



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 08:50 AM EST

PDB ID : 7T3P
EMDB ID : EMD-25667
Title : IP3 and ATP bound type 3 IP3 receptor in the pre-active A state
Authors : Schmitz, E.A.; Takahashi, H.; Karakas, E.
Deposited on : 2021-12-08
Resolution : 3.20 Å(reported)
Based on initial model : 6UQK

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
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

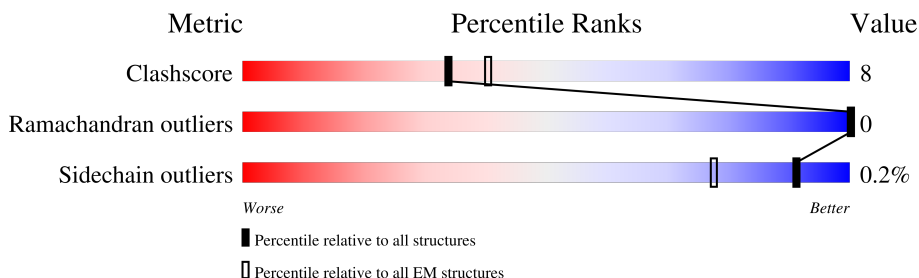
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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 ≥ 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	2633	<div> <div>6%</div> <div>64%</div> <div>14%</div> <div>22%</div> </div>
1	B	2633	<div> <div>7%</div> <div>64%</div> <div>14%</div> <div>22%</div> </div>
1	C	2633	<div> <div>6%</div> <div>64%</div> <div>14%</div> <div>22%</div> </div>
1	D	2633	<div> <div>6%</div> <div>64%</div> <div>14%</div> <div>22%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 66992 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.

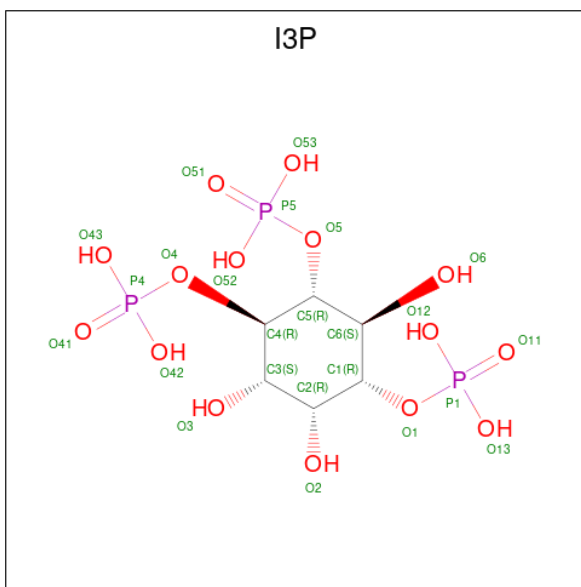
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		
1	B	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		
1	C	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		
1	D	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

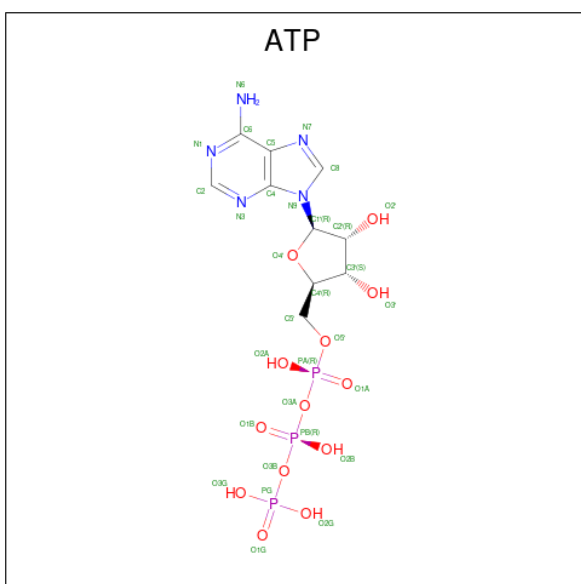
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: C₆H₁₅O₁₅P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			24	6	15	3	
3	B	1	Total	C	O	P	0
			24	6	15	3	
3	C	1	Total	C	O	P	0
			24	6	15	3	
3	D	1	Total	C	O	P	0
			24	6	15	3	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

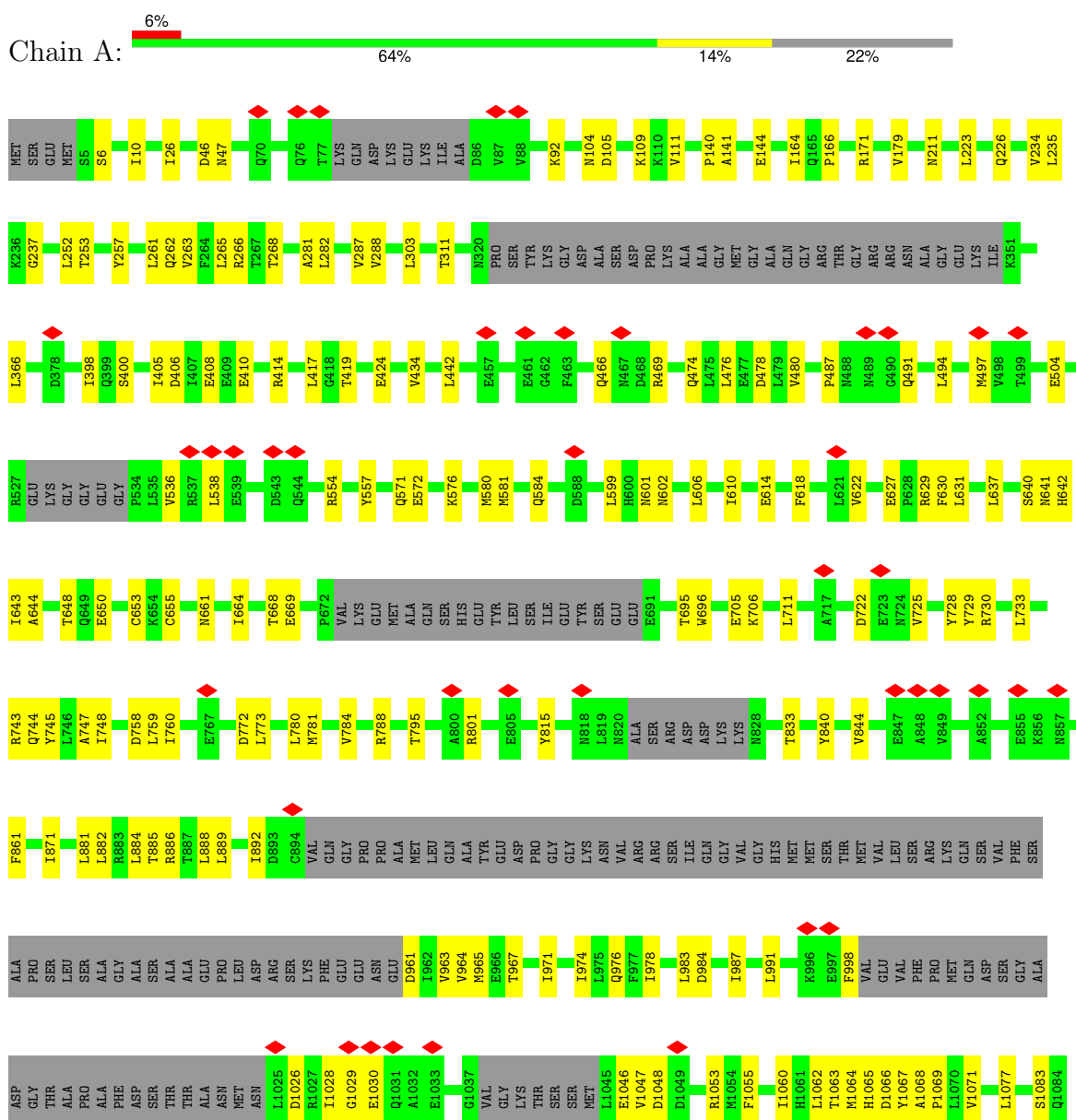


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0

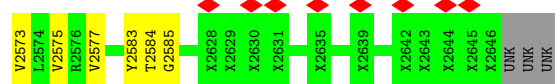
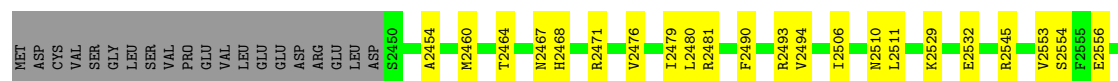
3 Residue-property plots

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.

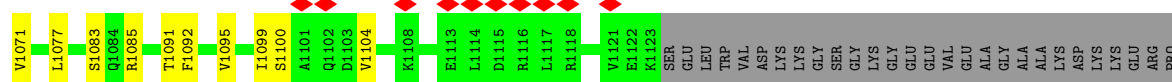
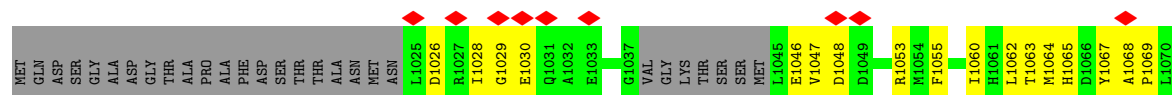
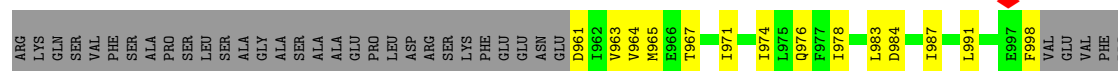
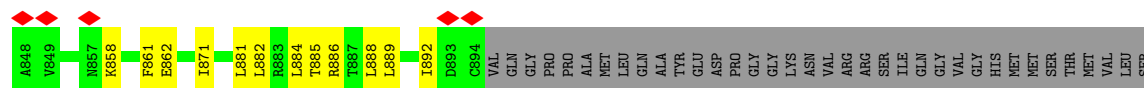
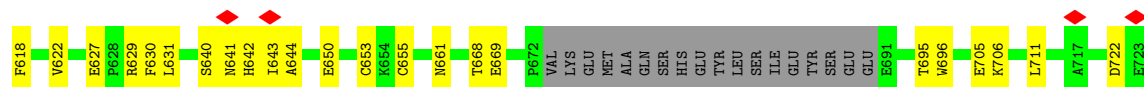
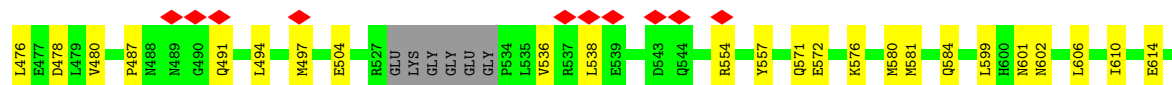
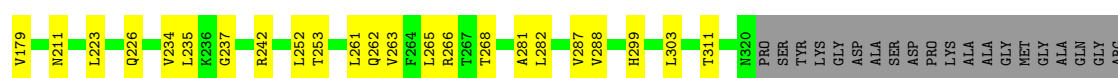
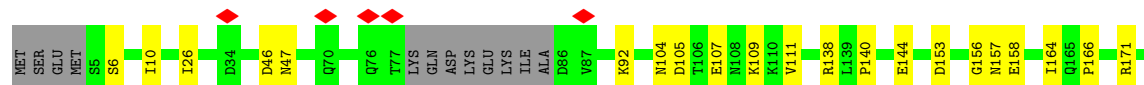
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3







• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





Q1273	S1279	E1280	P1281	V1282	L1283	Q1284	V1287	H1288	A1291	T1292	H1293	G1294	R1295	Q1298	D1301	T1305	V1306	I1307	K1312	Y1313	V1314	K1315	K1316	C1317	M1322	T1323	E1324	D1330	D1331	V1332	V1333	V1334	D1338	K1339	A1340	S1341	L1342	A1343	H1344	L1345	L1346	D1347	M1348	K1350	A1351	A1352	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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SER	T2261	L2264	F2307	ILE	ARG	GLY	TYR	ALA	MET	VAL	MET	P2318	L2321	Y2322	H2323	V2324	D2347	E2353	N2357	V2362	A2376	L2402	PRO	ASN	ASN	HIS	SER	THR	ALA	LEU	PRO	GLY	MET	PRO	HIS	GLY	ALA	ALA	ALA	VAL	ASP	THR	CYS	SER	GLY	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
LYS	MET	ASP	CYS	VAL	SER	GLY	LEU	VAL	VAL	LEU	GLU	ASP	ARG	GLU	LEU	ASP	A2454	M2460	T2464	N2467	H2468	R2471	V2476	T2479	L2480	R2481	F2490	R2493	V2494	I2506	I2507	V2508	L2509	N2510	L2511	K2529	E2532	R2545	V2553	S2554																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
F2555	E2556	V2573	L2574	V2575	P2576	V2577	Y2583	T2584	G2585	M2608	X2628	X2629	X2630	X2631	X2635	X2639	X2642	X2643	X2644	X2645	UNK	UNK	V2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2658	X2659	X2660	X2661	X2662	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2704	X2705	X2706	X2707	X2708	X2709	X2710	X2711	X2712	X2713	X2714	X2715	X2716	X2717	X2718	X2719	X2720	X2721	X2722	X2723	X2724	X2725	X2726	X2727	X2728	X2729	X2730	X2731	X2732	X2733	X2734	X2735	X2736	X2737	X2738	X2739	X2740	X2741	X2742	X2743	X2744	X2745	X2746	X2747	X2748	X2749	X2750	X2751	X2752	X2753	X2754	X2755	X2756	X2757	X2758	X2759	X2760	X2761	X2762	X2763	X2764	X2765	X2766	X2767	X2768	X2769	X2770	X2771	X2772	X2773	X2774	X2775	X2776	X2777	X2778	X2779	X2780	X2781	X2782	X2783	X2784	X2785	X2786	X2787	X2788	X2789	X2790	X2791	X2792	X2793	X2794	X2795	X2796	X2797	X2798	X2799	X2800	X2801	X2802	X2803	X2804	X2805	X2806	X2807	X2808	X2809	X2810	X2811	X2812	X2813	X2814	X2815	X2816	X2817	X2818	X2819	X2820	X2821	X2822	X2823	X2824	X2825	X2826	X2827	X2828	X2829	X2830	X2831	X2832	X2833	X2834	X2835	X2836	X2837	X2838	X2839	X2840	X2841	X2842	X2843	X2844	X2845	X2846	X2847	X2848	X2849	X2850	X2851	X2852	X2853	X2854	X2855	X2856	X2857	X2858	X2859	X2860	X2861	X2862	X2863	X2864	X2865	X2866	X2867	X2868	X2869	X2870	X2871	X2872	X2873	X2874	X2875	X2876	X2877	X2878	X2879	X2880	X2881	X2882	X2883	X2884	X2885	X2886	X2887	X2888	X2889	X2890	X2891	X2892	X2893	X2894	X2895	X2896	X2897	X2898	X2899	X2900	X2901	X2902	X2903	X2904	X2905	X2906	X2907	X2908	X2909	X2910	X2911	X2912	X2913	X2914	X2915	X2916	X2917	X2918	X2919	X2920	X2921	X2922	X2923	X2924	X2925	X2926	X2927	X2928	X2929	X2930	X2931	X2932	X2933	X2934	X2935	X2936	X2937	X2938	X2939	X2940	X2941	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X2981	X2982	X2983	X2984	X2985	X2986	X2987	X2988	X2989	X2990	X2991	X2992	X2993	X2994	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3071	X3072	X3073	X3074	X3075	X3076	X3077	X3078	X3079	X3080	X3081	X3082	X3083	X3084	X3085	X3086	X3087	X3088	X3089	X3090	X3091	X3092	X3093	X3094	X3095	X3096	X3097	X3098	X3099	X3100	X3101	X3102	X3103	X3104	X3105	X3106	X3107	X3108	X3109	X3110	X3111	X3112	X3113	X3114	X3115	X3116	X3117	X3118	X3119	X3120	X3121	X3122	X3123	X3124	X3125	X3126	X3127	X3128	X3129	X3130	X3131	X3132	X3133	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3164	X3165	X3166	X3167	X3168	X3169	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3237	X3238	X3239	X3240	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3

Chain D:



S2554	T2555	E2556	V2573	L2574	V2575	R2576	V2577	Y2583	T2584	G2585	X2628	X2629	X2630	X2631	X2635	X2639	X2642	X2643	X2644	X2645	X2646	UNK	UNK	UNK																																
CYS	SER	GLY	ASP	LYS	MET	ASP	CYS	VAL	SER	GLY	LEU	SER	VAL	PRO	GLU	VAL	LEU	GLU	GLU	ASP	ARG	GLU	LEU	UNK																																
THR	LYS	ARG	TYR	SER	I2261	L2264	F2307	ILE	ARG	GLY	TYR	LYS	ALA	VAL	MET	MET	ASP	W2318	L2321	Y2322	H2323	V2324	D2347	E2353	N2357	V2362	A2376	L2402	PRO	ASN	ASN	ASN	HIS	SER	THR	ALA	SER	PRO	GLY	MET	PRO	HIS	GLY	ALA	ALA	PHE	THR									
GLU	E2111	E2118	T2121	S2122	Q2123	Q2135	L2155	E2163	L2178	W2184	L2188	R2200	W2204	A2212	N2216	Y2225	MET	GLU	GLY	ALA	GLU	GLY	THR	GLY	VAL	ASP	LEU	ASP	SER	VAL	LEU	ILE	SER	LEU	PHE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	PHE										
L2034	GLN	GLU	GLU	GLU	ARG	GLU	VAL	SER	ASN	SER	VAL	V2044	E2048	H2051	Y2054	L2058	Q2059	R2062	V2073	VAL	LYS	ARG	ILE	GLN	GLU	GLU	GLU	ALA	GLU	ILE	SER	SER	MET	LEU	SER	LEU	PHE	GLN	SER	ALA	PRO	ALA	GLN	GLU	GLU											
P1951	C1952	H1953	Q1956	L1957	C1958	I1959	V1960	T1961	H1962	H1963	S1964	N1965	D1968	I1969	L1973	I1974	D1977	ILE	SER	PRO	LEU	CYS	LYS	TYR	M1986	D1987	L1988	L1992	L1999	L2000	L2001	A2002	M2003	M2004	E2005	S2006	R2007	E2014	I2018	S2019	L2020	R2021	V2025	L2026	D2027	V2028	K2031									
LEU	ARG	ARG	GLY	HIS	GLU	VAL	SER	GLU	VAL	GLN	SER	SER	GLU	MET	G1864	Q1871	P1872	R1886	Q1895	ASN	ASN	LYS	THR	ASN	Y1901	E1906	D1987	L1988	L1992	C1915	G1916	S1917	THR	THR	GLY	GLY	LEU	G1923	L1924	L1925	M1933	V1934	V1937	L1941	T1945	E1946	Y1947	C1948								
H1773	N1774	M1776	R1784	F1785	F1786	K1787	V1788	R1792	Q1797	T1803	VAL	ALA	VAL	ASN	MET	ASP	ASP	LEU	GLY	SER	GLN	GLM	PRO	HIS	GLU	ARG	ASP	GLU	VAL	PRO	THR	LYS	THR	GLY	VAL	VAL	SER	PHE	ILE	PRO	GLY	SER	SER	ARG	TYR	SER	LEU	PRO	SER							
D1681	R1682	R1687	L1695	G1696	ASN	LYS	THR	SER	THR	ARG	ASP	GLY	ASP	LEU	PRO	ASP	PRO	ILE	THR	GLY	LEU	ASP	ASP	PRO	TRP	ASN	L1626	L1627	G1631	R1637	C1638	E1639	K1646	H1650	T1651	L1654	H1655	E1656	E1659	V1665	L1674	LYS	LYS	THR	LYS	F1679	G1680									
THR	PRO	THR	ASN	GLN	TRP	ASP	TYR	K1589	I1592	E1593	K1594	I1598	E1603	K1607	V1610	E1613	L1617	V1618	D1619	V1620	L1621	L1626	L1627	G1631	R1637	C1638	E1639	K1646	H1650	T1651	L1654	H1655	E1656	E1659	V1665	L1674	LYS	LYS	THR	LYS	F1679	G1680														
GLY	SER	VAL	ALA	CYS	ILE	ARG	THR	THR	ALA	ASP	P1462	T1463	E1465	K1466	Y1467	L1468	L1469	L1473	A1478	S1481	S1482	P1483	F1484	S1485	E1486	N1487	S1488	S1489	S1490	L1491	Q1492	T1493	H1494	Q1495	T1496	I1497	V1498	Q1500	L1501	SER	TYR	LYS	Q1503	S1504	T1505	T1506	F1444	T1445	L1446	L1447	M1448	A1449	R1450	L1451	CYS	SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	116925	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.847	Depositor
Minimum map value	-1.846	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	397.44, 397.44, 397.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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: ZN, I3P, ATP

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	0.29	0/16897	0.47	0/22813
1	B	0.29	0/16897	0.47	0/22813
1	C	0.29	0/16897	0.47	0/22813
1	D	0.29	0/16897	0.47	0/22813
All	All	0.29	0/67588	0.47	0/91252

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16692	0	16773	272	0
1	B	16692	0	16773	281	0
1	C	16692	0	16773	281	0
1	D	16692	0	16773	274	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	9	2	0
3	C	24	0	9	2	0
3	D	24	0	9	2	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
All	All	66992	0	67176	1071	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 8.

The worst 5 of 1071 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:C:801:ARG:NH2	1:C:984:ASP:OD1	2.09	0.86
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.09	0.86
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.09	0.85
1:A:627:GLU:OE1	1:A:629:ARG:NH1	2.10	0.84
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.09	0.84

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	1995/2633 (76%)	1913 (96%)	82 (4%)	0	100	100
1	B	1995/2633 (76%)	1912 (96%)	83 (4%)	0	100	100
1	C	1995/2633 (76%)	1913 (96%)	82 (4%)	0	100	100
1	D	1995/2633 (76%)	1913 (96%)	82 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7980/10532 (76%)	7651 (96%)	329 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	1865/2329 (80%)	1861 (100%)	4 (0%)	92	97
1	B	1865/2329 (80%)	1861 (100%)	4 (0%)	92	97
1	C	1865/2329 (80%)	1861 (100%)	4 (0%)	92	97
1	D	1865/2329 (80%)	1861 (100%)	4 (0%)	92	97
All	All	7460/9316 (80%)	7444 (100%)	16 (0%)	91	97

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1735	LYS
1	D	1682	ARG
1	C	1443	ASN
1	D	1443	ASN
1	B	1933	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1243	GLN
1	B	1243	GLN
1	C	1243	GLN
1	D	1243	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 12 ligands modelled in this entry, 4 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$
3	I3P	C	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
4	ATP	B	2703	-	28,33,33	0.69	0	34,52,52	0.90	2 (5%)
4	ATP	C	2703	-	28,33,33	0.69	0	34,52,52	0.91	2 (5%)
3	I3P	D	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
4	ATP	A	2703	-	28,33,33	0.70	0	34,52,52	0.91	2 (5%)
4	ATP	D	2703	-	28,33,33	0.70	0	34,52,52	0.91	2 (5%)
3	I3P	B	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
3	I3P	A	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	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
3	I3P	C	2702	-	-	4/15/39/39	0/1/1/1
4	ATP	B	2703	-	-	4/18/38/38	0/3/3/3
4	ATP	C	2703	-	-	4/18/38/38	0/3/3/3
3	I3P	D	2702	-	-	3/15/39/39	0/1/1/1
4	ATP	A	2703	-	-	4/18/38/38	0/3/3/3
4	ATP	D	2703	-	-	4/18/38/38	0/3/3/3
3	I3P	B	2702	-	-	3/15/39/39	0/1/1/1
3	I3P	A	2702	-	-	3/15/39/39	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2702	I3P	P4-O4	3.10	1.65	1.59
3	A	2702	I3P	P4-O4	3.07	1.64	1.59
3	C	2702	I3P	P4-O4	3.07	1.64	1.59
3	D	2702	I3P	P4-O4	3.07	1.64	1.59
3	A	2702	I3P	P5-O5	2.99	1.64	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2703	ATP	C5-C6-N6	2.33	123.86	120.31
4	B	2703	ATP	C5-C6-N6	2.33	123.86	120.31
4	C	2703	ATP	C5-C6-N6	2.33	123.86	120.31
4	D	2703	ATP	C5-C6-N6	2.33	123.86	120.31
4	C	2703	ATP	O3'-C3'-C2'	-2.03	105.32	111.82

