



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:16 AM UTC

PDB ID : 8UXH / pdb_00008uxh
EMDB ID : EMD-42764
Title : Structure of PKA phosphorylated human RyR2-R420W in the primed state
in the presence of calcium
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.52 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:

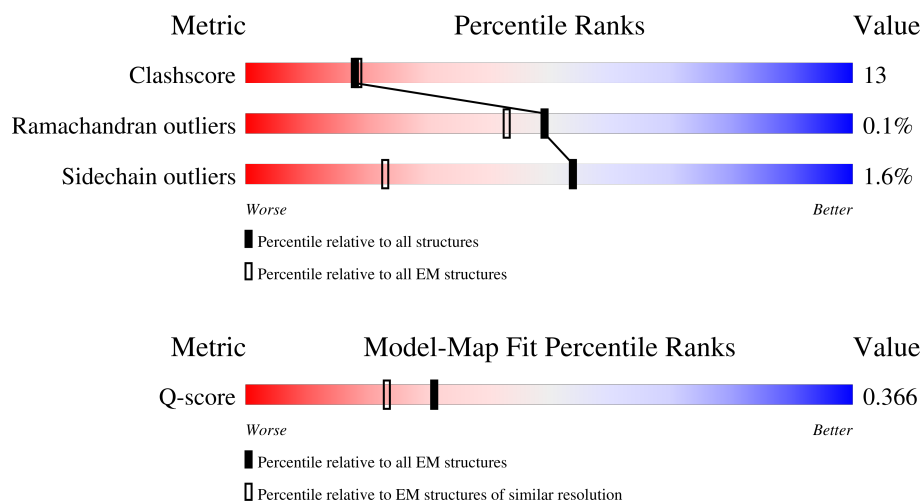
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 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	13017 (3.02 - 4.02)

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	10% 56% 23% • 19%
1	B	4967	10% 56% 24% • 19%
1	C	4967	10% 56% 24% • 19%
1	D	4967	11% 57% 23% • 19%

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Mol	Chain	Length	Quality of chain
2	E	108	 78%20%..
2	F	108	 80%19%..
2	G	108	 79%19%..
2	H	108	 79%19%..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 131656 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	4004	Total	C	N	O	S	2	0
			32032	20411	5451	5955	215		
1	B	4004	Total	C	N	O	S	2	0
			32032	20411	5451	5955	215		
1	C	4004	Total	C	N	O	S	2	0
			32032	20411	5451	5955	215		
1	D	4004	Total	C	N	O	S	2	0
			32032	20411	5451	5955	215		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

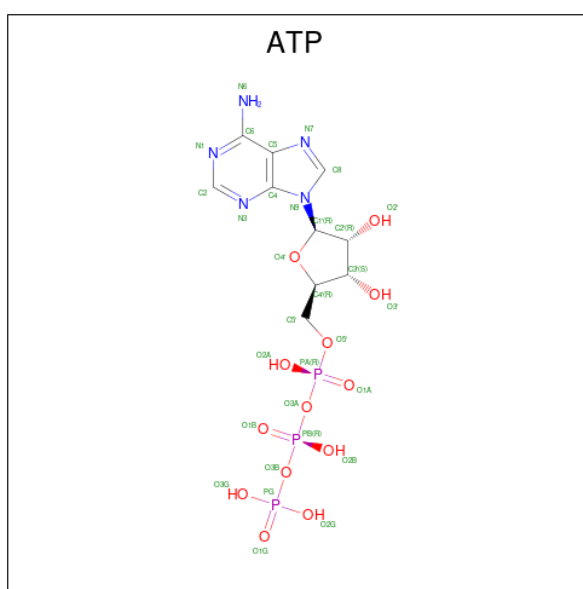
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 3 is ZINC ION (CCD ID: 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 (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
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
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

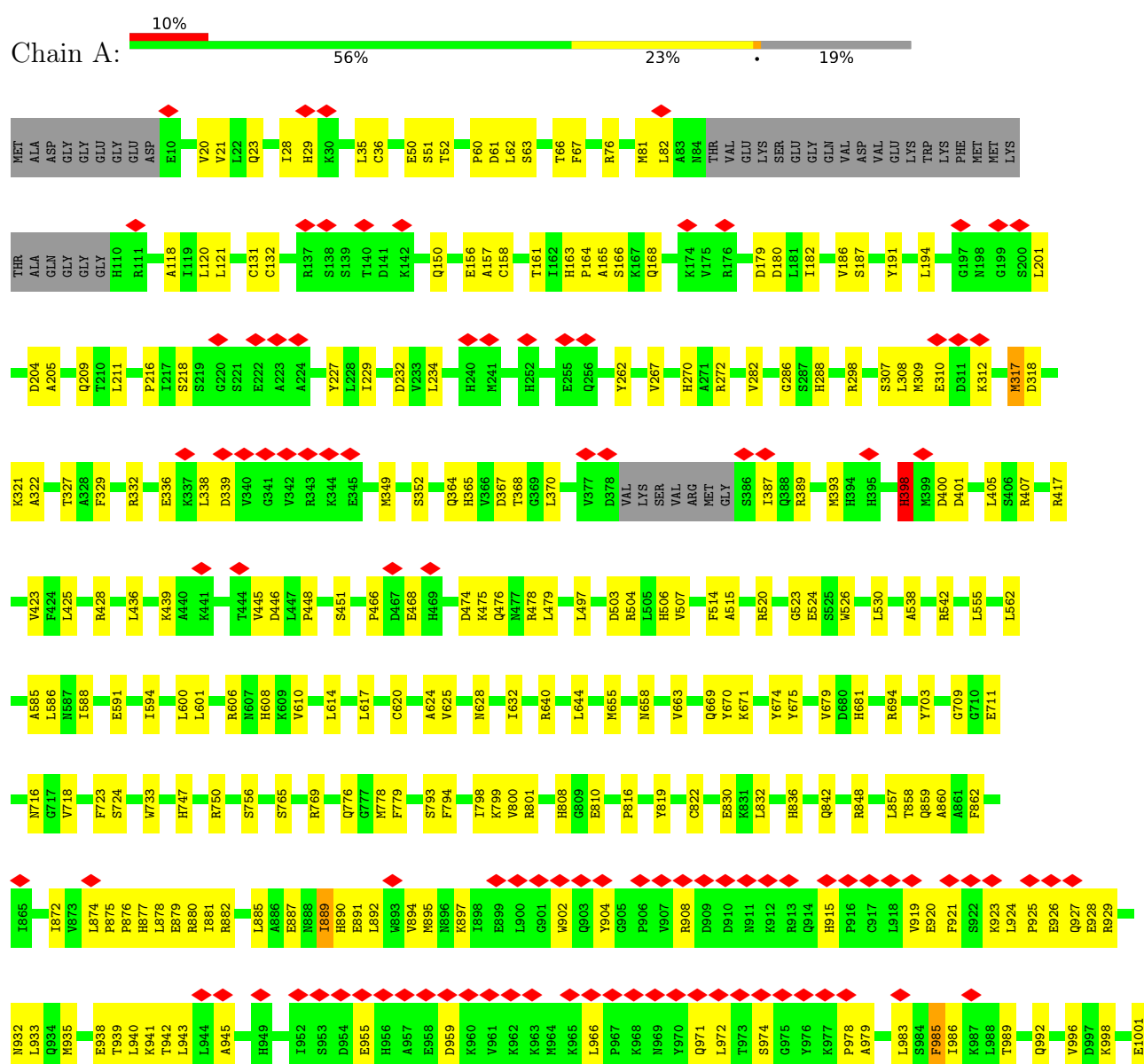
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

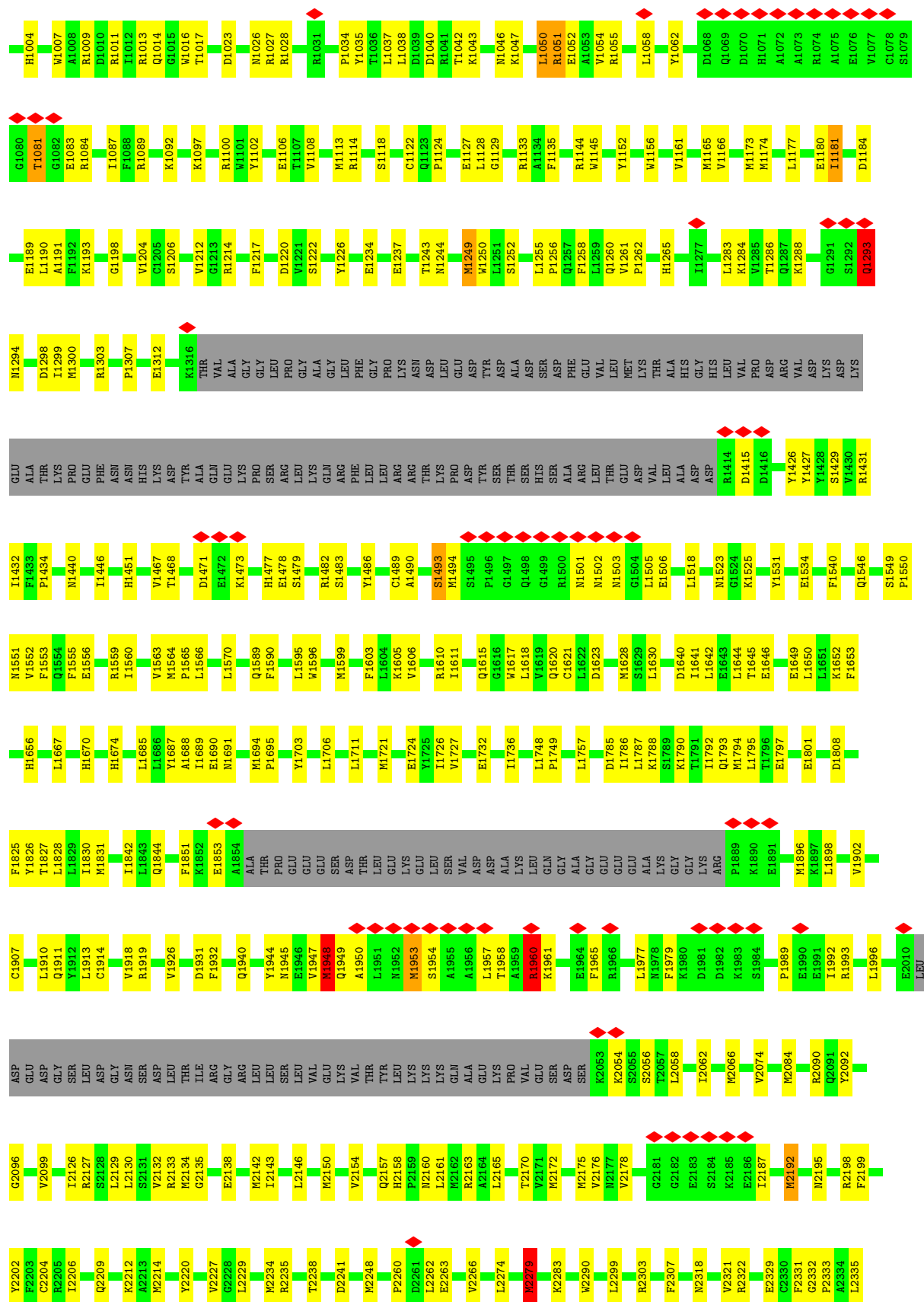
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

