



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 09:46 AM EDT

PDB ID : 8UQ5
EMDB ID : EMD-42461
Title : Structure of human RyR2-S2808D in the primed state in the presence of Rapamycin
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-10-23
Resolution : 3.96 Å(reported)
Based on initial model : 7UA5

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

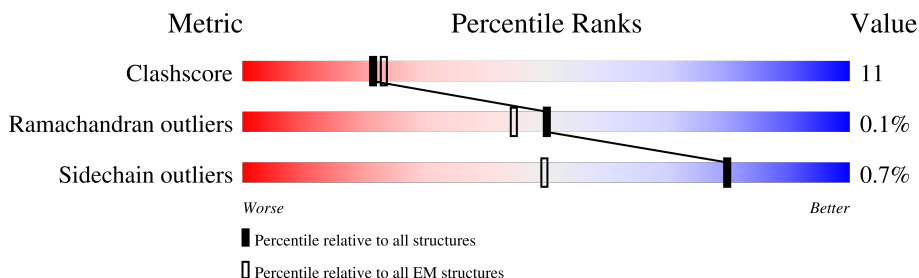
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.96 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	4967	<div> <div>16%</div> <div>62%</div> <div>23%</div> <div>15%</div> </div>
1	B	4967	<div> <div>16%</div> <div>62%</div> <div>23%</div> <div>15%</div> </div>
1	C	4967	<div> <div>16%</div> <div>62%</div> <div>23%</div> <div>15%</div> </div>
1	D	4967	<div> <div>16%</div> <div>62%</div> <div>23%</div> <div>15%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 135336 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

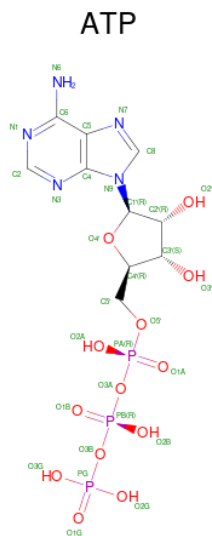
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2808	ASP	SER	engineered mutation	UNP Q92736
B	2808	ASP	SER	engineered mutation	UNP Q92736
C	2808	ASP	SER	engineered mutation	UNP Q92736
D	2808	ASP	SER	engineered mutation	UNP Q92736

- 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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

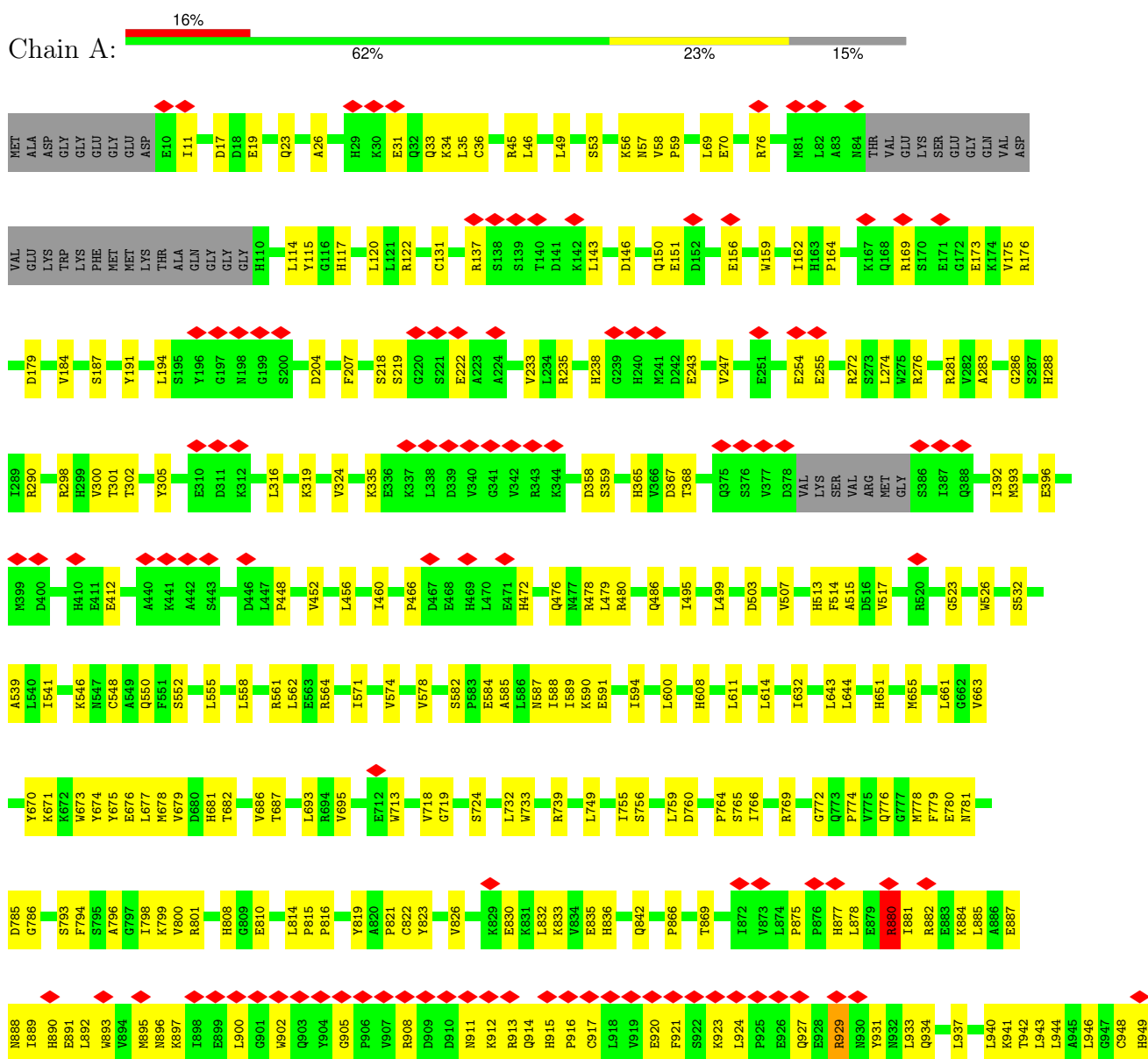


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10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

