



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 01:14 PM UTC

PDB ID : 7U9X / pdb_00007u9x
EMDB ID : EMD-26409
Title : Structure of PKA phosphorylated human RyR2-R2474S in the closed state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 2.58 Å(reported)
Based on initial model : 7TZC

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:

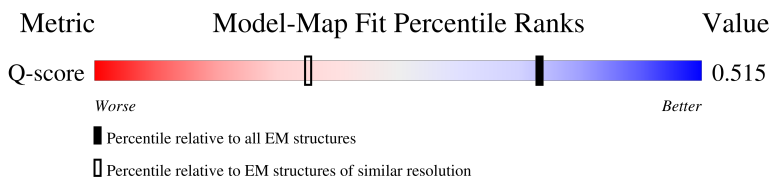
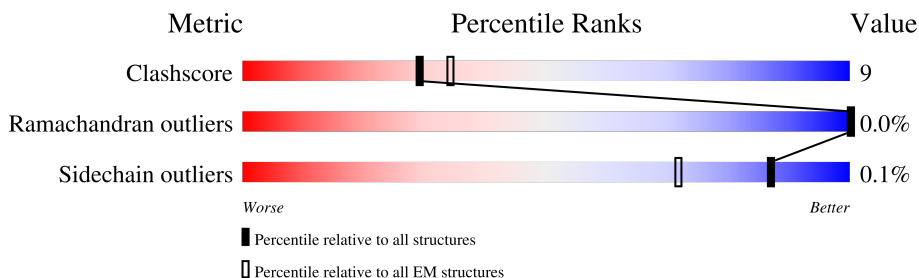
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.58 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	7675 (2.08 - 3.08)

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	8% 66% 19% 15%
1	B	4967	8% 66% 19% 15%
1	C	4967	8% 66% 19% 15%
1	D	4967	8% 66% 19% 15%

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Mol	Chain	Length	Quality of chain
2	E	108	 76%22%..
2	F	108	 76%22%..
2	G	108	 76%22%..
2	H	108	 75%23%..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 138588 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
			33766	21513	5742	6281	230		
1	B	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	C	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	D	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2474	SER	ARG	variant	UNP Q92736
B	2474	SER	ARG	variant	UNP Q92736
C	2474	SER	ARG	variant	UNP Q92736
D	2474	SER	ARG	variant	UNP Q92736

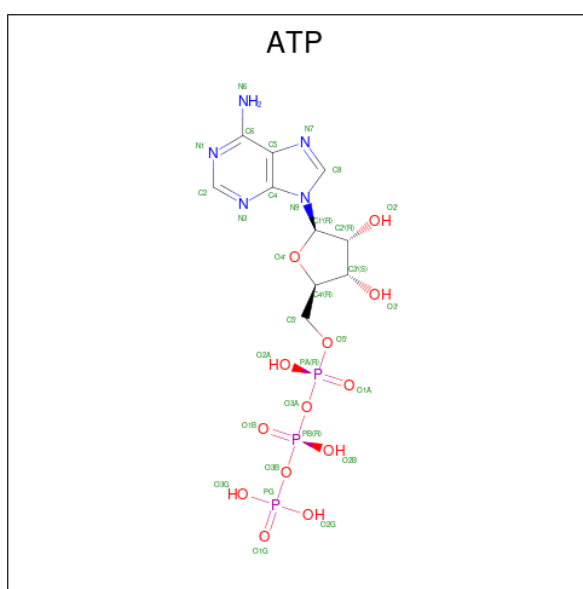
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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	

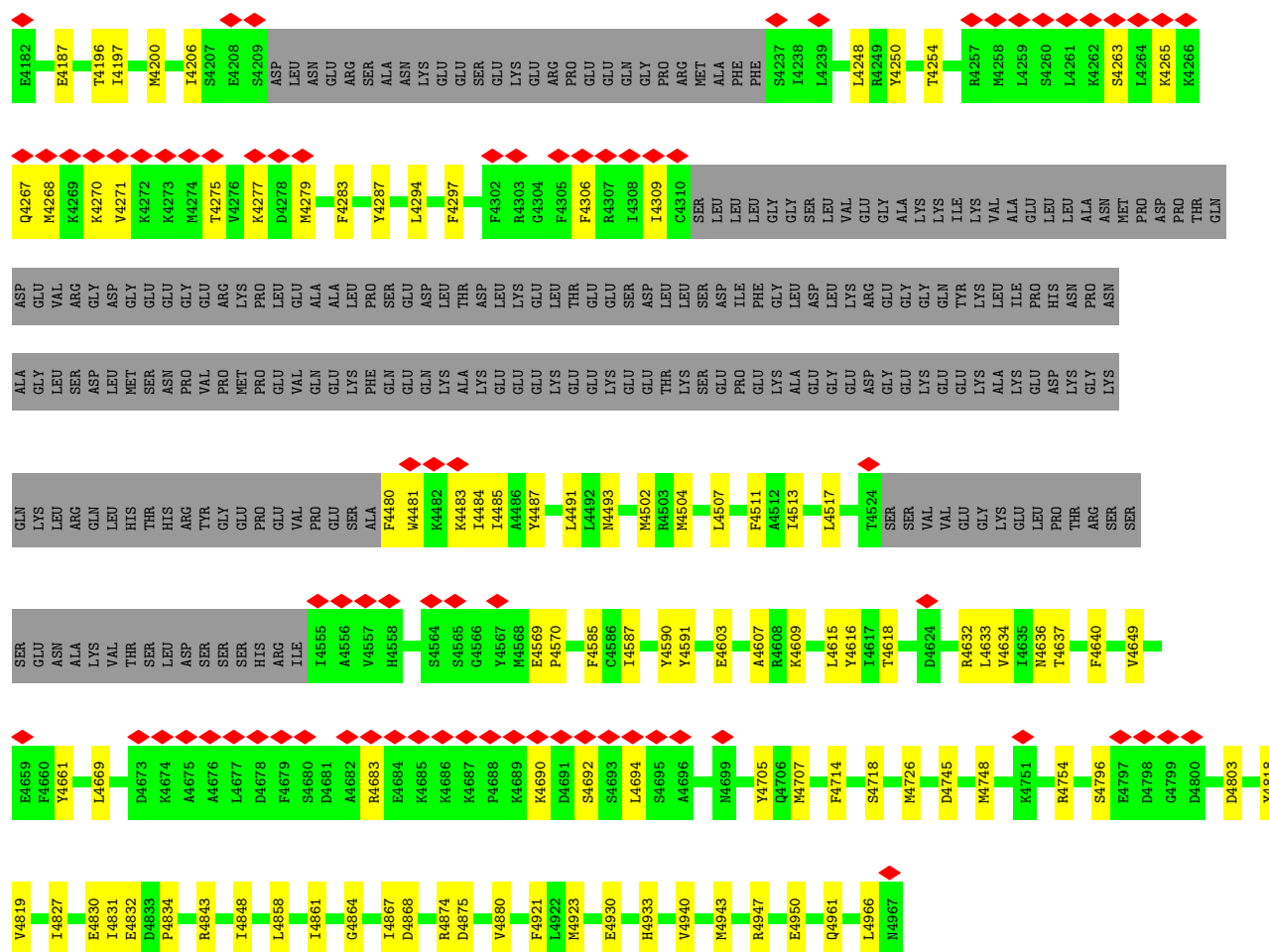
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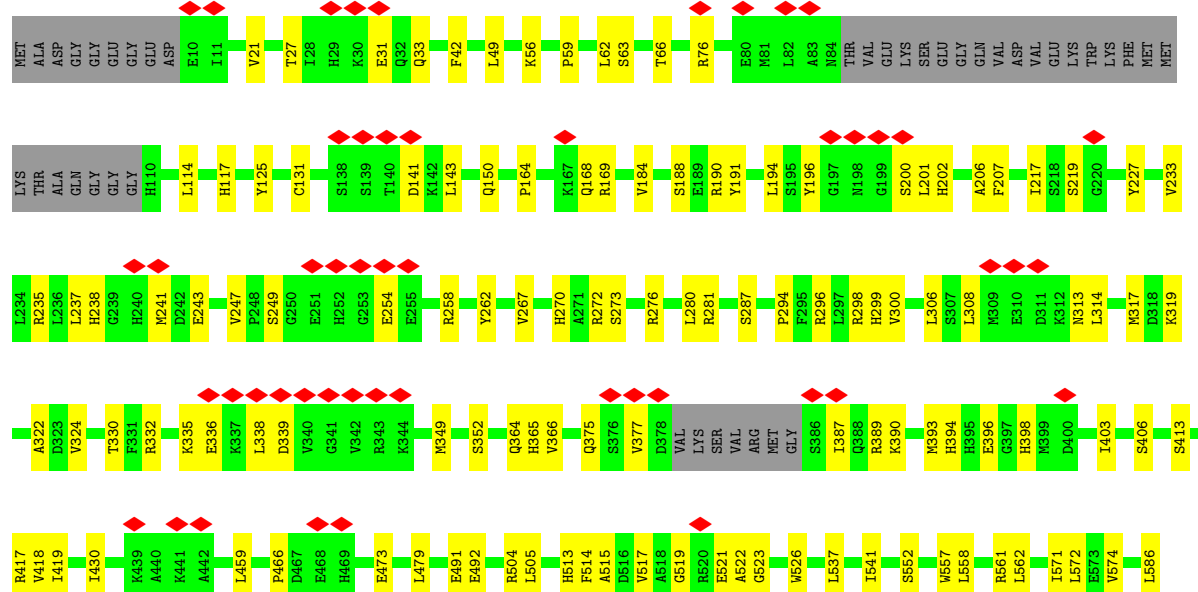
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	D	1	31	10	5	13	3	0





