



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 04:22 PM EDT

PDB ID : 9ZN7 / pdb_00009zn7
EMDB ID : EMD-74437
Title : Structure of rabbit RyR1 complexed with FKBP12.6 and calmodulin in the presence of ATP, ADP, and Mg²⁺ (mimicking muscle fatigue)
Authors : Kim, K.; Clarke, O.B.
Deposited on : 2025-12-12
Resolution : 2.23 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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.dev133
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) : 2.50

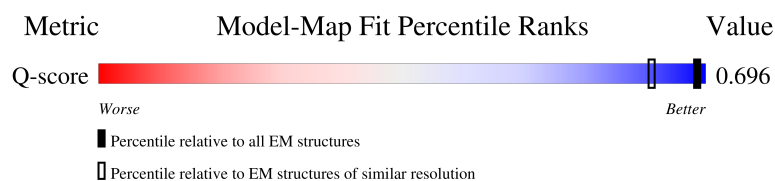
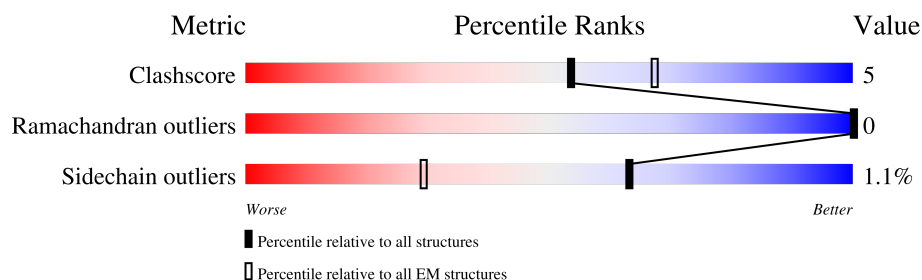
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.23 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.



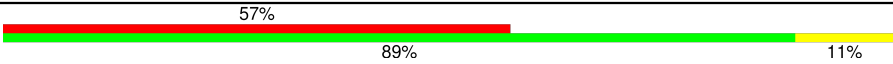
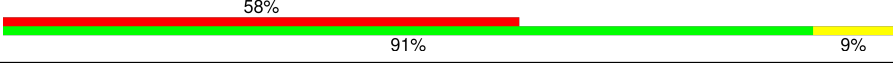
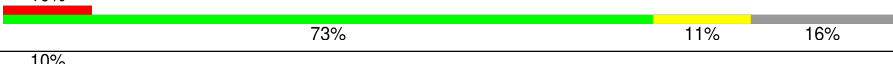
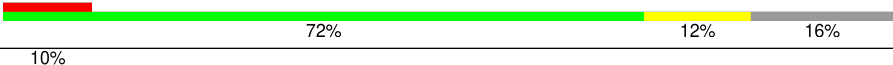
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3335 (1.73 - 2.73)

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	E	107	 79% 21%
1	F	107	 80% 19%
1	G	107	 79% 21%
1	H	107	 78% 22%

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Mol	Chain	Length	Quality of chain
2	I	148	
2	J	148	
2	K	148	
2	L	148	
3	A	5037	
3	B	5037	
3	C	5037	
3	D	5037	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 148402 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	F	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
2	J	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
2	K	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
2	L	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	HIS	-	expression tag	UNP P0DP23
J	-1	HIS	-	expression tag	UNP P0DP23
K	-1	HIS	-	expression tag	UNP P0DP23
L	-1	HIS	-	expression tag	UNP P0DP23

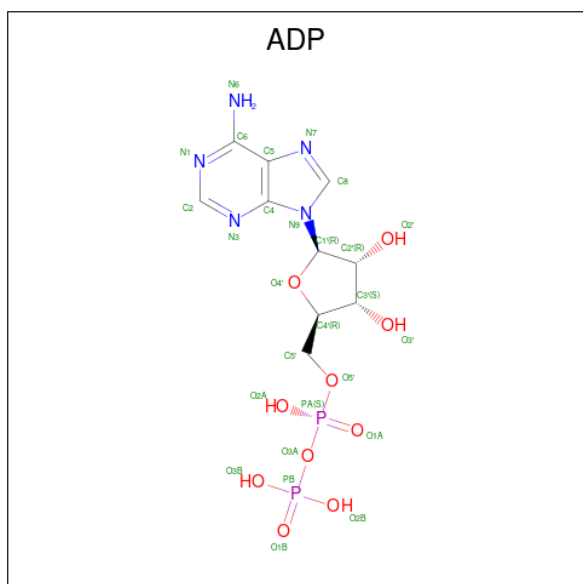
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	A	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	B	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	C	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



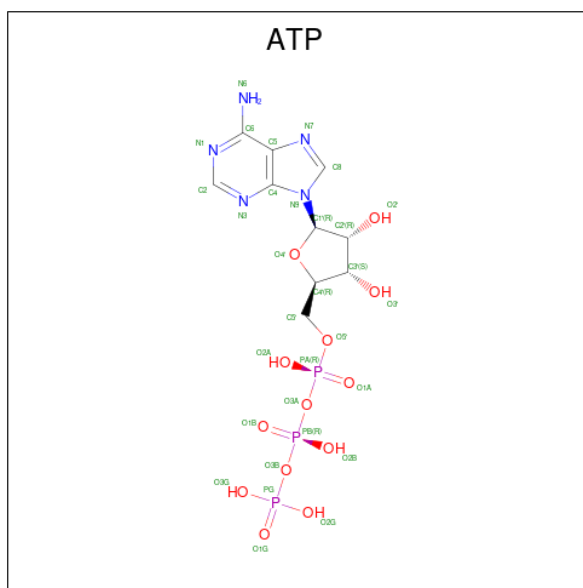
Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total 1	Mg 1	0
7	A	1	Total 1	Mg 1	0
7	B	1	Total 1	Mg 1	0
7	C	1	Total 1	Mg 1	0

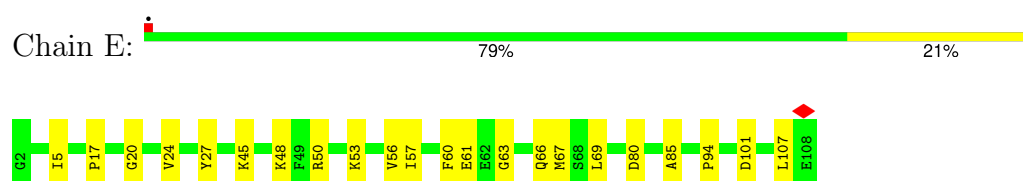
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	E	22	Total 22	O 22	0
8	F	20	Total 20	O 20	0
8	G	20	Total 20	O 20	0
8	H	24	Total 24	O 24	0
8	I	55	Total 55	O 55	0
8	J	58	Total 58	O 58	0
8	K	56	Total 56	O 56	0
8	L	62	Total 62	O 62	0
8	D	1225	Total 1225	O 1225	0
8	A	1213	Total 1213	O 1213	0
8	B	1213	Total 1213	O 1213	0
8	C	1226	Total 1226	O 1226	0

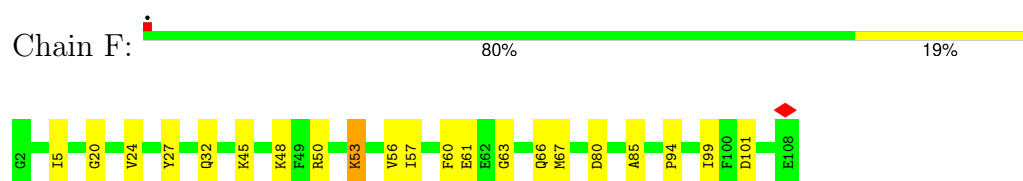
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

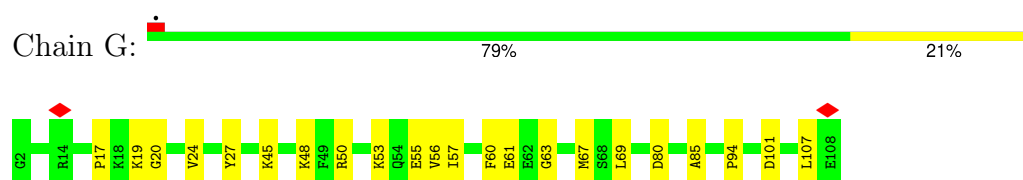
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



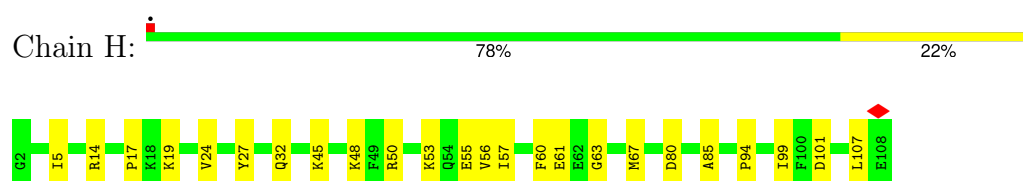
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



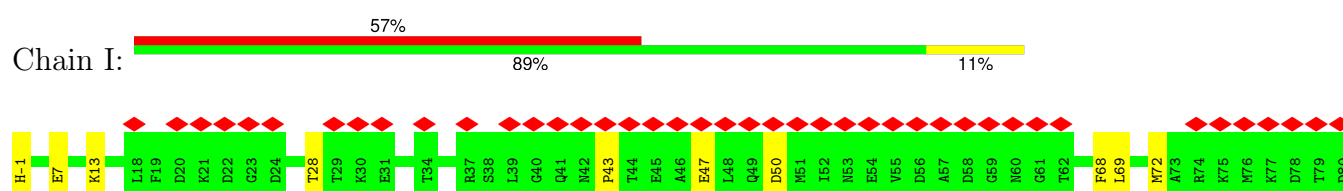
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

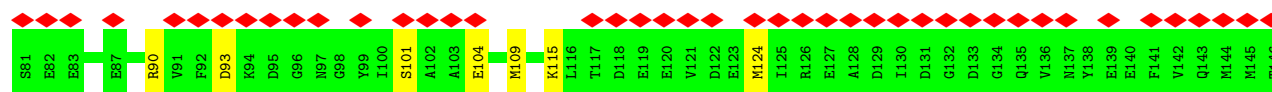


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

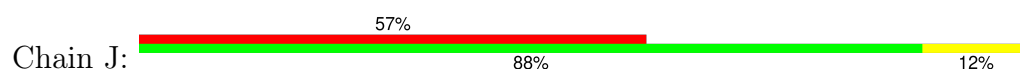


- Molecule 2: Calmodulin-1

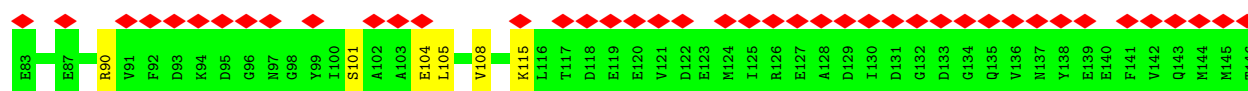
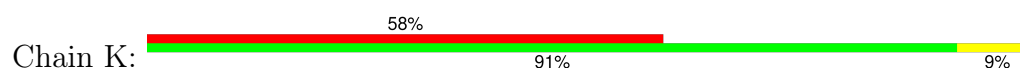




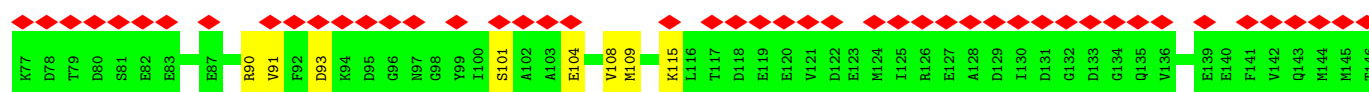
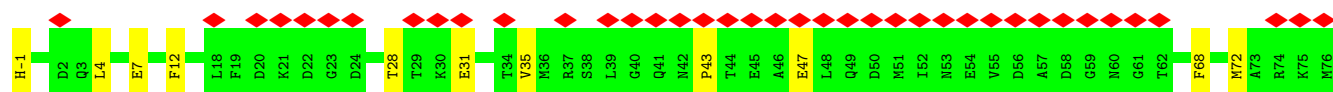
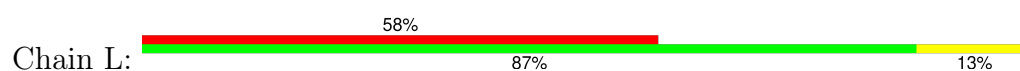
- Molecule 2: Calmodulin-1