3 Residue-property plots

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

• Molecule 1: Ryanodine receptor 2



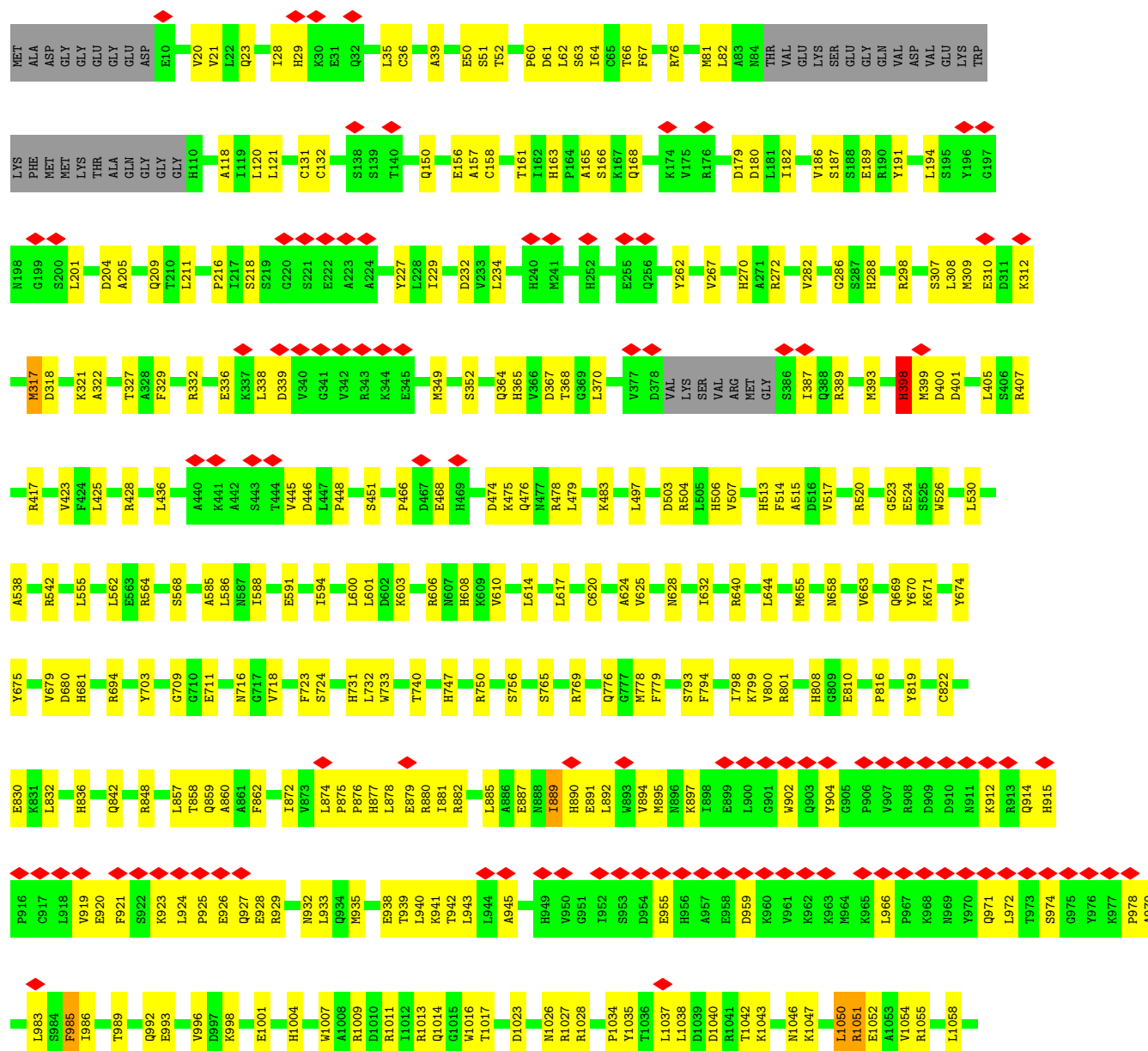








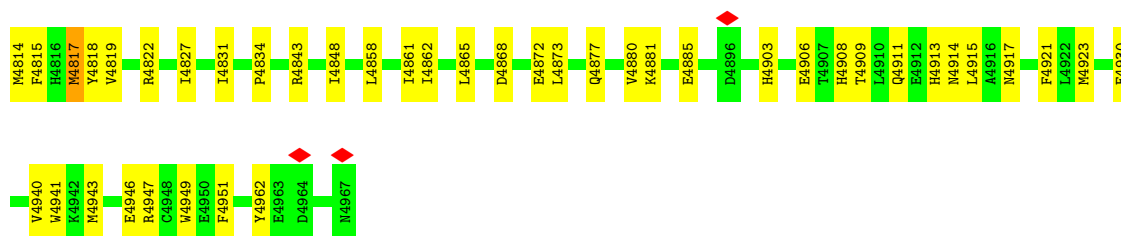
• Molecule 1: Ryanodine receptor 2



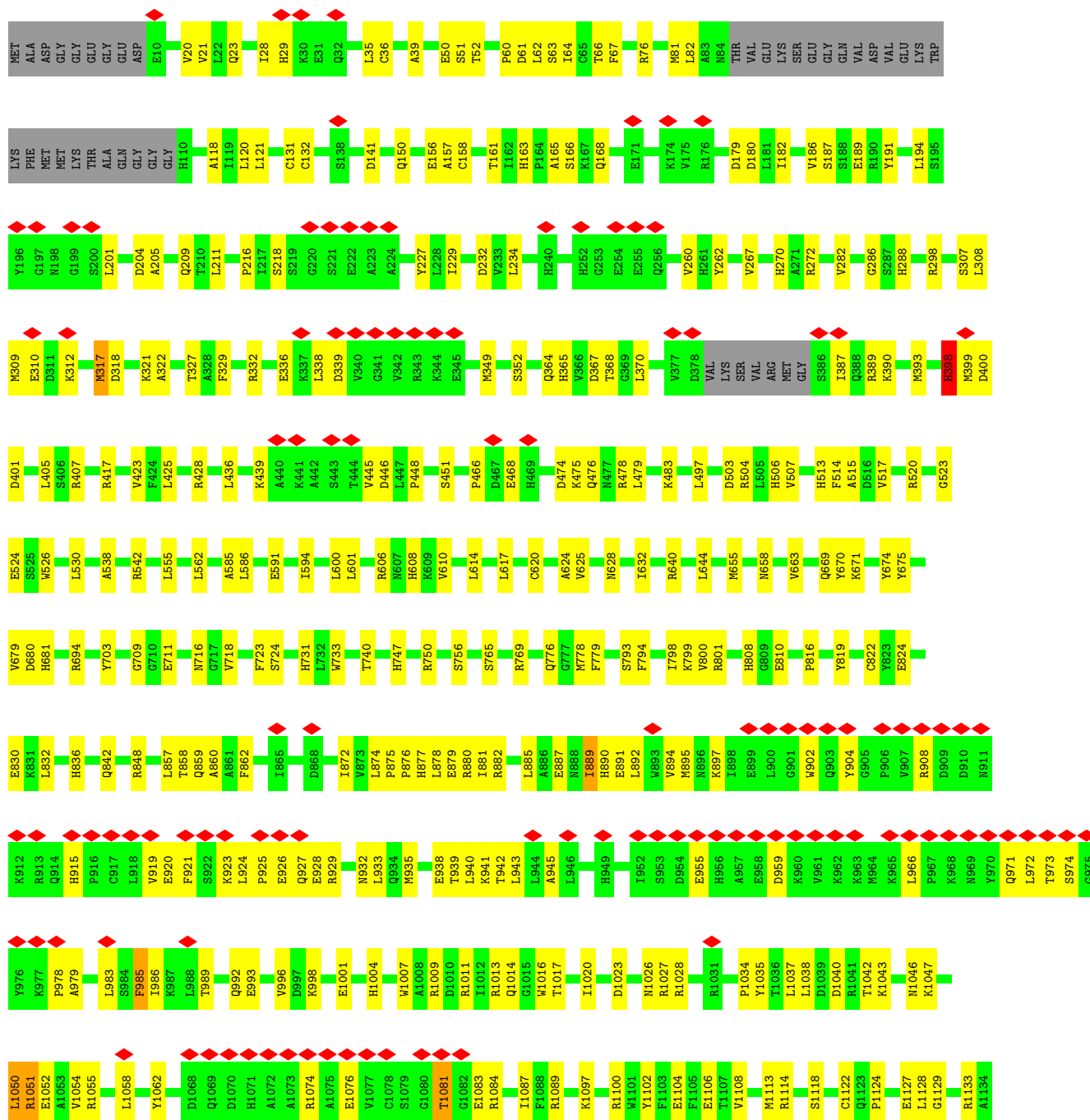


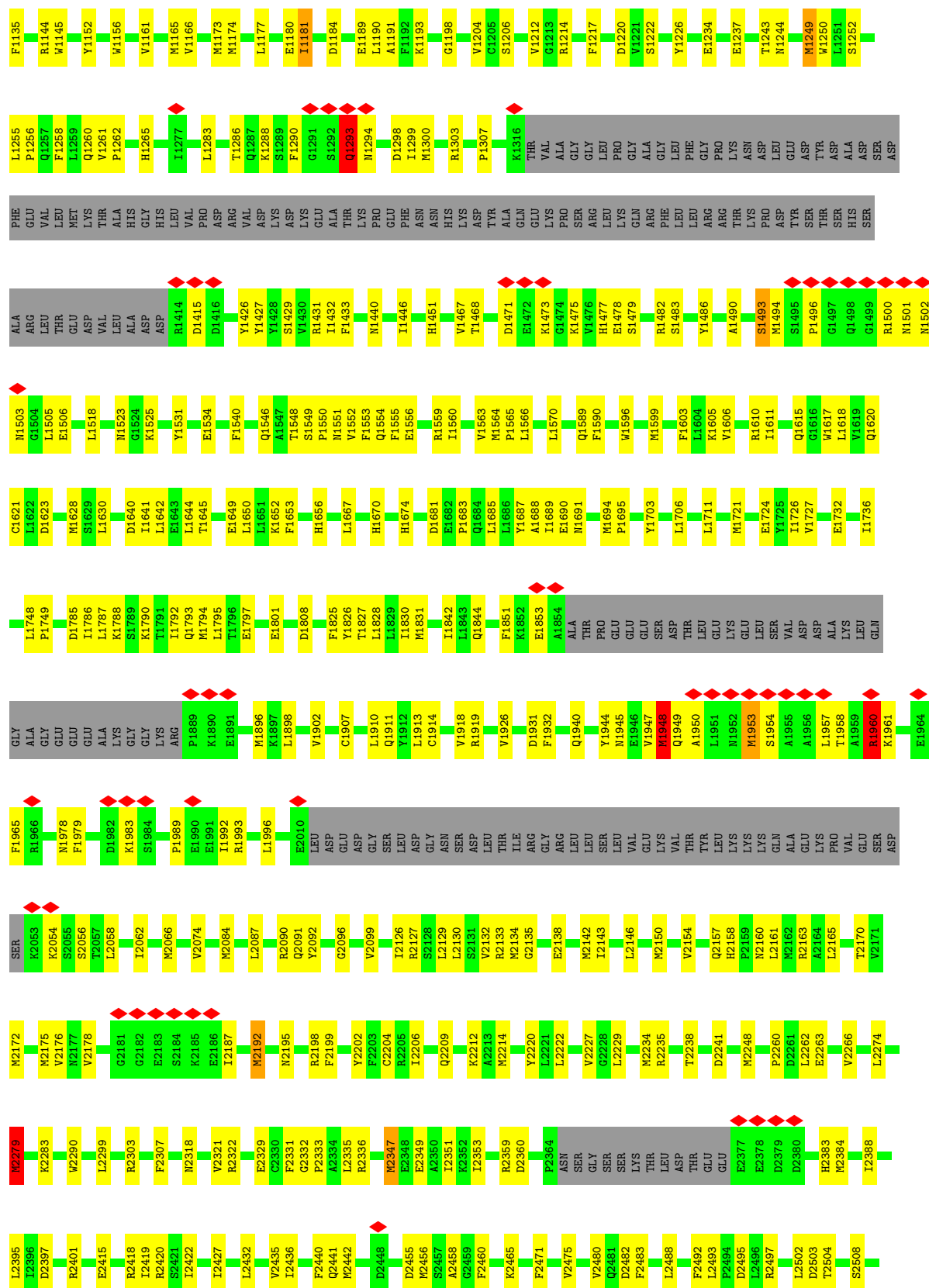
PRO	ILE	GLY	GLN	ASP	LEU	ILE	TRP	MET	LEU	HIS115	S3052	R2979	K2908	M2840	K2780	E2718	F2630	L2516
ILE	GLY	GLN	ASP	LEU	ASP	GLY	MET	VAL	ASP	Q3116	V3053	L2980	D2909	A2841	T2781	Y2719	E2635	C2521
ASN	PHE	ASN	PHE	LEU	HIS	K3054	LEU	ILE	ASN	F3117	Y2981	F2982	L2910	M2842	M2782	F2720	E2636	L2525
ALA	THR	ILE	VAL	PRO	ASN	L3057	LEU	ASP	ILE	GLY	A2985	A2986	L2912	M2844	L2783	I2721	P2526	P2526
VAL	THR	THR	VAL	MET	THR	R3058	LEU	THR	THR	ASP	S2987	A2988	D2913	A2852	V2785	Y2724	L2644	T2529
ALA	ALA	ILE	PHE	LEU	ILE	F3060	LEU	CYS	LEU	LEU	R2988	R2989	T2914	A2853	K2854	H2727	I2648	R2530
ASP	ASP	ASP	GLN	THR	THR	L3061	LEU	ASP	GLU	ASP	L2990	L2991	S2916	K2855	K2856	S2728	A2651	R2539
GLN	GLN	ASN	ILE	MET	THR	D3062	LEU	ASP	ASP	VAL	L2998	L2918	T2917	K2857	E2790	D2730	L2652	E2539
ASN	ALA	ASN	ASN	ARG	GLN	A3064	LEU	GLN	VAL	VAL	C2993	K2919	E2918	M2858	E2791	K2731	K2655	H2550
MET	ALA	LEU	LYS	ARG	VAL	A3065	VAL	VAL	VAL	THR	G2992	F2920	E2921	E2859	T2792	K2732	K2685	T2551
ILE	ALA	LEU	TRP	TRP	SER	E3066	SER	SER	CYS	THR	K2998	R2920	F2921	L2860	R2793	M2733	Q2659	Y2552
ALA	ALA	LEU	VAL	GLY	THR	D3067	GLY	THR	THR	THR	K2999	E2922	Y2923	E2861	E2794	S2734	Y2553	R2554
ASN	ASN	LEU	ALA	ALA	ARG	E3000	ALA	ILE	ILE	ILE	K3001	L2926	Q2927	S2862	D2796	K2736	L2666	K2557
THR	THR	THR	GLY	PRO	LEU	E3069	LEU	LEU	LEU	LEU	M3002	Q2928	Q2929	G2864	S2797	L2737	P2678	D2567
LYS	LYS	LYS	GLY	ASN	THR	K3070	LEU	THR	THR	THR	M3003	L2928	L2929	G2865	N2798	N2739	D2679	S2568
LYS	LYS	LYS	THR	ASN	SER	T3071	LEU	SER	SER	SER	M3004	Q2930	I2930	G2866	A2799	G2740	Y2680	E2570
ASN	ASN	THR	THR	THR	THR	M3072	THR	THR	THR	THR	M3005	L2930	I2930	N2867	L2801	W2741	V2571	C2572
ASN	ASN	THR	THR	THR	THR	E3073	ALA	ALA	ALA	ALA	L3007	V2933	V2933	H2868	M2802	I2742	L2573	I2576
THR	THR	THR	THR	THR	THR	N3074	VAL	VAL	VAL	VAL	F3008	L3007	H2937	P2869	ARG	Y2743	Y2685	L2580
ALA	ALA	ALA	ALA	ALA	ALA	L3075	GLY	GLY	GLY	GLY	C3009	L3010	H2937	L2870	THR	G2744	V2686	R2581
VAL	VAL	VAL	VAL	VAL	VAL	K3076	VAL	VAL	VAL	VAL	K3013	I2940	I2940	L2871	ARG	I2746	S2687	L2580
CYS	CYS	CYS	CYS	CYS	CYS	Q3077	VAL	VAL	VAL	VAL	V3013	I2940	I2940	L2871	THR	I2746	S2687	R2581
THR	THR	THR	THR	THR	THR	Q3078	VAL	VAL	VAL	VAL	H3016	F2943	F2943	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	H3017	VAL	VAL	VAL	VAL	R3016	D2944	D2944	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	Q3079	VAL	VAL	VAL	VAL	H3017	D2944	D2944	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	F3080	VAL	VAL	VAL	VAL	R3018	D2944	D2944	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	T3081	VAL	VAL	VAL	VAL	I3019	S2947	S2947	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	HIS	VAL	VAL	VAL	VAL	S3020	R2948	R2948	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	THR	VAL	VAL	VAL	VAL	L3021	G2949	G2949	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	ASN	VAL	VAL	VAL	VAL	F3022	G2950	G2950	L2871	THR	I2746	S2687	R2581
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ASN	ASN	ASN	ASN	ASN	ASN	PRO	VAL	VAL	VAL	VAL	I3029	H2953	H2953	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	K3088	VAL	VAL	VAL	VAL	H3034	V2956	V2956	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	G3089	VAL	VAL	VAL	VAL	H3034	V2956	V2956	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	V3090	VAL	VAL	VAL	VAL	I3035	E2957	E2957	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	L3036	VAL	VAL	VAL	VAL	L3036	Q2958	Q2958	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	G3037	VAL	VAL	VAL	VAL	G3037	E2959	E2959	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	Q3038	VAL	VAL	VAL	VAL	Q3038	I2960	I2960	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	T3039	VAL	VAL	VAL	VAL	T3039	F2962	F2962	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	L3040	VAL	VAL	VAL	VAL	L3040	F2962	F2962	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	D3041	VAL	VAL	VAL	VAL	D3041	A2964	A2964	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	R3042	VAL	VAL	VAL	VAL	R3042	K2965	K2965	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	R3043	VAL	VAL	VAL	VAL	R3043	V2966	V2966	L2871	THR	I2746	S2687	R2581
ASN	ASN	ASN	ASN	ASN	ASN	T3044	VAL	VAL	VAL	VAL	T3044	V2967	V2967	L2871	THR	I2746	S2687	R2581
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ASN	ASN	ASN	ASN	ASN	ASN	I3112	VAL	VAL	VAL	VAL	I3112	K2976	K2976	L2871	THR	I2746	S2687	R2581
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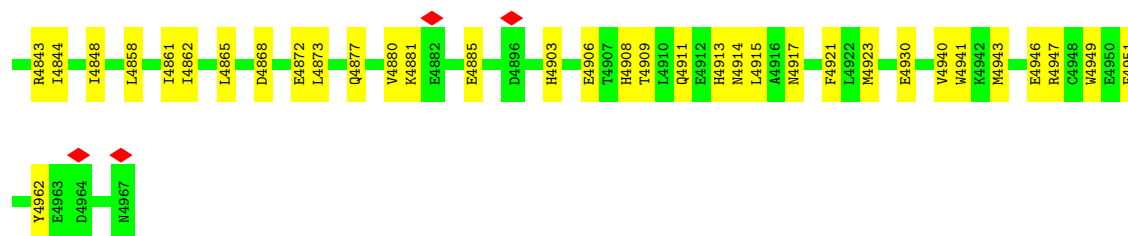
• Molecule 1: Ryanodine receptor 2