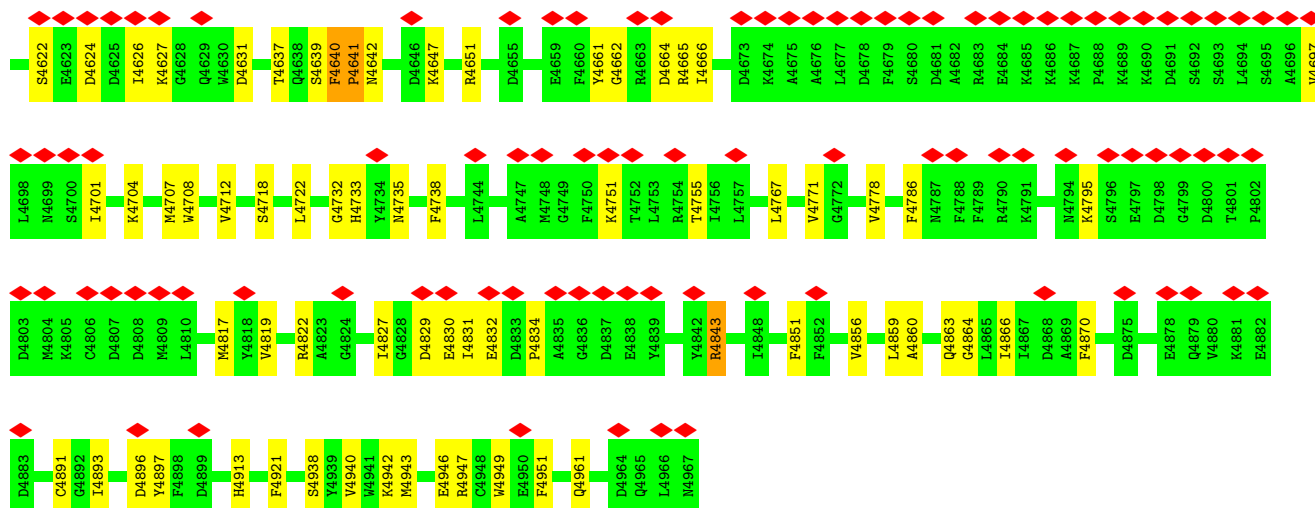
• Molecule 1: Ryanodine receptor 2



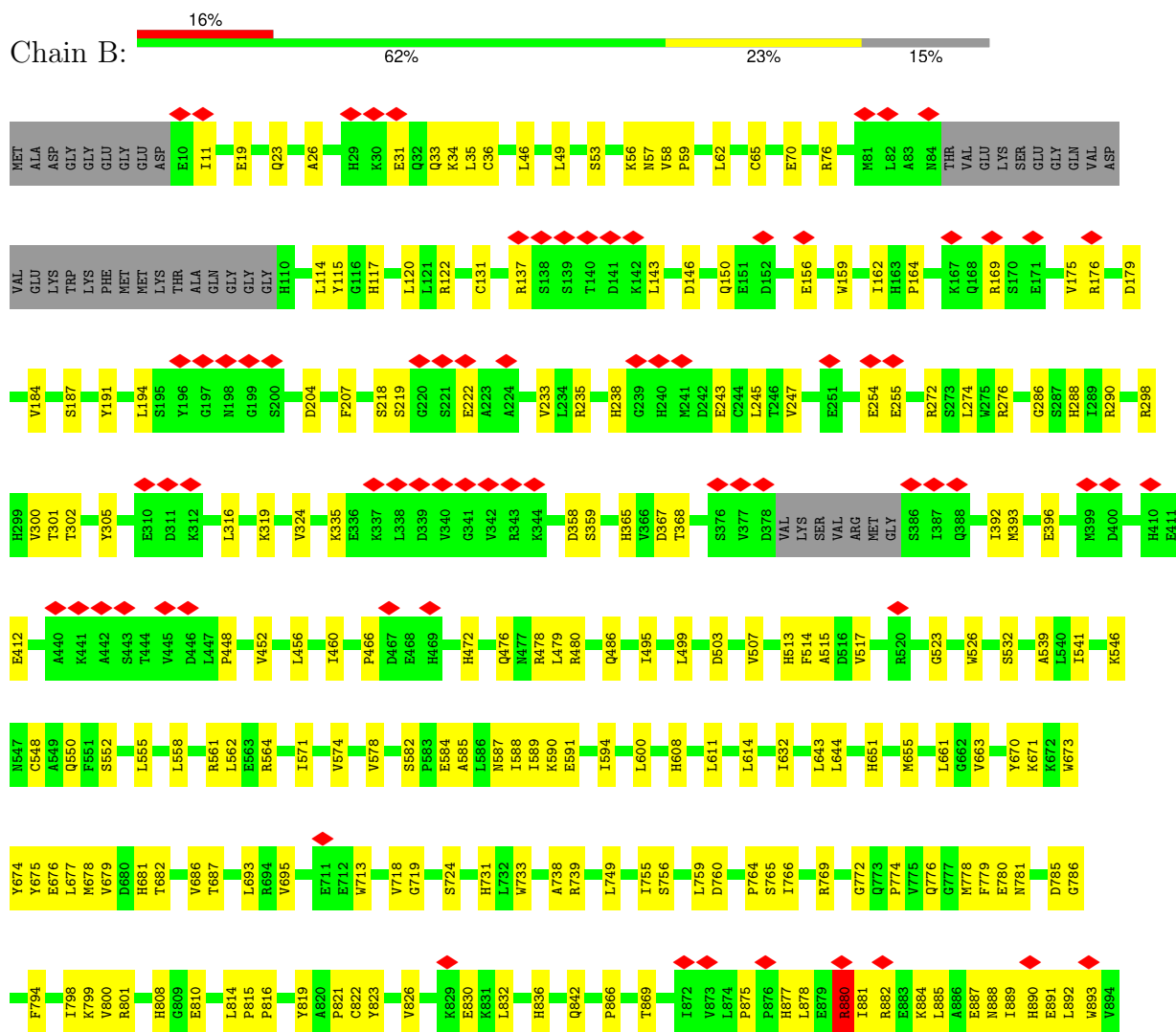


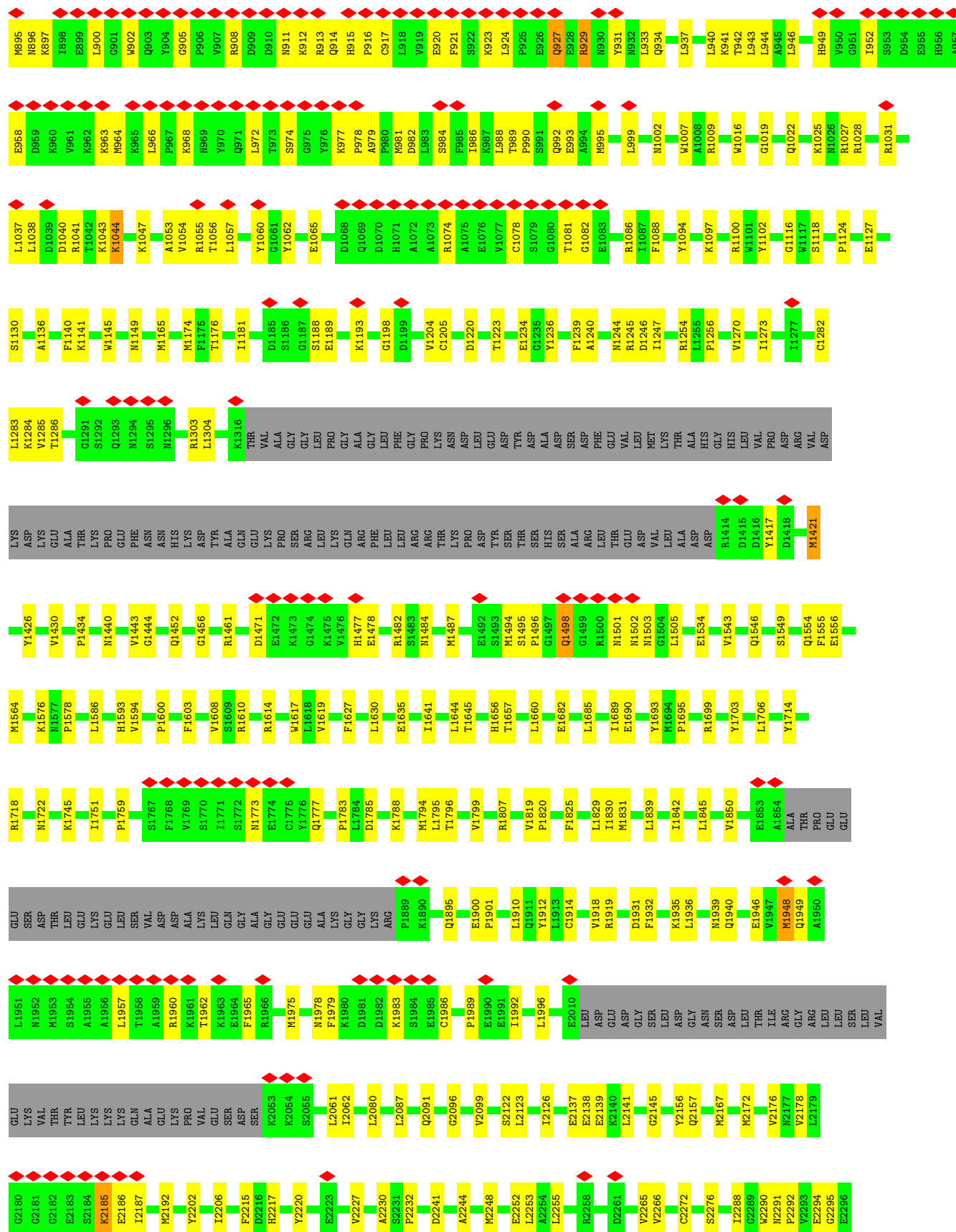


[illegible]