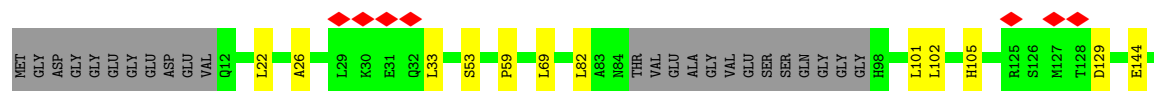
- Molecule 2: Calmodulin-1



- Molecule 2: Calmodulin-1

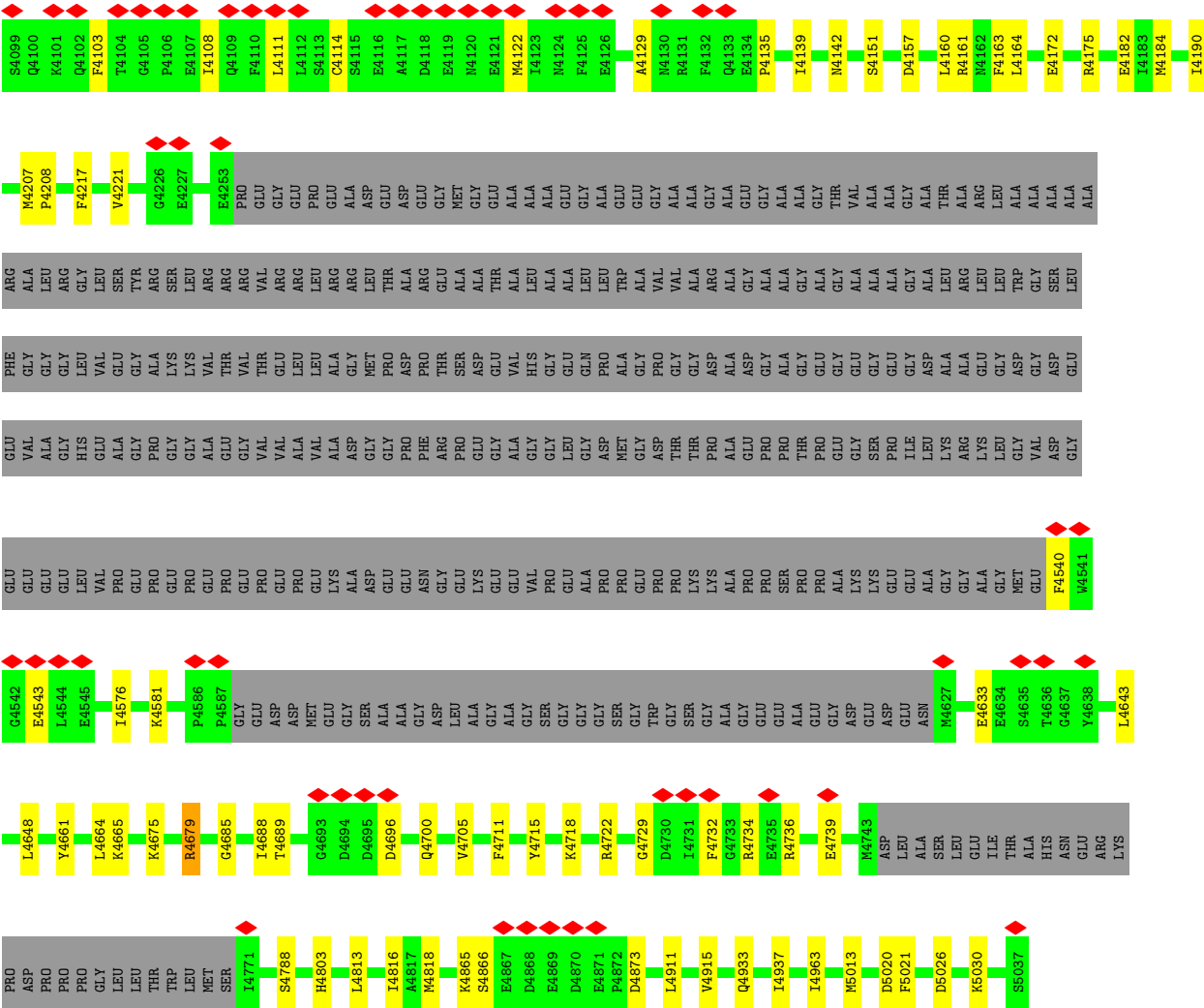


- Molecule 3: Ryanodine receptor 1

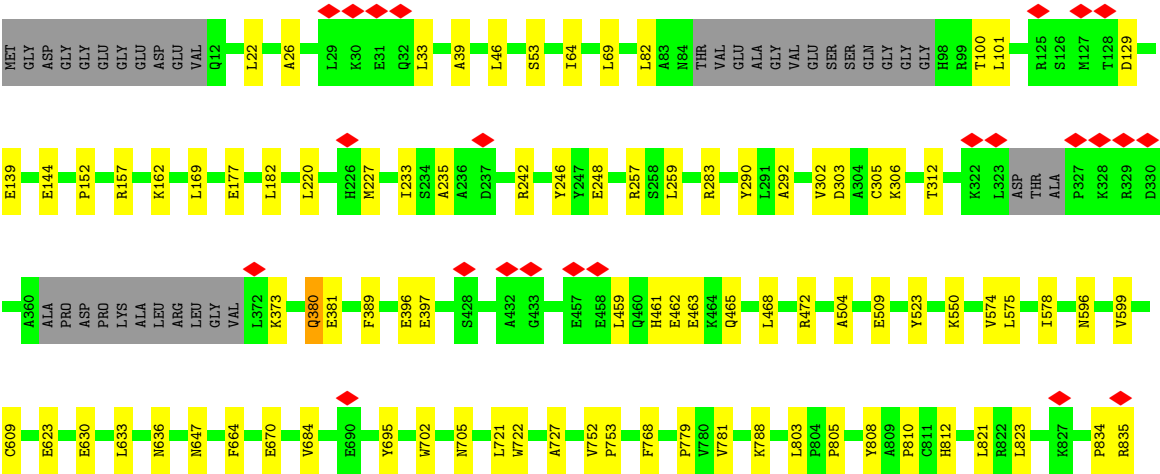




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S4008	M3816	E3682	L3365	T3177	T3040	K2928	S2868	P2808	P2748	K2638
Q4009		L3569	R3366	T3178	V3050	F2929	R2869	I2809	E2749	W2639
T4010	A3834	R3570	K3367	K3179	N3066	L2930	E2870	K2810	K2750	P2640
L4013	T3838	R3577	R3368	Y3182	T3070	Q2931	L2871	E2811	L2751	L2644
Q4020	Q3850	G3581	E3377	K3185	V3080	M2932	Q2872	S2812	L2752	L2644
K4021	V3859	R3582	Q3378	L3186	N3080	N2933	A2873	L2813	S2753	L2672
D4022	V3859	R3582	L3379	L3194	V3081	Q2934	M2874	K2814	F2754	
L4031	N3860	GLU	R3380	L3194	Q3082	Y2935	A2875	A2815	I2755	K2677
E3861	E3861	GLU	L3381	S3223	K3082	A2936	E2876	M2816	N2756	L2678
D3862	D3862	ASP	E3382	P3224	S3083	V2937	Q2877	I2817	K2757	F2679
		ALA	A3383	R3225	E3086	T2938	Q2878	A2818	F2758	K2690
V3865	V3865	L3710	K3384	R3225	K3089	R2939	A2879	W2819	A2759	Y2691
I3866	I3866	S3714	A3385	A3228	K3089	Q2940	E2880	E2820	E2760	E2694
ASN	ASN	K3715	A3385	I3229	L3092	L2941	M2881	TRP	Y2761	
ARG	ARG	L3721	E3386	L3230	K2942	K2942	Y2882	ILE	T2762	M2698
GLN	GLN	L3721	A3387	L3230	D2943	D2943	H2883	GLU	H2763	A2699
ASN	ASN	L3728	E3388	M3234	M2944	E2945	H2884	LYS	E2764	W2700
E3872	E3872	L3735	E3389	G3254	E2945	L2946	T2885	ALA	K2765	P2701
F3899	F3899	L3735	E3390	G3254	E2946	L2947	W2886	ARG	W2766	C2704
I3916	I3916	GLU	E3391	E3258	D2947	D2947	G2887	GLY	A2767	A2705
V3920	V3920	GLY	L3392	E3258	T2948	T2948	K2888	GLU	F2768	I2706
L3923	L3923	GLY	V3394	S3279	S2949	S2949	K2889	GLU	D2769	V2715
D3941	D3941	ASN	A3407	P3292	VAL	E2950	K2890	ARG	K2770	I2716
V3942	V3942	LYS	L3408	PRO	GLN	E2952	Q2891	THR	I2771	A2717
I3943	I3943	LYS	L3412	PRO	ALA	K2953	K2892	GLU	Q2772	S2718
S4074	S4074	LYS	V3416	PRO	THR	E2953	E2893	LYS	N2773	Y2719
E3945	E3945	ALA	R3420	ALA	GLN	K2953	E2894	LYS	N2774	S2720
Q3946	Q3946	VAL	L3434	GLY	VAL	E2953	E2896	ARG	W2775	S2721
R3949	R3949	LYS	M3437	ALA	K3123	S2970	K2897	LYS	S2776	K2722
K3959	K3959	LEU	H3449	P3301	Q3124	F2973	K2898	SER	Y2777	E2724
Q3960	Q3960	S3625	H3449	L3316	V3125	H2976	G2899	THR	G2778	K2725
V3961	V3961	K3626	R3453	V3324	G3126	L2977	G2900	ALA	N2779	LYS
G3971	G3971	K3627	R3453	L3327	Q3127	E2978	T2901	THR	V2781	THR
P3972	P3972	R3628	R3453	G3328	N3128	A2979	H2902	GLN	D2782	VAL
P4083	P4083	R3629	Q3456	I3329	L3129	V2980	P2903	TYR	E2783	ASP
R4085	R4085	R3630	E3463	A3332	L3136	V2981	L2905	PRO	E2784	ALA
Q4086	Q4086	A3631	I3464	T3333	Q3149	S2982	V2906	ARG	L2785	GLY
L4087	L4087	R3637	I3465	M3335	R3160	G2986	P2907	GLY	K2786	N2734
S4089	S4089	M3638	M3467	F3341	Q3151	R2986	Y2908	N2856	H2788	F2735
Q4090	Q4090	S3656	T3471	P3344	V3163	E2987	D2909	P2857	P2789	P2737
K4091	K4091	Y3657	ALA	I3345	R3167	K2988	T2910	Q2858	M2790	R2738
D4092	D4092	K3658	ASP	V3346	L3168	E2988	L2912	P2859	L2791	V2740
Q4094	Q4094	L3663	SER	F3358	L3175	S2989	T2911	P2860	R2792	E2741
K4095	K4095	D3666	LYS			L3003	A2913	D2861	P2793	E2741
A4096	A4096		SER			P3004	E2915	L2862	Y2794	T2742
M4097	M4097		NET			Q3008	K2916	S2863	K2795	L2743
D4098	D4098		ALA			S3027	A2917	G2864	F2797	L2744
						K3036	R2918	V2865	S2798	V2745
							D2919	T2866	E2799	I2746
							R2920		K2800	
							E2921		D2801	
							K2922		K2802	
							A2923		E2803	
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									R2806	



● Molecule 3: Ryanodine receptor 1

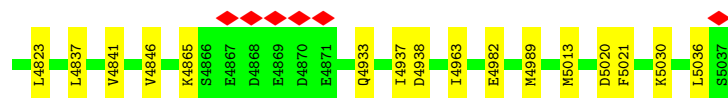




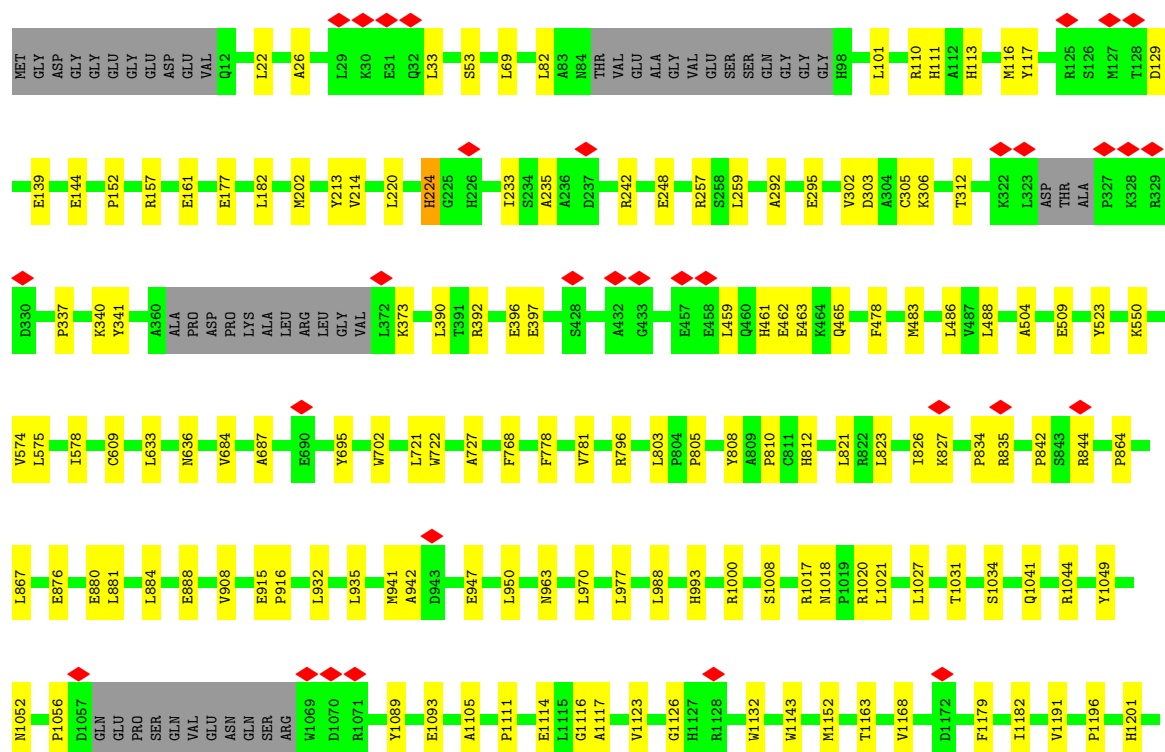
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										THR	ILE	GLU	LYS	ALA	ARG	GLU	GLY	GLU	GLU	GLU	THR	GLN	THR	ALA	GLN	GLN	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881					
Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	D2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	P2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	G2940	L2941
K2942	D2943	M2944	E2945	L2946	D2947	T2948	S2949	S2950	T2951	E2952	K2953	L2963	M2967	S2970	F2973	L2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	L3003	P3004	Q3008	S3027	K3036	T3039	T3040	L3049	N3066	L3070	V3080	K3082														
S3083	K3089	L3092	E3101	K3105	M3106	V3107	E3108	R3111	L3112	G3113	LYS	VAL	SER	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	K3127	M3128	L3129	T3132	L3136	Q3151	L3157	L3158	V3163	R3167	T3169	L3169	T3177	T3178	K3179	Y3182	K3185	L3186	L3194	V3203																
N3214	S3223	P3224	R3225	A3228	I3229	L3230	N3234	G3254	E3258	L3277	C3278	S3279	P3289	P3292	PRO	ALA	LEU	PRO	ALA	GLY	ALA	P3301	T3308	L3312	L3316	L3327	C3328	L3329	V3332	T3333	V3334	M3335	F3341	P3344	T3345	V3346	S3347	R3348																					
F3358	I3362	L3365	R3366	K3367	R3368	A3369	V3373	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	A3407	L3408	V3416	R3420	L3434	M3437	H3449	R3453	Q3456	N3457	Q3461	N3462	E3463	T3464	N3465	N3466	M3467	T3471	ALA															
ASP	SER	LYS	SER	LYS	MET	ALA	LYS	ALA	GLN	SER	GLY	SER	ASP	GLN	GLU	ARG	THR	GLU	GLU	ASP	ALA	D3587	P3588	P3589	E3590	K3591	L3592	V3593	R3594	R3595	Y3604	Q3608	T3609	E3610	H3611	P3612	TYR	LYS	SER	LYS	LYS	ALA	VAL	TRP	HIS	LYS	LEU	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	M3638			
K3562	V3563	E3564	G3565	S3566	P3567	S3568	L3569	R3570	M3573	A3574	L3575	R3576	R3577	G3581	R3582	GLU	GLU	ASP	ALA	D3587	P3588	P3589	E3590	K3591	L3592	V3593	R3594	R3595	Y3604	Q3608	T3609	E3610	H3611	P3612	TYR	LYS	SER	LYS	LYS	ALA	VAL	TRP	HIS	LYS	LEU	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	M3638					
Y3642	S3656	L3663	D3666	E3682	GLN	GLU	GLU	GLU	GLU	GLU	VAL	GLU	K3693	L3710	K3715	E3718	K3731	L3735	GLU	GLY	GLY	GLU	ASN	GLY	T3699	D3941	V3942	L3943	E3944	E3945	Q3946	R3949	G3971	P3972	A3981	R3984	F3996	A3997	M4000	L4003	A4004	Q4005	D4006																
S4007	S4008	Q4009	I4010	L4013	Q4020	M4026	I4040	S4053	E4056	M4057	I4058	L4059	K4060	M4064	K4067	L4068	K4069	D4070	I4071	V4072	G4073	S4074	E4075	A4076	F4077	Q4078	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	G4086	L4087	I4088	S4089	K4090	K4091	D4092	F4093	Q4094	K4095	A4096	M4097	D4098	S4099	Q4100	K4101	Q4102	F4103								
T4104	G4105	P4106	E4107	I4108	Q4109	F4110	L4111	L4112	S4115	E4116	A4117	D4118	E4119	M4120	E4121	M4122	I4123	F4125	E4126	A4129	M4130	M4131	F4132	P4135	I4139	S4151	V4154	D4157	L4160	L4164	E4165	L4166	E4182	M4207	P4208	F4217	V4221	G4226	E4227	M4231	E4253	PRO																	

