



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:09 PM UTC

PDB ID : 9E1H / pdb_00009e1h
EMDB ID : EMD-47394
Title : Structure of RyR1 in the primed state in the presence of oxopyricid
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 3.26 Å(reported)
Based on initial model : 7TZC

This is a wwPDB EM 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/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>.

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

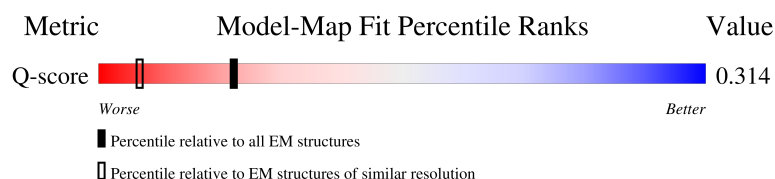
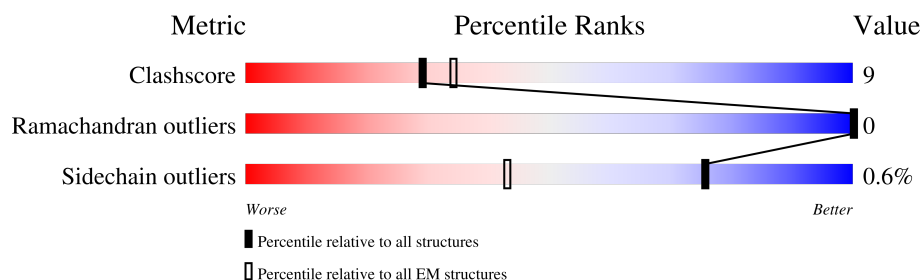
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14557 (2.76 - 3.76)

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 ≥ 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	5037	38% 69% 18% 13%
1	B	5037	38% 69% 18% 13%
1	C	5037	38% 69% 18% 13%
1	D	5037	38% 69% 18% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	74% 67% 31% ..
2	F	108	73% 66% 31% ..
2	G	108	73% 68% 31% ..
2	H	108	75% 67% 31% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144120 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	D	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	C	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	G	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	D	1	Total Ca 1 1	0
4	C	1	Total Ca 1 1	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

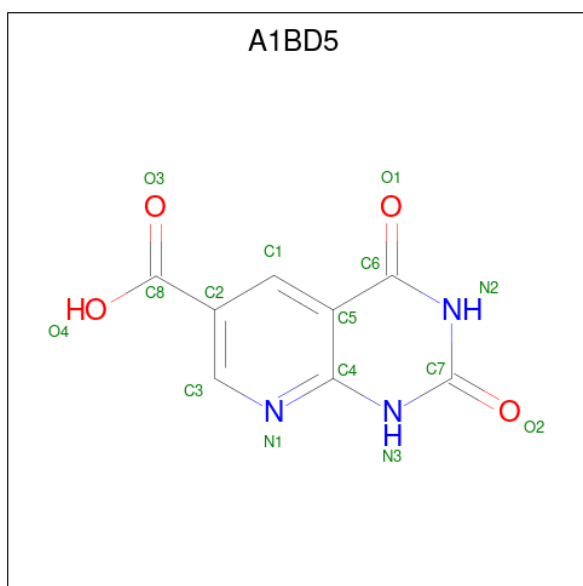
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	

- Molecule 6 is oxopyridicid (CCD ID: A1BD5) (formula: C₈H₅N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			15	8	3	4	
6	B	1	Total	C	N	O	0
			15	8	3	4	
6	D	1	Total	C	N	O	0
			15	8	3	4	
6	C	1	Total	C	N	O	0
			15	8	3	4	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	
7	B	1	Total	O	0
			1	1	

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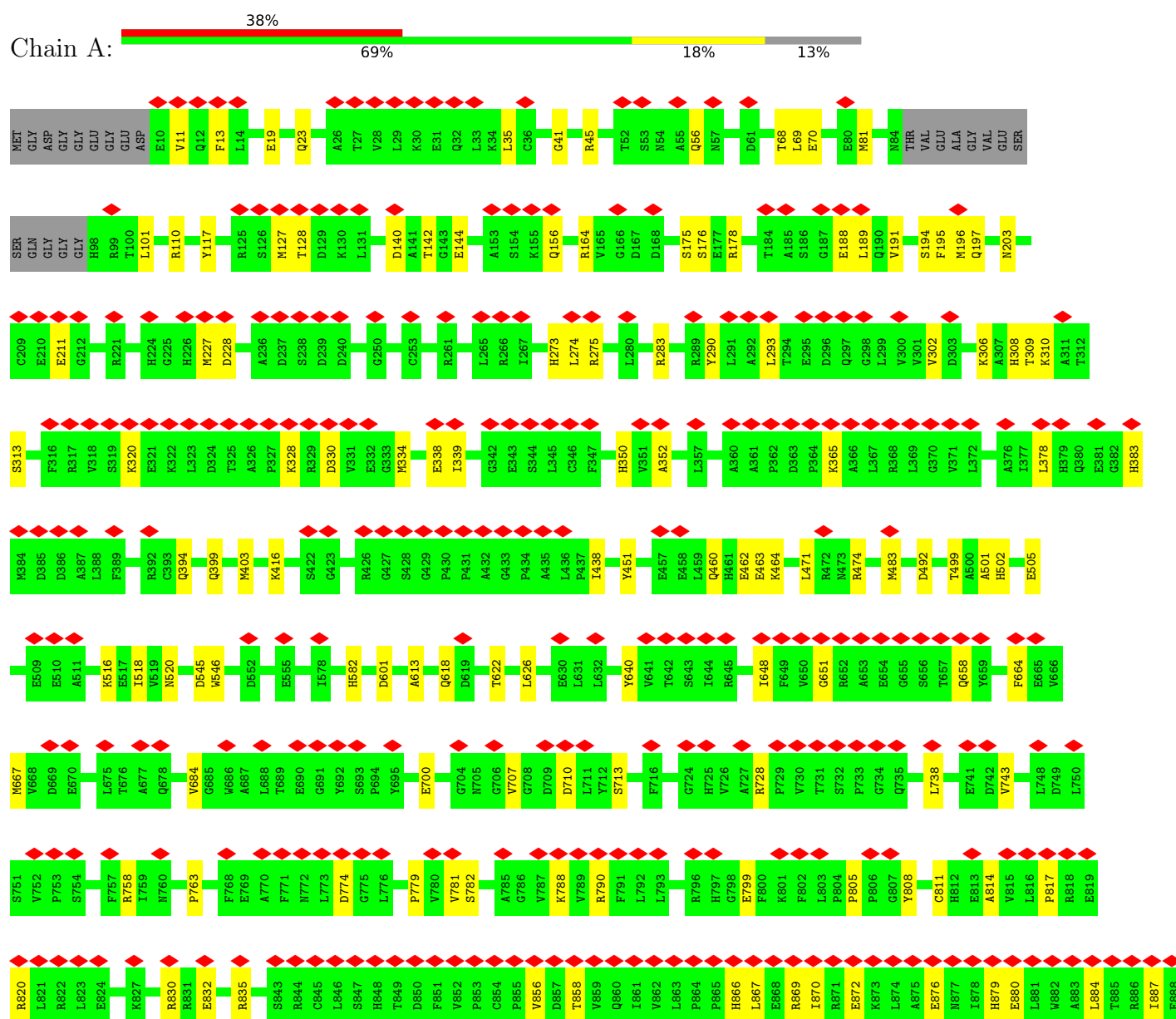
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Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total 1	O 1	0
7	C	1	Total 1	O 1	0

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 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.

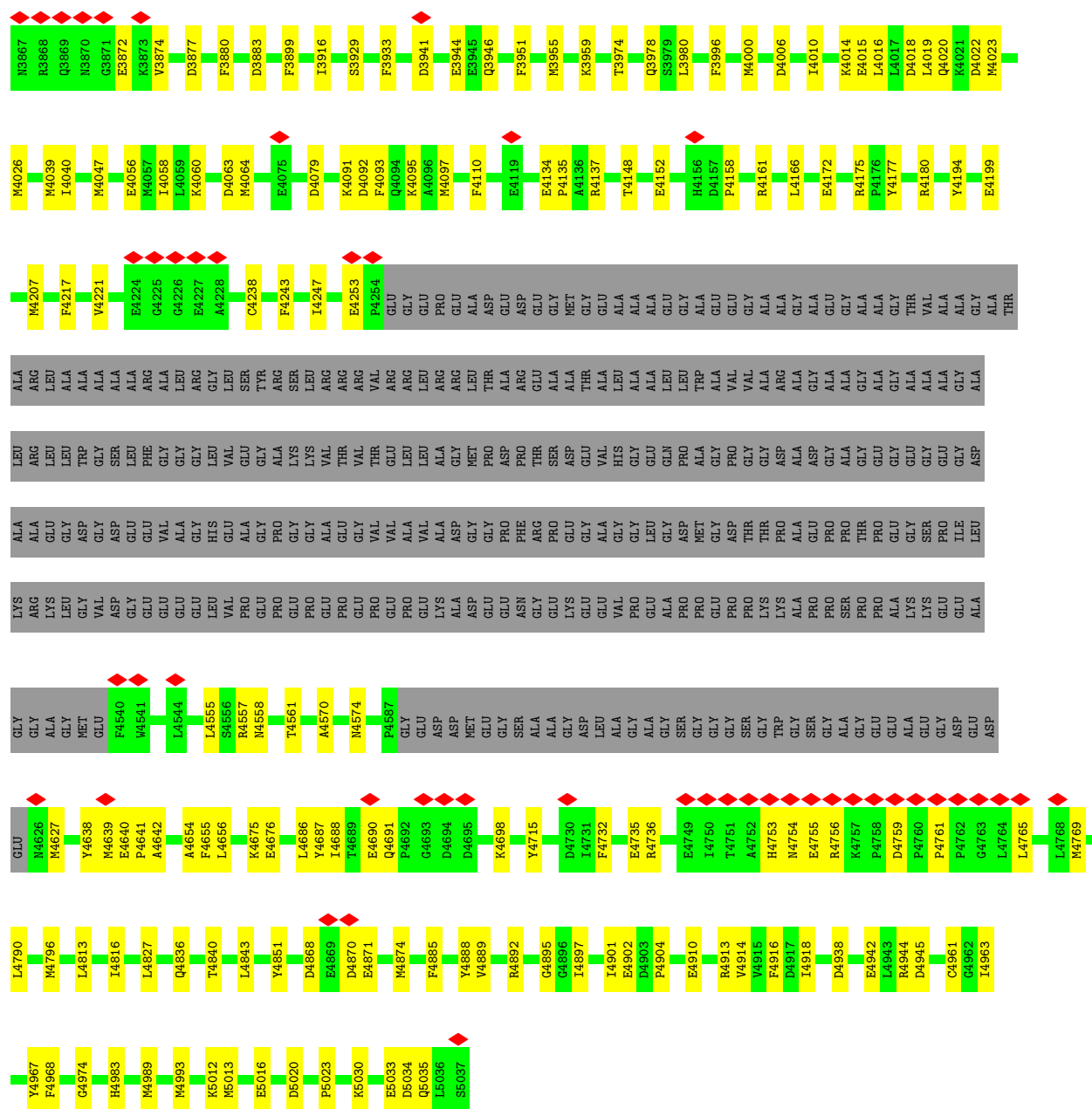
• Molecule 1: Ryanodine receptor 1



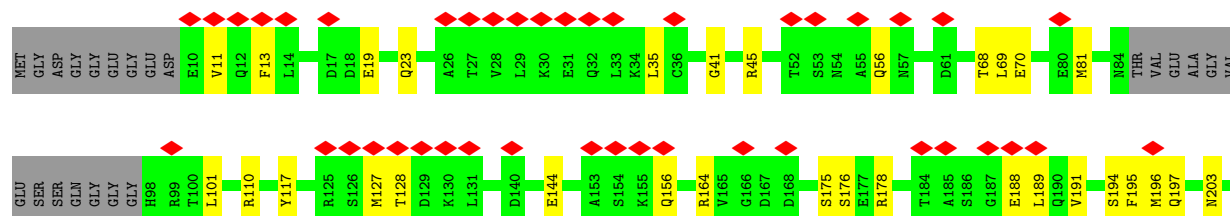
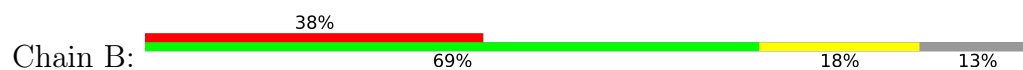
Q889	G890	W891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948
M949	L950	K951	K952	T953	K954	L955	P956	K957	T958	P1023	Y959	M960	M961	S962	M963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	E990	N991	A997	R998	D999	R1000	V1001	A1002	Q1003	G1004	M1005	S1006	Y1007	S1008	A1009	V1010	Q1011	D1012
T1013	P1014	A1015	R1016	R1017	N1018	P1019	R1020	L1021	V1022	Y1023	Y1024	R1025	L1026	D1027	L1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	P1055	P1056	D1057	Q1058	R1059	P1060	S1061	Q1062	V1063	G1064	M1065	Q1066	S1067	R1068	V1069	D1070	R1071	V1072
E1078	K1079	G1086	E1093	A1094	V1095	T1096	E1099	M1100	R1101	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	F1124	N1125	H1127	A1128	W1132	F1139	Q1144	S1145	G1146	D1147	G1150	D1154	L1155	T1156	E1157	T1163	L1164	M1165	E1167	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176														
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N1281	S1282	L1283	V1284	E1285	M1286	L1287	F1288	L1289	L1293	F1297	H1298	Q1299	F1300	R1301	R1302	C1303	T1304	ALA	GLY	THR	ARG	PRO	LEU	ALA	ASN	GLU	PRO	LYS	GLY	ALA	GLN	PRO	THR	GLU	ASP	ALA	ARG	PRO	ASP	TYR	GLU	ASN	LEU	ARG	SER	ALA	GLY	TRP	GLY	GLU									
ALA	GLU	GLY	LYS	GLU	THR	ALA	GLY	THR	PRO	GLY	THR	PRO	GLN	PRO	GLY	VAL	GLU	ALA	GLN	PRO	VAL	ARG	ALA	GLU	ASN	GLU	LYS	GLY	ALA	GLN	THR	THR	GLU	LYS	ASN	PHE	GLY	PHE	LYS	ALA	LYS	ALA	ALA	GLU	PRO	PRO	ALA												
THR	PRO	ALA	LEU	PRO	ARG	GLU	PRO	THR	ALA	D1419	M1420	R1421	D1422	D1423	P1424	E1425	I1426	I1427	L1428	N1429	Y1434	Y1435	S1436	A1441	C1447	V1448	G1451	T1454	P1455	D1456	Y1457	H1458	Q1459	H1460	D1461	M1462	N1463	D1465	K1468	V1469	R1470	A1471	V1472	M1476	G1477	D1478	E1479												
Q1480	G1481	M1482	V1483	H1484	S1485	S1486	L1487	L1488	C1489	S1490	M1491	C1492	Y1493	M1494	V1495	V1496	G1497	G1498	D1499	F1500	V1501	S1502	P1503	G1504	Q1505	Q1506	G1507	R1508	S1510	H1511	T1512	D1513	L1514	V1515	I1516	G1517	C1518	L1519	G1525	L1526	F1529	T1530	M1531	G1532	G1533	E1534	S1535	S1536	M1537	T1538	F1539	F1540	Q1541	V1542	E1543	P1544			
N1545	T1546	K1547	L1548	A1551	V1552	F1553	V1554	L1555	Q1559	N1560	V1561	I1562	E1565	L1566	G1567	K1568	Q1569	N1570	N1571	L1572	L1575	M1579	K1585	N1586	P1587	A1588	P1589	Q1590	C1591	R1594	L1595	E1596	M1601	Q1614	V1615	E1616	T1617	R1618	R1619	A1620	G1621	E1622	R1623	L1624	G1625	V1626	A1627	V1628	Q1629	V1630									
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L1786	P1787	A1788	A1789	G1790	V1791	A1792	E1793	A1794	P1795	A1796	R1797	E1805	R1808	E1817	A1818	V1819	R1820	D1821	G1822	Q1824	H1825	A1826	R1827	D1828	T1853	F1854	Q1861	K1864	M1865	V1870	F1871	T1872	E1873	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP										
GLU	GLU	LYS	GLU	ASP	GLU	GLU	GLU	GLU	LYS	GLU	ASP	LYS	GLU	GLU	ALA	PRO	GLU	GLY	LYS	GLU	ASP	L1922	E1923	E1924	G1925	L1926	M1929	M1939	L1943	E1956	Q1970	R1974	S1975	R1976	L1979	L1980	M1981	R1982	A1983	F1984	T1985	M1986	S1987	A1988															