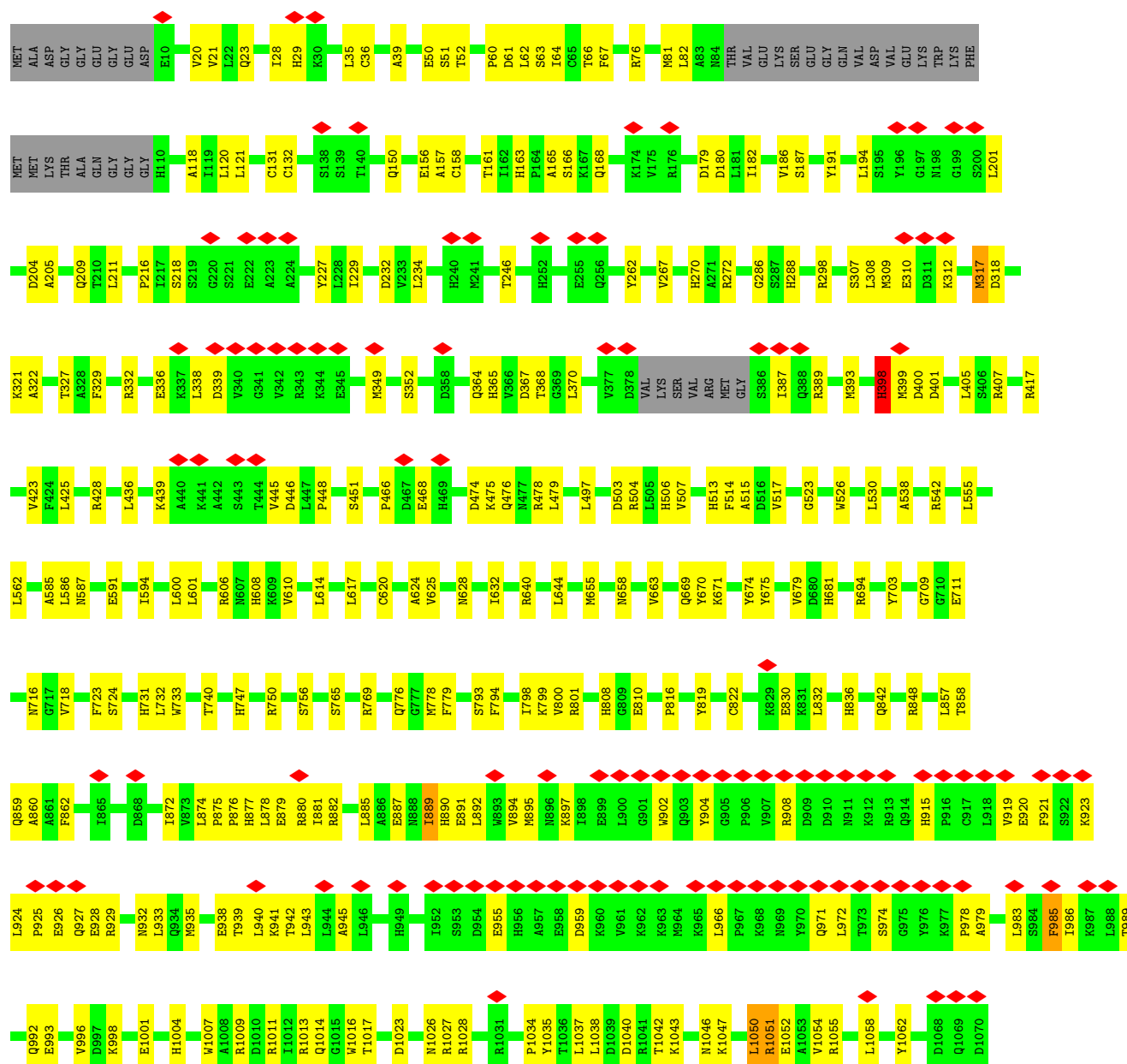


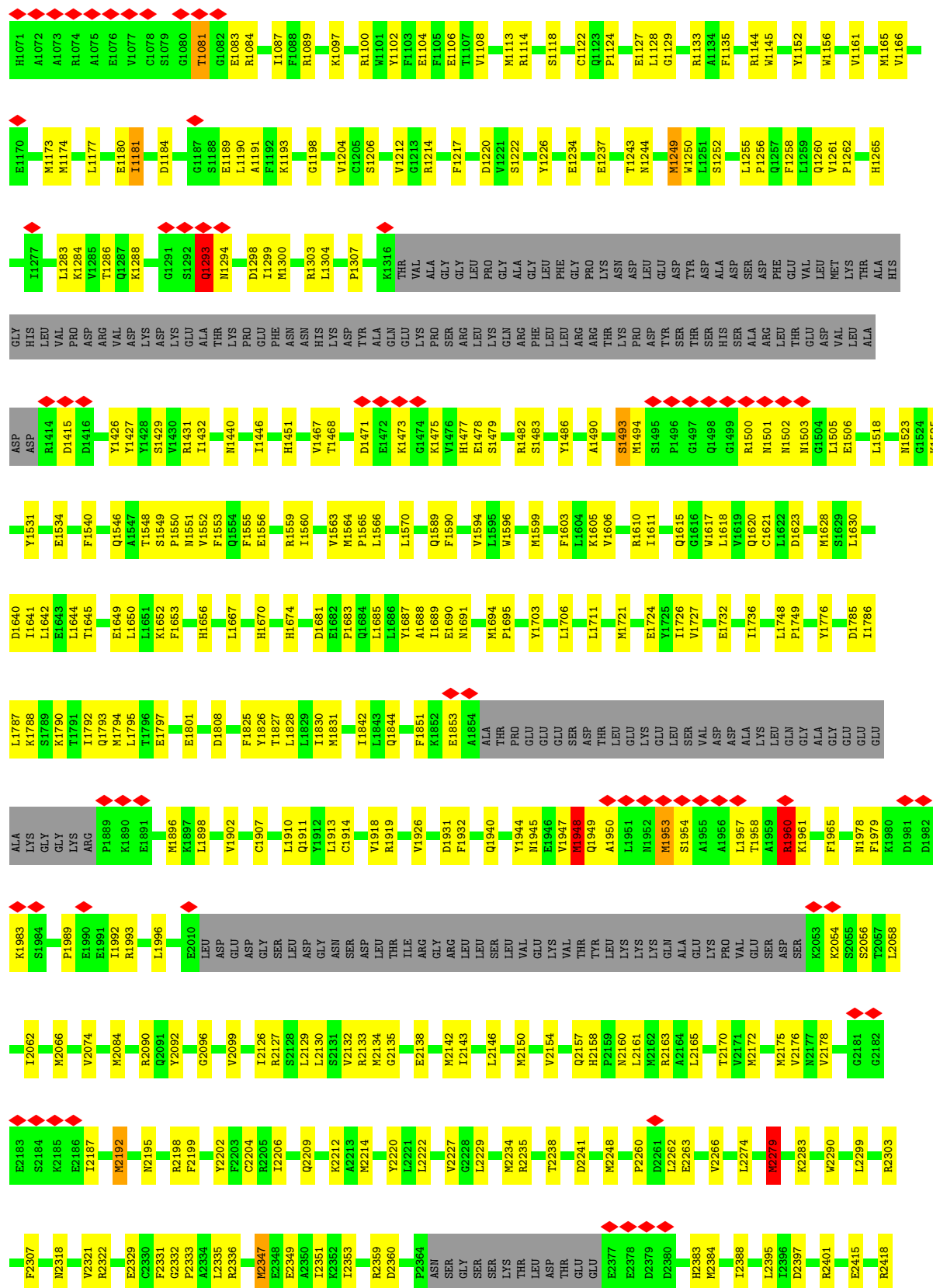






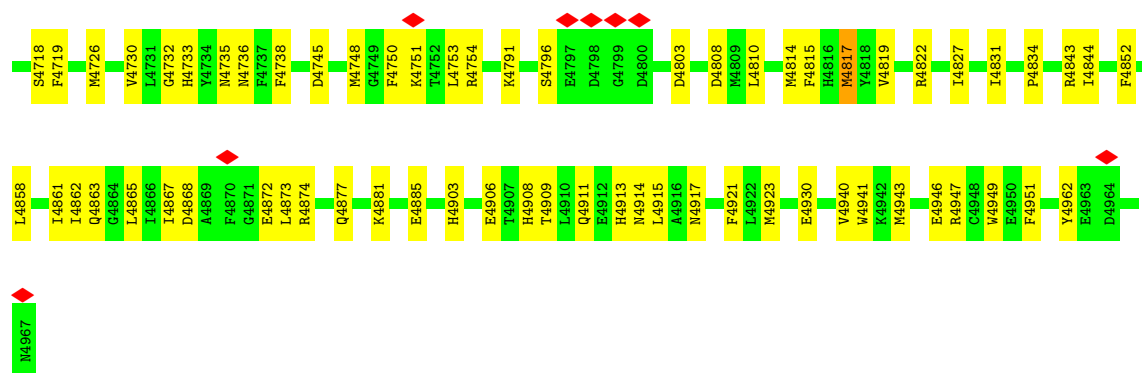
• Molecule 1: Ryanodine receptor 2





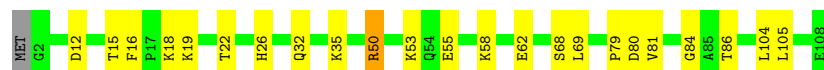
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- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 78% 20% ..