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

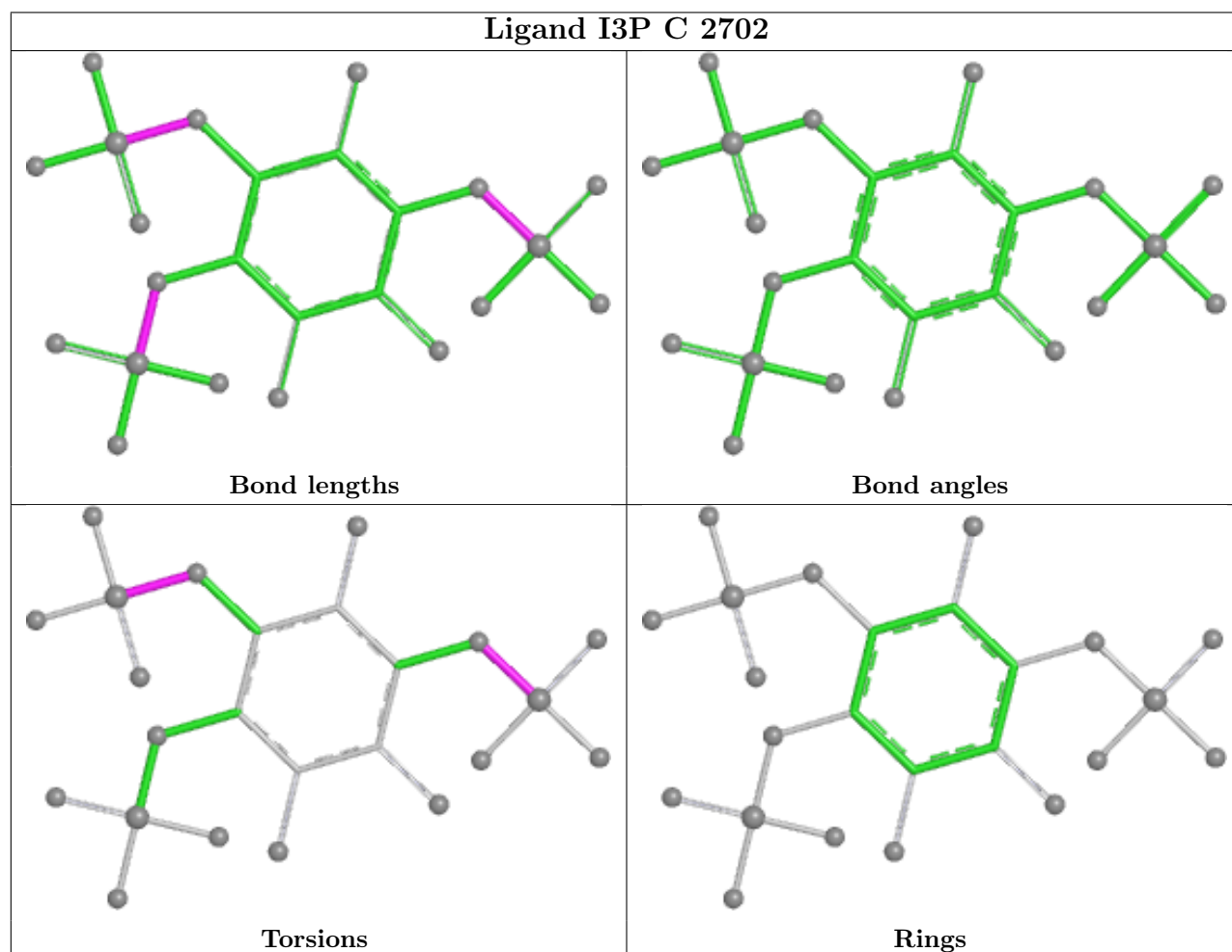
Mol	Chain	Res	Type	Atoms
4	A	2703	ATP	O4'-C4'-C5'-O5'
4	B	2703	ATP	O4'-C4'-C5'-O5'
4	C	2703	ATP	O4'-C4'-C5'-O5'
4	D	2703	ATP	O4'-C4'-C5'-O5'
4	A	2703	ATP	PB-O3A-PA-O5'

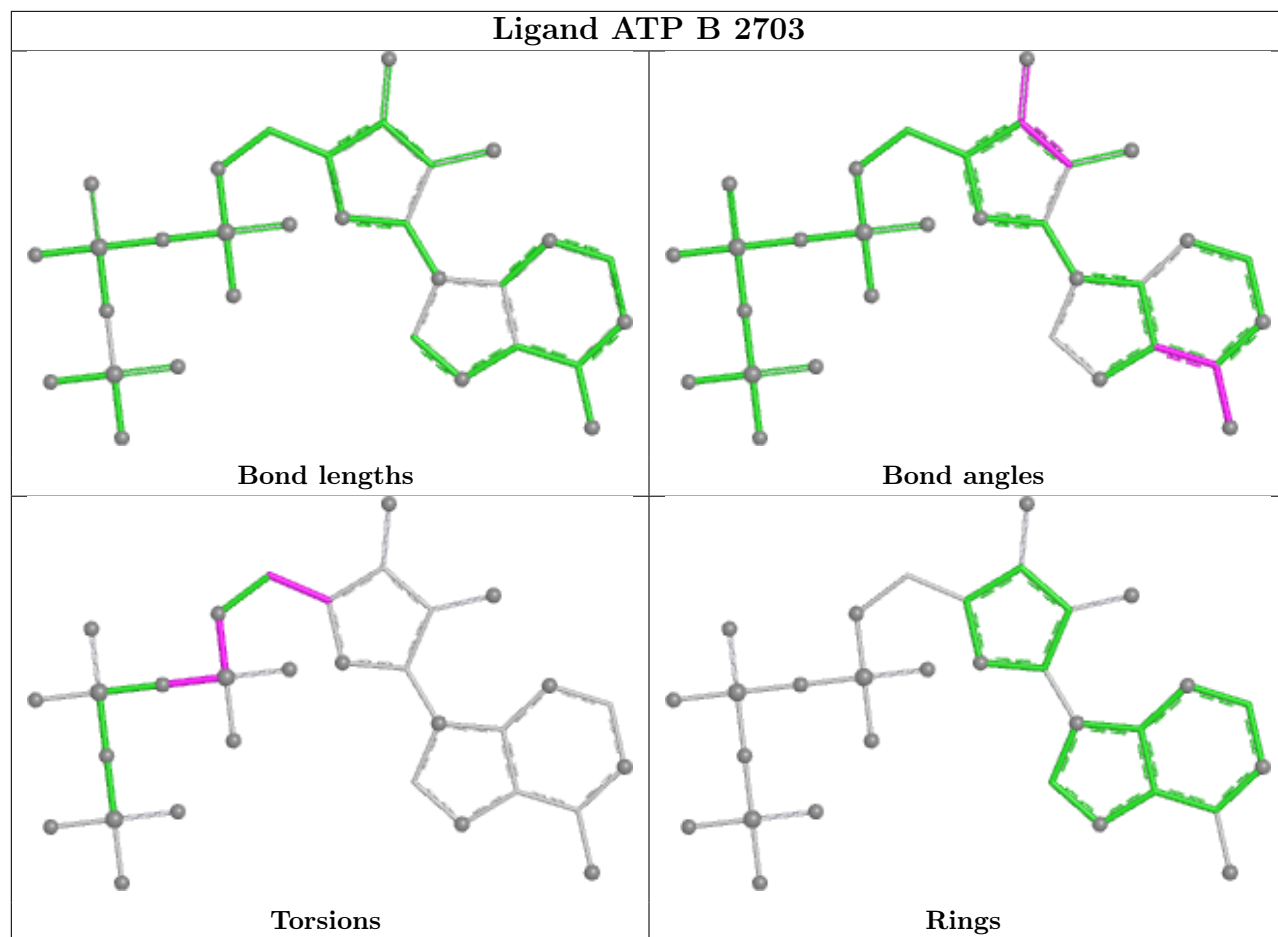
There are no ring outliers.

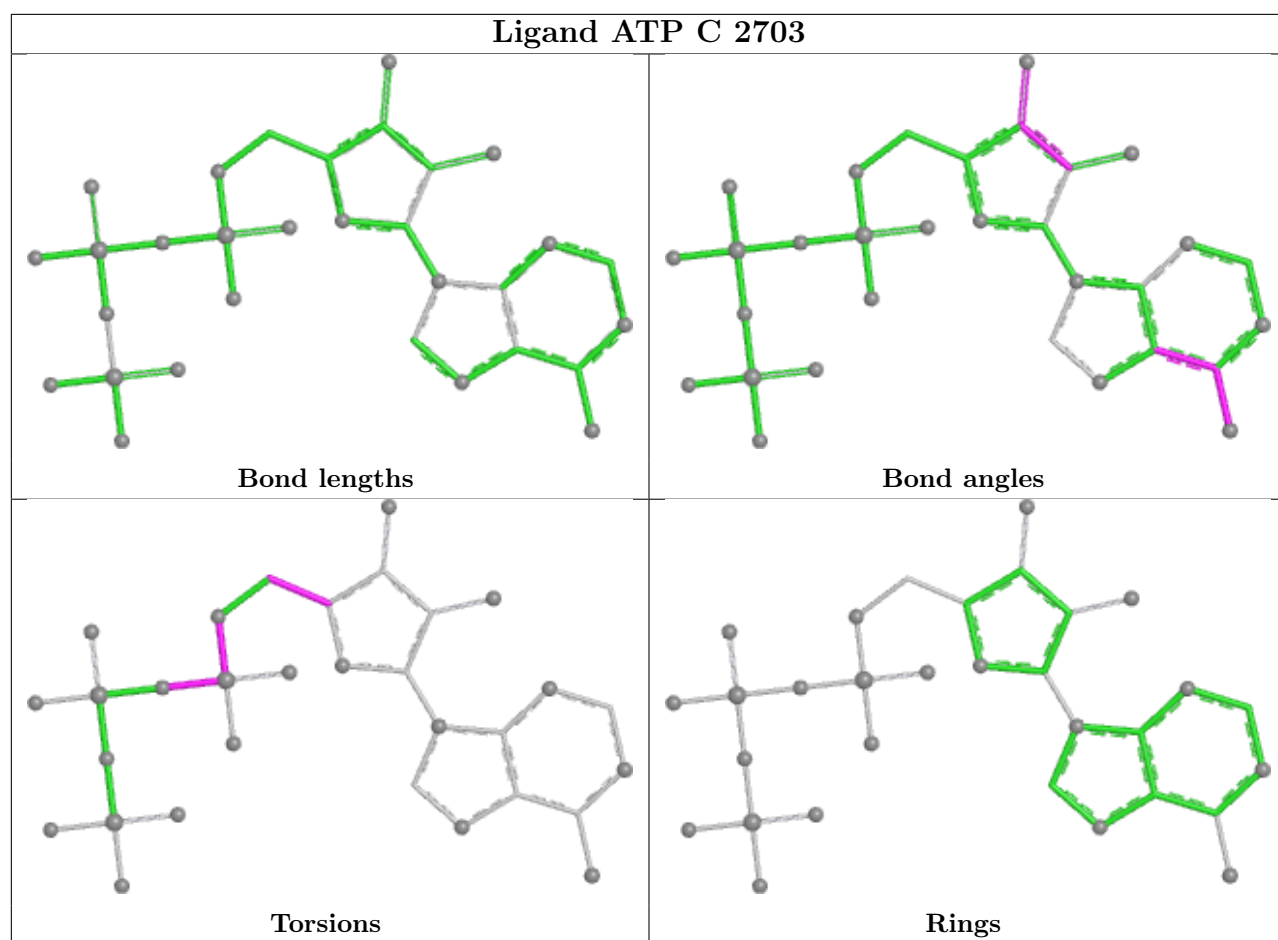
4 monomers are involved in 8 short contacts:

