU	VAL	A1672	M1482	M1482
R2644	GLU	S2261	L2179	L2179	GLU	GLU	GLU	ALA	V1673	V1483	V1483
R2645	GLU	G2262	Q2180	Q2180	K2089	K2089	GLU	E1793	L1676	H1484	H1484
R2646	GLU	L2263	I2182	I2182	L2094	L2094	GLU	R1797	M1678	S1485	S1485
R2647	GLU	G2264	G2264	G2264	Q2095	Q2095	GLU	L1798	R1680	C1489	C1489
R2648	GLU	L2265	M2184	M2184	E2096	E2096	GLU	S1799	F1580	F1580	F1580
R2649	GLU	M2267	M2185	M2185	H2100	H2100	GLU	P1800	R1584	R1584	R1584
R2650	GLU	Q2268	M2186	M2186	H2101	H2101	LYS	P1804	H1683	M1494	M1494
R2651	GLU	P2272	K2189	K2189	H2104	H2104	GLU	L1804	L1694	Y1496	Y1496
R2652	GLU	L2273	G2375	G2375	R2104	R2104	GLU	R1808	L1698	G1497	G1497
R2653	GLU	L2274	L2273	L2273	H2035	H2035	ASP	D1809	L1698	D1499	D1499

F3982	F3885	Q3766	PHE	R3550	K3475	H3268	T3178	P3004	T2912	THR	F2768
L3983	R3886	Q3767	ARG	E3551	SER	V3269	V3183	N3007	A2913	GLU	D2769
H5994	F3887	S3768	MET	F3552	LYS	I3270	V3183	N3007	K2914	LYS	K2770
F3996	F3888	R3769	P3640	L3553	ALA	P3275	L3186	C3014	E2915	THR	L2771
H3998	Q3888	L3770	R3648	V3563	LYS	C3278	R3187	L3015	K2916	ARG	Q2772
M4000	L3890	T3772	N3651	P3667	ALA	A3189	R3189	L3018	R2920	LYS	M2773
M4001	C3892	R3773	M3652	S3568	GLY	L3190	L3190	P3021	Q2924	ILE	M2774
M4002	E3893	G3774	M3655	L3569	ASP	W3284	G3191	A3022	K2928	SER	M2775
L4017	H3895	A3775	E3655	R3570	ALA	P3289	A3192	K3023	F2929	THR	Y2777
K4021	Q3900	M3778	T3664	M3571	GLN	P3289	C3193	V3024	L2930	ALA	Q2778
D4022	R3904	V3779	I3674	L3579	SER	A3295	L3194	L3025	Q2931	THR	E2779
M4023	T3905	L3780	I3674	P3580	GLY	L3296	A3195	L3025	L2930	GLN	M2780
V4024	T3905	G3788	K3679	G3581	SER	P3297	R3197	S3030	Y2935	TYR	Y2781
V4025	Q3906	E3789	K3679	R3582	ASP	P3297	L3197	A3031	D2782	ASP	Y2782
M4026	N3909	T3790	K3679	A3586	GLU	P3302	M3201	N3033	R2939	ARG	E2783
L4027	M3909	I3802	K3694	P3589	THR	P3303	P3202	N3033	GLY	GLU	K2786
L4028	I3916	L3805	P3695	E3590	ARG	C3804	V3203	K3034	L2946	LYS	Y2855
M4040	T3920	N3806	H3699	K3591	LYS	T3305	N3214	E3035	ASP	ASP	M2856
M4041	D3921	G3807	Q3700	L3592	LYS	T3305	Y3219	K3036	MET	GLU	H2788
M4042	R3925	G3808	L3701	V3593	ARG	N3312	Y3219	E3037	GLU	P2859	P2789
M4044	R3925	V3812	K3713	R3594	ARG	K3222	K3222	S3041	L2946	GLU	K2790
M4045	S3929	M3816	L3716	R3595	ASP	P3224	P3224	L3042	P2860	LYS	L2791
M4047	Y3936	Q3833	D3717	V3601	TYR	R3225	R3225	F3043	P2860	GLY	R2792
M4048	Y3937	A3834	L3716	A3602	TYR	E3226	E3226	K3045	S2863	LYS	Y2794
M4049	K3940	M3836	Y3720	L3603	S3504	L3327	A3228	L3049	K2953	GLY	Y2794
V4055	K3940	M3836	M3723	H3604	L3609	G3828	L3229	V3050	R2954	GLU	K2795
L4059	R3949	N3837	A3724	L3606	P3510	I3329	L3230	R3051	P2955	GLU	T2796
F4061	F3951	T3838	Y3725	E3607	L3511	L3329	G3291	V3054	F2957	LYS	Y2796
F4062	M3955	L3842	I3728	P3612	K3512	K3336	M3239	V3054	G2958	GLU	S2798
D4063	M3955	D3843	K3731	TYR	K3515	R3337	C3240	F3057	F2959	GLU	E2799
M4064	F3961	L3844	S3732	L3606	M3517	I3329	C3240	L3068	L2960	GLU	K2800
L4065	F3962	N3845	L3735	H3605	L3518	W3334	T3243	L3068	Q2961	GLU	D2801
L4066	F3962	A3846	L3735	L3518	M3524	M3335	V3244	L3068	Q2962	GLU	K2802
L4067	S3864	R3849	E3740	L3518	C3525	K3336	L3246	L3068	L2964	LYS	E2803
L4068	L3965	Q3850	ASN	L3518	C3525	R3337	D3247	L3068	R2965	GLU	R2806
V4071	T3966	N3851	GLY	L3518	I3533	F3341	R3248	L3068	N2861	LYS	I2809
V4072	E3967	K3852	GLU	L3518	I3533	Q3343	L3249	L3070	Y2882	GLU	K2810
V4081	Y3968	L3856	GLU	L3518	I3533	I3345	M3250	A3072	H2883	GLU	L2813
L4087	Q3970	V3865	GLU	L3518	I3533	S3347	A3251	R3073	N2884	GLU	A2815
L4088	N3976	I3866	GLY	L3518	I3533	R3348	M3250	A3072	K2891	LYS	K2814
S4089	R3984	N3867	ARG	L3518	I3533	A3349	A3251	R3073	Q2892	GLU	A2815
K4090	L3985	R3868	ARG	L3518	I3533	R3350	D3252	L3075	E2972	LYS	W2819
M4097	W3885	G3871	ALA	L3518	I3533	L3353	I3253	D3076	A2975	GLU	E2820
F4103	V3989	K3872	ALA	L3518	I3533	L3353	I3253	T3079	L2894	LYS	W2821
		V3874	CYS	V3549	T3471	R3368	P3257	V3080	L2977	GLU	T2822
								G3084	V2980	GLU	L2823
								V3088	V2981	GLU	E2824
								R3083	R2985	GLU	K2825
									L3003	GLU	A2826
										ARG	E2828
										ARG	G2829
										ARG	E2830



- Molecule 2: Ryanodine receptor 1



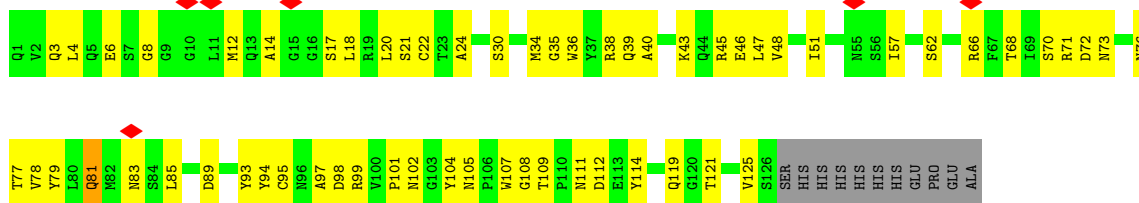
K424	K650	T657	D774	I878	H993	R1073	S1175	P1294	GLY	VAL	R1619	I1718	Q1837
P431	L651	T657	D774	H879	H993	I1074	E1176	P1297	THR	PRO	A1620	H1719	F1838
L443	D852	G660	P779	R886	M996	F1075	A1177	H1298	PRO	ALA	G1621	G1621	V1839
I449	R553	K661	P779	I887	M996	R1076	A1178	Q1299	GLY	ASP	E1622	R1727	P1940
E453	L564	K662	S762	M891	R1000	A1077	F1179	R1421	THR	R1420	R1624	M1730	V1941
Q460	E555	Y663	F763	M892	M1005	E1078	E1181	R1302	PRO	D1422	G1625	L1731	L1849
E463	I560	F664	S764	T892	S1006	Y1081	I1182	C1303	GLN	P1423	W1626	S1732	V1850
R469	L561	F665	F768	Y893	S1006	T1082	F1188	T1304	ALA	E1425	A1627	E1733	M1851
S470	L561	F665	F768	G894	Y1007	V1083	L1189	GLY	ALA	I1426	M1637	I1735	G1852
L471	V563	D669	V769	R897	S1008	G1086	C1192	ALA	GLU	T1431	A1638	P1740	F1854
R472	V574	A677	F791	K901	I1013	R1087	P1196	THR	ALA	T1432	L1639	P1740	D1858
M473	E480	T680	L792	R902	R1016	F1092	P1196	PRO	GLN	T1432	H1640	R1743	I1862
Q475	I578	T680	L792	L903	R1017	V1095	A1178	ALA	PRO	Y1433	I1641	R1743	I1862
E480	H582	L682	G795	H904	M1018	M1100	R1178	ALA	ALA	Y1434	P1642	P1749	M1865
G482	I583	R683	R796	P905	M1018	R1101	G1200	PRO	ALA	Y1435	E1644	R1758	I1866
M483	I587	R688	H797	C906	L1021	R1101	D1207	GLY	GLU	V1439	M1645	R1759	F1871
L486	S588	L688	E799	L907	P1022	W1104	S1210	GLN	ASN	Q1443	R1646	P1763	F1871
V487	F800	W702	F800	H911	L1026	L1115	F1223	PRO	GLU	C1447	E1652	L1771	E1874
L491	L589	W702	F802	S912	L1027	G1116	F1223	ALA	LYS	W1448	L1653	R1772	GLU
D492	E481	D717	F808	L913	L1027	G1116	A1227	ASP	THR	W1449	L1653	P1773	GLU
Y497	G482	D717	Y808	E917	K1032	Y1122	A1227	THR	THR	V1450	R1656	H1776	GLU
A501	M483	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	V1451	R1656	H1776	GLU
H502	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	W1452	Q1660	H1776	GLU
F503	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	W1453	R1661	V1783	GLU
E505	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	T1454	H1662	V1783	GLU
W515	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	P1455	H1663	L1786	GLU
I530	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	M1462	H1663	L1786	GLU
R531	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	M1476	S1664	F1787	GLU
G532	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	G1477	S1666	ALA	GLU
N533	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	D1478	T1666	GLY	GLU
R534	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	M1478	Y1670	VAL	GLU
A535	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	M1482	A1671	ALA	GLU
N536	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	V1483	V1673	LYS	GLU
L539	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	S1485	L1676	GLU	GLU
F540	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	C1489	R1680	P1800	LYS
S541	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	M1494	L1694	L1804	GLU
D545	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	V1495	L1694	L1804	GLU
W546	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	M1496	L1698	R1808	ASP
V547	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	G1497	L1698	D1809	GLU
S549	K592	W722	Y808	E917	K1032	Y1122	A1227	THR	THR	G1498	L1703	K1810	GLU
	K654	E769	N877	L984	V985	V1168	S1171	GLU	VAL	D1498	P1704	M1814	GLU
						V1169	S1171	GLU	VAL	F1500	R1708	L1814	GLU
						V1170	S1171	GLU	VAL	V1501	L1708	L1815	GLU
						V1171	S1171	GLU	VAL	S1502	R1708	L1816	GLU
						V1172	S1171	GLU	VAL	F1503	L1711	R1827	ASP
						V1173	S1171	GLU	VAL	G1504	Y1712	R1827	ASP
						V1174	S1171	GLU	VAL	GLN	V1615	V1830	GLU
						V1175	S1171	GLU	VAL	GLN	E1616	L1714	LYS
						V1176	S1171	GLU	VAL	GLY	H1617	L1715	GLU
						V1177	S1171	GLU	VAL	R1508	R1618	F1836	GLU