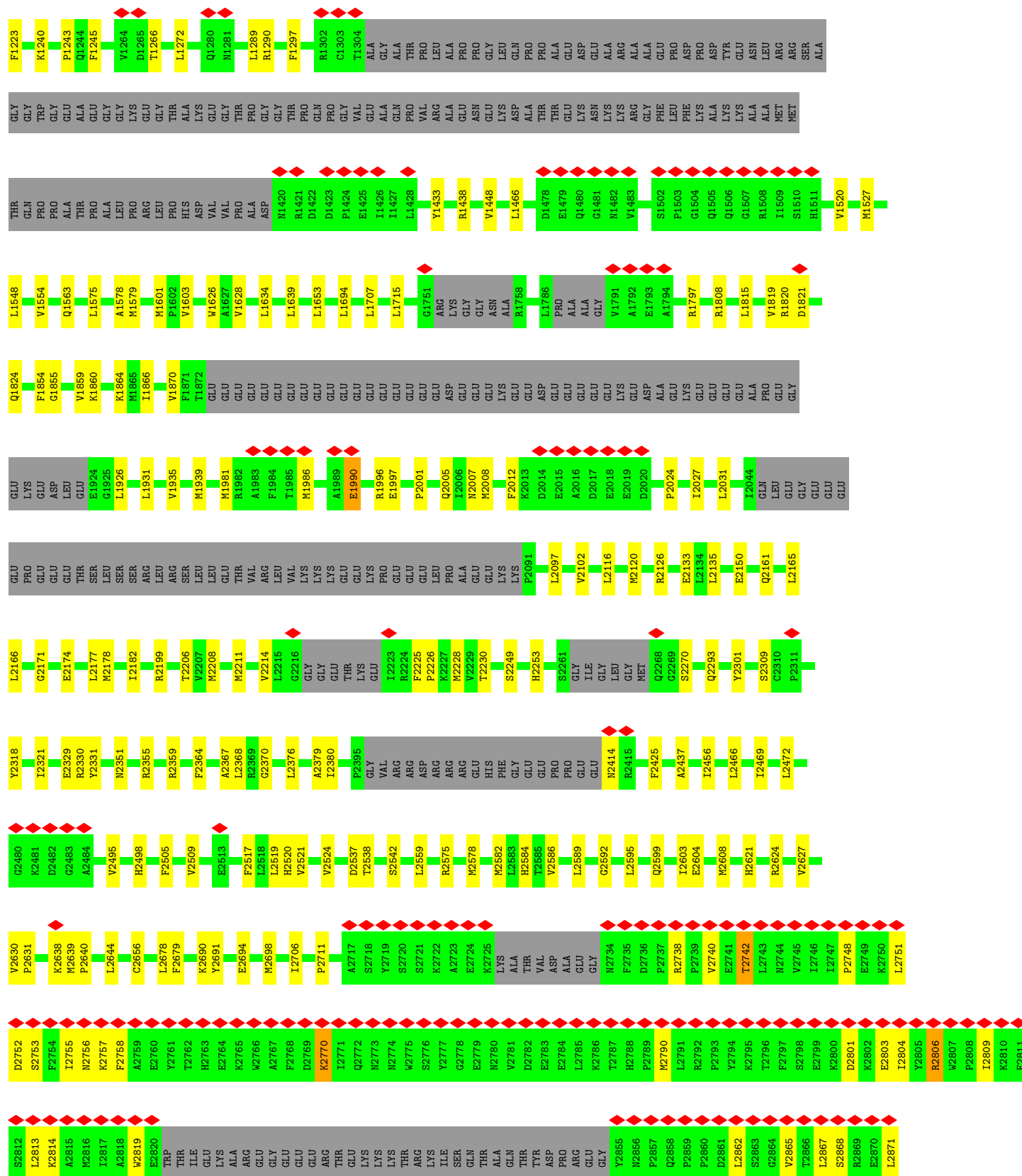


PRO	L4112	M4039	E3861	D3686	LYS	G3390	ALA	H3150	K2988	E2915	Y2855
GLU	S4115	I4040	D3862	P3689	ARG	E3391	GLY	Q3151	S2989	K2916	H2856
ALA	A4116	Q4043	T3866	E3590	GLY	L3392	ALA	D3159	K3027	A2917	F2857
ASP	A4117	S4052	T3866	K3591	ASP	L3393	ASP	V3163	S3027	R2918	Q2858
GLU	D4118	S4053	ASN	V3593	ASP	V3394	T3308	R3167	K3036	D2919	F2859
GLY	E4119	E4056	ARG	R3594	ASP	L3408	L3312	T3168	I3039	R2920	P2860
MET	E4120	M4057	GLN	R3595	ASP	L3412	L3316	L3169	D3060	E2921	D2861
GLY	N4121	M4057	ASN	Y3604	ASP	V3416	L3322	G3175	D3060	K2922	L2862
ALA	E4122	K4060	GLY	Q3608	Y3603	V3416	I3323	G3176	V3064	A2923	S2863
ALA	M4123	F4061	L3716	P3609	S3504	R3420	I3323	T3177	V3065	Q2924	G2864
ALA	N4124	M4064	D3717	E3610	Q3506	R3420	V3324	T3178	N3066	E2925	V2865
GLY	F4125	L4067	K3751	H3611	T3507	L3434	L3327	K3179	I3070	L2927	T2866
ALA	E4126	L4068	L3735	P3612	L3509	L3434	G3328	G3182	V3080	K2928	L2867
GLU	E4127	L4068	GLU	TYR	K3516	K3437	G3328	V3182	V3081	K2928	S2868
GLU	F4128	K4069	GLY	SER	M3517	L3453	I3329	K3185	K3081	F2929	R2869
GLY	A4129	D4070	GLY	LYS	D3531	R3453	A3332	K3186	K3082	L2930	E2870
ALA	N4130	I4071	ASN	LYS	K3543	H3449	T3333	L3186	S3083	Q2931	D2871
GLY	R4131	V4072	GLY	ALA	D3544	K3452	K3334	L3194	E3086	M2932	L2872
ALA	F4132	G4073	GLU	VAL	T3545	R3452	K3335	V3203	K3089	N2933	A2873
GLY	E4133	S4074	GLU	TRP	D3546	R3453	F3341	A3204	K3089	G2934	H2874
ALA	E4134	E4075	GLU	LEU	E3547	Q3456	P3344	F3205	L3092	A2935	A2875
ALA	I4139	A4076	GLU	L3624	E3548	E3463	P3344	L3206	L3092	A2936	E2876
GLY	G4140	F4077	GLU	S3625	R3549	T3464	F3344	E3207	K3105	V2937	Q2877
THR	F4141	Q4078	VAL	K3626	R3550	K3466	V3346	F3208	M3106	T2938	L2878
VAL	V4145	D4079	GLU	Q3627	E3551	K3466	S3347	Q3209	V3107	R2939	A2879
ALA	S4151	Y4080	V3751	R3629	F3552	K3467	R3348	N3214	E2880	G2940	E2880
ALA	V4154	Y4081	E3754	R3630	L3553	T3471	F3358	S2223	R3111	L2941	H2881
ARG	H4155	T4082	E3755	R3630	Q3554	ALA	I3362	P3224	L3112	K2942	Y2882
LEU	P4156	D4083	K3756	R3630	N3555	ASP	G3563	R3224	H2883	D2943	H2883
ALA	D4157	P4084	E3757	A3631	N3556	SER	R3364	R3225	N2884	M2944	N2884
ALA	P4158	R4085	M3758	M3638	L3557	LYS	L3366	A3228	T2885	E2945	T2885
ALA	R4159	G4086	Q3767	Y3642	H3558	LYS	R3367	I3229	V2886	L2946	V2886
ALA	L4160	L4087	Q3768	S3656	G3561	SER	R3368	L3230	G2887	D2947	G2887
ALA	L4161	K4090	H3771	S3656	K3562	LYS	A3369	N3234	R2888	T2948	R2888
ARG	L4164	K4091	L3798	L3663	V3563	MET	V3372	G3254	K2889	S2949	K2889
LEU	R4192	D4092	L3798	S3668	E3564	LYS	V3373	E3254	K2890	S2950	K2890
ARG	F4093	F4093	I3804	S3668	E3564	ALA	E3377	G3254	D2891	I2951	D2891
GLY	Q4094	Q4094	E3662	E3662	S3566	GLY	Q3378	E3254	Q2892	E2952	Q2892
LEU	K4095	K4095	GLN	GLN	S3566	ASP	L3379	E3258	E2893	K2953	E2893
SER	A4096	A4096	GLU	GLU	P3567	GLN	R3380	M3266	L2894	L2963	L2894
TYR	M4097	M4097	GLU	GLU	S3568	SER	L3381	M3266	E2895	M2967	E2895
SER	D4098	D4098	GLU	GLU	L3569	GLY	E3382	L3277	A2896	S2970	A2896
LEU	S4099	S4099	GLU	GLU	R3570	SER	A3383	P3289	K2897	F2973	K2897
ARG	Q4100	Q4100	GLU	GLU	M3573	ASP	K3384	P3289	G2898	Y3131	G2898
ARG	K4101	K4101	VAL	VAL	R3577	GLN	A3385	P3292	G2899	F2973	G2899
VAL	E4226	E4227	GLU	GLU	G3581	THR	E3386	PRO	G2900	H2976	G2900
ARG	A4228	A4228	GLU	GLU	R3582	ARG	A3387	ALA	T2901	L2977	T2901
ARG	E4253	E4253	GLU	GLU	GLU	LYS	A3388	LEU	H2902	E2978	H2902
PRO	PRO	G4105	GLU	GLU	GLU	LYS	E3388	PRO	A2979	A2979	T2903
GLY	GLY	P4106	GLU	GLU	GLU	LYS	E3388	PRO	V2980	V2980	L2904
GLU	GLU	E4107	GLU	GLU	GLU	LYS	E3388	PRO	V2981	V2981	L2905
GLU	GLU	T4108	GLU	GLU	GLU	LYS	E3388	PRO	S2982	S2982	L2905
GLU	GLU	Q4109	GLU	GLU	GLU	LYS	E3388	PRO	S2983	S2983	V2906
GLU	GLU	F4110	GLU	GLU	GLU	LYS	E3388	PRO	G2984	G2984	F2907
GLU	GLU	L4111	GLU	GLU	GLU	LYS	E3388	PRO	R2985	R2985	Y2908
GLU	GLU	L4111	GLU	GLU	GLU	LYS	E3388	PRO	D2909	D2909	D2909
GLU	GLU	L4111	GLU	GLU	GLU	LYS	E3388	PRO	T2910	T2910	T2910
GLU	GLU	L4111	GLU	GLU	GLU	LYS	E3388	PRO	T2911	T2911	T2911
GLU	GLU	L4111	GLU	GLU	GLU	LYS	E3388	PRO	A2913	A2913	A2913
GLU	GLU	L4111	GLU	GLU	GLU	LYS	E3388	PRO	K2914	K2914	K2914



Chain C:









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224598	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	7.779	Depositor
Minimum map value	0.000	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	E	0.13	0/835	0.33	0/1123
1	F	0.13	0/835	0.36	0/1123
1	G	0.13	0/835	0.33	0/1123
1	H	0.14	0/835	0.35	0/1123
2	I	0.11	0/1026	0.28	0/1386
2	J	0.10	0/1026	0.26	0/1386
2	K	0.11	0/1026	0.27	0/1386
2	L	0.11	0/1026	0.27	0/1386
3	A	0.15	0/34640	0.32	0/46902
3	B	0.15	0/34640	0.32	0/46902
3	C	0.15	0/34640	0.32	0/46902
3	D	0.15	0/34640	0.32	0/46902
All	All	0.14	0/146004	0.32	0/197644

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	E	819	0	821	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	819	0	821	11	0
1	G	819	0	821	13	0
1	H	819	0	821	14	0
2	I	1017	0	841	13	0
2	J	1017	0	841	12	0
2	K	1017	0	841	8	0
2	L	1017	0	841	13	0
3	A	33879	0	33511	343	0
3	B	33879	0	33511	355	0
3	C	33879	0	33511	370	0
3	D	33879	0	33511	348	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	54	0	24	0	0
5	B	54	0	24	0	0
5	C	54	0	24	0	0
5	D	54	0	24	0	0
6	A	31	0	12	0	0
6	B	31	0	12	0	0
6	C	31	0	12	0	0
6	D	31	0	12	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
8	A	1213	0	0	4	0
8	B	1213	0	0	3	0
8	C	1226	0	0	2	0
8	D	1225	0	0	3	0
8	E	22	0	0	0	0
8	F	20	0	0	0	0
8	G	20	0	0	0	0
8	H	24	0	0	0	0
8	I	55	0	0	0	0
8	J	58	0	0	0	0
8	K	56	0	0	0	0
8	L	62	0	0	0	0
All	All	148402	0	140836	1478	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 5.