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THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	L2866	L2867	S2868	R2869	W2870	P2871	Q2872	A2873	M2874	A2875	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	Q2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904		
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S2535	L2536	D2537	T2538	A2539	T2540	F2541	S2542	E2545	M2546	A2547	R2552	Y2553	L2554	C2555	L2556	L2559	P2560	L2562	T2563	K2564	C2565	A2566	F2569	A2570	T2571	T2572	E2573	H2574	R2575	A2576	L2577	M2578	V2579	D2580	S2581	M2582	L2583	H2584	T2585	V2586	Y2587	R2588	L2589	S2590	D2591	C2592	R2593	S2594	L2595	A2598	Q2599	R2600	D2601							
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	S3019	S3019	V3139	A3198	E3258	I3319	L3379	G3439		L3559	K3622		
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	P3021	P3021	T3141	A3200	K3260	R3321	L3381	T3441		G3561	L3624		
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	K3023	K3023	L3143	P3202	R3262	T3322	E3382	T3443		V3563	K3626		
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• Molecule 1: Ryanodine receptor 1





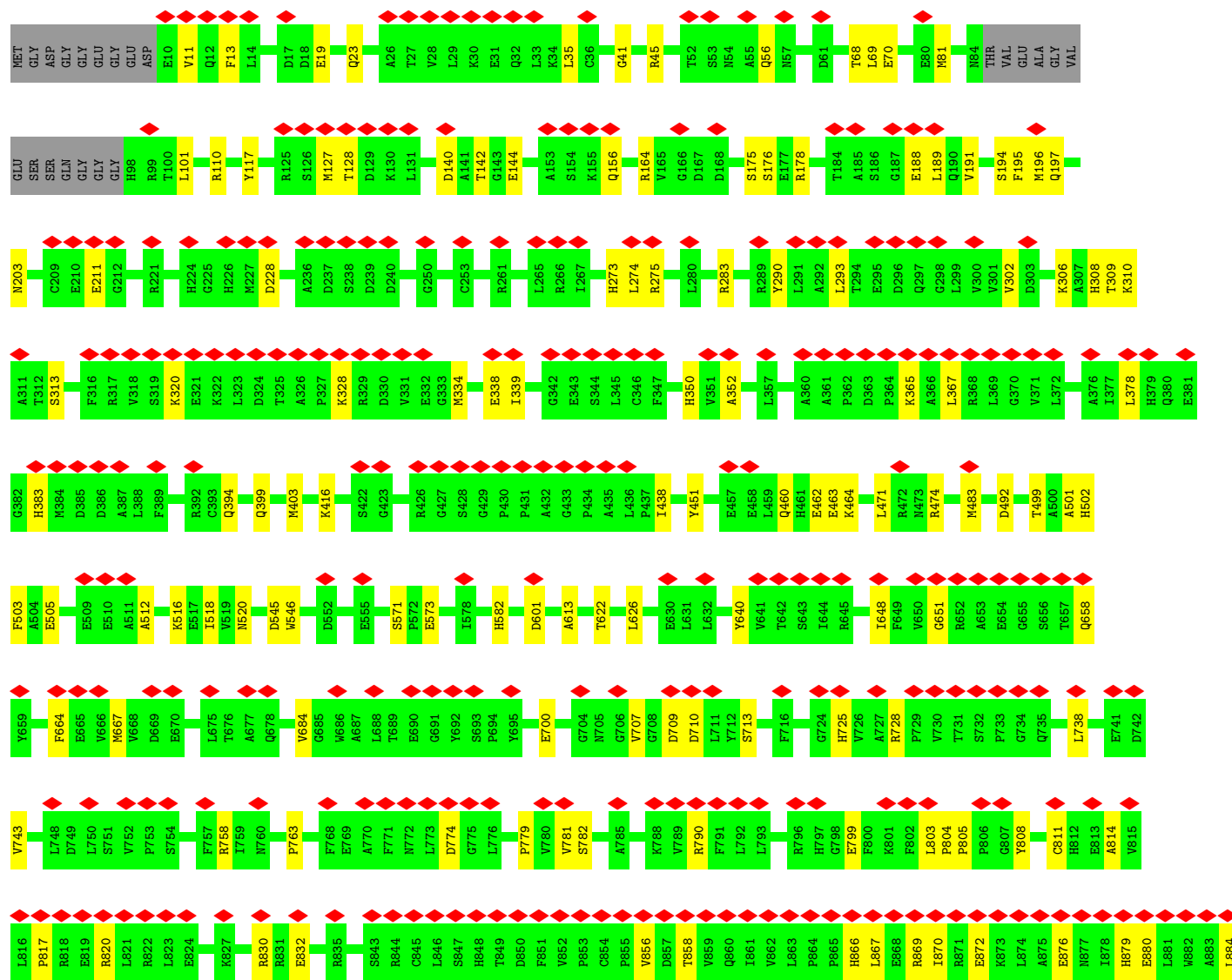
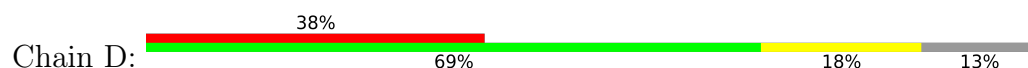


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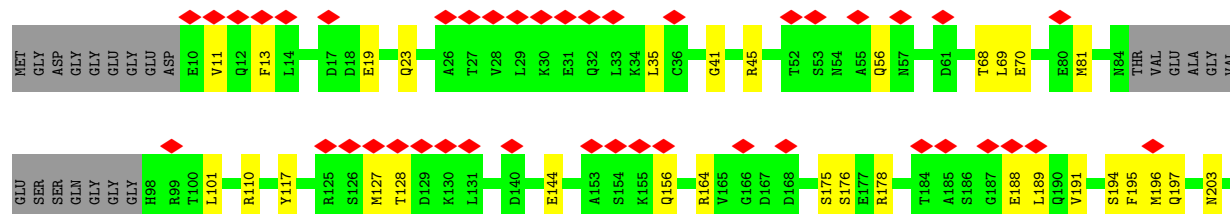
• Molecule 1: Ryanodine receptor 1





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LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	ASP	THR	VAL	ASP	ALA	GLY	T2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895						
S2776	Y2777	G2778	E2779	M2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	V2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	M2819	E2820	M2821	T2822	L2823	E2824	K2825	K2826	A2827	R2827	E2828	G2829	L2894	D2947	T2948	S2949	S2950	T2951	E2952	K2953	R2954	F2955
C2656	L2657	P2658	T2659	Y2660	V2661	A2662	N2663	F2664	G2665	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673	L2674	T2675	R2676	K2677	L2678	F2679	V2680	G2681	I2682	F2683	D2684	S2685	L2686	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	L2696	R2697	M2698	A2699	M2700	P2701	C2702	L2703	C2704	E2764	K2765	L2706	A2707	Q2708	A2709	D2769	K2770	L2771	Q2772	N2773	M2774	V2775			
G2592	R2593	S2594	L2595	A2598	Q2599	R2600	L2603	G2604	D2605	C2606	E2607	M2608	A2609	L2610	R2611	R2612	Y2613	L2614	R2615	P2616	S2617	M2618	L2619	Q2620	H2621	L2622	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	P2631	L2632	L2633	M2634	E2635	F2636	A2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	M2646	H2647	Y2648	R2649	C2651	Y2655									
F2526	L2527	P2528	D2529	M2530	R2531	A2532	A2533	A2534	S2535	L2536	T2537	T2538	A2539	P2540	F2541	S2542	E2545	M2546	A2547	Y2552	L2553	C2555	L2556	A2557	V2558	L2559	P2560	L2561	I2562	T2563	K2564	C2565	A2566	F2569	A2570	G2571	T2572	E2573	H2574	R2575	A2576	L2577	M2578	Y2579	D2580	S2581	M2582	L2583	H2584	Y2587	R2588	S2590	R2591											
G2446	K2447	G2448	E2449	T2456	S2459	L2460	V2461	T2462	L2463	D2464	D2465	L2466	S2471	L2472	F2473	L2474	Q2475	L2476	F2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	P2488	C2489	M2490	S2493	F2494	Y2495	F2496	D2497	H2498	F2499	M2502	T2512	E2513	N2514	Q2515	D2516	F2517	L2518	L2519	L2522	D2523														
R2369	Q2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	L2379	I2380	E2381	E2382	A2383	I2384	R2385	I2386	K2387	E2388	D2389	P2390	A2391	R2392	D2393	G2394	P2395	G2396	V2397	ARG	ASP	ARG	ARG	ARG	GLY	HIS	PHE	GLY	GLU	P2410	P2411	E2412	E2413	N2414	R2415	V2416	H2417	L2418	G2419	L2422	M2423	I2430	M2440	H2441	L2442										
L2258	E2259	M2260	S2261	G2262	T2263	G2264	L2265	G2266	M2267	G2268	G2269	L2288	D2294	L2295	E2296	K2297	V2298	A2303	Q2304	C2305	G2306	L2307	D2308	S2309	C2310	P2311	M2312	ARG	L2313	L2314	A2315	K2316	G2317	D2320	I2321	G2327	R2330	L2332	D2333	F2334	E2348	R2355	K2359	K2360	P2361	E2362	C2363	F2364	L2368															
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GLU	PRO	GLU	GLU	THR	SER	LEU	SER	ARG	ARG	LEU	THR	VAL	ARG	LEU	VAL	LYS	LYS	GLU	GLU	GLU	LYS	PRO	ALA	GLU	E2088	K2089	K2090	P2091	Q2095	M2101	V2102	W2105	E2108	L2116	M2120	L2123	Q2127	Y2128	V2149																									
M1981	R1982	A1983	F1984	T1985	M1986	S1987	A1988	A1989	E1990	T1991	M1992	R1993	R1994	T1995	R1996	E1997	F1998	R1999	S2000	P2001	Q2002	Q2003	E2004	Q2005	T2006	M2007	M2008	L2009	L2010	H2011	F2012	R2013	D2014	E2015	A2016	D2017	E2018	E2019	D2020	C2021	E2025	R2028	Q2029	D2030	L2031	Q2032	D2033	D2037	Q2045	L2046	GLU	GLY	GLU	GLU										

D3719	A3618	N3556	LYS	R3436	E3376	L3316	L3256	R3196	L3136	D3076	Y3016	A2956
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I3728	M3620	H3558	R3498	V3438	Q3378	N3318	E3258	A3198	F3138	R3078	L3018	G2958
K3731	H3621	L3559	R3499	G3439	L3379	I3319	S3259	A3199	V3139	T3079	S3019	F2959
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GLY	R3629	P3567	S3508	S2448	A3387	G3328	R3268	P3208	A3148	V3088	G3028	L2968
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A3634	A3634	A3574	T3513	R3453	L3392	T3333	T3273	Y3213	G3153	R3093	N3033	F2973
C3635	C3635	L3575	L3514	E3454	V3394	M3334	L3274	N3214	D3154	S3094	K3034	L2974
F3636	F3636	E3455	R3395	E3455	R3395	M3335	P3275	C3215	D3155	F3095	E3035	A2975
R3637	R3637	Q3456	D3396	Q3456	D3396	K3336	M3276	C3216	V3156	F3096	K3036	H2976
M3638	M3638	N3457	R3337	N3457	R3337	R3337	L3277	S3217	I3157	E3097	E3037	L2977
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E3670	E3670	Q3461	V3400	Q3461	F3398	A3339	Y3280	T3220	D3160	S3100	T3040	V2980
D3671	D3671	N3462	L3401	N3462	F3341	F3341	L3281	T3221	V3161	E3101	S3041	V2981
M3672	M3672	E3463	C3402	E3463	A3342	A3342	P3282	K3222	Q3162	D3102	L3042	S2982
D3676	D3676	L3464	R3403	L3464	P3344	P3344	R3283	P3224	V3163	T3103	F3043	S2983
G3681	G3681	N3465	D3404	N3465	I3345	I3345	N3284	R3225	S3164	E3104	C3044	G2984
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E3684	E3684	S3468	A3407	S3468	R3347	R3347	E3287	A3228	R3167	V3107	A3047	E2987
E3685	E3685	F3469	L3408	F3469	R3348	R3348	G3288	R3227	T3168	E3108	A3048	K2988
E3686	E3686	L3470	Y3409	L3470	A3349	A3349	P3289	I3229	L3169	N3109	L3049	S2989
E3687	E3687	T3471	P3410	T3471	R3350	R3350	E3290	L3230	G3170	L3110	V3050	P2990
E3688	E3688	D3473	L3411	D3473	P3351	P3351	A3291	G3231	S3171	R3111	R3051	H2991
E3689	E3689	S3474	L3413	S3474	E3352	E3352	P3292	L3232	I3172	L3112	H3052	E2992
V3690	V3690	K3475	R3414	K3475	L3353	L3353	P3293	P3233	T3173	G3113	R3053	Q2993
E3691	E3691	S3476	V3415	S3476	H3355	H3355	P3294	N3234	S3174	K3114	V3054	E2994
E3692	E3692	K3477	V3416	K3477	S3356	S3356	L3296	V3236	G3175	V3115	S3055	T2995
V3693	V3693	M3478	D3417	M3478	H3357	H3357	P3297	E3237	T3177	S3116	L3056	K2996
L3694	L3694	A3479	N3418	A3479	F3358	F3358	A3298	E3238	T3178	GLN	F3057	F2997
L3695	L3695	ALA	N3419	ALA	I3359	I3359	G3299	M3239	T3179	ALA	G3058	F2998
H3699	H3699	GLY	R3420	GLY	P3360	P3360	A3300	C3240	N3180	THR	G3059	A2999
F3705	F3705	ASP	A3421	ASP	T3361	T3361	P3301	P3241	T3181	GLN	T3060	K3000
T3708	T3708	GLN	H3422	GLN	I3362	I3362	P3302	D3242	T3182	VAL	A3061	K3001
K3714	K3714	GLN	V3423	GLN	G3363	G3363	P3303	D3243	V3183	K3123	P3062	L3002
S3715	S3715	GLY	L3424	GLY	R3364	R3364	C3304	P3244	E3184	G3124	A3063	L3003
L3716	L3716	GLY	T3425	GLY	L3365	L3365	T3305	V3245	K3185	G3125	V3064	F3004
D3717	D3717	SER	E3426	SER	R3366	R3366	A3306	L3246	L3186	Q3127	V3065	L3005
E3718	E3718	GLN	P3427	GLN	K3367	K3367	T3307	D3247	R3187	N3128	N3066	I3006
		ARG	A3428	ARG	R3368	R3368	T3308	R3248	P3188	L3129	C3067	N3007
		THR	N3429	THR	A3369	A3369	S3309	L3249	A3189	T3130	L3068	Q3008
		LYS	N3430	LYS	G3370	G3370	D3310	M3250	L3190	T3131	H3069	Y3009
			A3431		K3371	K3371	H3311	A3251	G3191	T3132	I3070	F3010
			E3432		V3372	V3372	L3312	D3252	E3192	T3133	L3071	N3012
			E3433		E3373	E3373	S3314	G3254	G3193	V3134	A3072	H3013
			L3434		E3375	E3375	S3314	G3254	L3194	A3135	R3074	C3014
			F3435				L3315		A3195		L3075	L3015