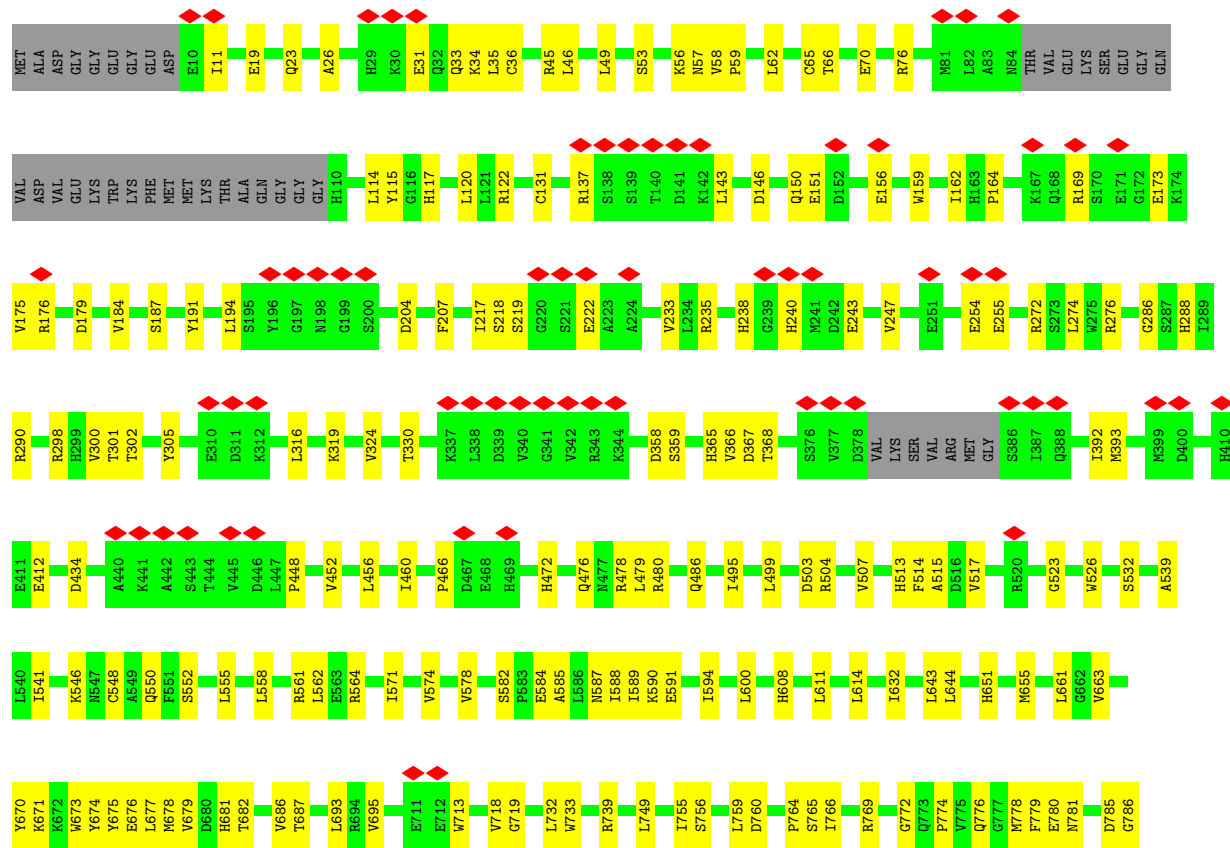
• Molecule 1: Ryanodine receptor 2

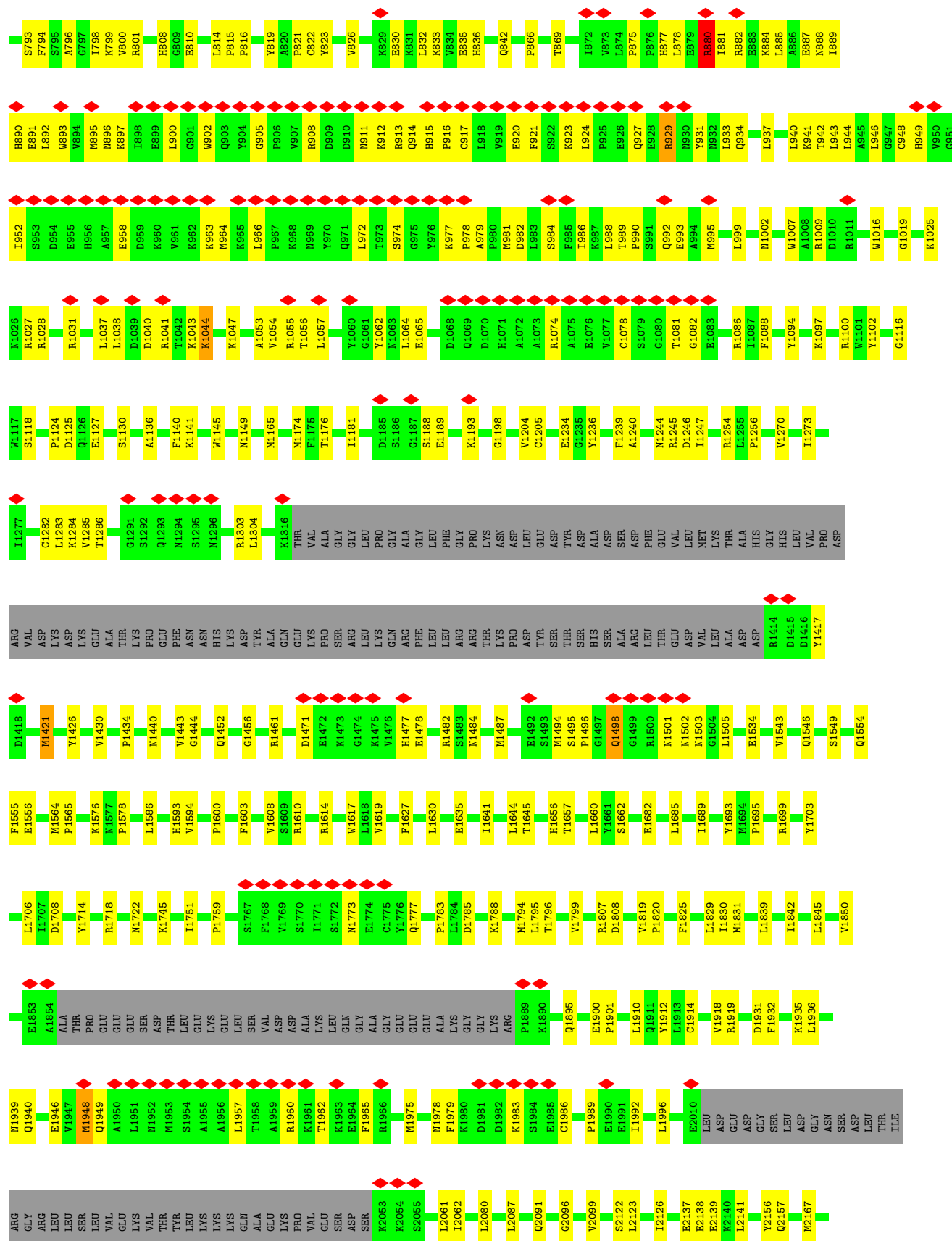






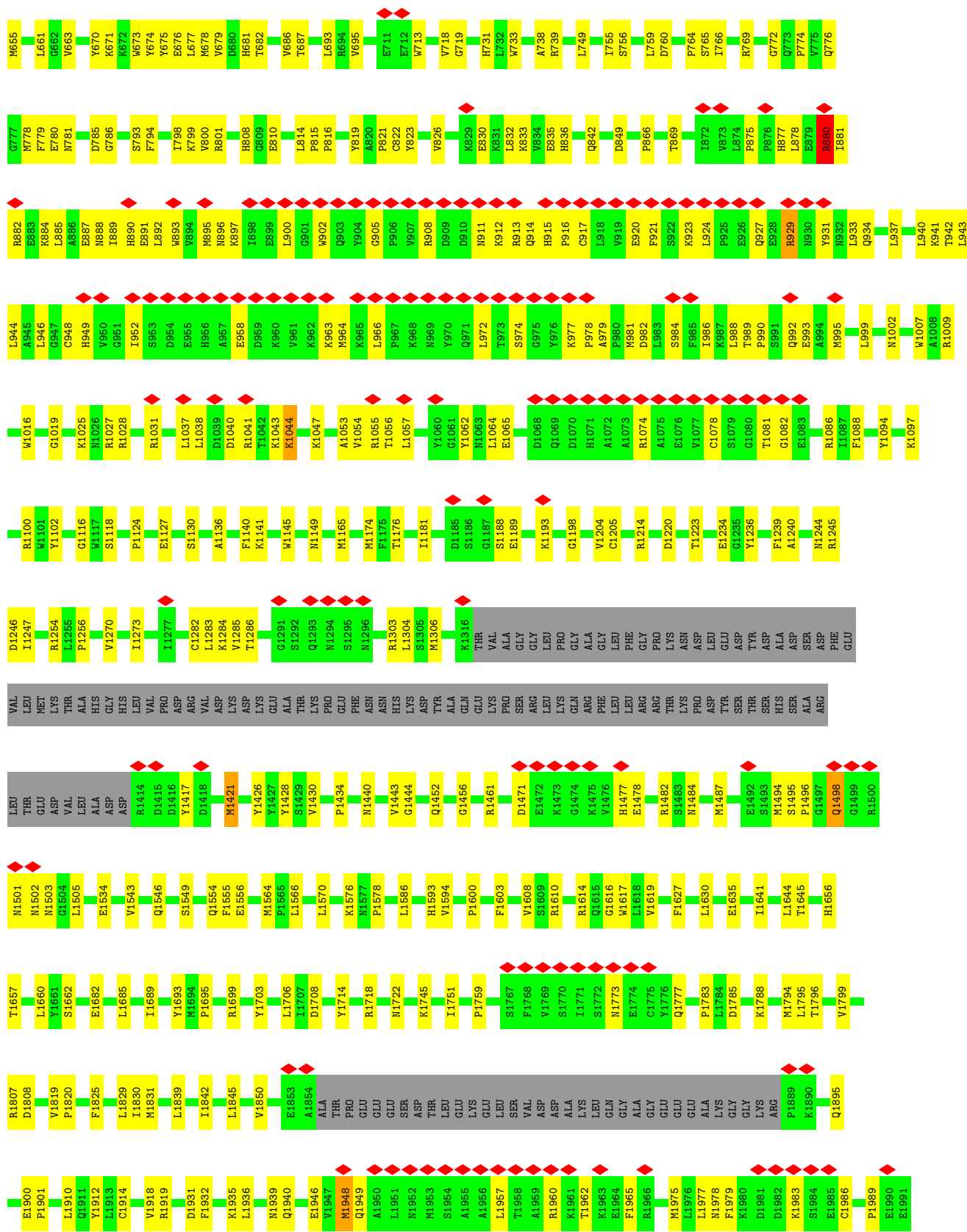




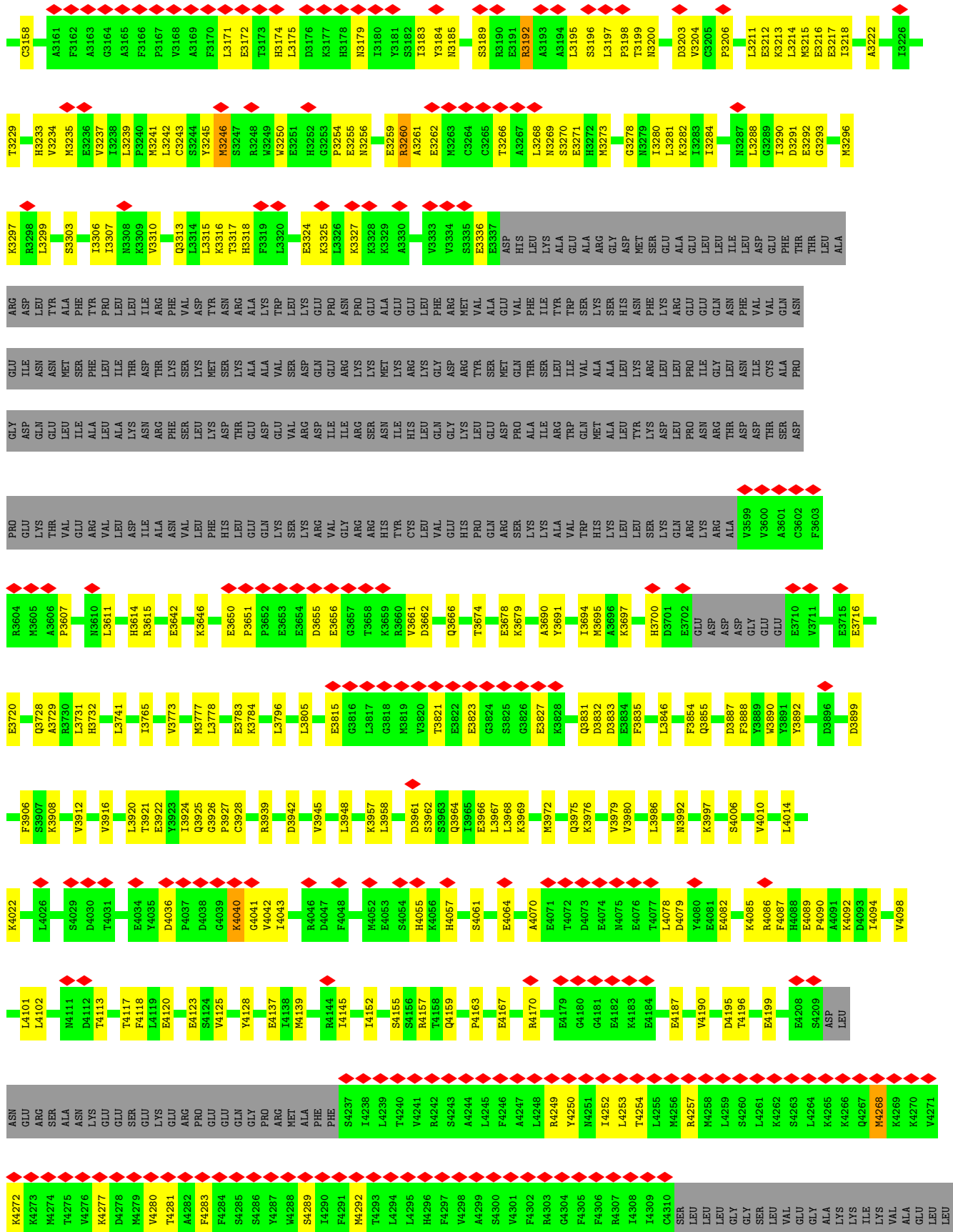








T3091	Q3092	I3093	Y3096	T3097	T3098	T3099	A3100	A3101	A3102	A3103	A3104	A3105	S3106	S3107	A3108	A3109	A3110	H3111	Q3114	A3115	F3117	A3118	A3119	D3120	L3121	I3122	L3123	E3124	D3125	V3126	Q3127	V3128	Y3131	A3132	A3133	T3071	M3072	T3135	S3136	L3137	L3140	G3141	T3142	S3143	A3144	S3145	L3146	F3147	V3148	E3149	R3150	Q3151	R3152	A3154		
D3025	A3026	T3027	S3028	I3029	V3030	N3031	C3032	A3033	H3034	A3035	L3036	G3037	Q3038	T3039	L3040	D3041	A3042	R3043	T3044	V3045	M3046	K3047	G3049	L3050	K3054	L3057	F3060	L3061	D3062	E3066	D3067	L3068	E3069	K3070	T3071	M3072	E3073	N3074	L3075	K3076	Q3077	G3078	Q3079	F3080	HIS	THR	ARG	ASN	GLN	PRO	K3088	G3089	V3090			
G2951	E2952	H2953	F2954	F2955	T2956	K2961	K2965	K2966	V2967	L2968	P2969	D2972	Q2973	T2974	F2975	R2979	F2982	L2983	S2984	A2985	A2986	S2987	R2988	P2989	L2990	C2991	S2992	G2993	T2994	H2995	A2996	S2997	N2998	K2999	M3000	K3001	E3002	T3005	S3006	L3007	F3008	G3009	K3010	V3013	R3016	H3017	R3018	R3019	S3020	N3024						
D2885	R2886	E2887	K2888	A2889	D2890	D2891	I2892	L2893	K2894	F2895	L2896	Q2897	I2898	N2899	G2900	Y2901	A2902	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913	T2914	P2915	R2920	F2921	A2922	Y2923	S2924	Q2928	L2929	I2930	R2931	Y2932	V2933	D2934	E2935	A2936	H2937	Q2938	Y2939	I2940	L2941	E2942	F2943	D2944	G2945	G2946	S2947	R2948	G2949	K2950
G2951	E2952	H2953	F2954	F2955	T2956	K2961	K2965	K2966	V2967	L2968	P2969	D2972	Q2973	T2974	F2975	R2979	F2982	L2983	S2984	A2985	A2986	S2987	R2988	P2989	L2990	C2991	S2992	G2993	T2994	H2995	A2996	S2997	N2998	K2999	M3000	K3001	E3002	T3005	S3006	L3007	F3008	G3009	K3010	V3013	R3016	H3017	R3018	R3019	S3020	N3024						
D3025	A3026	T3027	S3028	I3029	V3030	N3031	C3032	A3033	H3034	A3035	L3036	G3037	Q3038	T3039	L3040	D3041	A3042	R3043	T3044	V3045	M3046	K3047	G3049	L3050	K3054	L3057	F3060	L3061	D3062	E3066	D3067	L3068	E3069	K3070	T3071	M3072	E3073	N3074	L3075	K3076	Q3077	G3078	Q3079	F3080	HIS	THR	ARG	ASN	GLN	PRO	K3088	G3089	V3090			
E2745	I2746	Y2747	S2748	D2749	S2750	S2751	K2752	Q2753	Q2754	P2755	L2756	K2757	K2758	P2759	Y2760	K2761	L2762	L2763	S2764	K2768	E2769	I2770	Y2771	R2772	W2773	K2776	L2779	M2782	R2788	E2789	E2790	R2793	E2794	A2799	L2800	Y2801	N2802	ARG	THR	ARG	ASP	ILE	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA					
E2682	S2683	N2684	Y2685	V2686	S2687	M2688	M2689	E2690	K2691	Q2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	N2700	F2701	N2702	P2703	Q2704	P2705	V2706	D2707	T2708	S2709	N2710	L2711	T2712	I2713	P2714	E2715	K2716	L2717	F2720	I2721	N2722	K2723	E2726	H2727	S2728	K2731	W2732	S2733	M2734	D2735	L2736	L2737	A2738	N2739	G2740	W2741	Y2743	K2744	
E2745	I2746	Y2747	S2748	D2749	S2750	S2751	K2752	Q2753	Q2754	P2755	L2756	K2757	K2758	P2759	Y2760	K2761	L2762	L2763	S2764	K2768	E2769	I2770	Y2771	R2772	W2773	K2776	L2779	M2782	R2788	E2789	E2790	R2793	E2794	A2799	L2800	Y2801	N2802	ARG	THR	ARG	ASP	ILE	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA					
ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	T2826	D2827	M2828	S2829	N2830	V2831	T2832	L2833	S2834	R2835	D2836	L2837	H2838	A2841	E2842	M2843	N2844	E2845	R2846	N2847	H2849	K2854	K2855	M2858	E2859	L2860	E2861	S2862	K2863	G2864	G2865	G2866	N2867	H2868	P2869	L2870	Y2874	D2875	T2876	L2877	T2878	A2879	K2881	K2882	A2883	K2884			
D2885	R2886	E2887	K2888	A2889	D2890	D2891	I2892	L2893	K2894	F2895	L2896	Q2897	I2898	N2899	G2900	Y2901	A2902	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913	T2914	P2915	R2920	F2921	A2922	Y2923	S2924	Q2928	L2929	I2930	R2931	Y2932	V2933	D2934	E2935	A2936	H2937	Q2938	Y2939	I2940	L2941	E2942	F2943	D2944	G2945	G2946	S2947	R2948	G2949	K2950
G2951	E2952	H2953	F2954	F2955	T2956	K2961	K2965	K2966	V2967	L2968	P2969	D2972	Q2973	T2974	F2975	R2979	F2982	L2983	S2984	A2985	A2986	S2987	R2988	P2989	L2990	C2991	S2992	G2993	T2994	H2995	A2996	S2997	N2998	K2999	M3000	K3001	E3002	T3005	S3006	L3007	F3008	G3009	K3010	V3013	R3016	H3017	R3018	R3019	S3020	N3024						
D3025	A3026	T3027	S3028	I3029	V3030	N3031	C3032	A3033	H3034	A3035	L3036	G3037	Q3038	T3039	L3040	D3041	A3042	R3043	T3044	V3045	M3046	K3047	G3049	L3050	K3054	L3057	F3060	L3061	D3062	E3066	D3067	L3068	E3069	K3070	T3071	M3072	E3073	N3074	L3075	K3076	Q3077	G3078	Q3079	F3080	HIS	THR	ARG	ASN	GLN	PRO	K3088	G3089	V3090			





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18232	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.473	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	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, 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	A	0.25	0/34511	0.50	4/46614 (0.0%)
1	B	0.25	0/34511	0.50	4/46614 (0.0%)
1	C	0.25	0/34511	0.50	4/46614 (0.0%)
1	D	0.25	0/34511	0.50	4/46614 (0.0%)
All	All	0.25	0/138044	0.50	16/186456 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1948	MET	CB-CG-SD	7.23	134.09	112.40
1	B	1948	MET	CB-CG-SD	7.22	134.07	112.40
1	C	1948	MET	CB-CG-SD	7.22	134.07	112.40
1	A	1948	MET	CB-CG-SD	7.22	134.06	112.40
1	A	880	ARG	CA-CB-CG	6.59	127.90	113.40

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3192	ARG	Sidechain
1	A	4640	PHE	Peptide
1	A	880	ARG	Sidechain
1	B	3192	ARG	Sidechain
1	B	880	ARG	Sidechain

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	33771	0	33455	790	0
1	B	33771	0	33455	785	0
1	C	33771	0	33455	790	0
1	D	33771	0	33455	800	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	62	0	24	1	0
3	B	62	0	24	2	0
3	C	62	0	24	1	0
3	D	62	0	24	1	0
All	All	135336	0	133916	3086	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 11.