The worst 5 of 1478 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)
3:B:2175:GLU:HG3	3:B:2228:MET:HB2	1.51	0.91
3:A:1980:LEU:HD11	3:A:1994:ARG:HB3	1.68	0.75
3:D:915:GLU:HG3	3:D:916:PRO:HD3	1.68	0.75
1:H:50:ARG:HB2	1:H:53:LYS:HG3	1.68	0.75
3:B:4207:MET:HE3	3:B:4208:PRO:HD2	1.69	0.75

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	E	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
1	F	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
1	G	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
1	H	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	I	146/148 (99%)	140 (96%)	6 (4%)	0	100	100
2	J	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
2	K	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
2	L	146/148 (99%)	143 (98%)	3 (2%)	0	100	100
3	A	4198/5037 (83%)	4126 (98%)	72 (2%)	0	100	100
3	B	4198/5037 (83%)	4126 (98%)	72 (2%)	0	100	100
3	C	4198/5037 (83%)	4130 (98%)	68 (2%)	0	100	100
3	D	4198/5037 (83%)	4128 (98%)	70 (2%)	0	100	100
All	All	17796/21168 (84%)	17487 (98%)	309 (2%)	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	E	88/88 (100%)	87 (99%)	1 (1%)	65	74
1	F	88/88 (100%)	85 (97%)	3 (3%)	32	38
1	G	88/88 (100%)	85 (97%)	3 (3%)	32	38
1	H	88/88 (100%)	87 (99%)	1 (1%)	65	74
2	I	82/127 (65%)	80 (98%)	2 (2%)	43	51
2	J	82/127 (65%)	80 (98%)	2 (2%)	43	51
2	K	82/127 (65%)	79 (96%)	3 (4%)	30	35
2	L	82/127 (65%)	80 (98%)	2 (2%)	43	51
3	A	3696/4276 (86%)	3659 (99%)	37 (1%)	68	76
3	B	3696/4276 (86%)	3661 (99%)	35 (1%)	70	78
3	C	3696/4276 (86%)	3656 (99%)	40 (1%)	65	74
3	D	3696/4276 (86%)	3660 (99%)	36 (1%)	68	76
All	All	15464/17964 (86%)	15299 (99%)	165 (1%)	63	74

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	3394	VAL
3	C	3107	VAL
3	B	3899	PHE
3	C	821	LEU
3	C	3359	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	473	ASN
3	C	4156	HIS
3	C	911	HIS
3	C	2858	GLN

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Mol	Chain	Res	Type
3	A	911	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ADP	B	5604	7	28,29,29	1.40	4 (14%)	43,45,45	1.81	9 (20%)
5	ADP	A	5602	-	28,29,29	1.40	4 (14%)	43,45,45	1.85	9 (20%)
5	ADP	D	5604	7	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
5	ADP	C	5602	-	28,29,29	1.38	4 (14%)	43,45,45	1.85	9 (20%)
6	ATP	D	5603	-	32,33,33	0.31	0	48,52,52	0.43	0
5	ADP	D	5602	-	28,29,29	1.39	4 (14%)	43,45,45	1.85	9 (20%)
5	ADP	A	5604	7	28,29,29	1.40	4 (14%)	43,45,45	1.81	9 (20%)
6	ATP	A	5603	-	32,33,33	0.31	0	48,52,52	0.43	0
5	ADP	B	5602	-	28,29,29	1.40	4 (14%)	43,45,45	1.85	9 (20%)
6	ATP	C	5603	-	32,33,33	0.31	0	48,52,52	0.43	0
5	ADP	C	5604	7	28,29,29	1.39	4 (14%)	43,45,45	1.82	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ATP	B	5603	-	32,33,33	0.31	0	48,52,52	0.43	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
5	ADP	B	5604	7	-	5/16/32/32	0/3/3/3
5	ADP	A	5602	-	-	7/16/32/32	0/3/3/3
5	ADP	D	5604	7	-	5/16/32/32	0/3/3/3
5	ADP	C	5602	-	-	8/16/32/32	0/3/3/3
6	ATP	D	5603	-	-	3/22/38/38	0/3/3/3
5	ADP	D	5602	-	-	7/16/32/32	0/3/3/3
5	ADP	A	5604	7	-	5/16/32/32	0/3/3/3
6	ATP	A	5603	-	-	3/22/38/38	0/3/3/3
5	ADP	B	5602	-	-	7/16/32/32	0/3/3/3
6	ATP	C	5603	-	-	4/22/38/38	0/3/3/3
5	ADP	C	5604	7	-	5/16/32/32	0/3/3/3
6	ATP	B	5603	-	-	5/22/38/38	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5604	ADP	C5-C4	4.63	1.47	1.39
5	B	5604	ADP	C5-C4	4.62	1.47	1.39
5	D	5604	ADP	C5-C4	4.61	1.47	1.39
5	C	5604	ADP	C5-C4	4.58	1.47	1.39
5	B	5602	ADP	C5-C4	4.55	1.47	1.39

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5602	ADP	C5-C4-N3	-6.01	118.44	126.72
5	A	5602	ADP	C5-C4-N3	-6.01	118.45	126.72
5	B	5602	ADP	C5-C4-N3	-6.00	118.46	126.72
5	D	5602	ADP	C5-C4-N3	-6.00	118.46	126.72
5	D	5604	ADP	C5-C4-N3	-5.77	118.77	126.72

There are no chirality outliers.

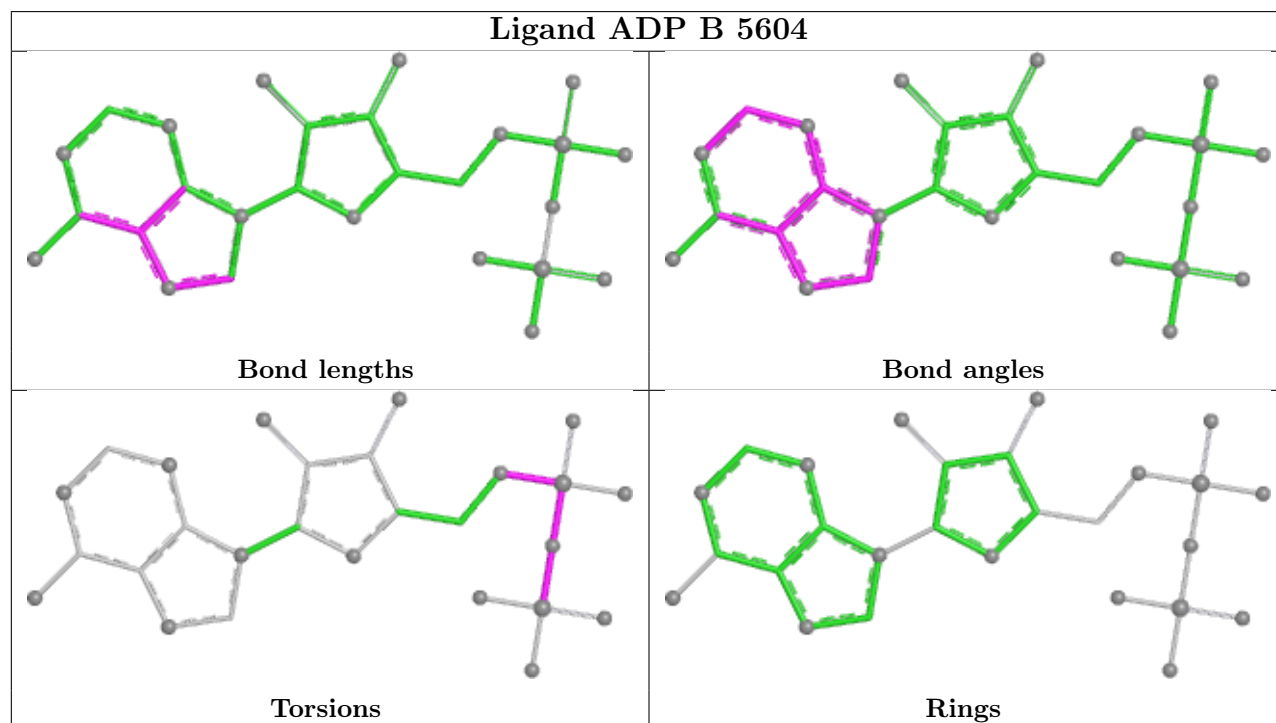
5 of 64 torsion outliers are listed below:

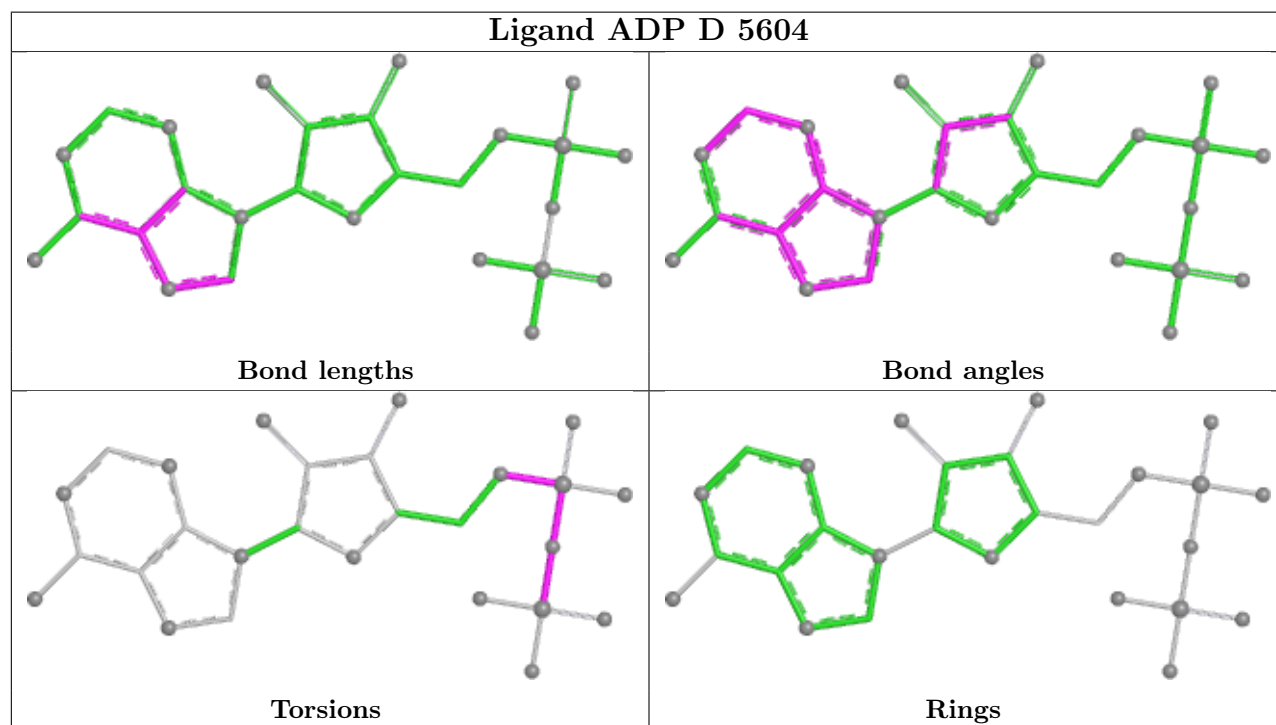
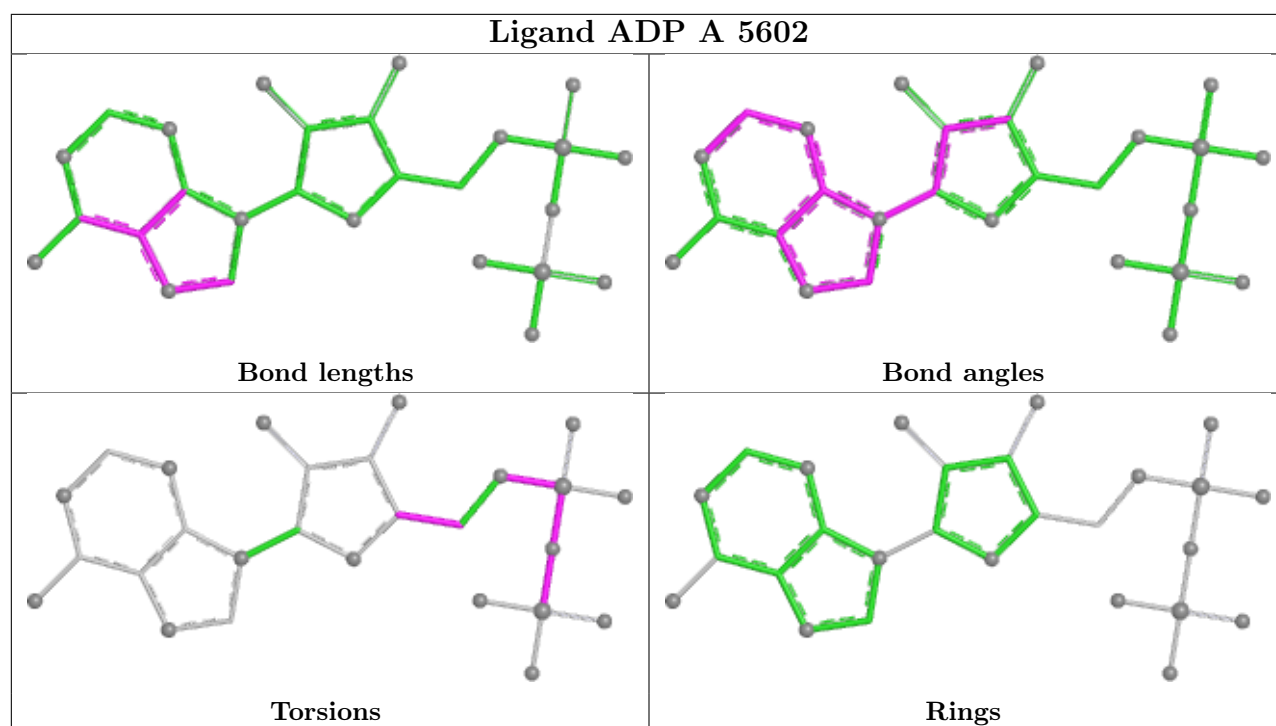
Mol	Chain	Res	Type	Atoms
5	D	5602	ADP	C5'-O5'-PA-O2A
5	D	5602	ADP	C5'-O5'-PA-O3A
5	D	5604	ADP	C5'-O5'-PA-O2A
5	D	5604	ADP	C5'-O5'-PA-O3A
5	A	5602	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