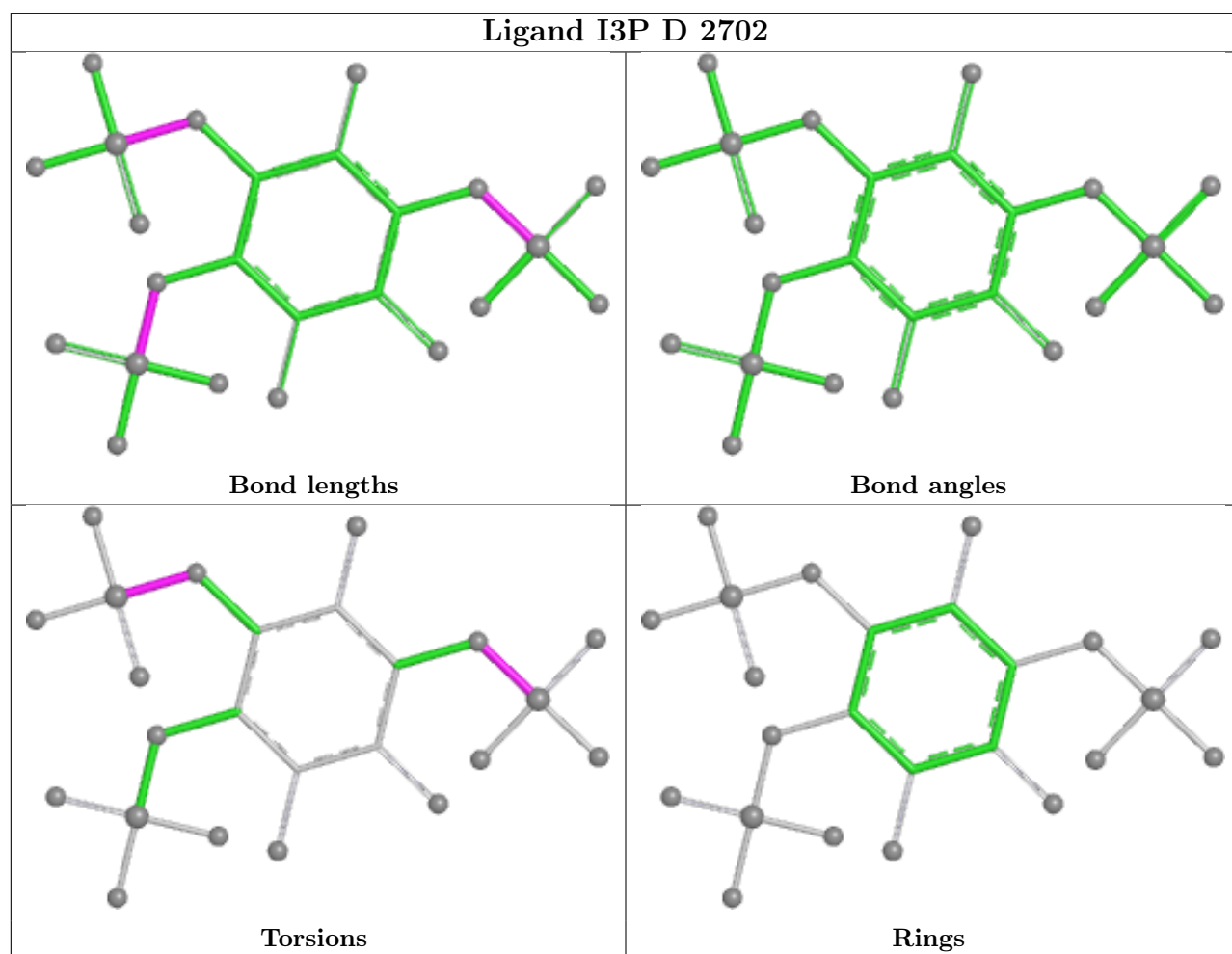
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2702	I3P	2	0
3	D	2702	I3P	2	0
3	B	2702	I3P	2	0
3	A	2702	I3P	2	0

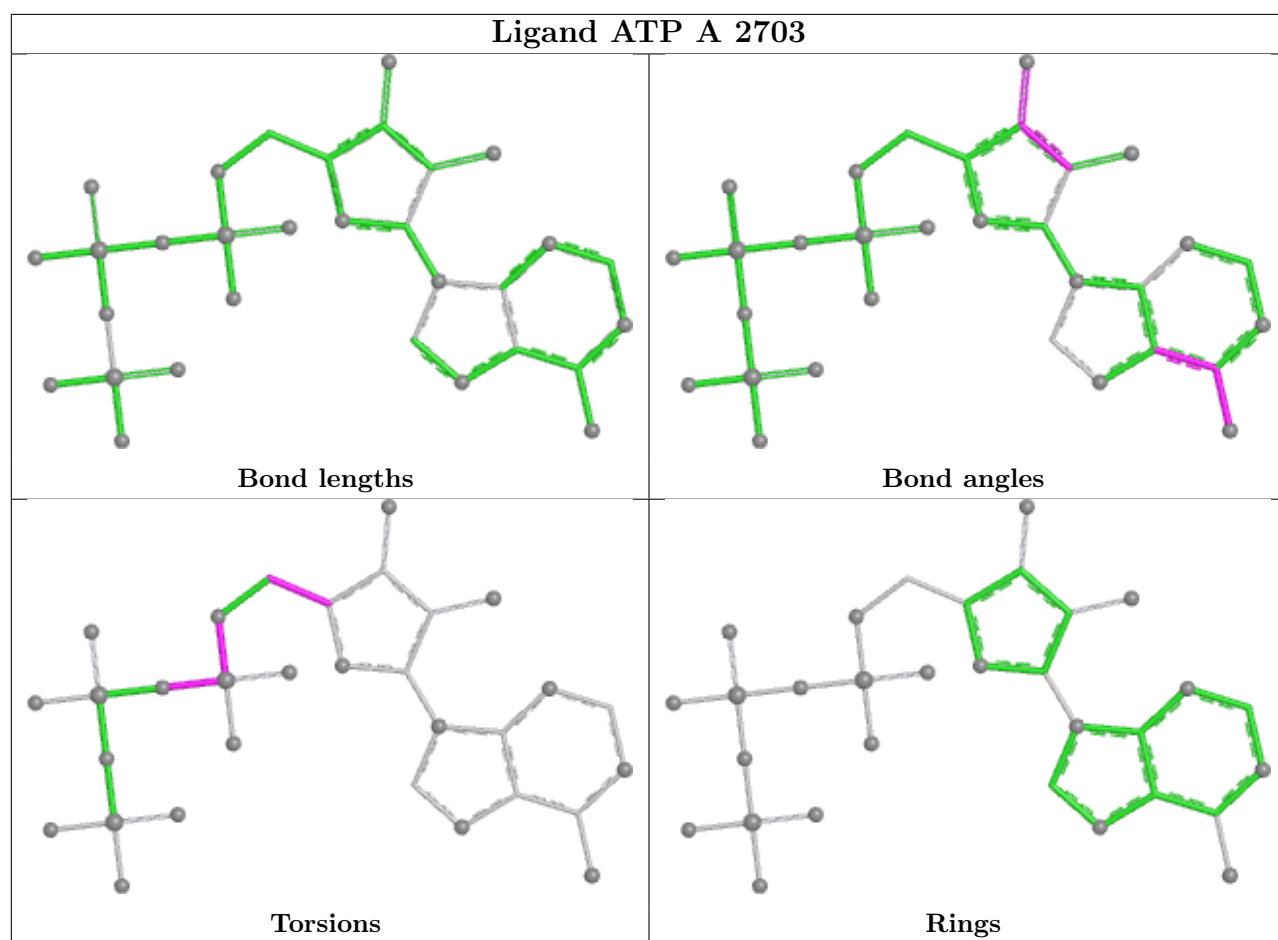
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