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 80% 19% ..



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 79% 19% ..



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 79% 19% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55886	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	0.564	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	0/32738	0.49	18/44213 (0.0%)
1	B	0.18	0/32738	0.49	18/44213 (0.0%)
1	C	0.18	0/32738	0.49	18/44213 (0.0%)
1	D	0.18	0/32738	0.49	18/44213 (0.0%)
2	E	0.14	0/834	0.39	0/1123
2	F	0.14	0/834	0.39	0/1123
2	G	0.14	0/834	0.40	0/1123
2	H	0.14	0/834	0.39	0/1123
All	All	0.18	0/134288	0.49	72/181344 (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 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2279	MET	CB-CG-SD	10.64	144.62	112.70
1	C	2279	MET	CB-CG-SD	10.64	144.61	112.70
1	B	2279	MET	CB-CG-SD	10.63	144.60	112.70
1	D	2279	MET	CB-CG-SD	10.63	144.58	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2788	ARG	CB-CG-CD	8.98	131.96	111.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2530	ARG	Sidechain
1	A	2788	ARG	Sidechain
1	A	398	HIS	Peptide
1	B	2530	ARG	Sidechain
1	B	398	HIS	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	A	32032	0	31689	881	0
1	B	32032	0	31689	883	0
1	C	32032	0	31689	868	0
1	D	32032	0	31689	866	0
2	E	818	0	821	14	0
2	F	818	0	821	12	0
2	G	818	0	821	13	0
2	H	818	0	821	13	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	0	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	131656	0	130136	3472	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 3472 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4814:MET:HE1	1:D:4844:ILE:HD13	1.35	1.03
1:D:2857:LYS:HE3	1:D:2871:LEU:HD23	1.52	0.92
1:A:2857:LYS:HE3	1:A:2871:LEU:HD23	1.52	0.92
1:C:2857:LYS:HE3	1:C:2871:LEU:HD23	1.52	0.91
1:B:2857:LYS:HE3	1:B:2871:LEU:HD23	1.52	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3978/4967 (80%)	3861 (97%)	113 (3%)	4 (0%)	48	79
1	B	3978/4967 (80%)	3862 (97%)	112 (3%)	4 (0%)	48	79
1	C	3978/4967 (80%)	3861 (97%)	113 (3%)	4 (0%)	48	79
1	D	3978/4967 (80%)	3862 (97%)	112 (3%)	4 (0%)	48	79
2	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	16332/20300 (80%)	15850 (97%)	466 (3%)	16 (0%)	49	79

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2988	ARG

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Mol	Chain	Res	Type
1	A	3927	PRO
1	A	4641	PRO
1	B	2988	ARG
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	3513/4358 (81%)	3459 (98%)	54 (2%)	57	71
1	B	3513/4358 (81%)	3459 (98%)	54 (2%)	57	71
1	C	3513/4358 (81%)	3459 (98%)	54 (2%)	57	71
1	D	3513/4358 (81%)	3459 (98%)	54 (2%)	57	71
2	E	88/89 (99%)	85 (97%)	3 (3%)	32	58
2	F	88/89 (99%)	85 (97%)	3 (3%)	32	58
2	G	88/89 (99%)	85 (97%)	3 (3%)	32	58
2	H	88/89 (99%)	85 (97%)	3 (3%)	32	58
All	All	14404/17788 (81%)	14176 (98%)	228 (2%)	54	70

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4504	MET
1	D	4208	GLU
1	C	2530	ARG
1	D	4046	ARG
1	D	2652	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 230 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	288	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4075	ASN
1	C	2722	ASN
1	D	4009	ASN
1	D	2158	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, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.28	0
4	ATP	D	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	A	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	B	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	A	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	D	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	C	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	C	5004	-	32,33,33	0.26	0	48,52,52	0.27	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
4	ATP	B	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5004	-	-	9/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	B	5004	-	-	9/22/38/38	0/3/3/3
4	ATP	A	5004	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	C	5004	-	-	9/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

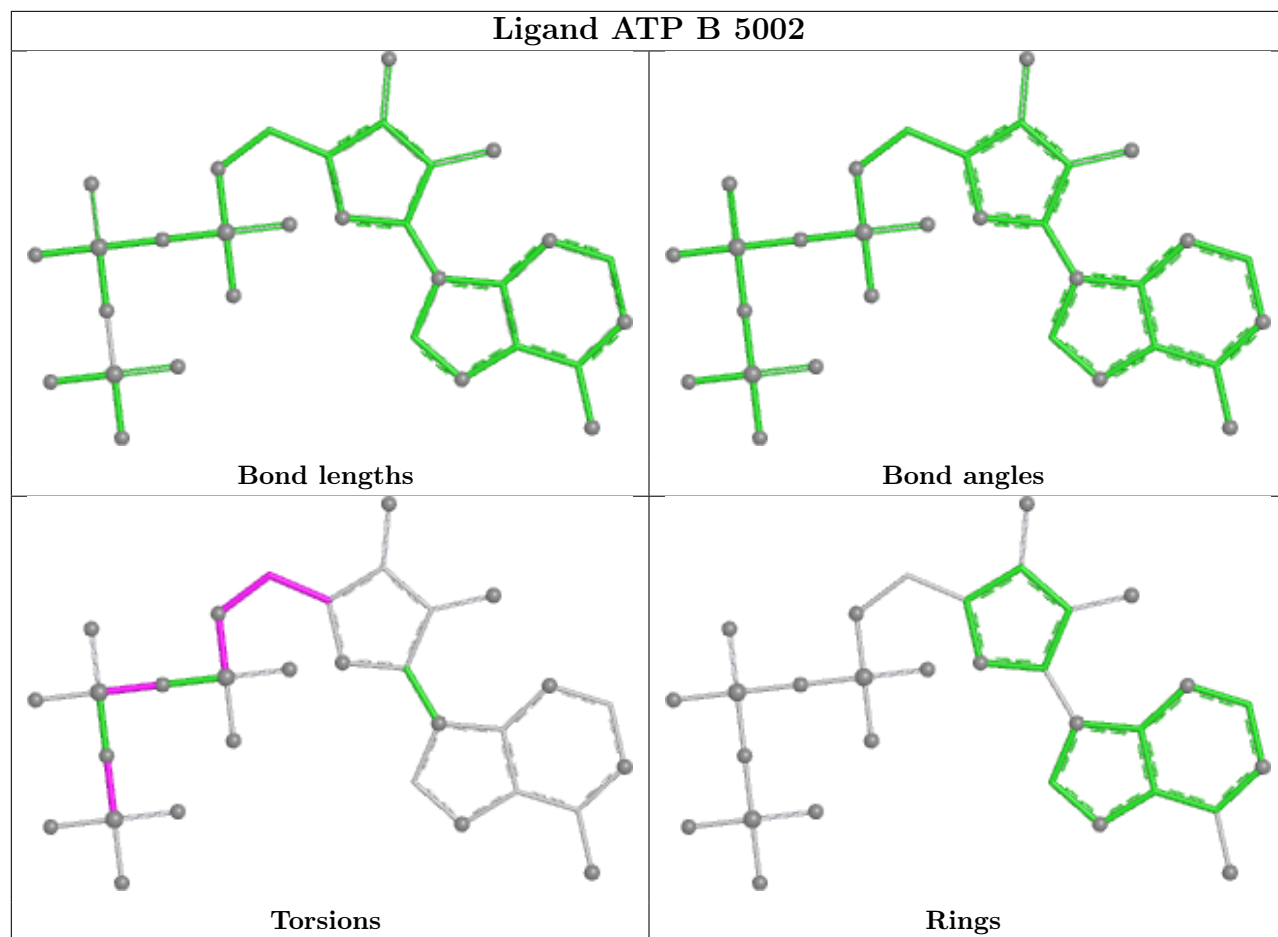
5 of 72 torsion outliers are listed below:

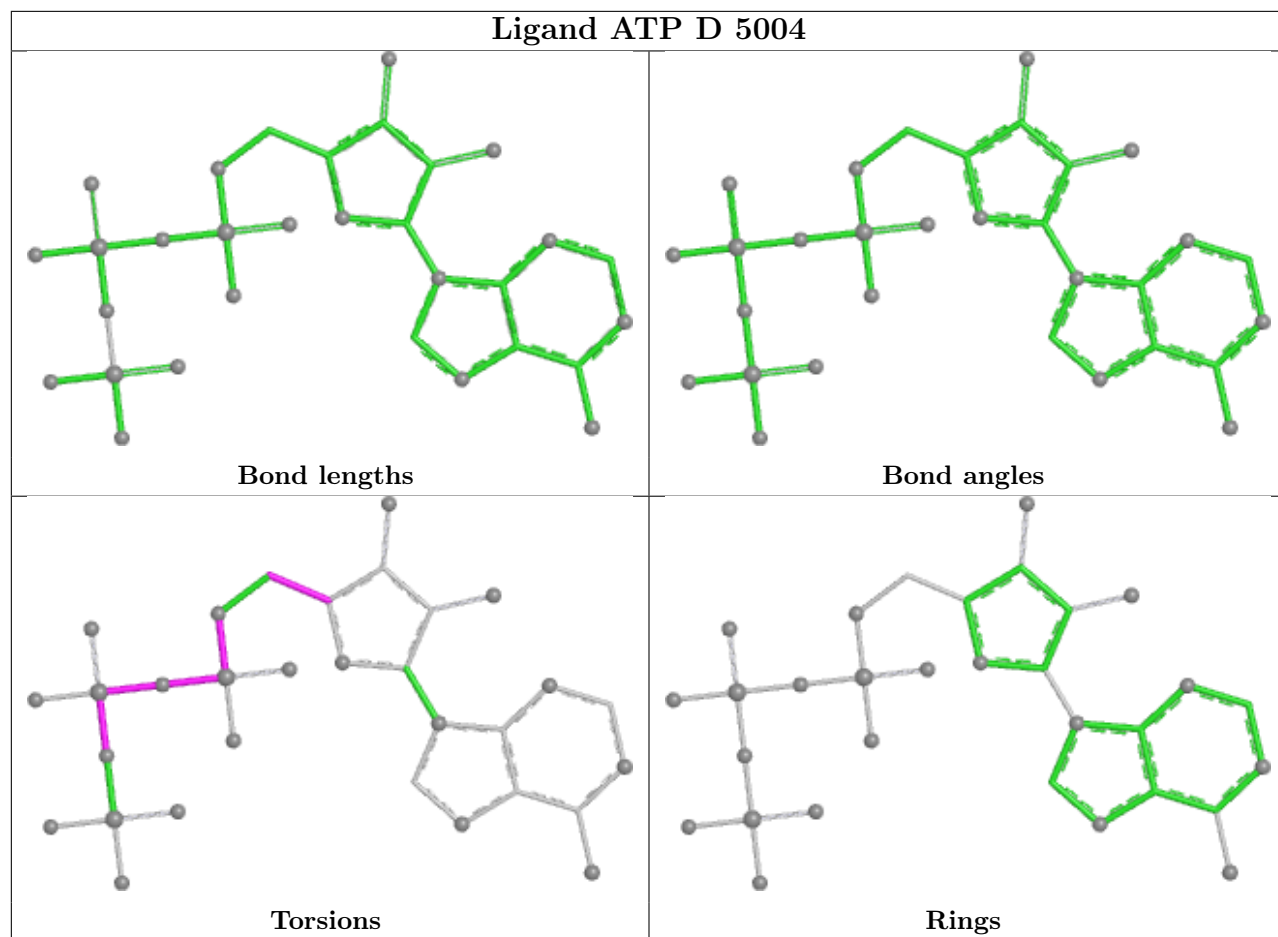
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5004	ATP	C5'-O5'-PA-O2A