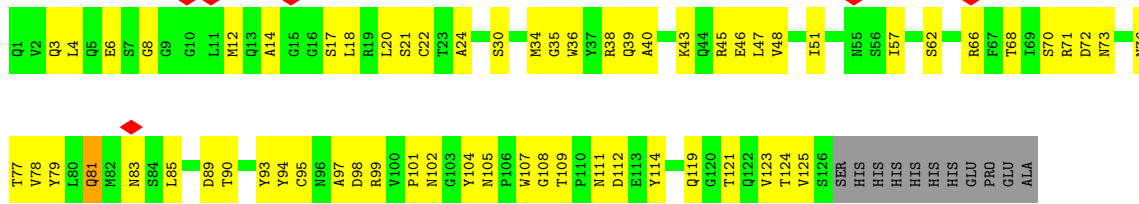




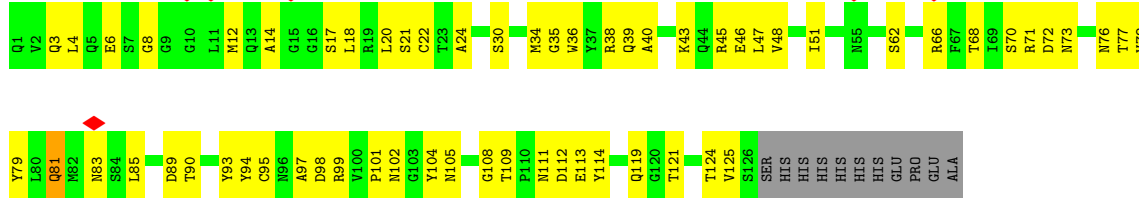
• Molecule 3: Nanobody 9657



• Molecule 3: Nanobody 9657

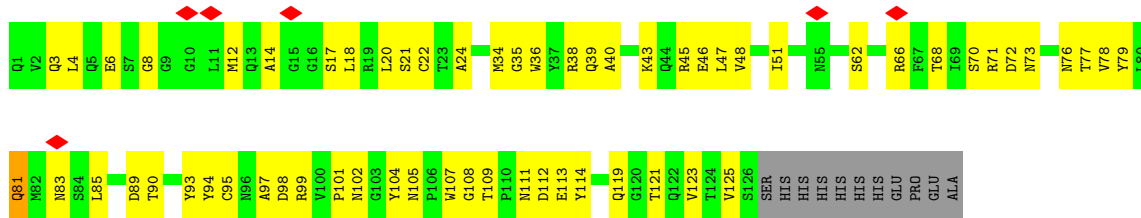


• Molecule 3: Nanobody 9657



• Molecule 3: Nanobody 9657







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16530	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.003	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.044	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	504.0, 504.0, 504.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.5, 1.5, 1.5	Depositor

## 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: ATP, CA, ZN, CFF

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	0.25	0/834	0.54	0/1123
1	D	0.25	0/834	0.54	0/1123
1	H	0.25	0/834	0.54	0/1123
1	I	0.25	0/834	0.54	0/1123
2	B	0.25	0/34916	0.51	1/47328 (0.0%)
2	E	0.25	0/34916	0.51	1/47328 (0.0%)
2	G	0.25	0/34923	0.51	1/47336 (0.0%)
2	J	0.25	0/34916	0.51	1/47328 (0.0%)
3	C	0.26	0/987	0.56	0/1340
3	F	0.26	0/987	0.56	0/1340
3	K	0.26	0/987	0.56	0/1340
3	M	0.26	0/987	0.56	0/1340
All	All	0.25	0/146955	0.51	4/199172 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1503	PRO	N-CA-CB	5.77	110.23	103.30
2	E	1503	PRO	N-CA-CB	5.77	110.23	103.30
2	G	1503	PRO	N-CA-CB	5.77	110.23	103.30
2	J	1503	PRO	N-CA-CB	5.77	110.23	103.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	818	0	824	26	0
1	D	818	0	824	28	0
1	H	818	0	824	29	0
1	I	818	0	824	28	0
2	B	34143	0	33531	1049	0
2	E	34143	0	33531	1047	0
2	G	34150	0	33542	1050	0
2	J	34143	0	33531	1042	0
3	C	967	0	916	58	0
3	F	967	0	916	59	0
3	K	967	0	916	58	0
3	M	967	0	916	57	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	B	31	0	12	1	0
5	E	31	0	12	1	0
5	G	31	0	12	1	0
5	J	31	0	12	1	0
6	B	14	0	10	0	0
6	E	14	0	10	0	0
6	G	14	0	10	0	0
6	J	14	0	10	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
All	All	143907	0	141183	4467	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 16.

The worst 5 of 4467 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)
2:E:3416:VAL:HG11	2:E:3516:LYS:HD3	1.51	0.93
2:E:248:GLU:HB2	2:E:373:LYS:HD2	1.51	0.92
2:B:248:GLU:HB2	2:B:373:LYS:HD2	1.52	0.91
2:J:3416:VAL:HG11	2:J:3516:LYS:HD3	1.51	0.91
2:B:3416:VAL:HG11	2:B:3516:LYS:HD3	1.51	0.91

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 EM 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	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	D	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
1	H	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
1	I	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	B	4280/5027 (85%)	4144 (97%)	136 (3%)	0	100	100
2	E	4280/5027 (85%)	4142 (97%)	138 (3%)	0	100	100
2	G	4280/5027 (85%)	4142 (97%)	138 (3%)	0	100	100
2	J	4280/5027 (85%)	4140 (97%)	140 (3%)	0	100	100
3	C	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	F	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	K	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	M	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
All	All	18036/21084 (86%)	17434 (97%)	602 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 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 EM 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	88/88 (100%)	88 (100%)	0	100	100
1	D	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	88 (100%)	0	100	100
1	I	88/88 (100%)	88 (100%)	0	100	100
2	B	3672/4270 (86%)	3665 (100%)	7 (0%)	92	94
2	E	3672/4270 (86%)	3665 (100%)	7 (0%)	92	94
2	G	3674/4270 (86%)	3667 (100%)	7 (0%)	92	94
2	J	3672/4270 (86%)	3665 (100%)	7 (0%)	92	94
3	C	104/114 (91%)	103 (99%)	1 (1%)	73	82
3	F	104/114 (91%)	103 (99%)	1 (1%)	73	82
3	K	104/114 (91%)	103 (99%)	1 (1%)	73	82
3	M	104/114 (91%)	103 (99%)	1 (1%)	73	82
All	All	15458/17888 (86%)	15426 (100%)	32 (0%)	91	94

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	81	GLN
3	F	81	GLN
2	E	3262	ARG
2	E	2914	LYS
3	K	81	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	3889	GLN
3	K	3	GLN
2	J	3970	GLN
3	C	73	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	M	3	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	ATP	E	5102	-	26,33,33	0.60	0	31,52,52	0.79	2 (6%)
6	CFF	B	5103	-	8,15,15	1.02	0	8,23,23	2.44	2 (25%)
6	CFF	G	5103	-	8,15,15	1.03	0	8,23,23	2.43	2 (25%)
5	ATP	J	5102	-	26,33,33	0.60	0	31,52,52	0.80	2 (6%)
6	CFF	J	5103	-	8,15,15	1.01	0	8,23,23	2.43	2 (25%)
5	ATP	G	5102	-	26,33,33	0.60	0	31,52,52	0.79	2 (6%)
6	CFF	E	5103	-	8,15,15	1.03	0	8,23,23	2.42	2 (25%)
5	ATP	B	5102	-	26,33,33	0.60	0	31,52,52	0.79	2 (6%)

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	ATP	E	5102	-	-	5/18/38/38	0/3/3/3
6	CFF	B	5103	-	-	-	0/2/2/2
6	CFF	G	5103	-	-	-	0/2/2/2
5	ATP	J	5102	-	-	5/18/38/38	0/3/3/3
6	CFF	J	5103	-	-	-	0/2/2/2
5	ATP	G	5102	-	-	5/18/38/38	0/3/3/3
6	CFF	E	5103	-	-	-	0/2/2/2
5	ATP	B	5102	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	5103	CFF	C5-C6-N1	-5.77	112.05	118.20
6	B	5103	CFF	C5-C6-N1	-5.76	112.06	118.20
6	J	5103	CFF	C5-C6-N1	-5.76	112.06	118.20
6	E	5103	CFF	C5-C6-N1	-5.75	112.07	118.20
6	B	5103	CFF	C4-C5-C6	3.53	122.22	119.96