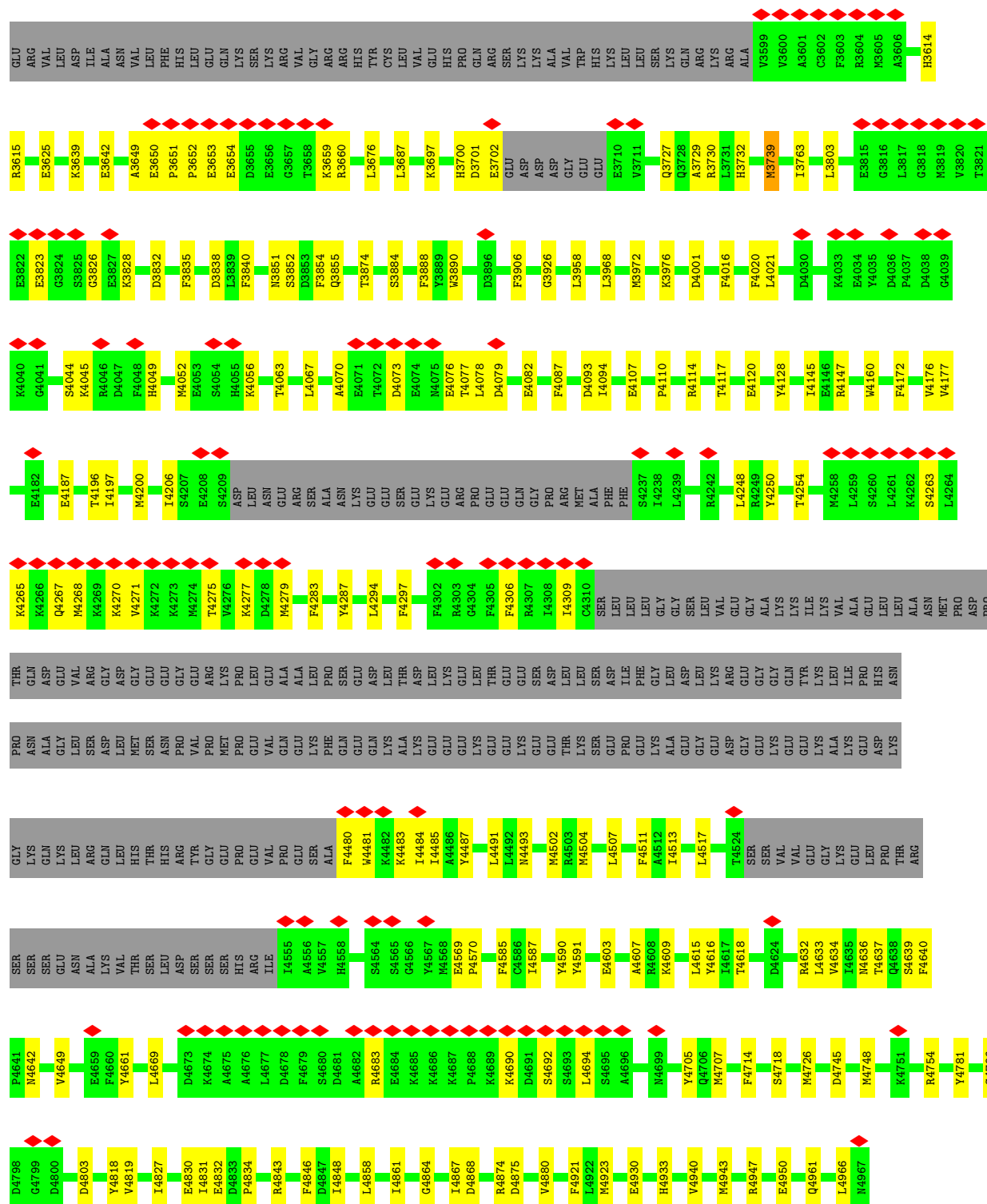


• Molecule 1: Ryanodine receptor 2

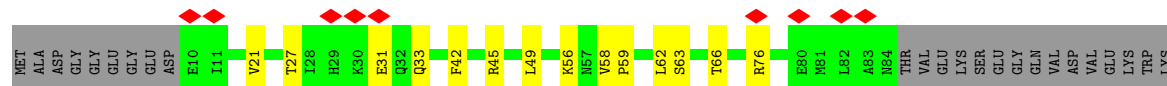


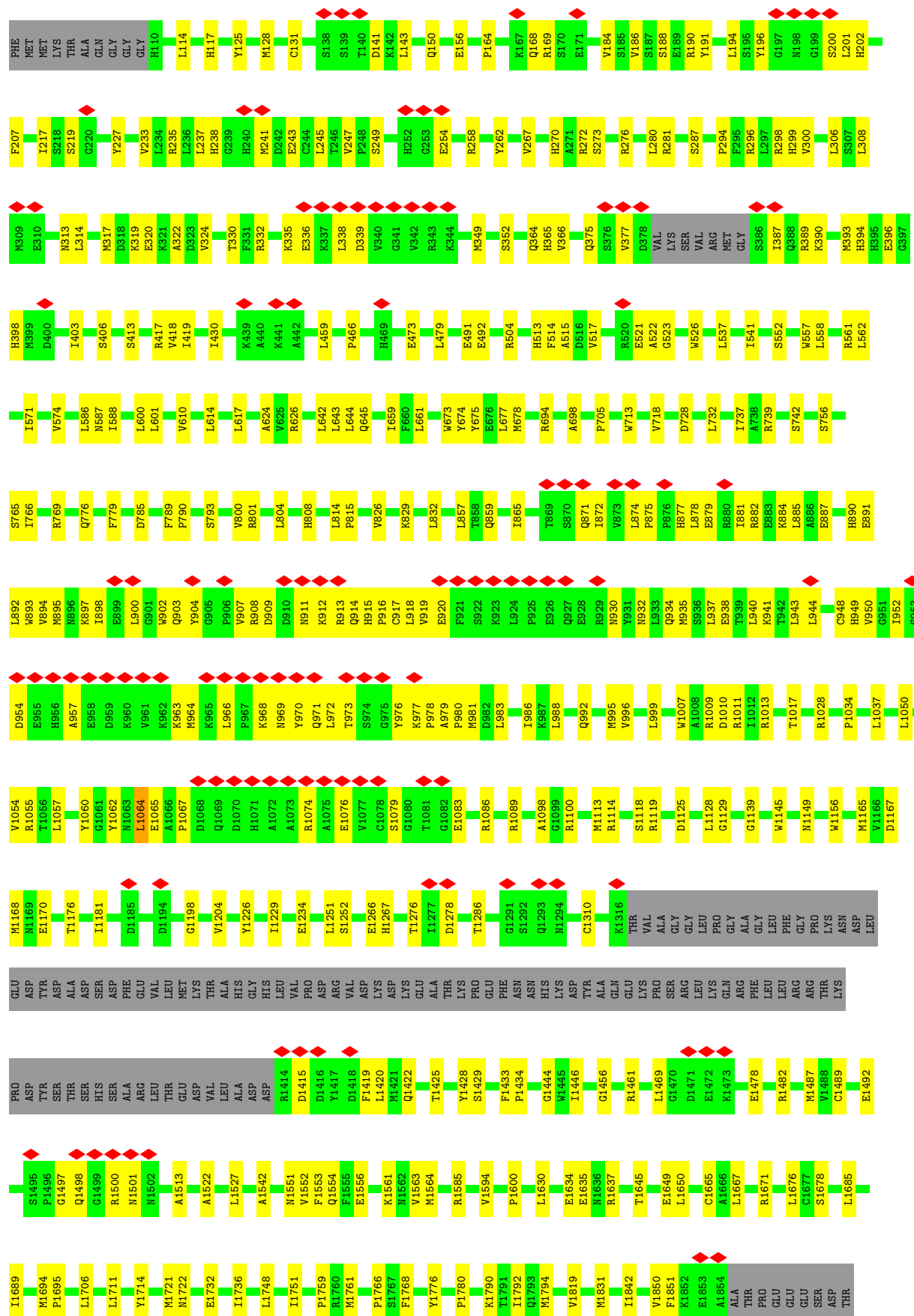


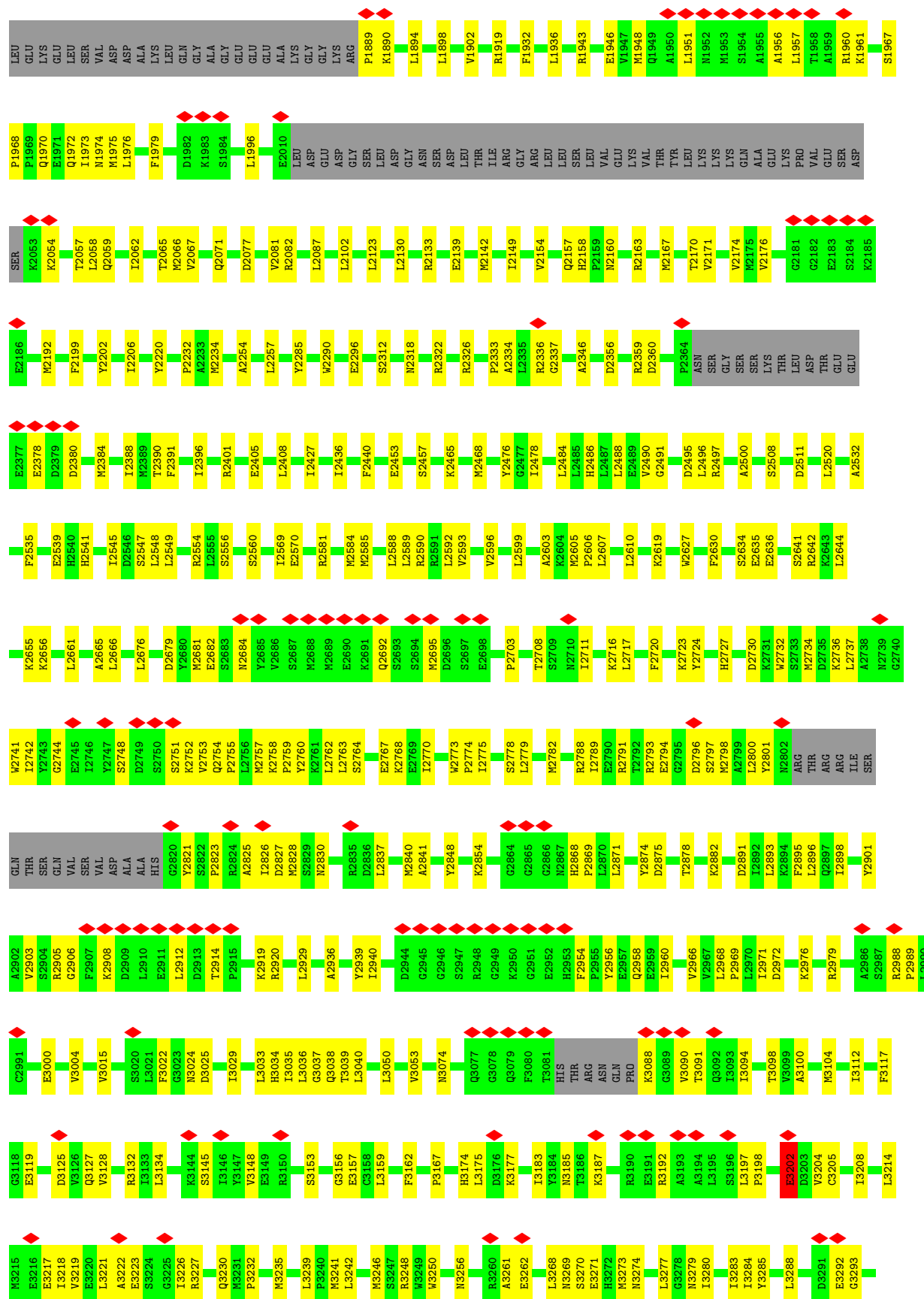




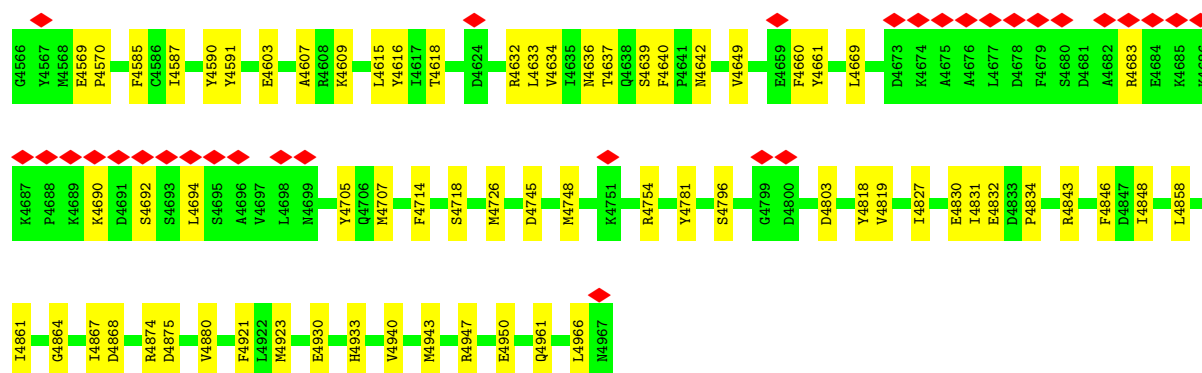
• Molecule 1: Ryanodine receptor 2



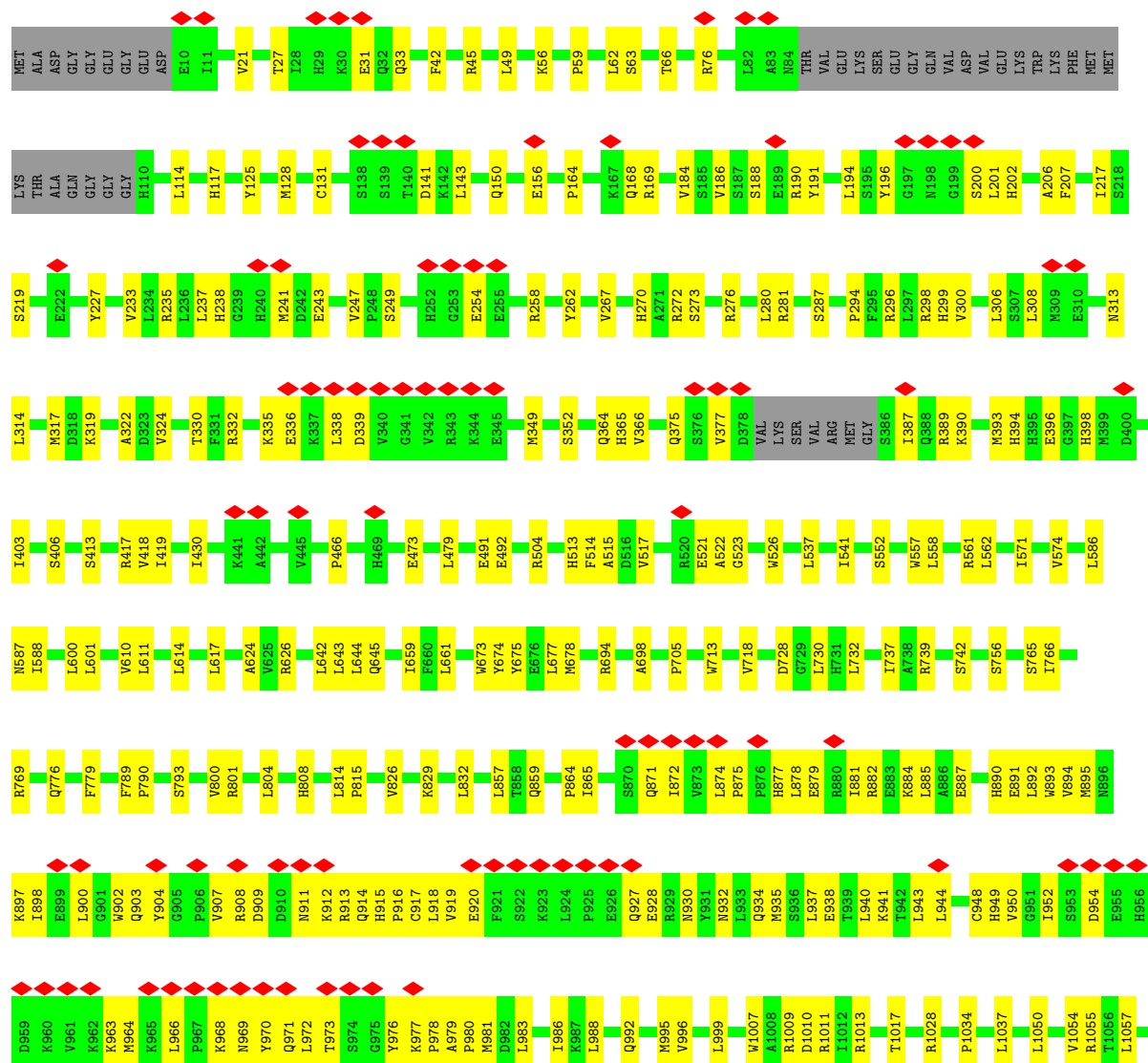


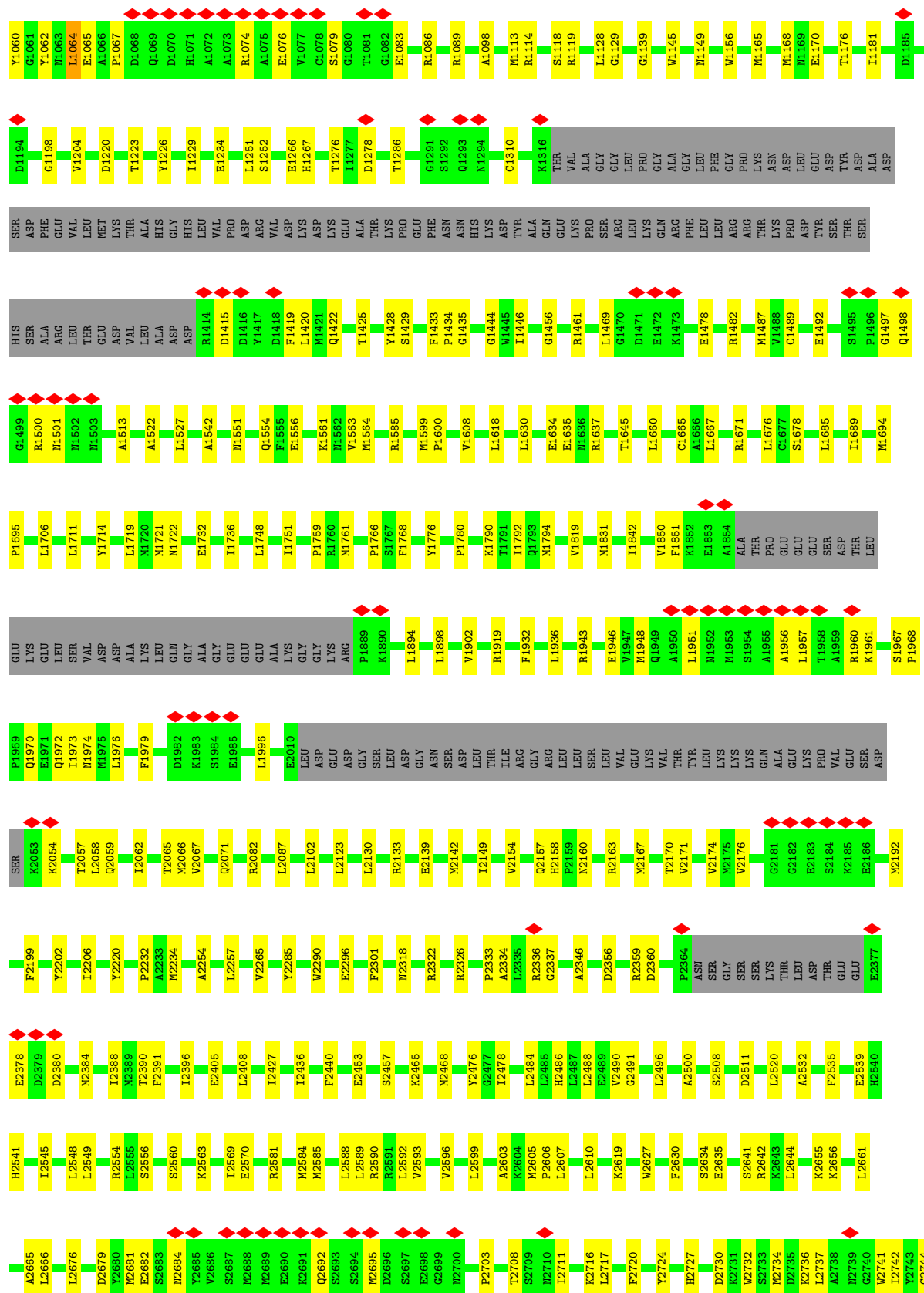




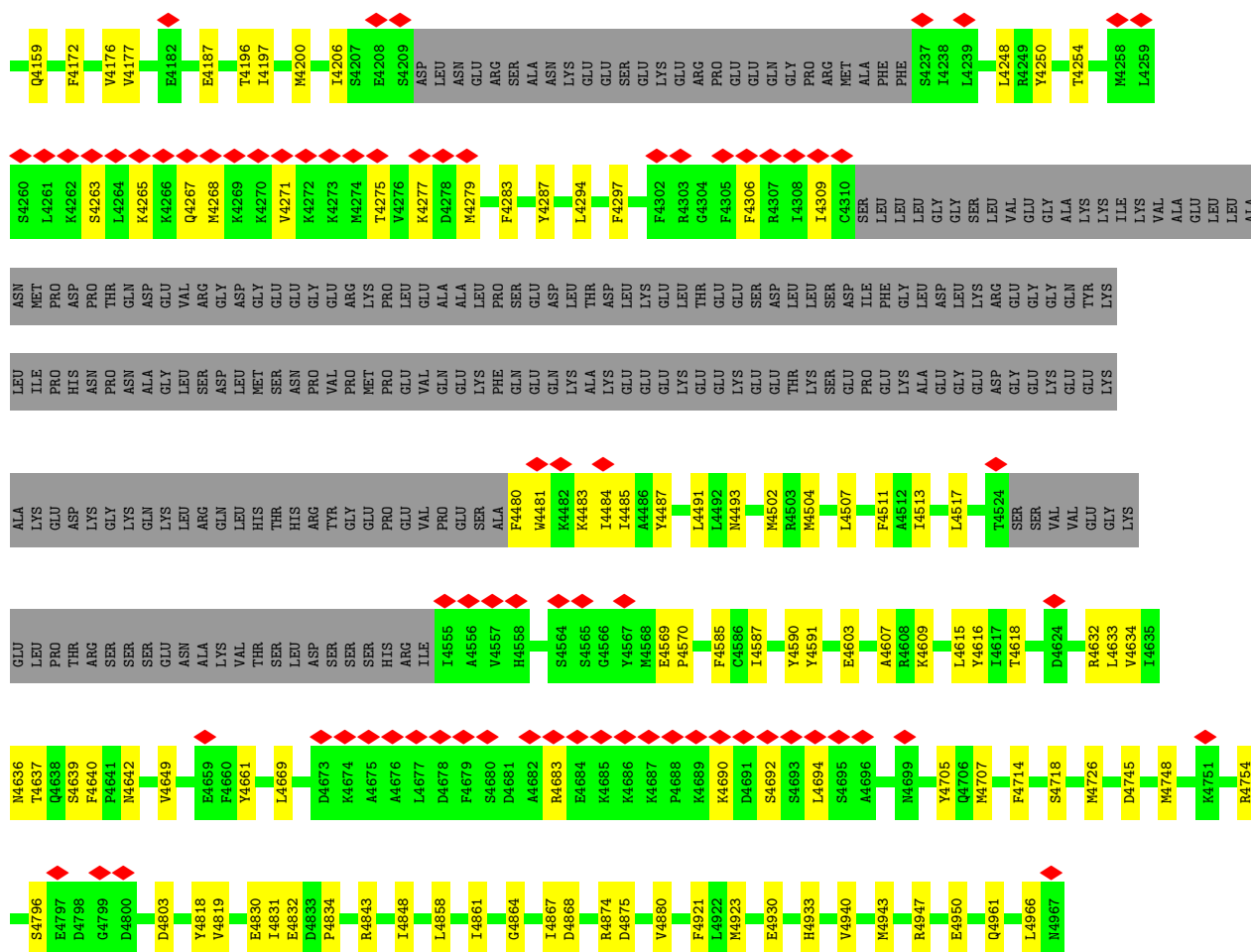


• Molecule 1: Ryanodine receptor 2





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VAL	SER	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	L2826	D2827	N2830	R2835	D2836	L2837	M2840	A2841	K2854	G2864	G2865	G2866	N2867	H2868	P2869	L2870	L2871	Y2874	D2875	T2878	K2882	D2891	L2892	L2893	K2894	F2895	L2896	Q2897	I2898	Y2901	A2902	V2903	S2904	R2905	G2906	F2907	K2908					
D2909	L2910	E2911	L2912	L2913	T2914	P2915	K2919	R2920	L2929	A2936	Y2939	I2940	F2943	D2944	G2945	S2947	R2948	G2949	K2950	G2951	E2952	H2953	F2954	P2955	Y2956	G2957	Q2958	E2959	I2960	V2966	L2968	P2969	L2970	I2971	D2972	R2979	A2986	S2987	R2988	P2989	L2990	C2991	L3011	V3015	S3020	L3021								
F3022	G3023	K3024	D3025	T3029	L3033	H3034	I3035	L3036	G3037	Q3038	L3040	L3050	V3053	N3074	Q3077	G3078	Q3079	F3080	T3081	HIS	THR	ARG	ASN	GLN	PRO	K3088	G3089	V3090	T3091	Q3092	I3093	I3094	T3098	V3099	A3100	M3104	T3112	F3117	G3118	E3119	D3125	V3126	Q3127	V3128	R3132	I3133								
L3134	K3144	S3145	V3148	S3153	G3156	E3157	G3158	L3159	F3162	P3167	H3174	L3175	D3176	K3177	I3183	Y3184	N3185	T3186	K3187	R3190	G3278	E3191	R3192	A3193	S3196	L3197	P3198	E3202	D3203	V3204	C3205	I3208	L3214	I3218	V3219	L3221	A3222	S3224	G3225	L3226	R3227	Q3230	K3231											
