



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 09:57 PM EDT

PDB ID : 8UXE
EMDB ID : EMD-42761
Title : Structure of PKA phosphorylated human RyR2-R420Q in the closed state in the presence of ARM210
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.53 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

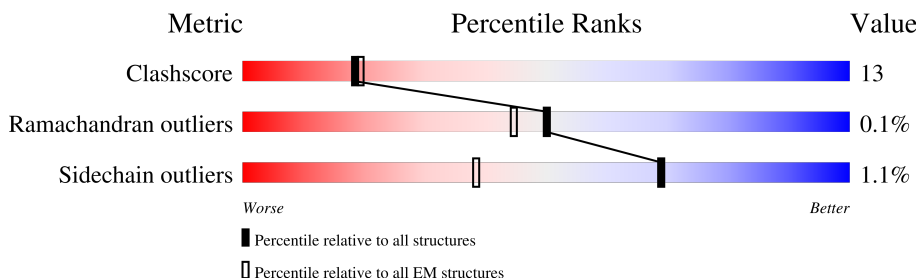
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 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	E	108	
1	F	108	
1	G	108	
1	H	108	
2	A	4967	
2	B	4967	
2	C	4967	
2	D	4967	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 138692 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
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
2	B	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
2	C	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
2	D	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		

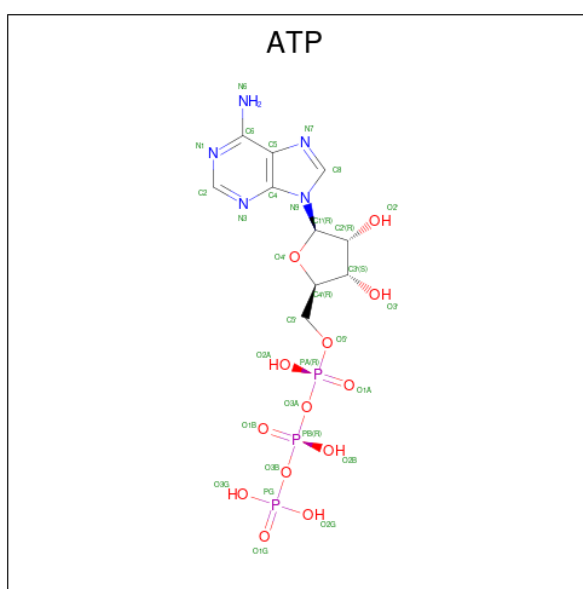
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLN	ARG	conflict	UNP Q92736
B	420	GLN	ARG	conflict	UNP Q92736
C	420	GLN	ARG	conflict	UNP Q92736
D	420	GLN	ARG	conflict	UNP Q92736

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- 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).



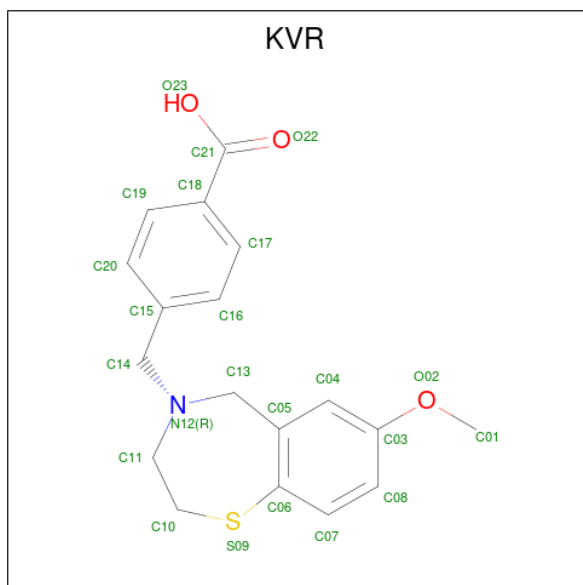
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10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

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

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: C₁₈H₁₉NO₃S) (labeled as "Ligand of Interest" by depositor).

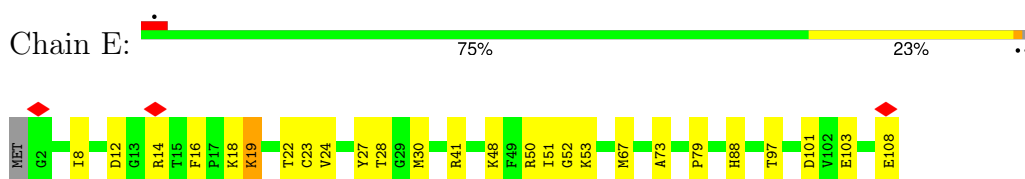


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	A	1	23	18	1	3	1	0
5	B	1	23	18	1	3	1	0
5	C	1	23	18	1	3	1	0
5	D	1	23	18	1	3	1	0

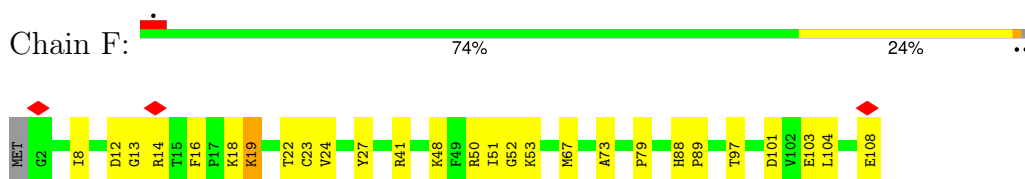
3 Residue-property plots [i](#)

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

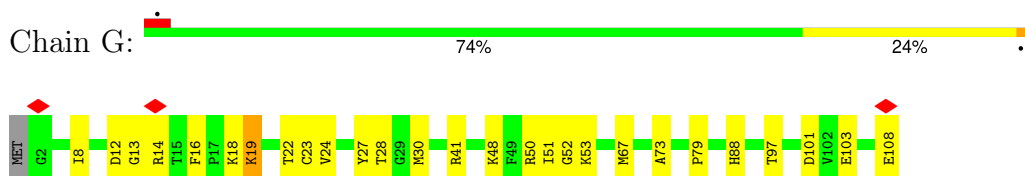
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



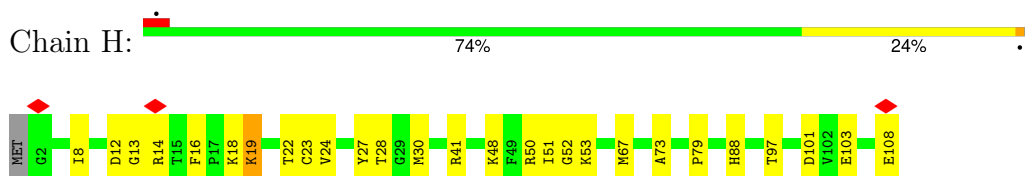
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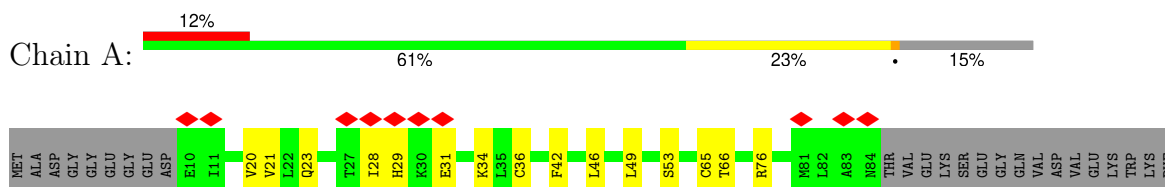
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



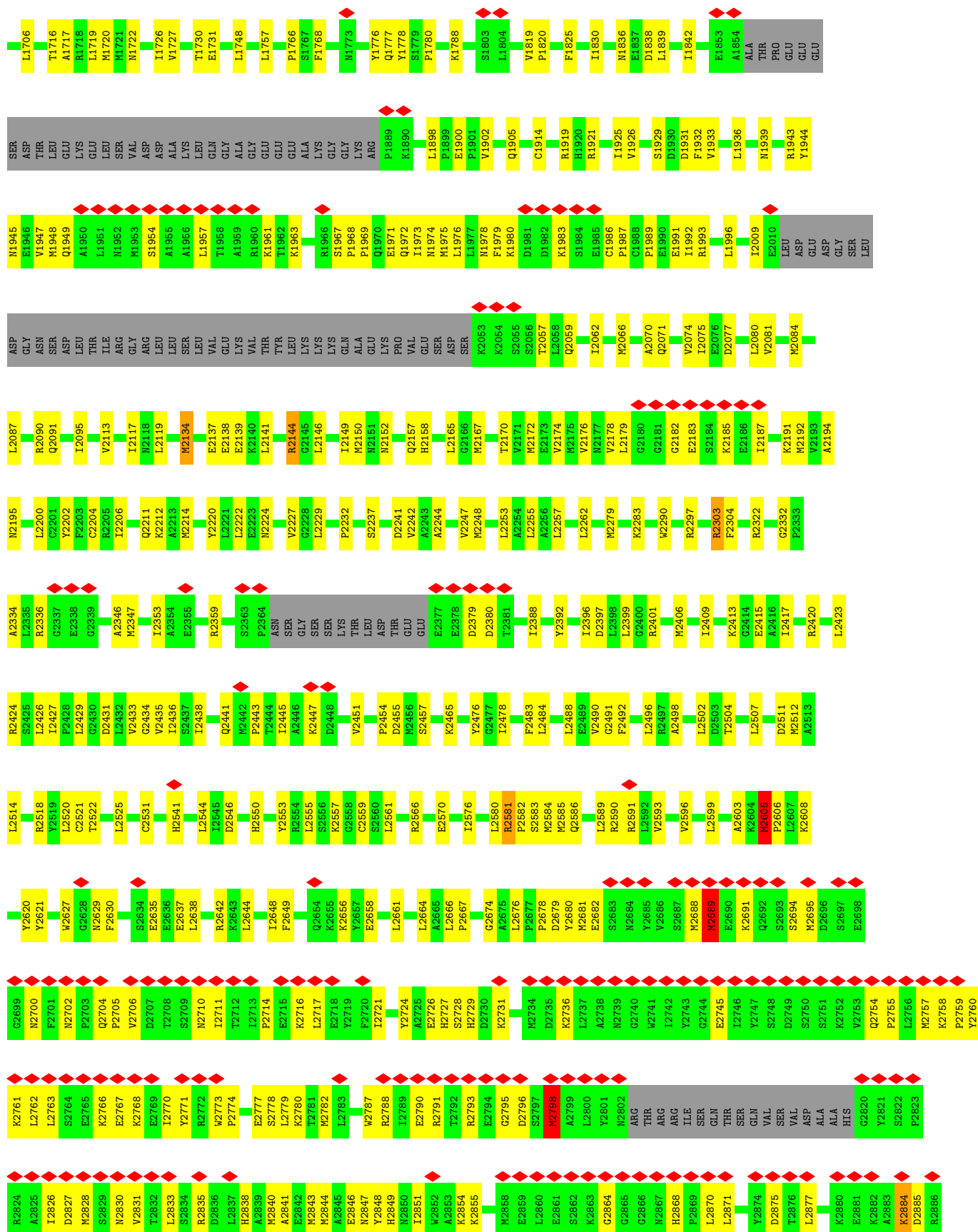
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