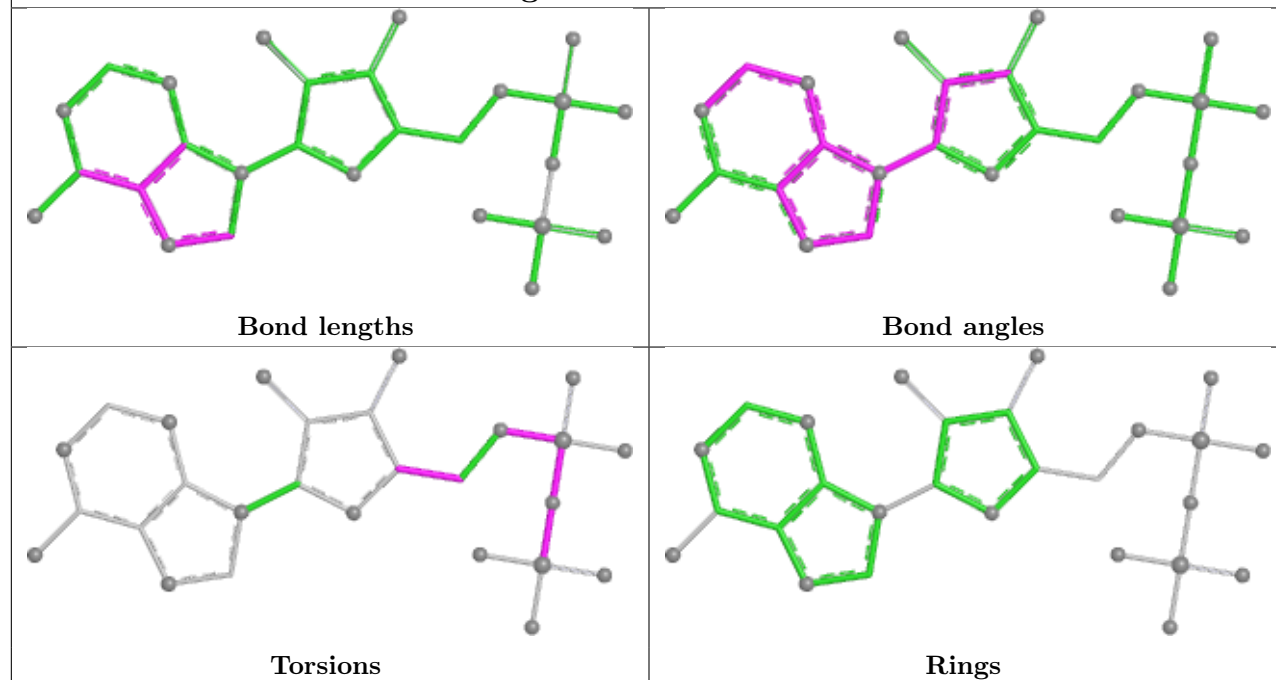
No monomer is involved in short contacts.

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.