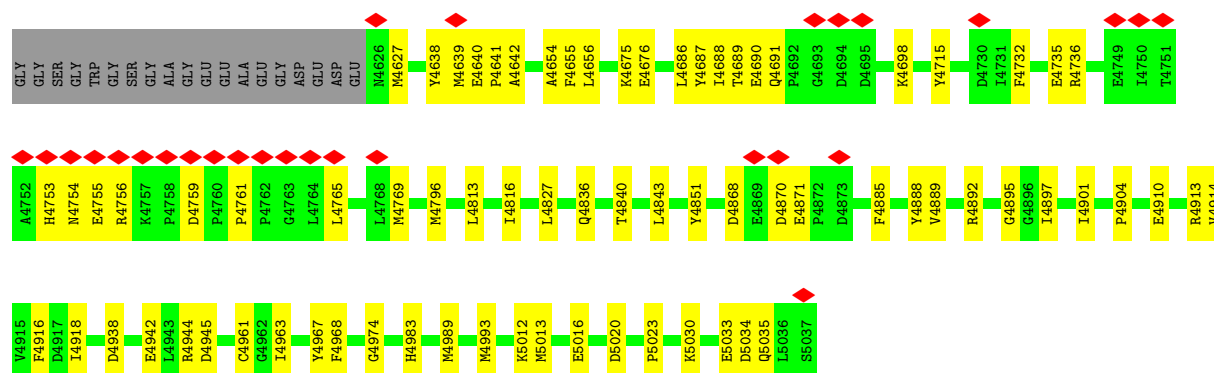




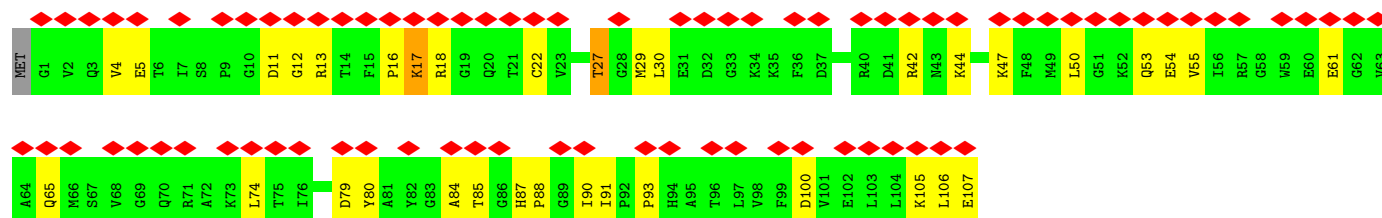


S3314	G3254	L3194	V3134	S3074	C3014	R2954	L2894	THR	N2774	Y2714	Y2655	C2590
L3315	G3255	A3195	A3135	L3075	L3015	P2955	E2895	GLU	W2775	V2715	Y2656	R2591
L3316	L3256	R3196	L3136	D3076	F3016	F2956	A2896	LYS	S2776	D2716	C2656	G2592
A3257	A3257	L3197	L3137	A3077	F3017	P2957	K2897	LYS	Y2777	A2717	L2657	R2593
E3258	E3258	A3198	P3138	R3078	L3018	G2958	G2898	THR	G2778	S2718	P2658	S2594
S3259	S3259	A3199	V3139	T3079	S3019	P2959	G2899	ARG	E2779	Y2719	T2659	L2595
G3260	G3260	A3200	V3139	V3079	S3019	P2959	G2899	LYS			G2660	
A3261	A3261	M3201	L3140	M3081	T3020	Q2961	T2901	SER	N2780	S2720	W2661	A2598
R3262	R3262	P3202	T3141	K3082	P3021	Q2962	T2902	GLN	V2781	S2721	W2662	Q2599
L3263	L3263	V3203	T3142	S3083	K3023	Q2962	H2902	THR	D2782	K2722	A2662	R2600
Y3263	Y3263	F3204	L3143	G3084	V3024	L2963	P2903	ALA	E2783	A2723	N2663	
T3264	T3264	A3204	F3144	G3084	V3024	L2964	E2784	GLN	E2784	E2724	F2664	I2603
E3265	E3265	F3205	Q3145	P3085	L3025	R2965	L2905	THR	L2785	K2725	G2665	E2604
M3266	M3266	L3206	H3146	E3086	G3026	W2966	V2906	TYR	K2786	K2725	V2666	D2605
P3267	P3267	E3207	I3147	I3087	S3027	W2967	P2907	ASP	T2787	LYS	T2667	D2606
H3268	H3268	F3208	A3148	V3088	G3028	D2968	Y2908	PRO	T2787	ALA	T2668	C2606
I3329	I3329	Q3209	Q3149	K3089	G3029	I2969	D2909	ARG	H2788	THR	S2668	C2606
V3269	V3269	L3210	H3150	K3089	G3029	I2969	D2909	GLU	P2789	ASP	E2669	L2607
I3270	I3270	N3211	H3150	A3090	H3030	S2970	T2910	GLY	M2790	ALA	E2670	N2608
E3271	E3271	K3211	Q3151	G3091	A3031	Q2971	L2911		L2791	GLU	E2671	A2609
L3272	L3272	F3212	F3152	L3092	S3032	E2972	T2912		T2912	GLY	L2672	L2610
T3273	T3273	G3213	G3153	R3093	N3033	F2973	A2913		N2734	N2734	H2673	C2611
L3274	L3274	N3214	D3154	S3094	K3034	I2974	K2914		P2735	P2735	H2674	R2612
P3275	P3275	A3215	D3155	F3095	E3035	A2975	E2915		D2736	D2736	T2675	T2614
M3276	M3276	C3216	V3156	F3096	E3035	A2975	E2915		P2737	P2737	R2676	R2615
K3277	K3277	S3217	I3157	E3097	K3037	H2976	T2916		R2738	R2738	K2677	P2616
L3278	L3278	V3218	L3158	S3098	M3038	L2978	A2917		F2739	F2739	L2678	S2617
C3279	C3279	Y3219	D3159	A3099	I3039	E2979	D2919		V2740	V2740	W2680	L2618
S3279	S3279	T3220	D3160	S3100	T3040	G2964	R2918		E2741	E2741	G2681	L2619
Y3280	Y3280	T3221	V3161	E3101	S3041	V2981	E2921		T2742	T2742	Q2620	Q2621
A3942	A3942	K3222	Q3162	D3102	L3042	S2982	K2922		L2743	L2743	F2683	H2621
K3943	K3943	S3223	V3163	L3103	F3043	S2983	A2923		N2744	N2744	D2684	L2622
P3944	P3944	P3224	S3164	E3104	C3044	G2984	A2924		V2745	V2745	S2685	L2623
L3345	L3345	R3225	C3165	K3105	K3045	R2985	Q2924		I2746	I2746	L2686	L2623
W3295	W3295	E3226	Y3166	M3106	L3046	V2986	E2925		L2747	L2747	A2687	R2625
R3287	R3287	R3227	R3167	V3107	A3047	E2987	L2926		P2748	P2748	H2688	L2626
G3288	G3288	A3228	T3168	E3108	A3048	K2988	L2927		E2749	E2749	K2689	V2627
P3289	P3289	L3169	L3169	N3109	L3049	S2989	P2929		K2750	K2750	K2690	F2628
E3290	E3290	L3230	C3170	L3110	V3050	P2990	L2930		L2751	L2751	Y2691	D2629
A3291	A3291	G3231	S3171	R3111	R3051	H2991	Q2931		D2752	D2752	D2692	V2630
P3292	P3292	L3232	I3172	L3112	H3052	E2992	M2932		S2753	S2753	Q2693	P2631
L3293	L3293	P3233	S3173	G3113	R3053	Q2993	N2933		F2754	F2754	E2694	L2632
P3294	P3294	N3234	S3174	K3114	V3054	E2994	L2934		N2756	N2756	L2695	L2633
A3295	A3295	S3235	L3175	V3115	S3055	I2995	Y2935		K2757	K2757	Y2696	N2634
L3296	L3296	V3236	G3176	S3116	L3056	K2996	A2936		F2758	F2758	R2697	E2635
P3297	P3297	E3237	T3177	GLN	F3057	P2997	V2937		A2637	A2637	M2698	F2636
T3298	T3298	ALA	T3178	ALA	F3057	P2997	V2937		L2817	L2817	A2699	Y2637
N3299	N3299	ARG	T3178	ARG	G3058	P2998	T2938		A2759	A2759	M2700	K2638
G3299	G3299	THR	K3179	THR	T3059	P2999	R2938		E2760	E2760	P2701	M2639
A3300	A3300	VAL	N3180	VAL	T3059	A2999	R2939		Y2761	Y2761	C2702	P2640
P3301	P3301		T3181		A3061	K3000	GLY		T2762	T2762	L2703	L2641
P3302	P3302		Y3182		P3062	L3002	LYS		H2763	H2763	C2704	L2641
P3303	P3303		V3183		A3063	L3003	ASP		E2764	E2764	A2705	L2643
C3304	C3304		E3184		V3064	P3004	MET		K2765	K2765	L2706	L2644
T3305	T3305		K3185		V3065	L3005	GLU		W2766	W2766	L2706	L2644
L3246	L3246		L3186		N3066	I3006	L2946		A2707	A2707	T2708	T2645
D3247	D3247		R3187		C3067	T3067	D2947		A2767	A2767	G2708	H2646
R3248	R3248		P3188		L3068	N3007	T2948		F2768	F2768	A2709	H2647
T3309	T3309		A3189		T3130	Q3008	S2949		D2769	D2769	L2710	Y2648
S3308	S3308		L3190		Y3131	Y3009	S2950		K2770	K2770	P2711	E2649
D3310	D3310		G3191		T3132	F3010	T2951		I2771	I2771	P2712	R2650
H3311	H3311		E3192		T3133	N3012	E2952		D2772	D2772	D2713	C2651
L3312	L3312		C3193			H3013	K2953		N2773	N2773		

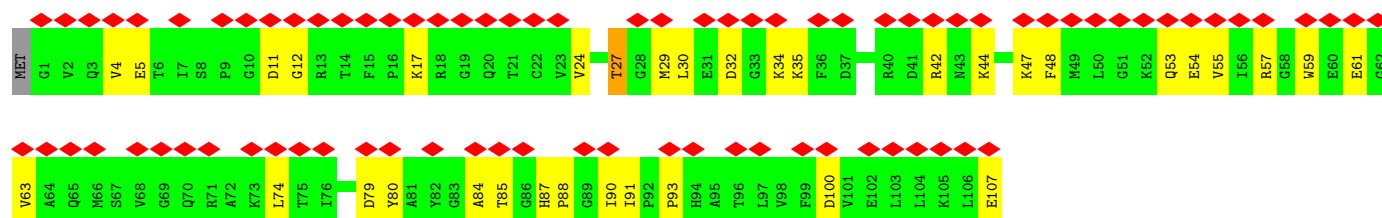
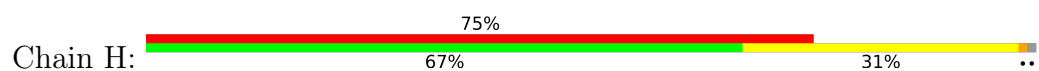




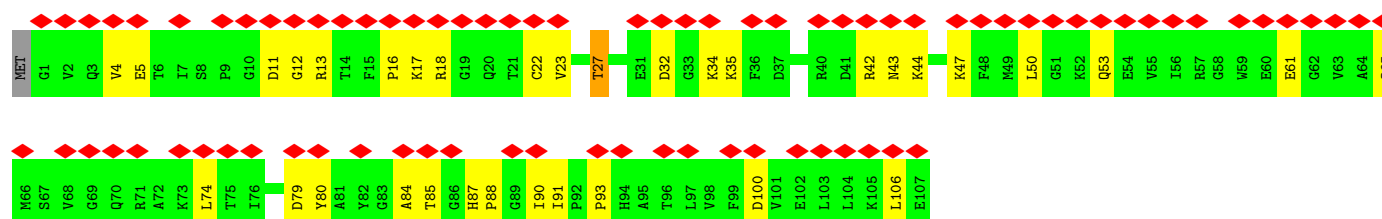
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

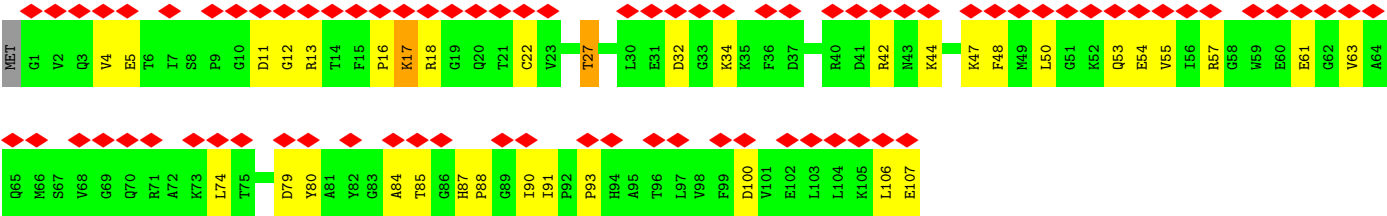


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.395	Depositor
Minimum map value	-0.215	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	423.424, 423.424, 423.424	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, ATP, A1BD5

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	0/35977	0.35	2/48726 (0.0%)
1	B	0.25	0/35977	0.35	2/48726 (0.0%)
1	C	0.25	0/35977	0.35	2/48726 (0.0%)
1	D	0.25	0/35977	0.35	2/48726 (0.0%)
2	E	0.23	0/850	0.42	0/1146
2	F	0.23	0/850	0.46	0/1146
2	G	0.23	0/850	0.41	0/1146
2	H	0.23	0/850	0.41	0/1146
All	All	0.25	0/147308	0.36	8/199488 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2639	MET	CB-CG-SD	5.15	128.16	112.70
1	C	2639	MET	CB-CG-SD	5.14	128.12	112.70
1	A	2639	MET	CB-CG-SD	5.14	128.11	112.70
1	B	2639	MET	CB-CG-SD	5.13	128.09	112.70
1	A	3603	LEU	CA-CB-CG	5.01	133.84	116.30

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	35150	0	34797	644	0
1	B	35150	0	34797	646	0
1	C	35150	0	34797	643	0
1	D	35150	0	34797	650	0
2	E	831	0	831	32	0
2	F	831	0	831	32	0
2	G	831	0	831	27	0
2	H	831	0	831	22	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	15	0	0	0	0
6	C	15	0	0	0	0
6	D	15	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	144120	0	142560	2658	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 9.