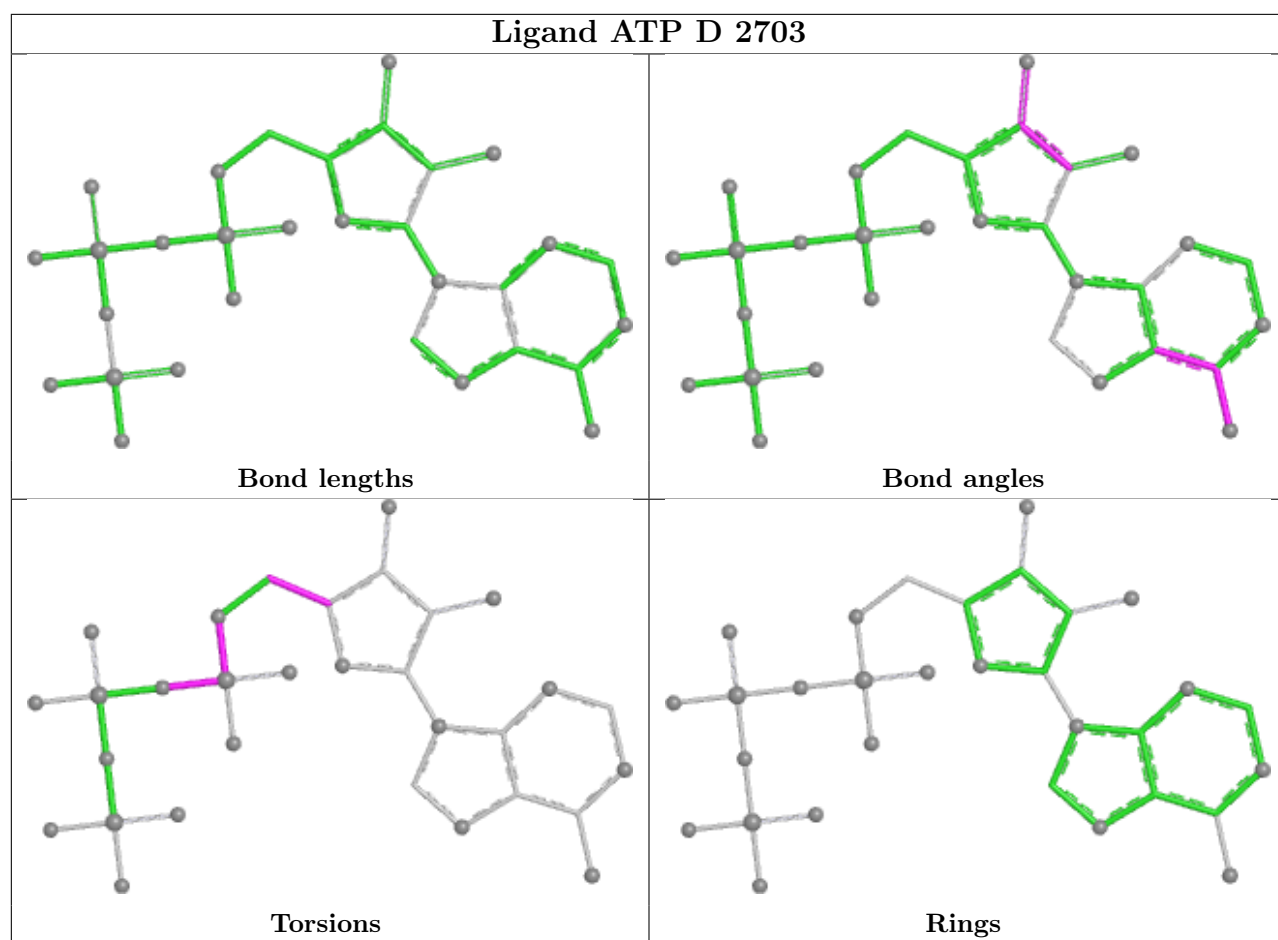


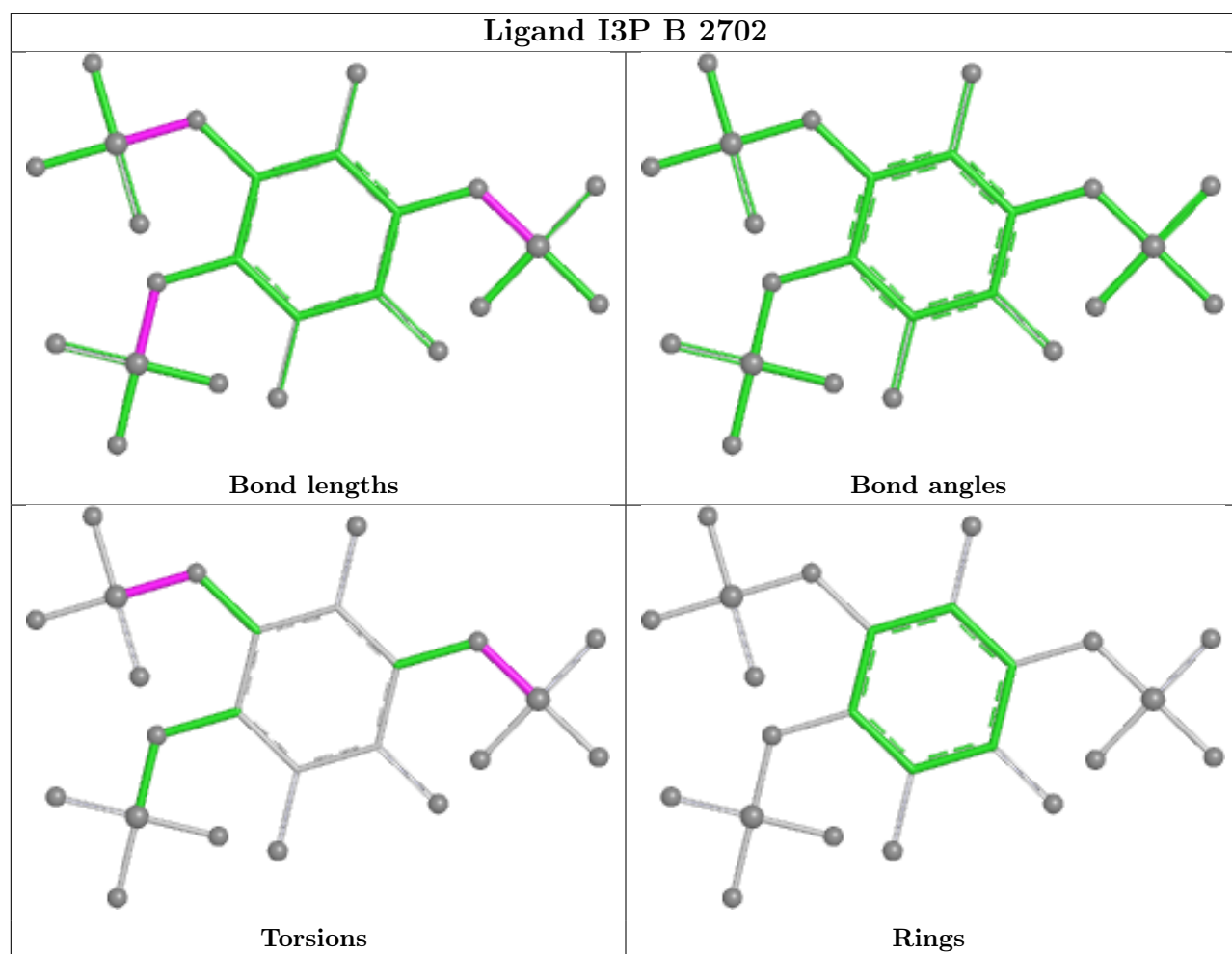


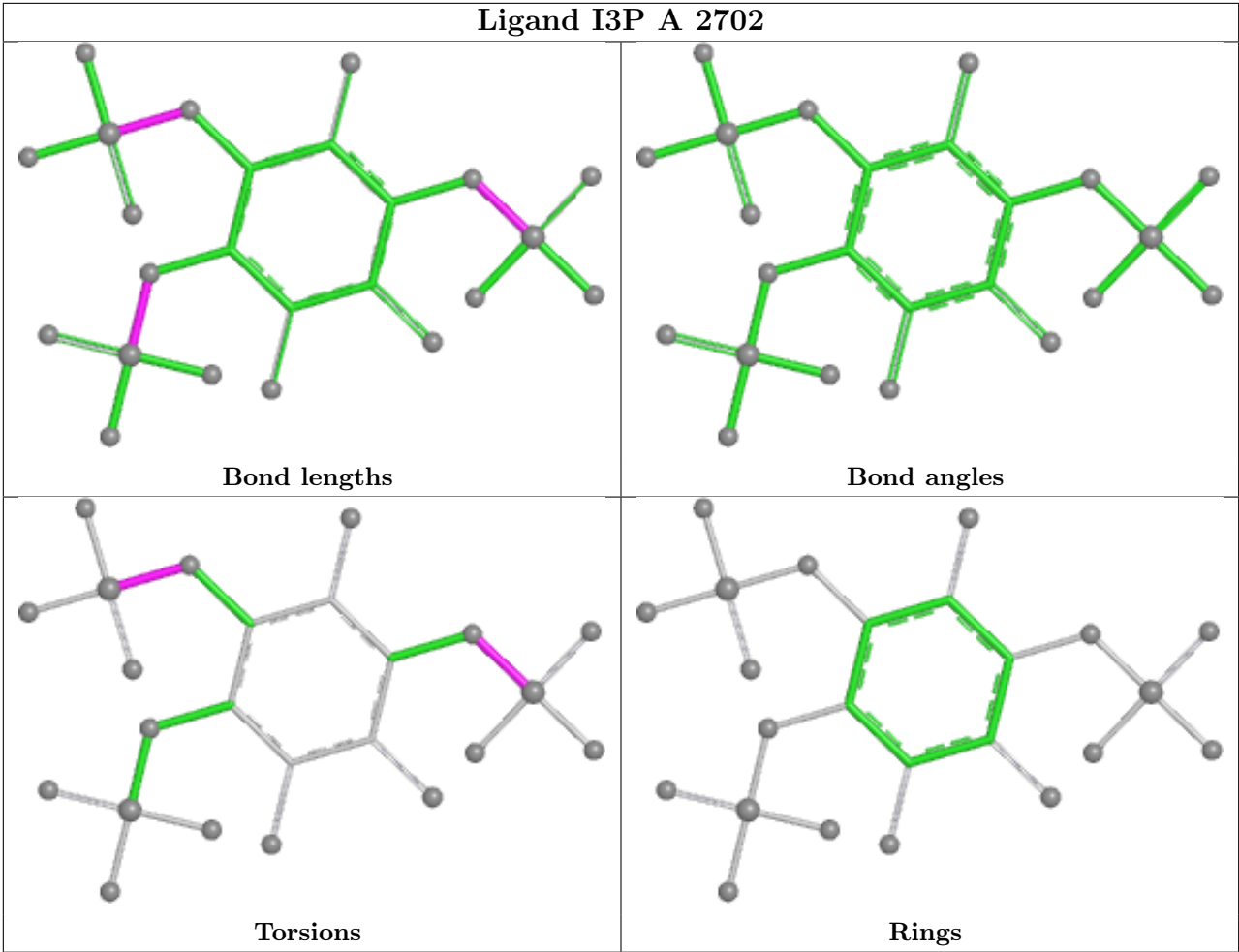












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2611:VAL	C	2628:UNK	N	25.33

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2611:VAL	C	2628:UNK	N	25.33
1	C	2611:VAL	C	2628:UNK	N	25.33
1	D	2611:VAL	C	2628:UNK	N	25.33

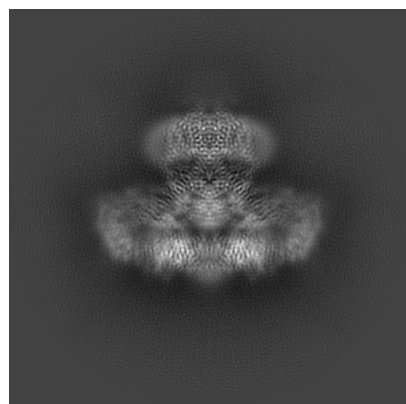
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25667. These allow visual inspection of the internal detail of the map and identification of artifacts.

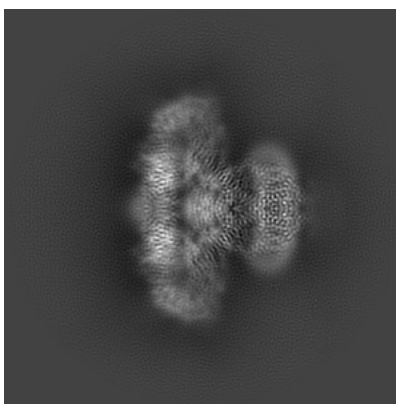
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

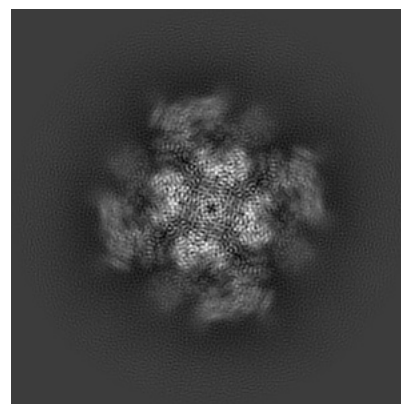
6.1.1 Primary map



X

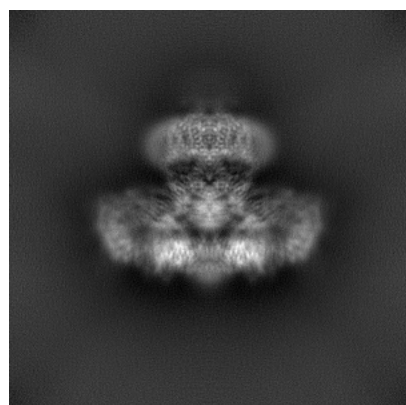


Y

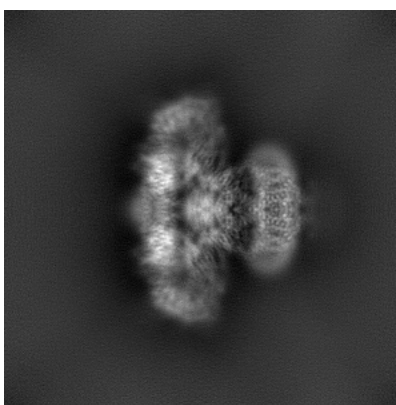


Z

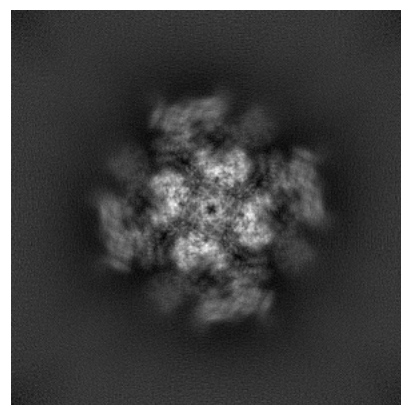
6.1.2 Raw map



X



Y

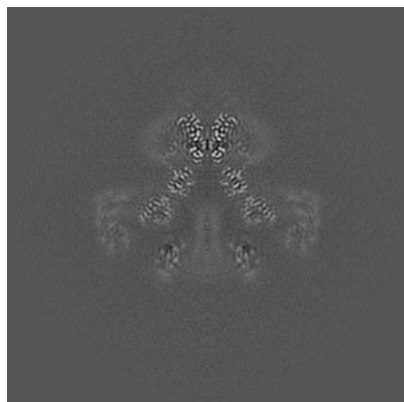


Z

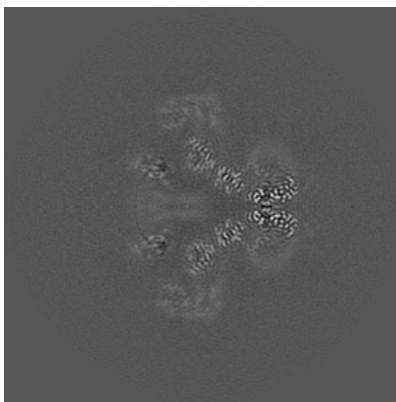
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