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

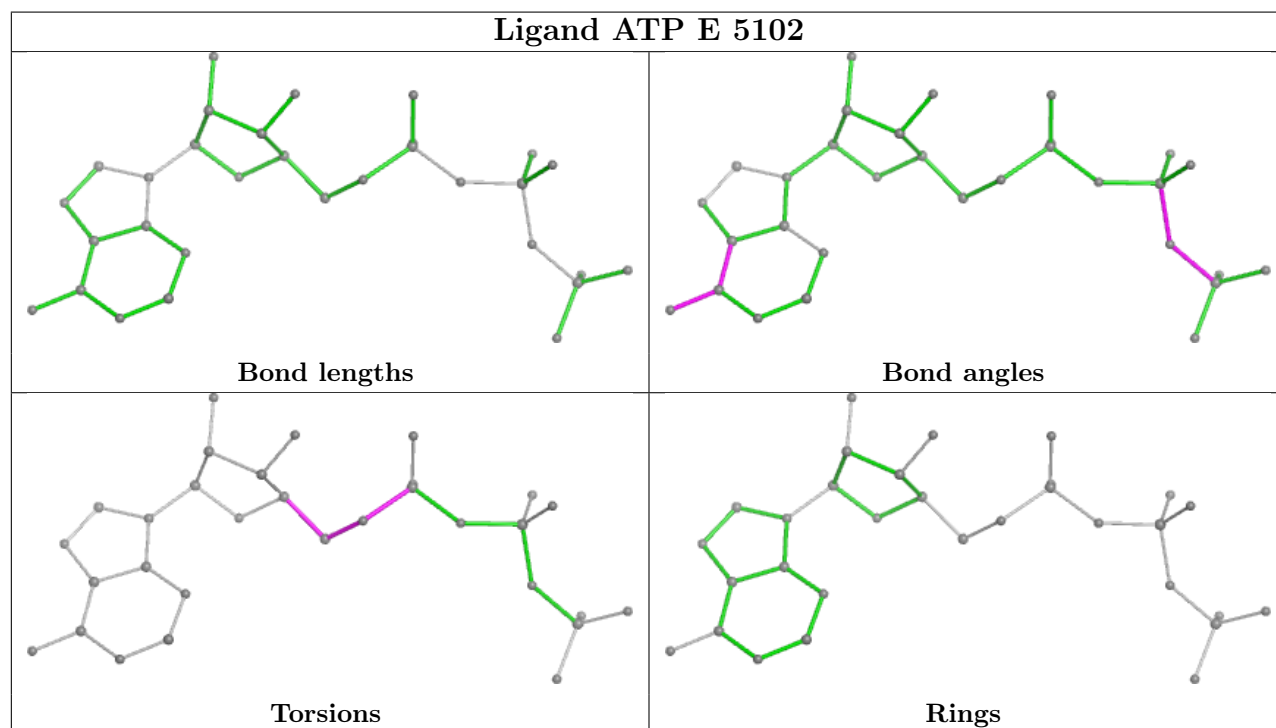
Mol	Chain	Res	Type	Atoms
5	B	5102	ATP	C5'-O5'-PA-O1A
5	B	5102	ATP	C5'-O5'-PA-O2A
5	E	5102	ATP	C5'-O5'-PA-O1A
5	E	5102	ATP	C5'-O5'-PA-O2A
5	G	5102	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

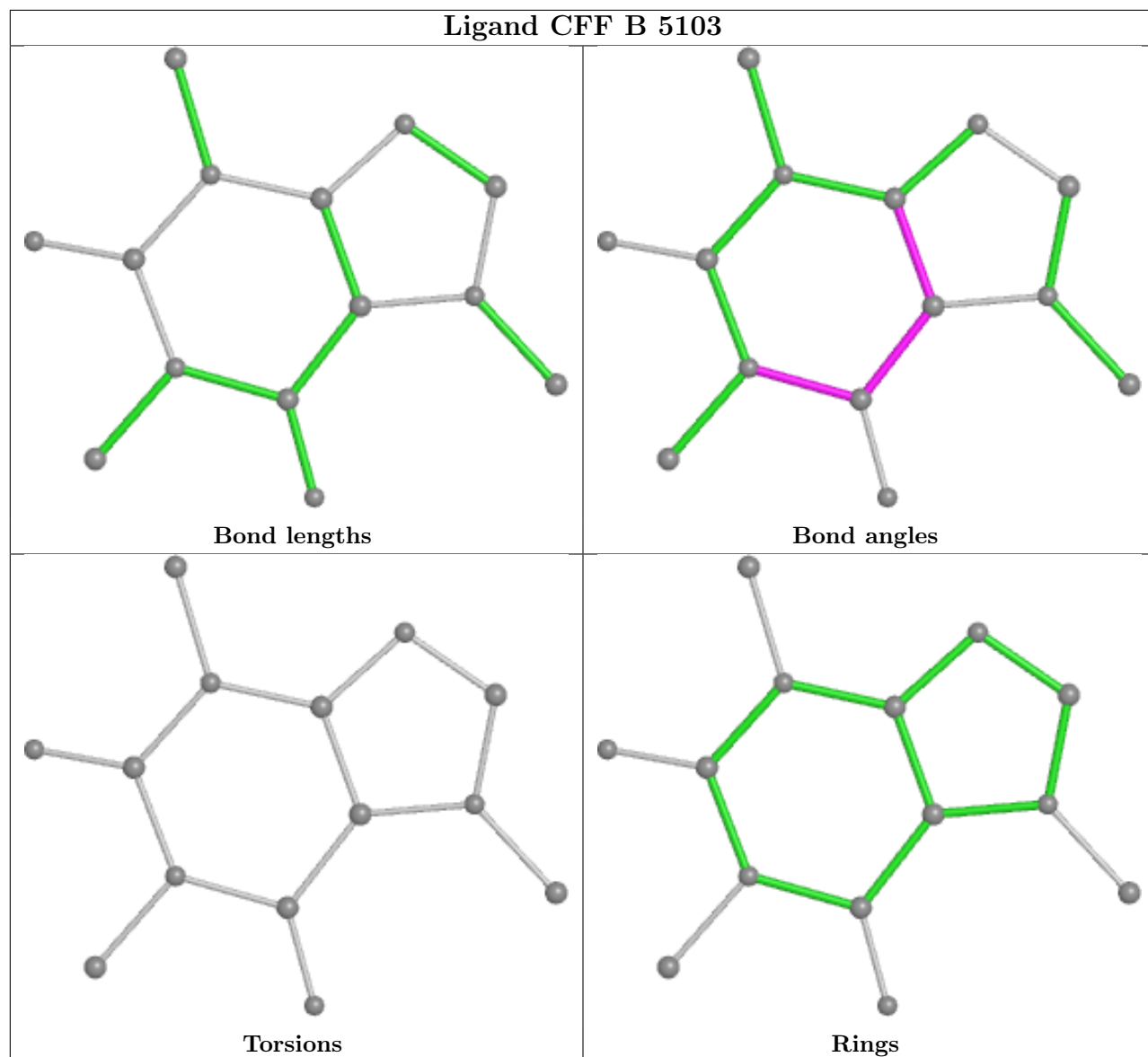
4 monomers are involved in 4 short contacts:

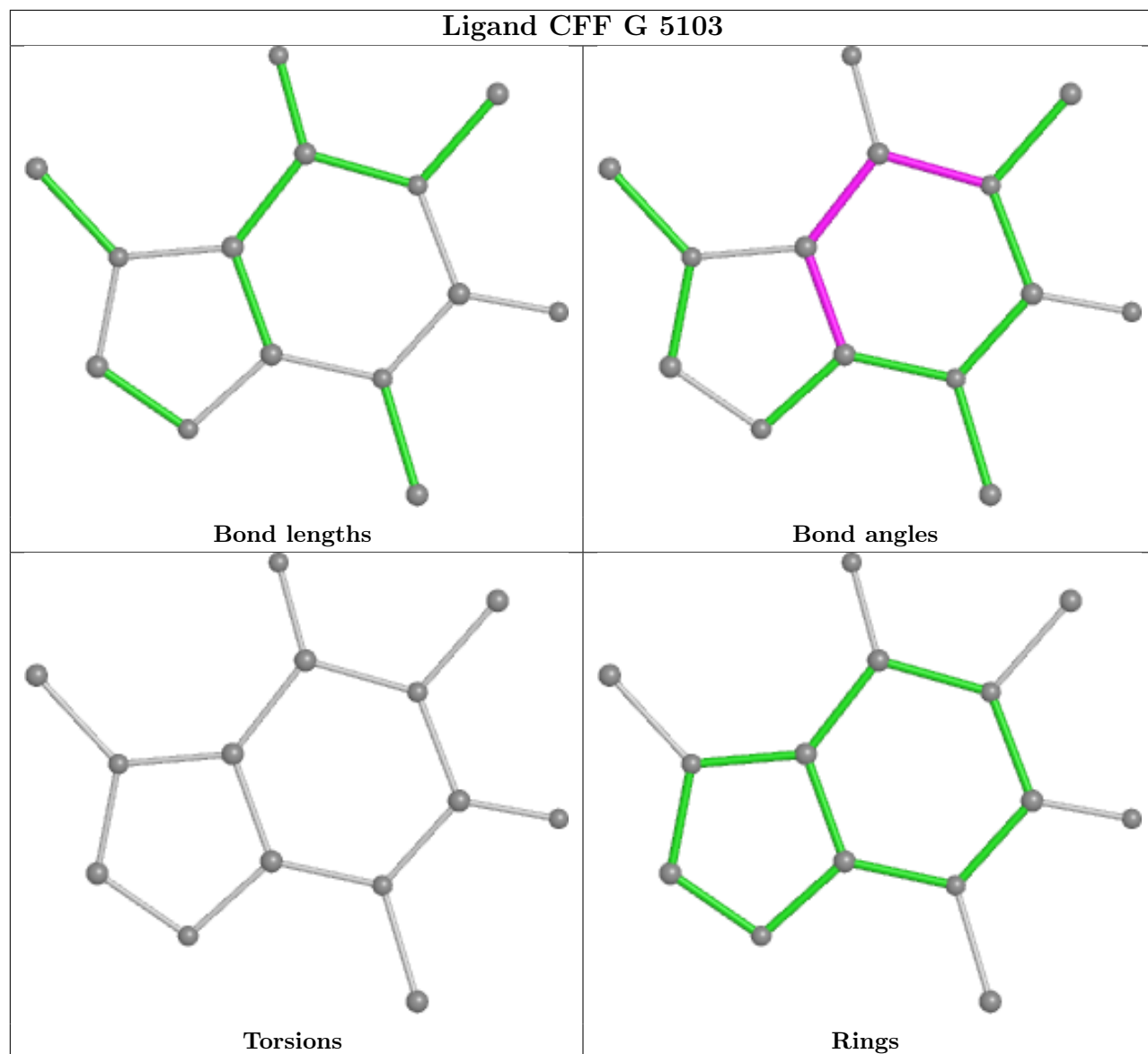
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	5102	ATP	1	0
5	J	5102	ATP	1	0
5	G	5102	ATP	1	0
5	B	5102	ATP	1	0