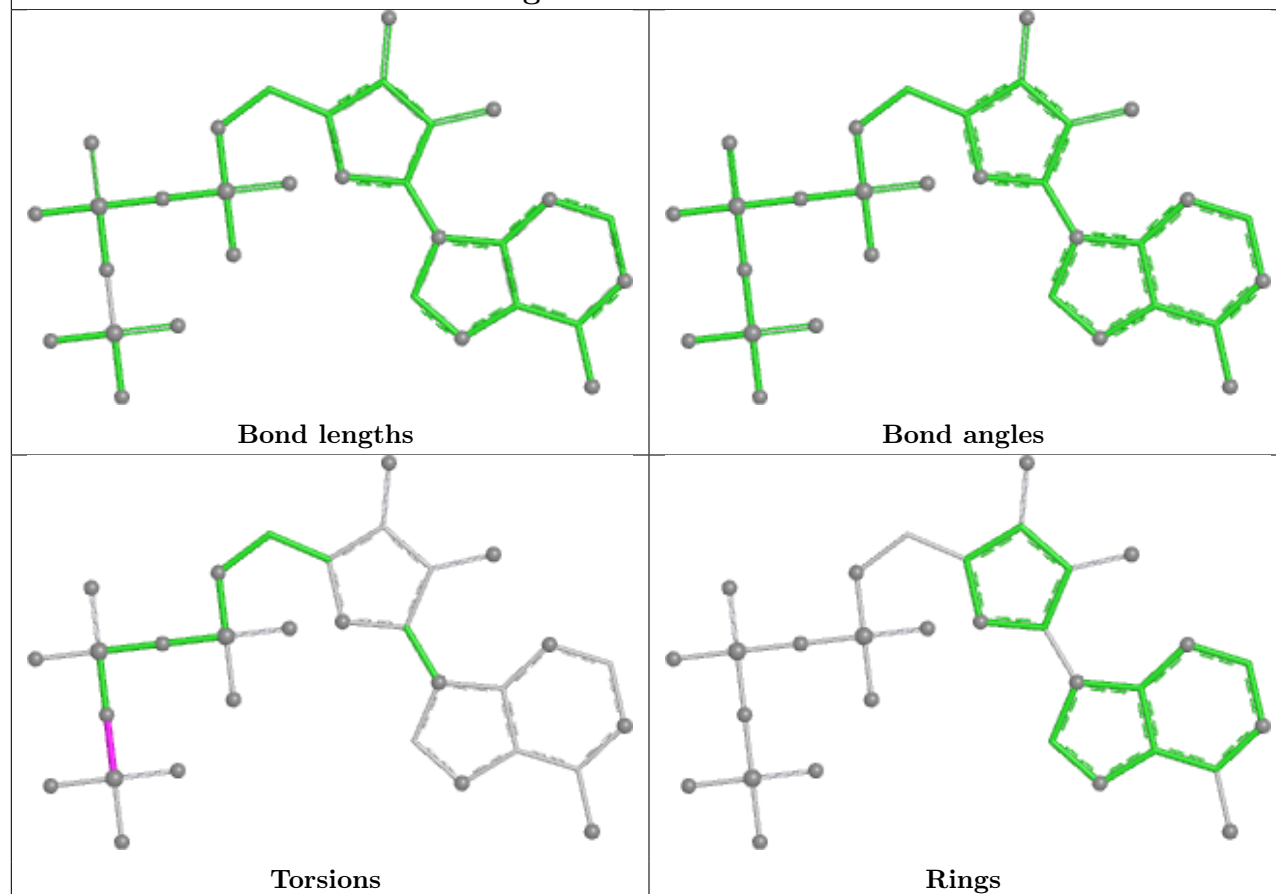




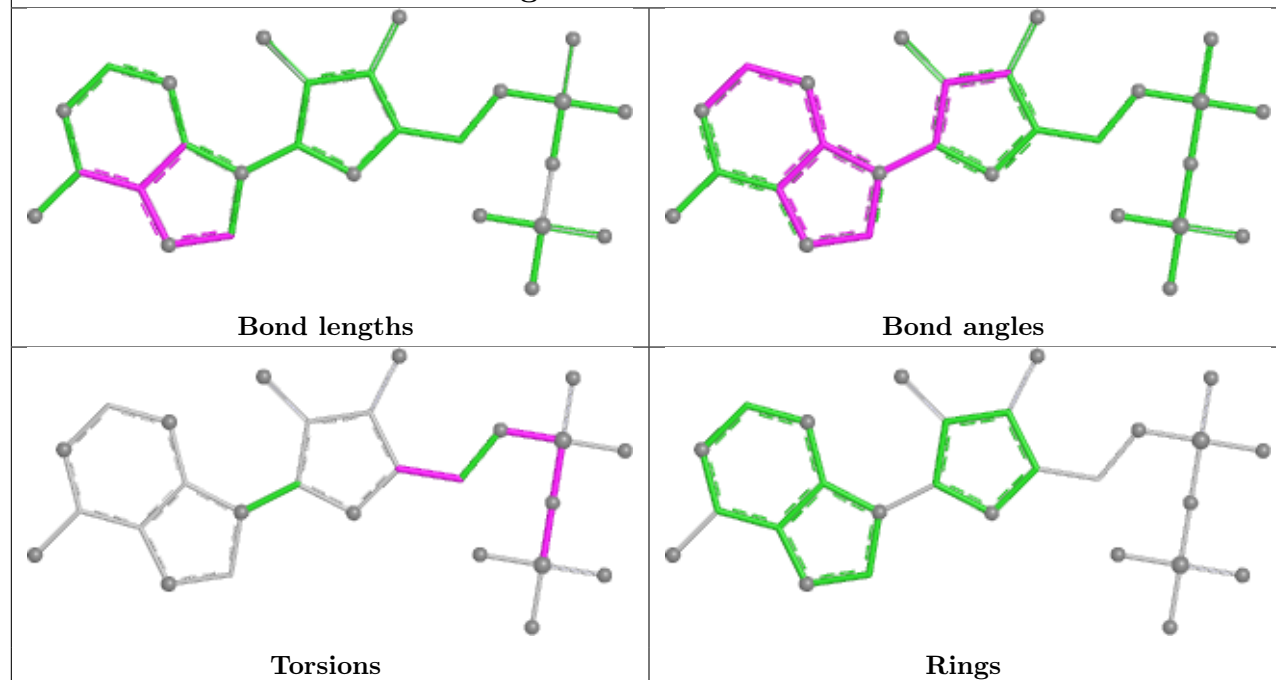
Ligand ADP C 5602



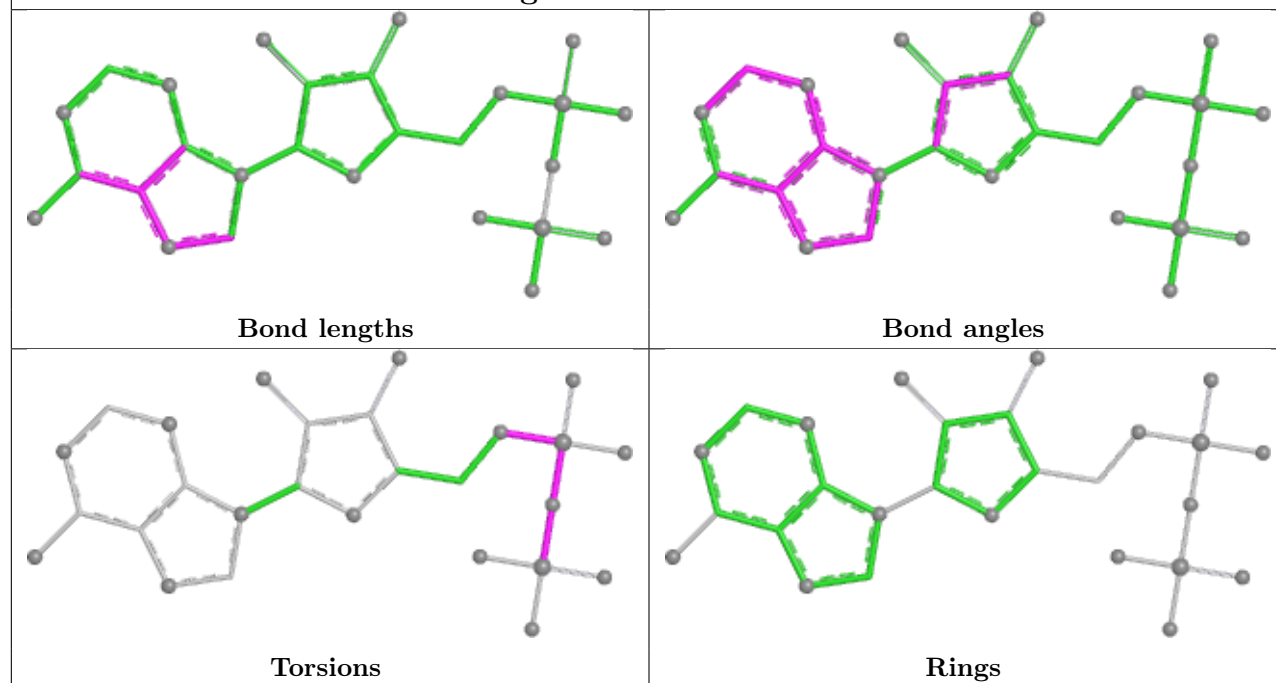
Ligand ATP D 5603

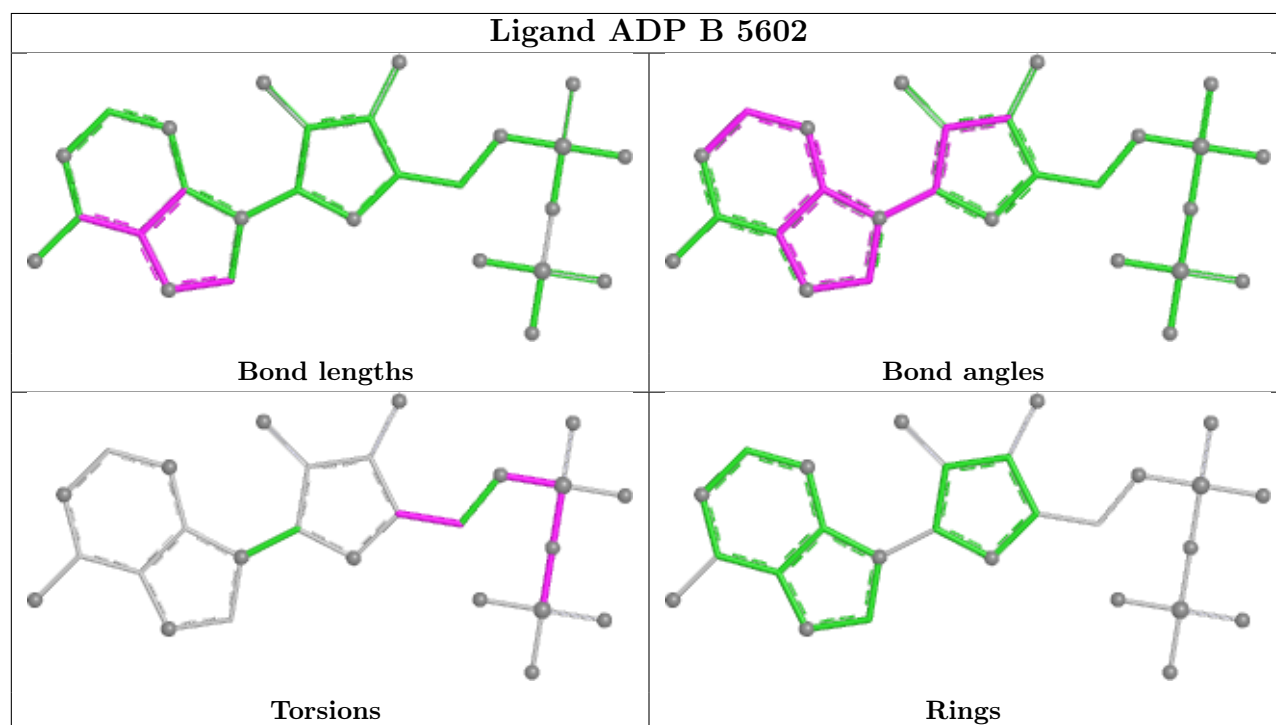
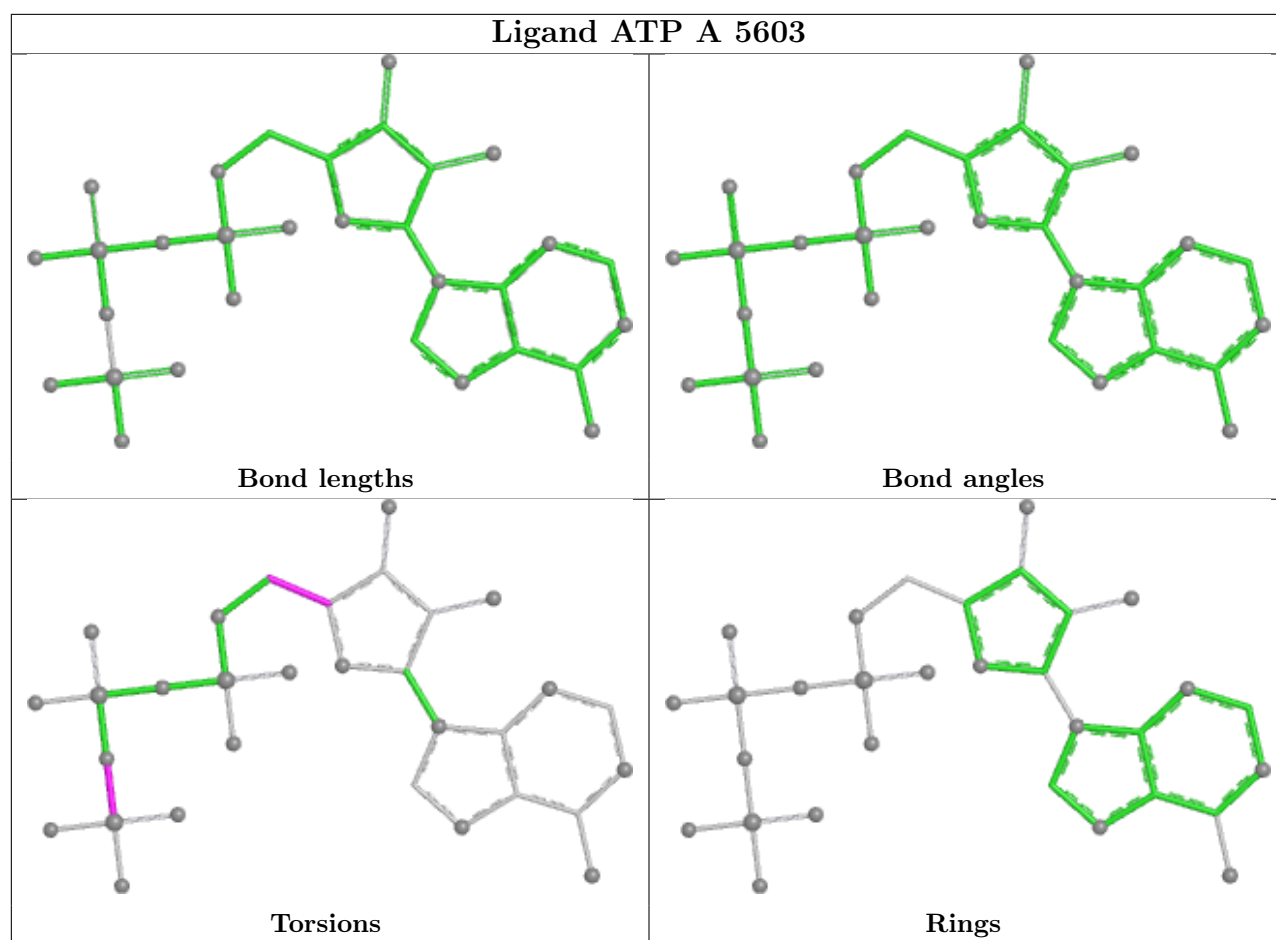


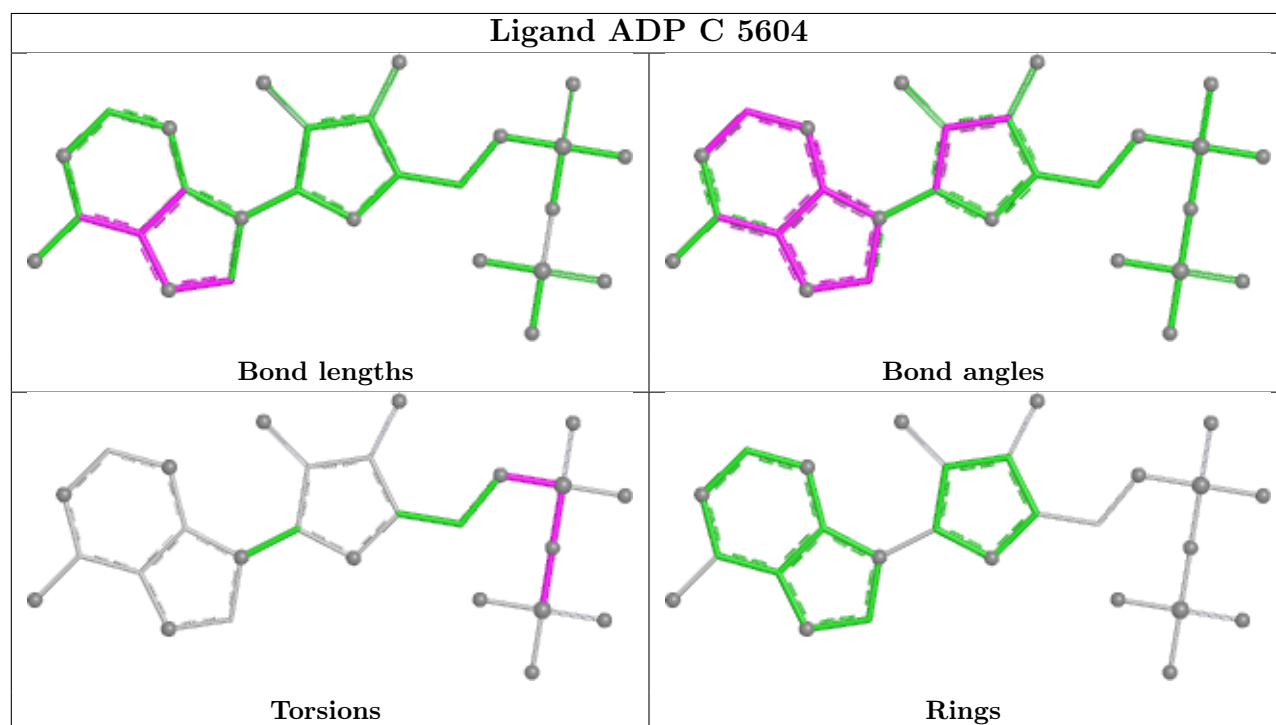
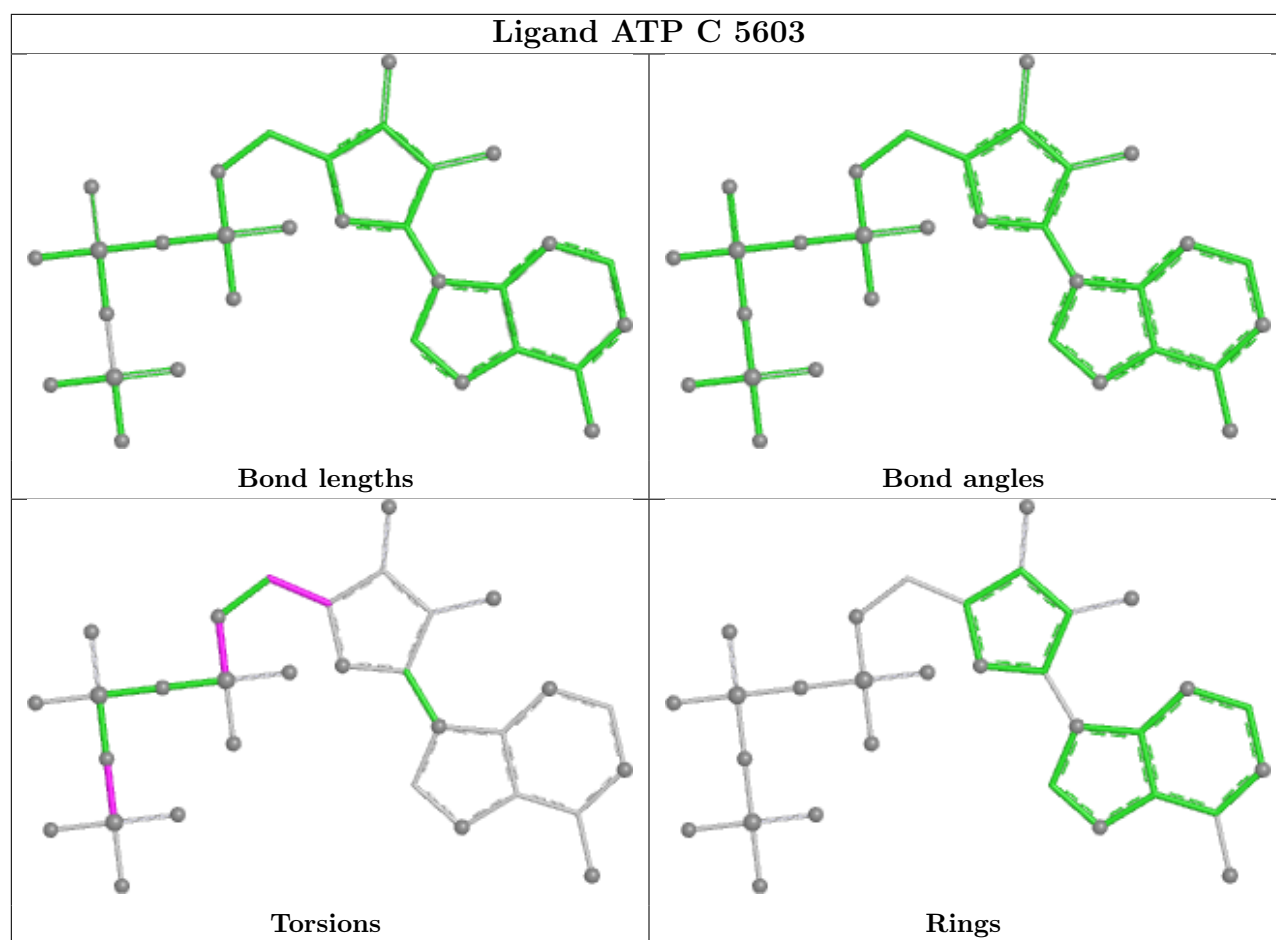
Ligand ADP D 5602

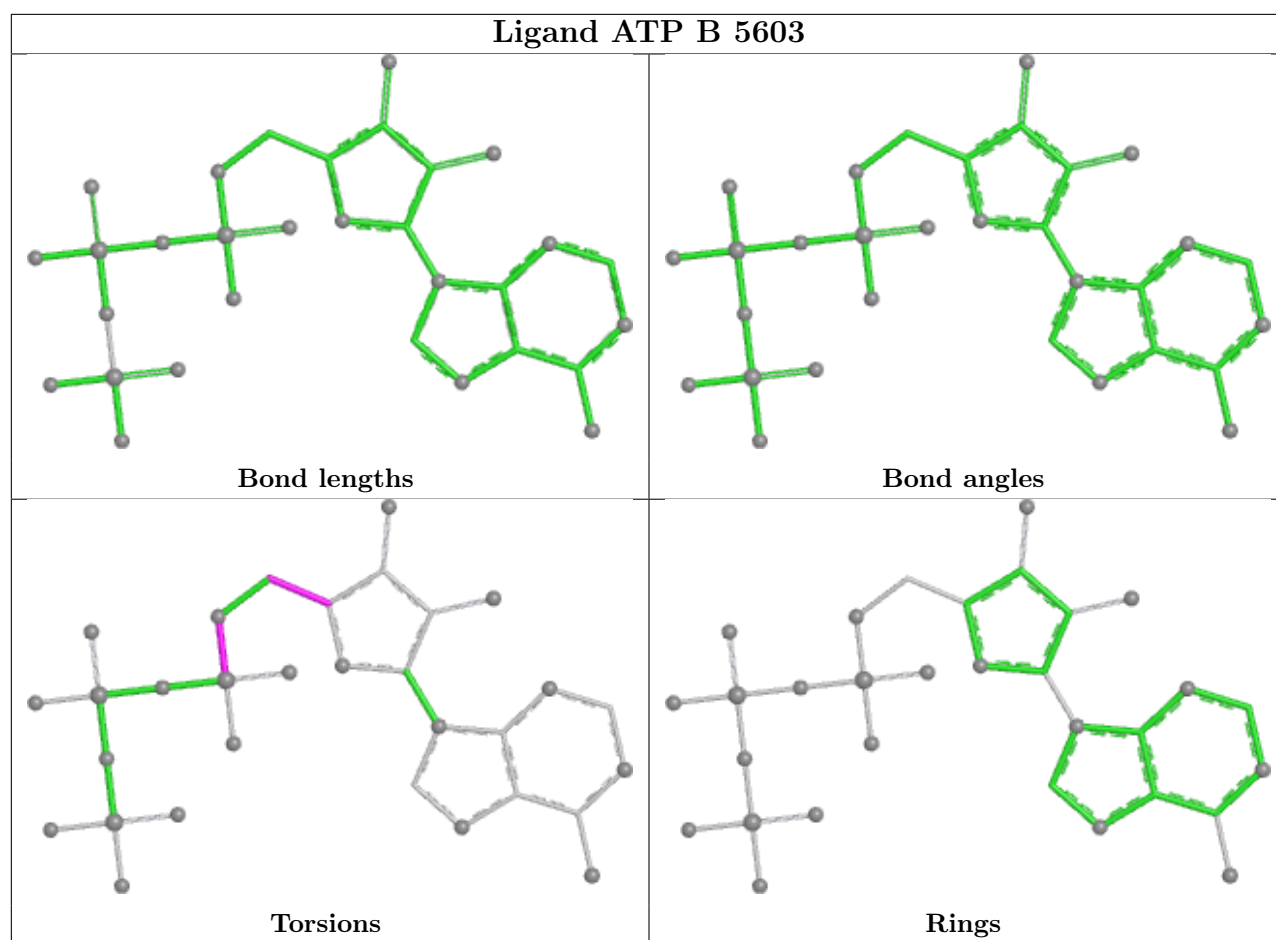


Ligand ADP A 5604









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.

