



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2023 – 12:50 PM EST

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.

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<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:

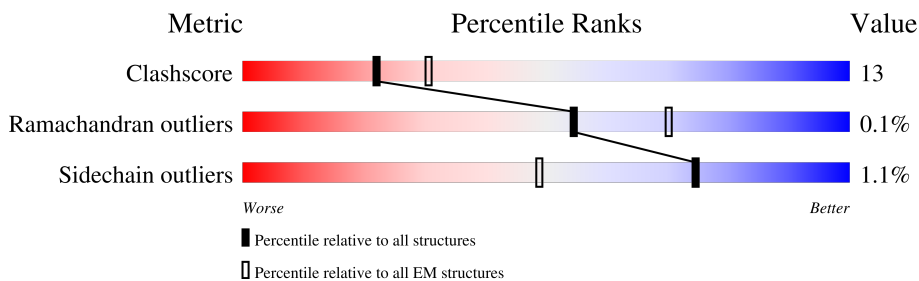
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 i

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
			Total	C	N	O	S		
1	E	107	818	516	144	154	4	0	0
1	F	107	818	516	144	154	4	0	0
1	G	107	818	516	144	154	4	0	0
1	H	107	818	516	144	154	4	0	0

- Molecule 2 is a protein called Ryanodine receptor 2.

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

There are 4 discrepancies between the modelled and reference sequences:

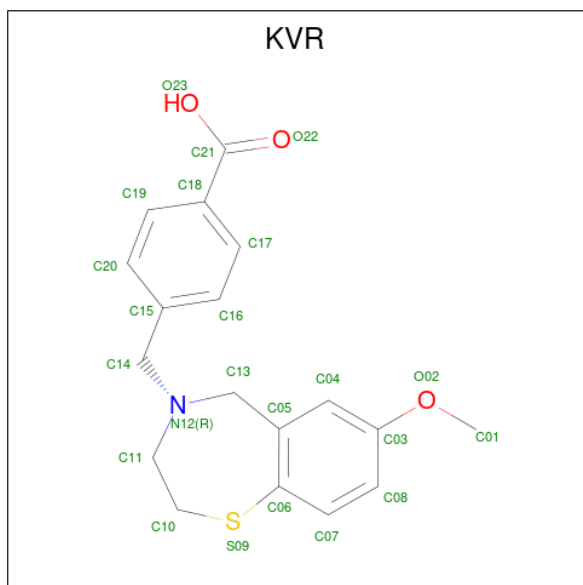
Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLN	ARG	conflict	UNP Q92736
B	420	GLN	ARG	conflict	UNP Q92736
C	420	GLN	ARG	conflict	UNP Q92736
D	420	GLN	ARG	conflict	UNP Q92736

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

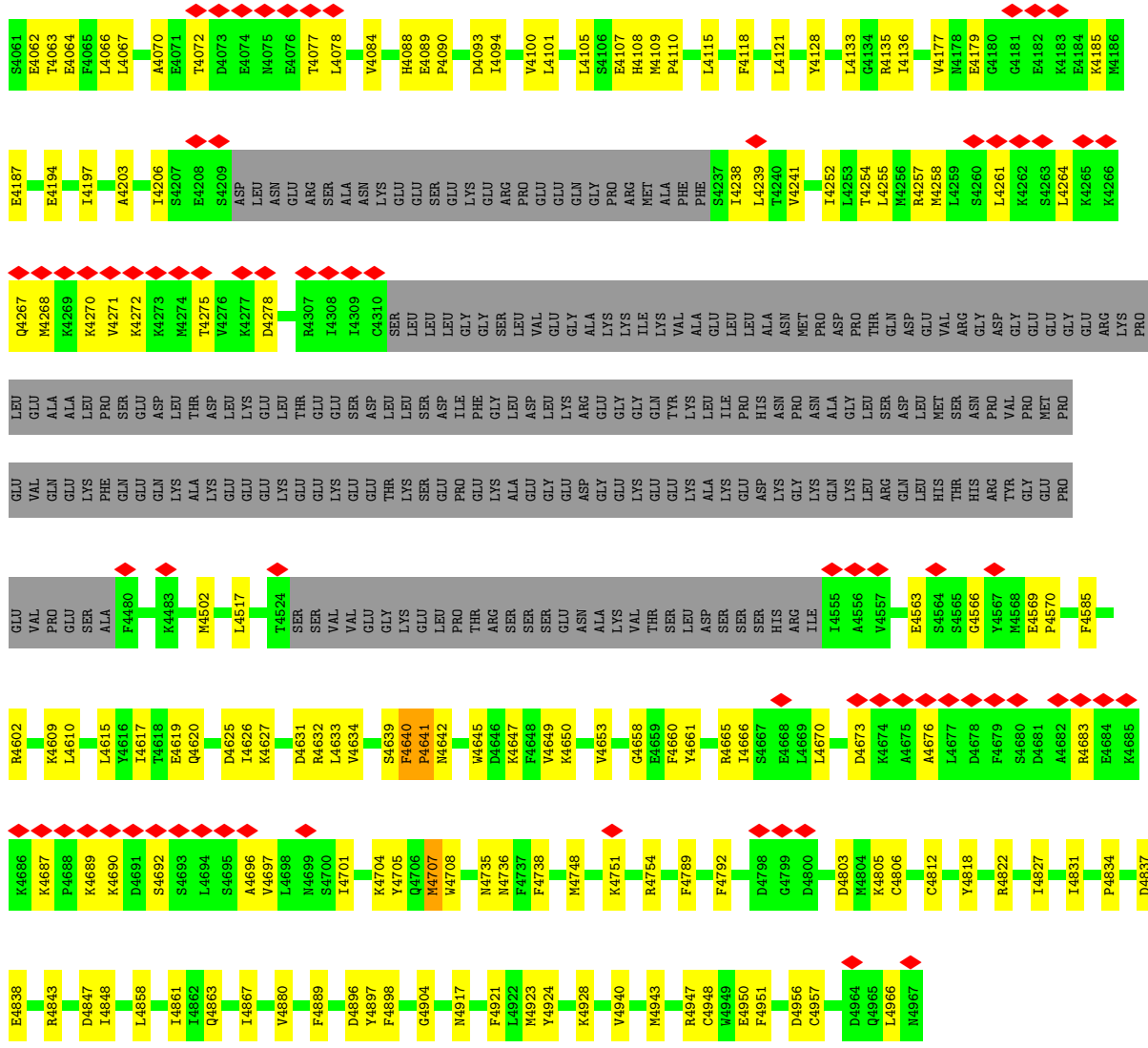
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	D	1	31	10	5	13	3	0