P3232	M3235	L3239	P3240	K3241	L3242	M3246	S3247	K3248	V3249	W3250	N3256	K3260	A3261	E3262	L3268	N3269	S3270	E3271	H3272	K3273	N3274	L3277	G3278	N3279	L3280	I3283	L3284	L3288	I3291	E3292	G3293	L3299	F3302	S3303	I3306	I3307	N3308	K3309	V3310	K3311	P3312	Q3313	L3314	L3315	K3316	T3317								
H3318	F3319	L3320	P3321	L3322	M3323	K3325	L3326	K3327	K3328	K3329	A3330	A3331	T3332	V3333	S3334	S3335	E3336	E3337	ASP	HIS	LEU	LYS	ALA	GLU	ALA	GLY	ARG	GLY	ASP	THR	ILE	THR	VAL	ASP	GLU	GLN	ASP	GLY	ASP	THR	VAL	ASP	GLU	GLN	ASP	GLY	ASP	THR	VAL					
ASP	TYR	ASN	ARG	ALA	LYS	LEU	TRP	LEU	ASP	LYS	GLU	PRO	ASN	ARG	LYS	PRO	GLU	ALA	GLU	GLY	ARG	GLU	GLY	ASP	THR	ILE	THR	VAL	ASP	GLU	GLN	ASP	GLY	ASP	THR	VAL	ASP	GLU	GLN	ASP	GLY	ASP	THR	VAL	ASP	GLU	GLN	ASP	GLY	ASP	THR	VAL		
LYS	MET	SER	LYS	ALA	VAL	SER	ASP	GLN	ARG	LYS	GLY	ASP	THR	ILE	THR	VAL	ASP	GLU	GLY	ARG	GLU	GLY	ASP	THR	ILE	THR	VAL	ASP	GLU	GLN	ASP	GLY	ASP	THR	VAL	ASP	GLU	GLN	ASP	GLY	ASP	THR	VAL	ASP	GLU	GLN	ASP	GLY	ASP	THR	VAL			
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LEU	PHE	HIS	GLN	LYS	SER	GLY	VAL	HIS	ARG	TYR	THR	ASP	GLU	PRO	GLN	ARG	ASP	GLU	GLY	ASP	THR	ILE	THR	VAL	ASP	GLU	GLY	ASP	THR	VAL	ASP	GLY	ASP	THR	VAL	ASP	GLY	ASP	THR	VAL	ASP	GLY	ASP	THR	VAL	ASP	GLY	ASP	THR	VAL				
LEU	PHE	HIS	GLN	LYS	SER	GLY	VAL	HIS	ARG	TYR	THR	ASP	GLU	PRO	GLN	ARG	ASP	GLU	GLY	ASP	THR	ILE	THR	VAL	ASP	GLU	GLY	ASP	THR	VAL	ASP	GLY	ASP	THR	VAL	ASP	GLY	ASP	THR	VAL	ASP	GLY	ASP	THR	VAL	ASP	GLY	ASP	THR	VAL				
LEU	PHE	HIS	GLN	LYS	SER	GLY	VAL	HIS	ARG	TYR	THR	ASP	GLU	PRO	GLN	ARG	ASP	GLU	GLY	ASP	THR																																	



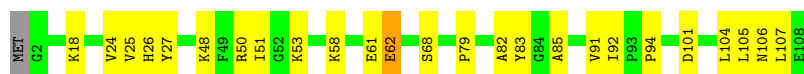
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 76% 22% ..