The worst 5 of 3086 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:B:4891:CYS:SG	1:B:4913:HIS:CE1	2.51	1.04
1:A:4891:CYS:SG	1:A:4913:HIS:CE1	2.51	1.02
1:D:4891:CYS:SG	1:D:4913:HIS:CE1	2.51	1.00
1:C:4891:CYS:SG	1:C:4913:HIS:CE1	2.51	1.00
1:A:4860:ALA:CB	1:D:4863:GLN:OE1	2.15	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	4198/4967 (84%)	4085 (97%)	109 (3%)	4 (0%)	48	81
1	B	4198/4967 (84%)	4085 (97%)	109 (3%)	4 (0%)	48	81
1	C	4198/4967 (84%)	4085 (97%)	109 (3%)	4 (0%)	48	81
1	D	4198/4967 (84%)	4084 (97%)	110 (3%)	4 (0%)	48	81
All	All	16792/19868 (84%)	16339 (97%)	437 (3%)	16 (0%)	50	81

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2770	ILE
1	A	3927	PRO
1	A	4641	PRO
1	B	2770	ILE
1	B	3927	PRO

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	3708/4358 (85%)	3682 (99%)	26 (1%)	81	86
1	B	3708/4358 (85%)	3682 (99%)	26 (1%)	81	86
1	C	3708/4358 (85%)	3682 (99%)	26 (1%)	81	86
1	D	3708/4358 (85%)	3682 (99%)	26 (1%)	81	86
All	All	14832/17432 (85%)	14728 (99%)	104 (1%)	80	86

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1044	LYS
1	C	3327	LYS
1	D	4085	LYS
1	C	1498	GLN
1	C	2884	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3949	HIS
1	D	3114	GLN
1	C	2550	HIS
1	D	2928	GLN
1	D	3949	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 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	ATP	B	5002	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
3	ATP	A	5002	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
3	ATP	C	5003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
3	ATP	D	5003	-	28,33,33	0.62	0	34,52,52	0.58	1 (2%)
3	ATP	B	5003	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
3	ATP	C	5002	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
3	ATP	A	5003	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
3	ATP	D	5002	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)

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	ATP	B	5002	-	-	4/18/38/38	0/3/3/3
3	ATP	A	5002	-	-	4/18/38/38	0/3/3/3
3	ATP	C	5003	-	-	6/18/38/38	0/3/3/3
3	ATP	D	5003	-	-	6/18/38/38	0/3/3/3
3	ATP	B	5003	-	-	6/18/38/38	0/3/3/3
3	ATP	C	5002	-	-	4/18/38/38	0/3/3/3
3	ATP	A	5003	-	-	6/18/38/38	0/3/3/3
3	ATP	D	5002	-	-	4/18/38/38	0/3/3/3

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(°)
3	A	5003	ATP	C5-C6-N6	2.32	123.85	120.31
3	B	5003	ATP	C5-C6-N6	2.32	123.85	120.31
3	C	5003	ATP	C5-C6-N6	2.32	123.85	120.31
3	B	5002	ATP	C5-C6-N6	2.32	123.85	120.31
3	C	5002	ATP	C5-C6-N6	2.32	123.85	120.31

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

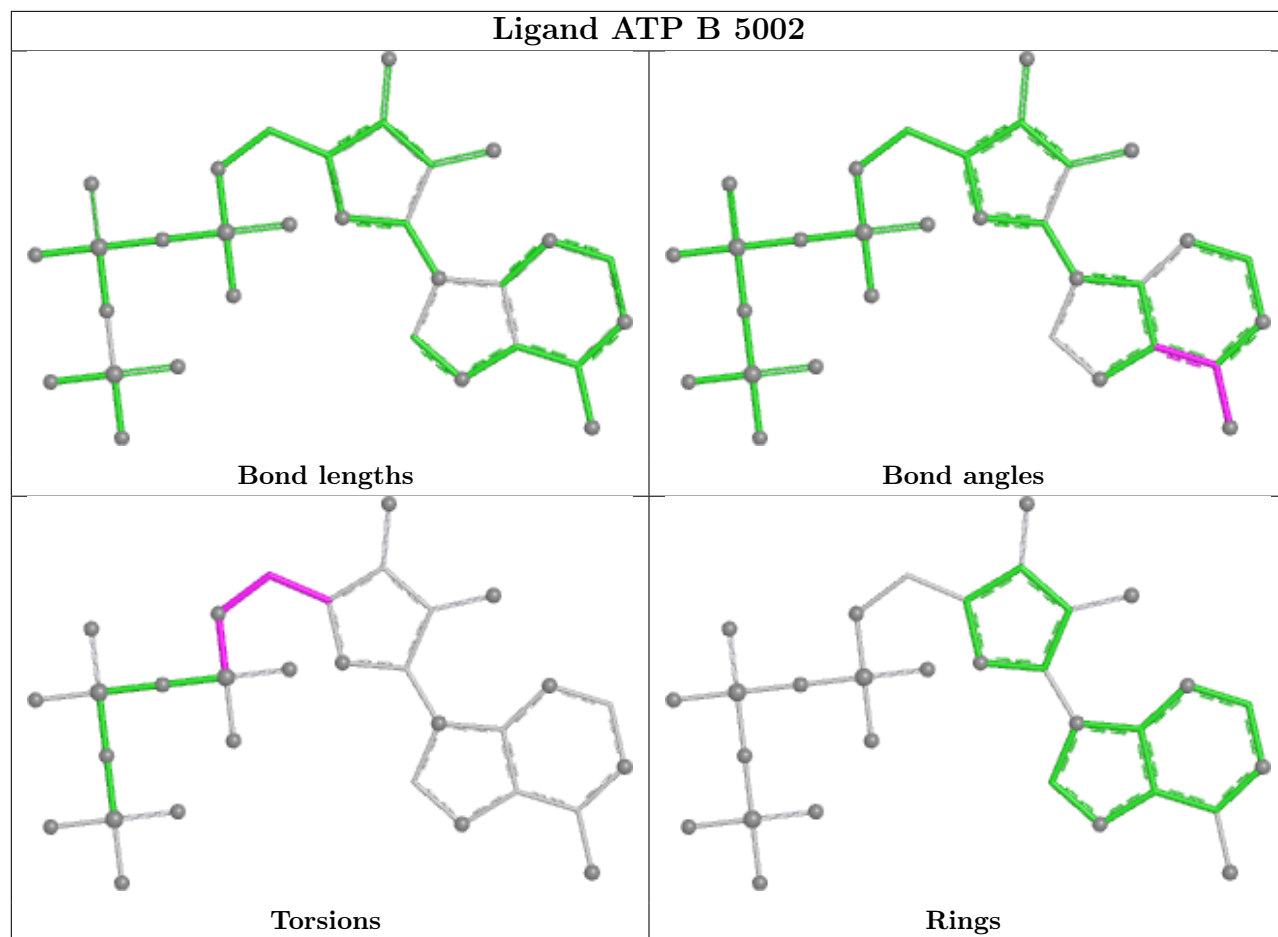
Mol	Chain	Res	Type	Atoms
3	A	5002	ATP	O4'-C4'-C5'-O5'
3	A	5002	ATP	C3'-C4'-C5'-O5'
3	A	5003	ATP	O4'-C4'-C5'-O5'
3	B	5002	ATP	O4'-C4'-C5'-O5'
3	B	5002	ATP	C3'-C4'-C5'-O5'

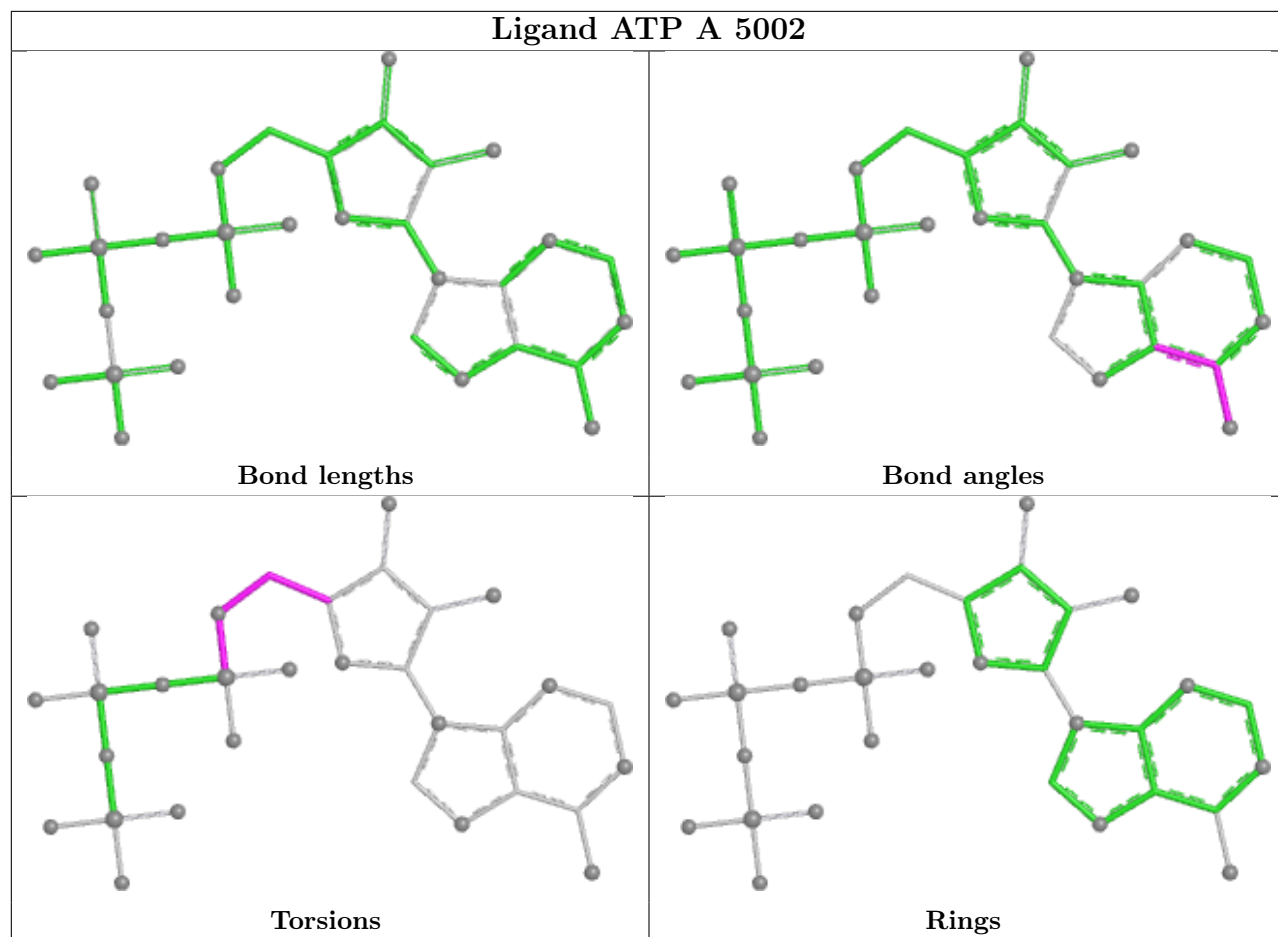
There are no ring outliers.