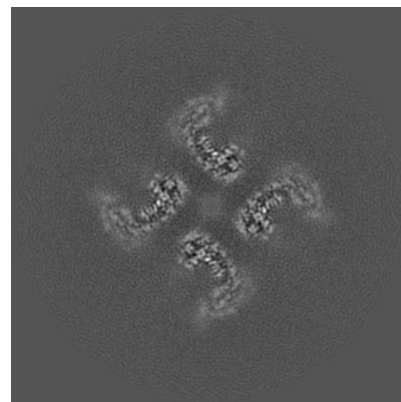
6.2.1 Primary map



X Index: 240

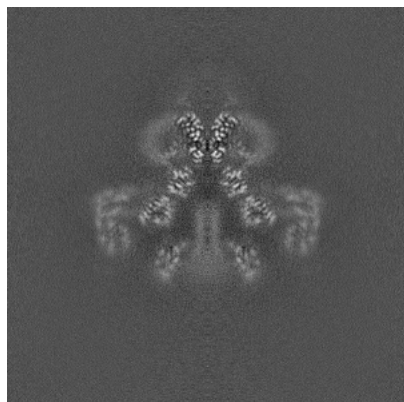


Y Index: 240

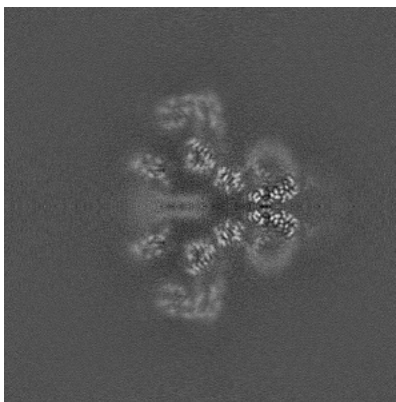


Z Index: 240

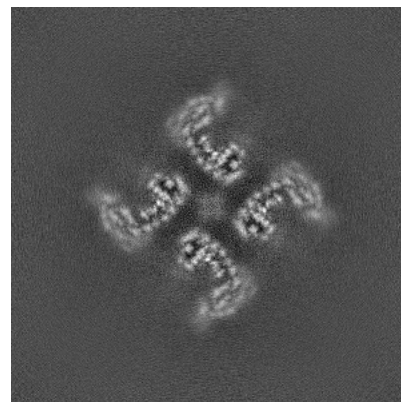
6.2.2 Raw map



X Index: 240



Y Index: 240

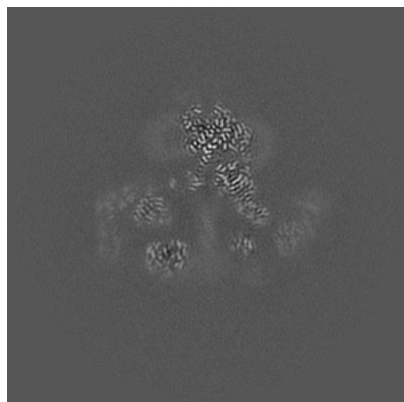


Z Index: 240

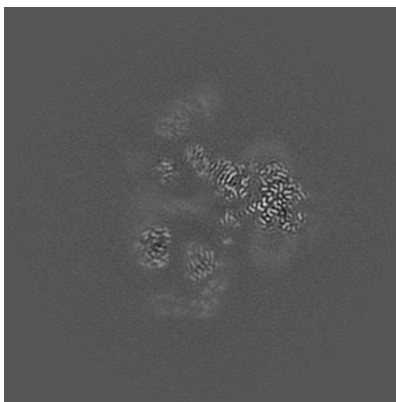
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

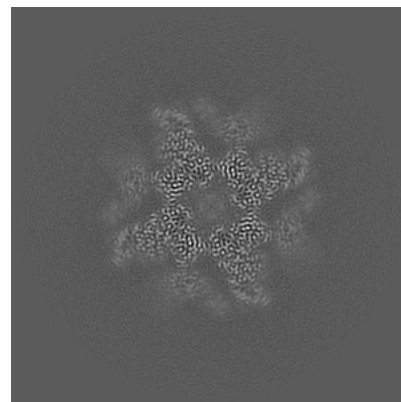
6.3.1 Primary map



X Index: 250

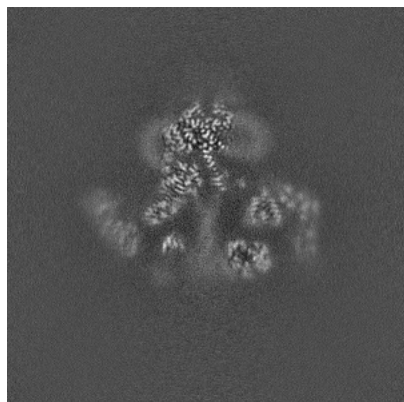


Y Index: 230

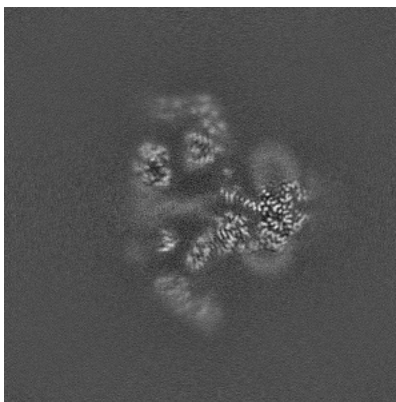


Z Index: 188

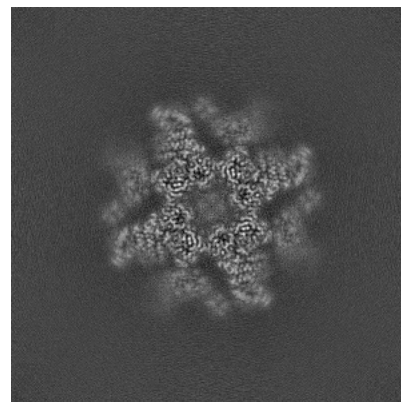
6.3.2 Raw map



X Index: 229



Y Index: 251

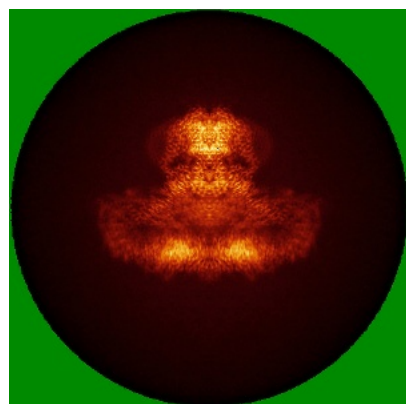


Z Index: 189

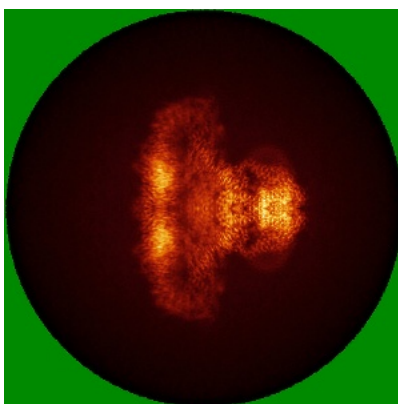
The images above show the largest variance slices of the map in three orthogonal directions.

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

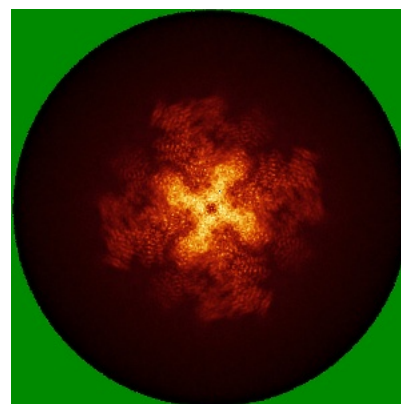
6.4.1 Primary map



X

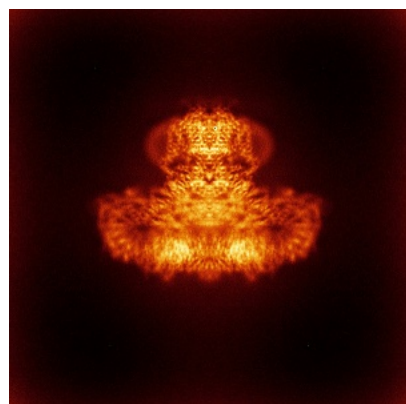


Y

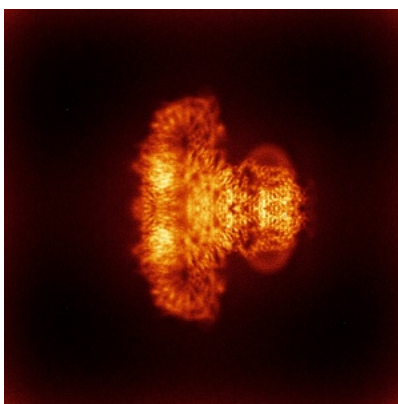


Z

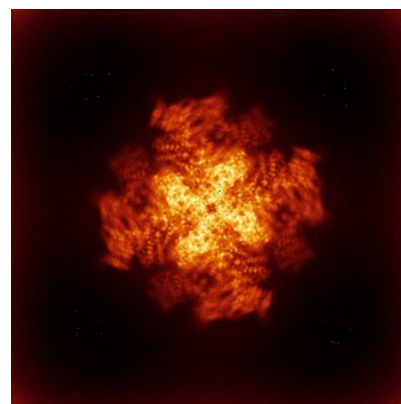
6.4.2 Raw map



X



Y

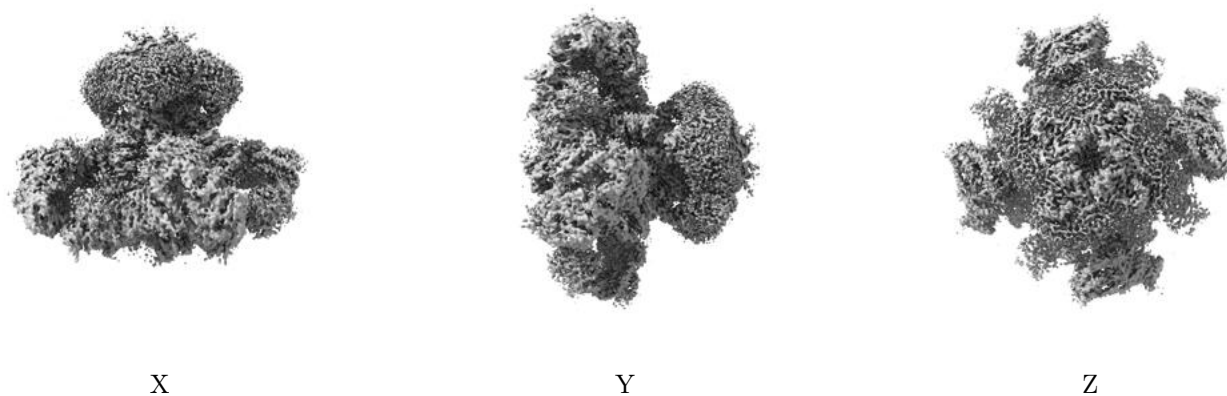


Z

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 0.2. 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.