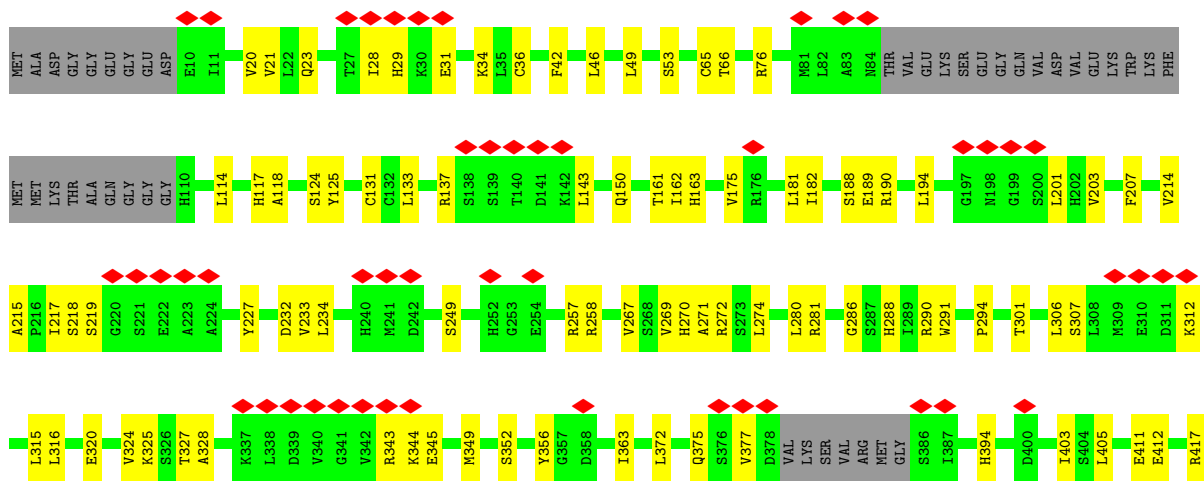
- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: C₁₈H₁₉NO₃S) (labeled as "Ligand of Interest" by depositor).

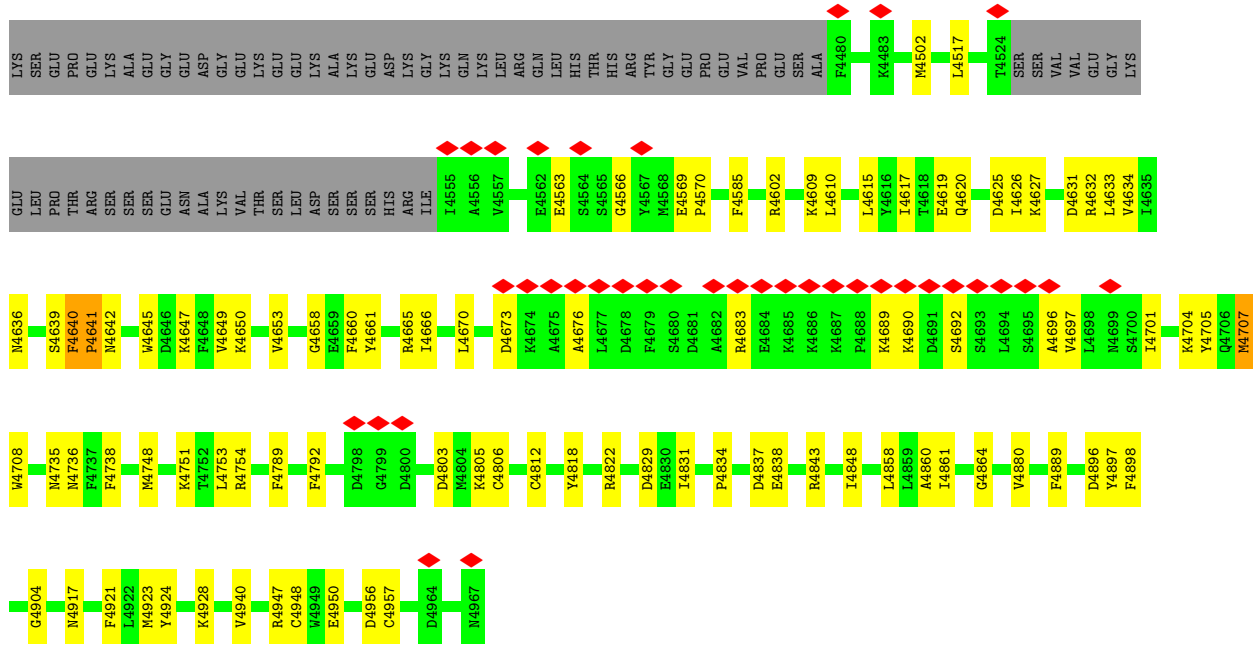


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	A	1	23	18	1	3	1	0
5	B	1	23	18	1	3	1	0
5	C	1	23	18	1	3	1	0
5	D	1	23	18	1	3	1	0