The worst 5 of 2658 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2765:LYS:HZ3	1:A:2857:PRO:HB2	1.38	0.85
1:B:2765:LYS:HZ2	1:B:2860:PRO:HA	1.41	0.85
2:F:18:ARG:HH21	2:F:50:LEU:HD22	1.43	0.83
1:D:3539:ARG:HH12	1:D:3542:LEU:HD22	1.43	0.83
2:E:61:GLU:OE2	2:E:61:GLU:N	2.12	0.82

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	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	B	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	C	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	D	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
2	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17960/20580 (87%)	17398 (97%)	562 (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	3836/4276 (90%)	3815 (100%)	21 (0%)	81	82
1	B	3836/4276 (90%)	3816 (100%)	20 (0%)	81	82
1	C	3836/4276 (90%)	3815 (100%)	21 (0%)	81	82
1	D	3836/4276 (90%)	3817 (100%)	19 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	89/90 (99%)	85 (96%)	4 (4%)	24	52
2	F	89/90 (99%)	85 (96%)	4 (4%)	24	52
2	G	89/90 (99%)	83 (93%)	6 (7%)	15	41
2	H	89/90 (99%)	84 (94%)	5 (6%)	19	46
All	All	15700/17464 (90%)	15600 (99%)	100 (1%)	76	81

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3759	GLU
1	D	2369[B]	ARG
1	C	4871	GLU
1	B	4871	GLU
1	D	960	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3704	HIS
1	C	2260	ASN
1	D	949	ASN
1	C	2253	HIS
1	C	4009	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
6	A1BD5	A	5304	-	16,16,16	0.97	0	21,23,23	0.73	0
6	A1BD5	D	5304	-	16,16,16	0.96	0	21,23,23	0.73	0
6	A1BD5	C	5304	-	16,16,16	0.96	0	21,23,23	0.73	0
3	ATP	D	5301	-	32,33,33	0.32	0	48,52,52	0.41	0
6	A1BD5	B	5304	-	16,16,16	0.96	0	21,23,23	0.73	0
3	ATP	A	5301	-	32,33,33	0.32	0	48,52,52	0.41	0
3	ATP	B	5301	-	32,33,33	0.32	0	48,52,52	0.41	0
3	ATP	C	5301	-	32,33,33	0.32	0	48,52,52	0.42	0

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
6	A1BD5	A	5304	-	-	0/4/4/4	0/2/2/2
6	A1BD5	D	5304	-	-	0/4/4/4	0/2/2/2
6	A1BD5	C	5304	-	-	0/4/4/4	0/2/2/2
3	ATP	D	5301	-	-	10/22/38/38	0/3/3/3
6	A1BD5	B	5304	-	-	0/4/4/4	0/2/2/2
3	ATP	A	5301	-	-	10/22/38/38	0/3/3/3
3	ATP	B	5301	-	-	10/22/38/38	0/3/3/3
3	ATP	C	5301	-	-	10/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

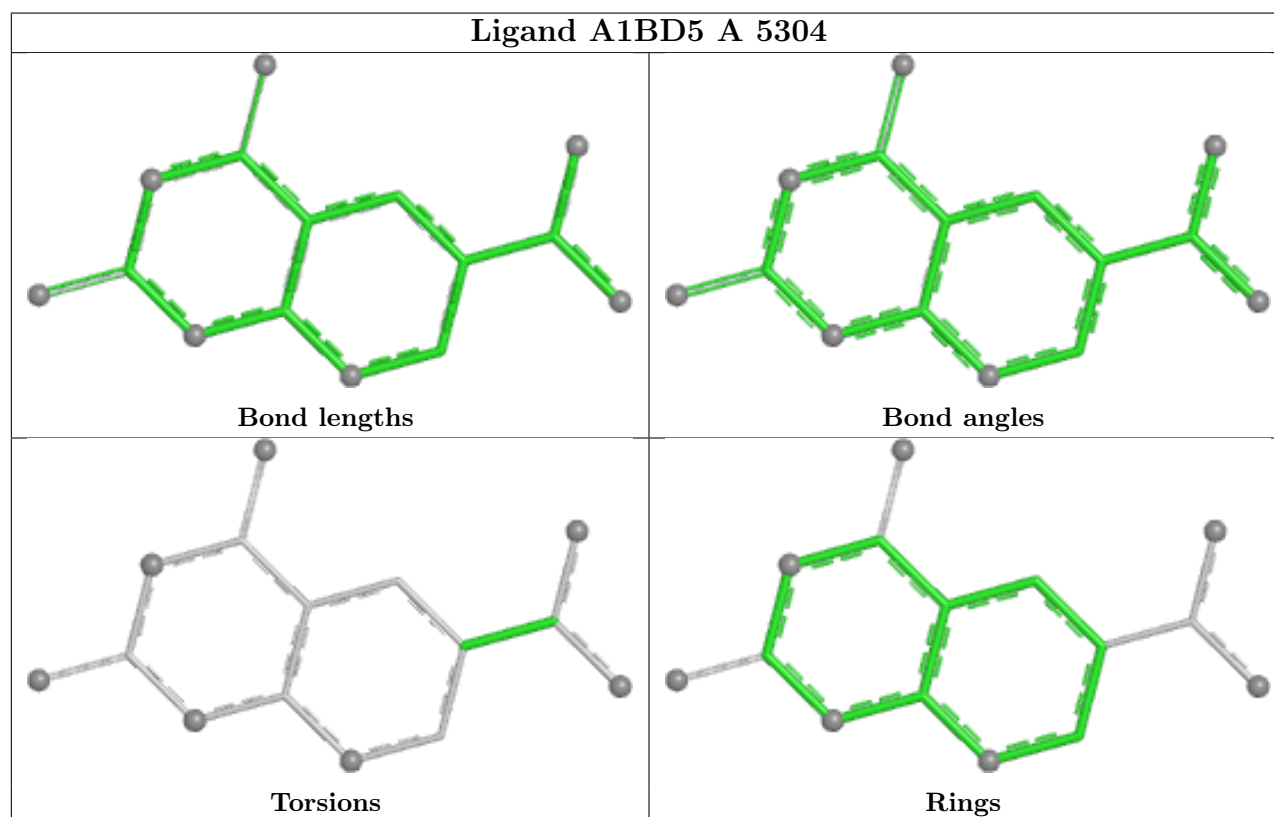
5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	PB-O3B-PG-O2G
3	A	5301	ATP	C5'-O5'-PA-O1A
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	PB-O3B-PG-O2G

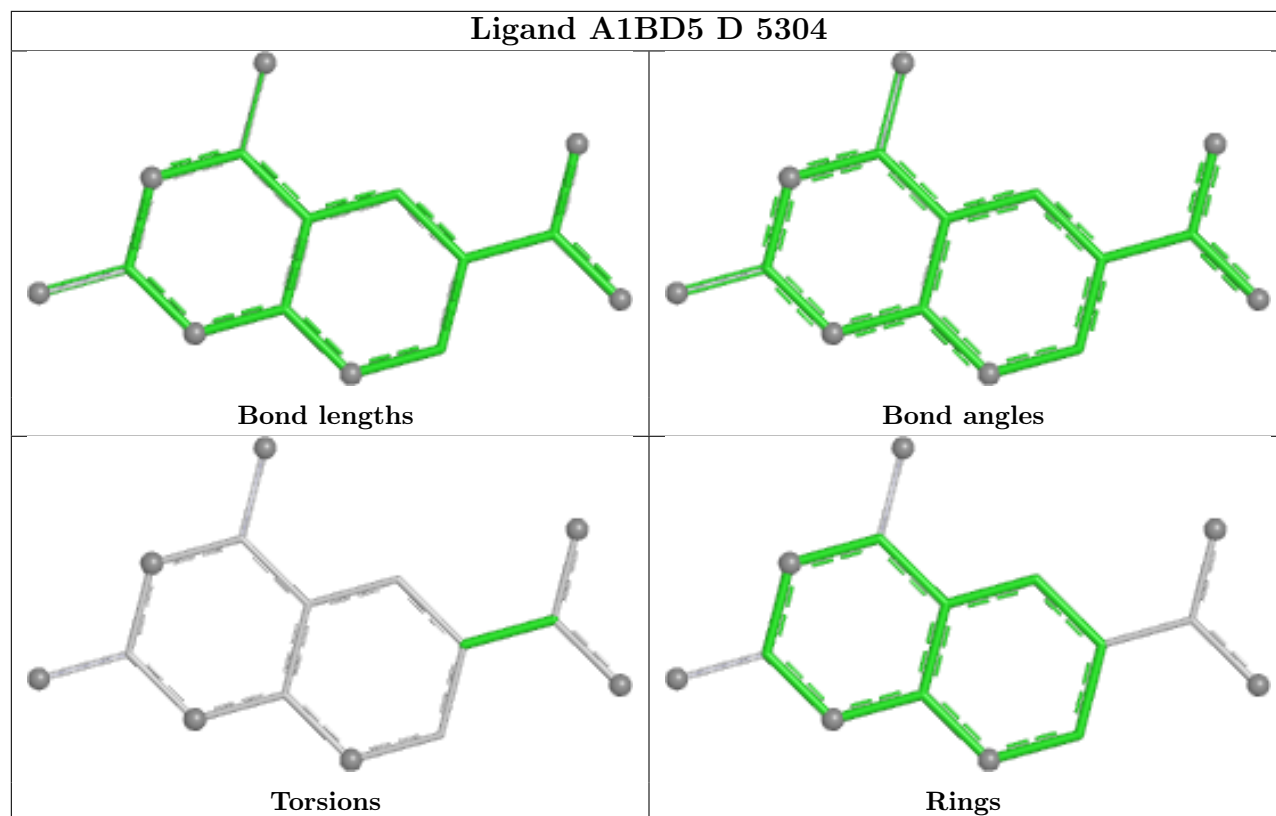
There are no ring outliers.

No monomer is involved in short contacts.

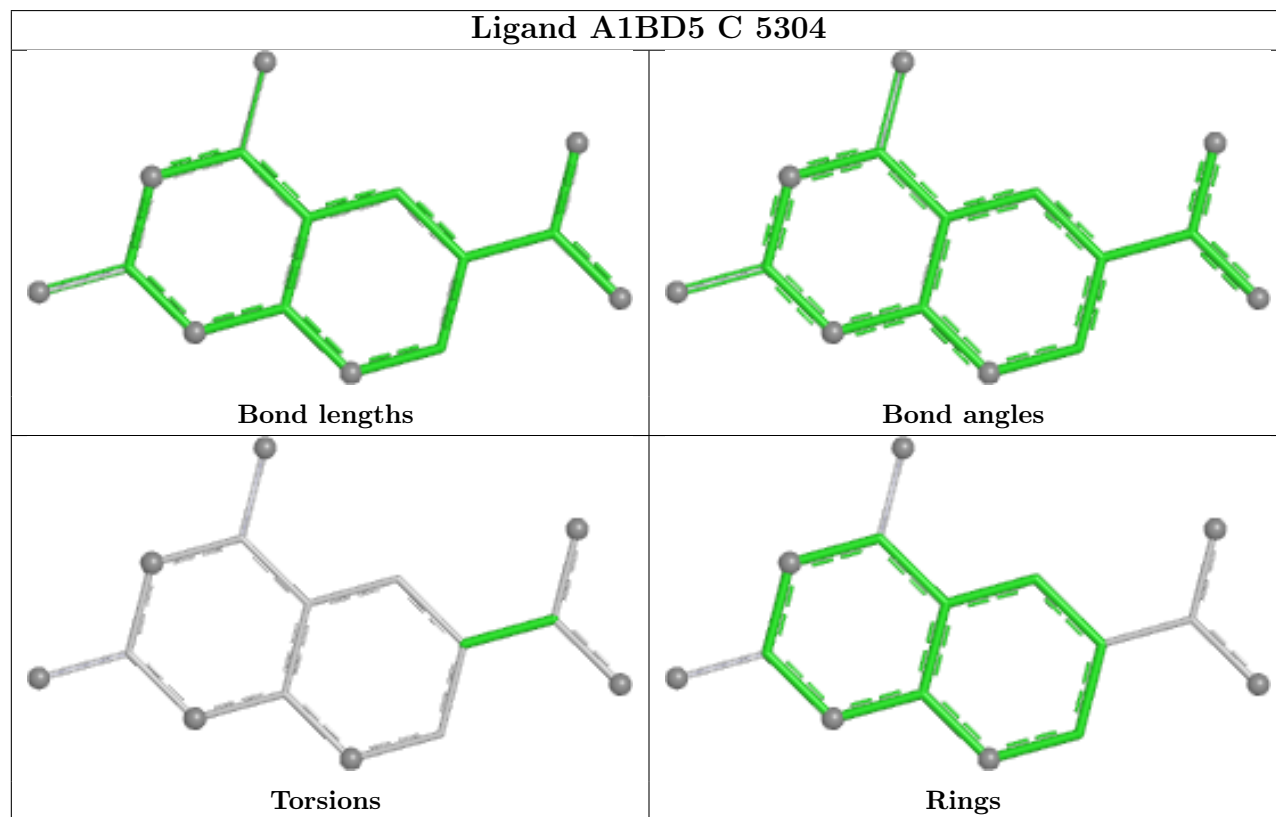
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