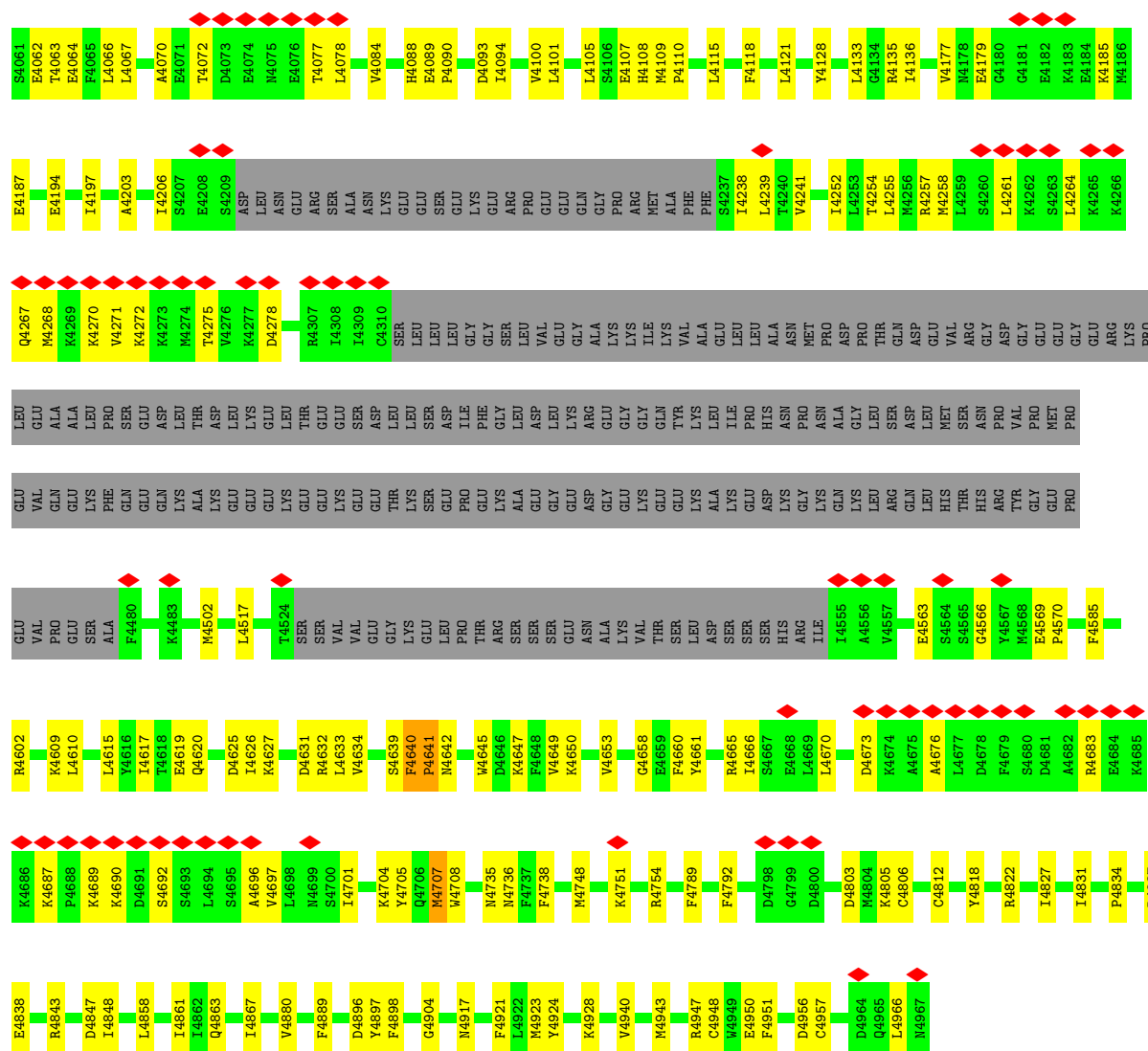
- Molecule 2: Ryanodine receptor 2



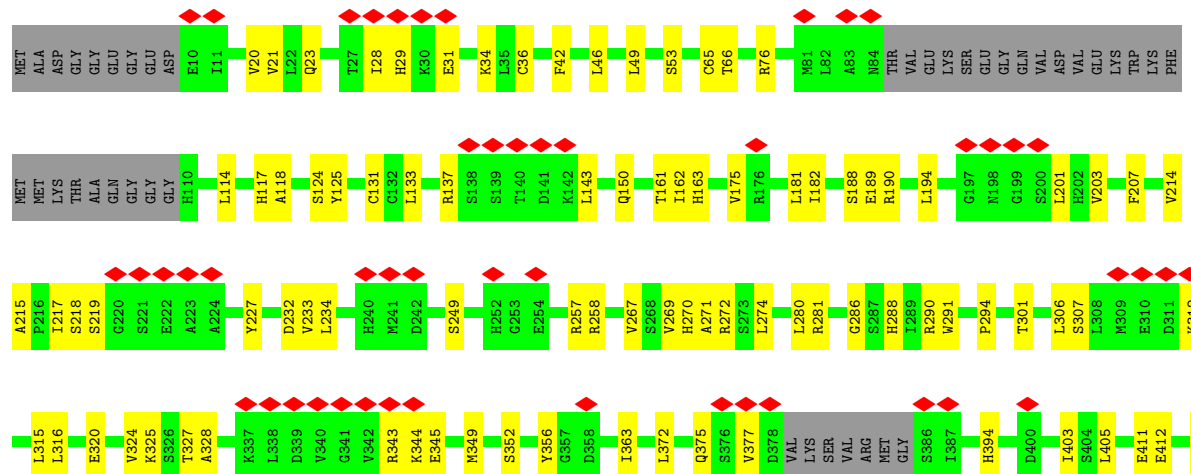
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THR	GLU	ASP	VAL	LEU	ALA	ASP	ASP	R1414	D1415	D1416	Y1417	D1418	T1425	S1429	V1430	R1431	G1435	P1438	A1439	N1440	G1444	W1445	I1446	H1451	D1471	E1472	K1473	G1474	K1475	M1487	V1488	C1489	E1492	S1495	P1496	G1497	Q1498	G1499	R1500	N1501	N1502	N1503	E1506	A1522	L1527											
LEU	MET	LYS	THR	ALA	HIS	GLY	HIS	LEU	VAL	PRO	ARG	VAL	ASP	LYS	LYS	GLU	ALA	THR	LYS	PRO	PHE	ASN	ASN	HIS	LYS	ASP	TYR	ALA	GLN	GLU	LYS	PRO	GLY	LEU	GLY	ARG	THR	LYS	ASP	ASP	TYR	GLU	ASP	THR	SER	HIS	SER	ALA	ARG	LEU						
P1067	D1068	Q1069	D1070	H1071	A1072	A1073	R1074	A1075	E1076	V1077	C1078	S1079	G1080	T1081	G1082	E1083	E1091	Y1094	K1097	R1100	S1118	G1129	W1145	V1161	D1167	M1168	N1169	E1170	H1171	T1172	I1181	E1189	G1198	V1204	V1209	R1214	K1225	Y1226	I1229	E1234	G1235															
Y1236	L1255	I1268	E1269	V1270	I1273	T1276	T1277	D1278	C1282	V1285	T1286	Q1287	G1291	S1292	Q1293	M1294	S1295	I1299	Y1302	K1316	THR	VAL	ALA	GLY	LEU	PRO	GLY	ALA	GLY	LEU	PHE	GLY	PRO	LYS	ASN	ASP	GLU	TYR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	VAL									
LEU	MET	LYS	THR	ALA	HIS	GLY	HIS	LEU	VAL	PRO	ARG	VAL	ASP	LYS	LYS	GLU	ALA	THR	LYS	PRO	PHE	ASN	ASN	HIS	LYS	ASP	TYR	ALA	GLN	GLU	LYS	PRO	GLY	LEU	GLY	ARG	THR	LYS	ASP	ASP	TYR	GLU	ASP	THR	SER	HIS	SER	ALA	ARG	LEU						
E310	D311	K312	L315	L316	E320	V324	K325	S326	A327	A328	K337	L338	D339	V340	G341	V342	R343	K344	E345	M349	S352	Y356	G357	D358	I363	L372	Q375	S376	V377	D378	VAL	LYS	SER	VAL	ARG	MET	GLY	S386	I387	H394	T403	S404	L405	E411	E412											
R417	K441	A442	S443	T444	V445	D446	L447	F448	L449	L456	L459	H469	D474	R478	K483	N484	R485	E491	K671	K672	W673	Y674	Y675	E676	L677	M678	V679	D680	R694	Y703	G717	V718	D720	D728	G729	L730	H731	L732	W733	A738	S742															
V574	V578	I588	R606	L614	A624	V625	N628	Q629	I632	M655	R656	P657	N658	I659	F660	L661	G662	V663	Y670	K671	K672	W673	Y674	Y675	E676	L677	M678	V679	D680	R694	Y703	G717	V718	D720	D728	G729	L730	H731	L732	W733	A738	S742														
Q746	H747	L748	R749	I751	T755	S756	R769	P774	F788	S793	F794	I798	K799	N800	R801	L804	H808	G809	E810	F811	Y819	A820	P821	C822	Y823	E824	Q825	V826	K831	L832	K833	D849	T858	P866	V867	D868	T869	S870	Q871	I872	V873	L874	P875	H877												
L878	E879	R880	T881	R882	V884	L885	A886	E887	N888	L889	H890	O891	L892	N893	V894	N895	N896	K897	I898	E899	G901	Q902	Y903	G905	P906	Y907	R908	D909	T910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	Q923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	N935	S936	L937		
K941	T942	L943	L944	A945	L946	G947	C948	H949	I952	S953	E954	E955	H956	A957	E958	D959	K960	V961	K962	K963	M964	K965	L966	P967	K968	N969	Y970	L972	T973	S974	G975	Y976	K977	P978	A979	P980	M981	D982	L983	S984	F985	L986	K987	T989	P990	Q991	Q992	M995	V996	L999	A1000	E1001	N1002	A1003		
H1004	H1005	W1007	A1008	R1009	D1010	R1011	I1012	R1013	Q1014	A1016	T1017	Y1018	G1019	I1020	Q1021	N1026	R1027	N1028	N1029	P1030	R1031	L1032	V1033	P1034	Y1035	T1036	L1037	L1038	D1039	D1040	R1041	T1042	K1043	S1044	N1045	N1046	A1047	D1048	S1049	L1050	R1051	E1052	A1053	V1054	R1055	T1056	L1057	L1058	G1059	Y1060	G1061	Y1062	N1063	L1064	E1065	A1066