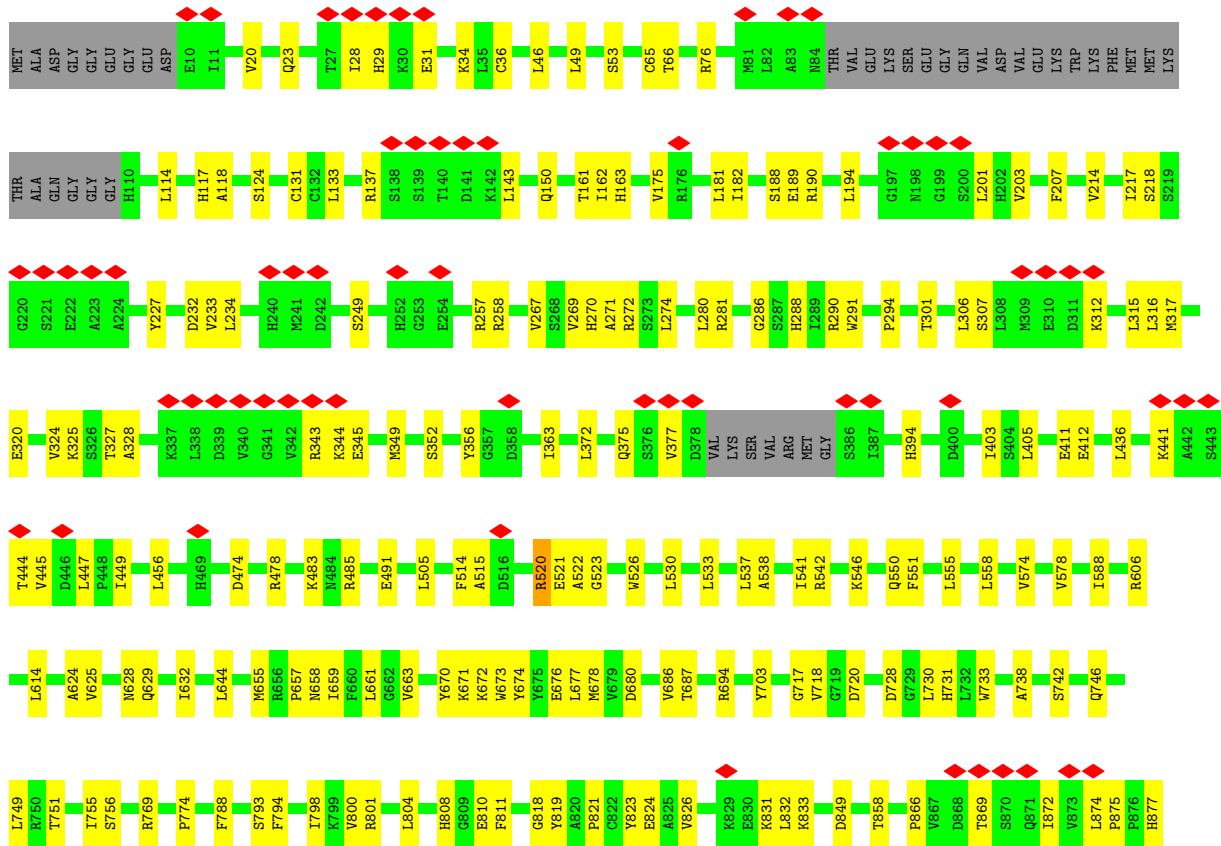


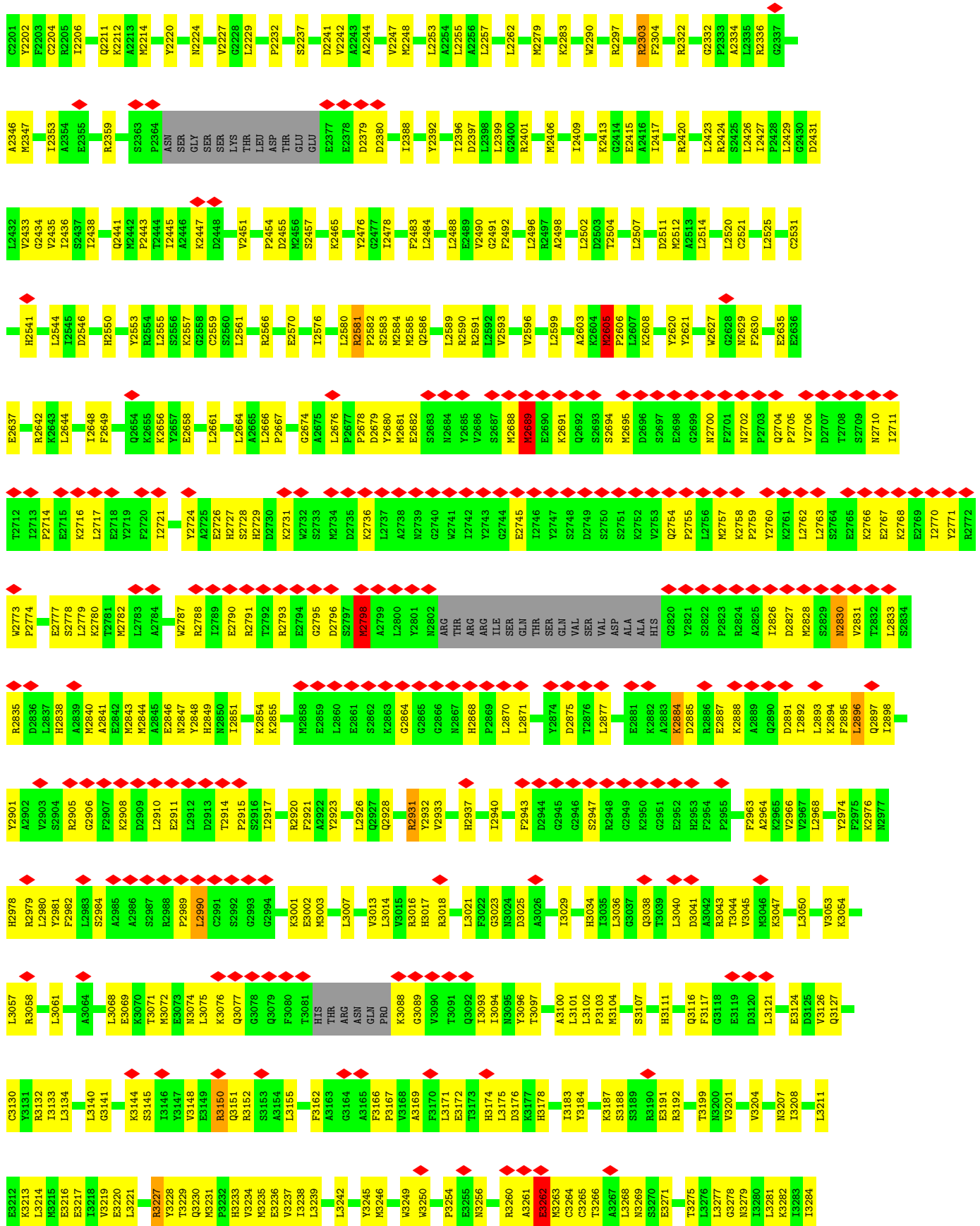
● Molecule 2: Ryanodine receptor 2

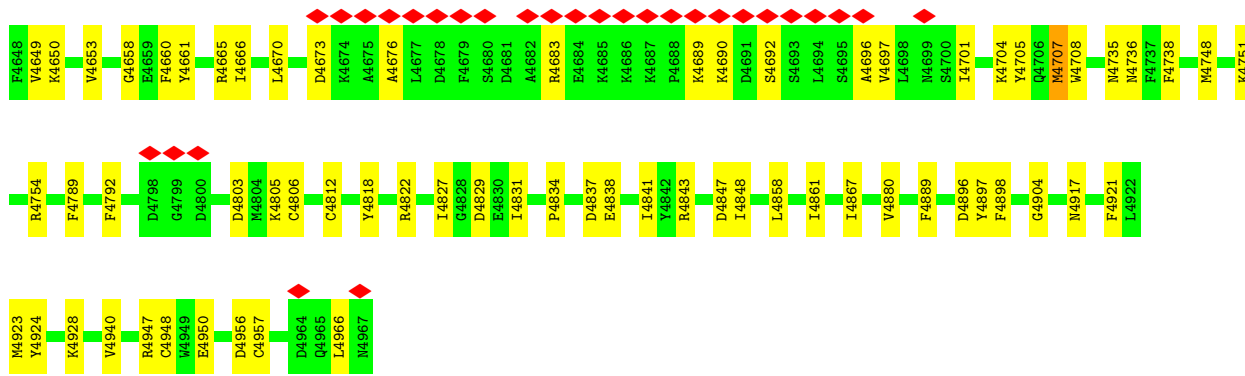




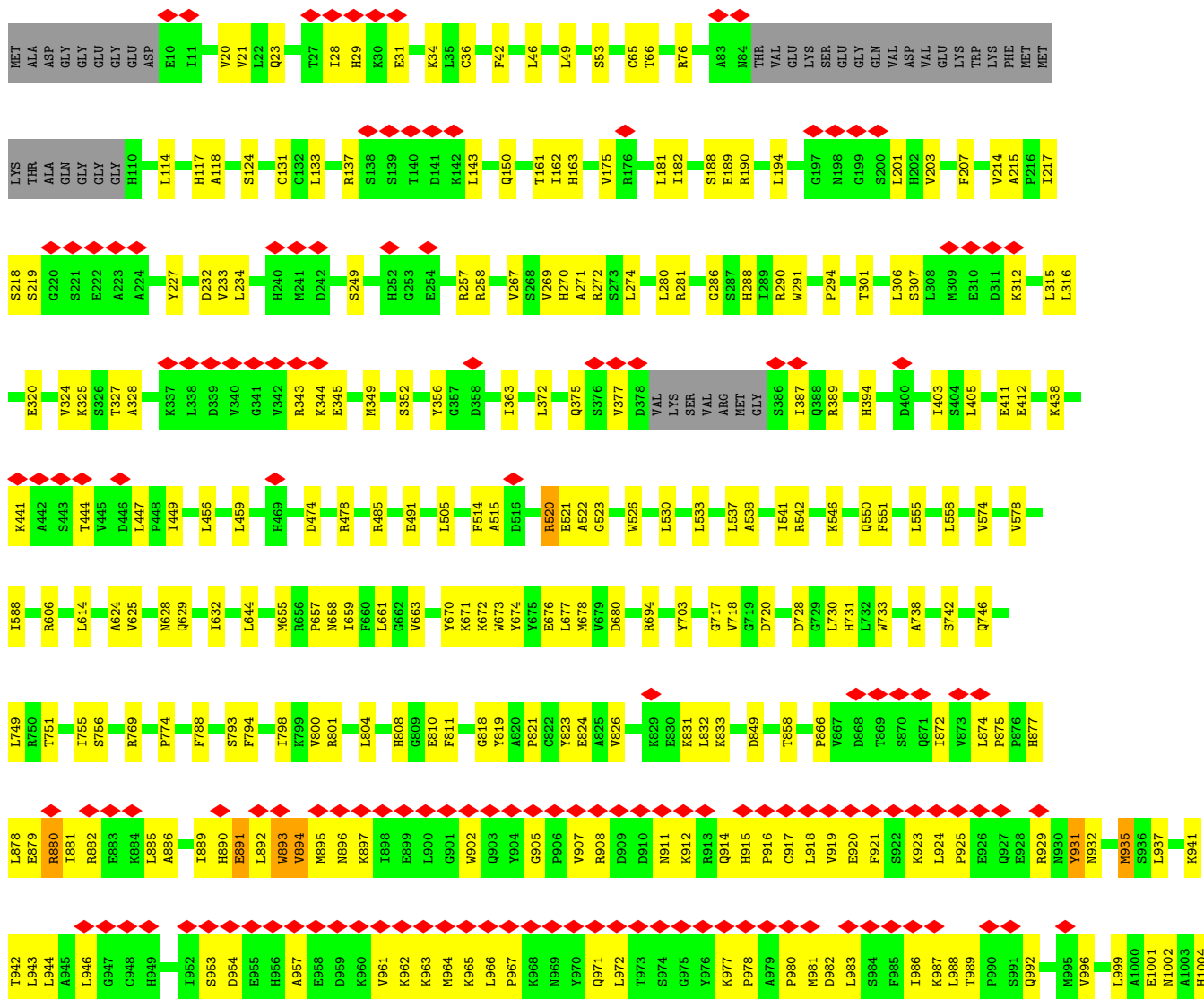
● Molecule 2: Ryanodine receptor 2

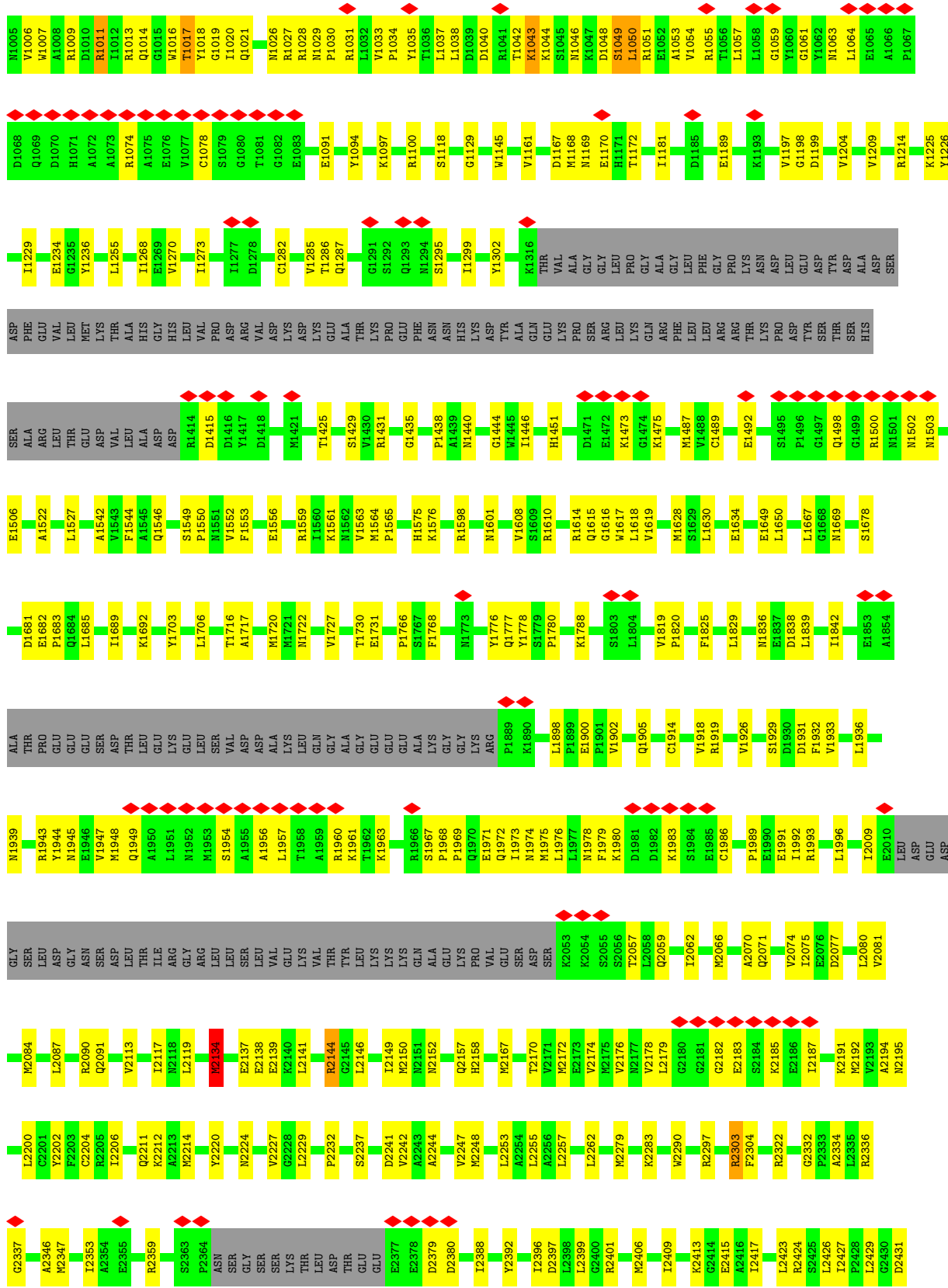




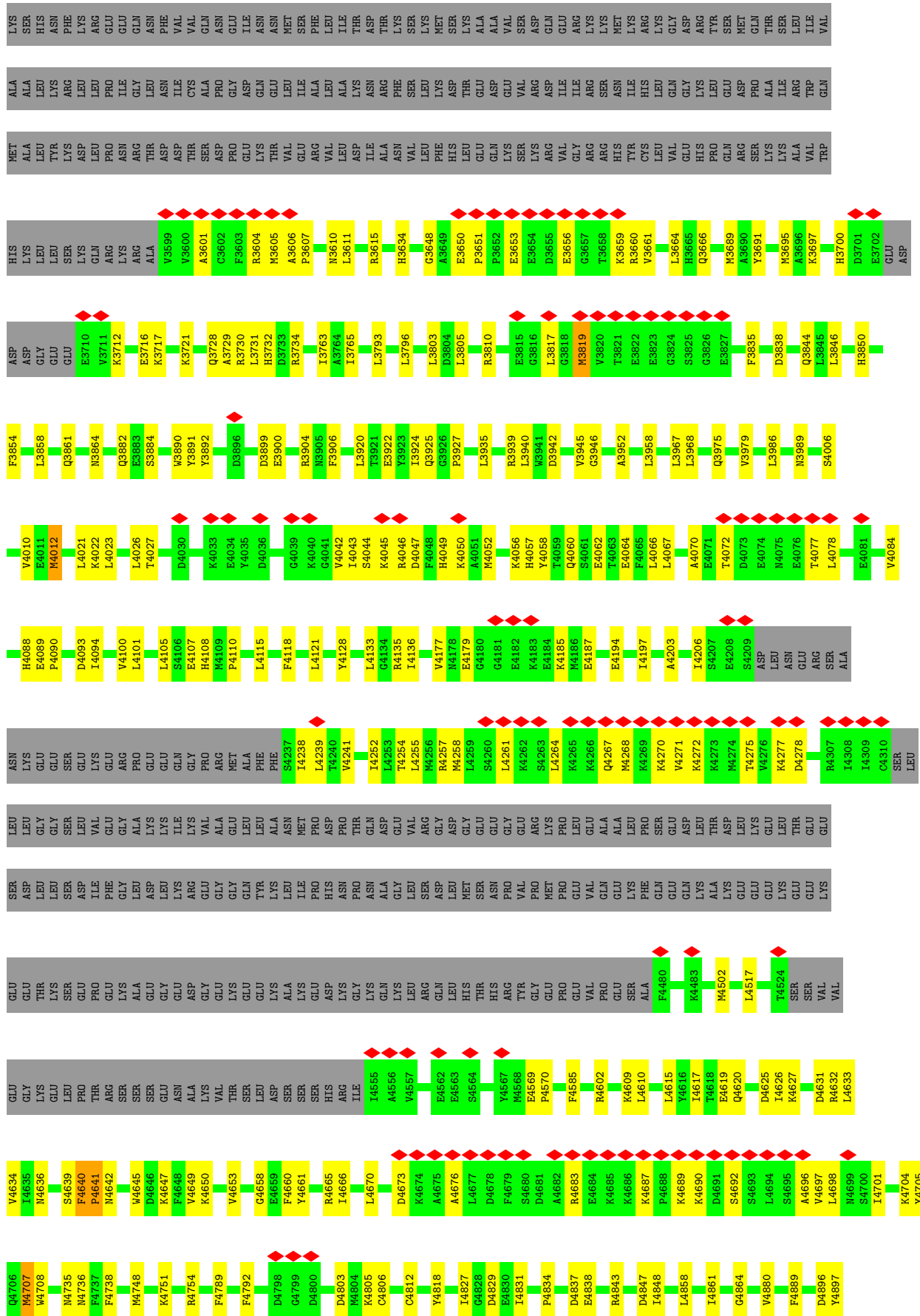


• Molecule 2: Ryanodine receptor 2





MET	I3280	V3126	K3054	K2976	Q2897	T2832	I2770	S2709	E2635	L2432
SER	L3281	Q3127	L3057	H2977	I2898	L2833	Y2771	N2710	E2636	V2433
GLU	K3282	C3130	R3058	R2978	Y2901	S2834	R2772	N2711	E2637	G2434
ALA	I3283	R3059	R3061	R2979	A2902	D2835	W2773	I2712	L2638	V2435
LEU	Y3284	L3061	L3064	L2980	V2903	R2836	W2774	T2713	I2639	I2436
LEU	Y3285	A3064	A3068	Y2981	S2904	L2837	P2774	I2714	S2437	S2437
ILE	N3286	L3068	L3069	L2983	R2905	H2838	E2777	P2715	I2438	I2438
LEU	K3287	E3069	E3070	S2984	R2906	A2839	S2778	E2716	Q2441	Q2441
ASP	N3288	E3071	E3072	A2985	G2907	N2840	K2779	K2716	L2442	L2442
ASP	G3289	M3072	M3073	A2986	F2908	K2841	K2780	L2717	P2443	P2443
GLU	K3290	T3071	T3072	S2987	K2909	N2843	T2781	E2718	T2444	T2444
PHE	I3291	R2988	R2989	K2988	D2909	M2844	M2782	Y2719	L2585	L2585
THR	E3292	E3073	E3074	L2910	L2910	N2844	L2783	F2720	K2557	K2557
LEU	M3293	N3074	N3075	L2911	E2911	E2845	Y2784	I2721	G2558	G2558
ALA	K3294	L3074	L3075	L2912	E2912	A2846	W2787	I2722	Y2560	Y2560