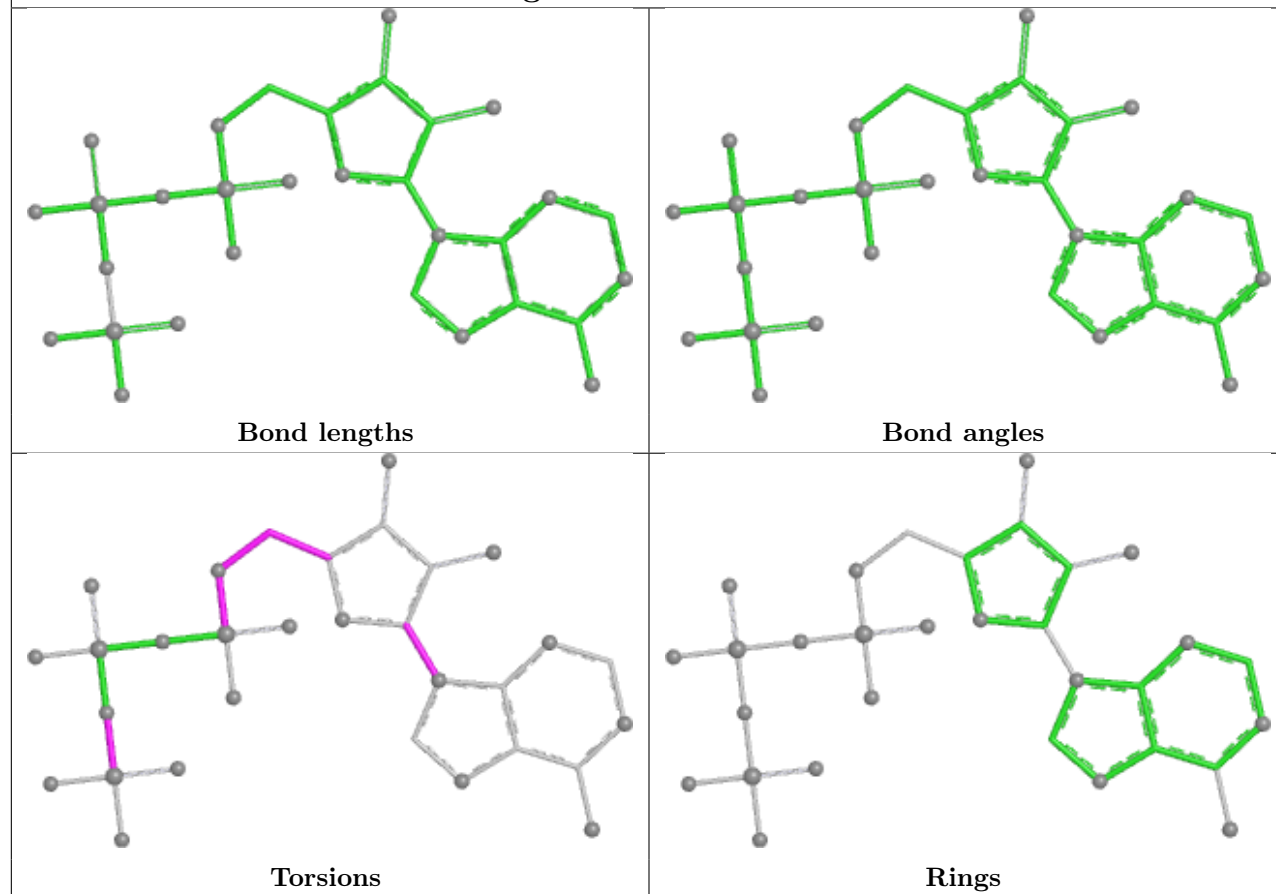
Ligand A1BD5 D 5304



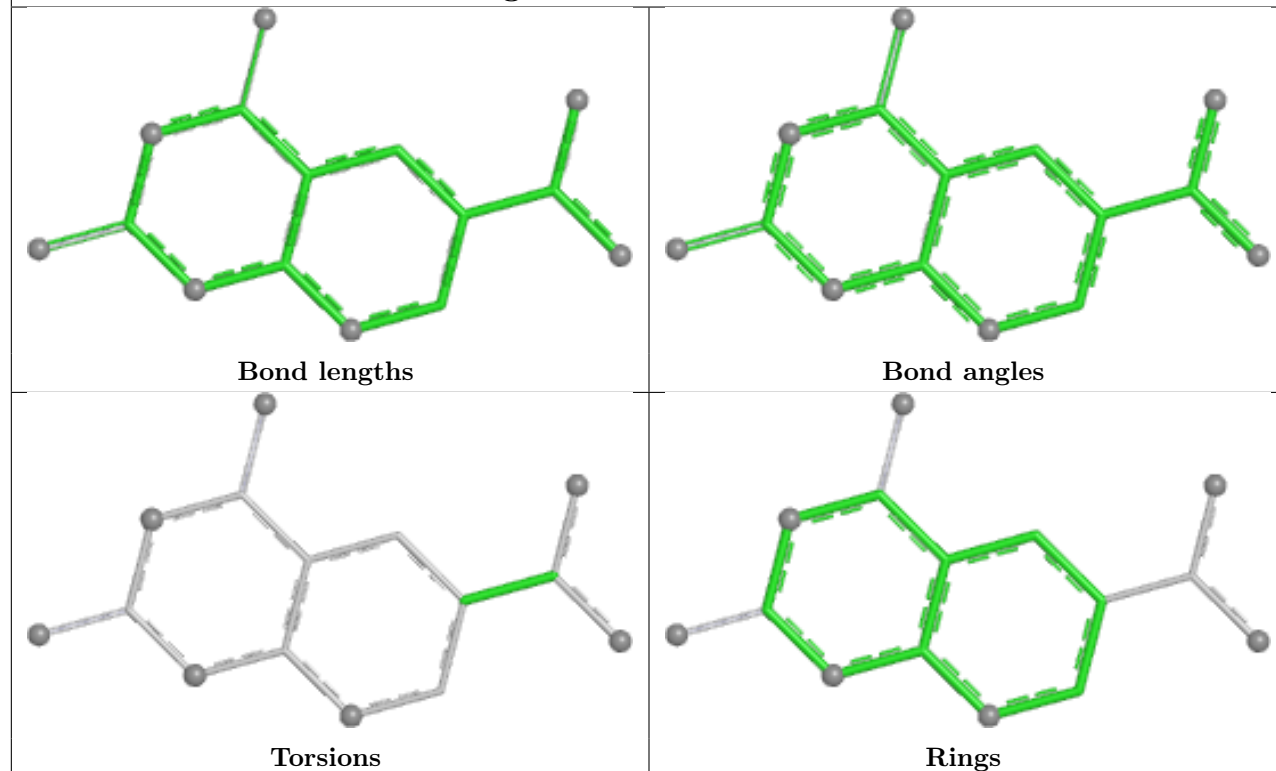
Ligand A1BD5 C 5304

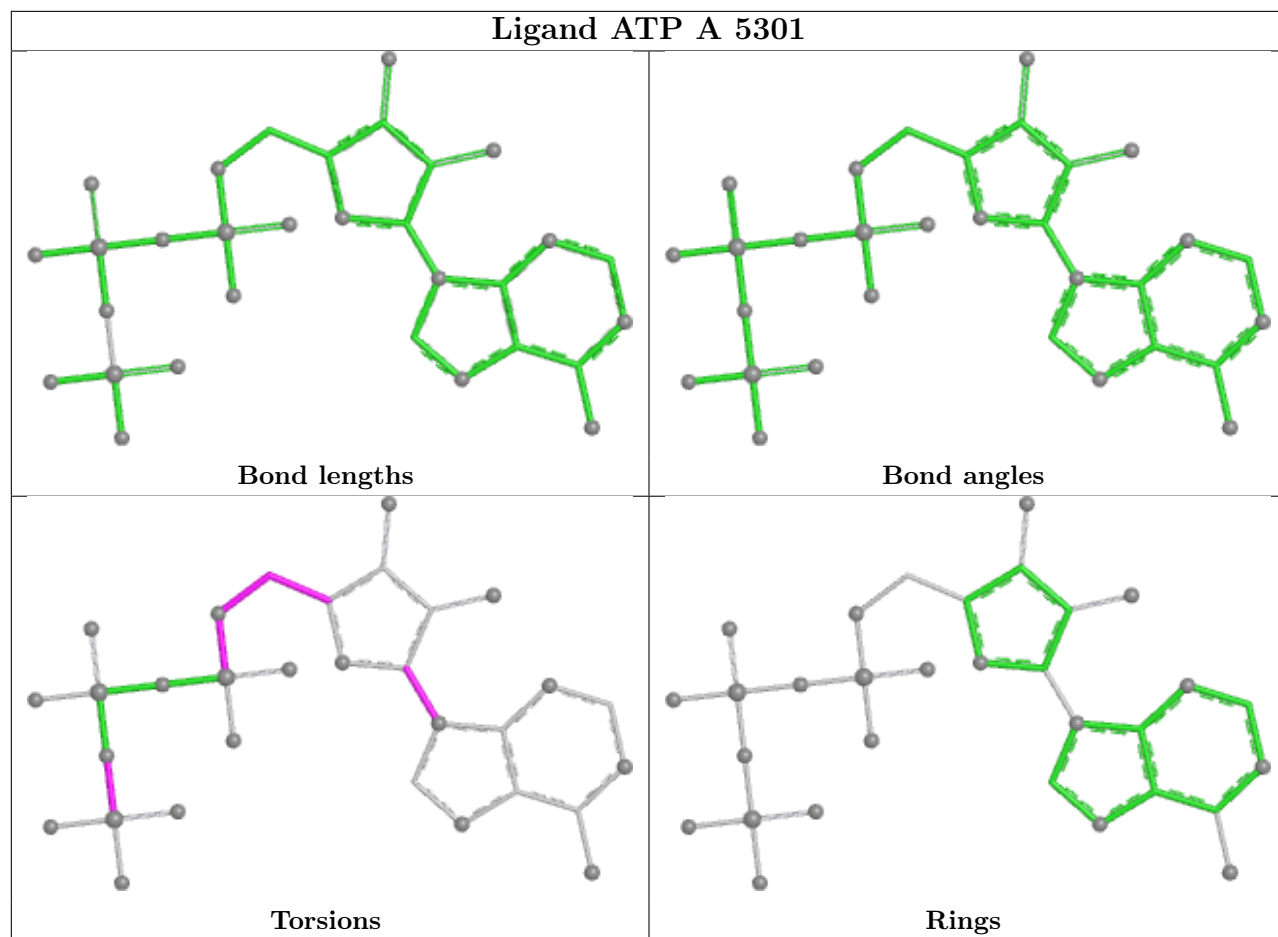


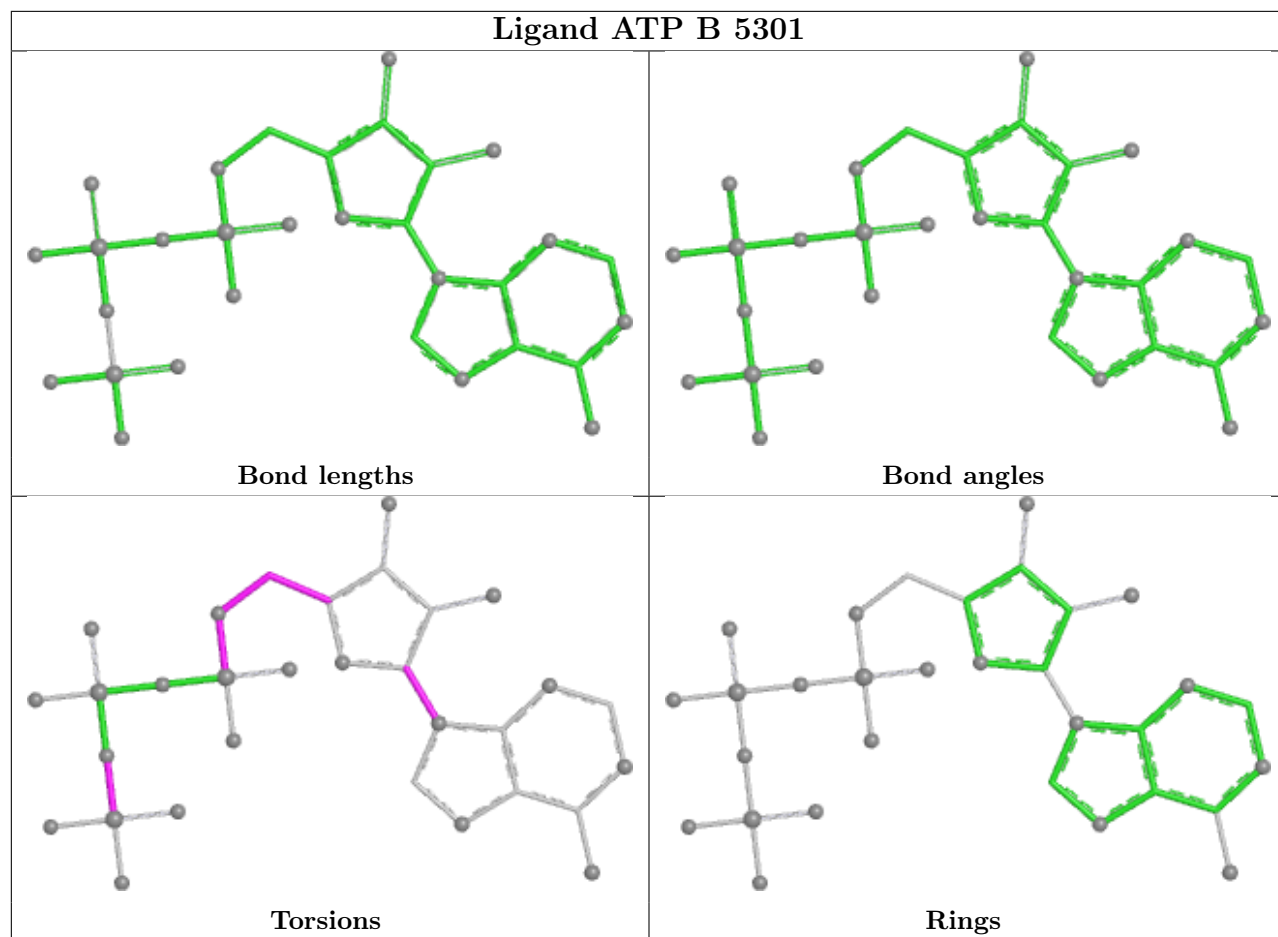
Ligand ATP D 5301

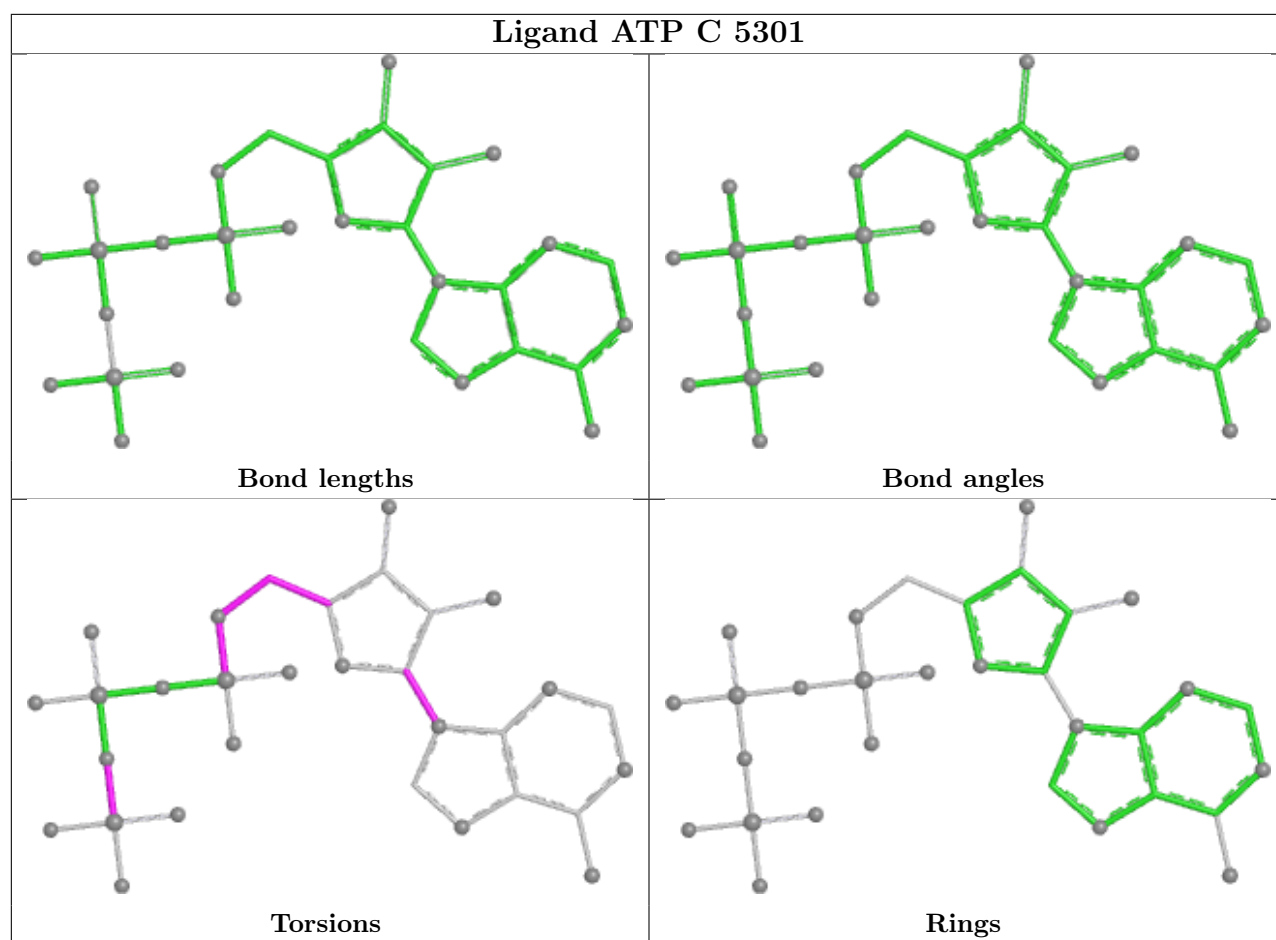


Ligand A1BD5 B 5304









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.

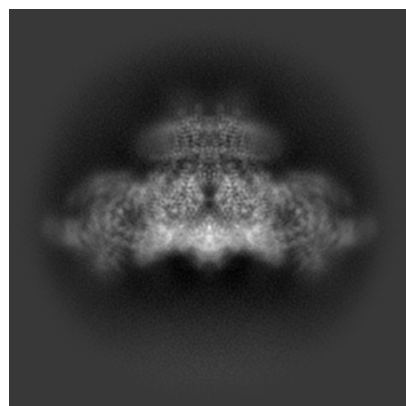
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47394. These allow visual inspection of the internal detail of the map and identification of artifacts.

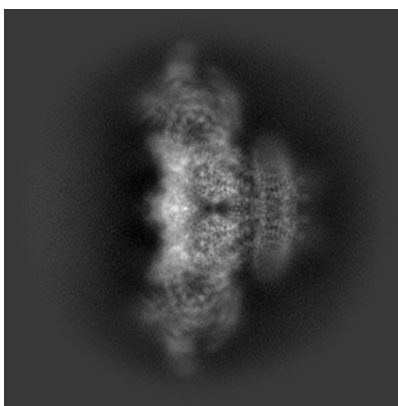
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

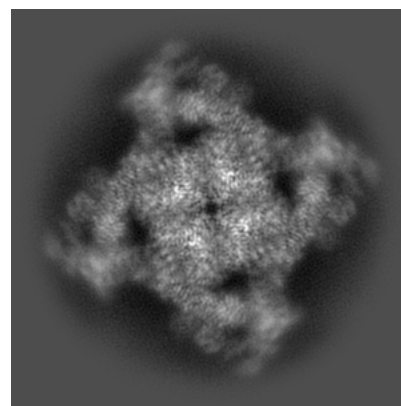
6.1.1 Primary map



X

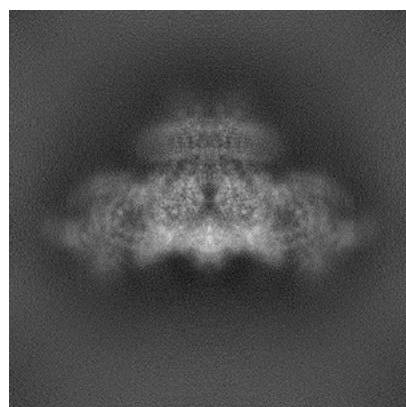


Y

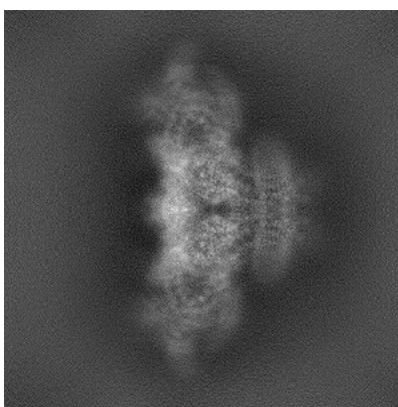


Z

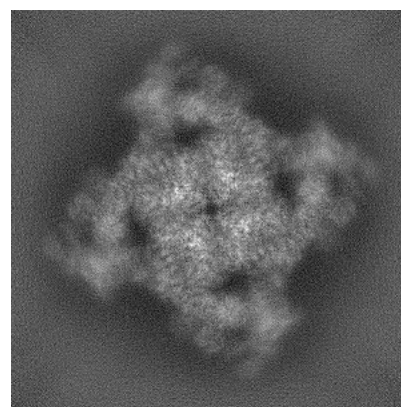
6.1.2 Raw map



X



Y

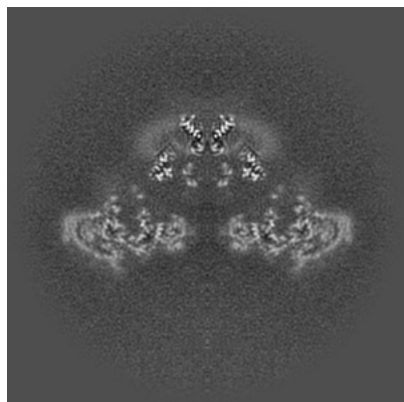


Z

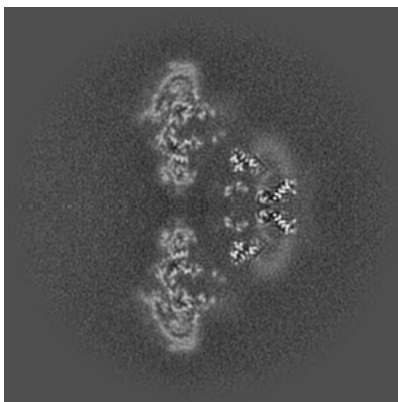