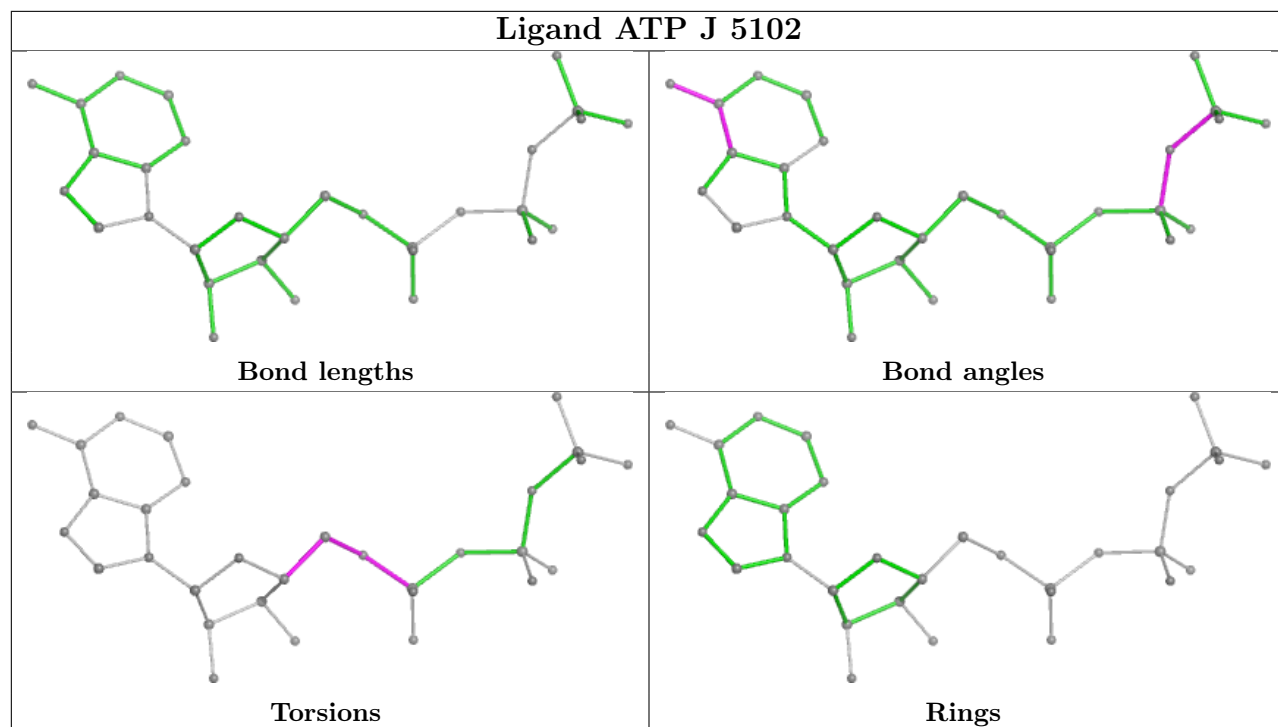
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