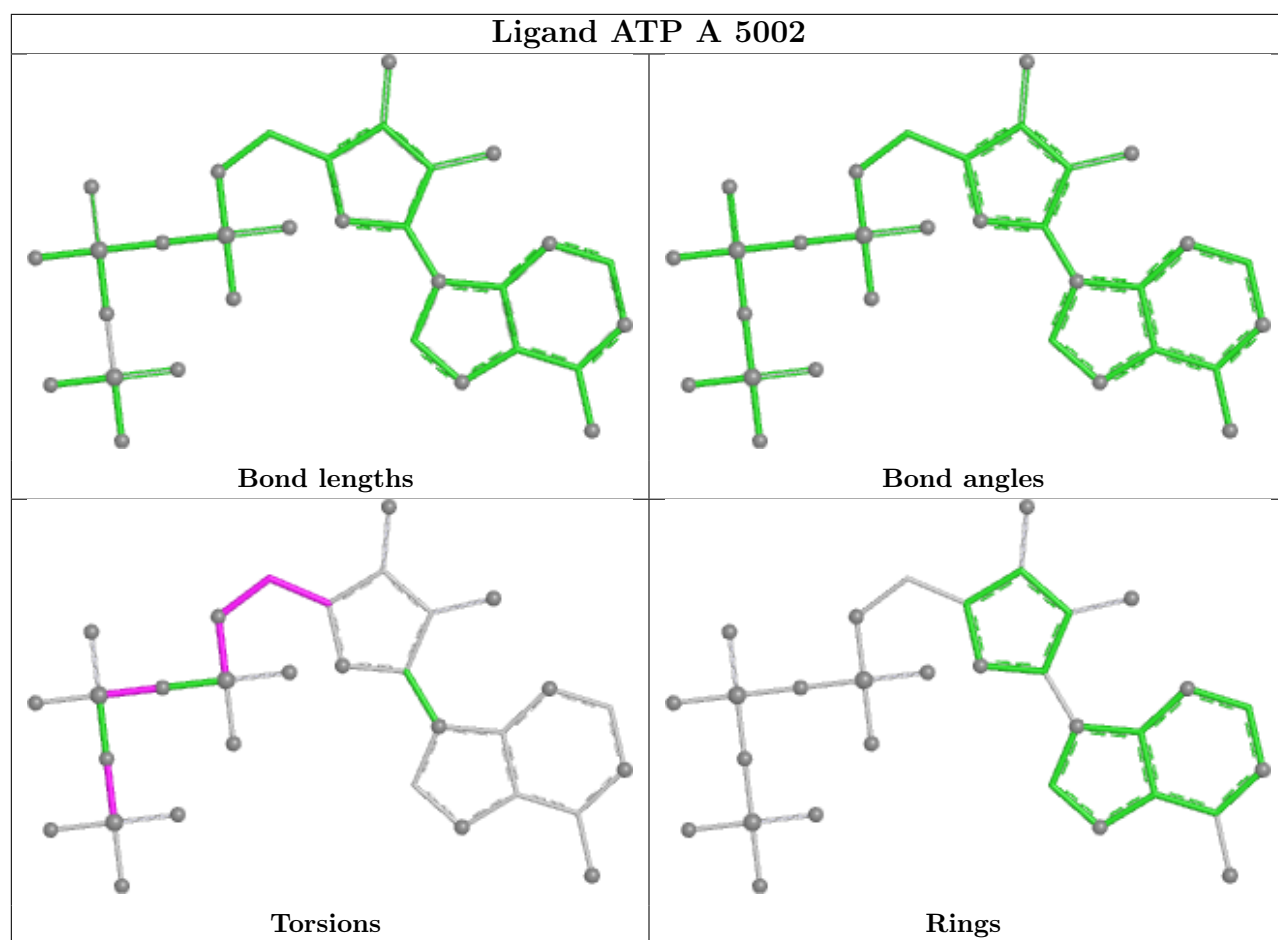
There are no ring outliers.

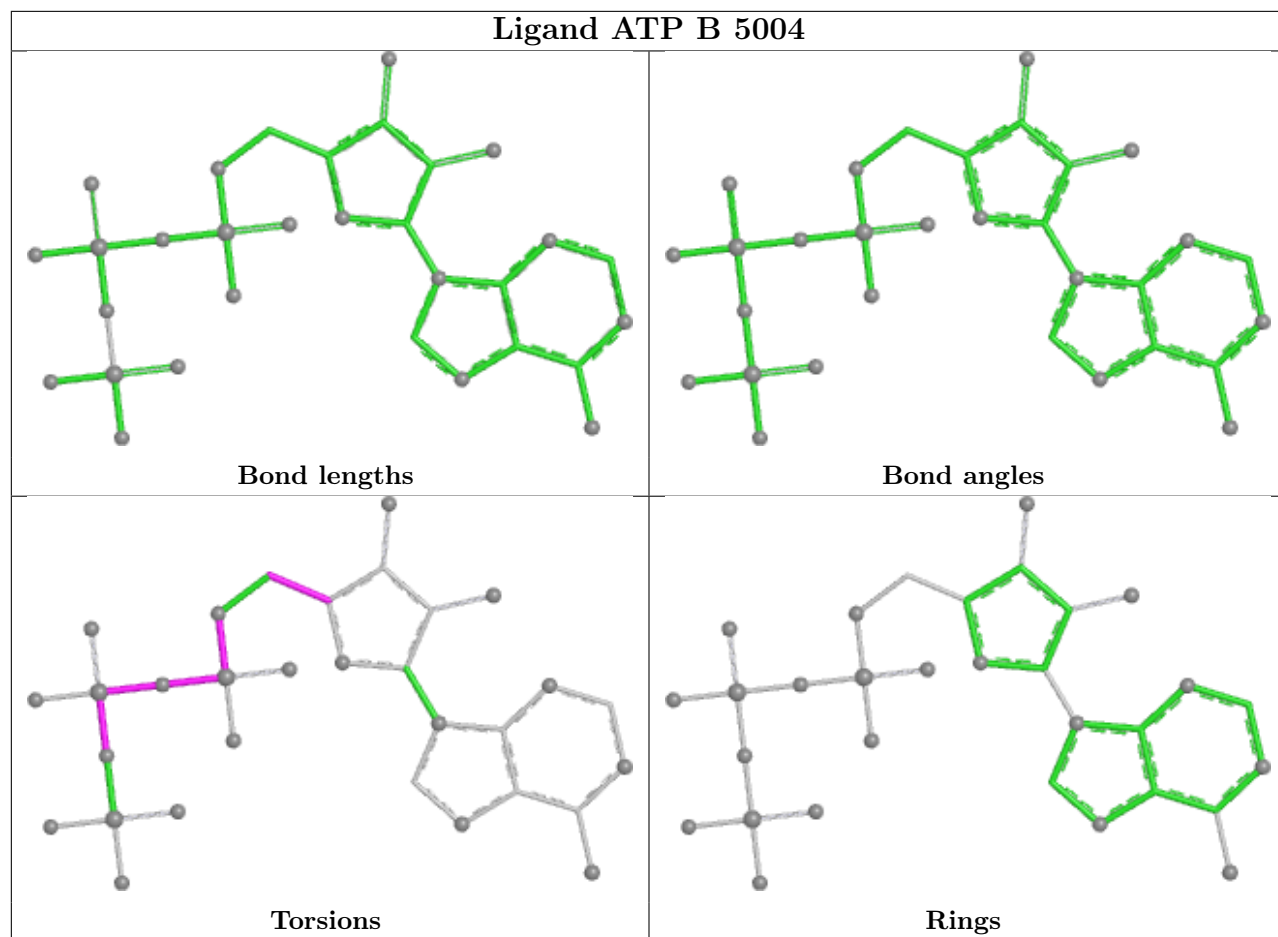
No monomer is involved in short contacts.

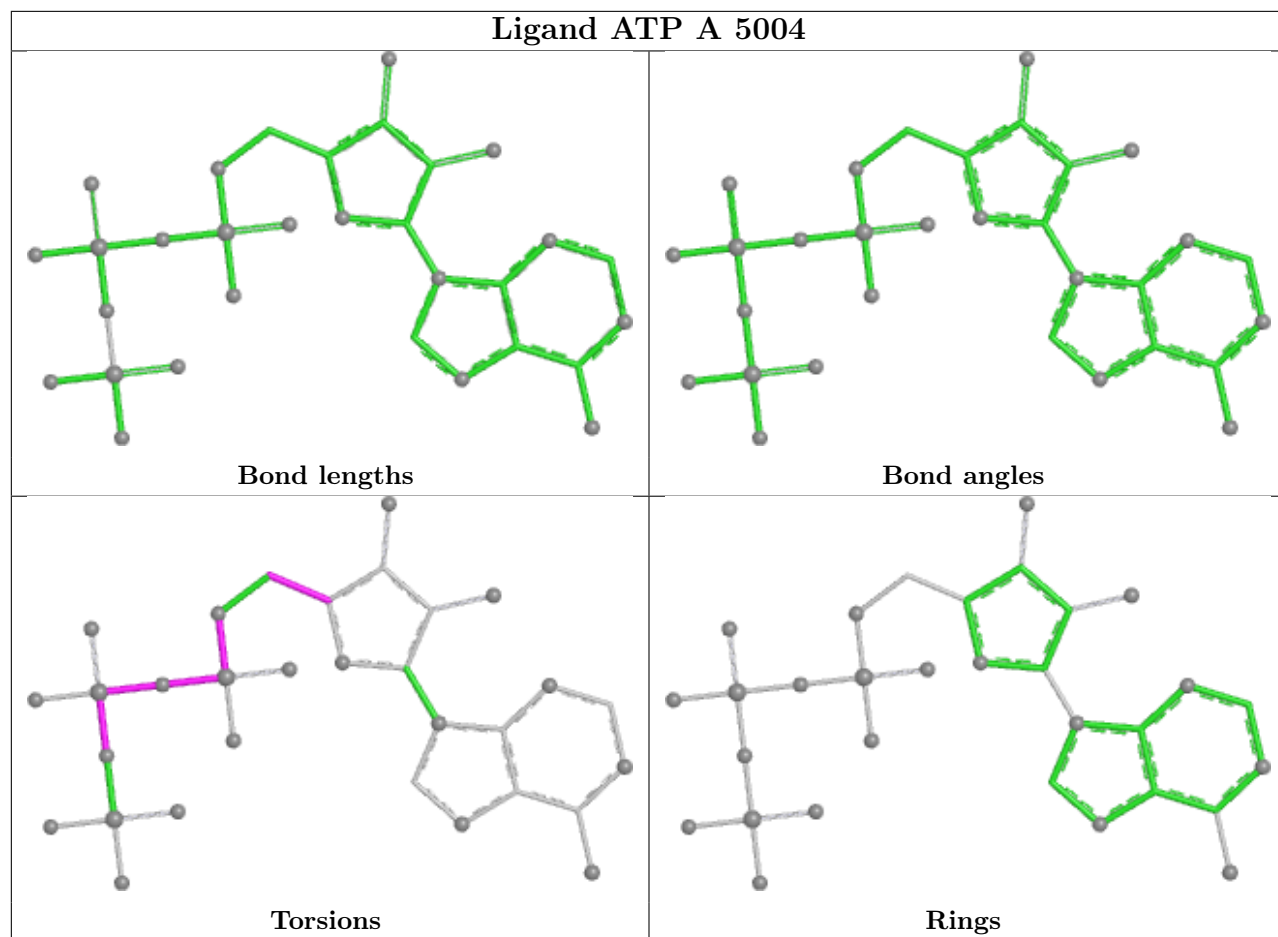
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