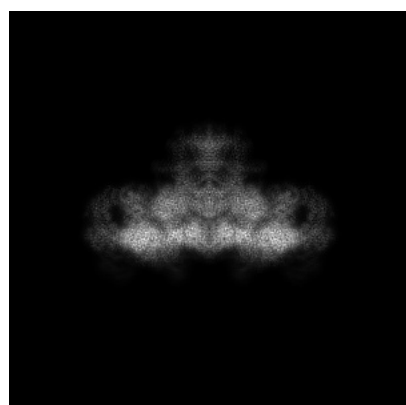
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74437. These allow visual inspection of the internal detail of the map and identification of artifacts.

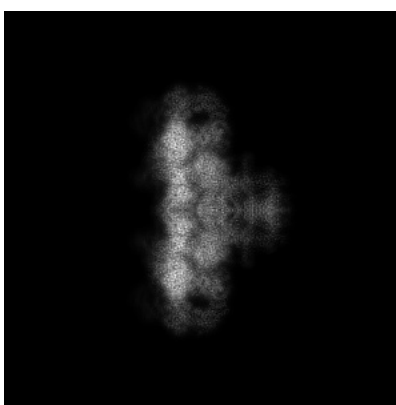
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

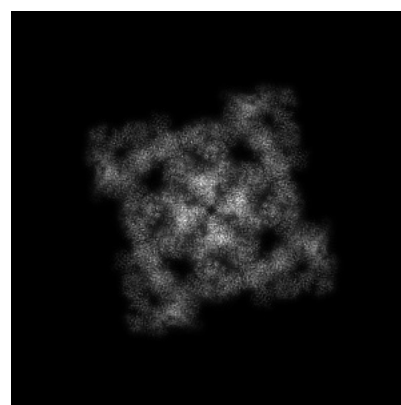
6.1.1 Primary map



X



Y

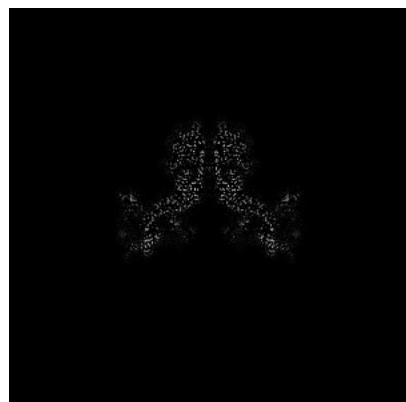


Z

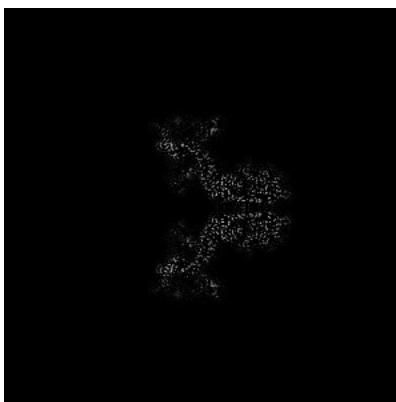
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

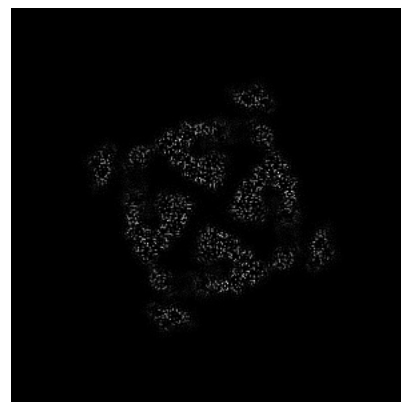
6.2.1 Primary map



X Index: 300



Y Index: 300

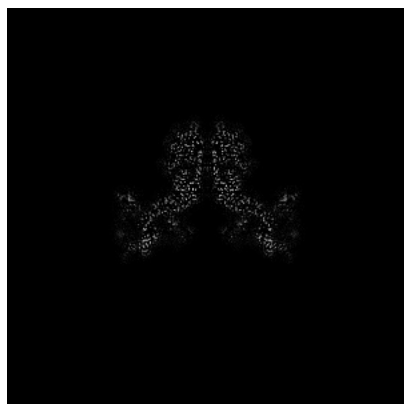


Z Index: 300

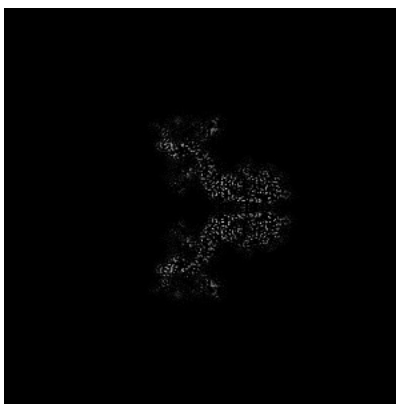
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

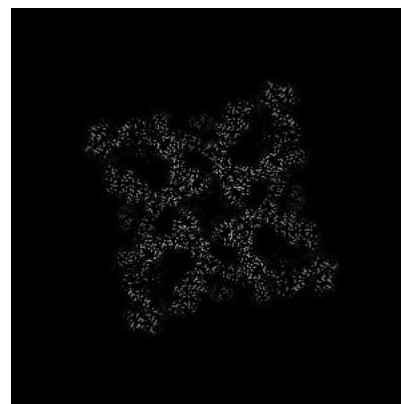
6.3.1 Primary map



X Index: 300



Y Index: 300

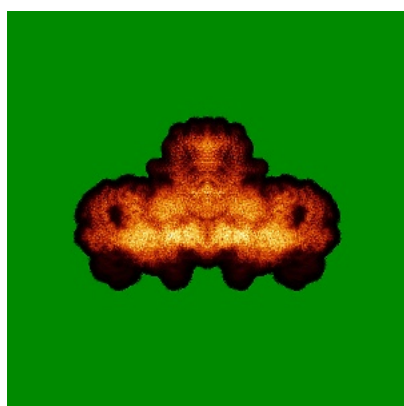


Z Index: 262

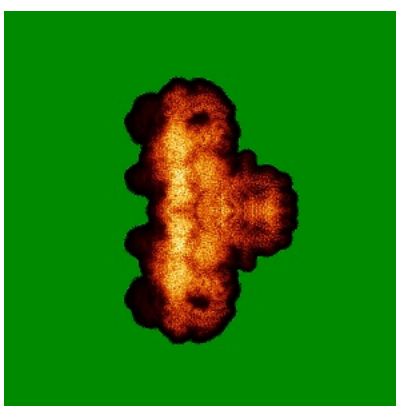
The images above show the largest variance slices of the map in three orthogonal directions.

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

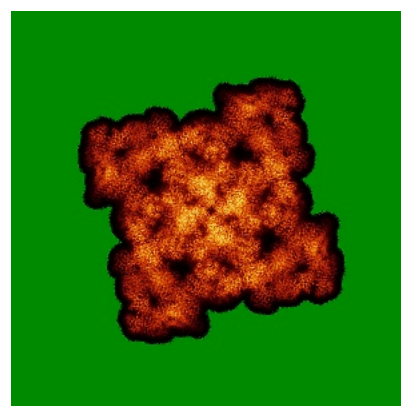
6.4.1 Primary map



X



Y

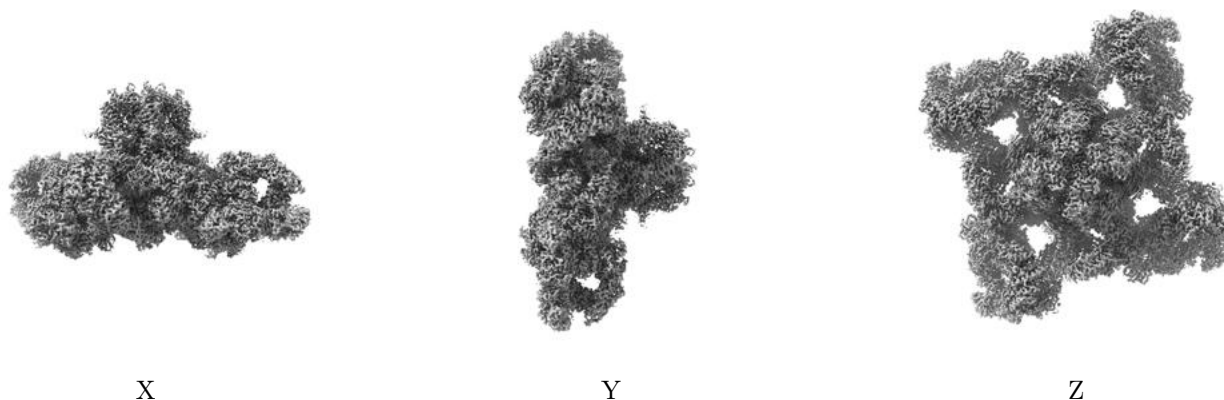


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

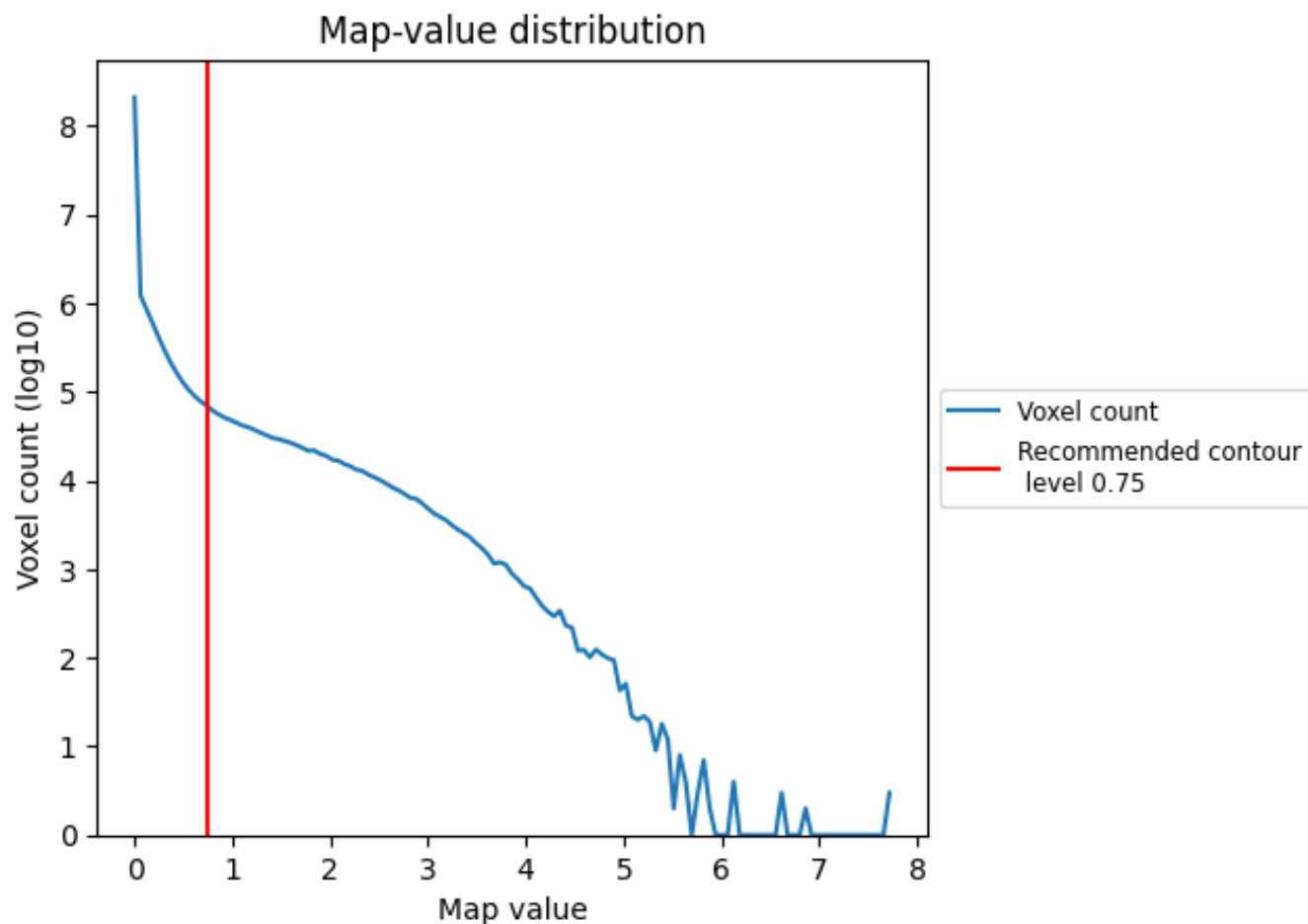
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

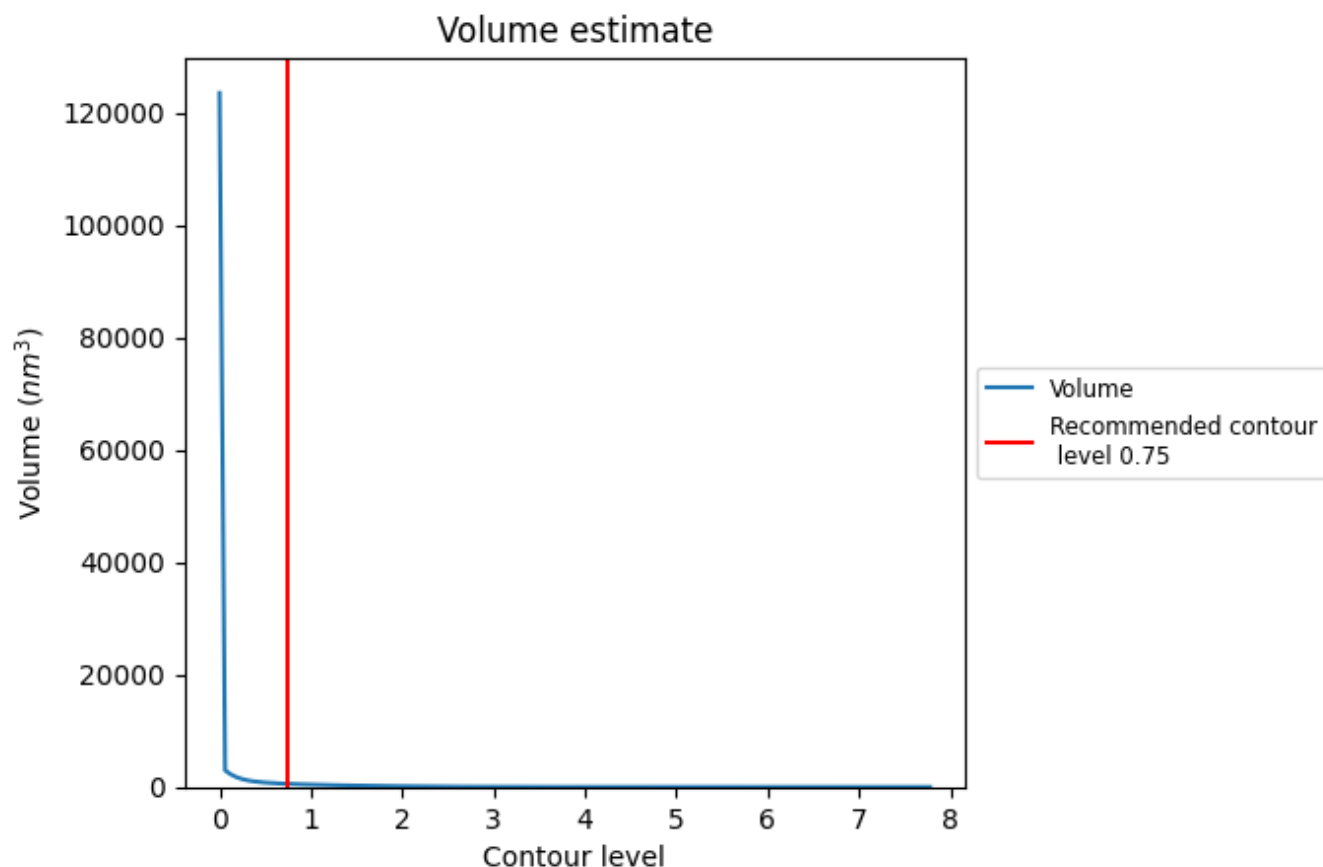
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