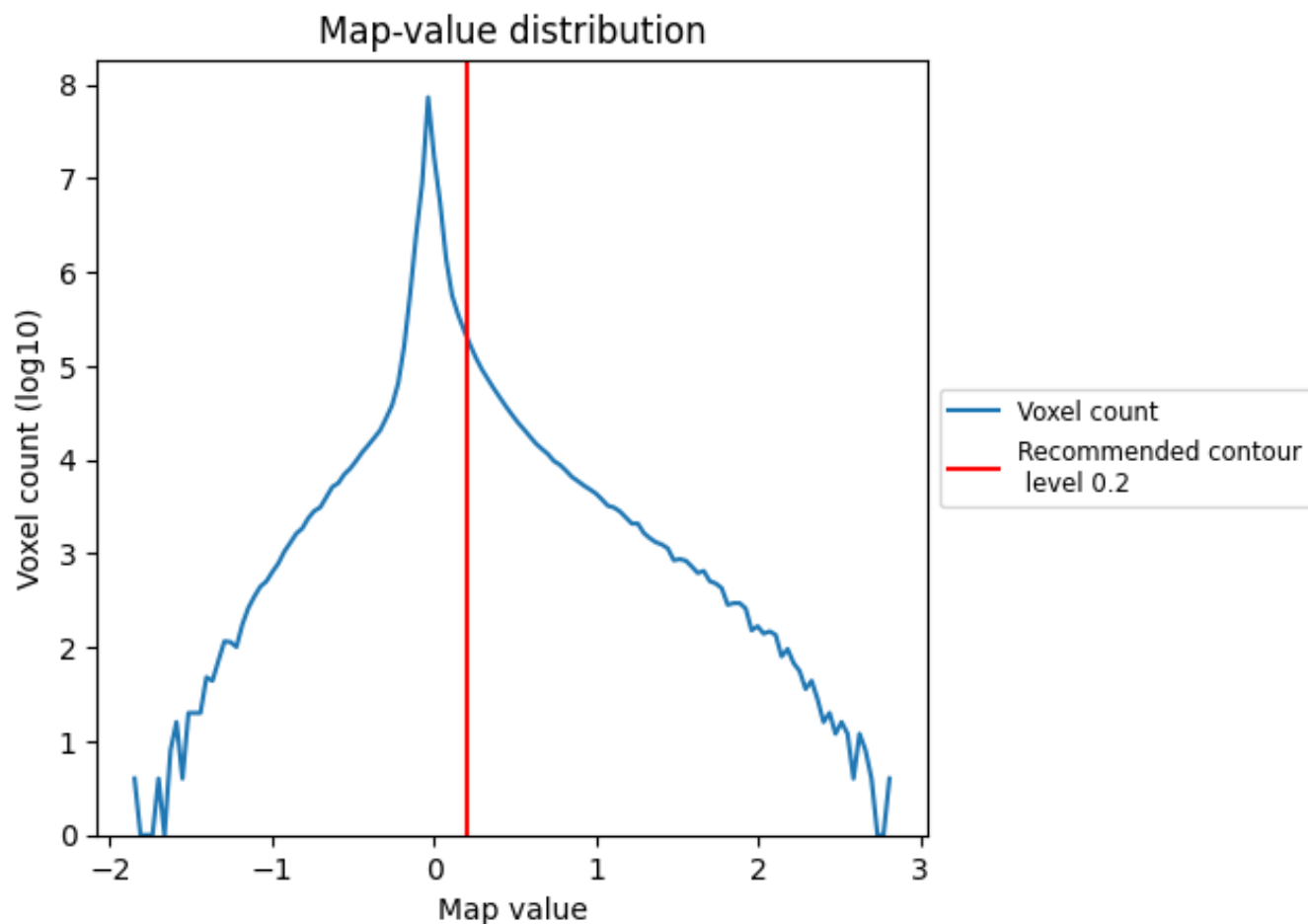
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

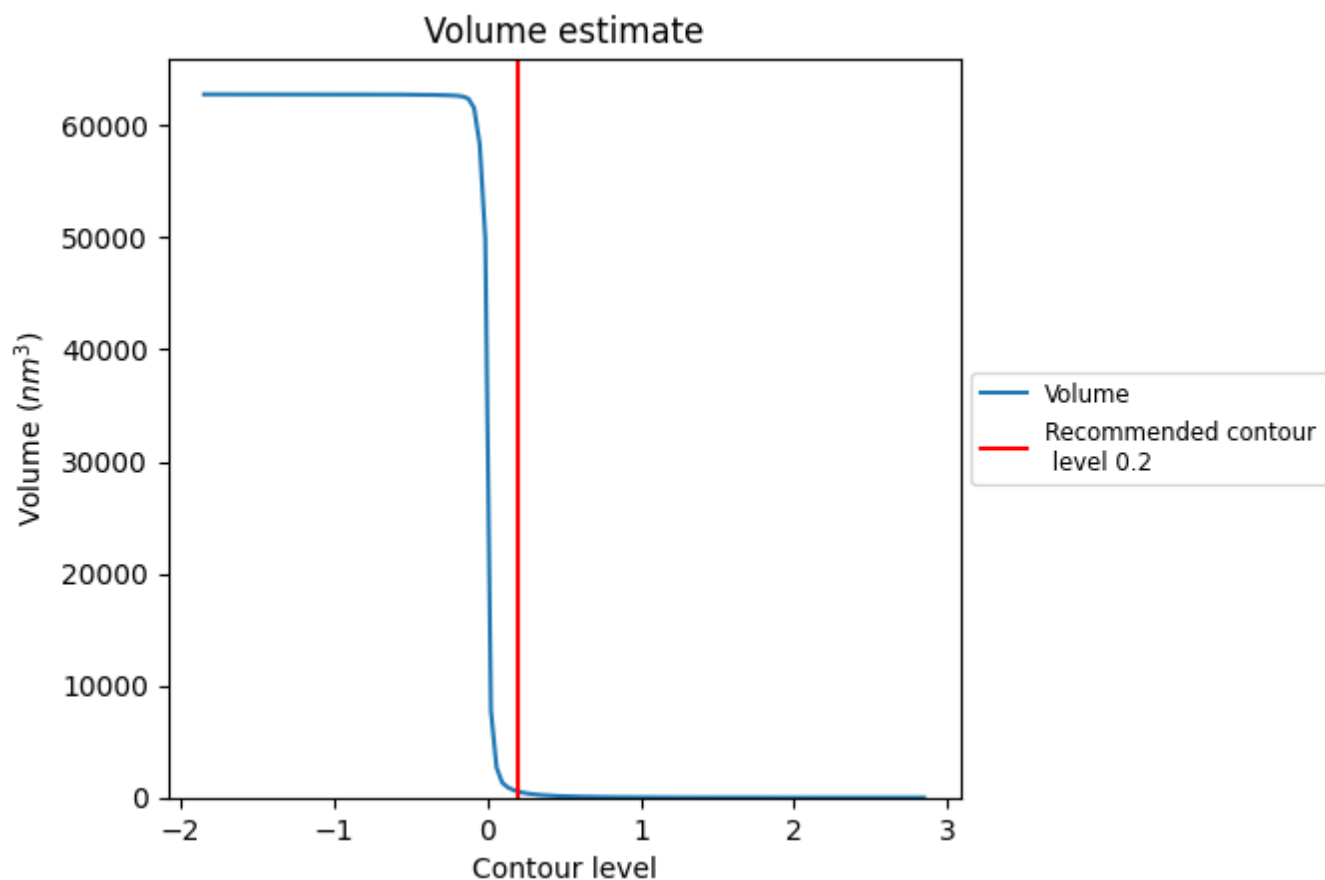
This section contains the results of statistical analysis of the map.

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.

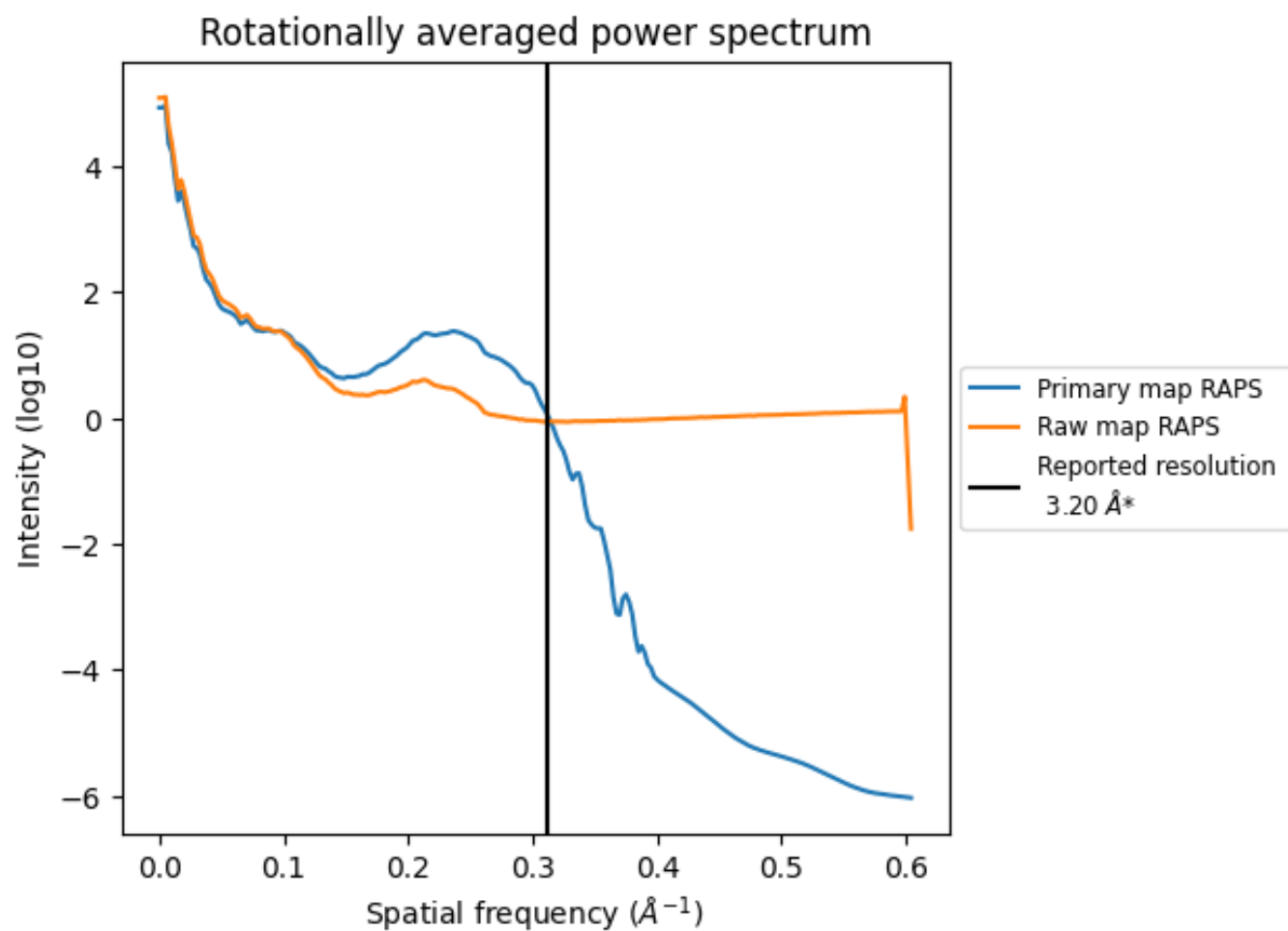
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 544 nm³; this corresponds to an approximate mass of 491 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 ⓘ