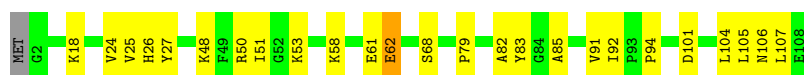
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 76% 22% ..



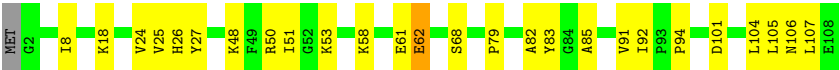
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 76% 22% ..



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

Chain H:  75% 23% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212141	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)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.859	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.832, 0.832, 0.832	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	0.14	1/34506 (0.0%)	0.35	1/46608 (0.0%)
1	B	0.14	1/34506 (0.0%)	0.35	1/46608 (0.0%)
1	C	0.14	1/34506 (0.0%)	0.35	1/46608 (0.0%)
1	D	0.14	1/34506 (0.0%)	0.35	1/46608 (0.0%)
2	E	0.24	0/834	0.45	0/1123
2	F	0.24	0/834	0.45	0/1123
2	G	0.24	0/834	0.45	0/1123
2	H	0.24	0/834	0.45	0/1123
All	All	0.14	4/141360 (0.0%)	0.35	4/190924 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1819	VAL	CA-CB	-5.14	1.51	1.54
1	B	1819	VAL	CA-CB	-5.10	1.51	1.54
1	D	1819	VAL	CA-CB	-5.10	1.51	1.54
1	C	1819	VAL	CA-CB	-5.01	1.51	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3202	GLU	CA-CB-CG	5.63	125.36	114.10
1	C	3202	GLU	CA-CB-CG	5.63	125.36	114.10
1	A	3202	GLU	CA-CB-CG	5.61	125.33	114.10
1	D	3202	GLU	CA-CB-CG	5.61	125.31	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3926	GLY	Peptide
1	B	3926	GLY	Peptide
1	C	3926	GLY	Peptide
1	D	3926	GLY	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	33766	0	33447	649	0
1	B	33766	0	33447	641	0
1	C	33766	0	33447	653	0
1	D	33766	0	33447	641	0
2	E	818	0	821	15	0
2	F	818	0	821	14	0
2	G	818	0	821	15	0
2	H	818	0	821	15	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	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0
All	All	138588	0	137168	2562	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 9.

The worst 5 of 2562 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:2149:ILE:HG21	1:B:2167:MET:HE1	1.53	0.90
1:A:2149:ILE:HG21	1:A:2167:MET:HE1	1.53	0.88
1:D:2149:ILE:HG21	1:D:2167:MET:HE1	1.53	0.88
1:C:2149:ILE:HG21	1:C:2167:MET:HE1	1.53	0.87
1:C:4834:PRO:HB3	1:C:4843:ARG:HD3	1.59	0.83

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	4198/4967 (84%)	4102 (98%)	96 (2%)	0	100	100
1	B	4198/4967 (84%)	4102 (98%)	96 (2%)	0	100	100
1	C	4198/4967 (84%)	4101 (98%)	97 (2%)	0	100	100
1	D	4198/4967 (84%)	4103 (98%)	95 (2%)	0	100	100
2	E	105/108 (97%)	102 (97%)	2 (2%)	1 (1%)	12	26
2	F	105/108 (97%)	102 (97%)	2 (2%)	1 (1%)	12	26
2	G	105/108 (97%)	102 (97%)	2 (2%)	1 (1%)	12	26
2	H	105/108 (97%)	102 (97%)	2 (2%)	1 (1%)	12	26
All	All	17212/20300 (85%)	16816 (98%)	392 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	61	GLU
2	H	61	GLU
2	E	61	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	61	GLU

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%)	3705 (100%)	3 (0%)	88	96
1	B	3708/4358 (85%)	3705 (100%)	3 (0%)	88	96
1	C	3708/4358 (85%)	3705 (100%)	3 (0%)	88	96
1	D	3708/4358 (85%)	3705 (100%)	3 (0%)	88	96
2	E	88/89 (99%)	87 (99%)	1 (1%)	65	83
2	F	88/89 (99%)	87 (99%)	1 (1%)	65	83
2	G	88/89 (99%)	87 (99%)	1 (1%)	65	83
2	H	88/89 (99%)	87 (99%)	1 (1%)	65	83
All	All	15184/17788 (85%)	15168 (100%)	16 (0%)	87	96

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

Mol	Chain	Res	Type
1	D	3202	GLU
1	D	1064	LEU
1	B	3202	GLU
1	C	3739	MET
1	B	1064	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 166 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3767	ASN
1	D	2059	GLN
1	C	3869	ASN
1	D	198	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3185	ASN

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	$\# Z > 2$
4	ATP	C	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	D	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	A	5003	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	D	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	B	5003	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	C	5003	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.30	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	C	5002	-	-	7/22/38/38	0/3/3/3
4	ATP	D	5002	-	-	7/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	7/22/38/38	0/3/3/3
4	ATP	A	5003	-	-	6/22/38/38	0/3/3/3
4	ATP	D	5003	-	-	6/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	6/22/38/38	0/3/3/3
4	ATP	C	5003	-	-	6/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

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

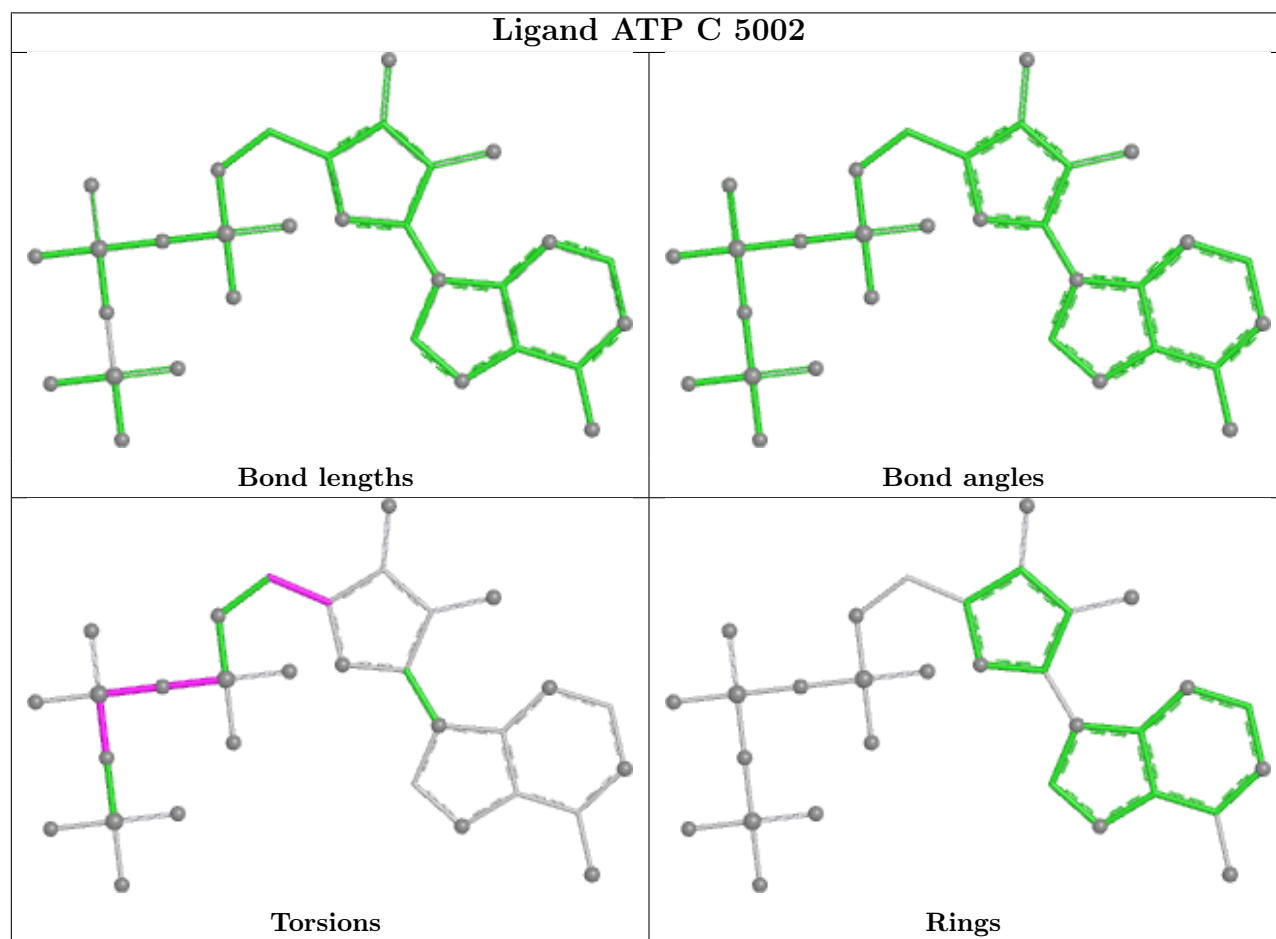
There are no ring outliers.

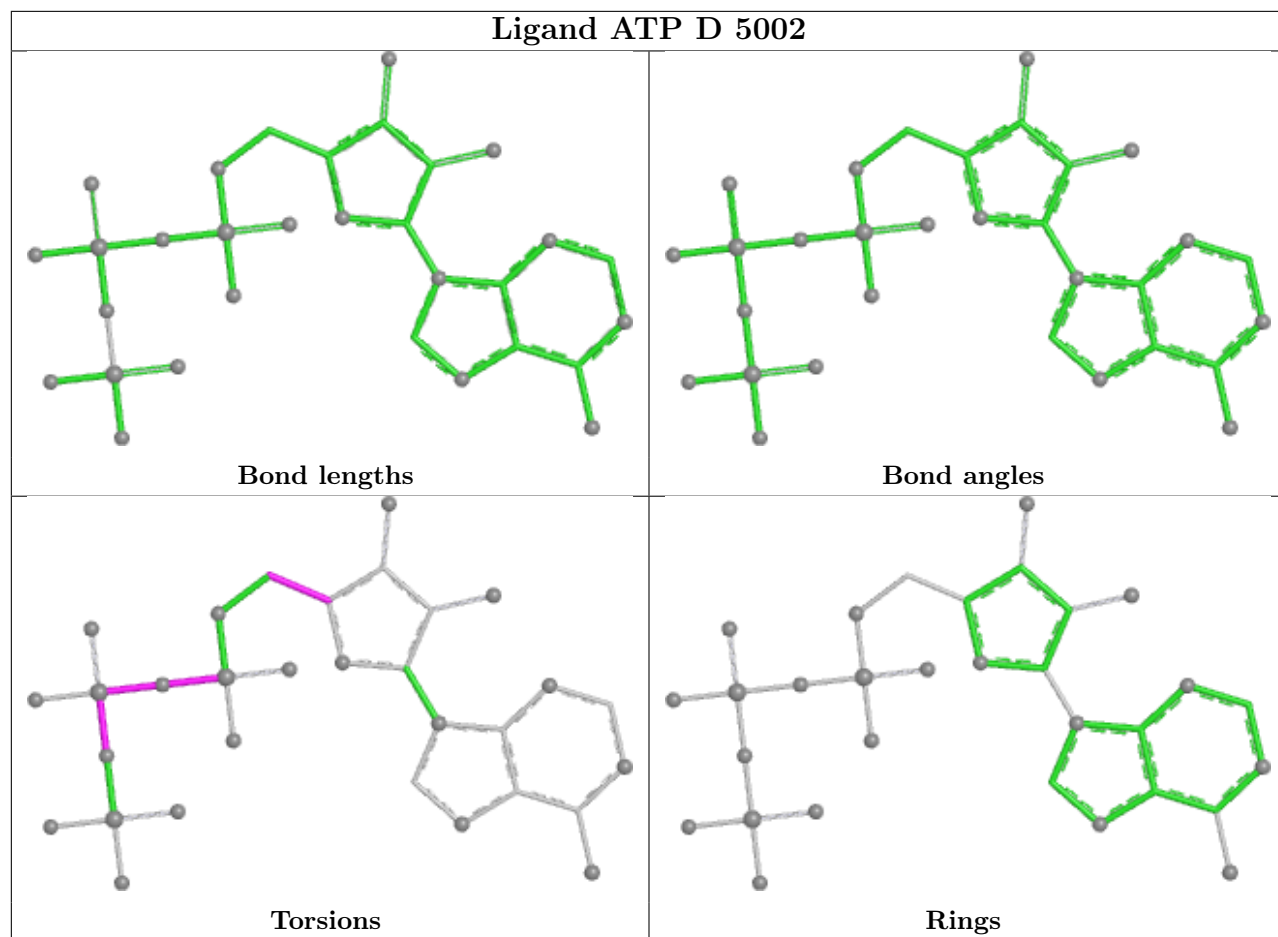
4 monomers are involved in 8 short contacts:

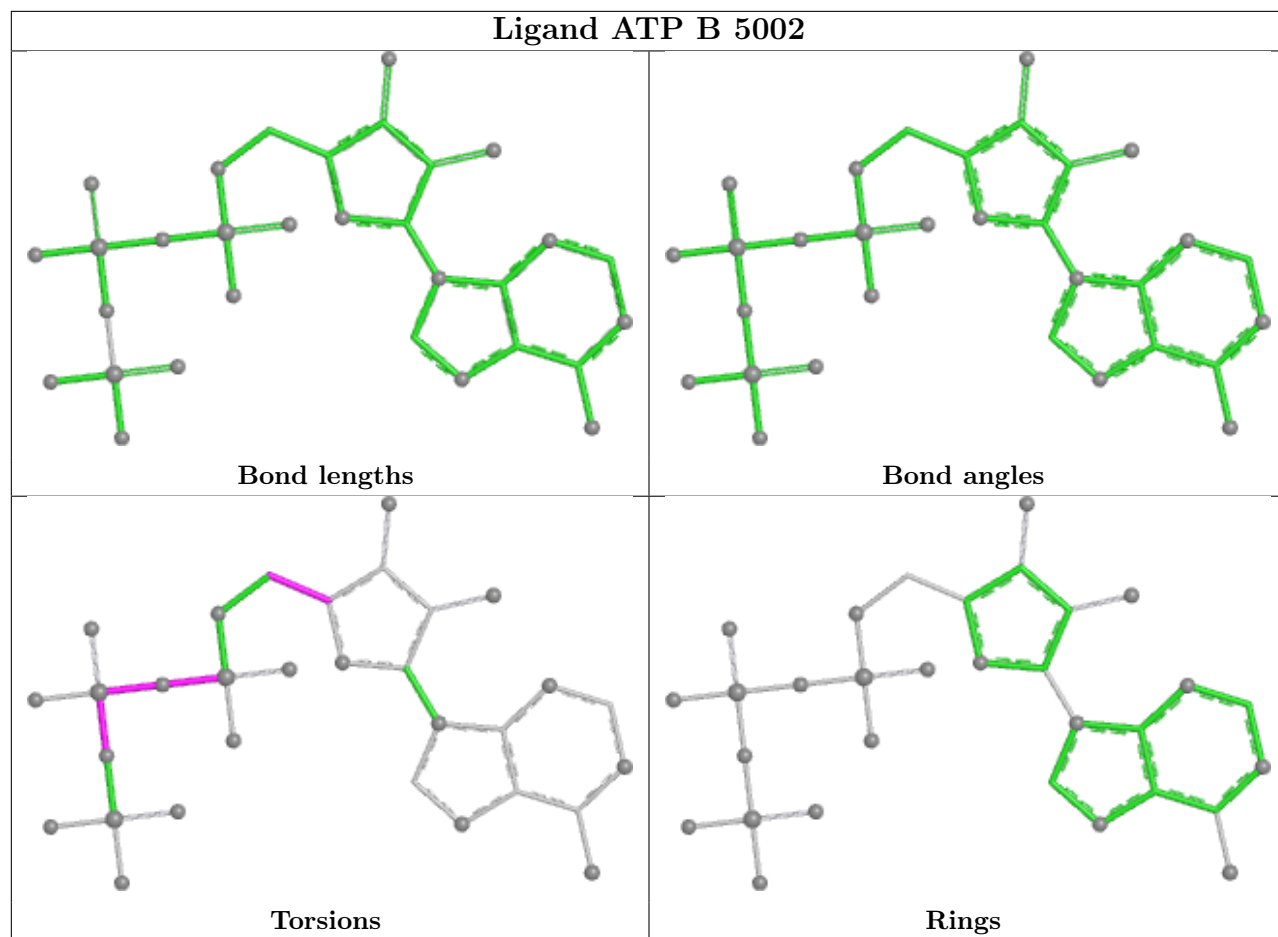
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5003	ATP	2	0
4	D	5003	ATP	2	0
4	B	5003	ATP	2	0
4	C	5003	ATP	2	0

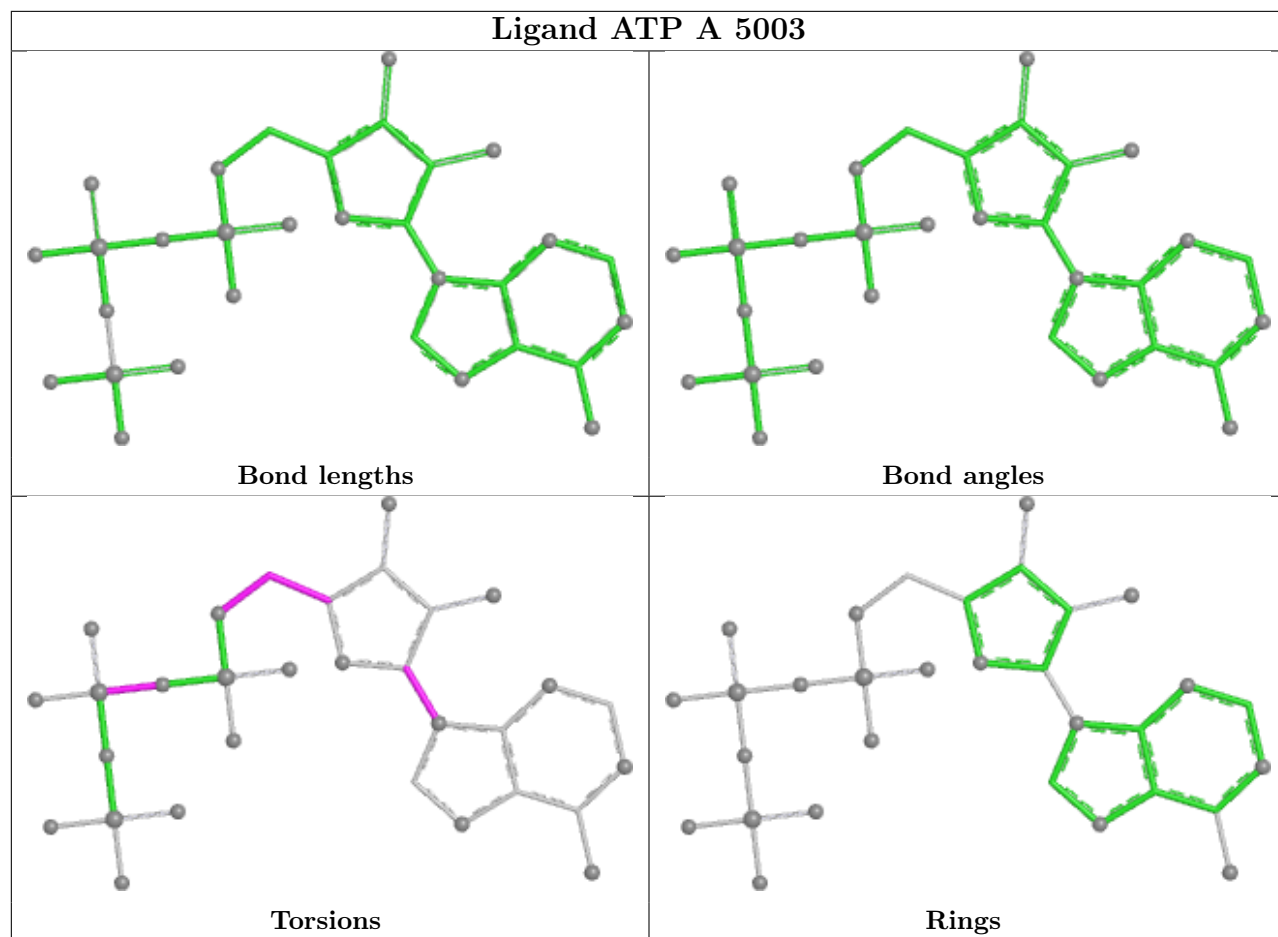
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

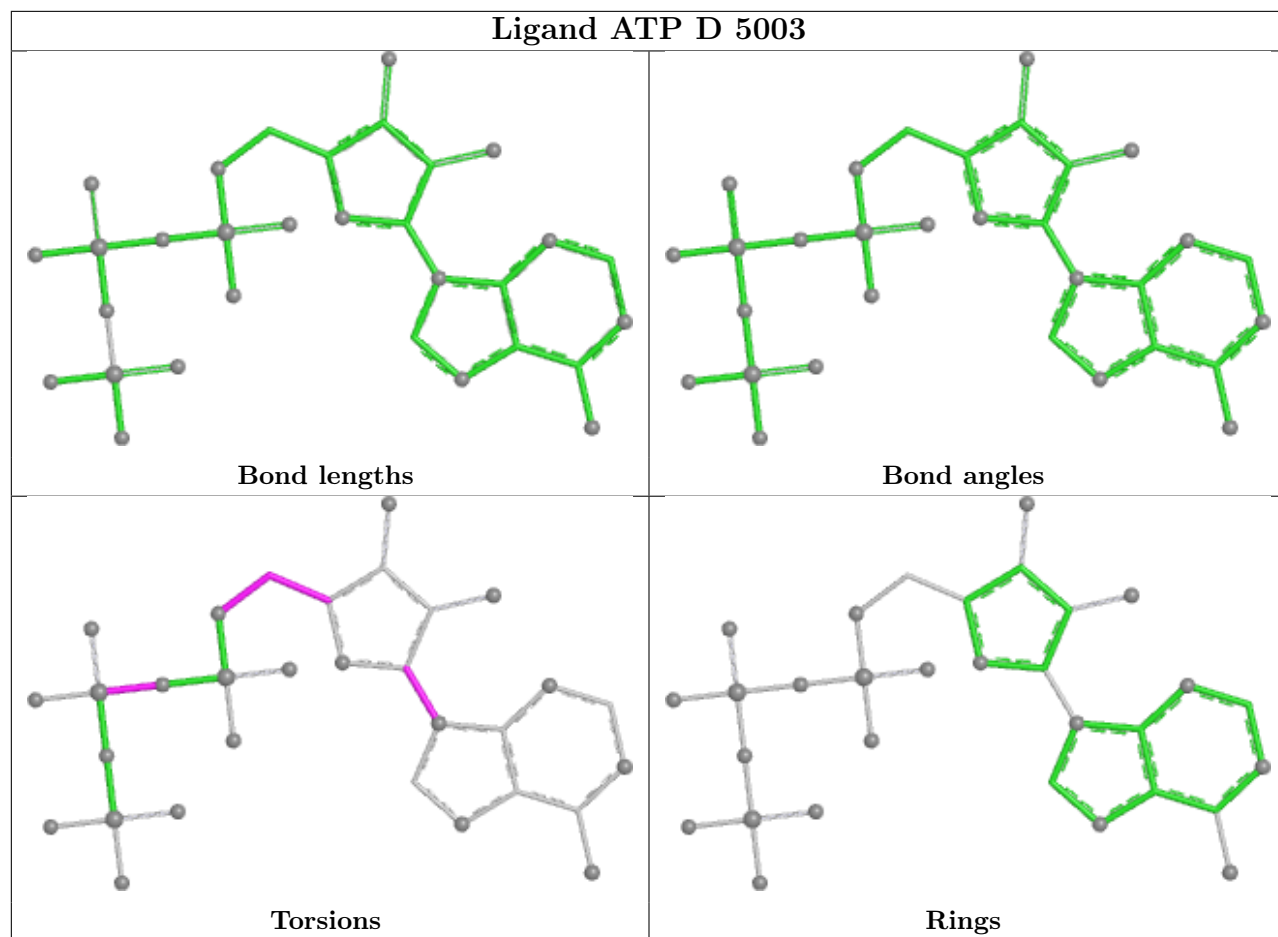
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