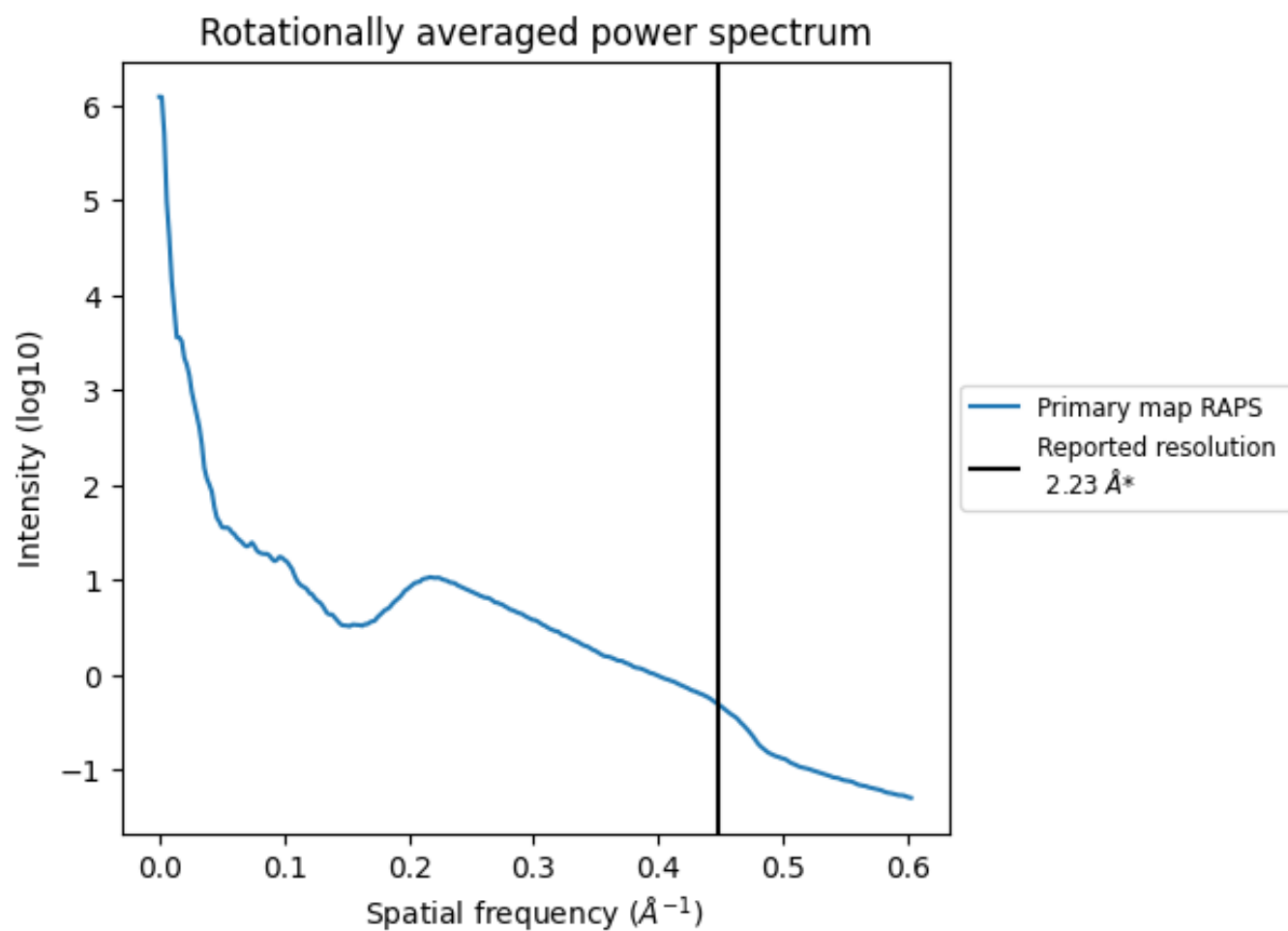
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 550 nm³; this corresponds to an approximate mass of 497 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 0.448 Å⁻¹

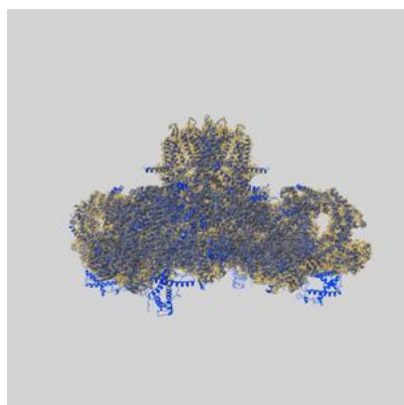
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

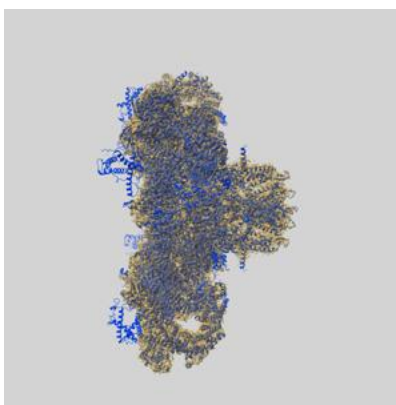
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74437 and PDB model 9ZN7. Per-residue inclusion information can be found in section [3](#) on page [8](#).

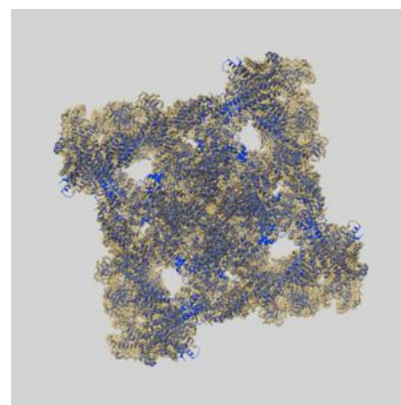
9.1 Map-model overlay [i](#)



X



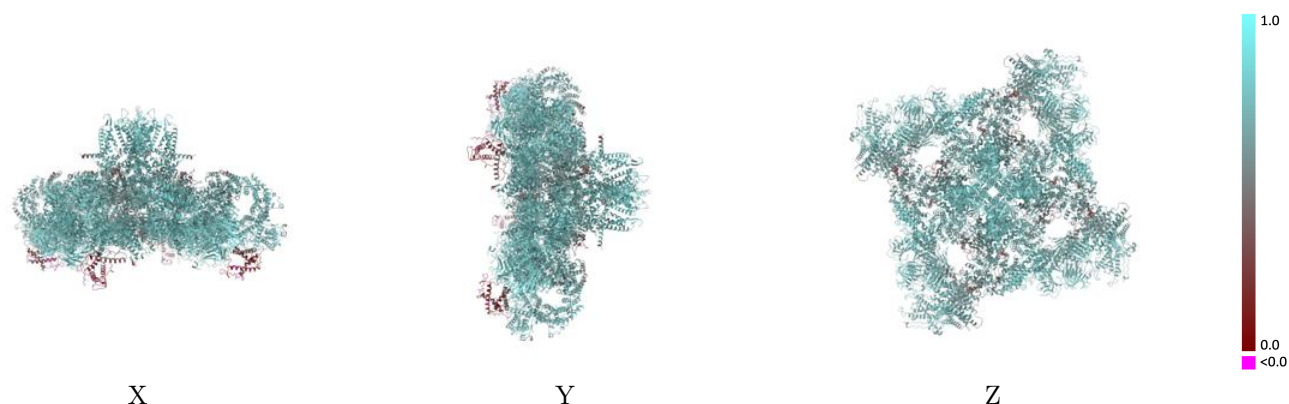
Y



Z

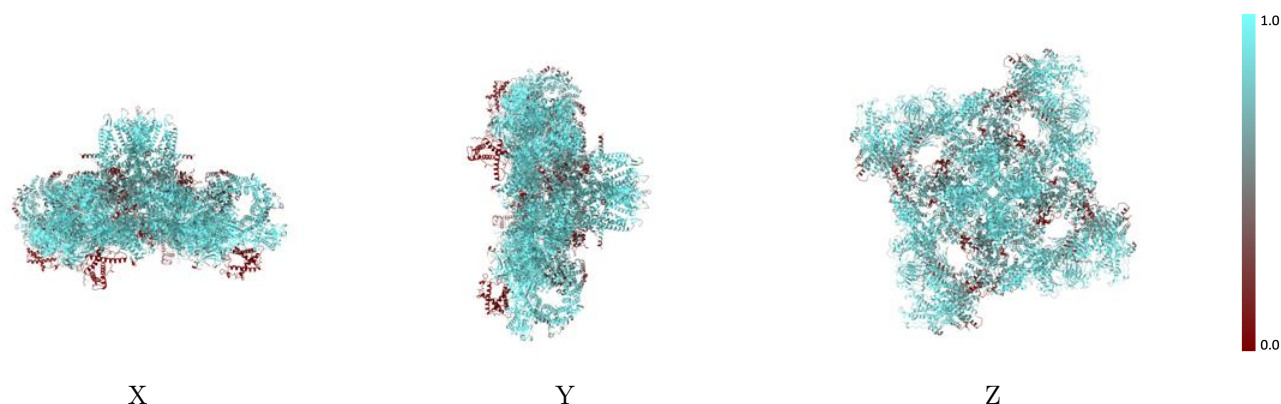
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



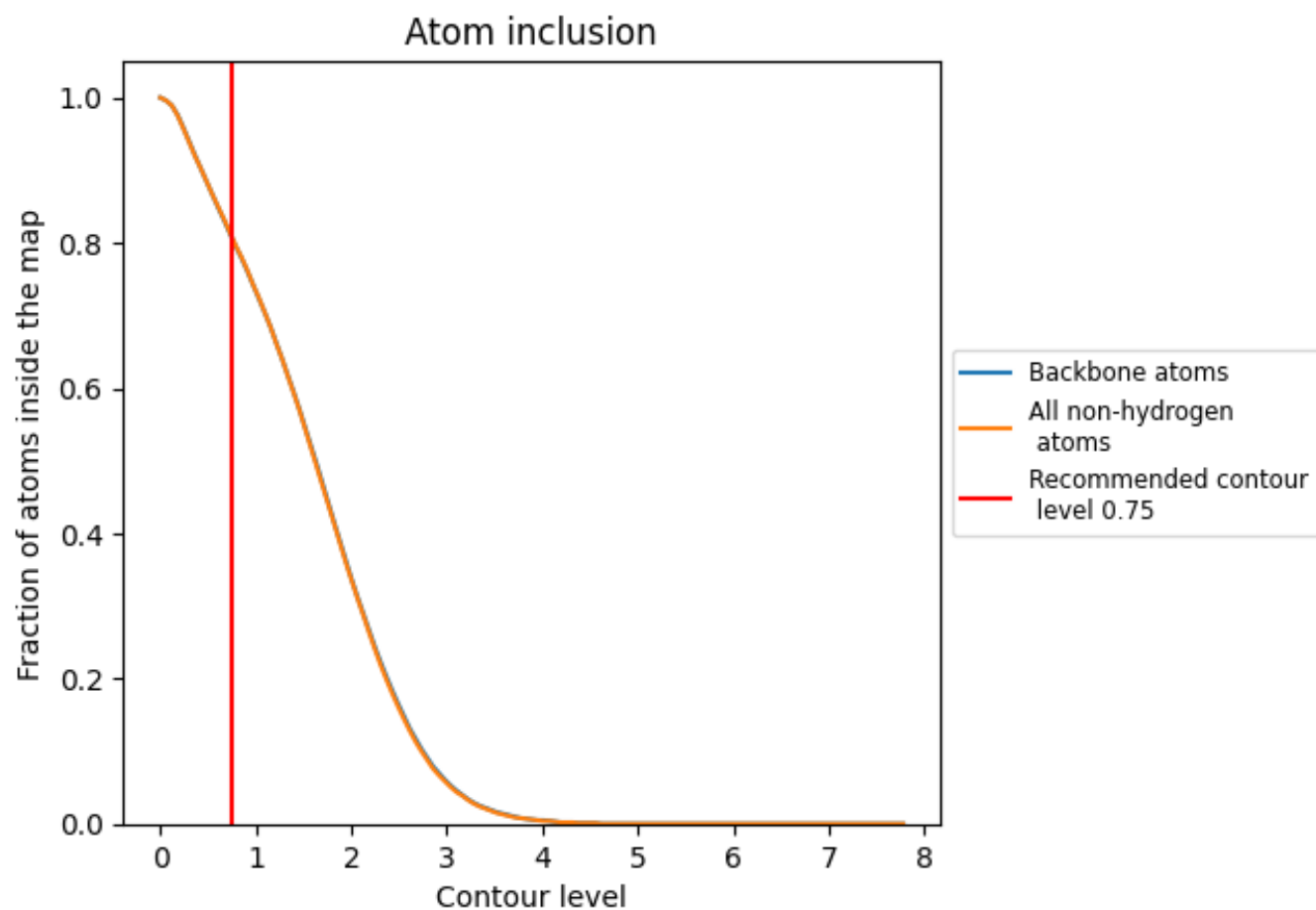
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.6960
A	0.8220	0.7000
B	0.8220	0.7000
C	0.8220	0.7000
D	0.8220	0.7000
E	0.8700	0.7170
F	0.8690	0.7160
G	0.8670	0.7160
H	0.8700	0.7140
I	0.4180	0.5500
J	0.4220	0.5500
K	0.4220	0.5500
L	0.4240	0.5490

1.0

0.0

<0.0