ALA	K3297	K3144	K3145	L2913	E2913	N2847	R2788	Y2724	L2561	L2561
ARG	Y3298	I3146	I3147	D2913	T2913	N2848	A2725	A2725	R2566	R2566
ASP	L3299	Y3148	Y3149	T2914	T2914	H2849	E2726	H2726	P2454	P2454
LEU	A3300	E3149	E3150	S2992	T2915	I2851	H2727	H2727	D2455	D2455
LEU	V3301	G3077	G3078	S2993	P2915	K2854	S2728	S2728	A2456	A2456
ALA	Q3304	Q3079	Q3080	G2994	I2917	L2855	R2729	H2729	S2457	S2457
PHE	I3307	R3081	R3082	K3001	I2917	K2854	D2730	D2730	I2576	I2576
PRO	N3308	HIS	HIS	E3002	R2920	K2855	K2731	K2731	K2465	K2465
LEU	K3309	THR	THR	E3003	F2921	M2858	W2732	W2732	R2581	R2581
LEU	V3310	ARG	ARG	M3003	A2922	E2859	S2733	S2733	Y2476	Y2476
ILE	K3311	ASN	ASN	L3007	Y2923	L2860	D2734	D2734	G2477	G2477
VAL	L3315	GLN	GLN	L3007	Y2923	E2861	W2735	W2735	S2583	S2583
ASP	L3242	PRO	PRO	V3013	L2926	S2862	K2736	K2736	M2584	M2584
ASN	Y3245	K3088	K3089	L3014	Q2927	S2863	L2737	L2737	F2483	F2483
ARG	M3246	G3088	G3089	V3015	Q2927	S2864	A2738	A2738	L2484	L2484
ALA	W3249	V3089	V3090	H3017	Q2928	G2865	M2739	M2739	L2468	L2468
TRP	W3250	T3091	T3092	R3018	Q2928	G2866	Y2801	Y2801	E2489	E2489
LEU	P3254	L3092	L3093	R3018	Y2933	G2866	L2800	L2800	V2490	V2490
GLU	E3255	F3022	F3023	R3022	Y2933	H2867	Y2802	Y2802	G2491	G2491
ASN	N3256	G3023	G3024	D3025	Y2933	H2868	N2802	N2802	F2492	F2492
PRO	R3260	H3024	H3025	D3025	Y2933	G2869	ARG	ARG	L2496	L2496