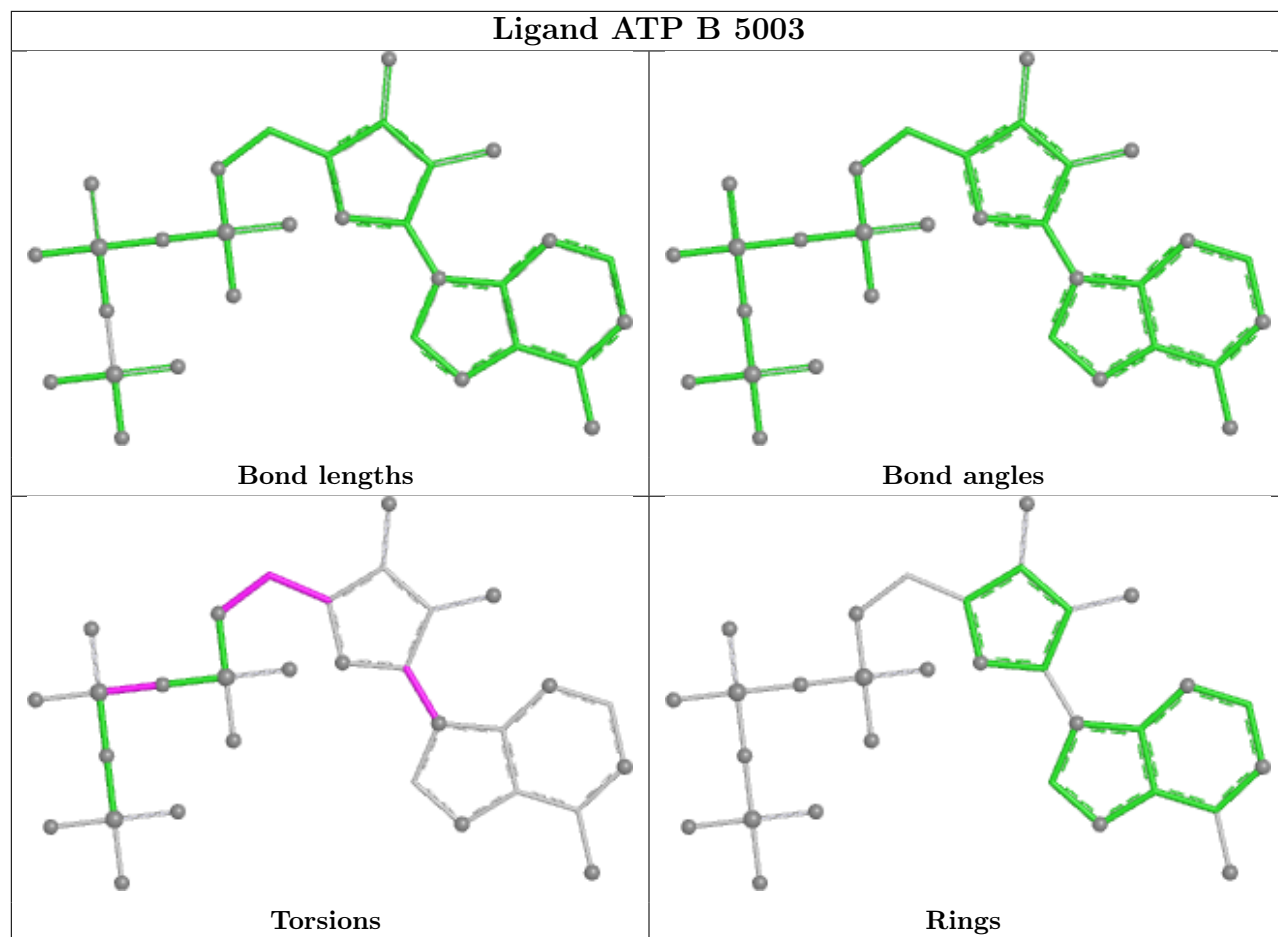


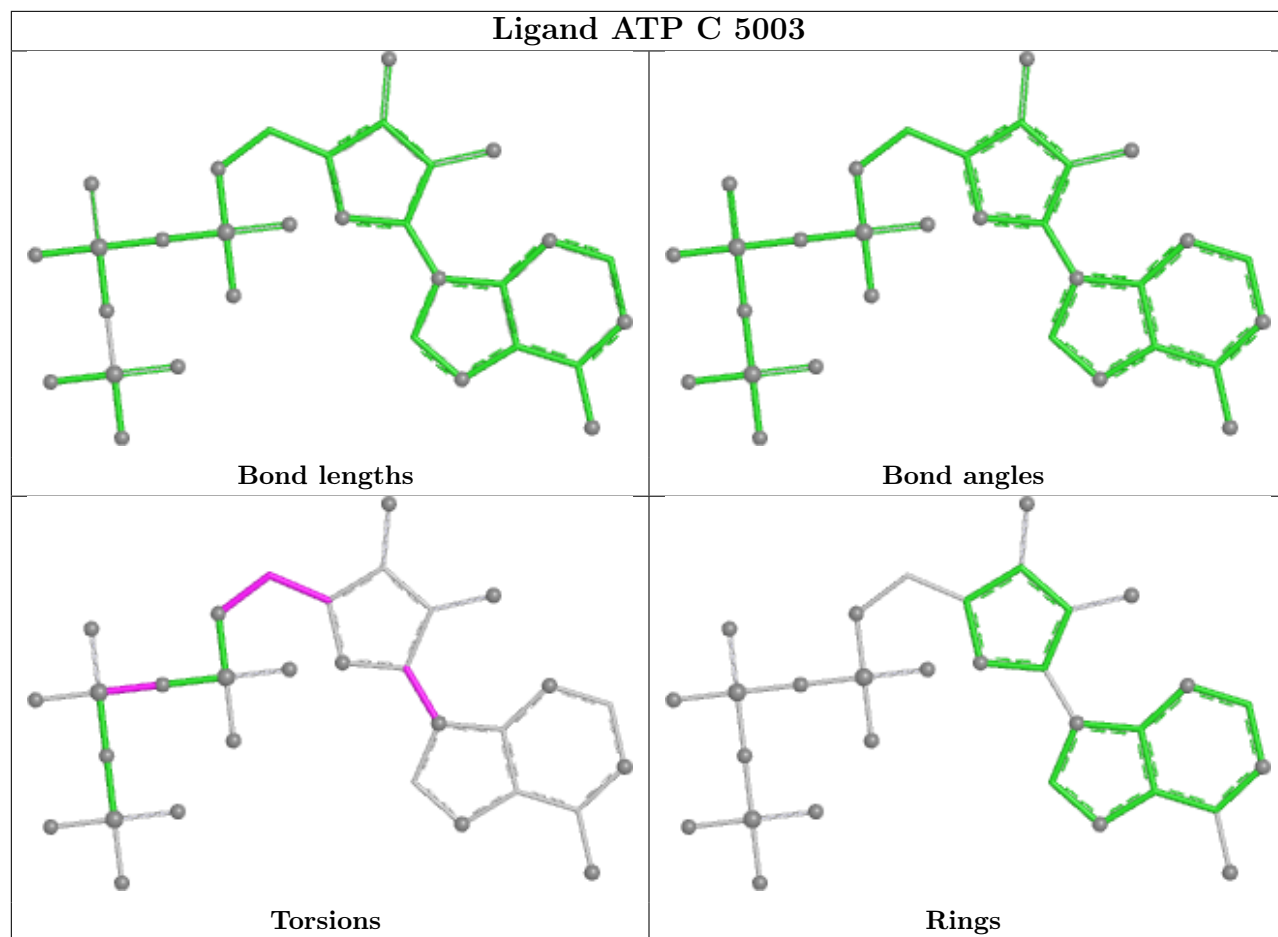


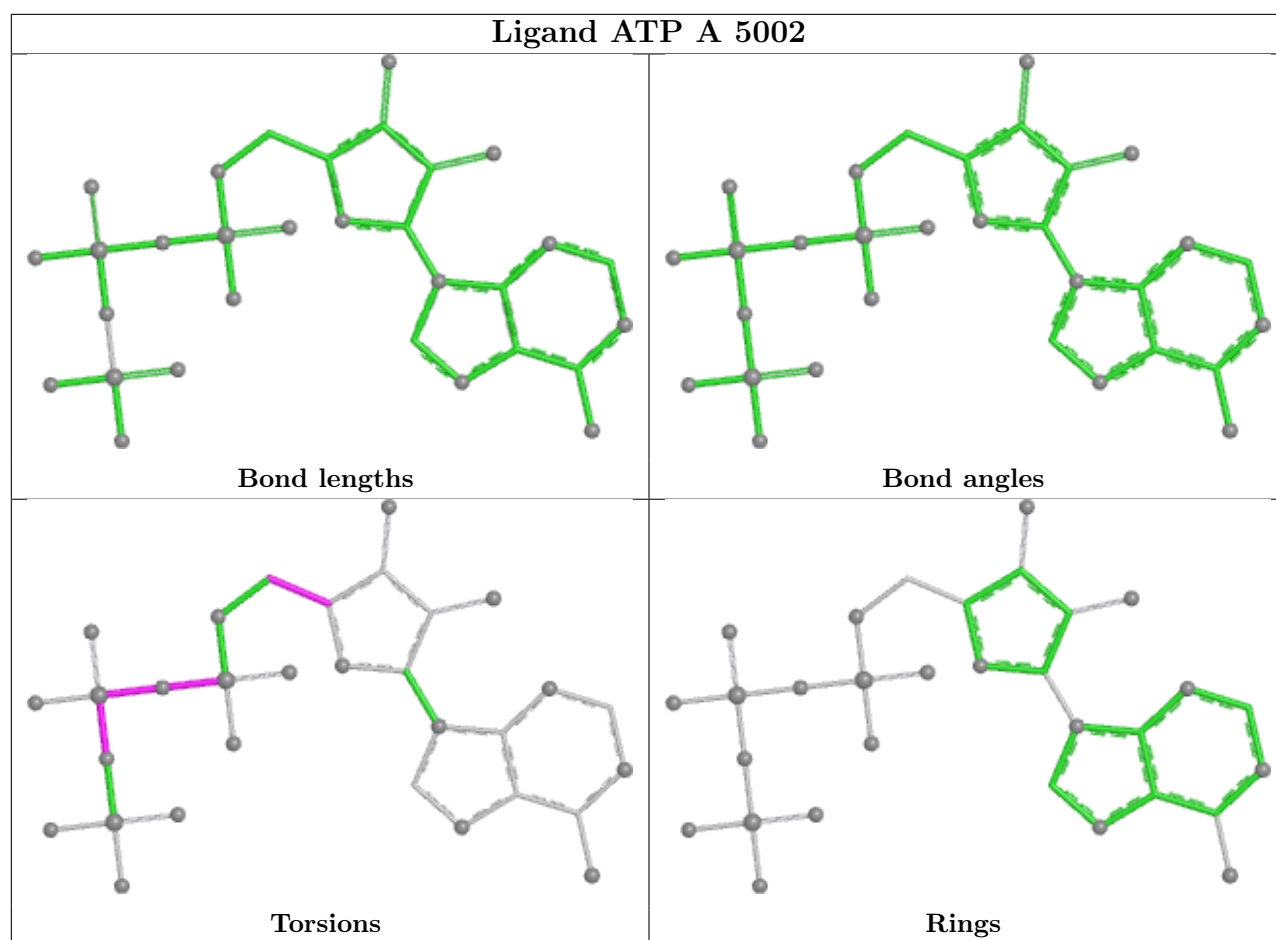












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

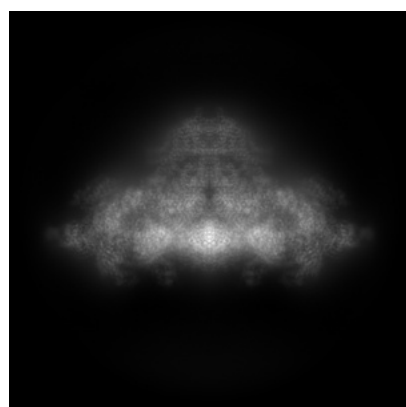
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26409. These allow visual inspection of the internal detail of the map and identification of artifacts.

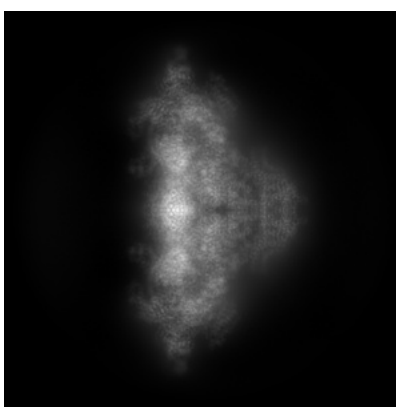
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

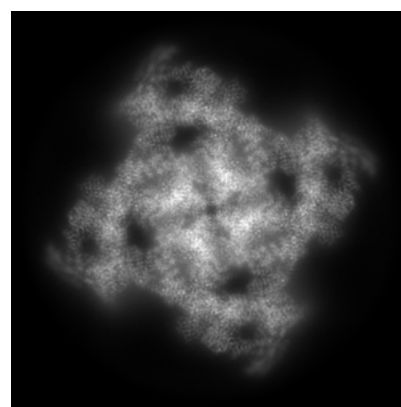
6.1.1 Primary map



X



Y

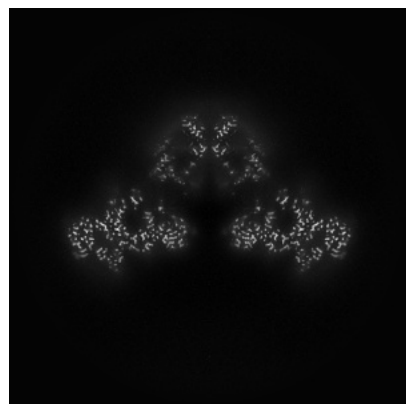


Z

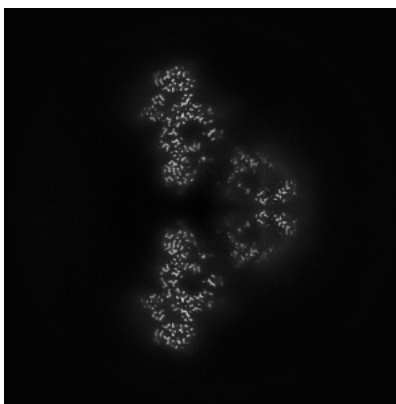
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