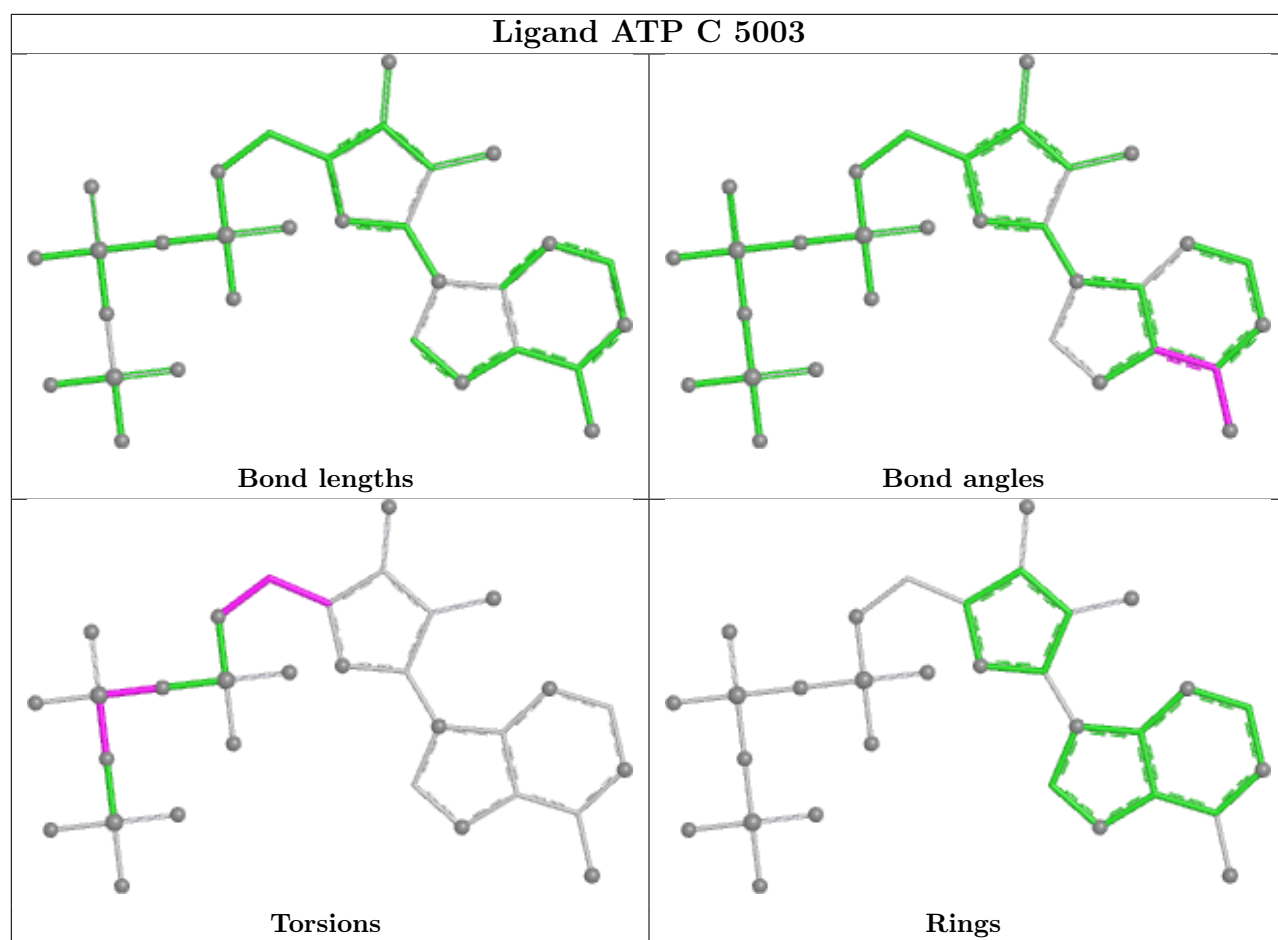
4 monomers are involved in 5 short contacts:

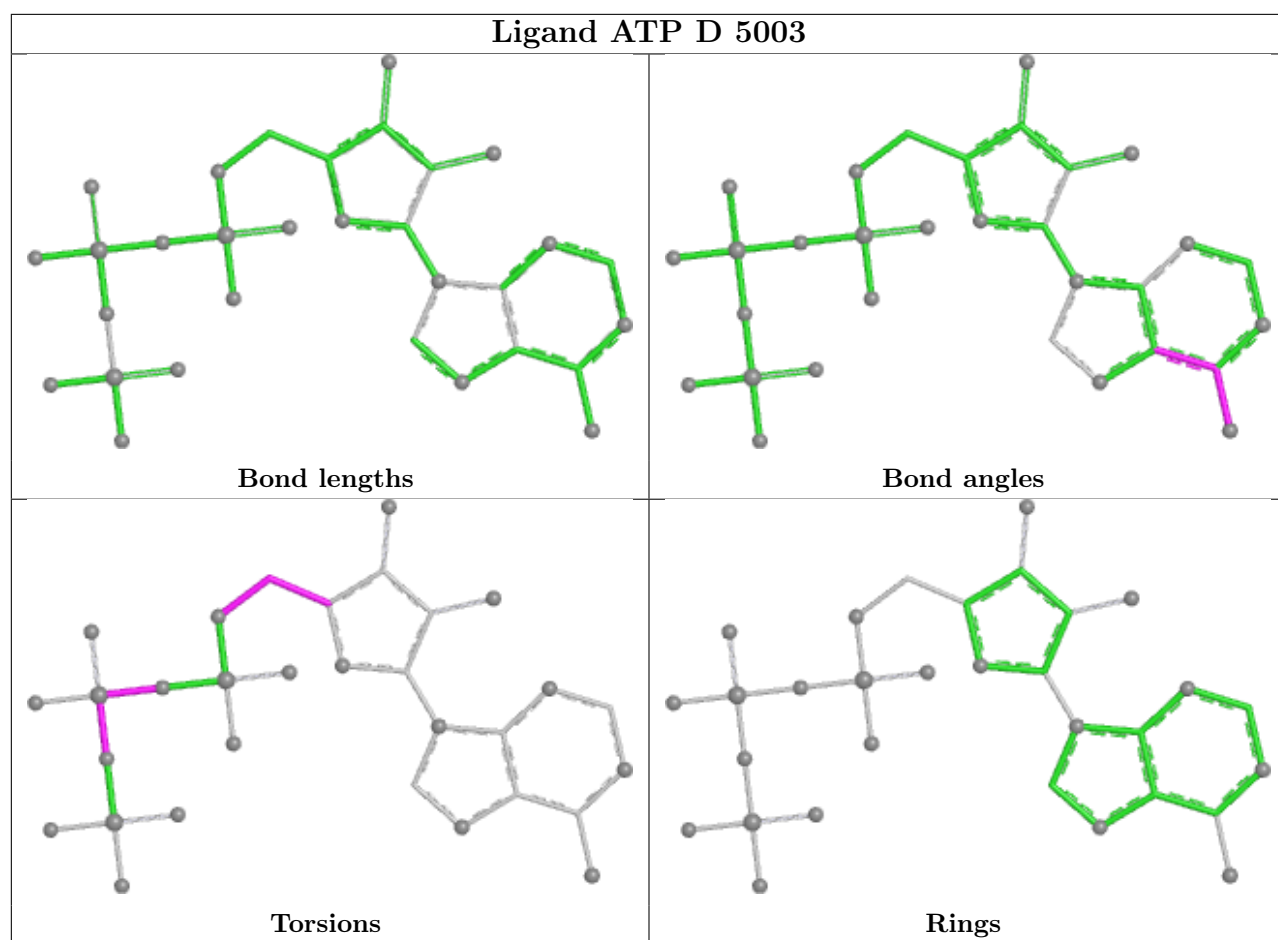
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5003	ATP	1	0
3	D	5003	ATP	1	0
3	B	5003	ATP	2	0
3	A	5003	ATP	1	0

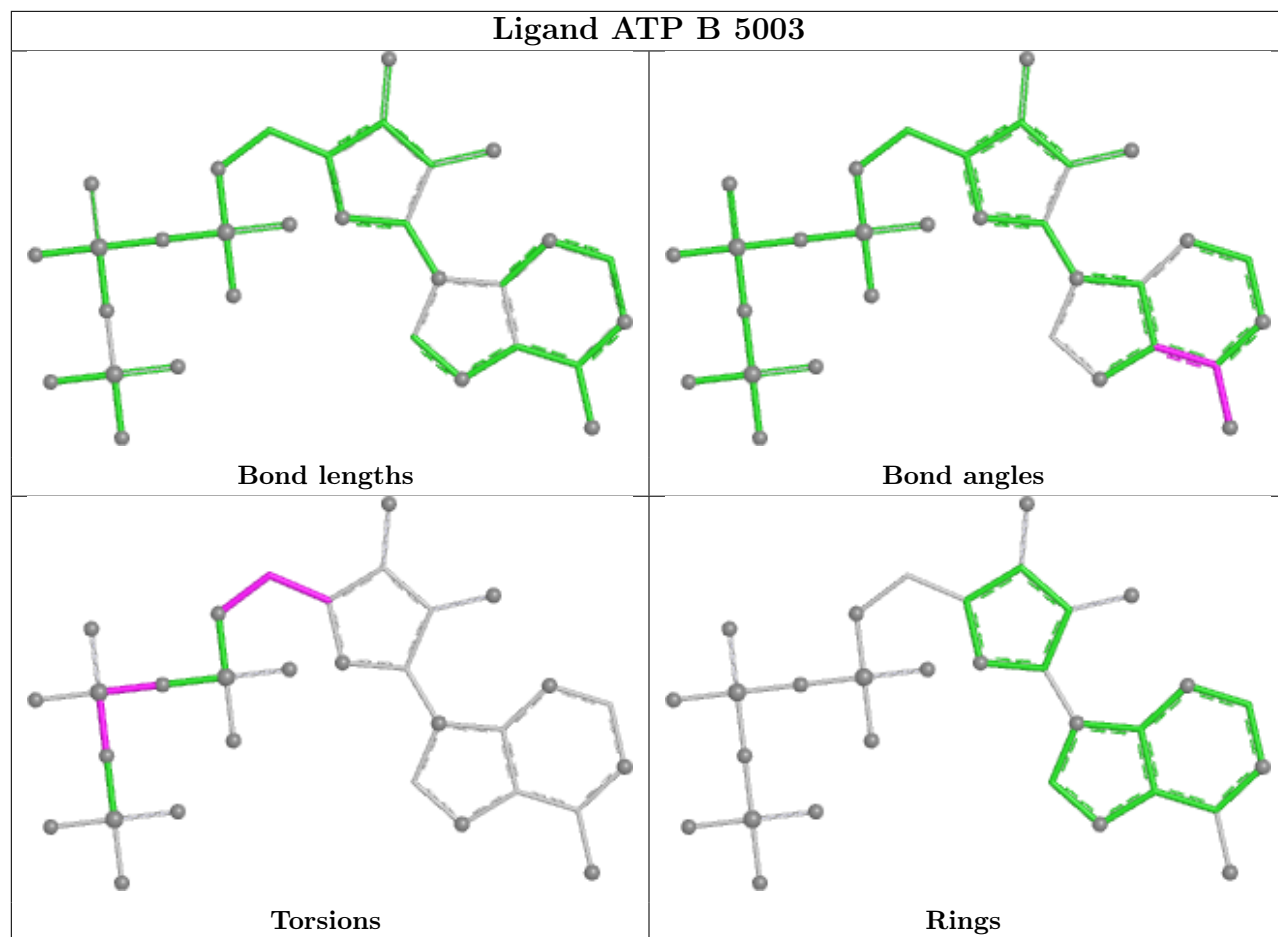
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