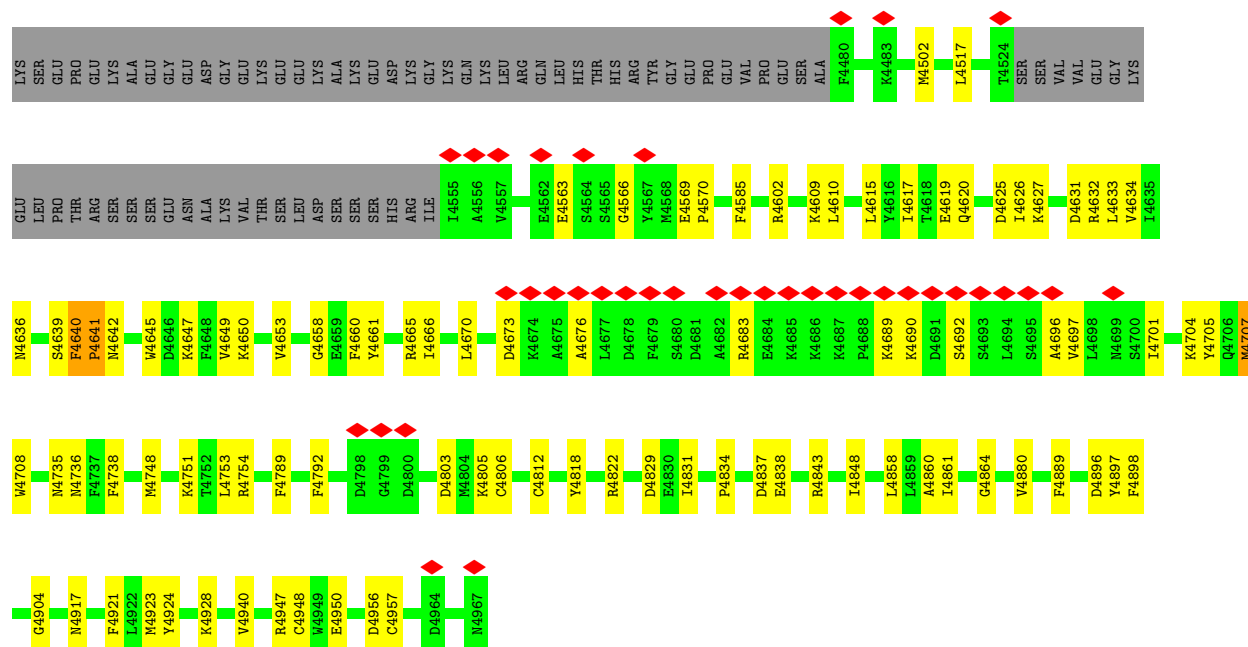
• Molecule 2: Ryanodine receptor 2



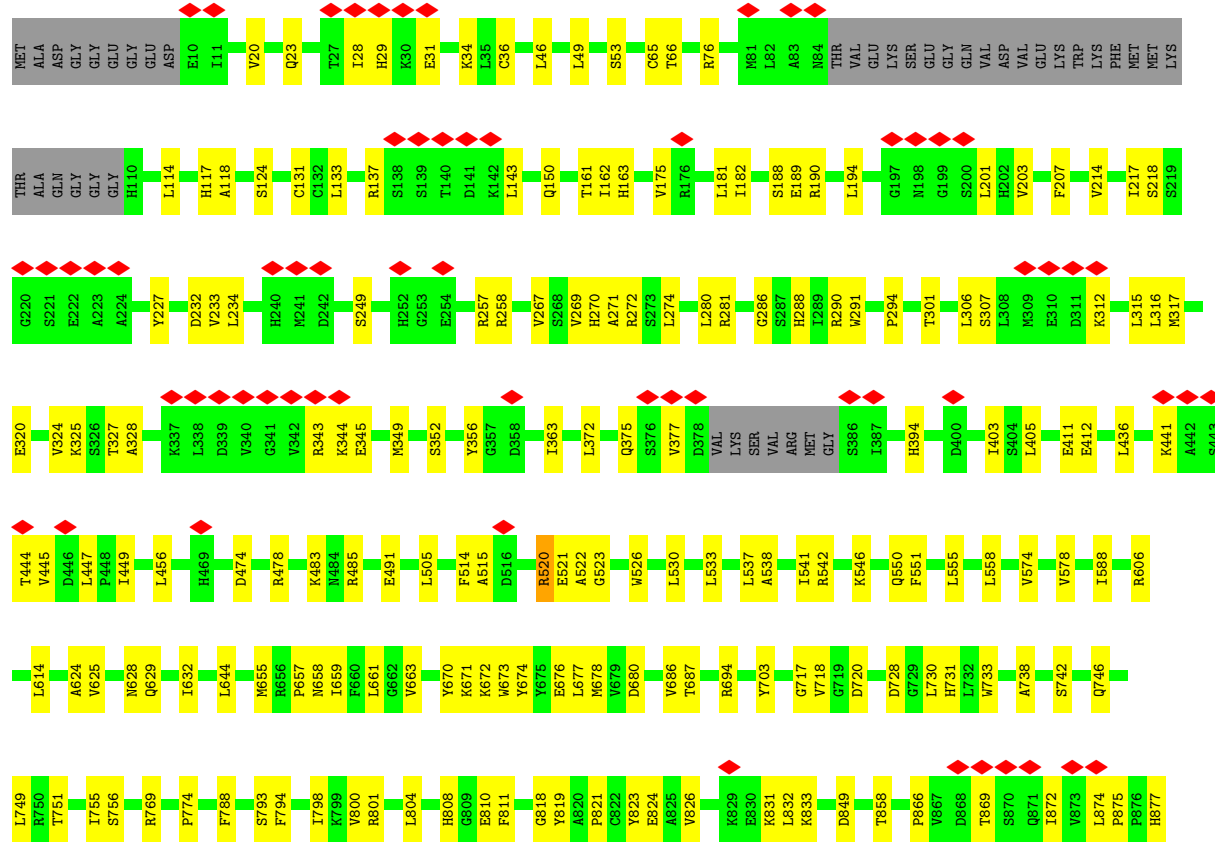








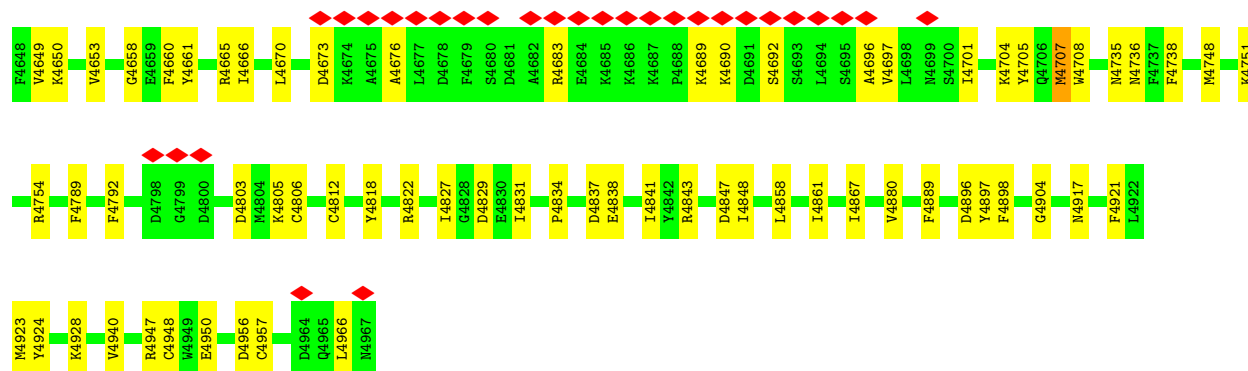
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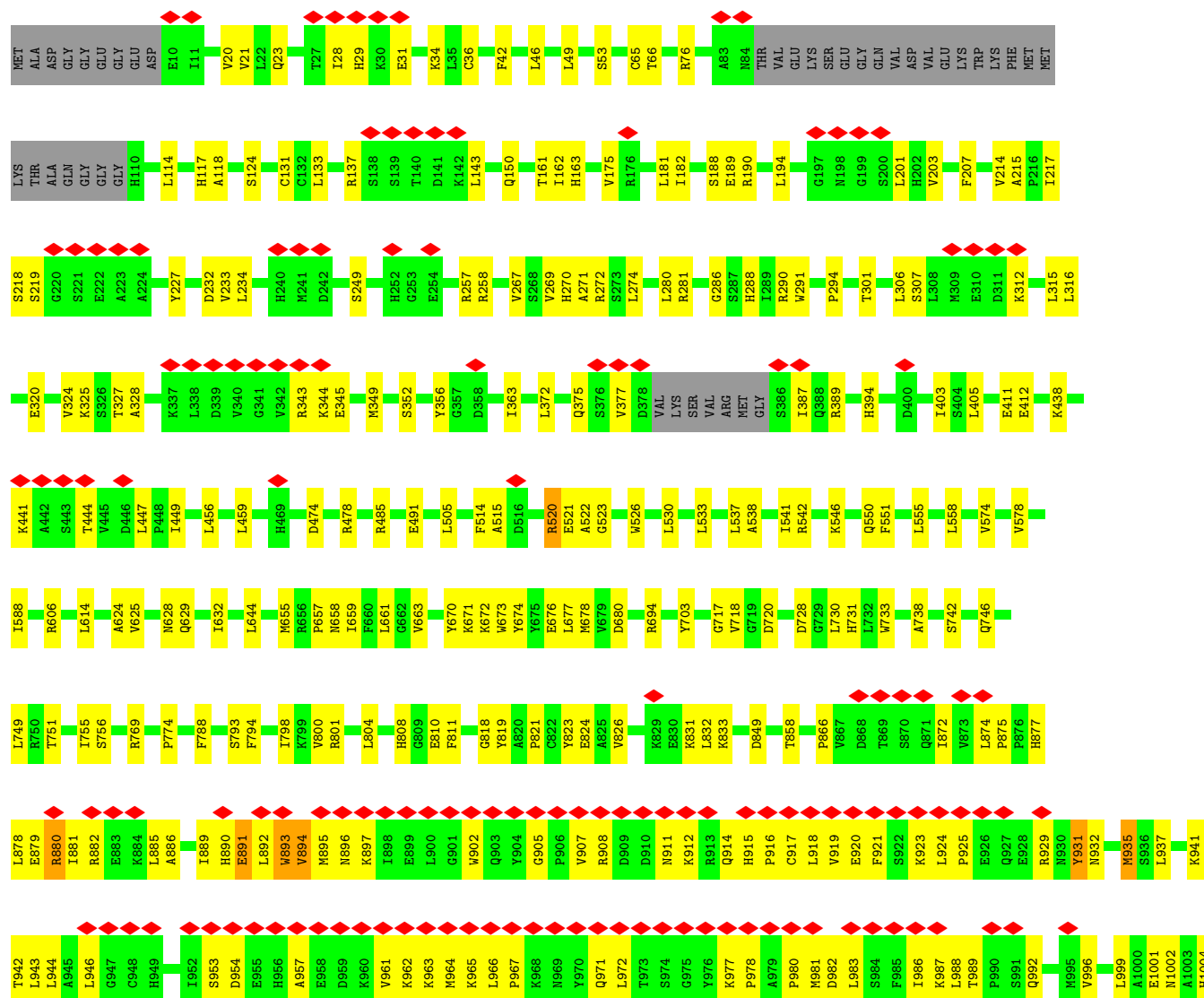


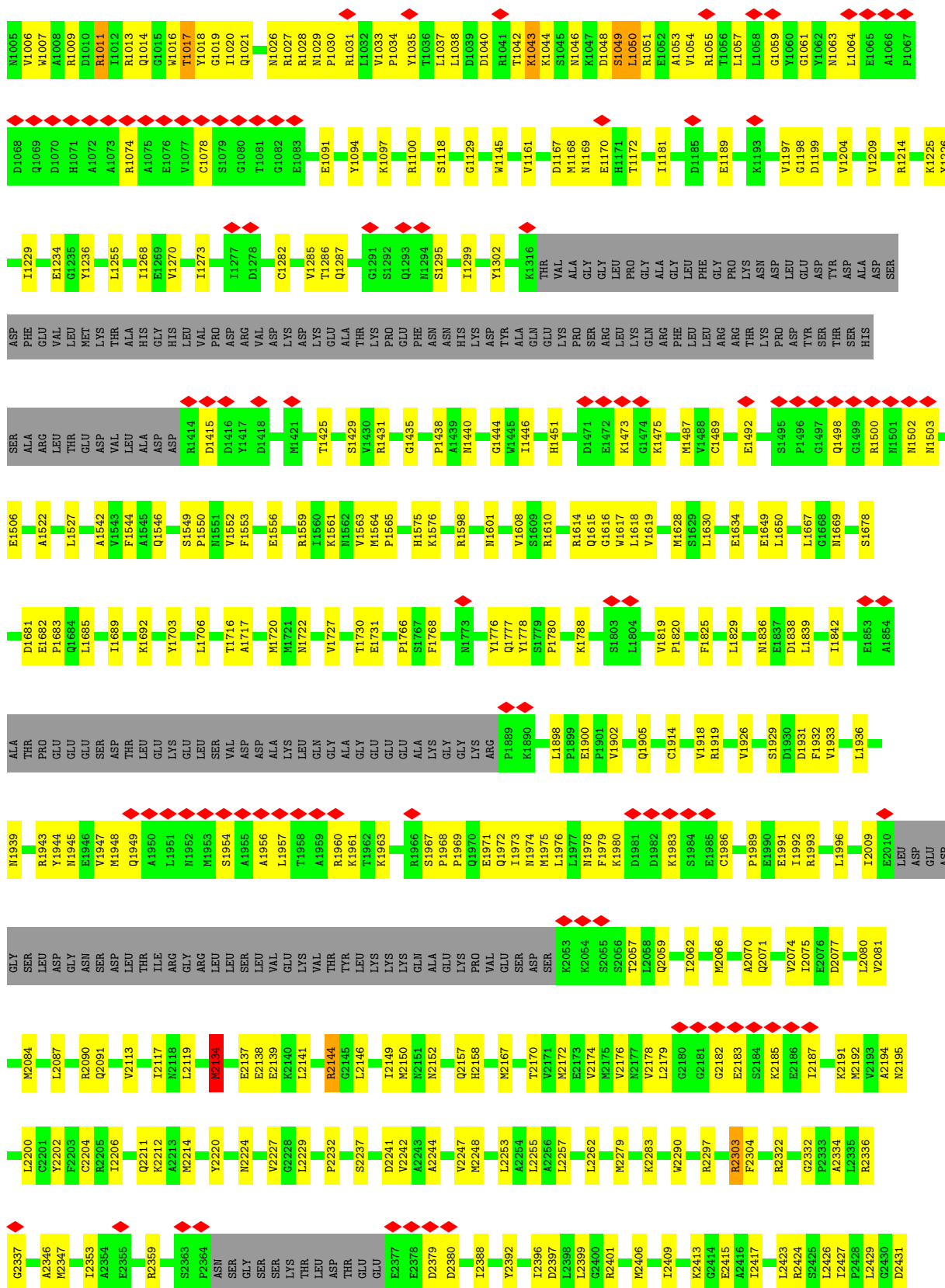
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A2346	M2347	I2363	A2364	E2365	R2369	S2363	P2364	ASN	SER	GLY	SER	LYS	THR	LEU	ASP	THR	GLU	E2377	E2378	D2379	D2380	L2388	Y2392	I2396	D2397	L2398	L2399	G2400	R2401	M2406	L2409	K2413	G2414	E2415	A2416	L2417	R2420	L2423	R2424	S2425	L2426	P2427	L2428	L2429	G2430	D2431												
L2432	V2433	G2434	V2435	S2437	L2438	Q2441	M2442	P2443	T2444	L2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	Y2476	G2477	L2478	P2483	L2484	L2488	E2489	V2490	G2491	F2492	L2496	R2497	A2498	L2502	D2503	T2504	L2507	D2511	M2512	L2514	L2520	C2521	L2525	C2531															
H2541	L2544	T2545	D2546	H2550	Y2553	K2554	L2555	S2556	K2557	G2558	S2560	L2561	R2566	E2570	L2576	L2580	P2581	S2582	S2583	M2584	M2585	Q2586	L2589	Y2590	R2591	L2592	V2593	Y2596	L2599	K2603	K2604	P2605	P2606	L2607	K2608	Y2620	Y2621	W2627	G2628	N2629	F2630	E2635	E2636															
E2637	R2642	L2644	L2648	F2649	Q2654	K2655	K2656	E2657	E2658	L2661	L2664	A2665	L2666	P2667	G2674	A2675	L2676	P2677	P2678	D2679	Y2680	M2681	E2682	S2683	N2684	Y2685	V2686	S2687	M2688	E2689	E2690	K2691	Q2692	S2693	S2694	M2695	S2697	E2698	G2699	N2700	F2701	N2702	P2703	Q2704	P2705	V2706	D2707	T2708	S2709	N2710	L2711							
T2712	T2713	P2714	E2715	T2716	L2717	E2718	T2719	F2720	T2721	Y2724	K2725	E2726	H2727	S2728	H2729	D2730	K2731	W2732	S2733	M2734	D2735	K2736	L2737	A2738	N2739	G2740	W2741	L2742	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749	S2750	S2751	K2752	V2753	Q2754	P2755	L2756	W2757	T2758	P2759	Y2760	K2761	L2762	L2763	S2764	E2765	E2766	E2767	K2768	E2769	L2770	Y2771	R2772
W2773	P2774	E2777	S2778	L2779	T2781	M2782	L2783	A2784	W2787	R2788	L2789	E2790	R2791	T2792	T2793	E2794	G2795	D2796	S2797	E2798	A2799	L2800	Y2801	N2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	I2826	D2827	M2828	S2829	N2830	V2831	T2832	L2833	S2834		
R2835	D2836	L2837	H2838	A2839	M2840	A2841	E2842	M2843	M2844	A2845	E2846	N2847	Y2848	H2849	L2851	K2854	K2855	M2858	E2859	L2860	E2861	S2862	K2863	G2864	G2865	G2866	H2867	H2868	P2869	L2870	L2871	Y2874	D2875	T2876	L2877	E2881	K2882	A2883	D2884	L2885	R2886	E2887	K2888	A2889	Q2890	D2891	T2892	L2893	K2894	F2895	L2896	Q2897	L2898					
Y2901	A2902	S2903	V2904	R2905	G2906	F2907	K2908	D2909	L2910	E2911	D2912	T2914	P2915	L2917	R2920	F2921	A2922	Y2923	L2926	Q2927	Q2928	E2931	Y2932	V2933	H2937	L2940	F2943	D2944	G2945	Q2946	S2947	R2948	G2949	K2950	G2951	E2952	H2953	F2954	P2955	F2963	K2965	V2966	V2967	L2968	Y2974	F2975	K2976	M2977										
H2978	R2979	L2980	Y2981	F2982	L2983	S2984	A2985	A2986	S2987	R2988	L2989	L2990	C2991	G2992	G2993	G2994	K3001	E3002	M3003	L3007	V3013	L3014	V3015	R3016	H3017	R3018	L3021	F3022	G3023	N3024	D3025	A3026	L3029	H3034	L3035	G3037	Q3038	T3039	L3040	D3041	R3043	T3044	V3045	M3046	K3047	L3050	V3053	K3054										
L3057	R3058	L3061	A3064	L3068	E3069	K3070	T3071	M3072	E3073	N3074	L3075	K3076	Q3077	Q3078	Q3079	F3080	T3081	HIS	THR	ASN	GLN	PRO	K3088	G3089	V3090	T3091	Q3092	I3093	L3094	N3095	Y3096	T3097	A3100	L3101	L3102	P3103	M3104	S3107	H3111	Q3116	F3117	G3118	E3119	D3120	L3121	E3124	L3125	V3126	Q3127									
C3130	Y3131	I3132	I3133	L3134	L3140	G3141	K3144	S3145	I3146	Y3147	V3148	E3149	R3150	K3151	R3152	S3153	E3154	L3155	F3162	A3163	G3164	A3165	F3166	F3167	A3168	A3169	F3170	L3171	E3172	T3173	H3174	L3175	D3176	K3177	H3178	I3183	Y3184	K3187	S3188	S3189	L3268	N3269	S3270	E3271	T3276	L3277	G3278	N3279	L3280	L3281	K3282	L3283	L3284					





• Molecule 2: Ryanodine receptor 2









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14924	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	0.660	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	426.752, 426.752, 426.752	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8335, 0.8335, 0.8335	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/834	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	G	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
2	A	0.28	0/34509	0.50	9/46612 (0.0%)
2	B	0.28	0/34509	0.50	9/46612 (0.0%)
2	C	0.28	0/34509	0.50	8/46612 (0.0%)
2	D	0.28	0/34509	0.50	9/46612 (0.0%)
All	All	0.28	0/141372	0.50	35/190940 (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
2	A	0	1
2	B	0	1
2	C	0	1
2	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2605	MET	CA-CB-CG	7.43	125.92	113.30
2	A	2605	MET	CA-CB-CG	7.42	125.92	113.30
2	C	2605	MET	CA-CB-CG	7.41	125.89	113.30
2	D	2605	MET	CA-CB-CG	7.40	125.88	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3262	GLU	CA-CB-CG	7.23	129.31	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	4640	PHE	Peptide
2	B	4640	PHE	Peptide
2	C	4640	PHE	Peptide
2	D	4640	PHE	Peptide

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	E	818	0	821	19	0
1	F	818	0	821	22	0
1	G	818	0	821	18	0
1	H	818	0	821	18	0
2	A	33769	0	33450	886	0
2	B	33769	0	33450	877	0
2	C	33769	0	33450	879	0
2	D	33769	0	33450	875	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	3	0
4	B	62	0	24	3	0
4	C	62	0	24	3	0
4	D	62	0	24	3	0
5	A	23	0	0	2	0
5	B	23	0	0	2	0
5	C	23	0	0	2	0
5	D	23	0	0	2	0
All	All	138692	0	137180	3541	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 13.