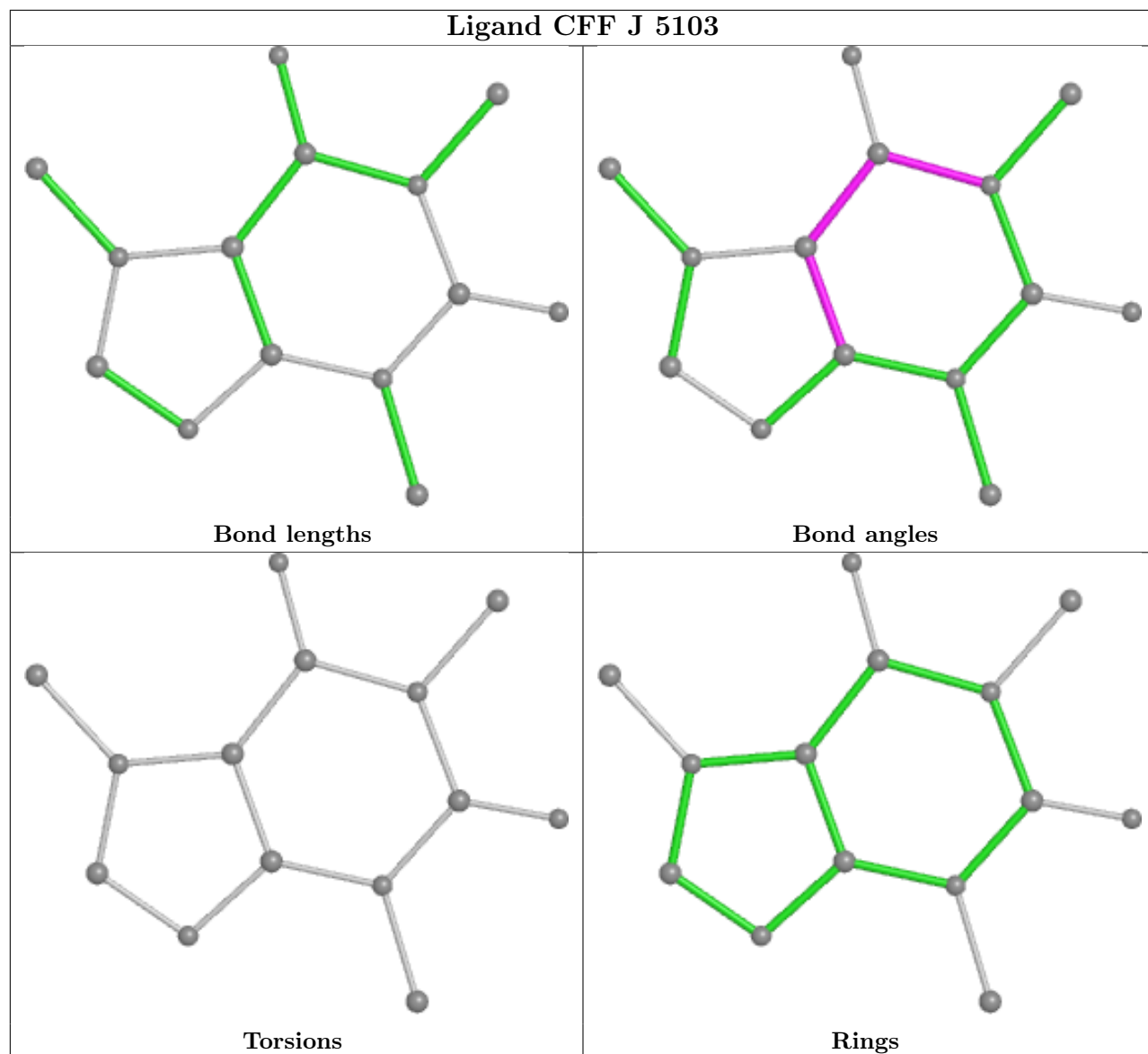


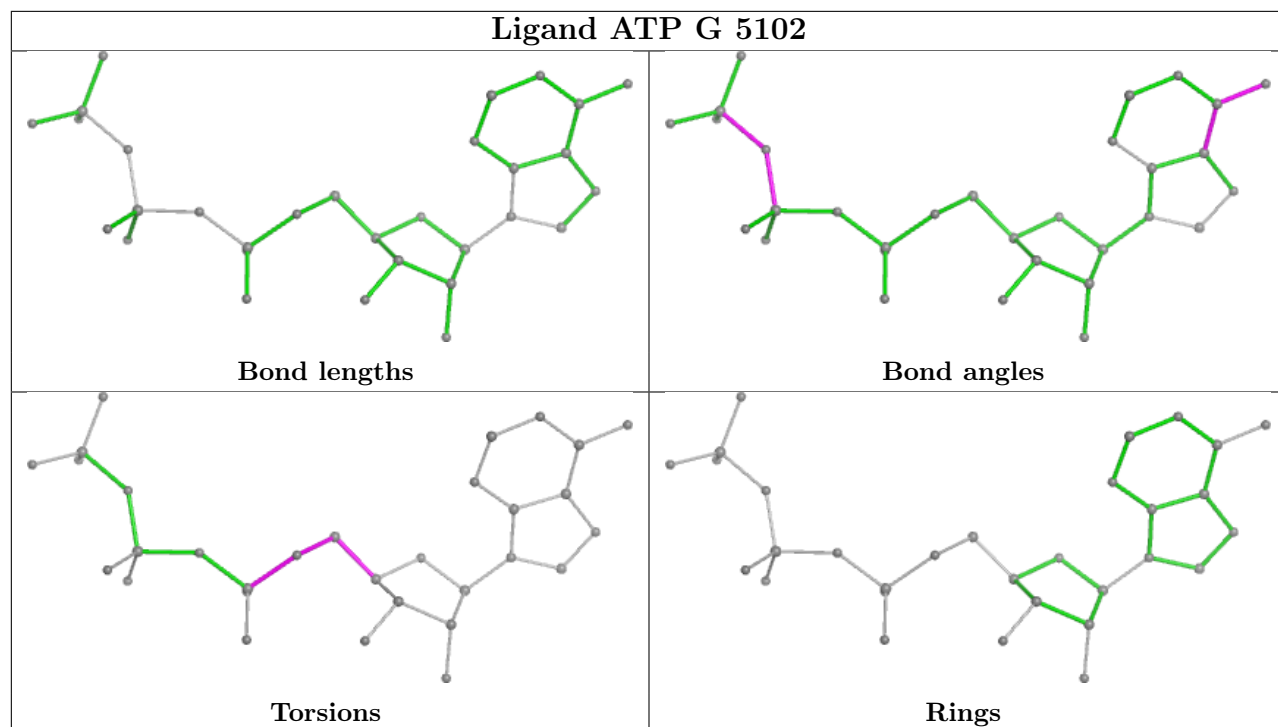


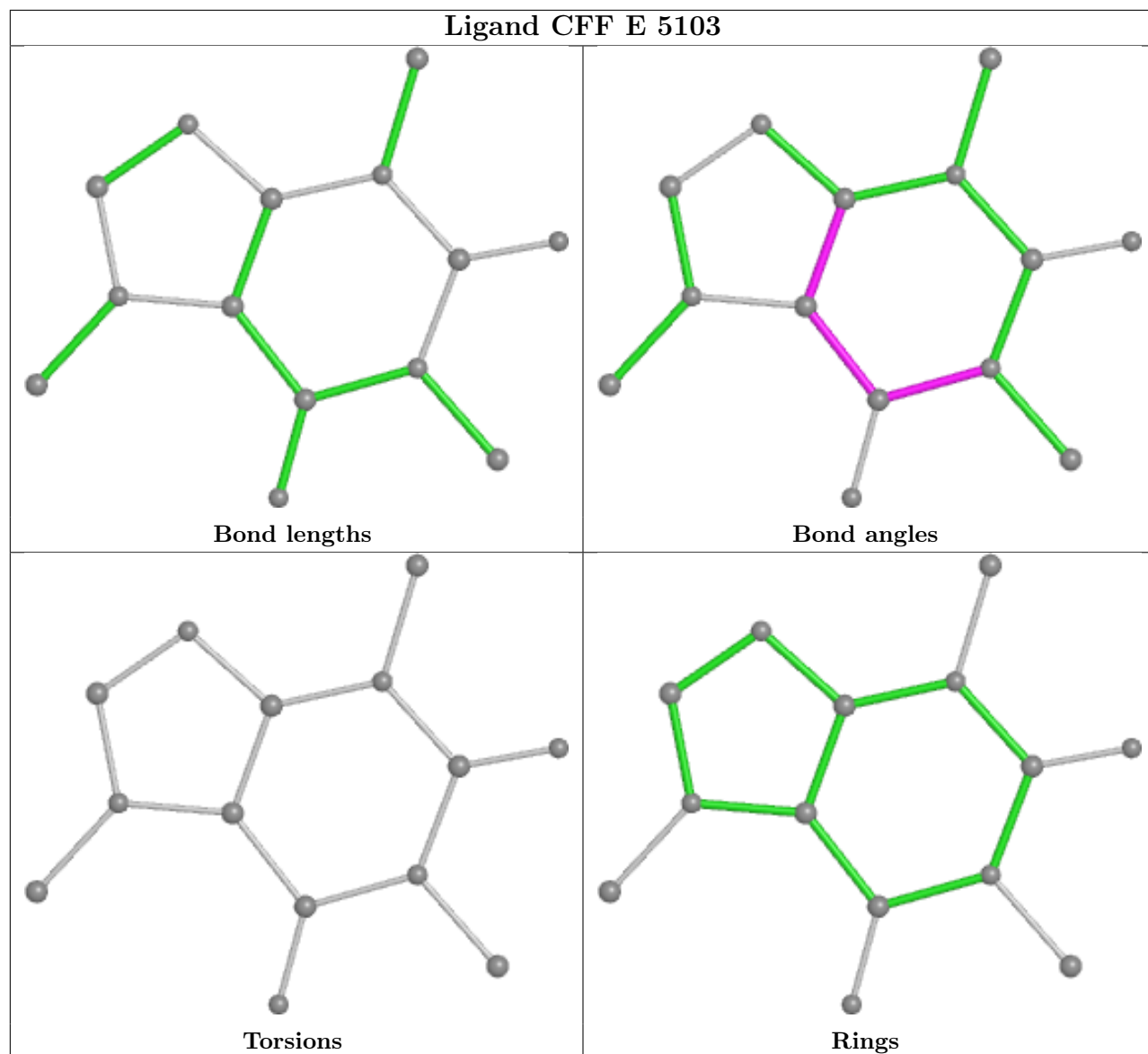


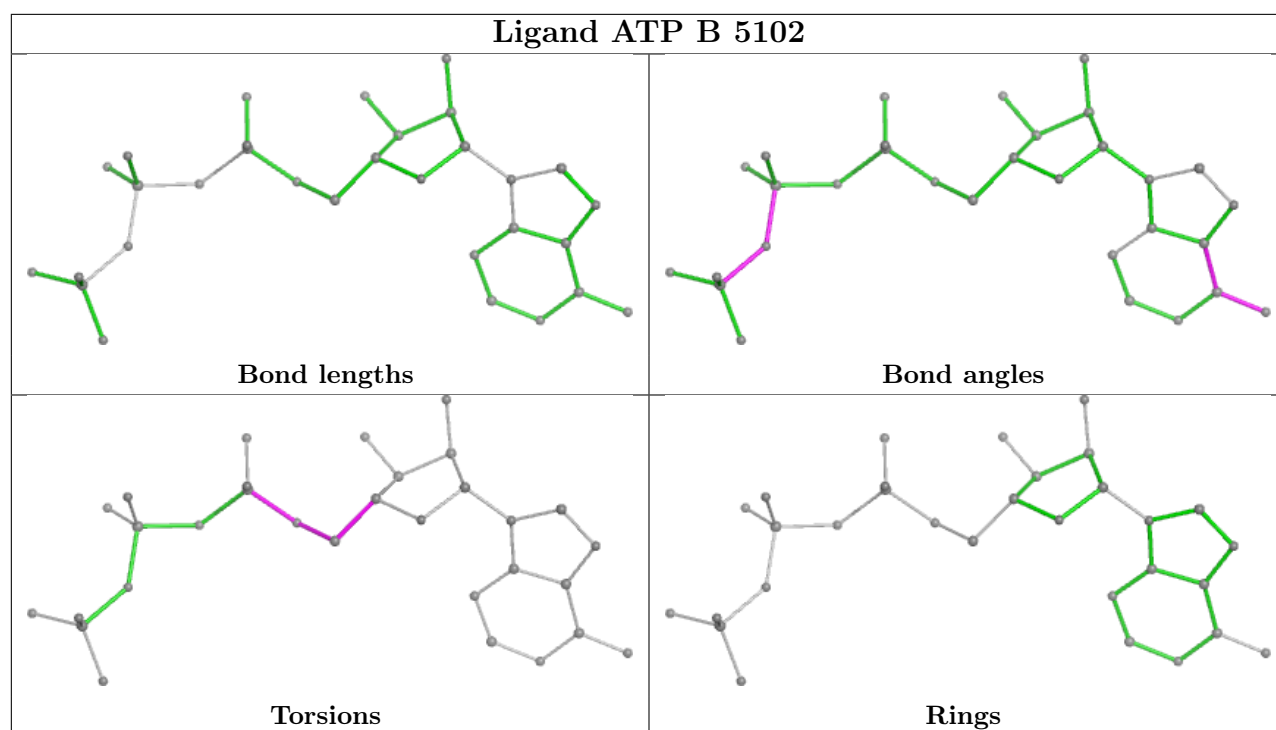












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

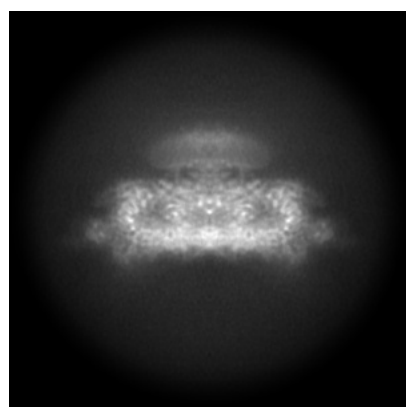
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19465. These allow visual inspection of the internal detail of the map and identification of artifacts.

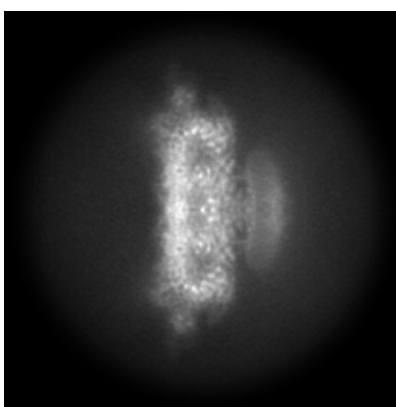
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

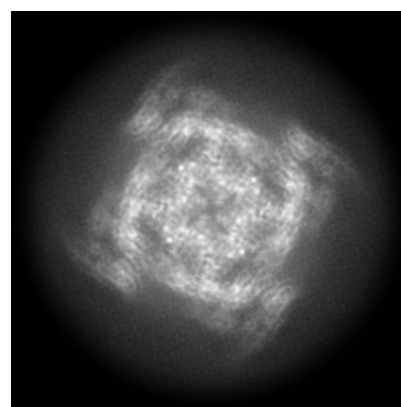
#### 6.1.1 Primary map



X



Y

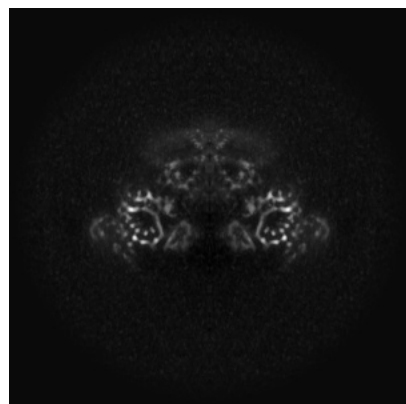


Z

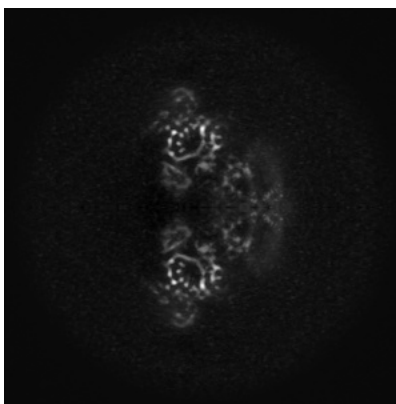
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