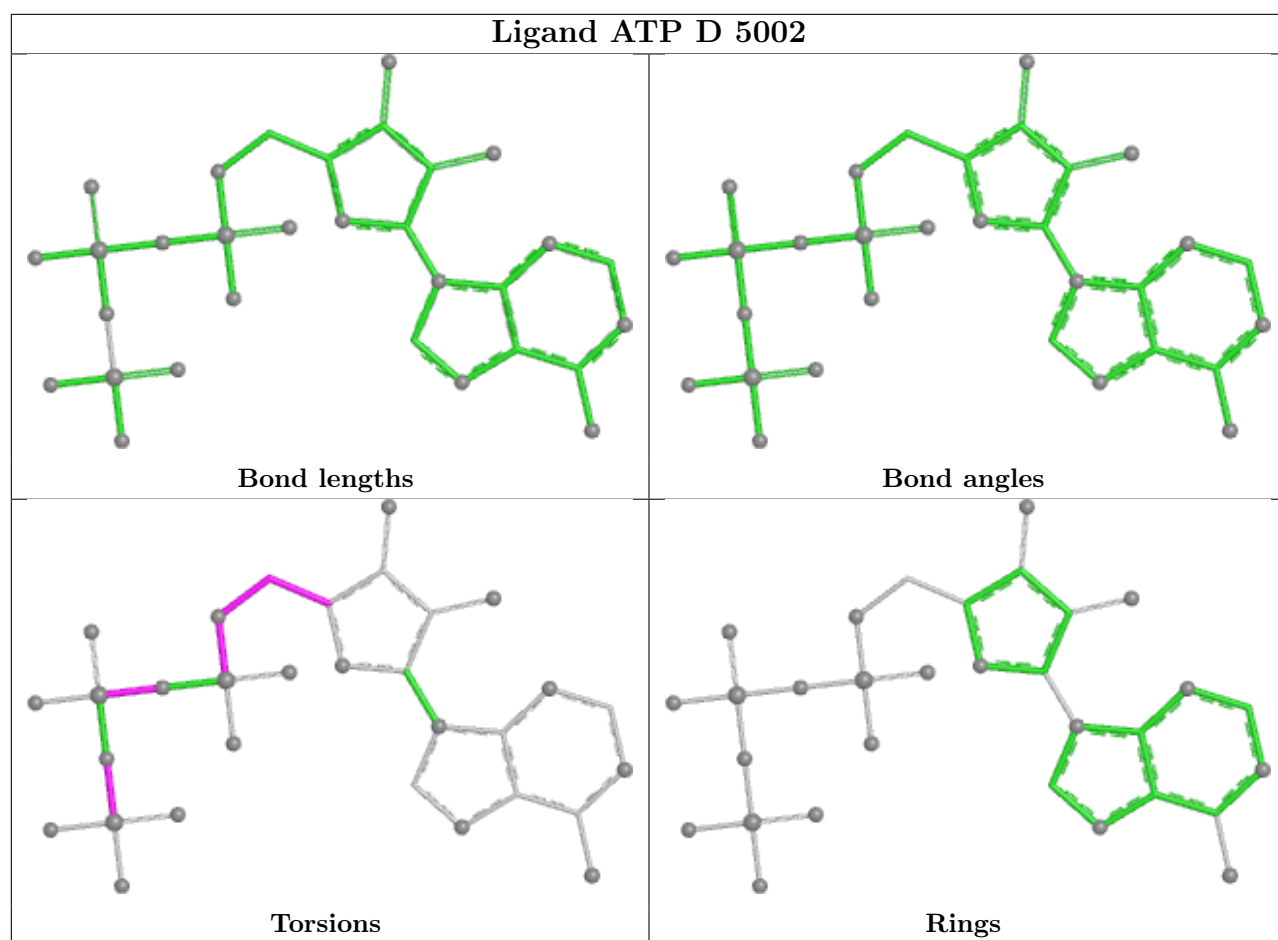


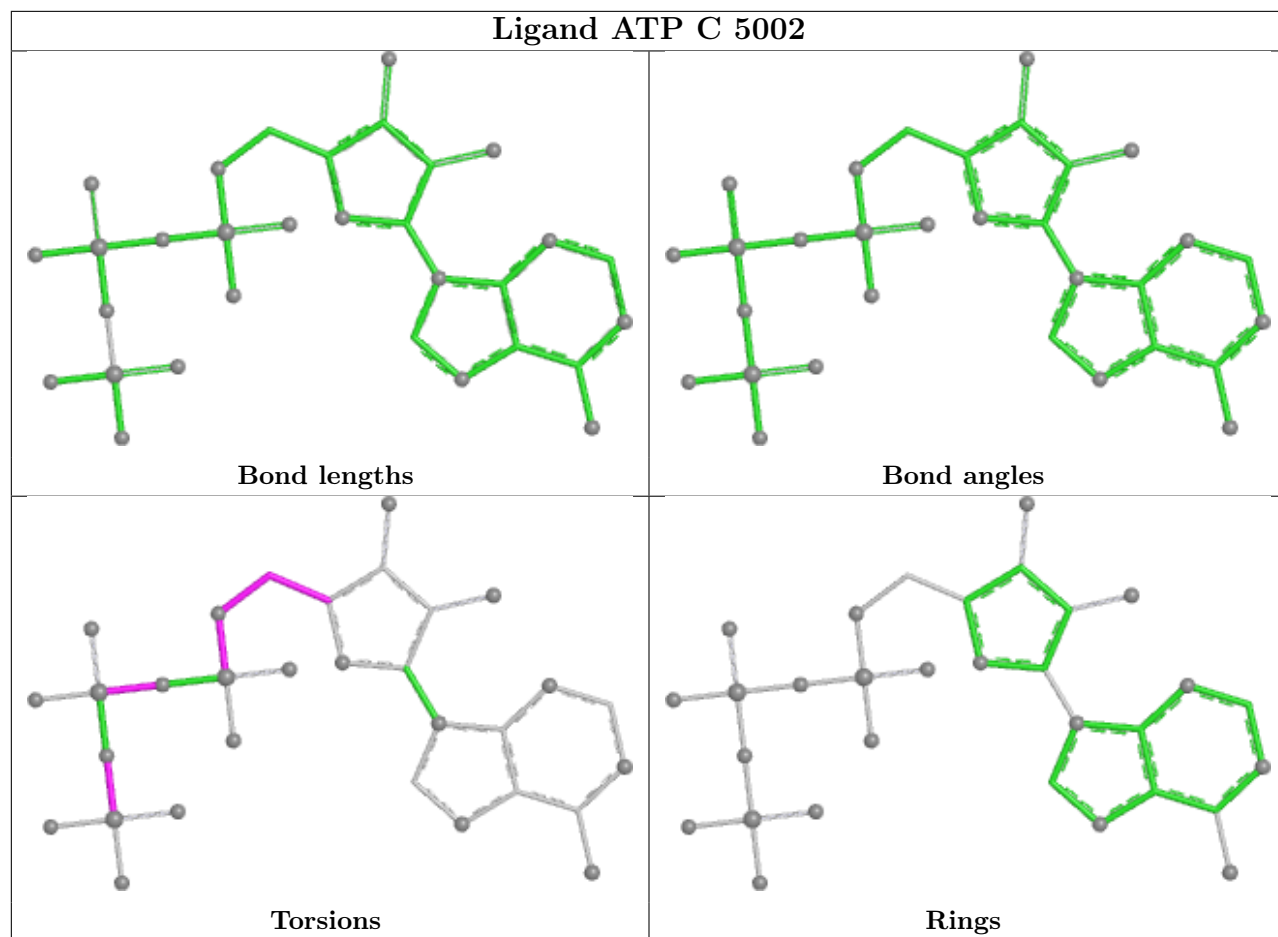


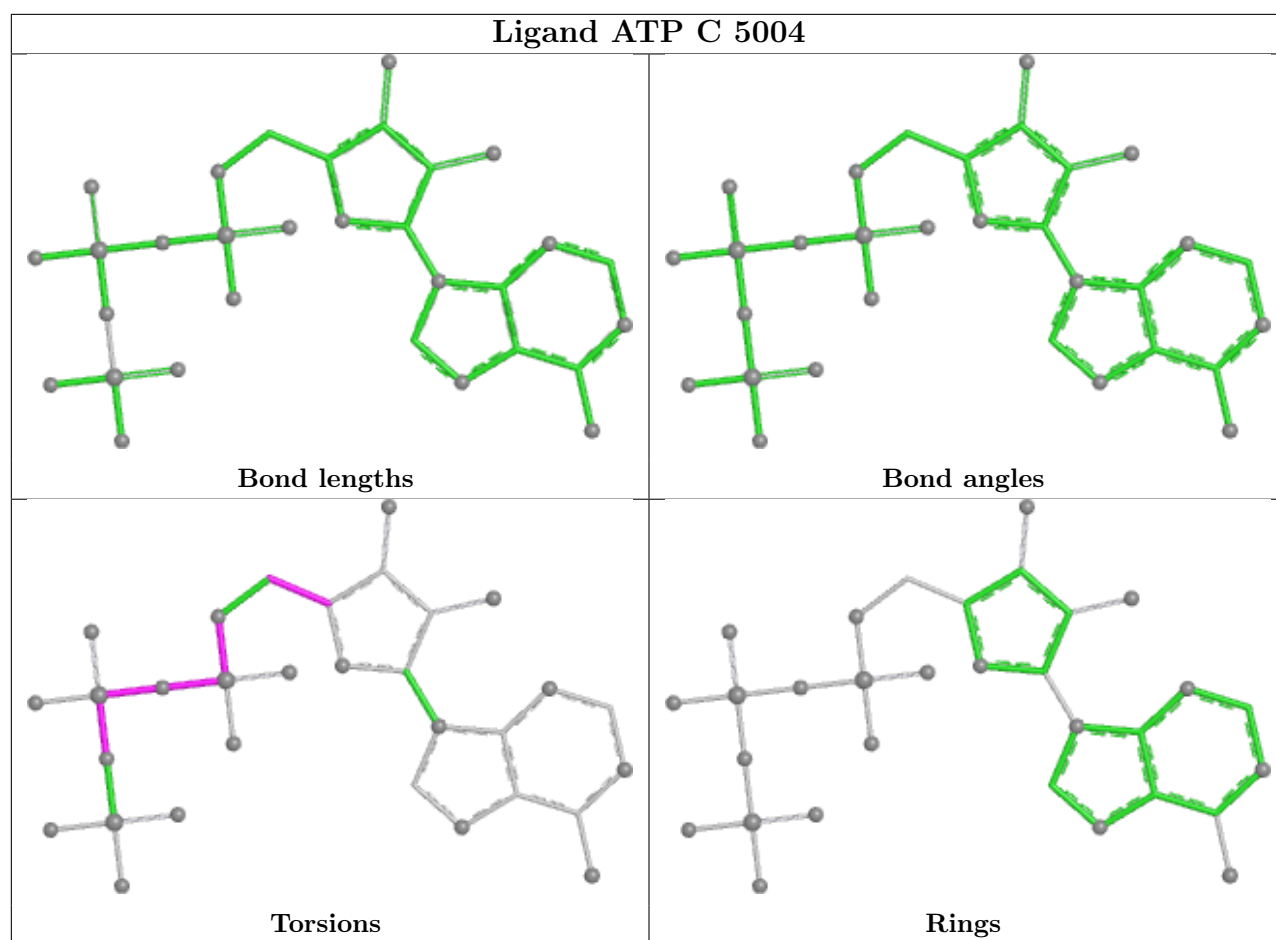












5.7 Other polymers [i](#)

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-42764. These allow visual inspection of the internal detail of the map and identification of artifacts.

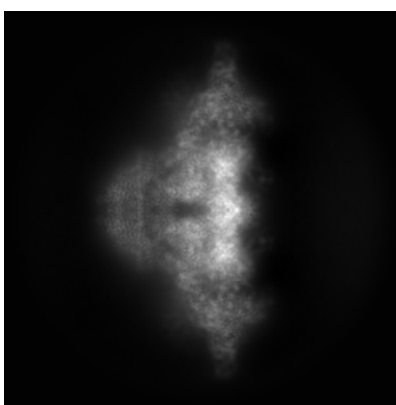
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

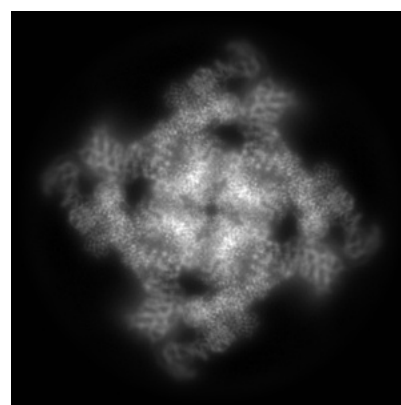
6.1.1 Primary map



X



Y

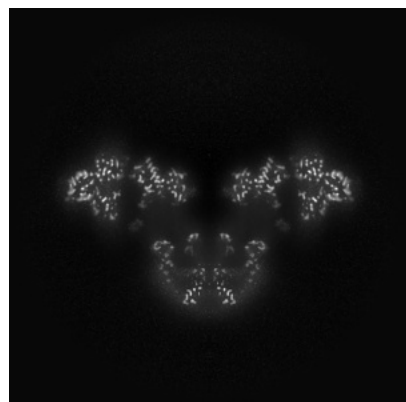


Z

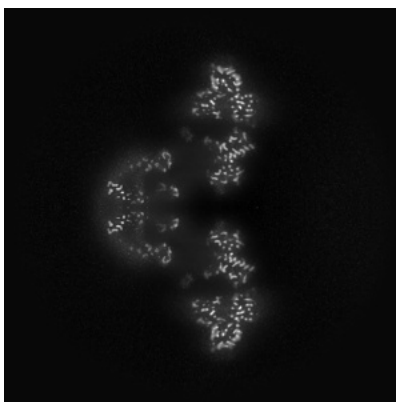
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