The worst 5 of 3541 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1031:ARG:HH21	2:B:1038:LEU:HD11	1.24	1.02
2:A:1031:ARG:HH21	2:A:1038:LEU:HD11	1.24	1.02
2:D:1031:ARG:HH21	2:D:1038:LEU:HD11	1.24	1.00
2:C:1031:ARG:HH21	2:C:1038:LEU:HD11	1.24	1.00
2:C:894:VAL:HG21	2:C:972:LEU:HD22	1.48	0.95

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	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	A	4198/4967 (84%)	4061 (97%)	132 (3%)	5 (0%)	48	79
2	B	4198/4967 (84%)	4061 (97%)	132 (3%)	5 (0%)	48	79
2	C	4198/4967 (84%)	4061 (97%)	132 (3%)	5 (0%)	48	79
2	D	4198/4967 (84%)	4060 (97%)	133 (3%)	5 (0%)	48	79
All	All	17212/20300 (85%)	16655 (97%)	537 (3%)	20 (0%)	50	79

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3927	PRO

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Mol	Chain	Res	Type
2	A	4641	PRO
2	B	3927	PRO
2	B	4641	PRO
2	C	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	E	88/89 (99%)	87 (99%)	1 (1%)	70	84
1	F	88/89 (99%)	87 (99%)	1 (1%)	70	84
1	G	88/89 (99%)	87 (99%)	1 (1%)	70	84
1	H	88/89 (99%)	87 (99%)	1 (1%)	70	84
2	A	3708/4358 (85%)	3667 (99%)	41 (1%)	70	84
2	B	3708/4358 (85%)	3667 (99%)	41 (1%)	70	84
2	C	3708/4358 (85%)	3667 (99%)	41 (1%)	70	84
2	D	3708/4358 (85%)	3667 (99%)	41 (1%)	70	84
All	All	15184/17788 (85%)	15016 (99%)	168 (1%)	69	84

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	2798	MET
2	D	1046	ASN
2	C	3088	LYS
2	D	880	ARG
2	D	2347	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1046	ASN

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Mol	Chain	Res	Type
2	C	3850	HIS
2	C	1974	ASN
2	C	2847	ASN
2	D	117	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 16 ligands modelled in this entry, 4 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	$\# Z > 2$
4	ATP	A	5002	-	28,33,33	0.65	0	34,52,52	0.77	2 (5%)
5	KVR	D	5004	-	24,25,25	0.50	0	31,34,34	0.83	2 (6%)
4	ATP	C	5002	-	28,33,33	0.65	0	34,52,52	0.77	2 (5%)
4	ATP	B	5003	-	28,33,33	0.73	0	34,52,52	0.77	1 (2%)
5	KVR	B	5004	-	24,25,25	0.49	0	31,34,34	0.82	2 (6%)
5	KVR	A	5004	-	24,25,25	0.51	0	31,34,34	0.83	2 (6%)
5	KVR	C	5004	-	24,25,25	0.52	0	31,34,34	0.83	2 (6%)
4	ATP	C	5003	-	28,33,33	0.73	0	34,52,52	0.77	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	D	5002	-	28,33,33	0.65	0	34,52,52	0.77	2 (5%)
4	ATP	D	5003	-	28,33,33	0.74	0	34,52,52	0.77	1 (2%)
4	ATP	A	5003	-	28,33,33	0.73	0	34,52,52	0.77	1 (2%)
4	ATP	B	5002	-	28,33,33	0.66	0	34,52,52	0.76	2 (5%)

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
4	ATP	A	5002	-	-	5/18/38/38	0/3/3/3
5	KVR	D	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	C	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	6/18/38/38	0/3/3/3
5	KVR	B	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	A	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	C	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	C	5003	-	-	6/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	6/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	6/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5004	KVR	C10-S09-C06	3.24	107.30	102.71
5	D	5004	KVR	C10-S09-C06	3.23	107.28	102.71
5	A	5004	KVR	C10-S09-C06	3.22	107.28	102.71
5	B	5004	KVR	C10-S09-C06	3.18	107.21	102.71
4	D	5002	ATP	C4'-O4'-C1'	-2.88	107.29	109.92

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

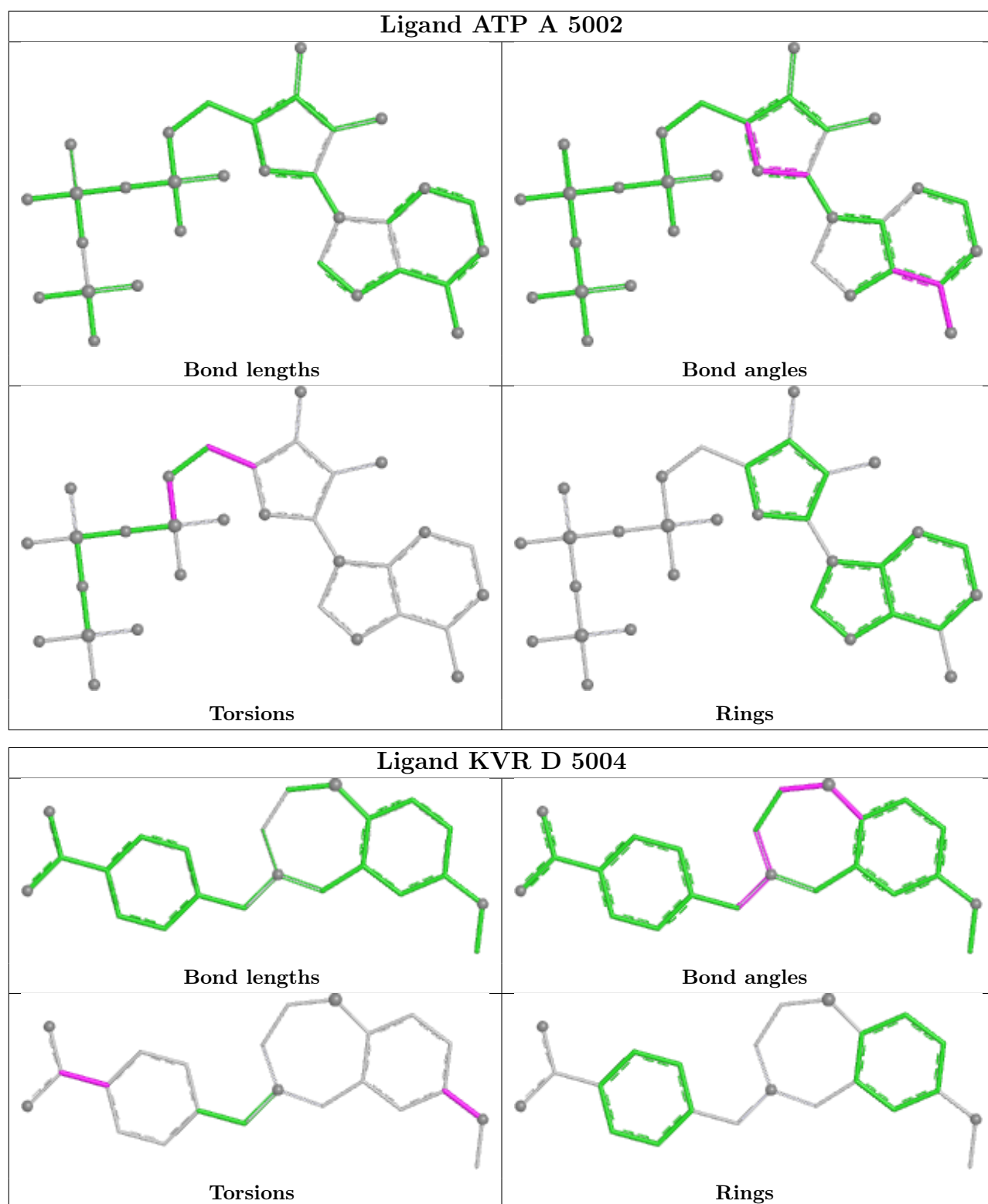
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	B	5002	ATP	C5'-O5'-PA-O2A

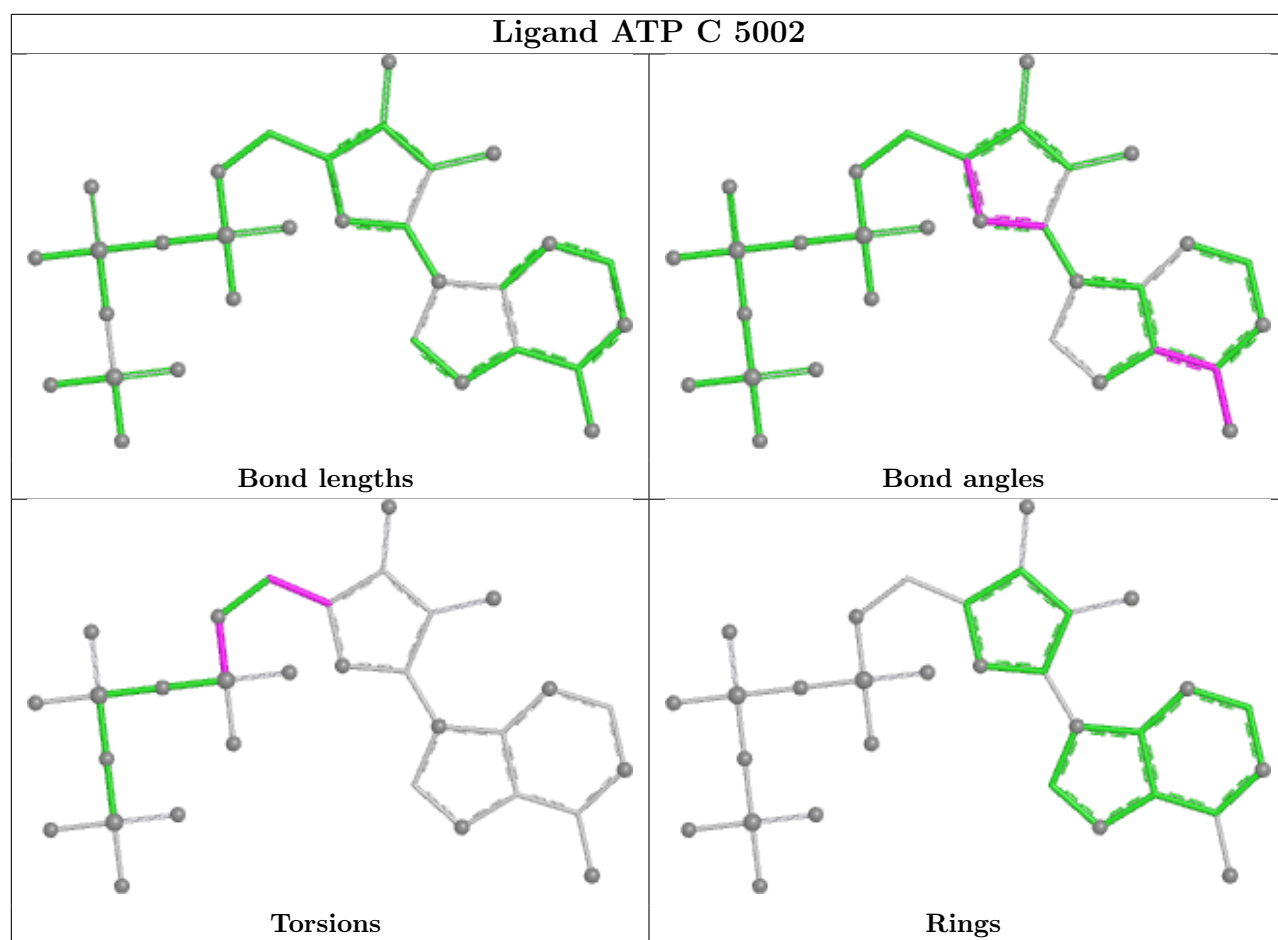
There are no ring outliers.