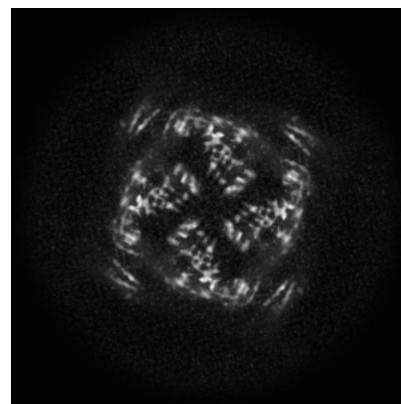
#### 6.2.1 Primary map



X Index: 168



Y Index: 168



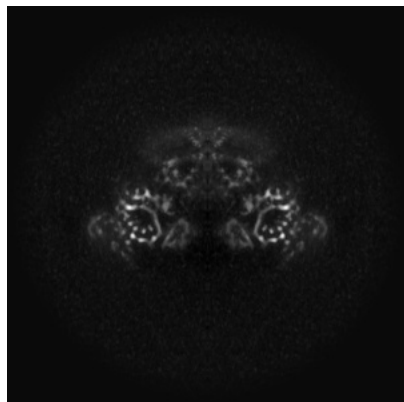
Z Index: 168



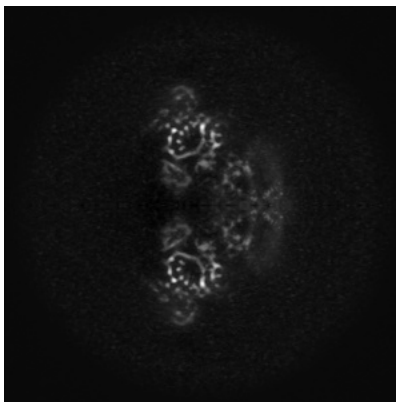
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

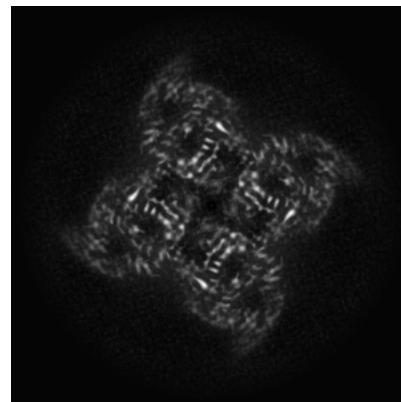
### 6.3.1 Primary map



X Index: 168



Y Index: 168

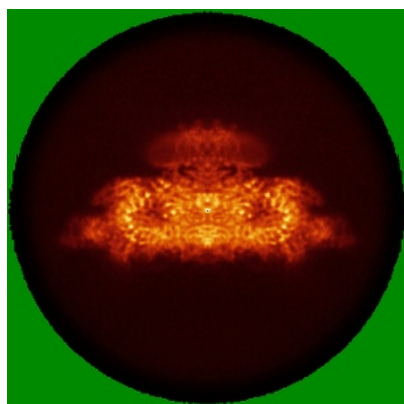


Z Index: 145

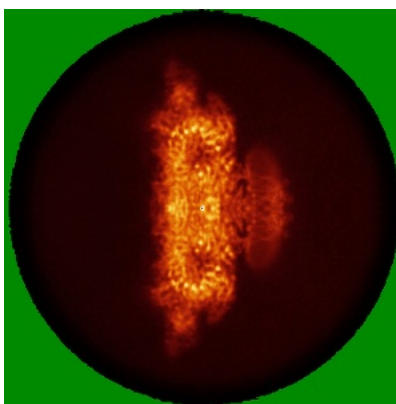
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

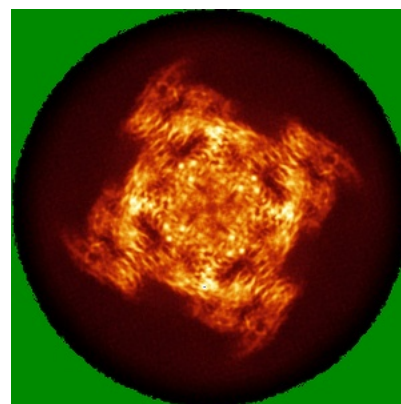
### 6.4.1 Primary map



X



Y

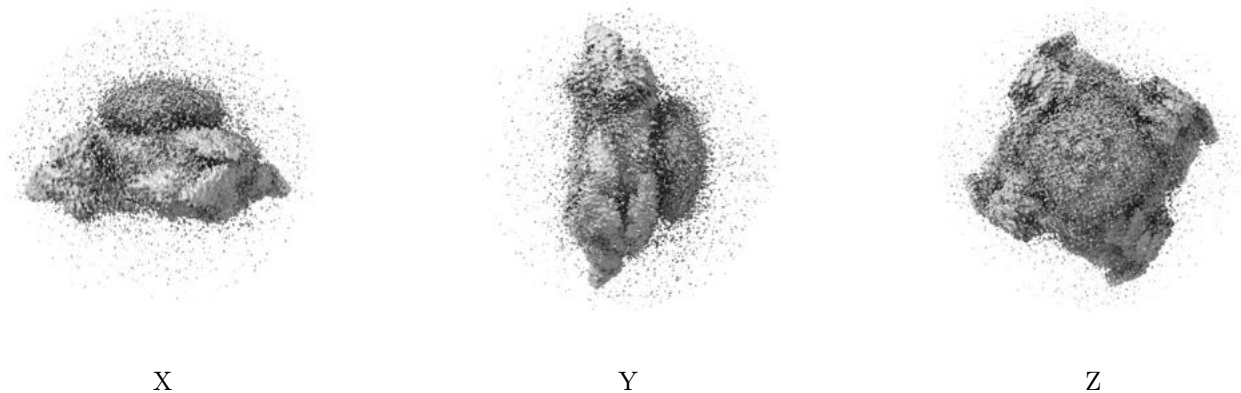


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

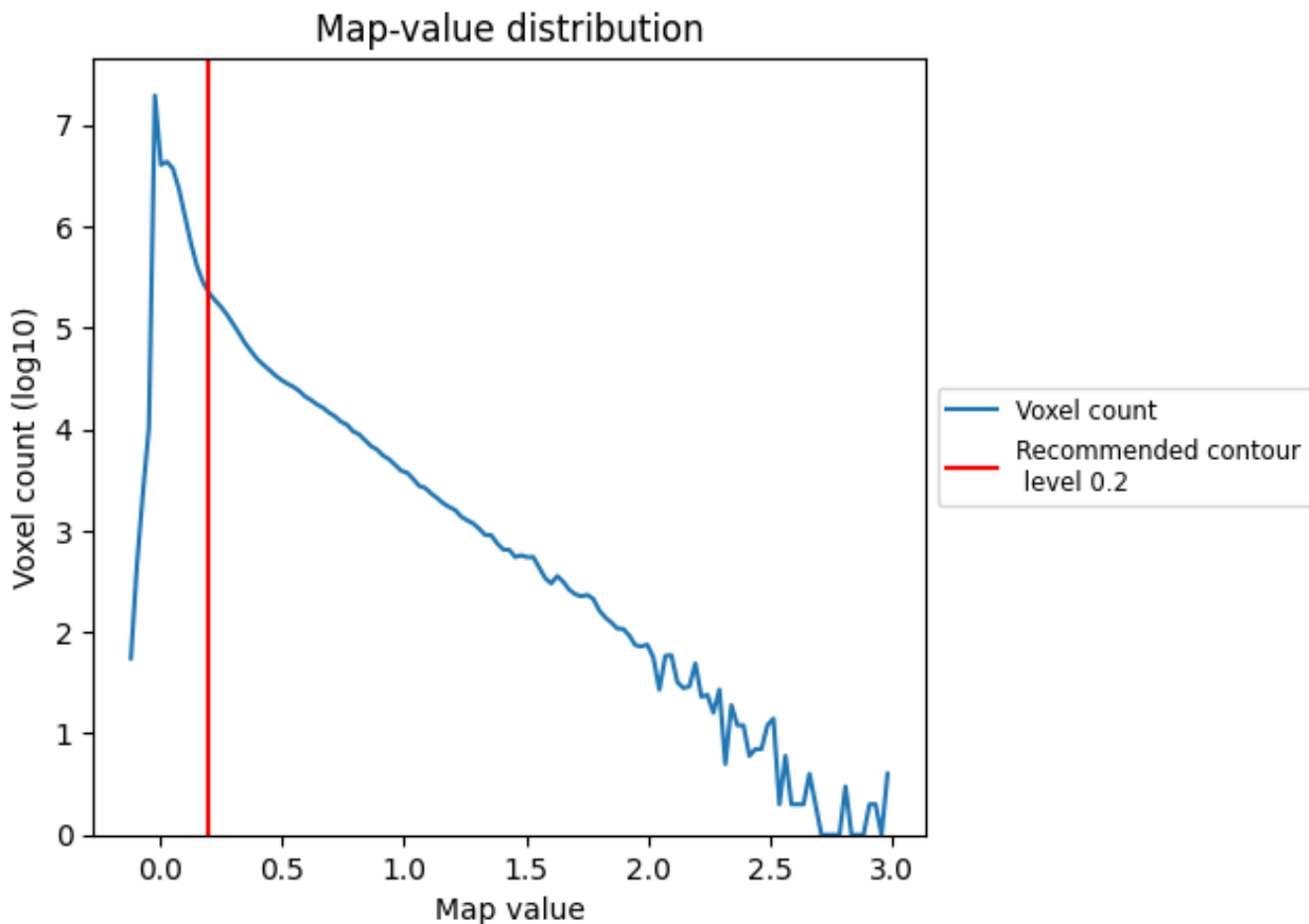
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