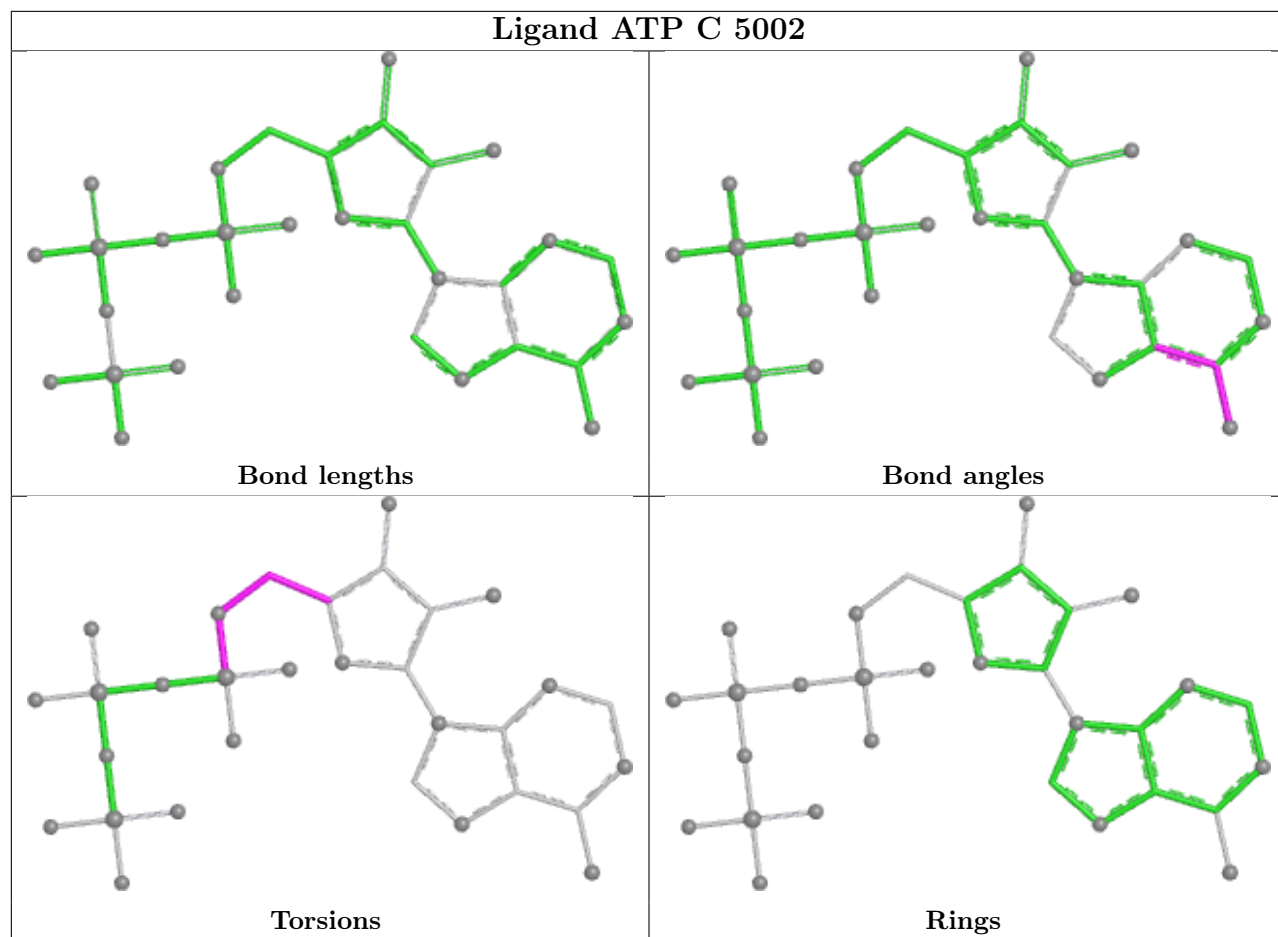


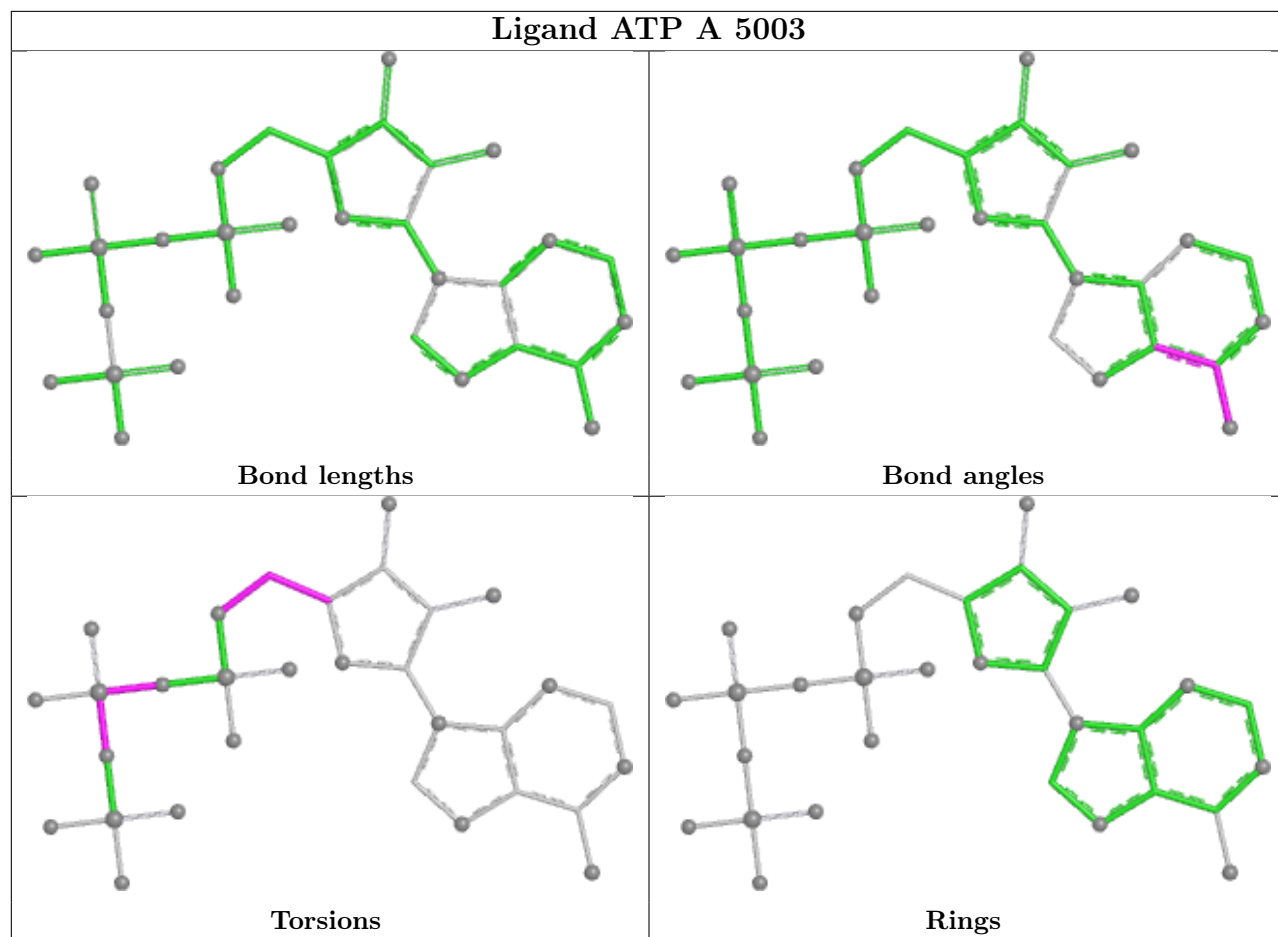


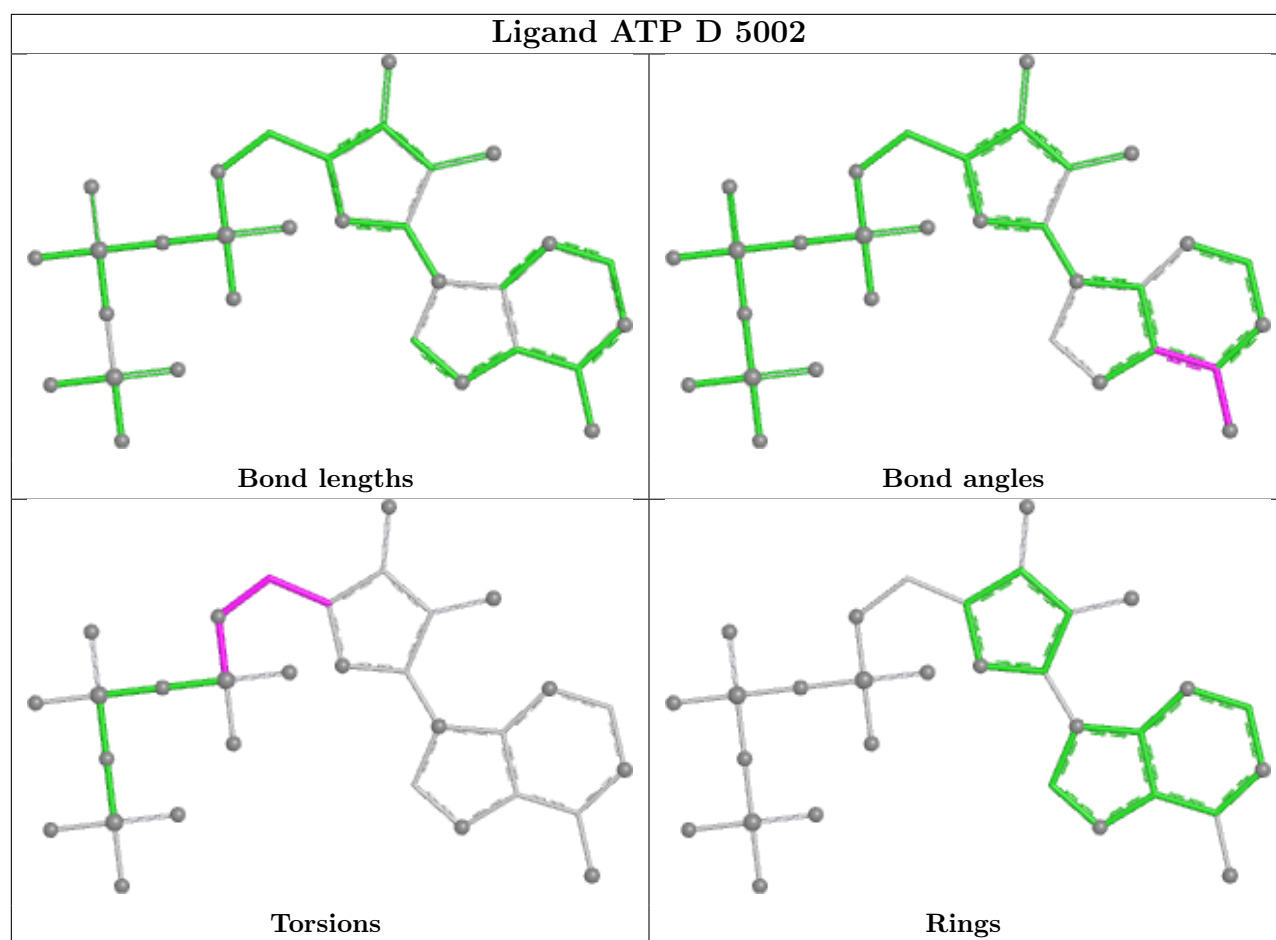












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

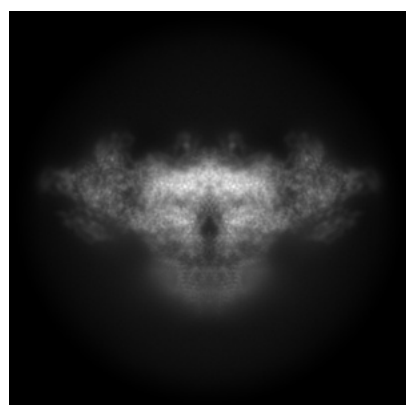
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42461. These allow visual inspection of the internal detail of the map and identification of artifacts.

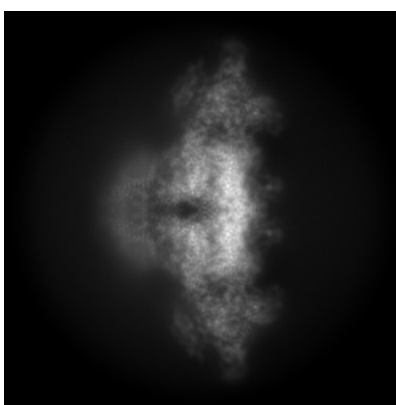
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

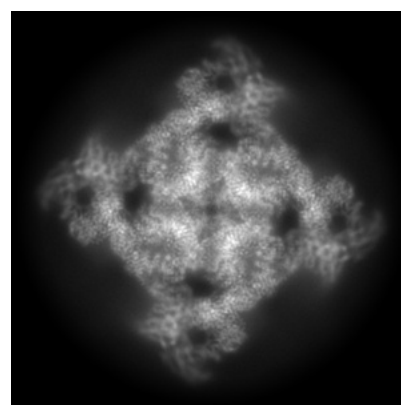
6.1.1 Primary map



X



Y

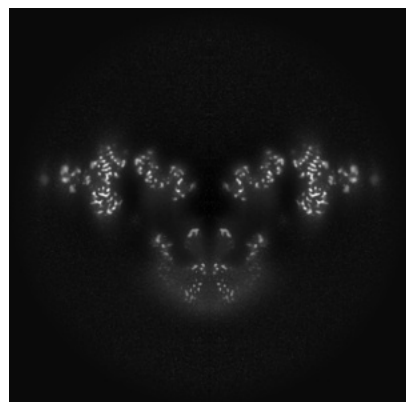


Z

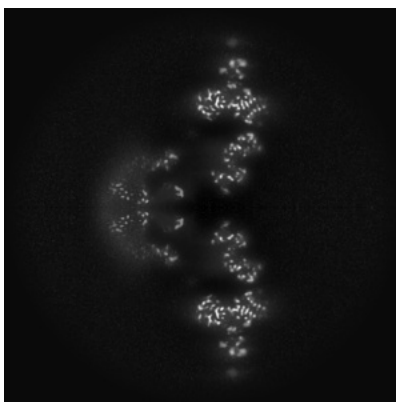
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