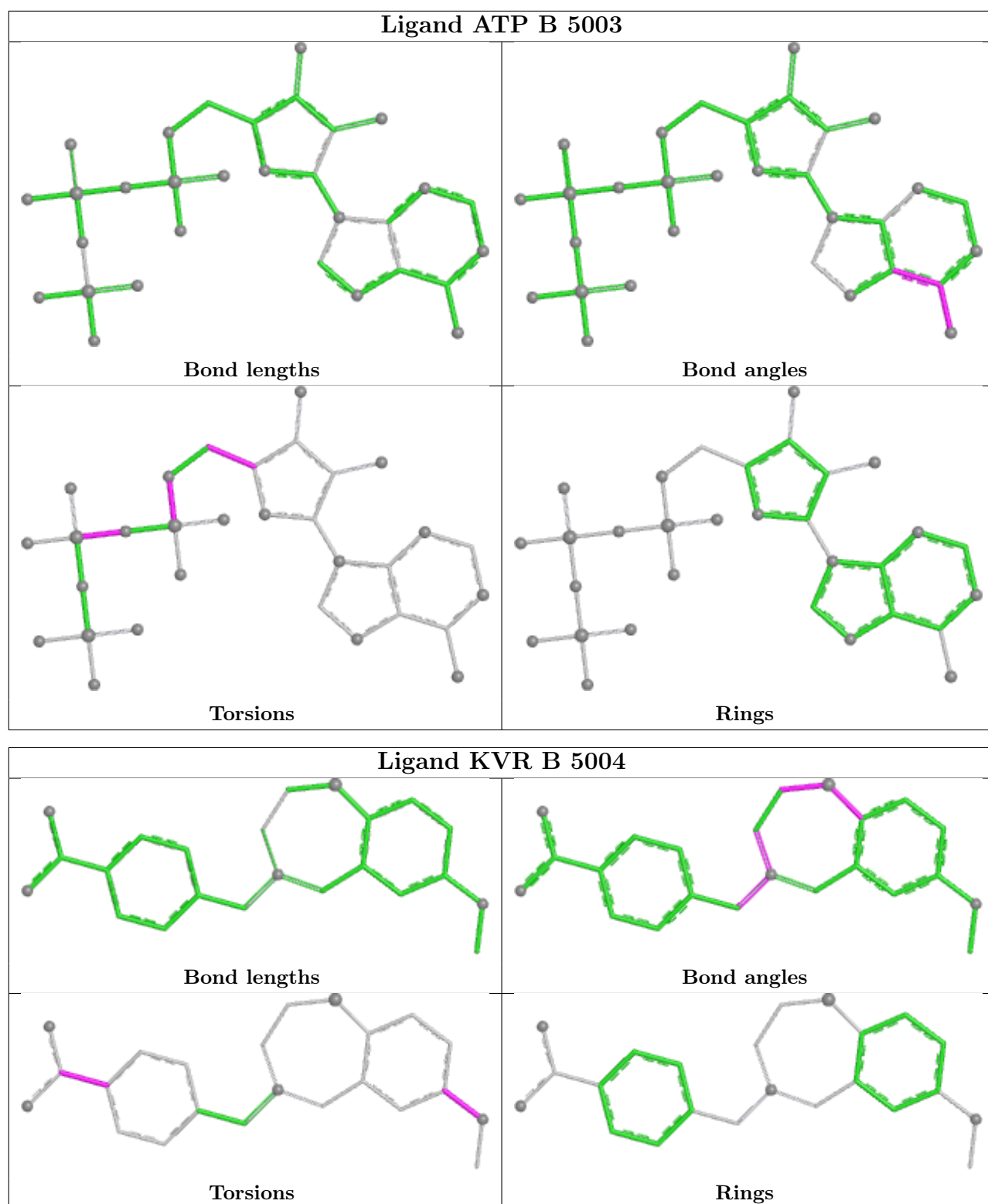
8 monomers are involved in 16 short contacts:

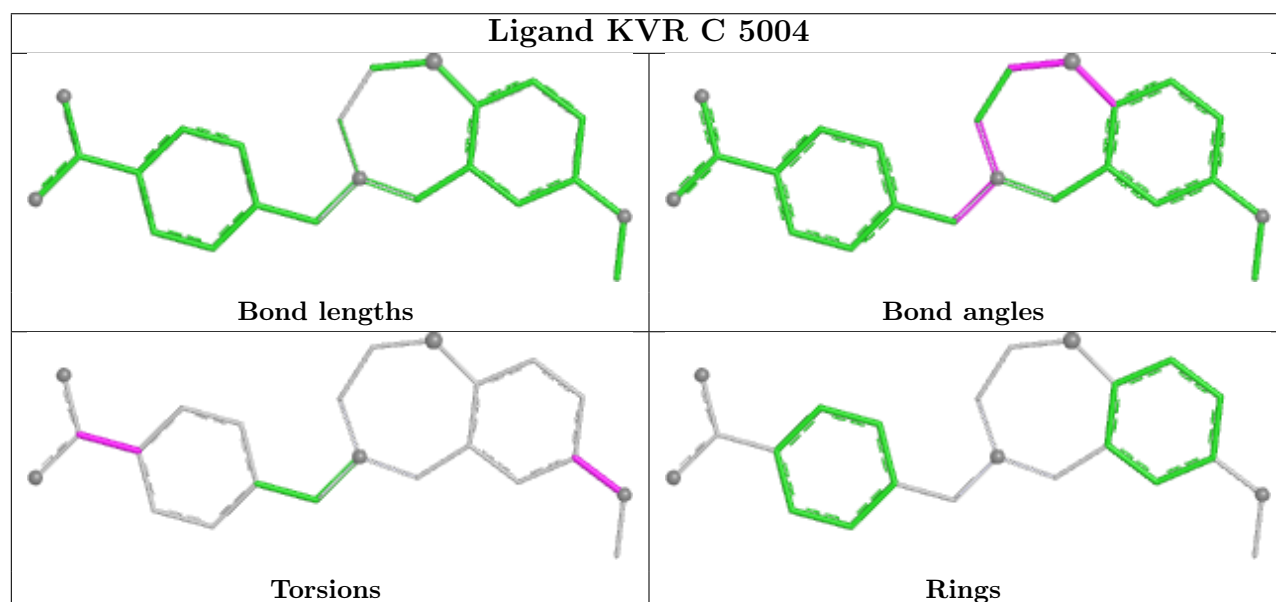
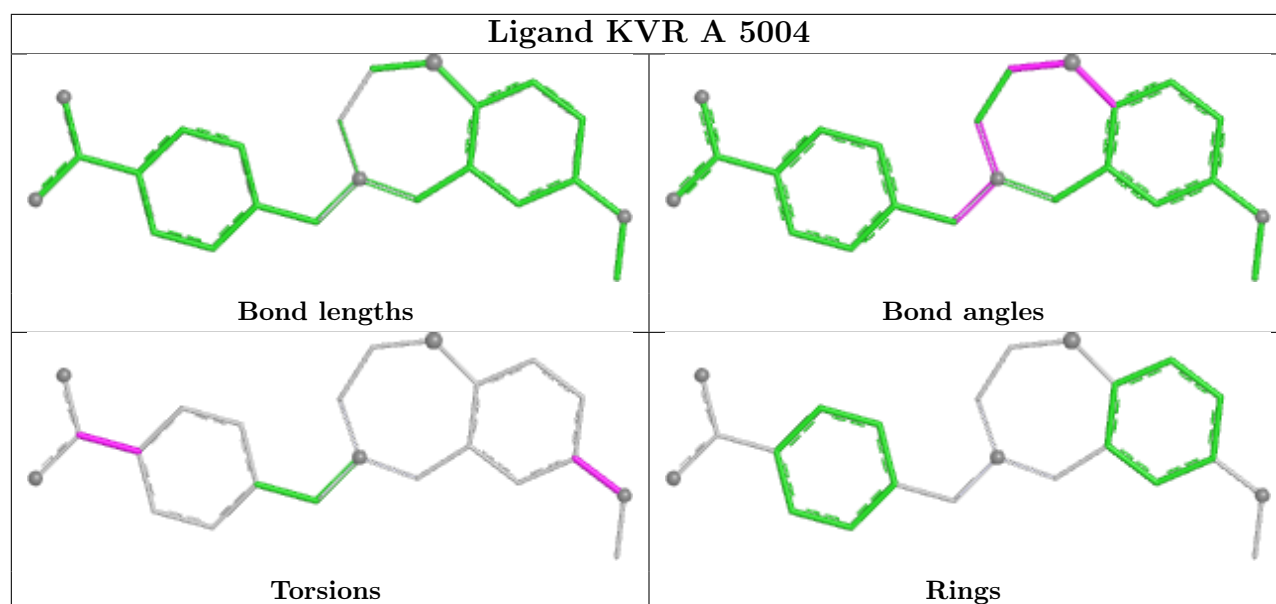
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	5004	KVR	2	0
4	B	5003	ATP	3	0
5	B	5004	KVR	2	0
5	A	5004	KVR	2	0
5	C	5004	KVR	2	0
4	C	5003	ATP	3	0
4	D	5003	ATP	3	0
4	A	5003	ATP	3	0

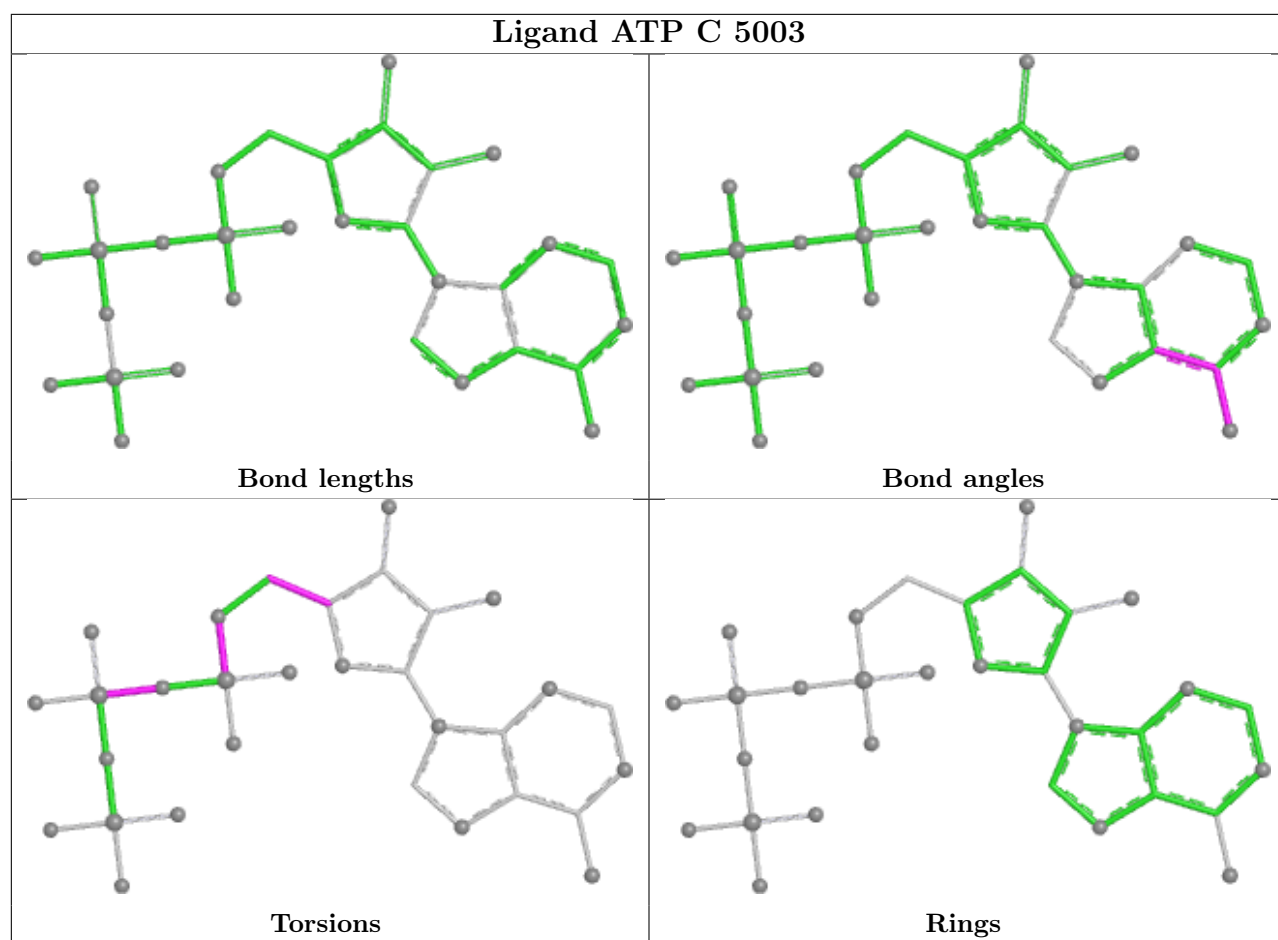
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