ALA	A3261	L3029	L3030	D3025	Y2933	H2869	THR	THR	R2497	R2497
GLU	K3262	L3101	L3102	D3025	Y2933	H2870	ILE	ILE	A2498	A2498
LEU	M3263	L3102	L3103	D3025	Y2933	L2871	GLN	GLN	L2502	L2502
PHE	T3266	M3104	M3105	D3025	Y2933	Y2874	THR	THR	D2603	D2603
ARG	T3266	S3107	S3108	D3025	Y2933	D2875	SER	SER	K2604	K2604
MET	K3267	K3187	K3188	D3025	Y2933	T2876	GLN	GLN	M2605	M2605
ALA	L3268	E3110	E3111	D3025	Y2933	L2877	SER	SER	T2504	T2504
ALA	N3269	H3111	H3112	D3025	Y2933	L2877	VAL	VAL	L2507	L2507
VAL	E3271	Q3116	Q3117	D3025	Y2933	E2881	ASP	ASP	P2511	P2511
PHE	T3275	G3118	G3119	D3025	Y2933	K2882	ALA	ALA	M2512	M2512
ILE	L3277	E3119	E3120	D3025	Y2933	A2883	ALA	ALA	K2619	K2619
TRP	G3278	F3117	F3118	D3025	Y2933	D2885	HIS	HIS	Y2620	Y2620
SER	N3279	M3046	M3047	D3025	Y2933	E2887	G2820	G2820	G2626	G2626
		L3050	L3053	D3025	Y2933	D2888	Y2821	Y2821	W2627	W2627
		V3204	V3053	D3025	Y2933	D2889	S2822	S2822	N2629	N2629
				D3025	Y2933	K2965	P2823	P2823	F2630	F2630
				D3025	Y2933	V2966	R2824	R2824		
				D3025	Y2933	L2968	A2825	A2825		
				D3025	Y2933	Y2974	D2827	D2827		
				D3025	Y2933	F2975	M2828	M2828		
				D3025	Y2933	L2893	L2762	L2762		
				D3025	Y2933	F2895	L2763	L2763		
				D3025	Y2933	L2896	S2764	S2764		
				D3025	Y2933		E2765	E2765		
				D3025	Y2933		K2766	K2766		
				D3025	Y2933		E2767	E2767		
				D3025	Y2933		K2768	K2768		
				D3025	Y2933		E2769	E2769		