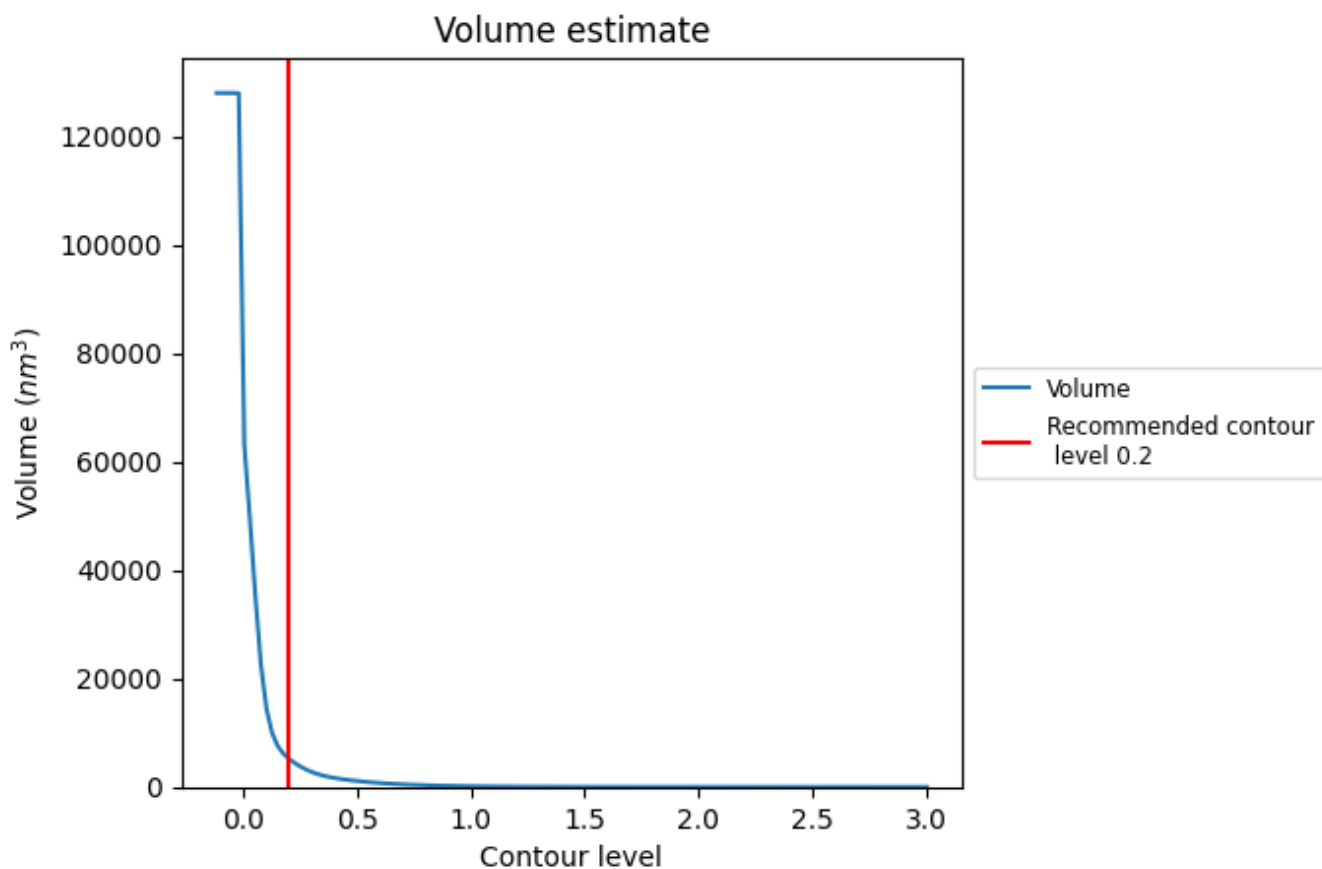
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

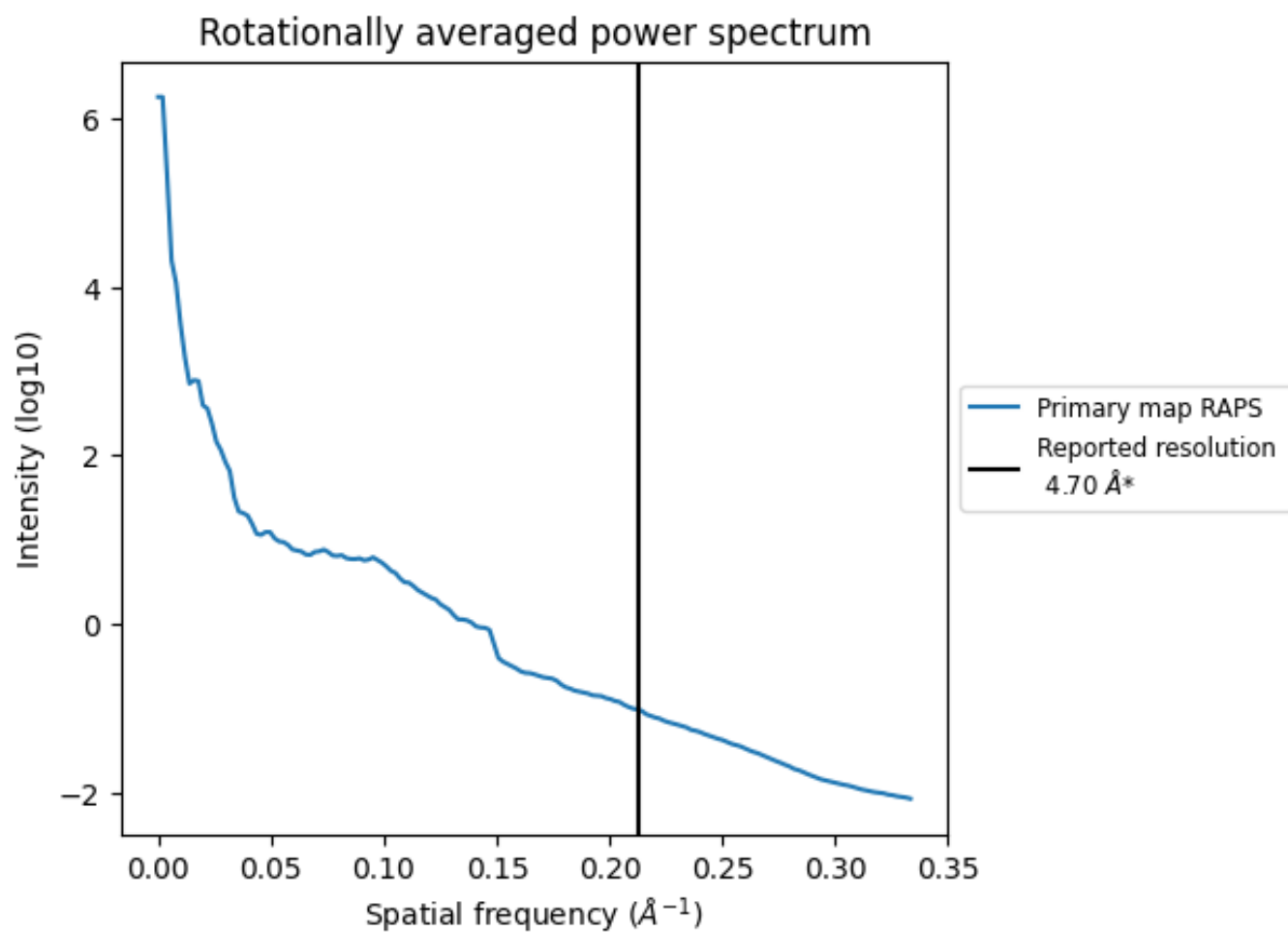
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 5220  $\text{nm}^3$ ; this corresponds to an approximate mass of 4715 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [\(i\)](#)

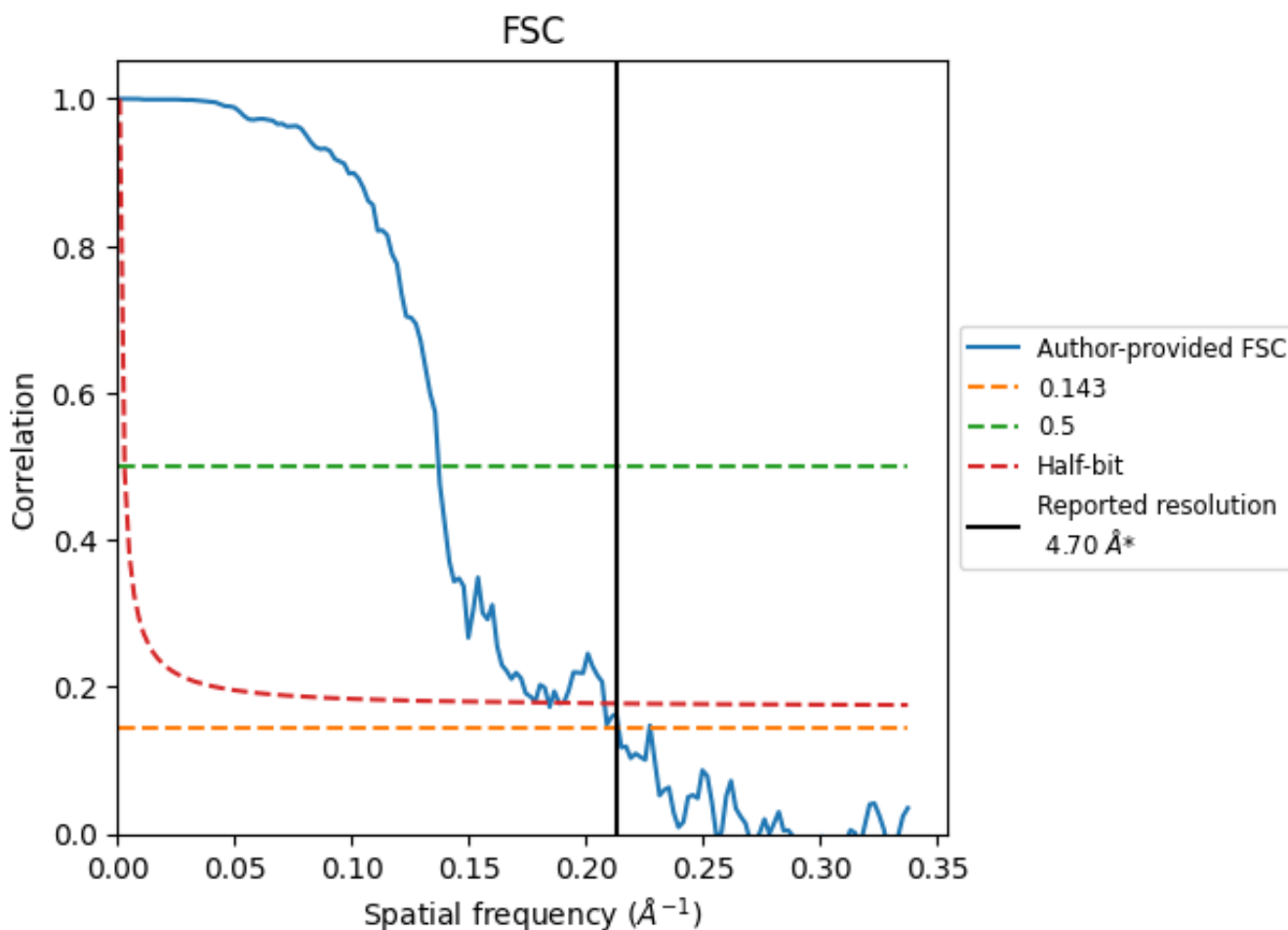


\*Reported resolution corresponds to spatial frequency of 0.213 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.213 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