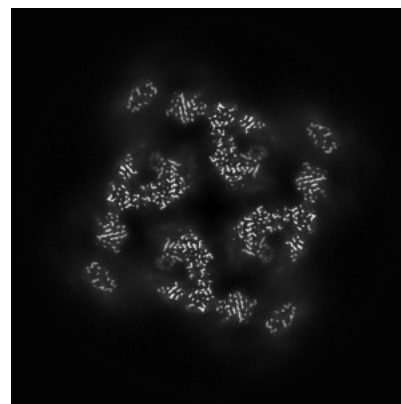
6.2.1 Primary map



X Index: 256



Y Index: 256

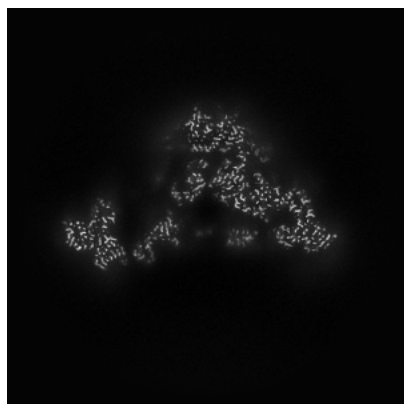


Z Index: 256

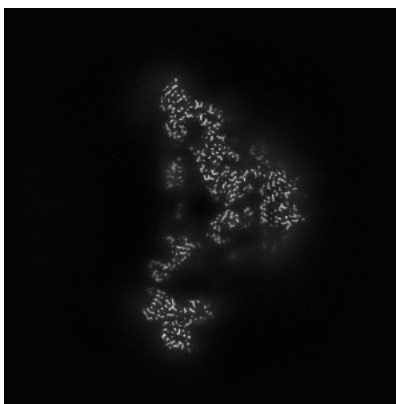
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

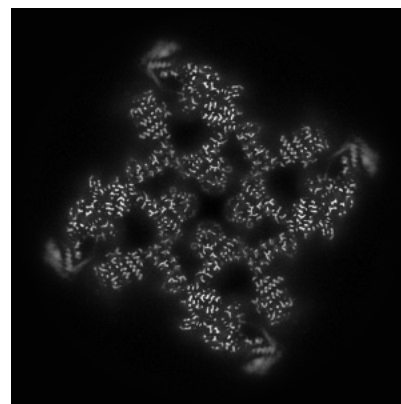
6.3.1 Primary map



X Index: 275



Y Index: 237

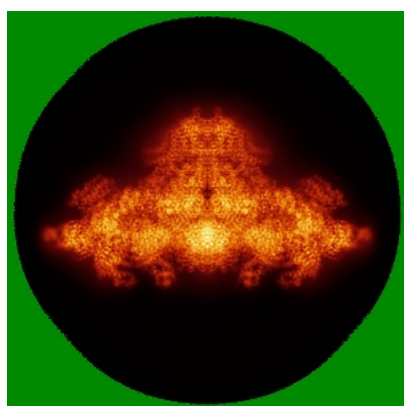


Z Index: 227

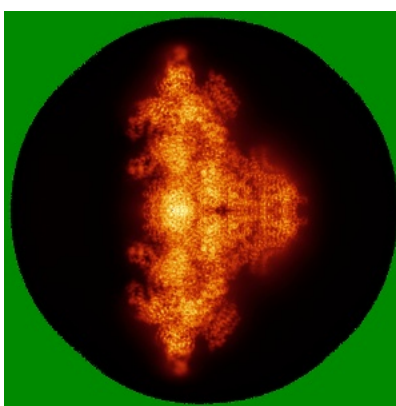
The images above show the largest variance slices of the map in three orthogonal directions.

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

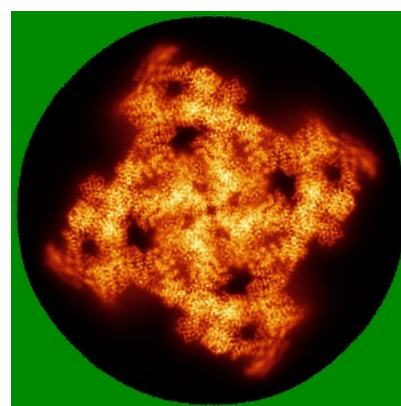
6.4.1 Primary map



X



Y

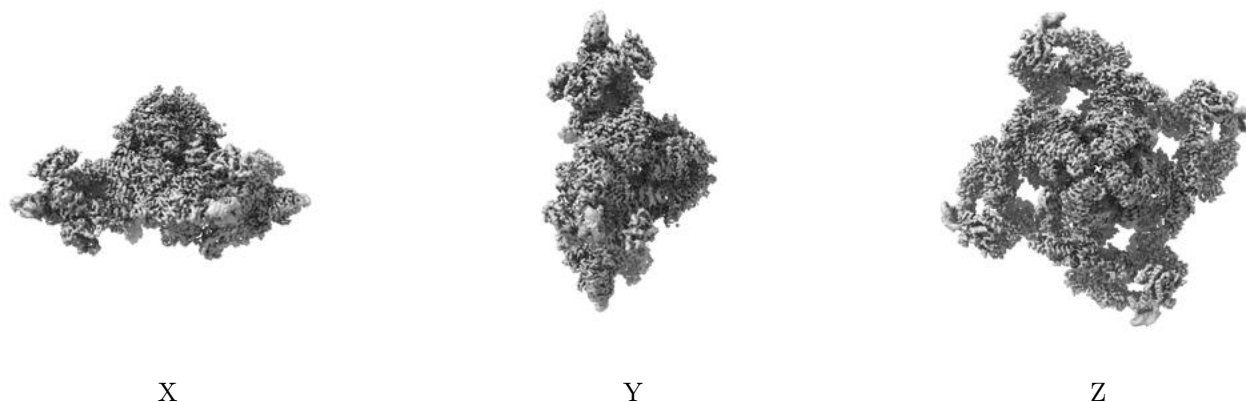


Z

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

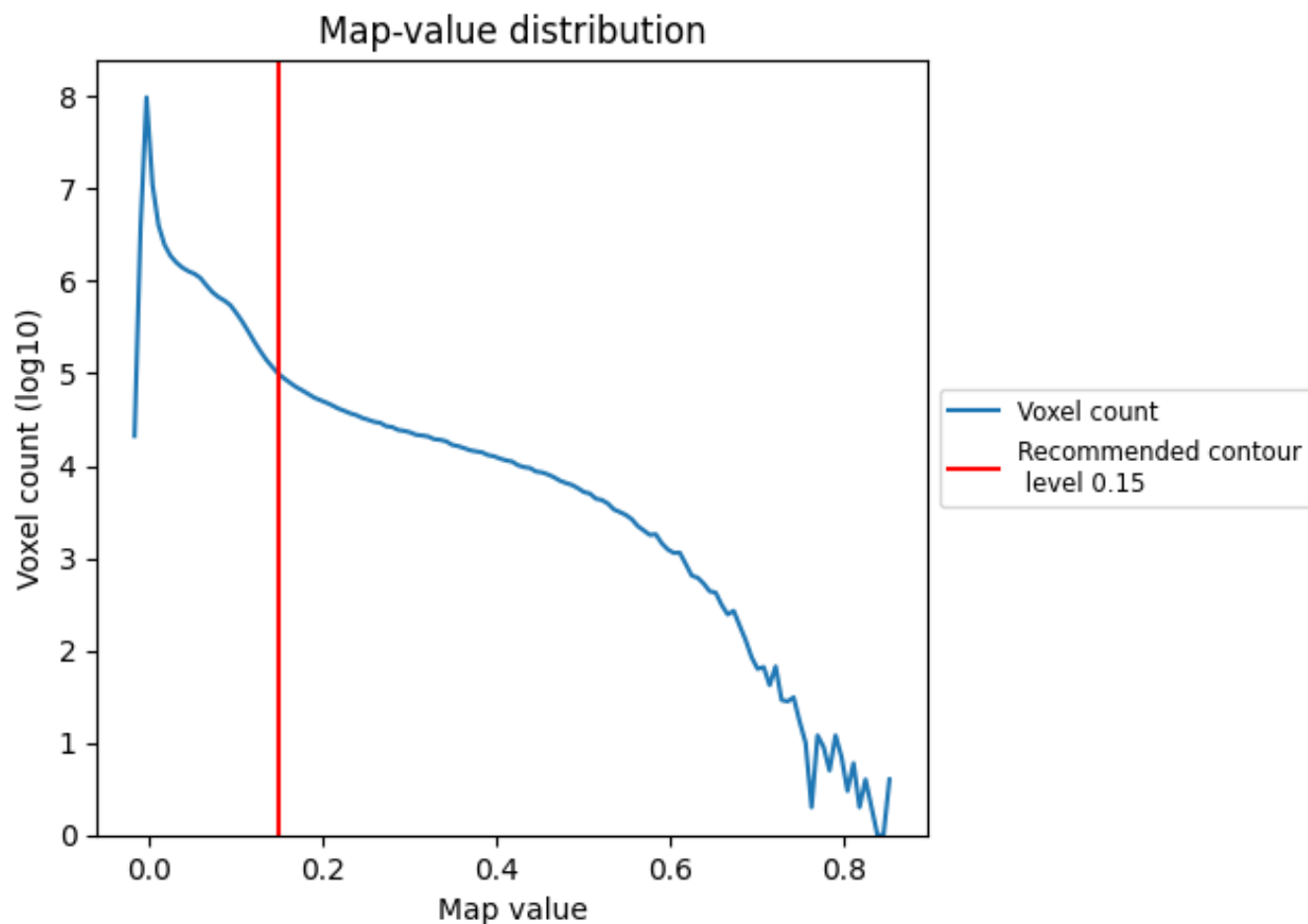
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

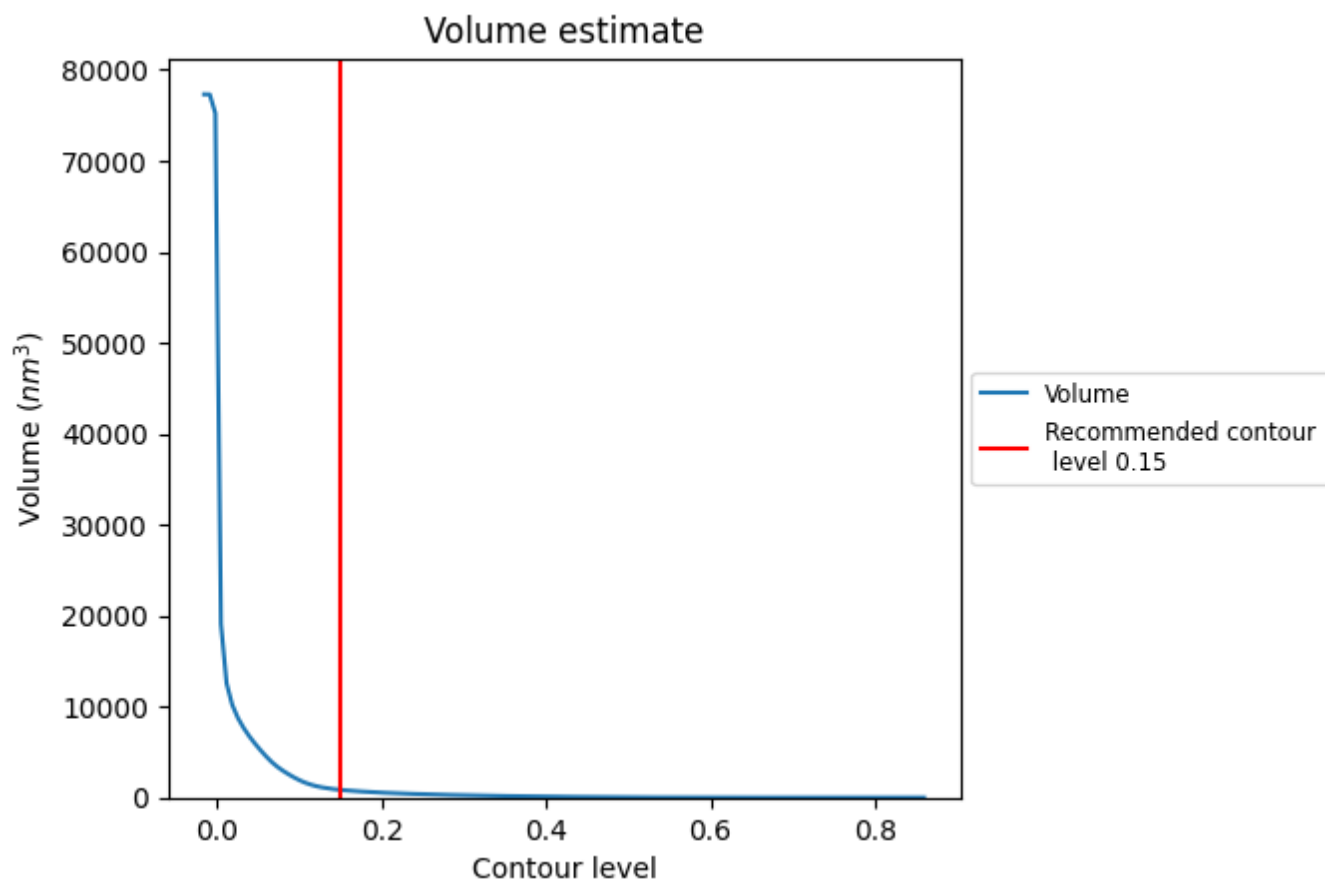
This section contains the results of statistical analysis of the map.

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.