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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.31	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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	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%)	51	84
2	B	4198/4967 (84%)	4061 (97%)	132 (3%)	5 (0%)	51	84
2	C	4198/4967 (84%)	4061 (97%)	132 (3%)	5 (0%)	51	84
2	D	4198/4967 (84%)	4060 (97%)	133 (3%)	5 (0%)	51	84
All	All	17212/20300 (85%)	16655 (97%)	537 (3%)	20 (0%)	54	84

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 [i](#)

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%)	73	88
1	F	88/89 (99%)	87 (99%)	1 (1%)	73	88
1	G	88/89 (99%)	87 (99%)	1 (1%)	73	88
1	H	88/89 (99%)	87 (99%)	1 (1%)	73	88
2	A	3708/4358 (85%)	3667 (99%)	41 (1%)	73	88
2	B	3708/4358 (85%)	3667 (99%)	41 (1%)	73	88
2	C	3708/4358 (85%)	3667 (99%)	41 (1%)	73	88
2	D	3708/4358 (85%)	3667 (99%)	41 (1%)	73	88
All	All	15184/17788 (85%)	15016 (99%)	168 (1%)	74	88

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 monosaccharides 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	D	5002	-	26,33,33	0.61	0	31,52,52	0.82	2 (6%)
4	ATP	C	5003	-	26,33,33	0.66	0	31,52,52	0.77	1 (3%)
5	KVR	C	5004	-	24,25,25	0.50	0	32,34,34	0.83	2 (6%)
4	ATP	D	5003	-	26,33,33	0.67	0	31,52,52	0.77	1 (3%)
4	ATP	C	5002	-	26,33,33	0.61	0	31,52,52	0.81	2 (6%)
4	ATP	B	5002	-	26,33,33	0.61	0	31,52,52	0.81	2 (6%)
4	ATP	A	5002	-	26,33,33	0.61	0	31,52,52	0.82	2 (6%)
4	ATP	A	5003	-	26,33,33	0.67	0	31,52,52	0.77	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	KVR	D	5004	-	24,25,25	0.49	0	32,34,34	0.83	2 (6%)
5	KVR	A	5004	-	24,25,25	0.49	0	32,34,34	0.83	2 (6%)
5	KVR	B	5004	-	24,25,25	0.48	0	32,34,34	0.83	2 (6%)
4	ATP	B	5003	-	26,33,33	0.67	0	31,52,52	0.77	1 (3%)

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	D	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	6/18/38/38	0/3/3/3
5	KVR	C	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	D	5003	-	-	6/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	6/18/38/38	0/3/3/3
5	KVR	D	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	A	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	B	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	B	5003	-	-	6/18/38/38	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	A	5002	ATP	C5-C6-N6	2.30	123.84	120.35