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

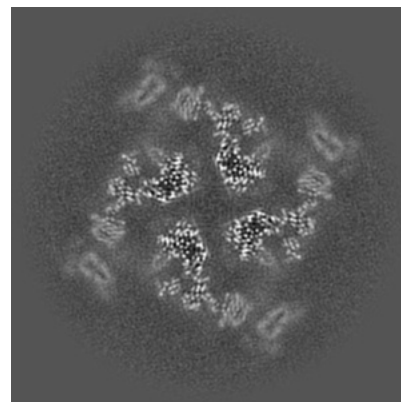
6.2.1 Primary map



X Index: 256

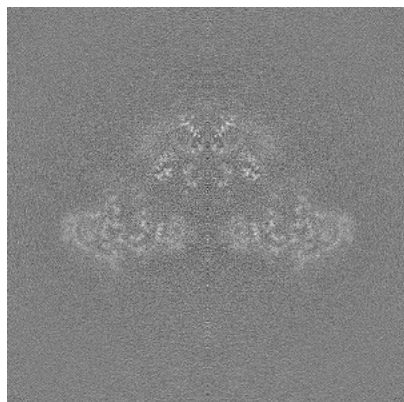


Y Index: 256

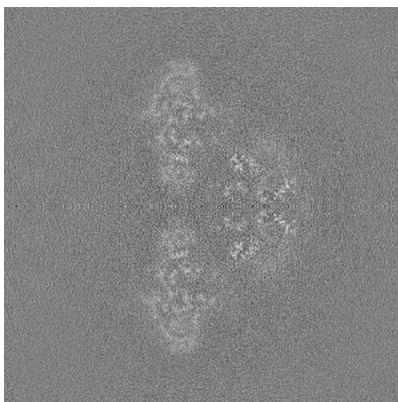


Z Index: 256

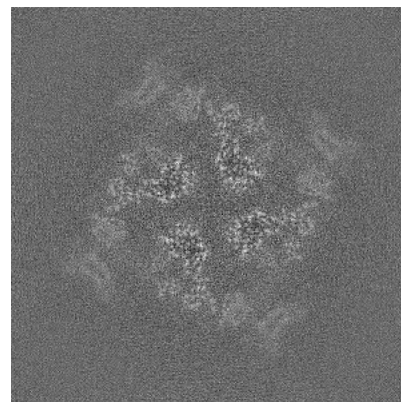
6.2.2 Raw map



X Index: 256



Y Index: 256

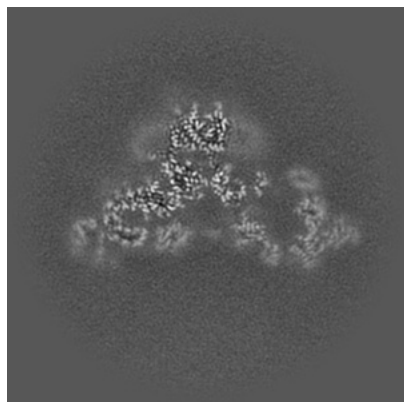


Z Index: 256

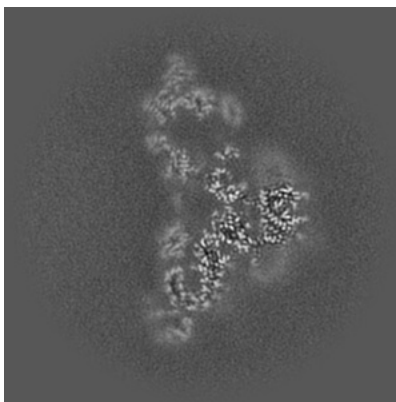
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

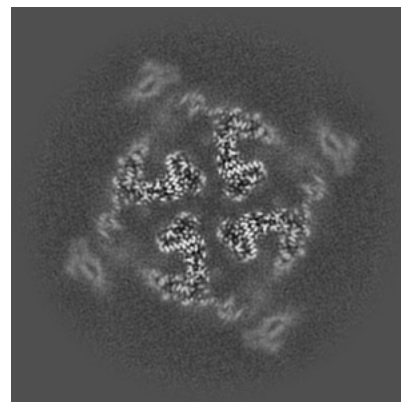
6.3.1 Primary map



X Index: 239

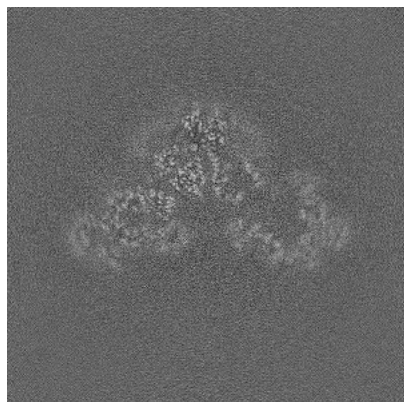


Y Index: 273

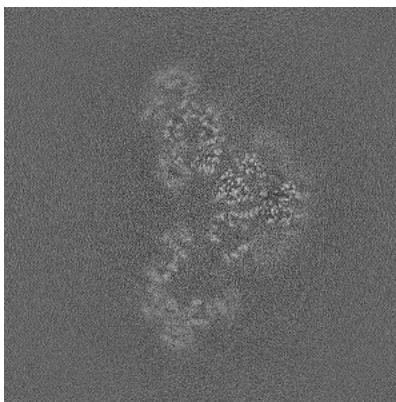


Z Index: 265

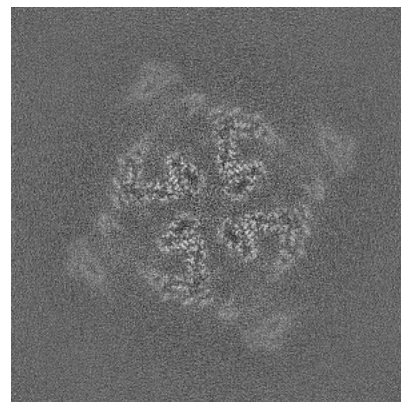
6.3.2 Raw map



X Index: 244



Y Index: 244

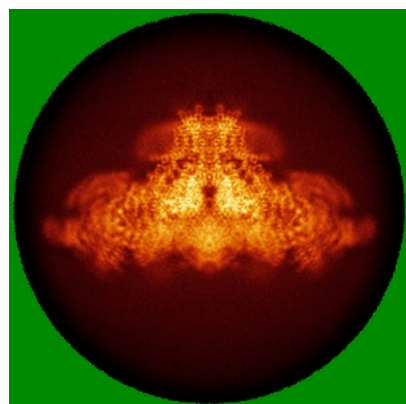


Z Index: 266

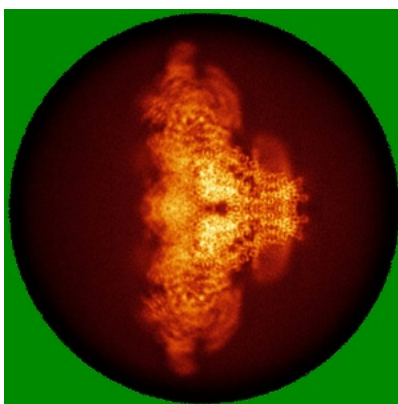
The images above show the largest variance slices of the map in three orthogonal directions.