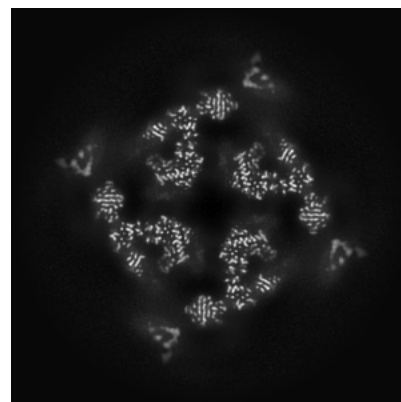
6.2.1 Primary map



X Index: 256



Y Index: 256

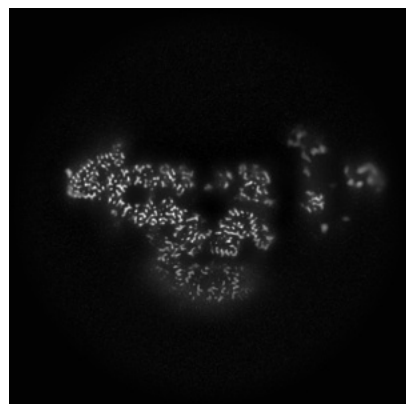


Z Index: 256

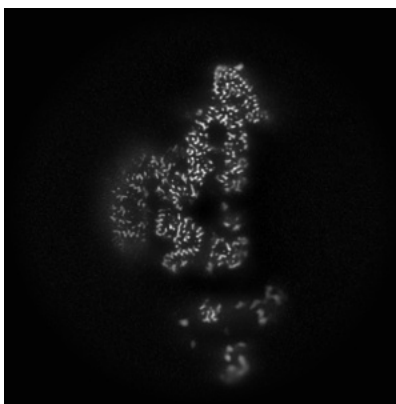
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

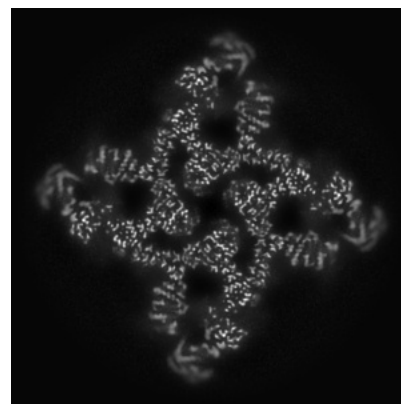
6.3.1 Primary map



X Index: 279



Y Index: 279



Z Index: 289

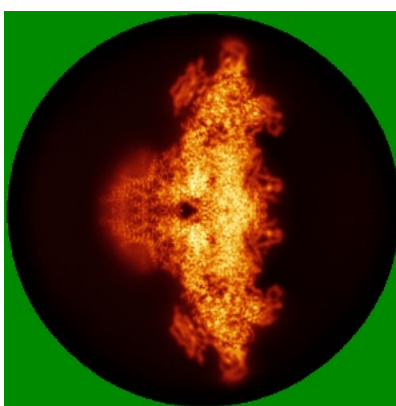
The images above show the largest variance slices of the map in three orthogonal directions.

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

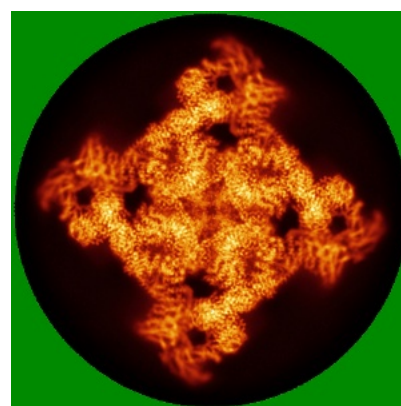
6.4.1 Primary map



X



Y

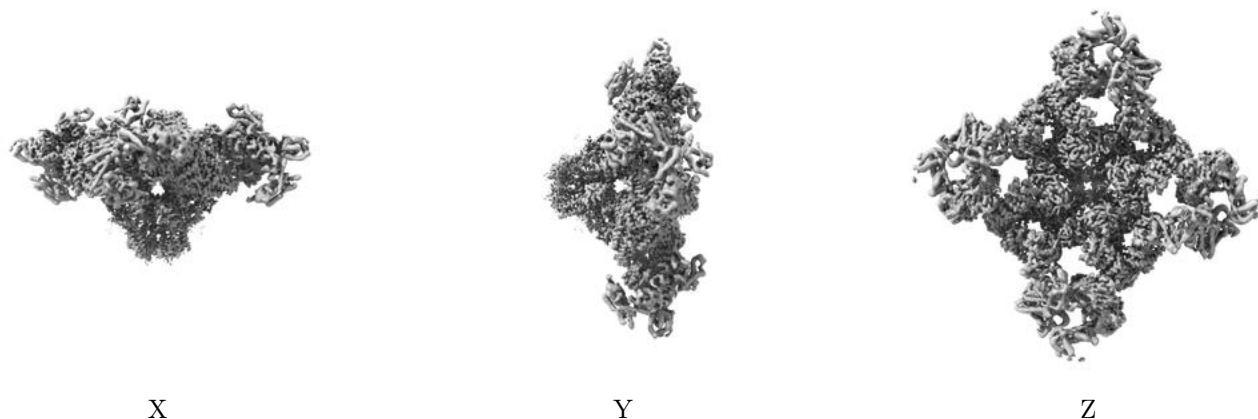


Z

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 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

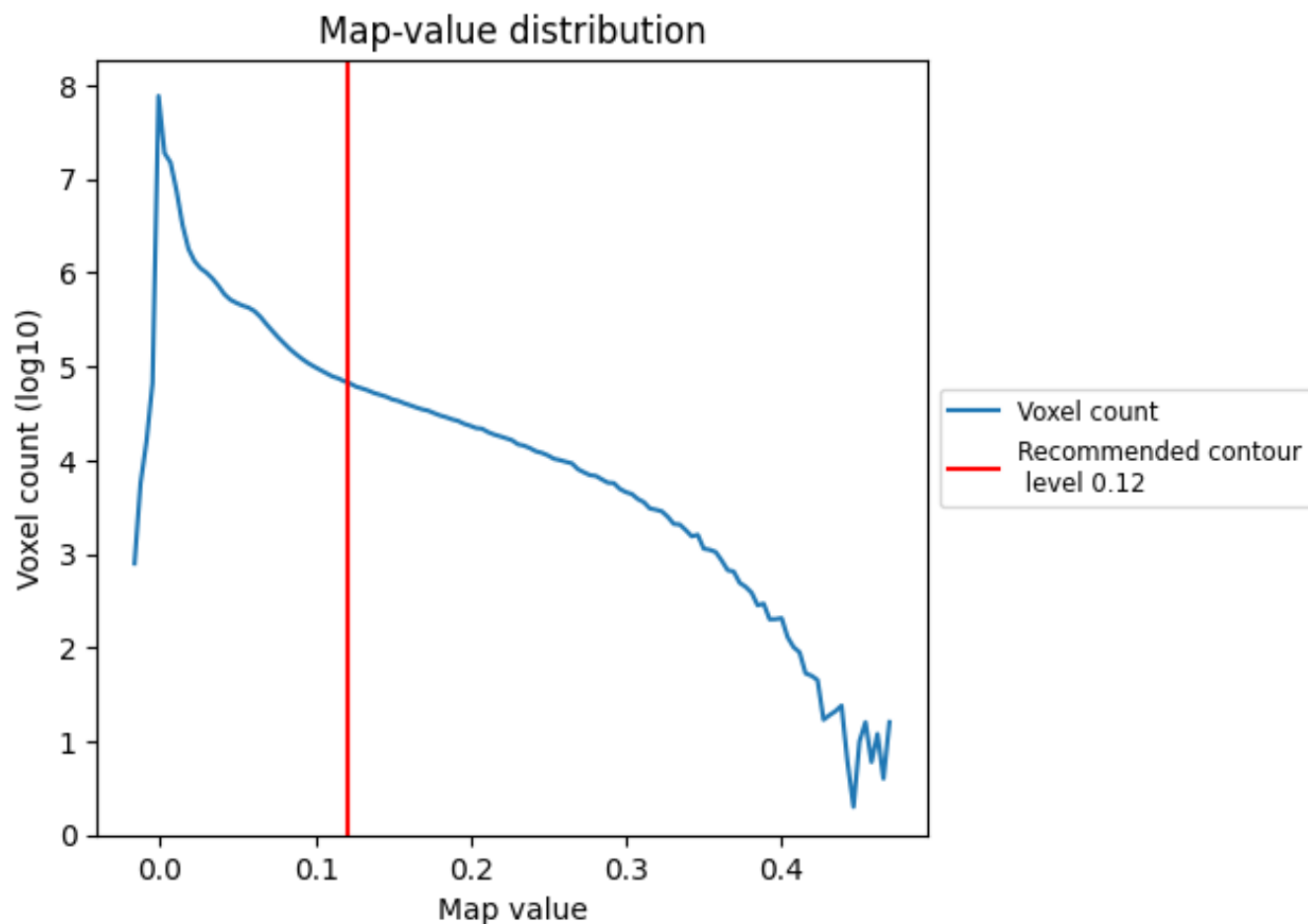
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

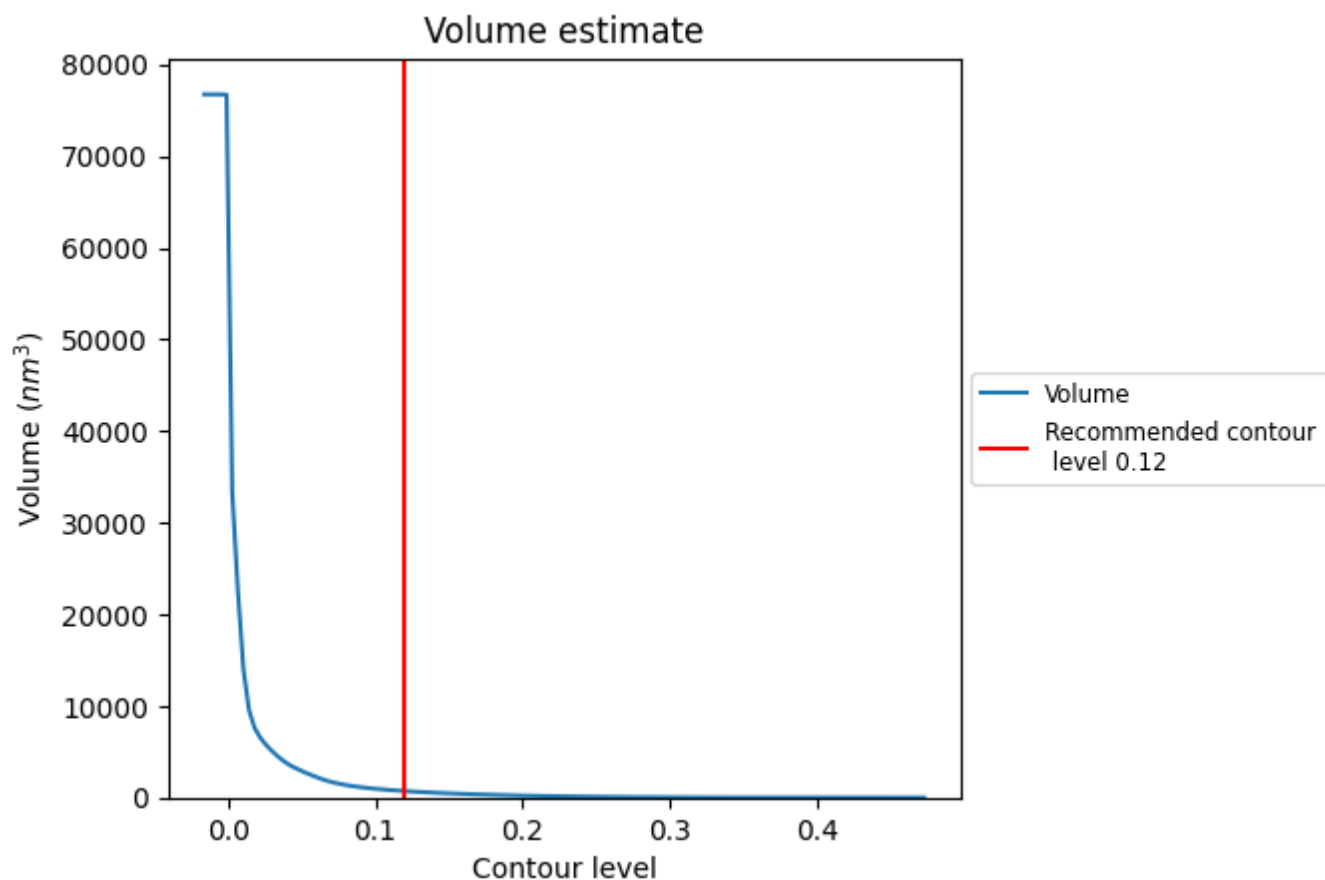
This section contains the results of statistical analysis of the map.

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.