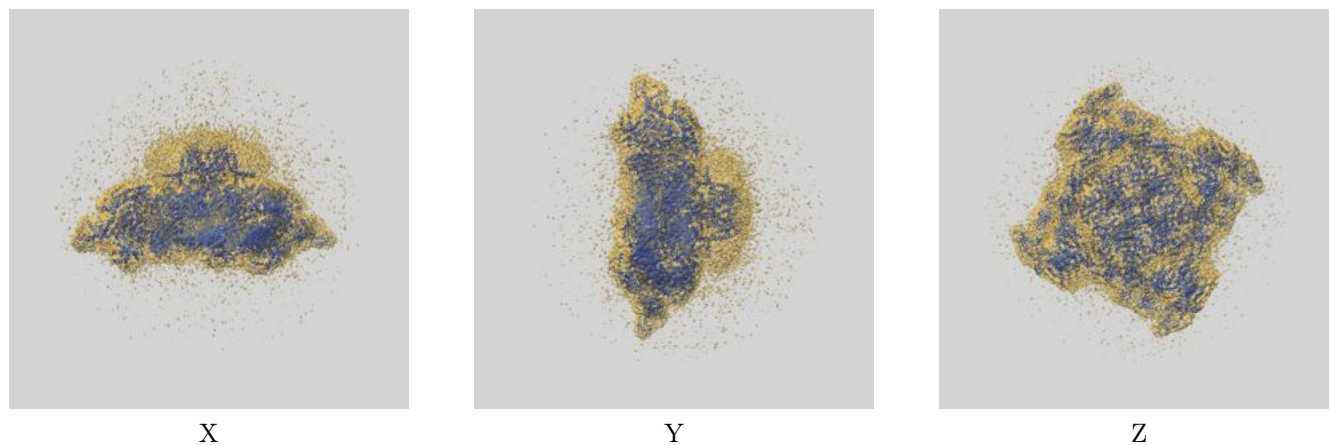
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.68	7.29	5.43
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19465 and PDB model 8RRU. Per-residue inclusion information can be found in section 3 on page 8.

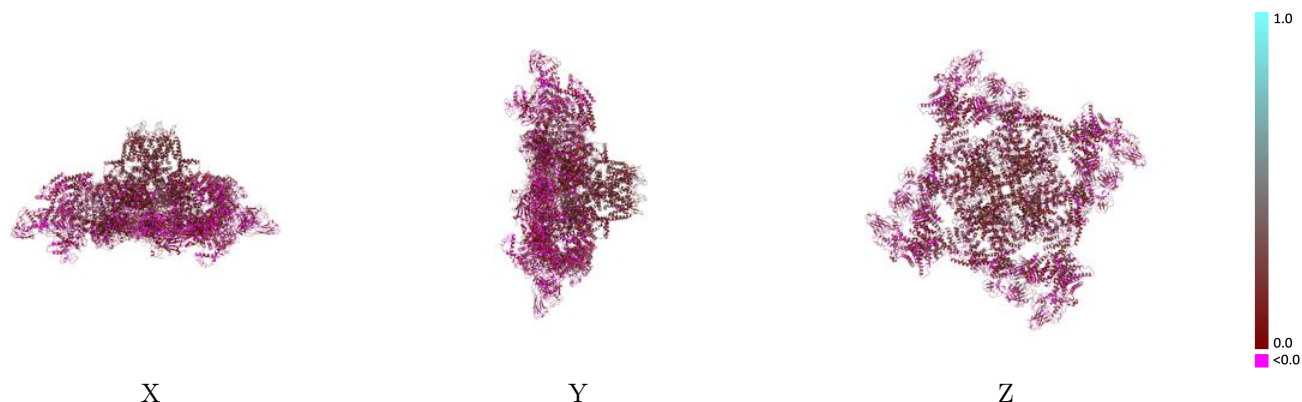
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

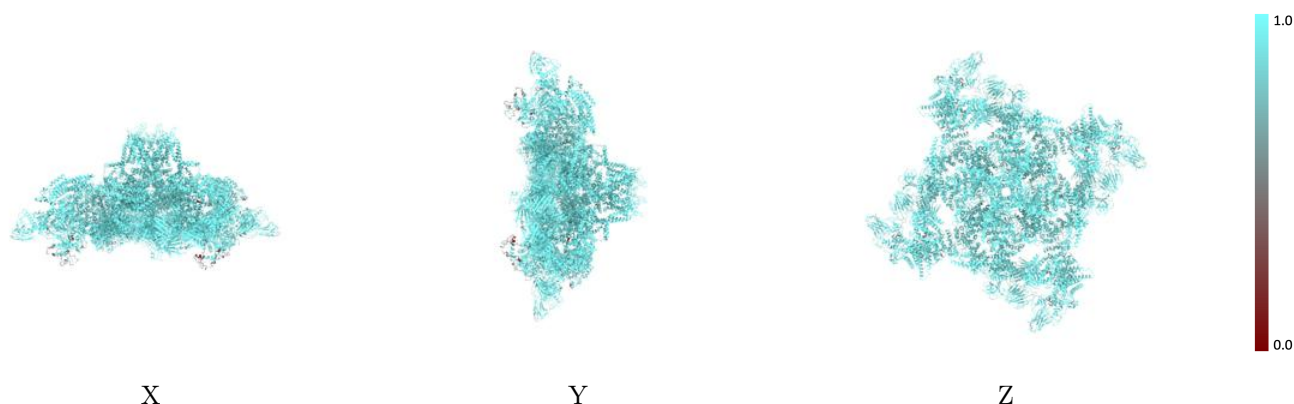


## 9.2 Q-score mapped to coordinate model [i](#)



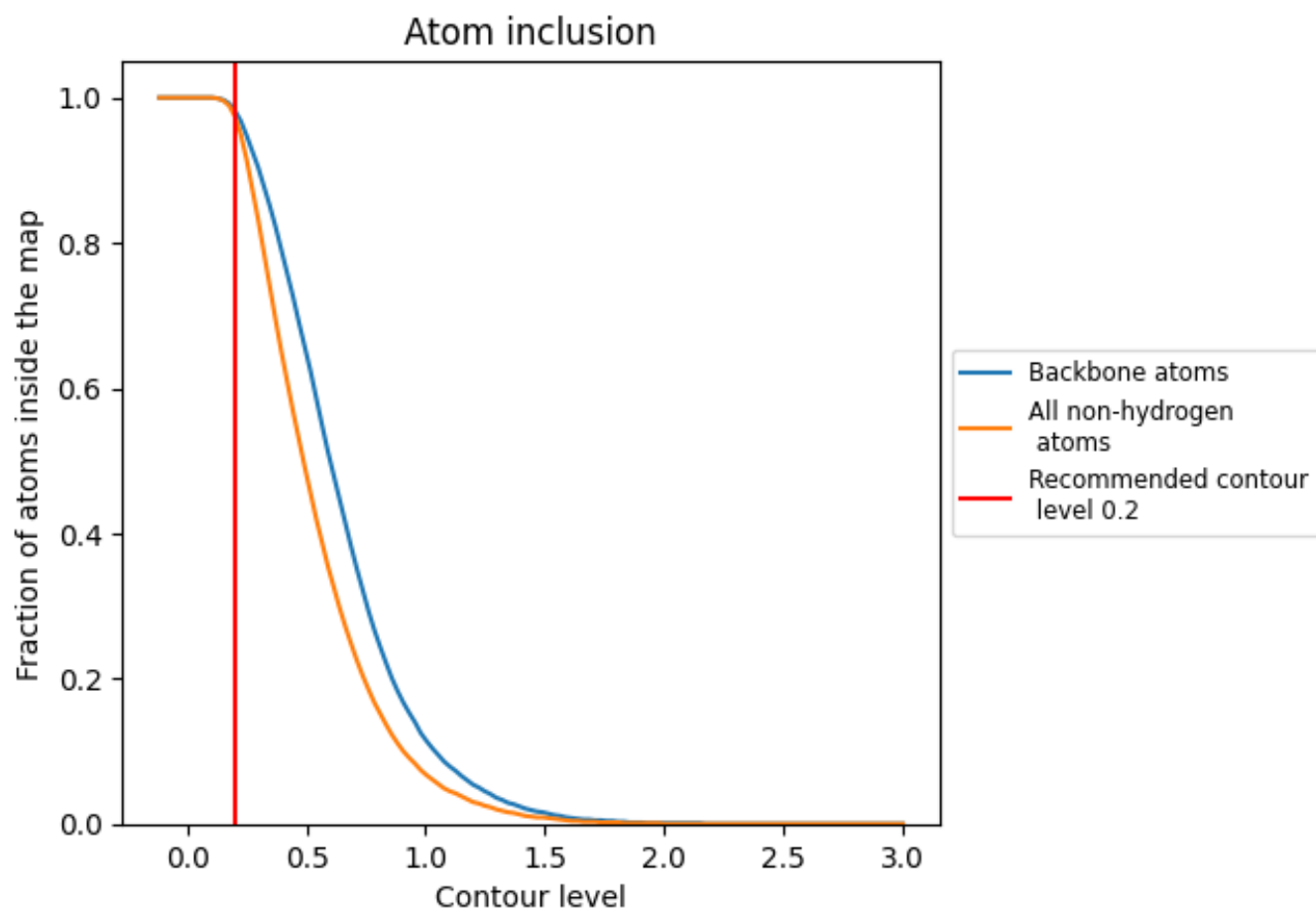
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9740	 0.1100
A	 0.9860	 0.0460
B	 0.9760	 0.1140
C	 0.9180	 0.0580
D	 0.9860	 0.0440
E	 0.9760	 0.1130
F	 0.9190	 0.0590
G	 0.9760	 0.1140
H	 0.9880	 0.0460
I	 0.9850	 0.0440
J	 0.9760	 0.1140
K	 0.9160	 0.0570
M	 0.9270	 0.0610