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

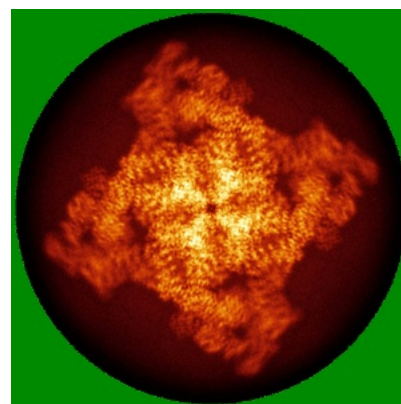
6.4.1 Primary map



X

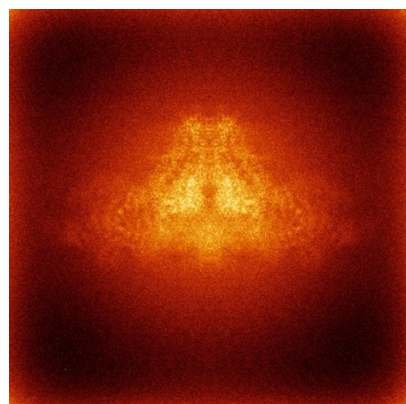


Y

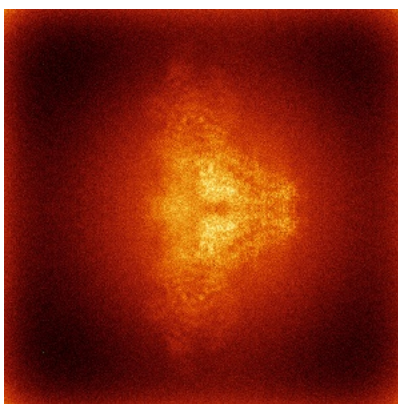


Z

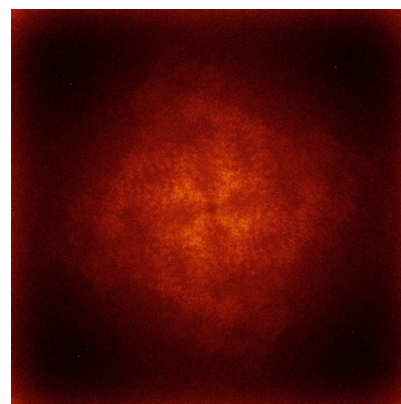
6.4.2 Raw map



X



Y

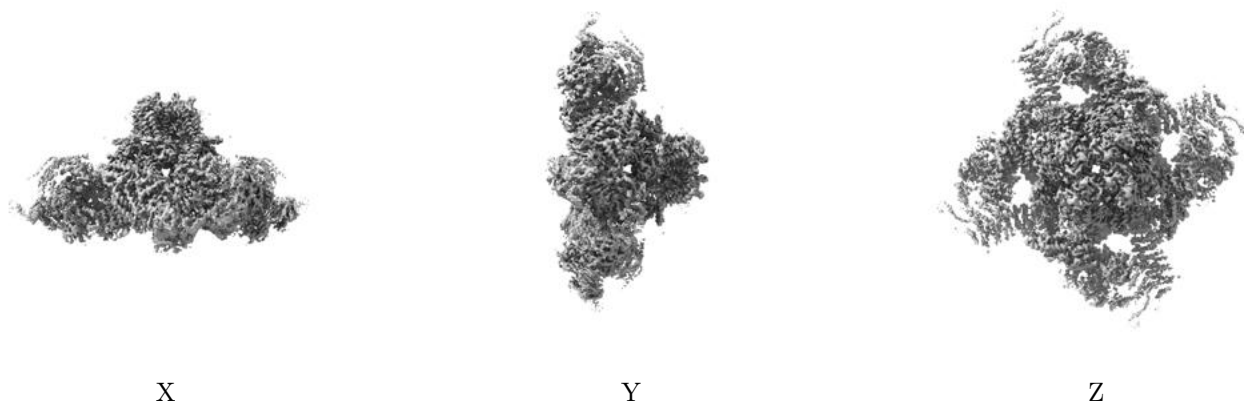


Z

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.

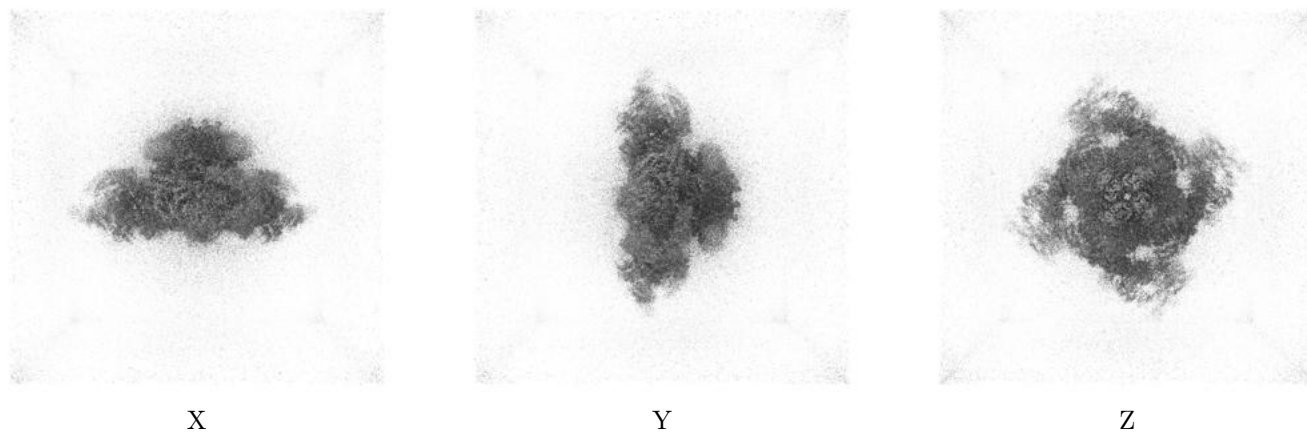
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

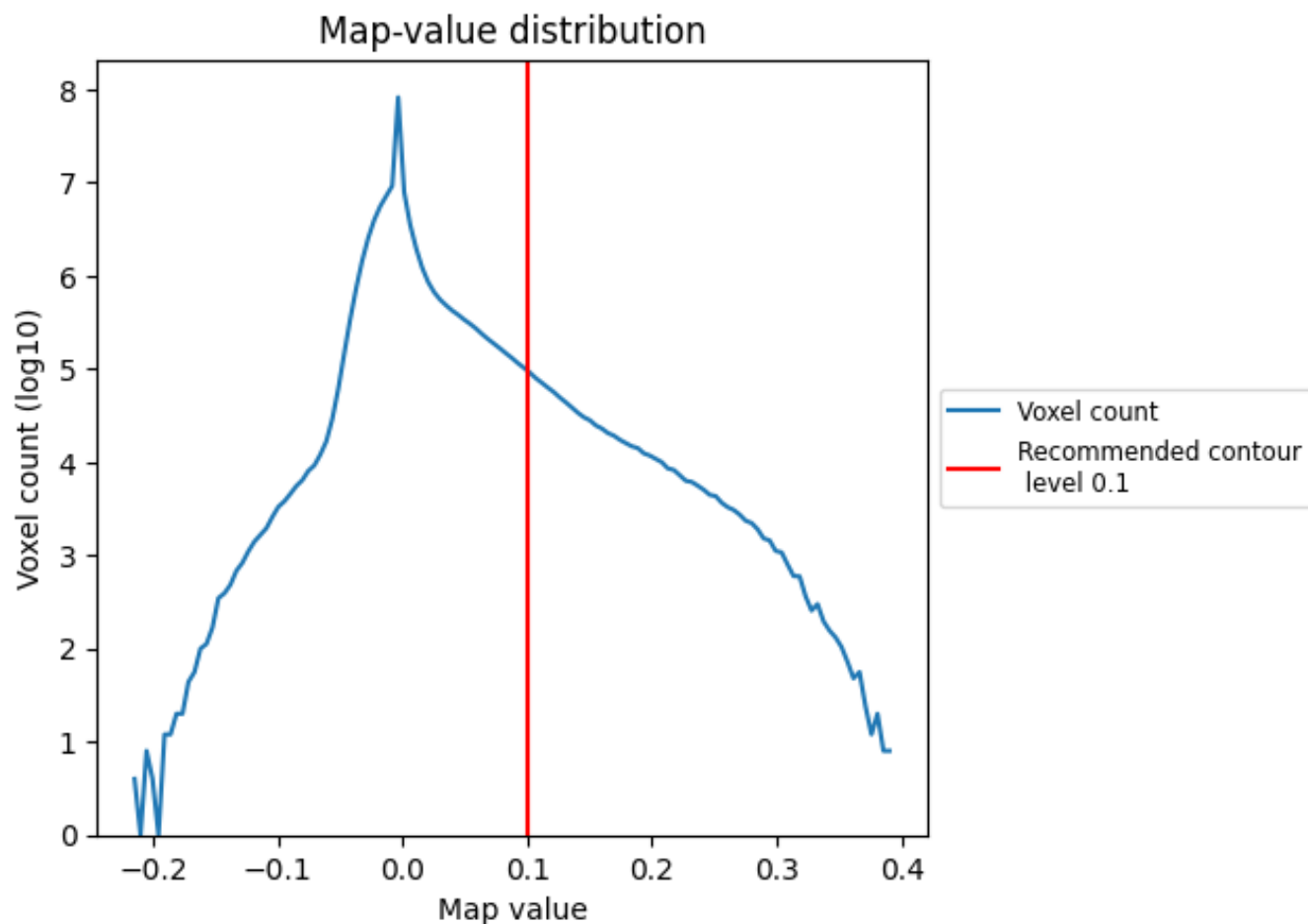
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

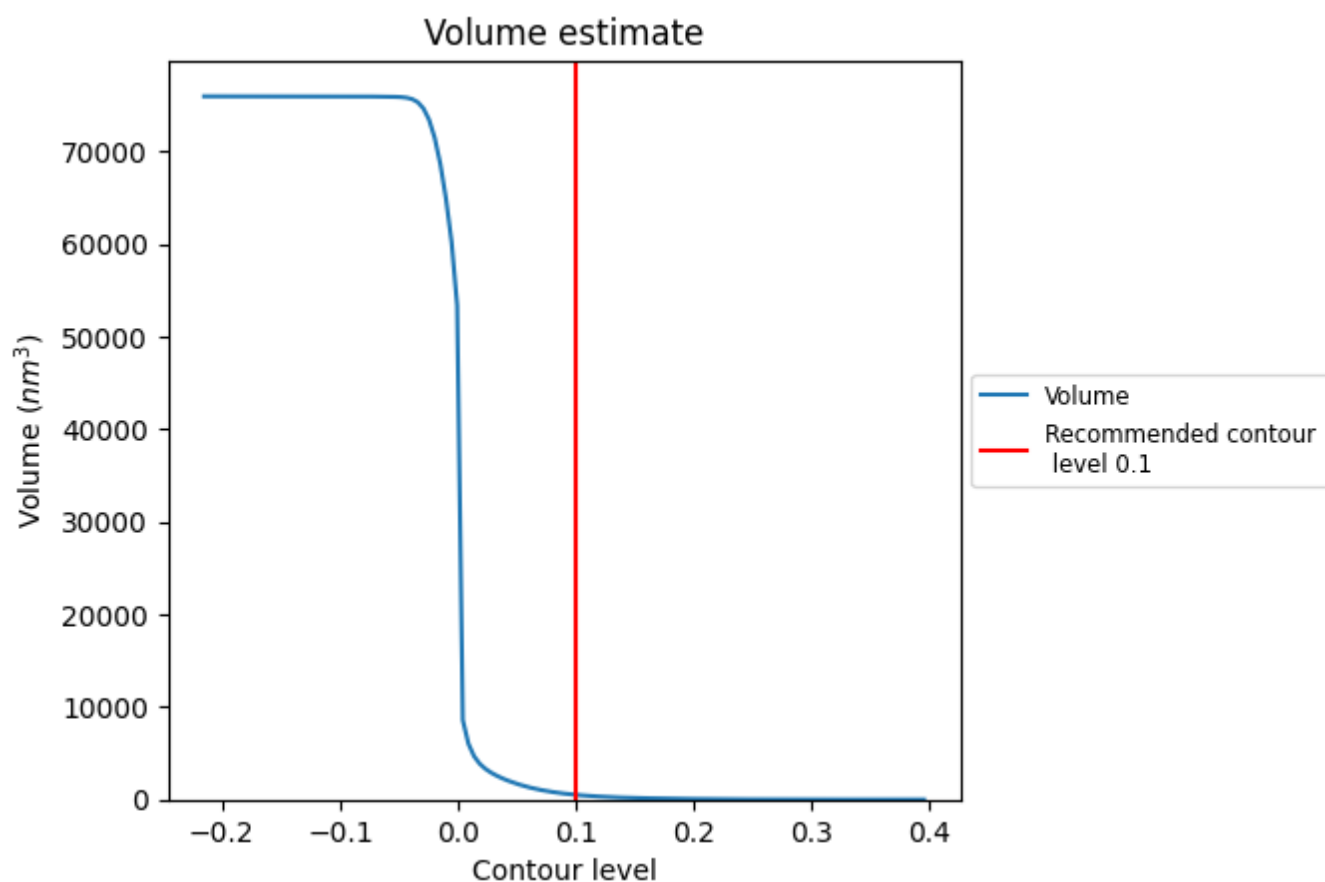
This section contains the results of statistical analysis of the map.

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.

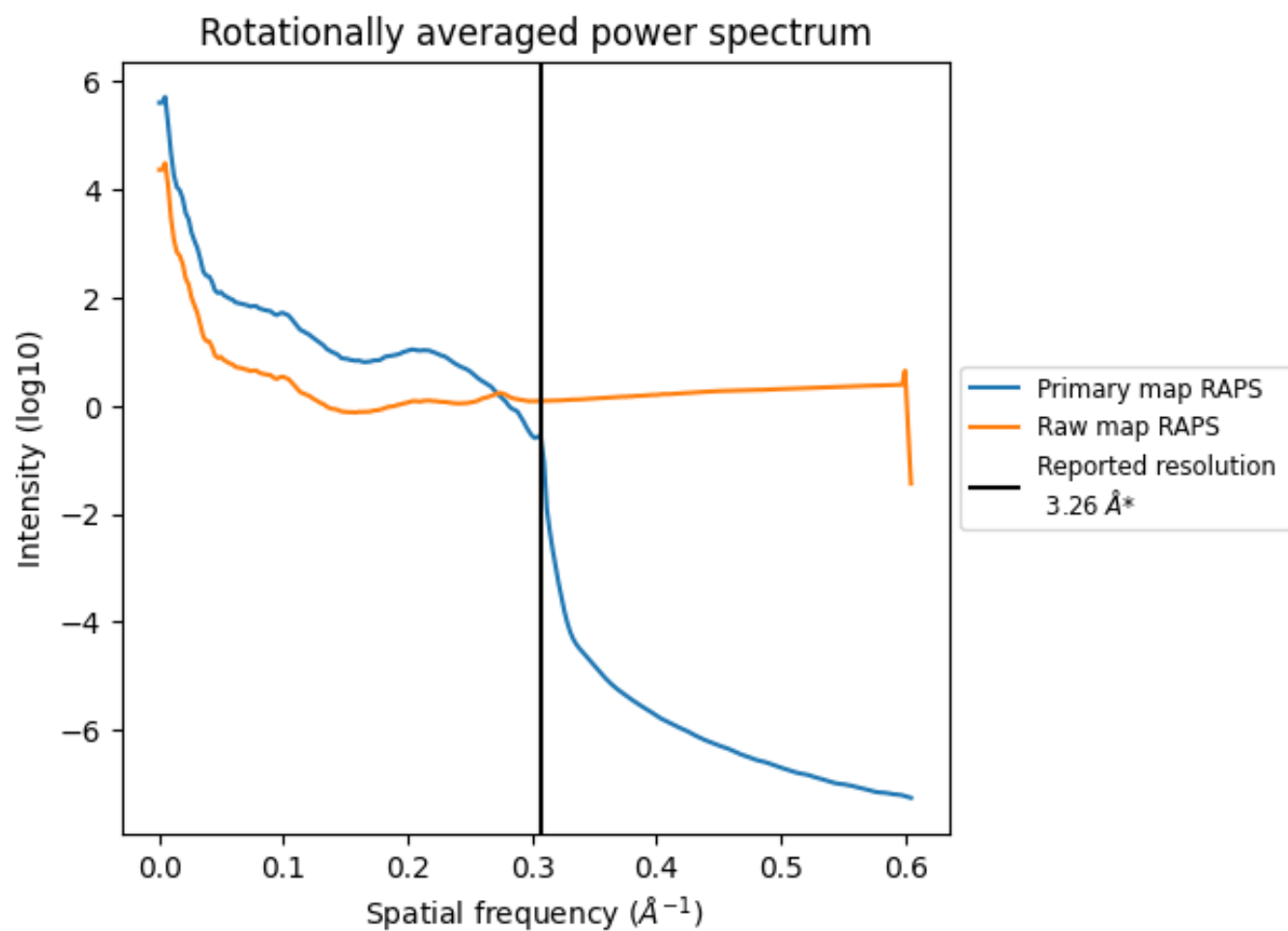
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm³; this corresponds to an approximate mass of 463 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 ⓘ