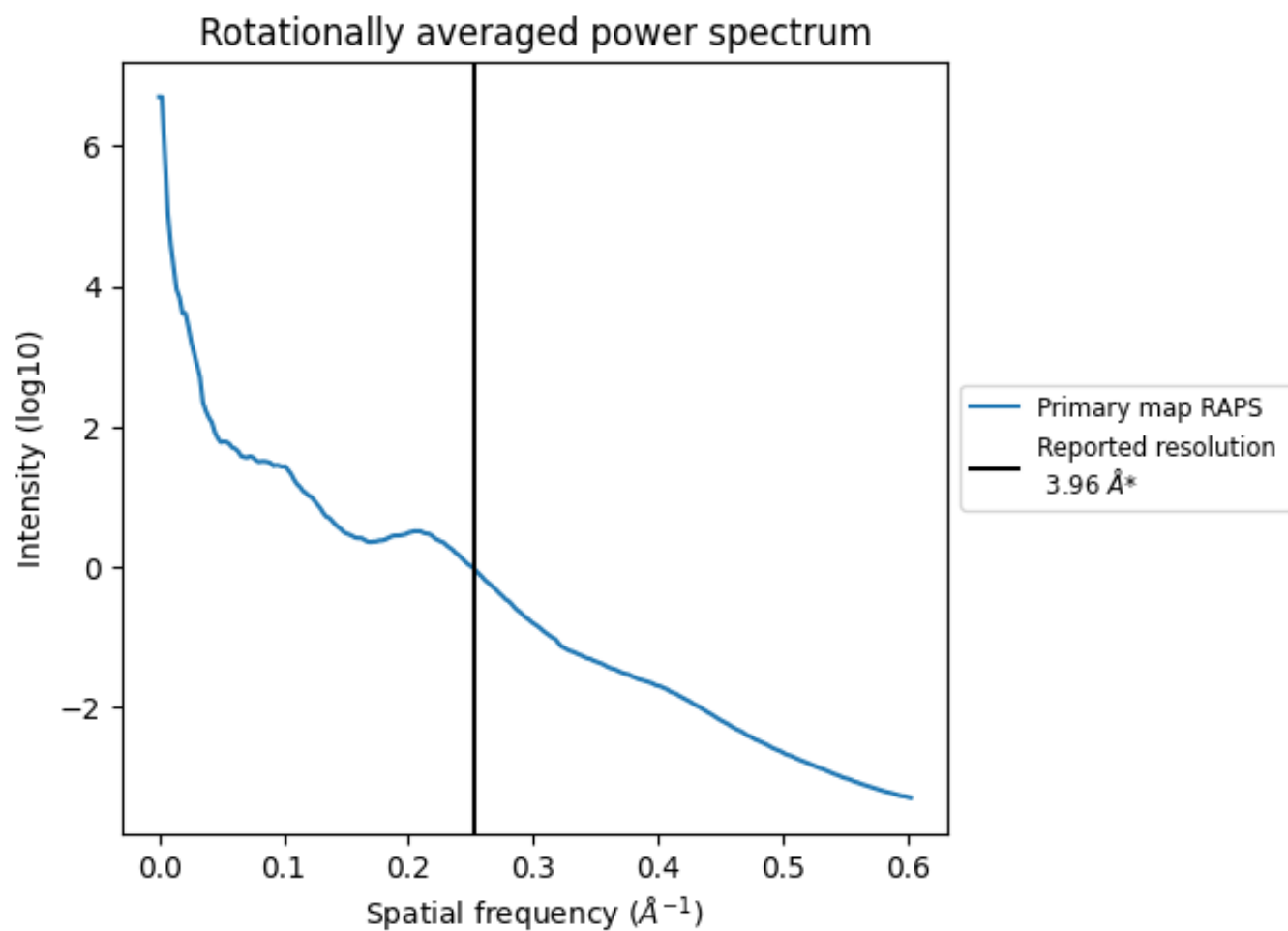
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 708 nm³; this corresponds to an approximate mass of 640 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 0.253 Å⁻¹

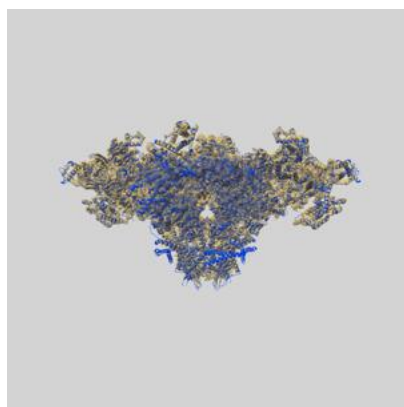
8 Fourier-Shell correlation ⓘ

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

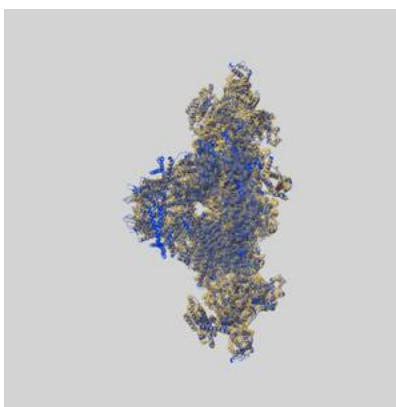
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42461 and PDB model 8UQ5. Per-residue inclusion information can be found in section [3](#) on page [5](#).

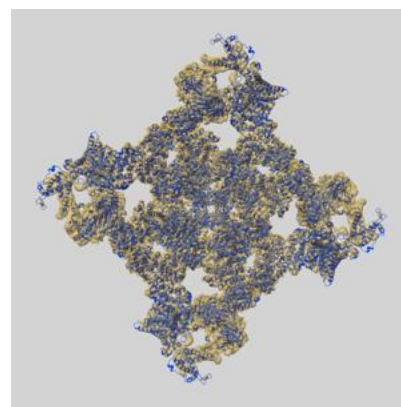
9.1 Map-model overlay [i](#)



X



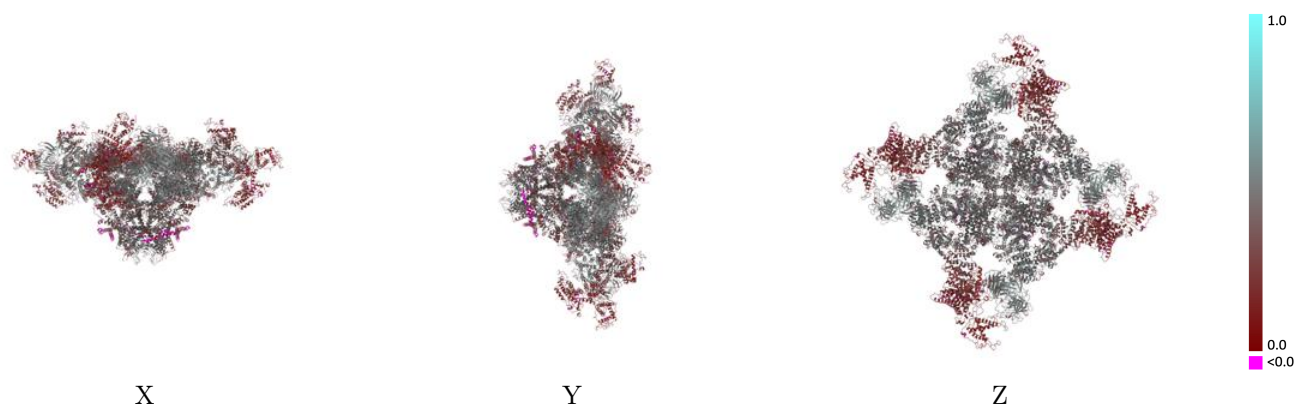
Y



Z

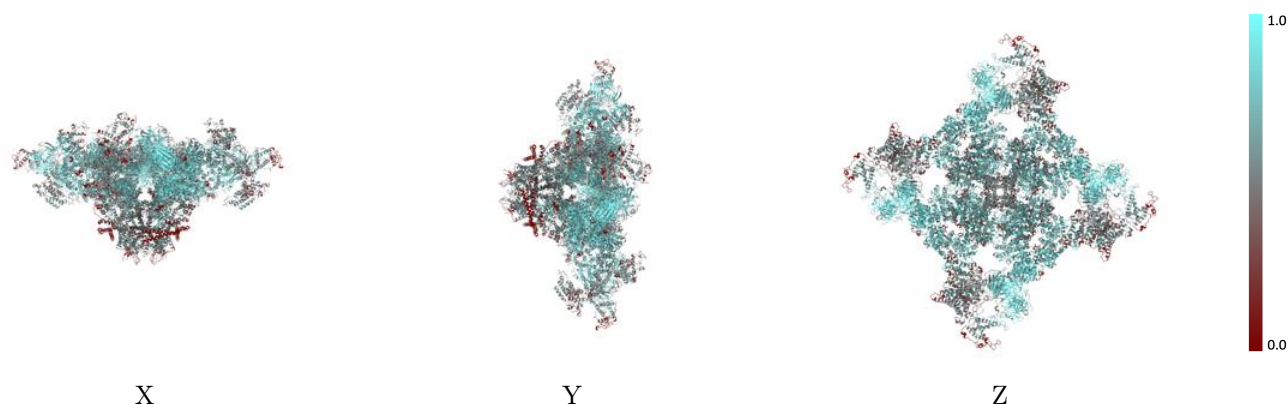
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



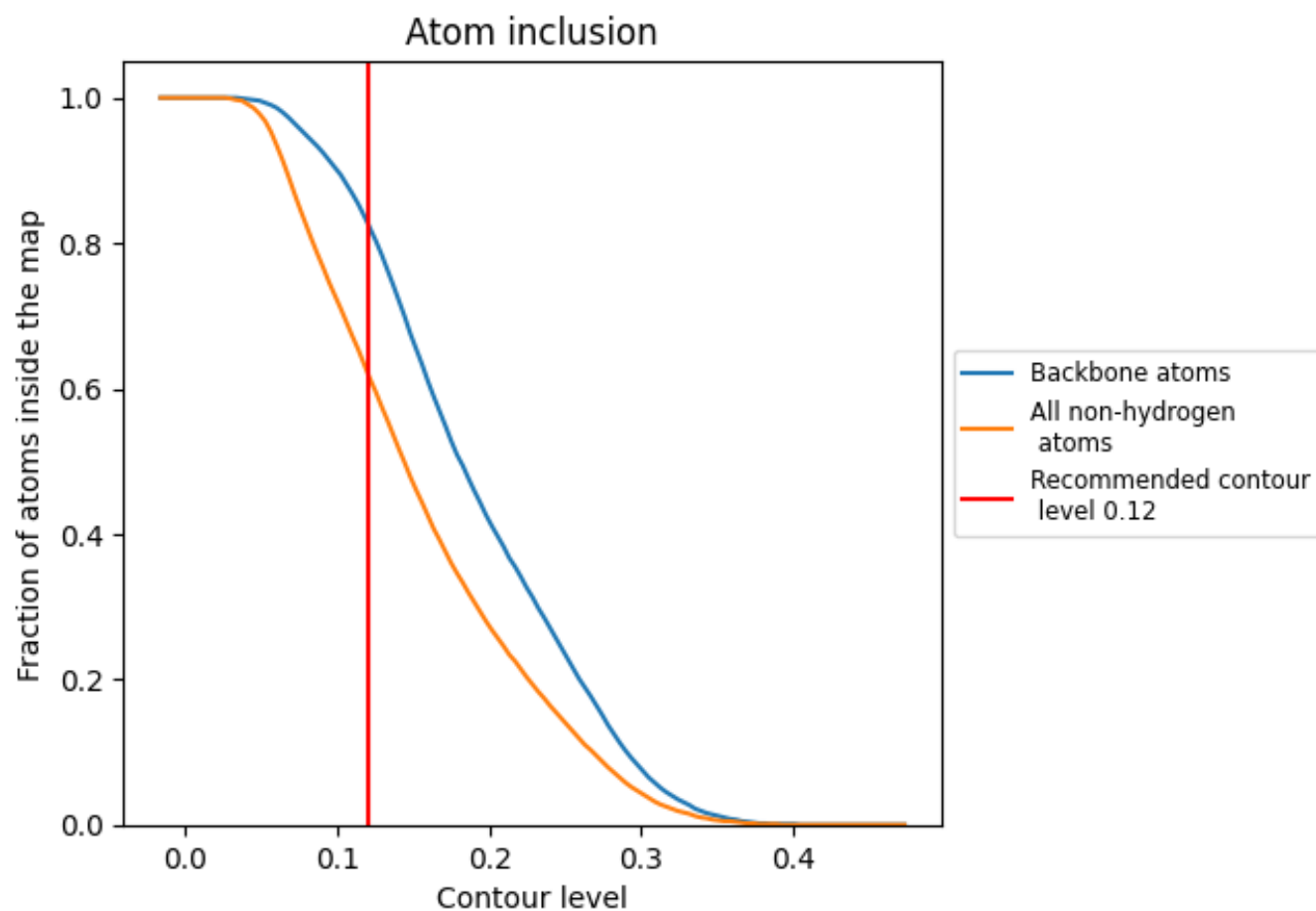
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 62% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6210	<div></div> 0.3710
A	<div></div> 0.6200	<div></div> 0.3710
B	<div></div> 0.6220	<div></div> 0.3710
C	<div></div> 0.6220	<div></div> 0.3710
D	<div></div> 0.6210	<div></div> 0.3720