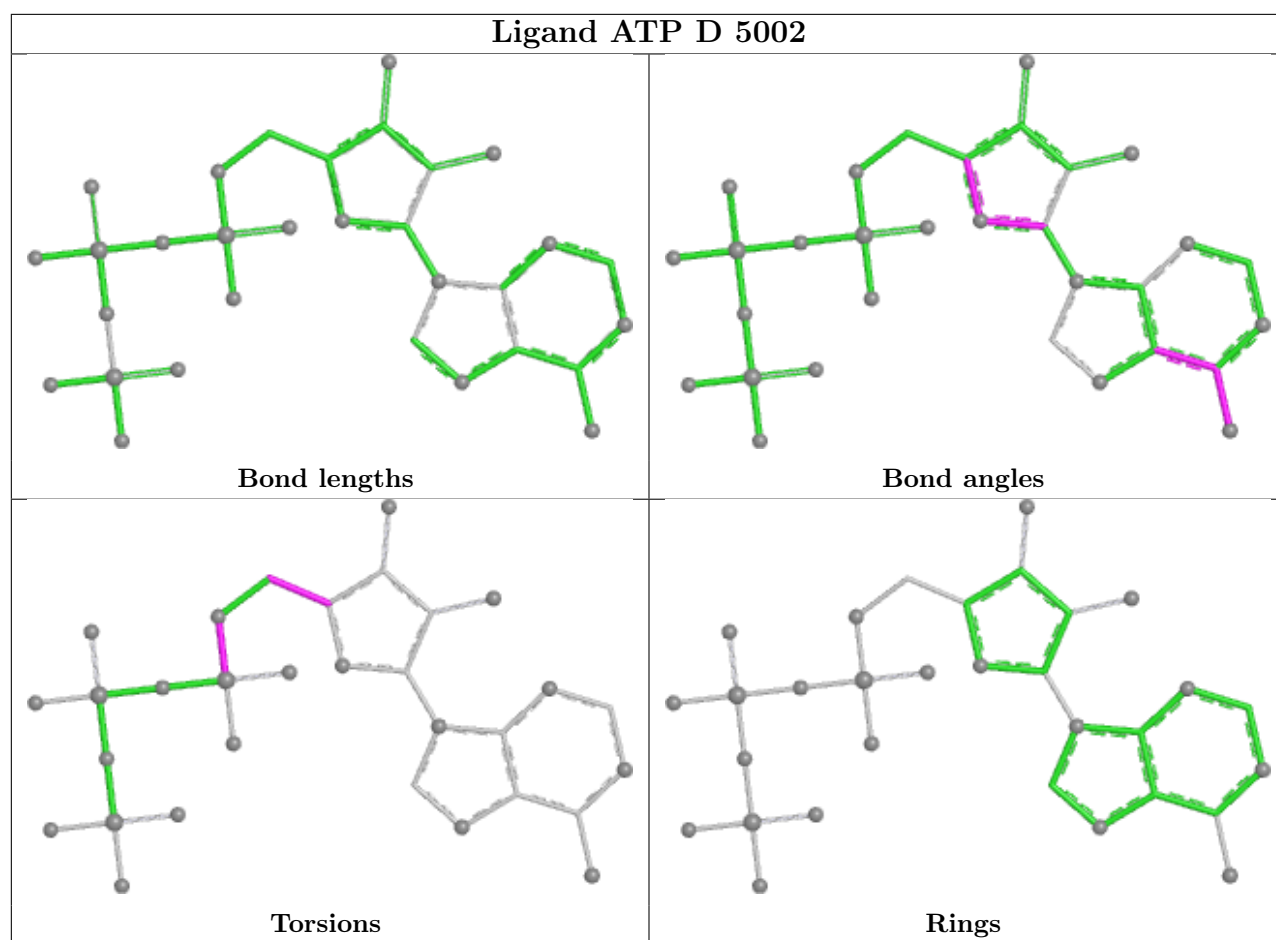


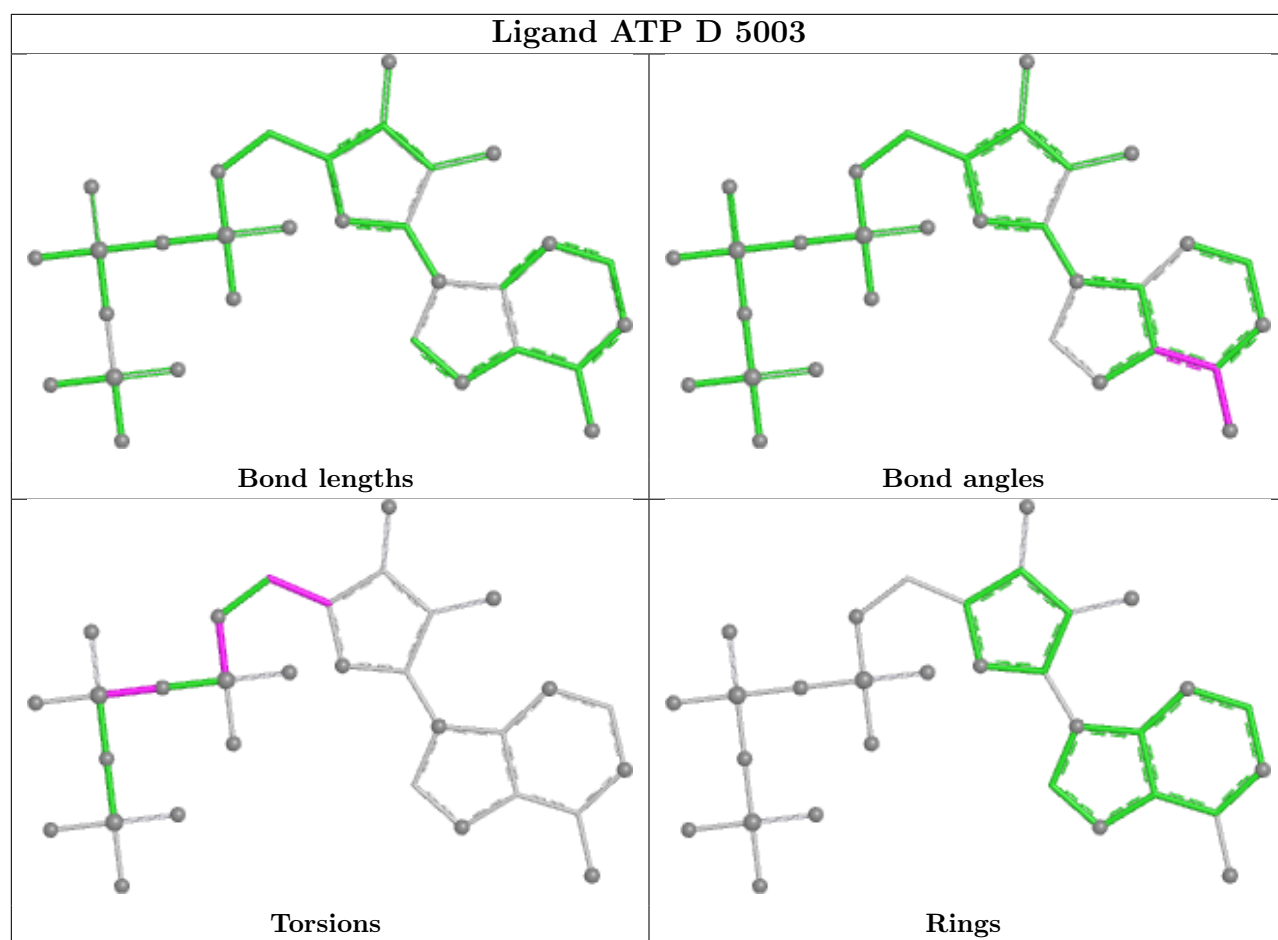


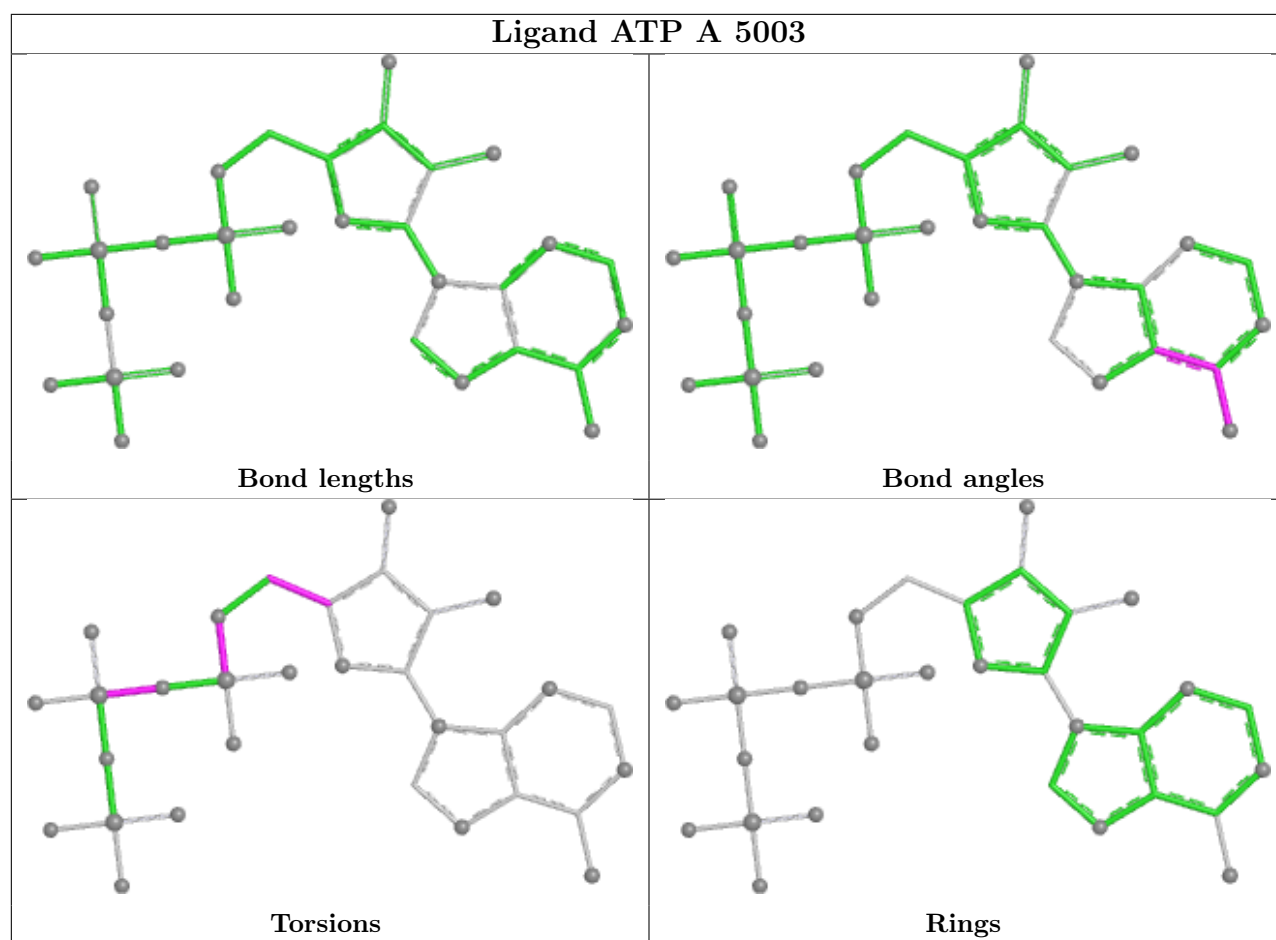


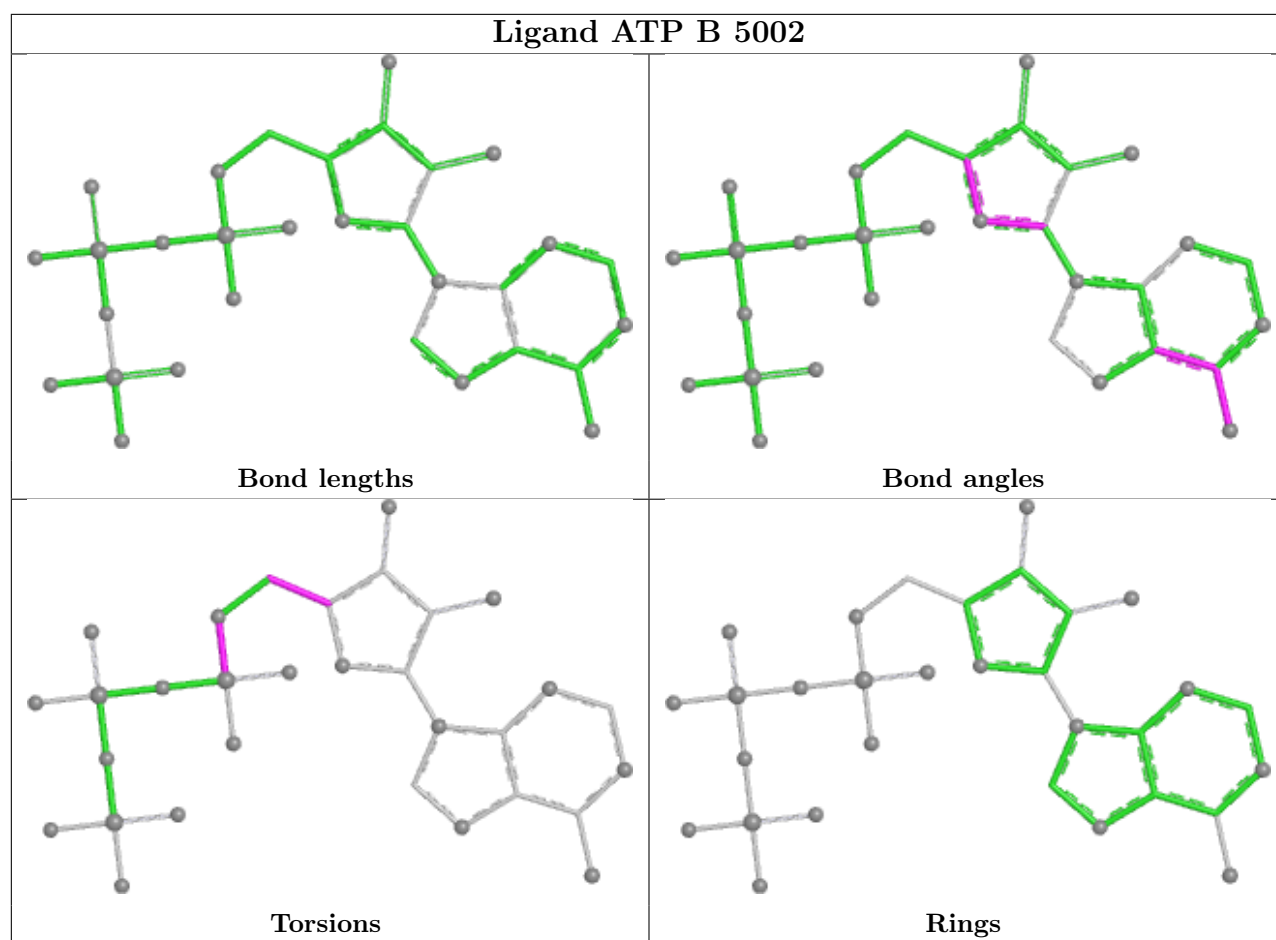












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

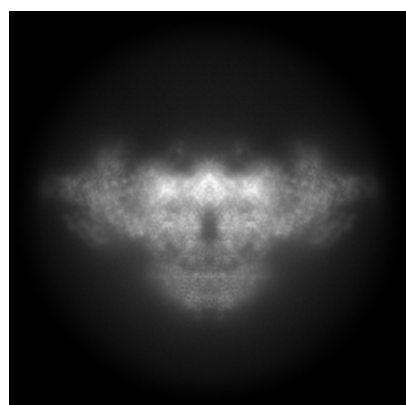
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42761. These allow visual inspection of the internal detail of the map and identification of artifacts.