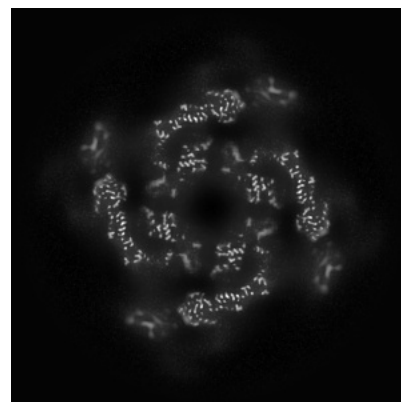
6.2.1 Primary map



X Index: 256



Y Index: 256

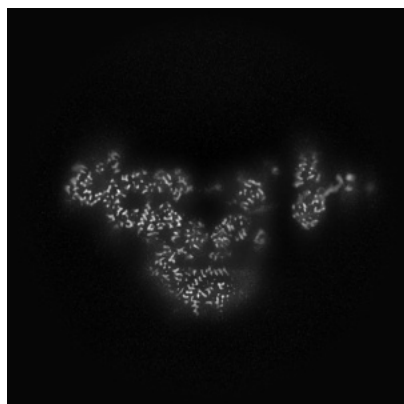


Z Index: 256

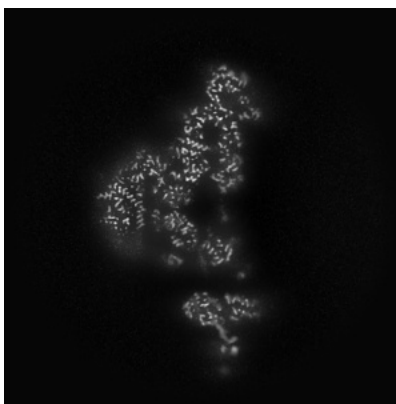
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

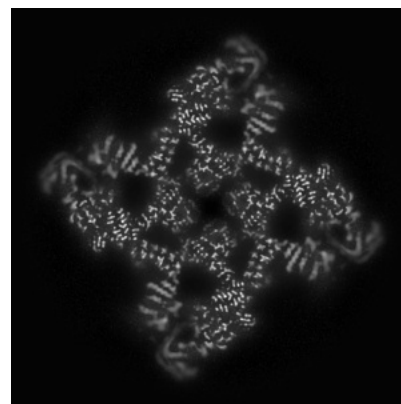
6.3.1 Primary map



X Index: 274



Y Index: 274



Z Index: 277

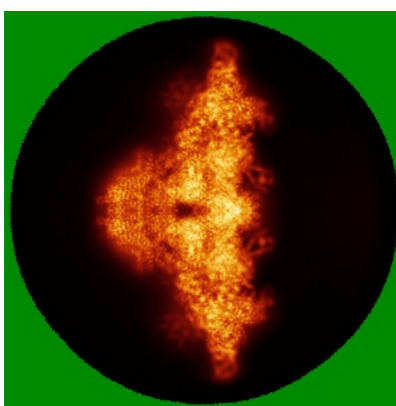
The images above show the largest variance slices of the map in three orthogonal directions.

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

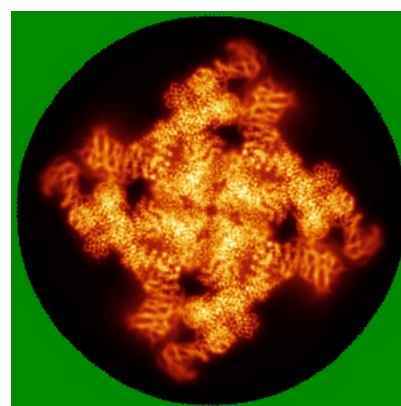
6.4.1 Primary map



X



Y

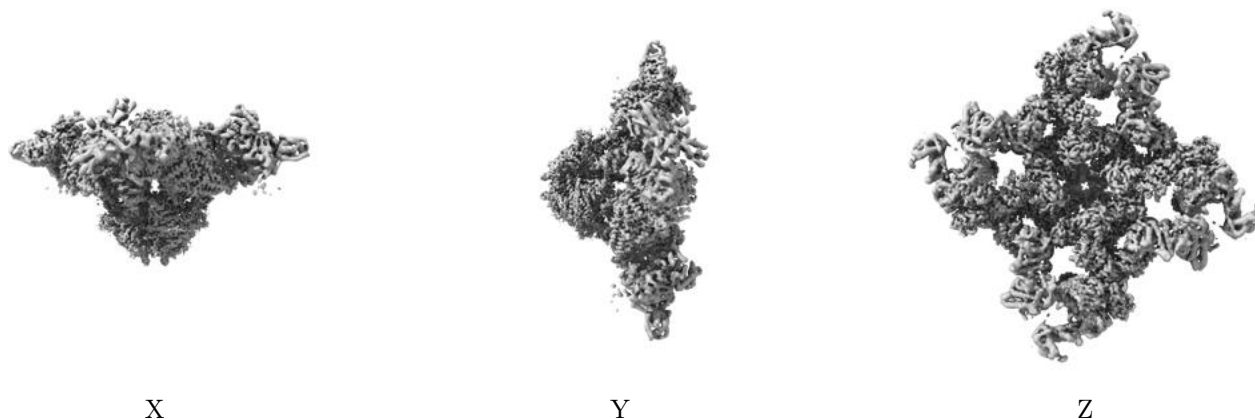


Z

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.

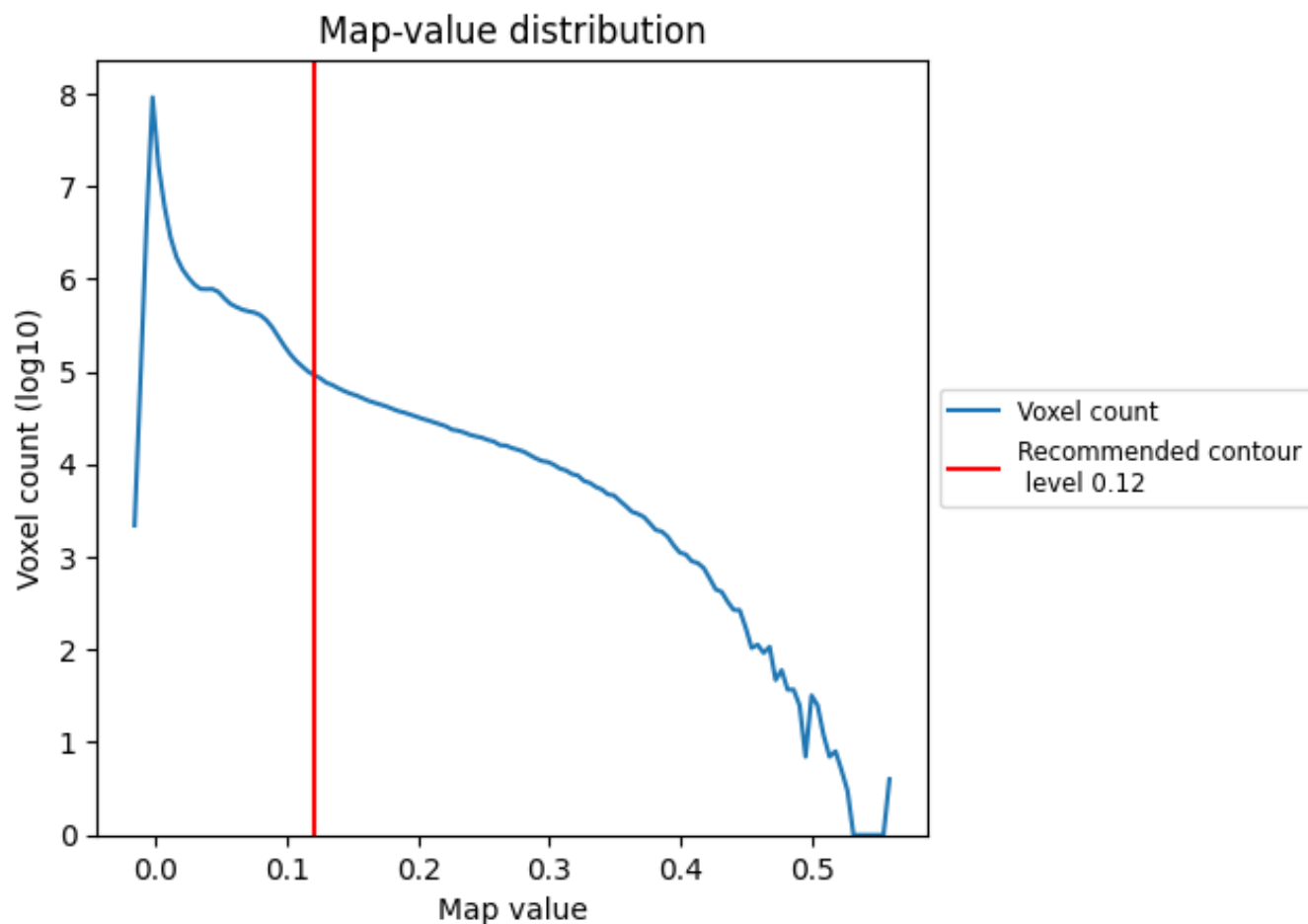
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

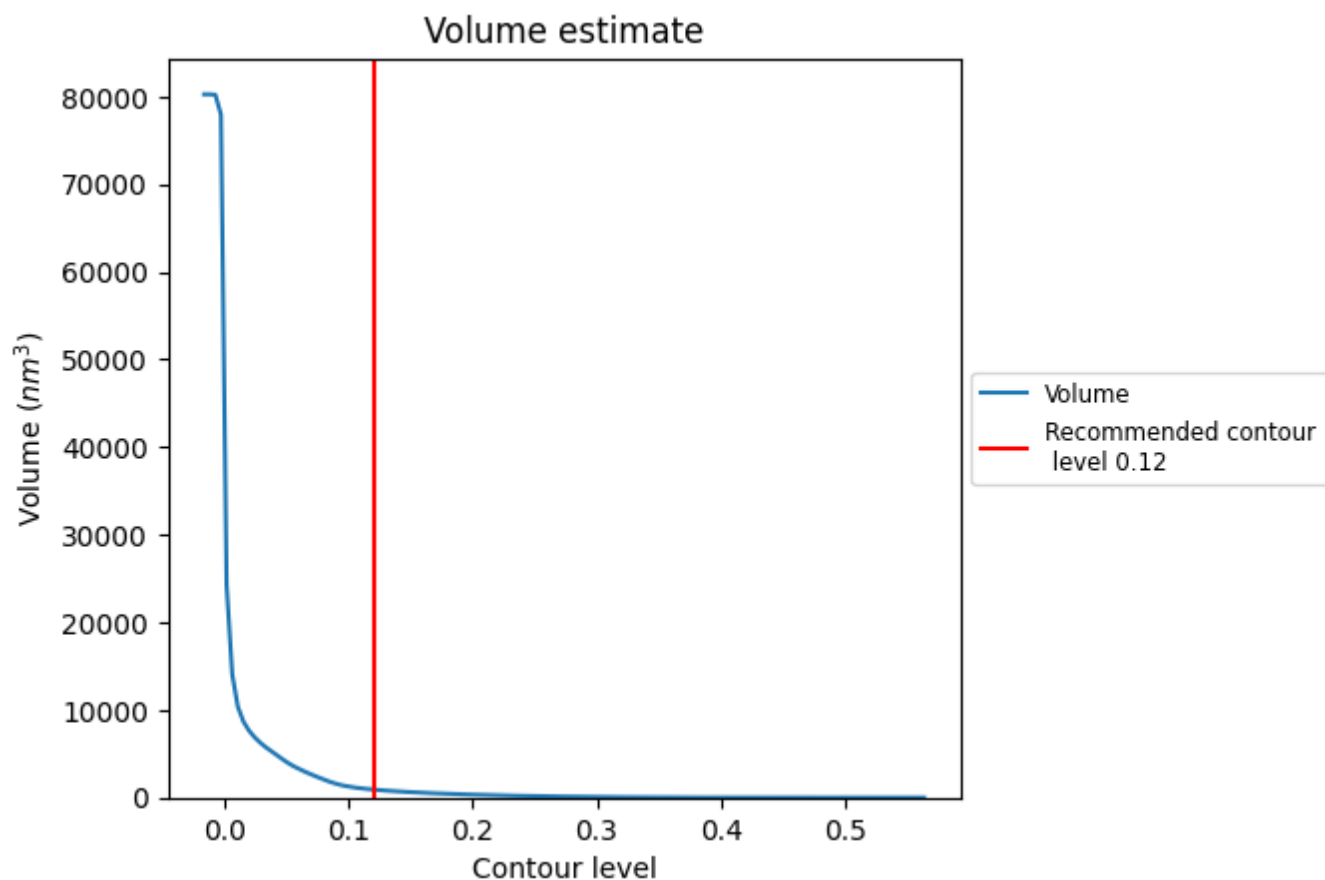
This section contains the results of statistical analysis of the map.

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.