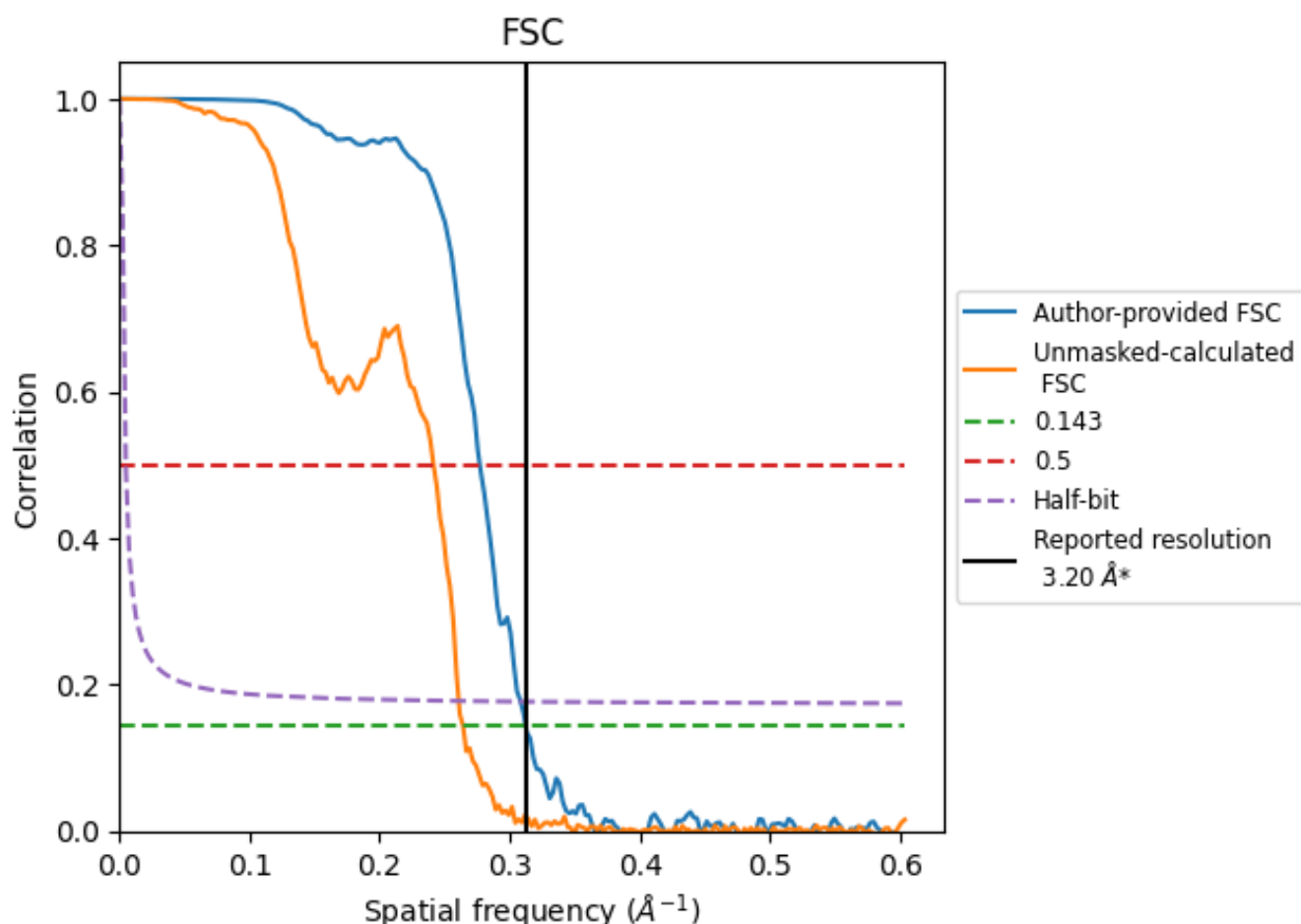


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

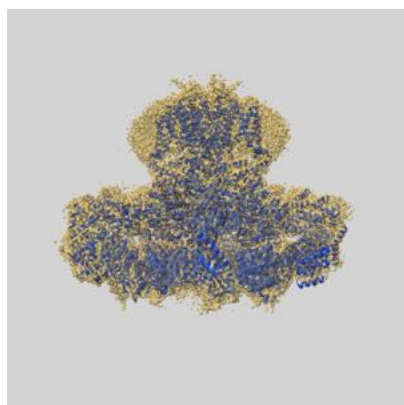
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.61	3.24
Unmasked-calculated*	3.79	4.14	3.83

*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 3.79 differs from the reported value 3.2 by more than 10 %

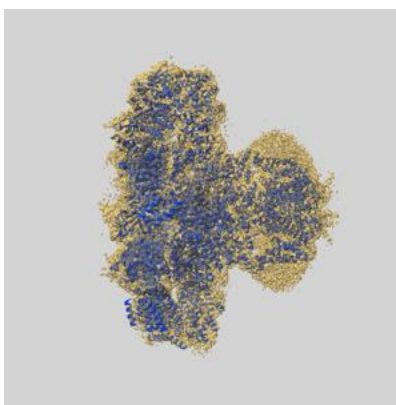
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25667 and PDB model 7T3P. Per-residue inclusion information can be found in section [3](#) on page [6](#).

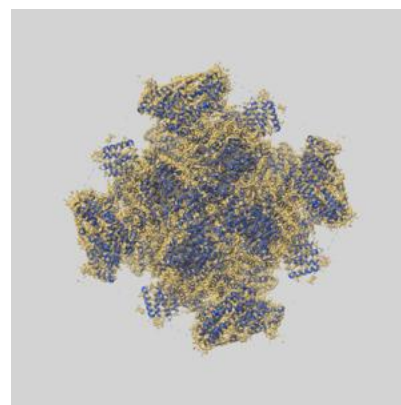
9.1 Map-model overlay [i](#)



X



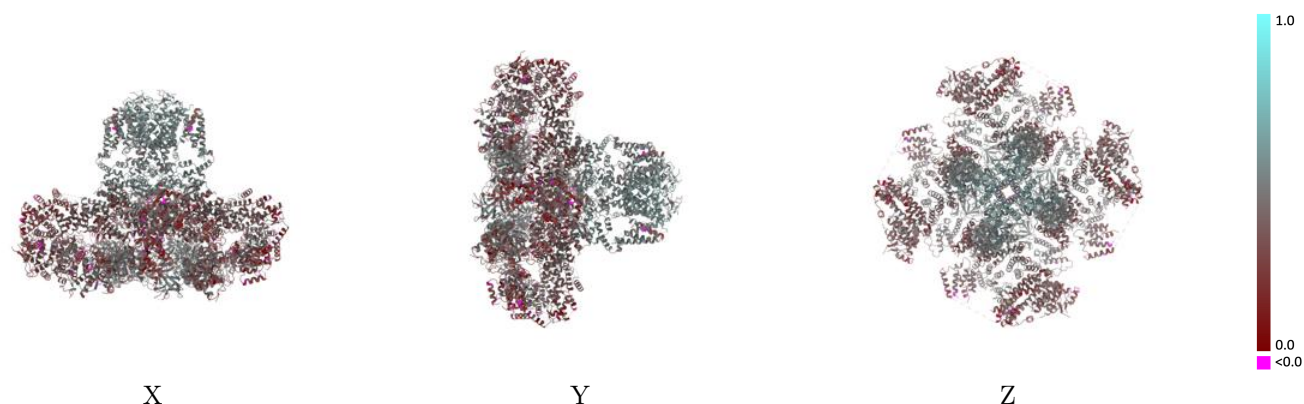
Y



Z

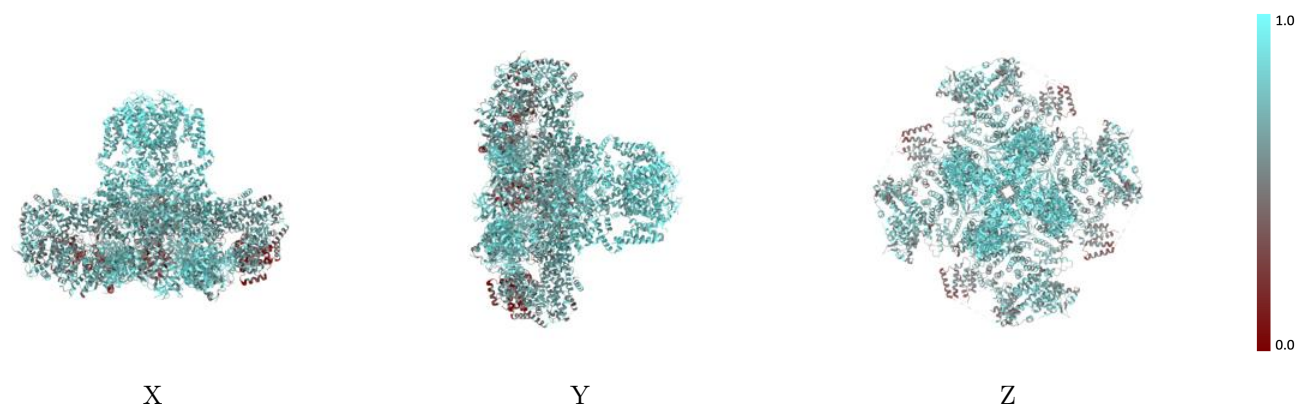
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



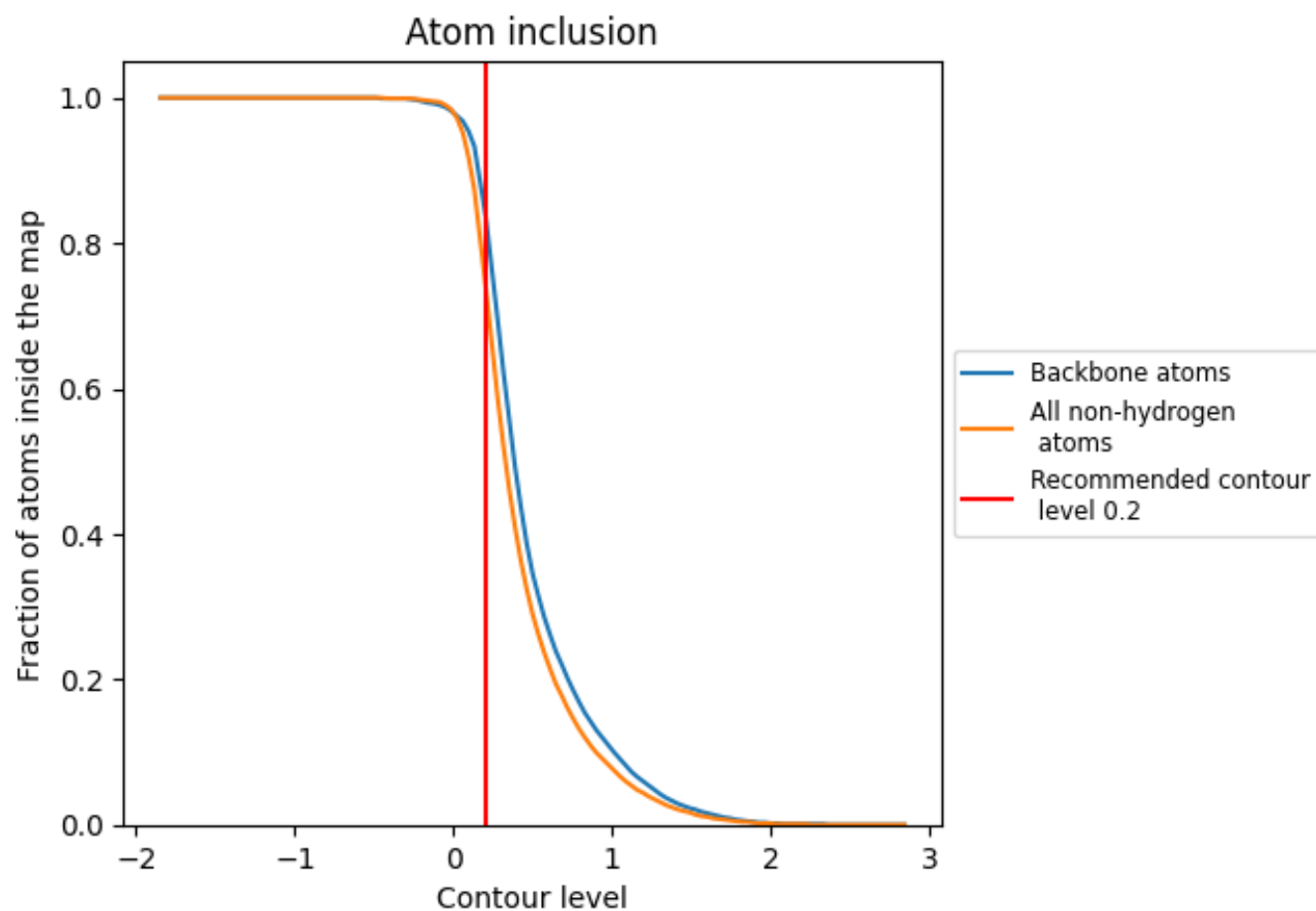
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 75% 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	<div></div> 0.7500	<div></div> 0.3990
A	<div></div> 0.7510	<div></div> 0.4020
B	<div></div> 0.7450	<div></div> 0.3910
C	<div></div> 0.7510	<div></div> 0.4020
D	<div></div> 0.7510	<div></div> 0.4020