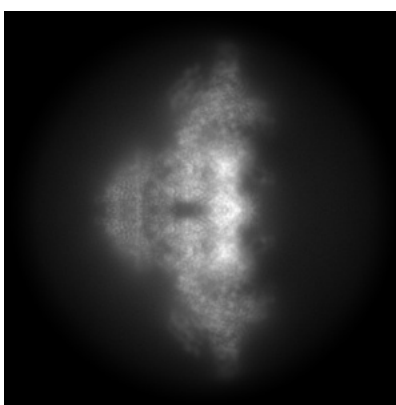
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

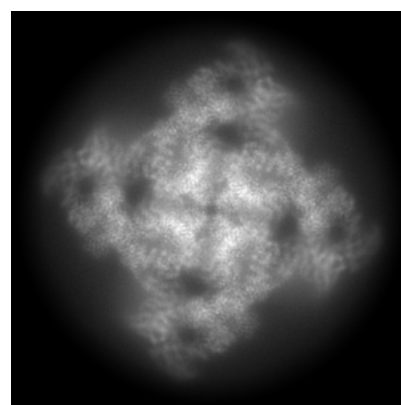
6.1.1 Primary map



X



Y

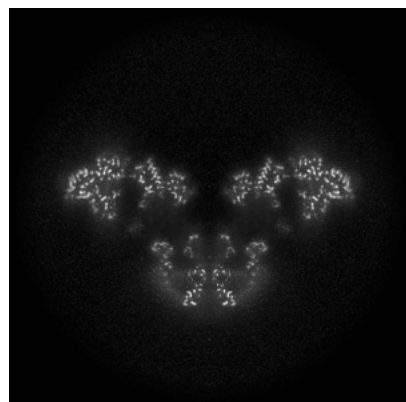


Z

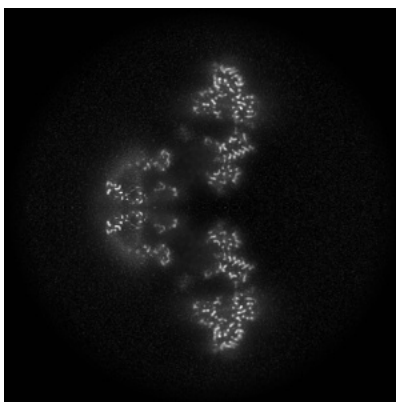
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

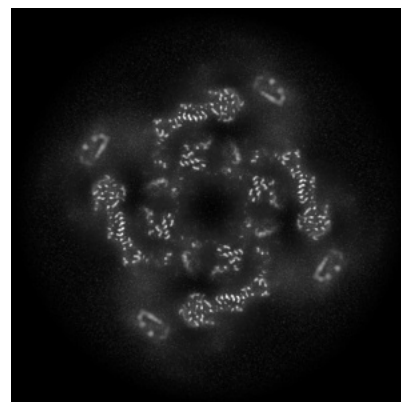
6.2.1 Primary map



X Index: 256



Y Index: 256

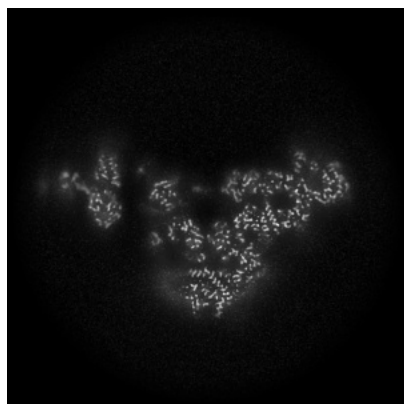


Z Index: 256

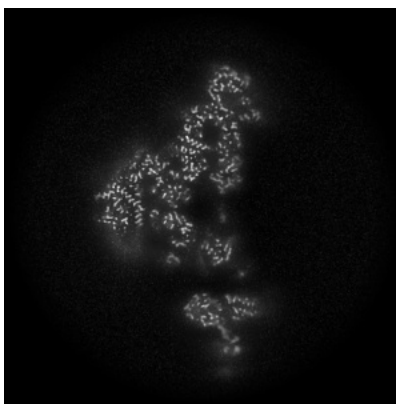
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

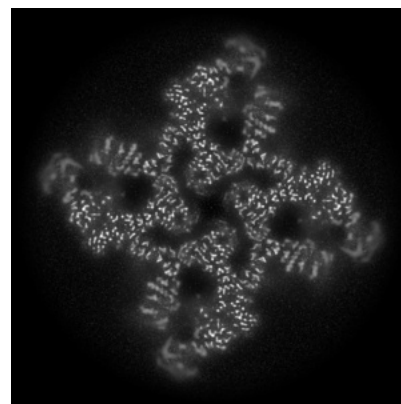
6.3.1 Primary map



X Index: 238



Y Index: 274

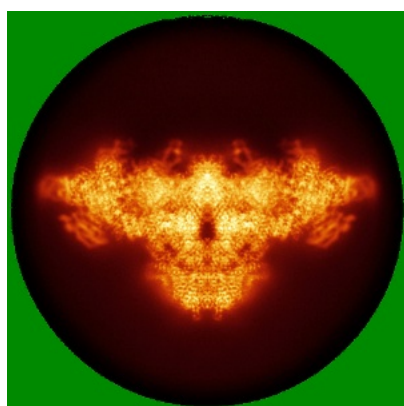


Z Index: 282

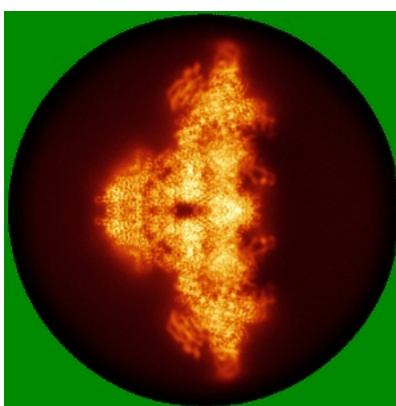
The images above show the largest variance slices of the map in three orthogonal directions.

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

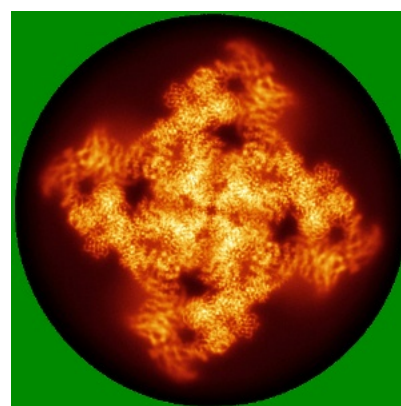
6.4.1 Primary map



X



Y

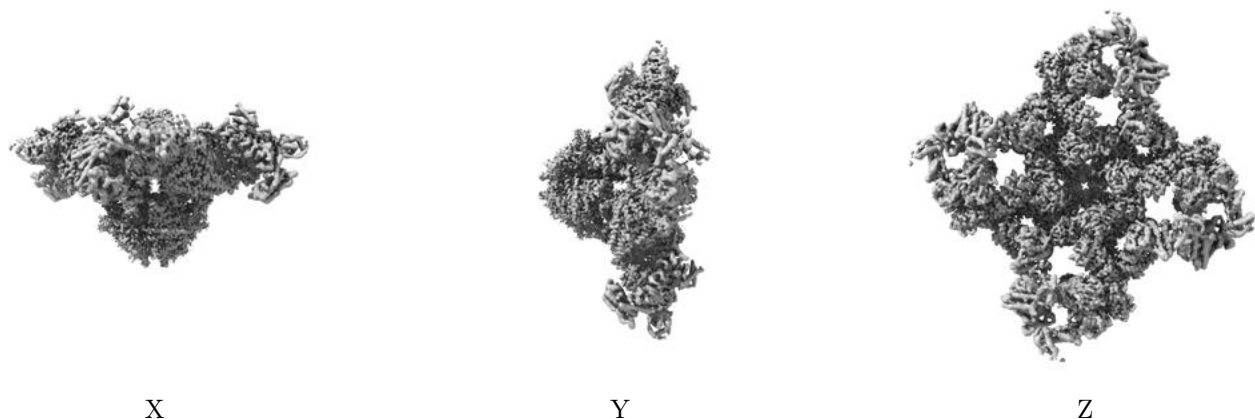


Z

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

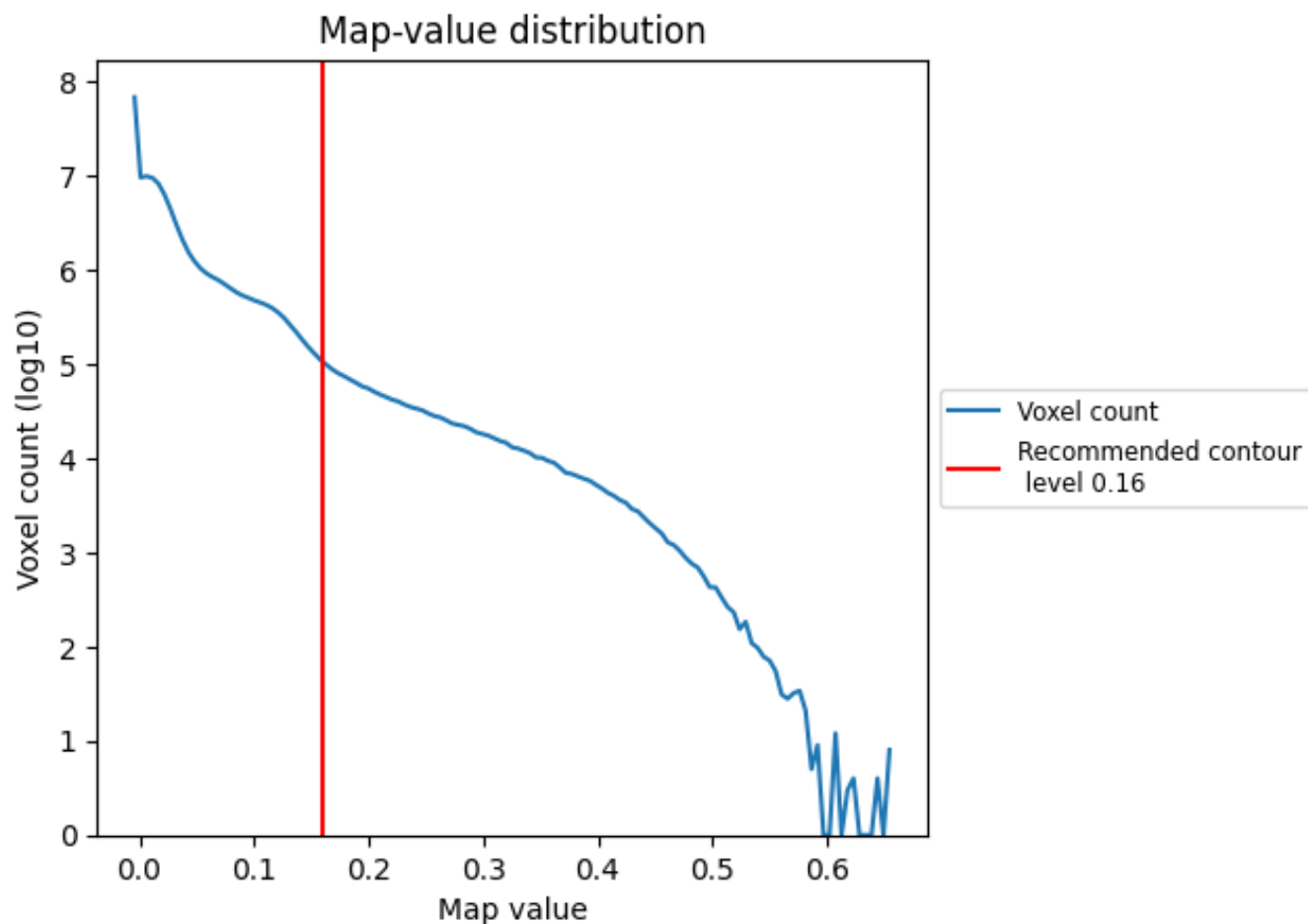
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

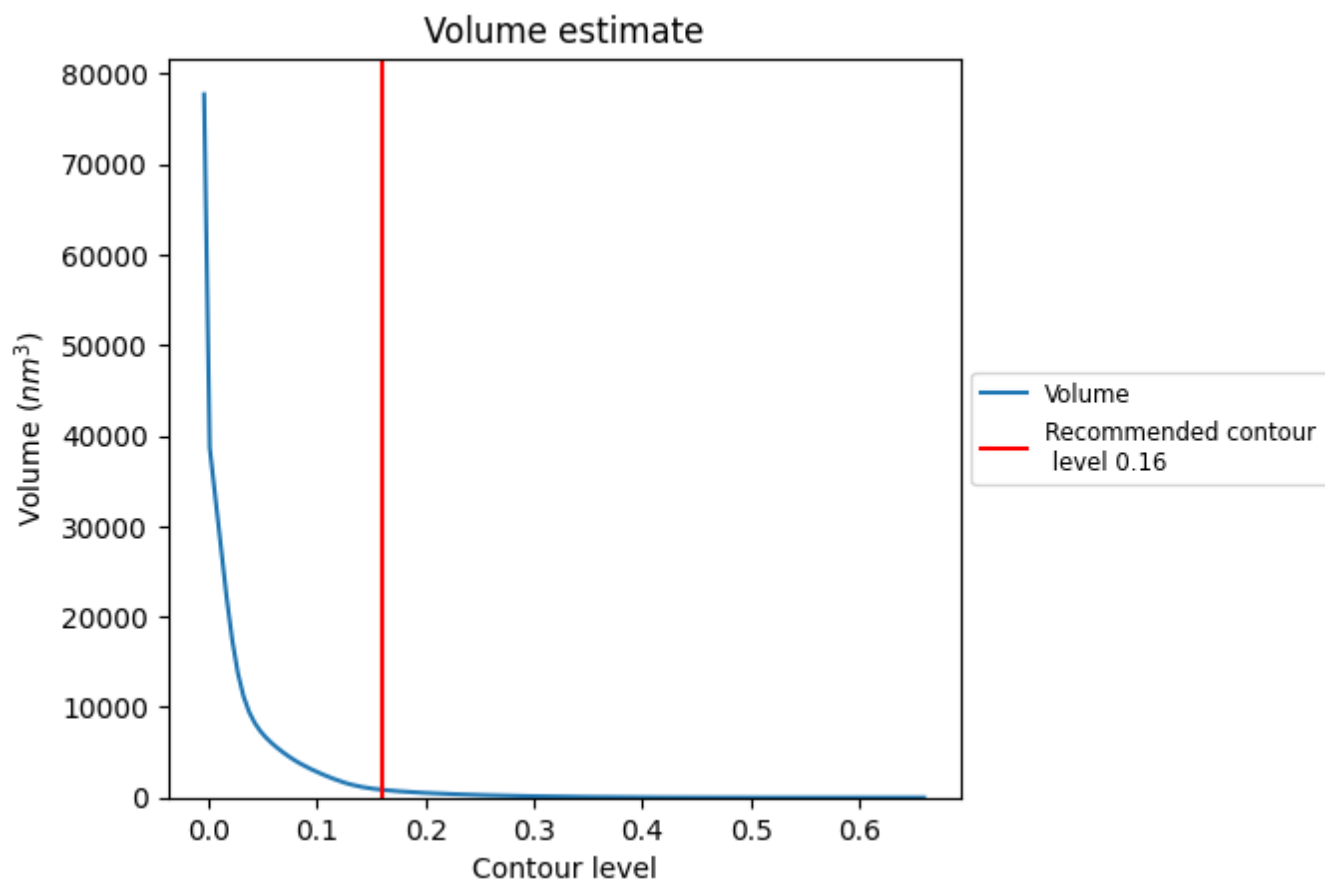
This section contains the results of statistical analysis of the map.