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

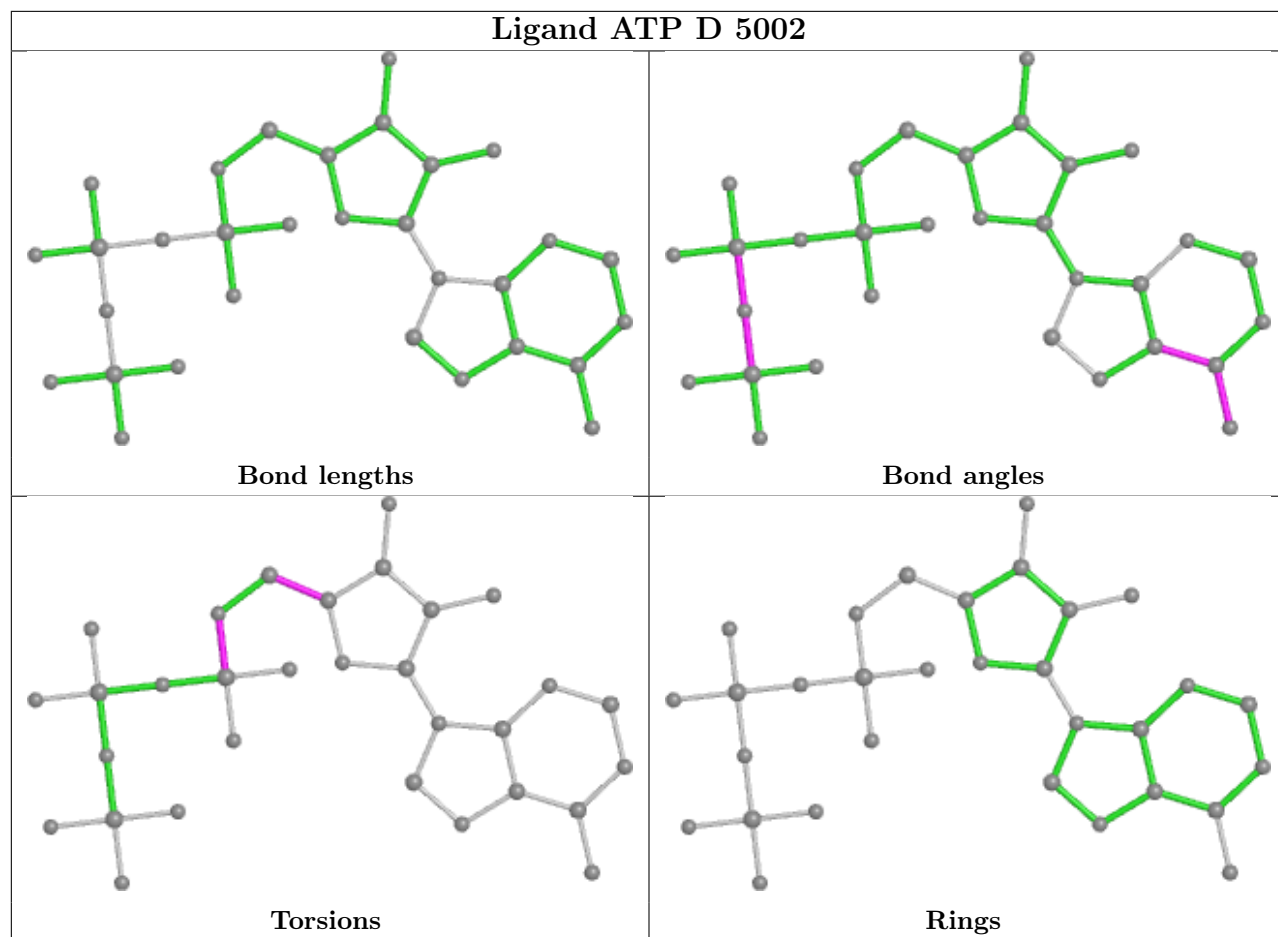
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	O4'-C4'-C5'-O5'

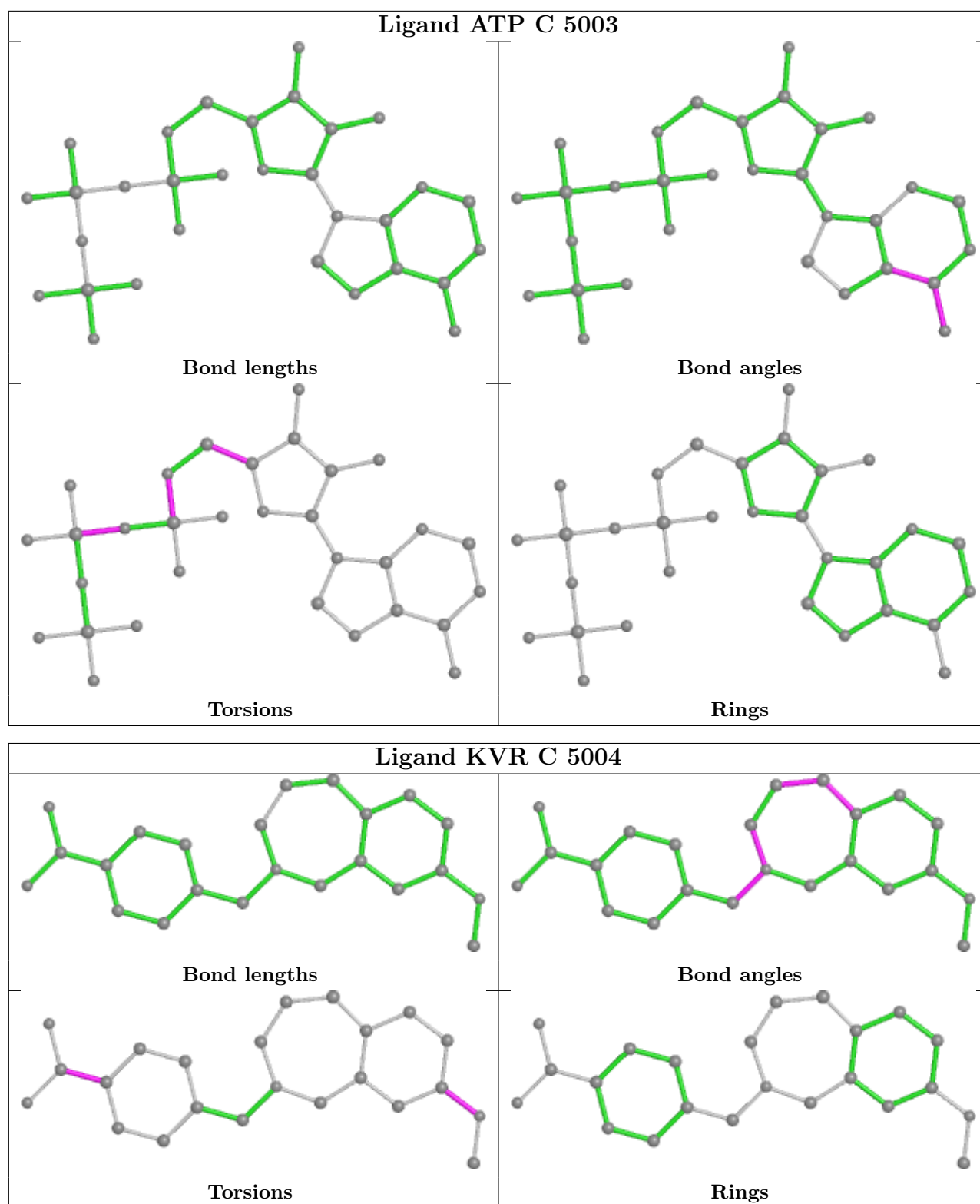
There are no ring outliers.