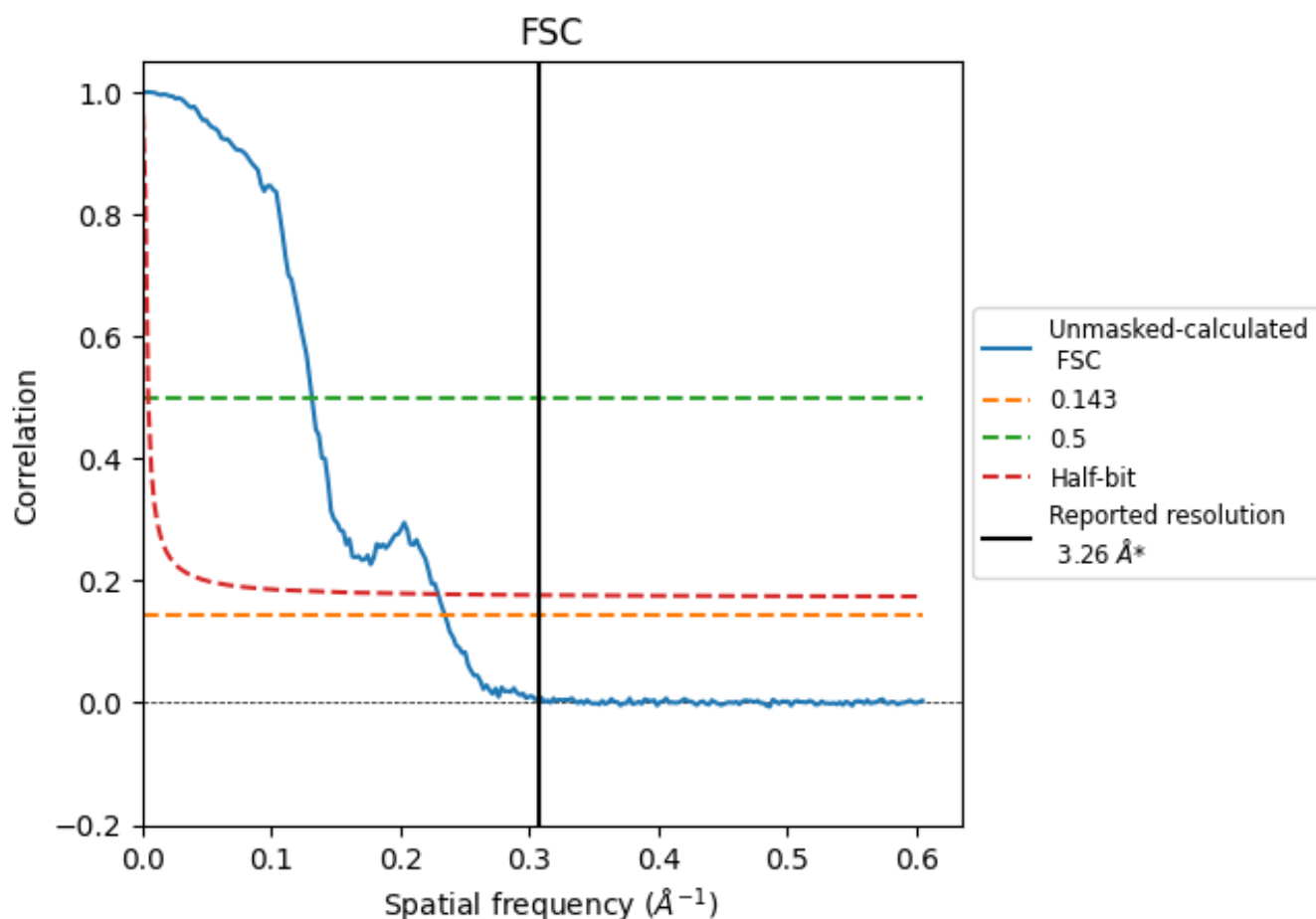


*Reported resolution corresponds to spatial frequency of 0.307 $\text{\AA}^{-1}$

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 0.307 Å⁻¹

8.2 Resolution estimates [i](#)

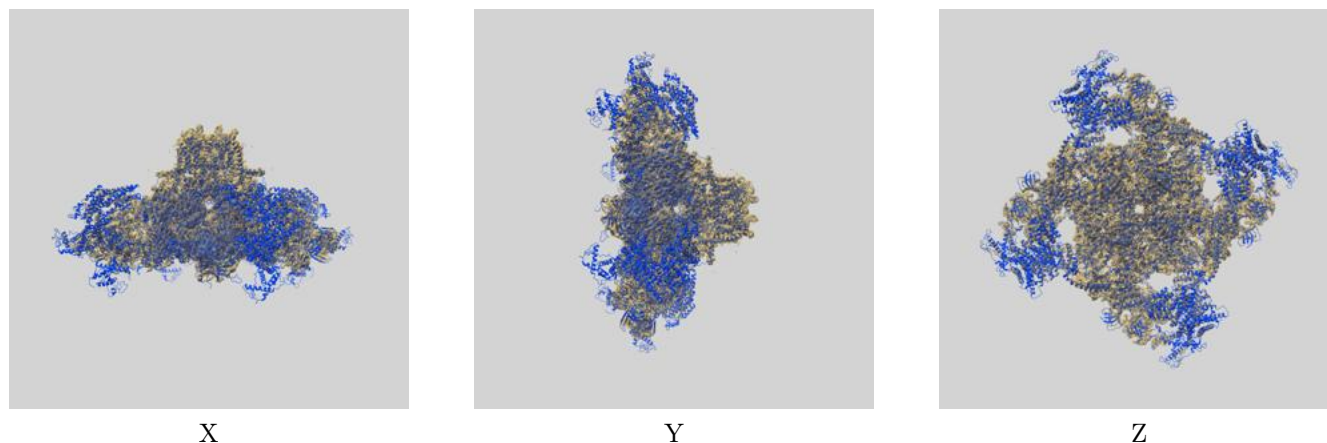
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.26	7.60	4.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

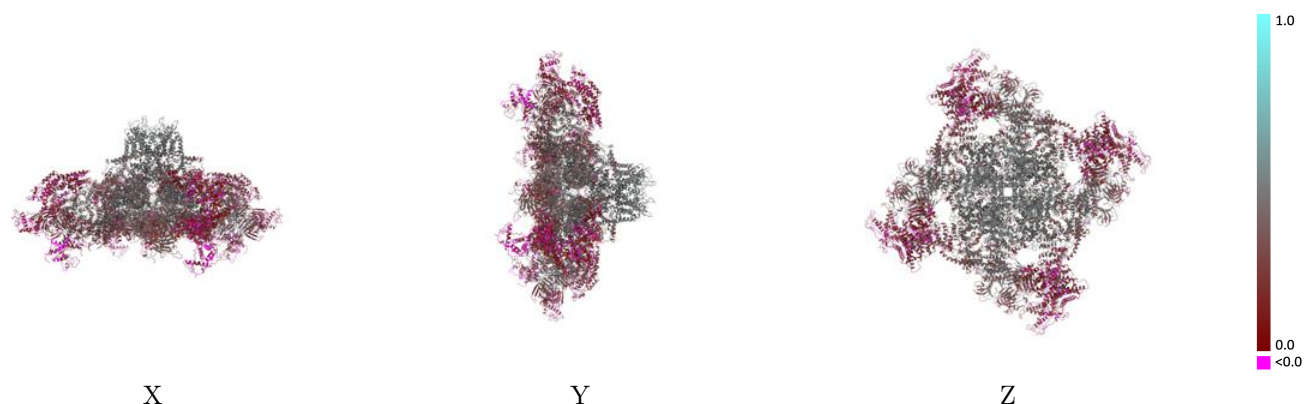
This section contains information regarding the fit between EMDB map EMD-47394 and PDB model 9E1H. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



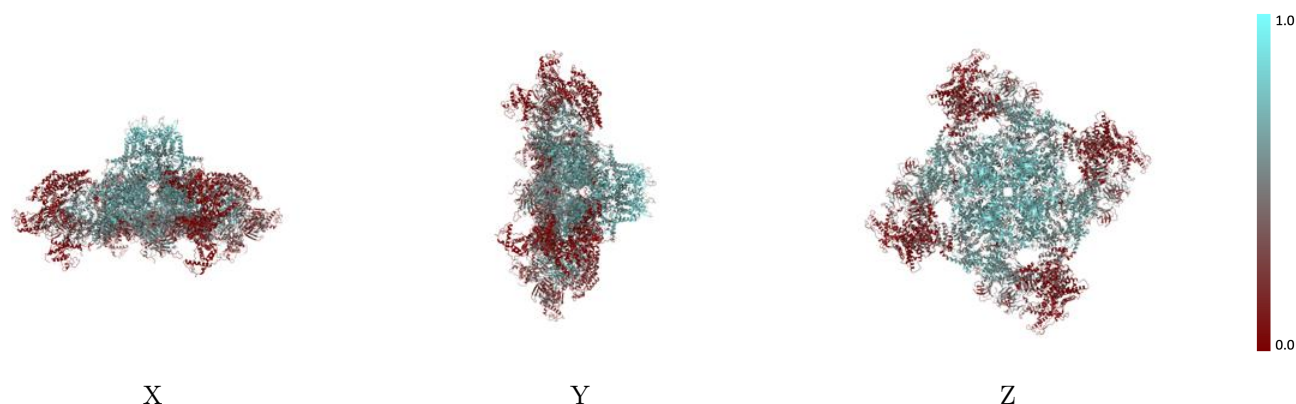
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



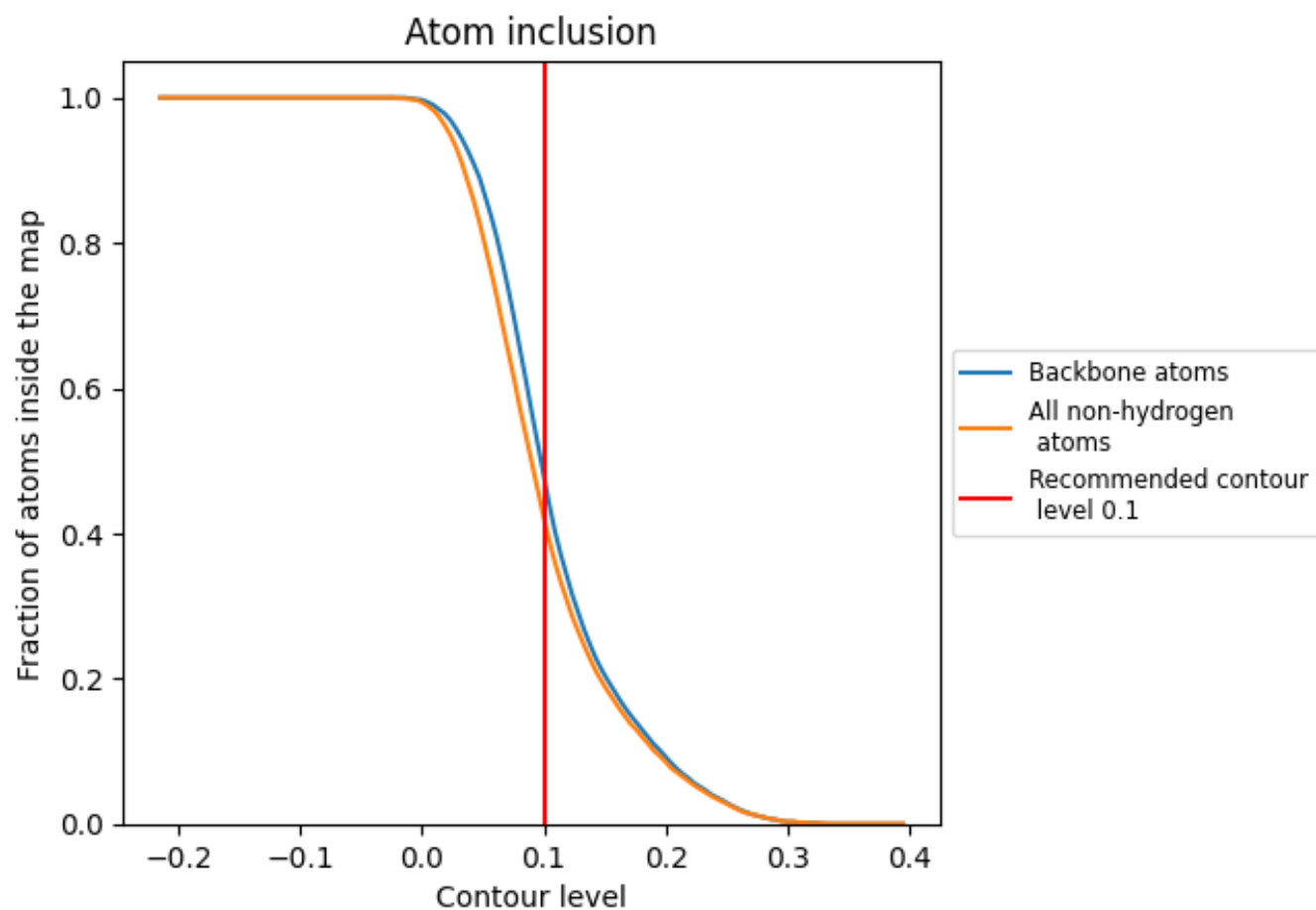
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 42% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4210	0.3140
A	0.4340	0.3130
B	0.4350	0.3130
C	0.4340	0.3130
D	0.4340	0.3130
E	0.2440	0.3570
F	0.2440	0.3560
G	0.2470	0.3530
H	0.2420	0.3560

1.0

0.0

<0.0