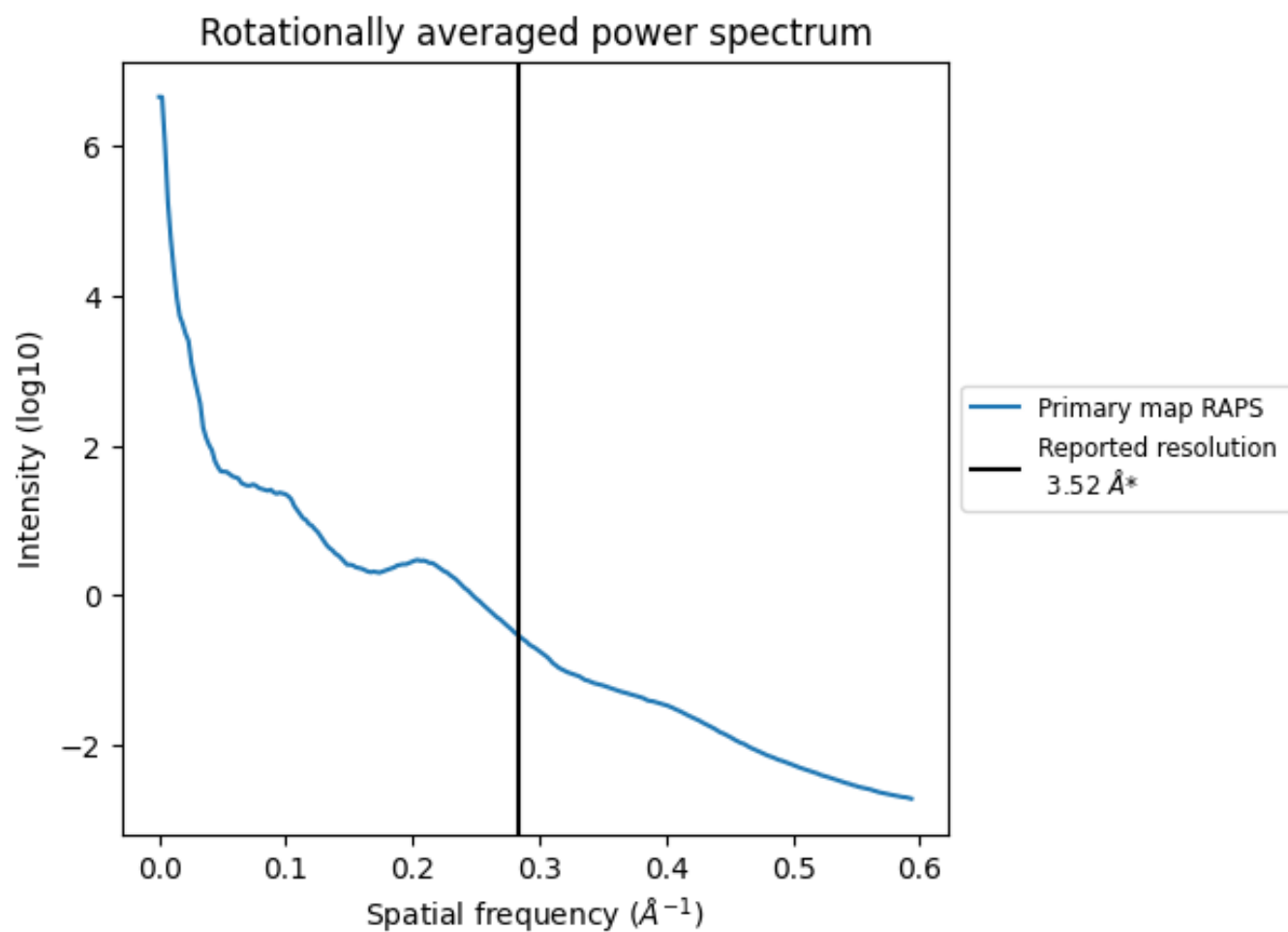
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 911 nm³; this corresponds to an approximate mass of 823 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 0.284 Å⁻¹

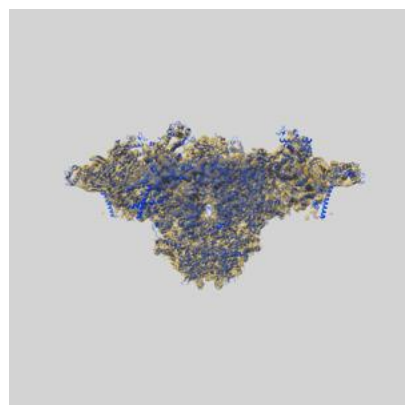
8 Fourier-Shell correlation ⓘ

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

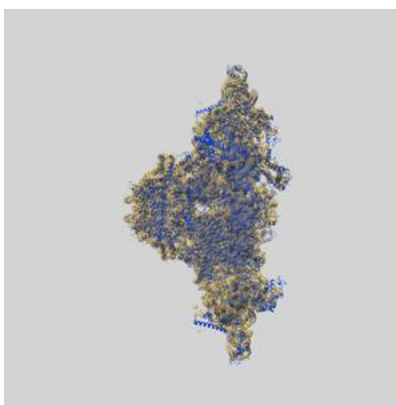
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42764 and PDB model 8UXH. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

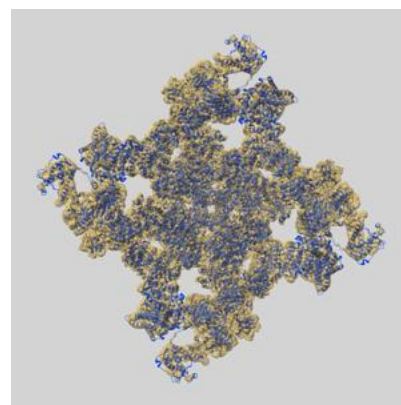
9.1 Map-model overlay [i](#)



X



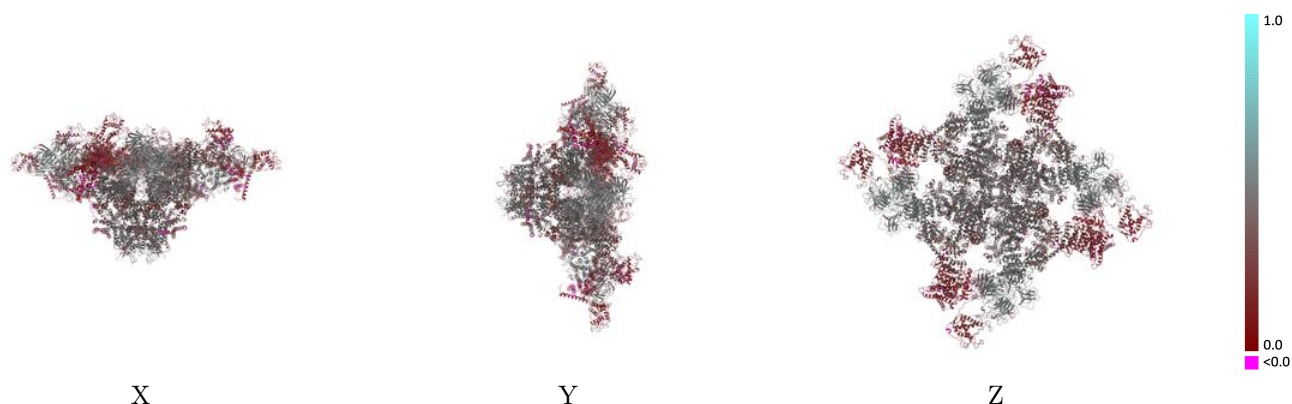
Y



Z

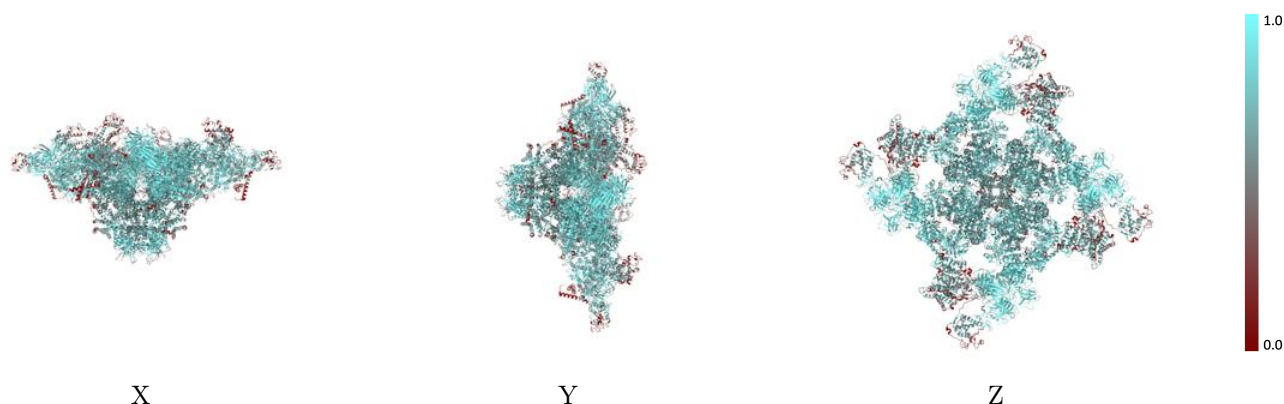
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



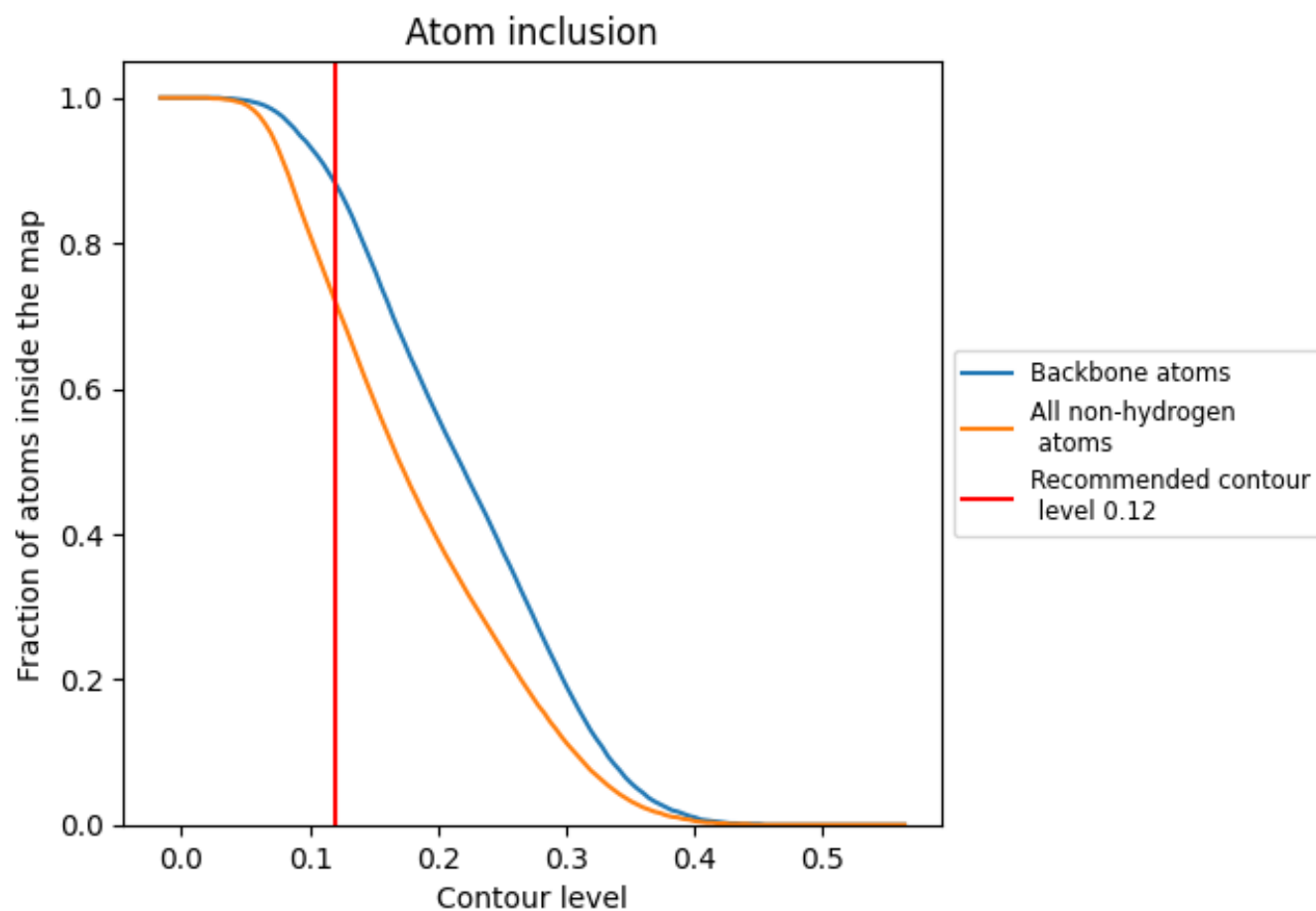
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 88% of all backbone atoms, 72% 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	0.7190	0.3660
A	0.7170	0.3650
B	0.7160	0.3640
C	0.7180	0.3660
D	0.7120	0.3560
E	0.8560	0.5050
F	0.8510	0.5030
G	0.8590	0.5060
H	0.8570	0.5040

1.0

0.0

<0.0