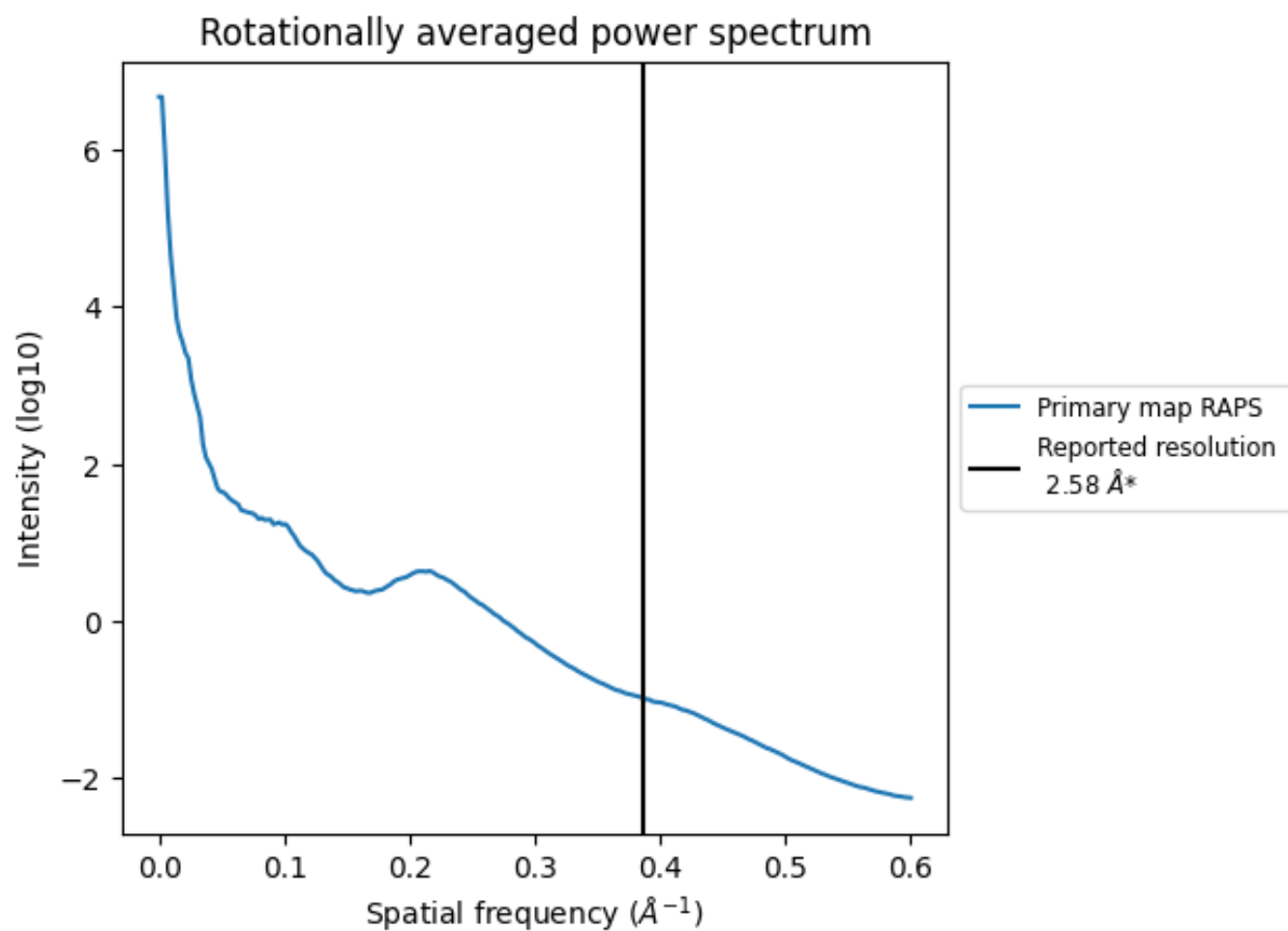
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 847 nm³; this corresponds to an approximate mass of 765 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 0.388 Å⁻¹

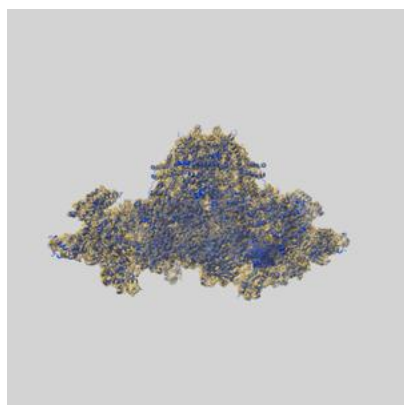
8 Fourier-Shell correlation ⓘ

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

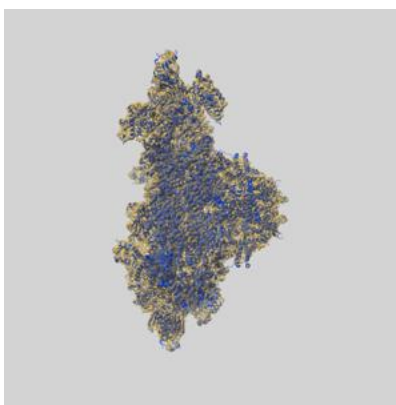
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26409 and PDB model 7U9X. Per-residue inclusion information can be found in section [3](#) on page [7](#).

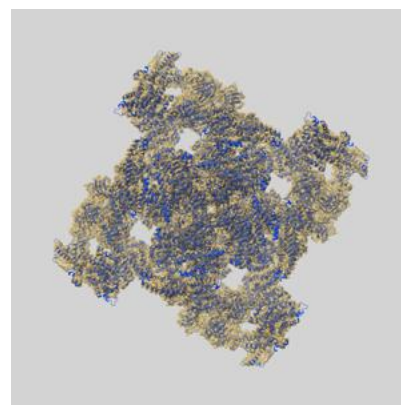
9.1 Map-model overlay [i](#)



X



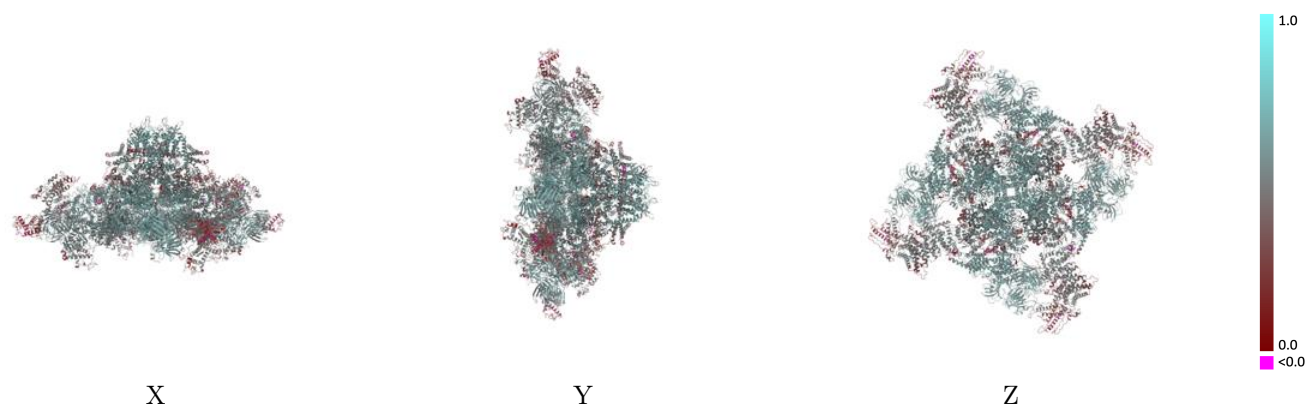
Y



Z

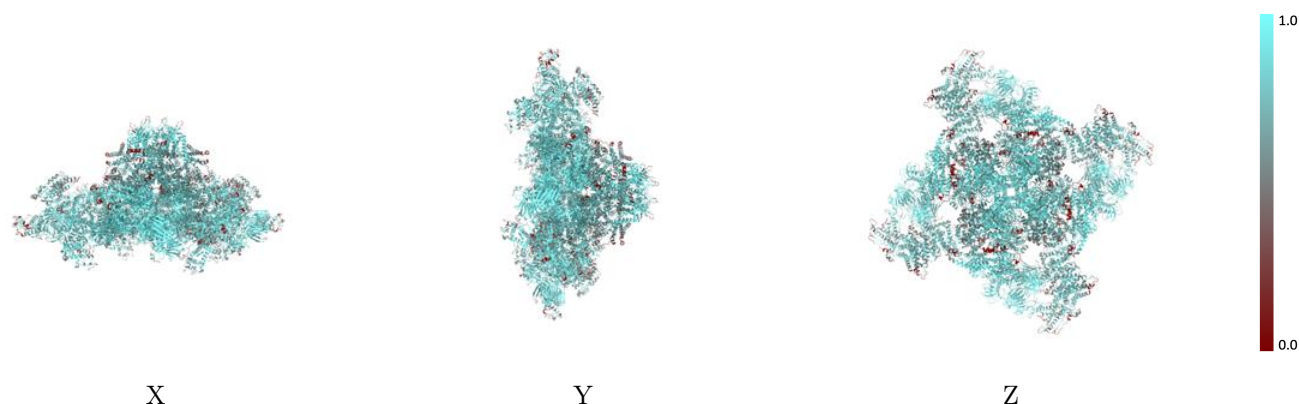
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



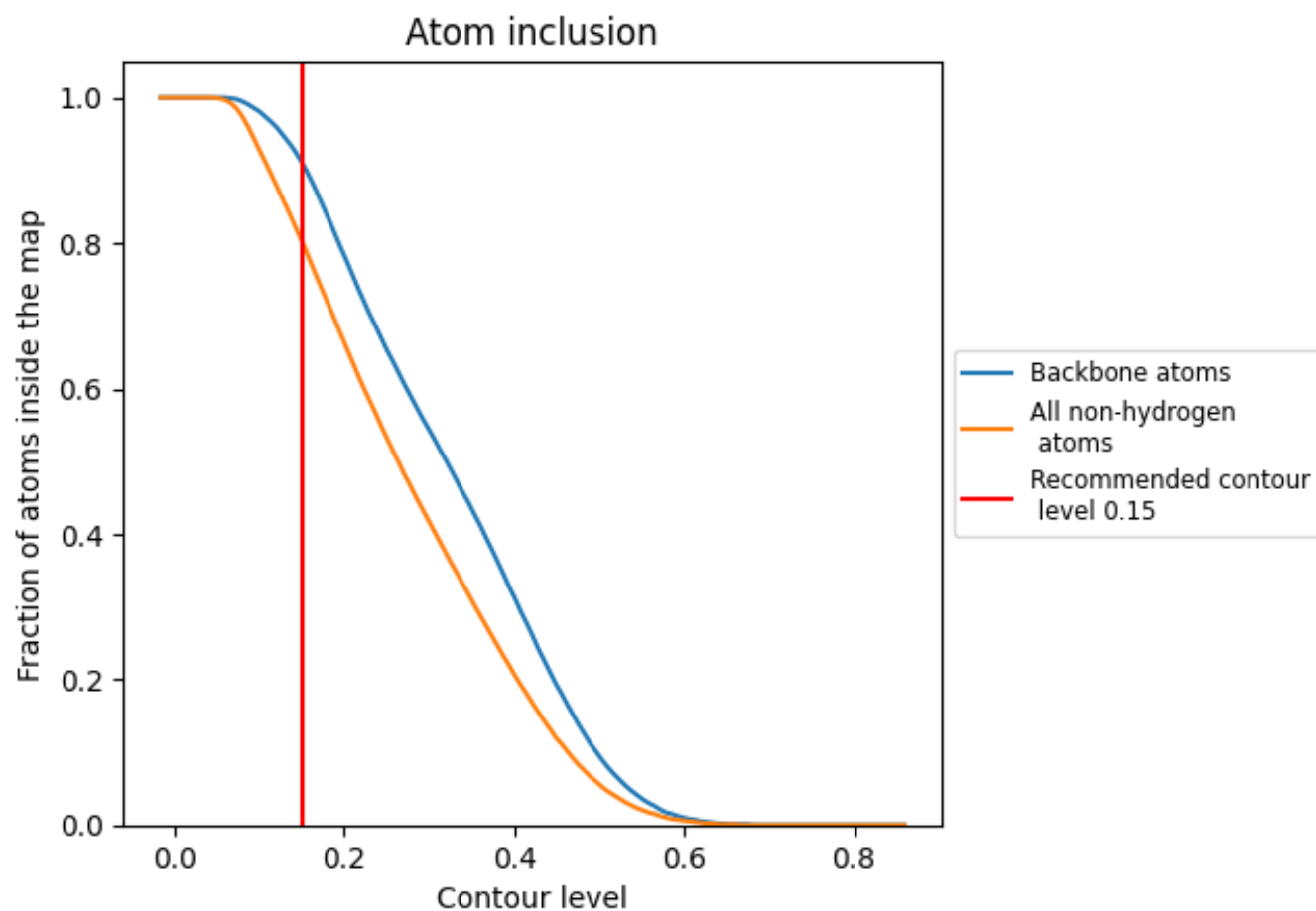
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 80% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.5150
A	0.8010	0.5150
B	0.8000	0.5100
C	0.8000	0.5100
D	0.8020	0.5170
E	0.9070	0.5880
F	0.8930	0.5750
G	0.9060	0.5720
H	0.9160	0.5910

1.0

0.0

<0.0