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.

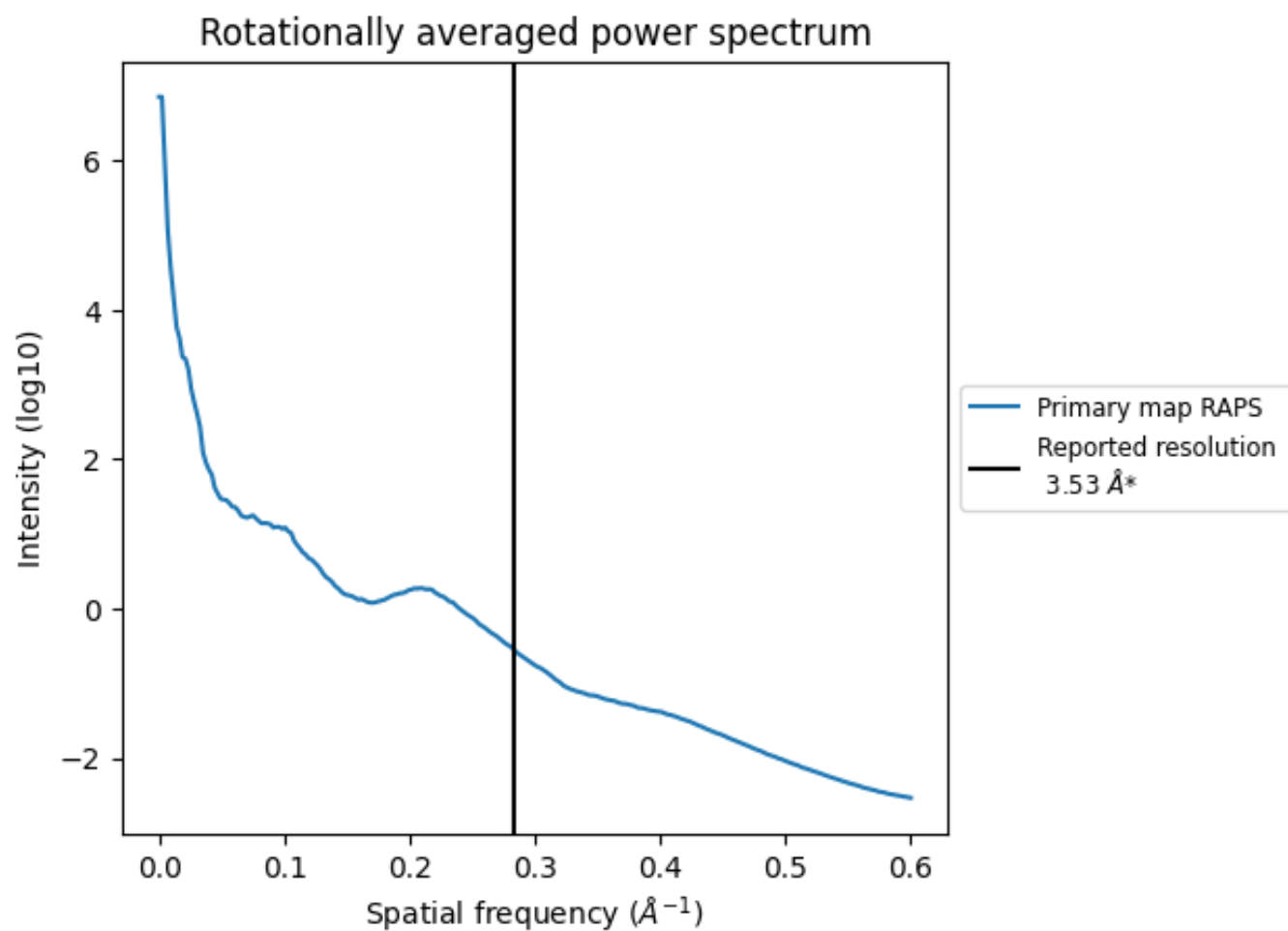
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 858 nm^3 ; this corresponds to an approximate mass of 775 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 0.283 Å⁻¹

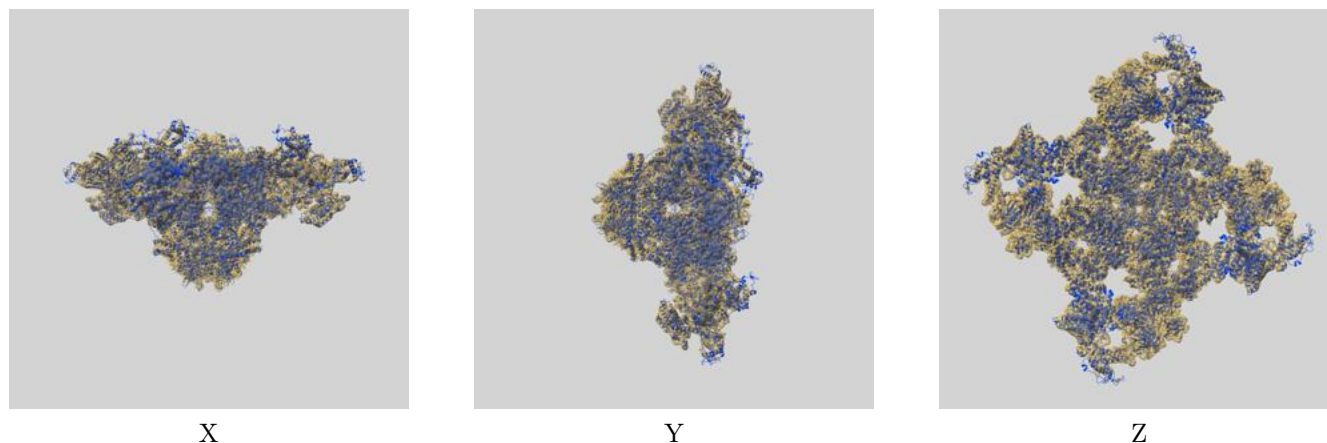
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

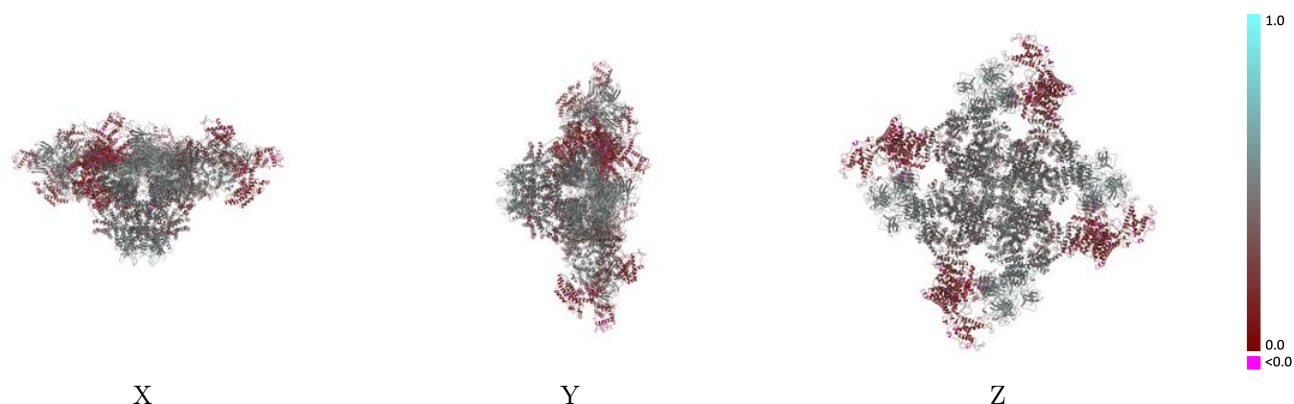
This section contains information regarding the fit between EMDB map EMD-42761 and PDB model 8UXE. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



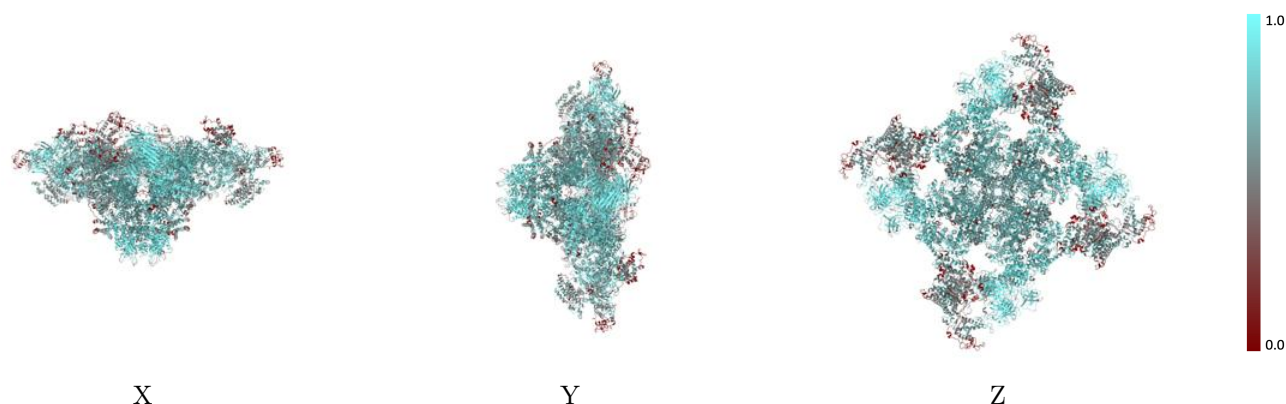
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



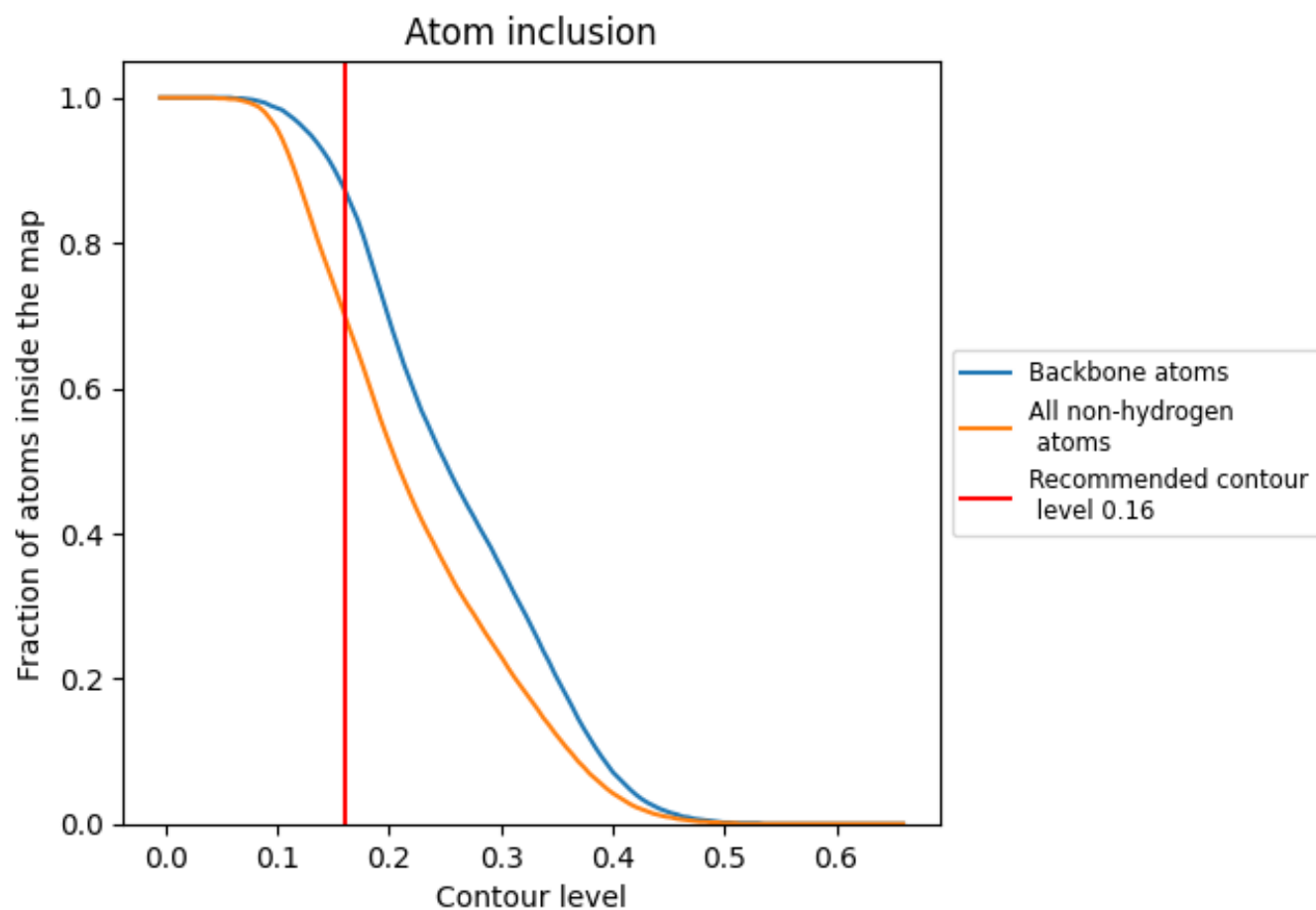
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7020	<div></div> 0.3910
A	<div></div> 0.6990	<div></div> 0.3870
B	<div></div> 0.7000	<div></div> 0.3900
C	<div></div> 0.7000	<div></div> 0.3900
D	<div></div> 0.7000	<div></div> 0.3900
E	<div></div> 0.8190	<div></div> 0.4810
F	<div></div> 0.8090	<div></div> 0.4800
G	<div></div> 0.8180	<div></div> 0.4790
H	<div></div> 0.8230	<div></div> 0.4800

1.0

0.0

<0.0