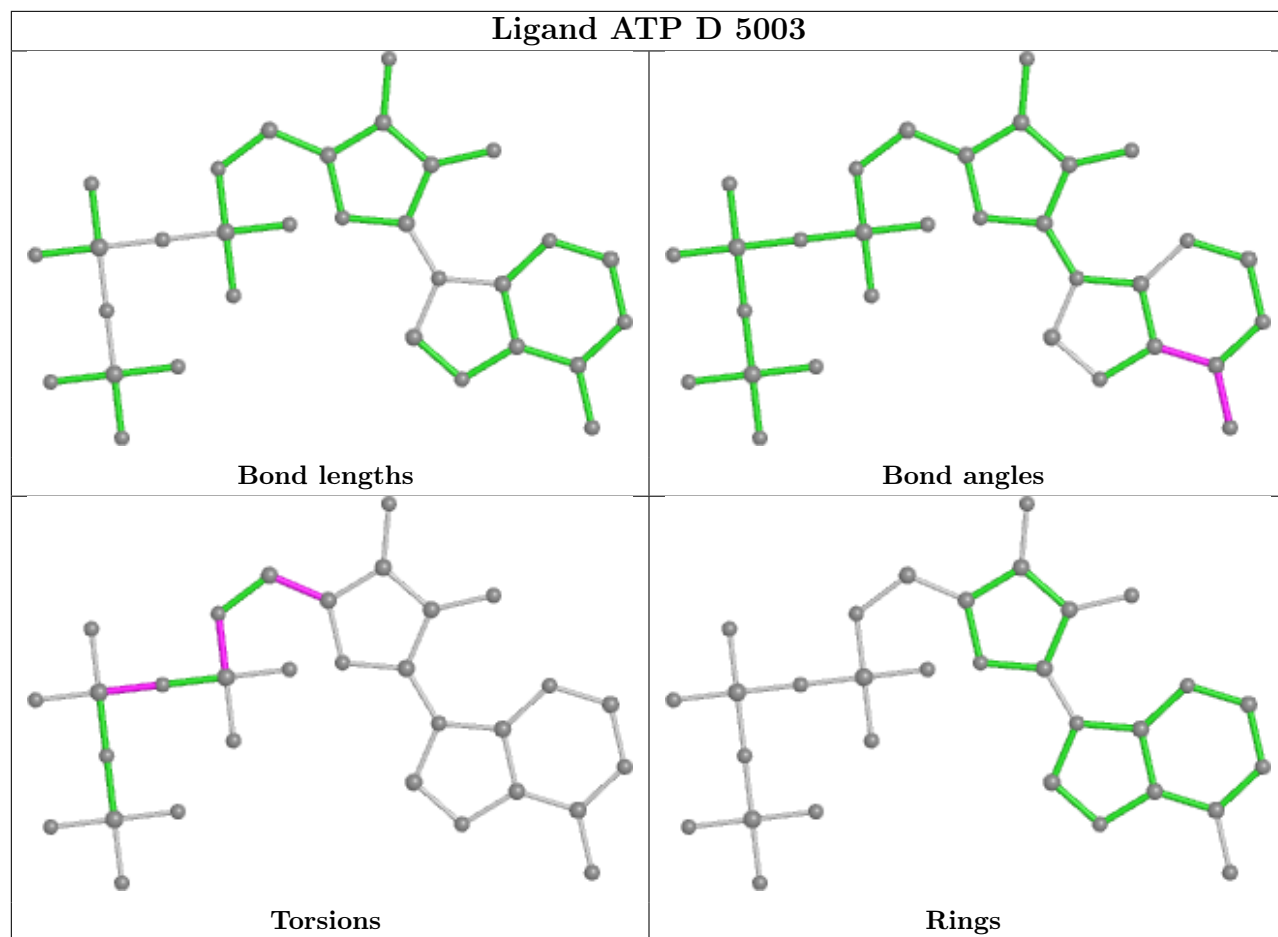
8 monomers are involved in 16 short contacts:

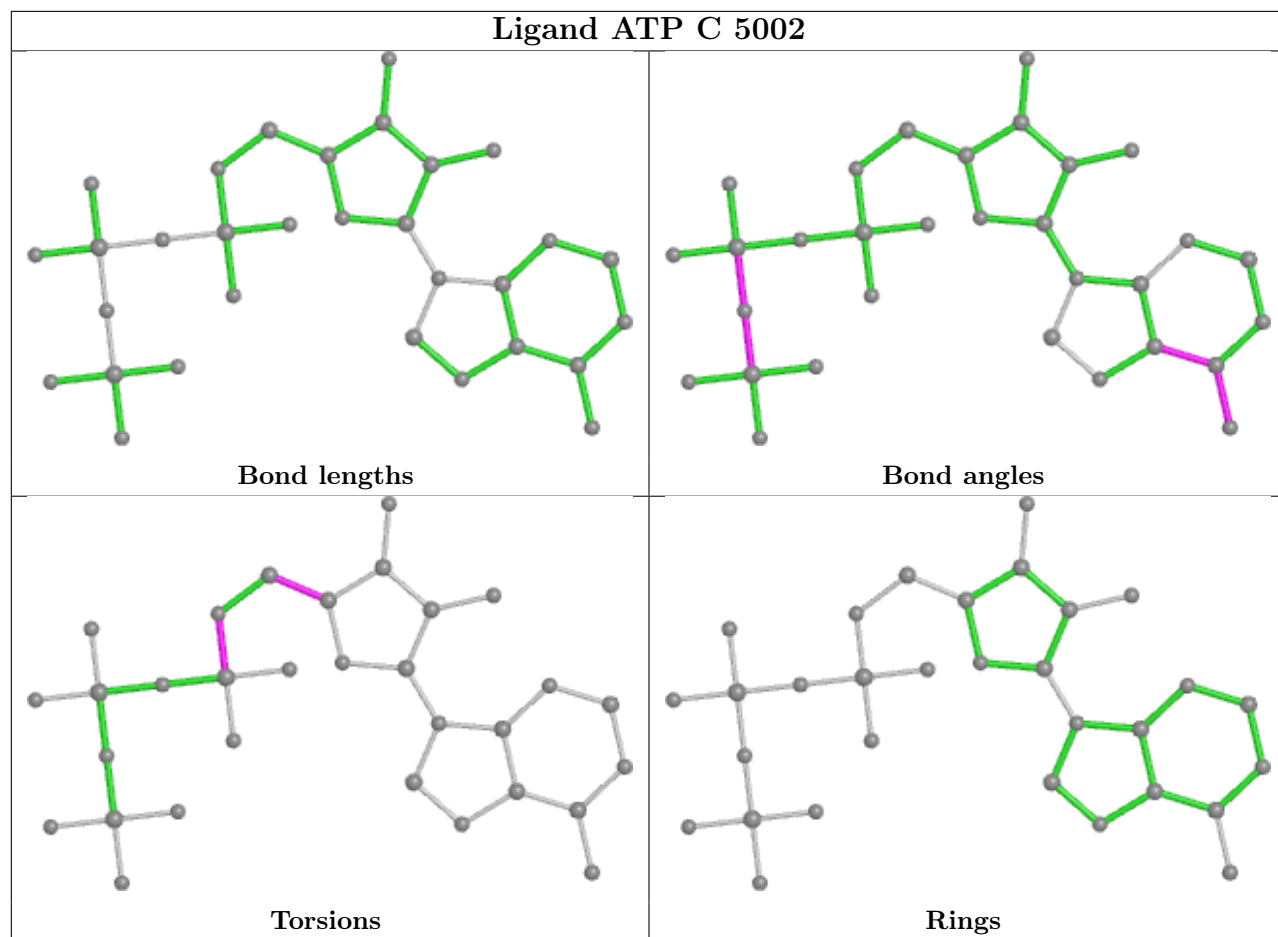
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5003	ATP	3	0
5	C	5004	KVR	2	0
4	D	5003	ATP	3	0
4	A	5003	ATP	3	0
5	D	5004	KVR	2	0
5	A	5004	KVR	2	0
5	B	5004	KVR	2	0
4	B	5003	ATP	3	0

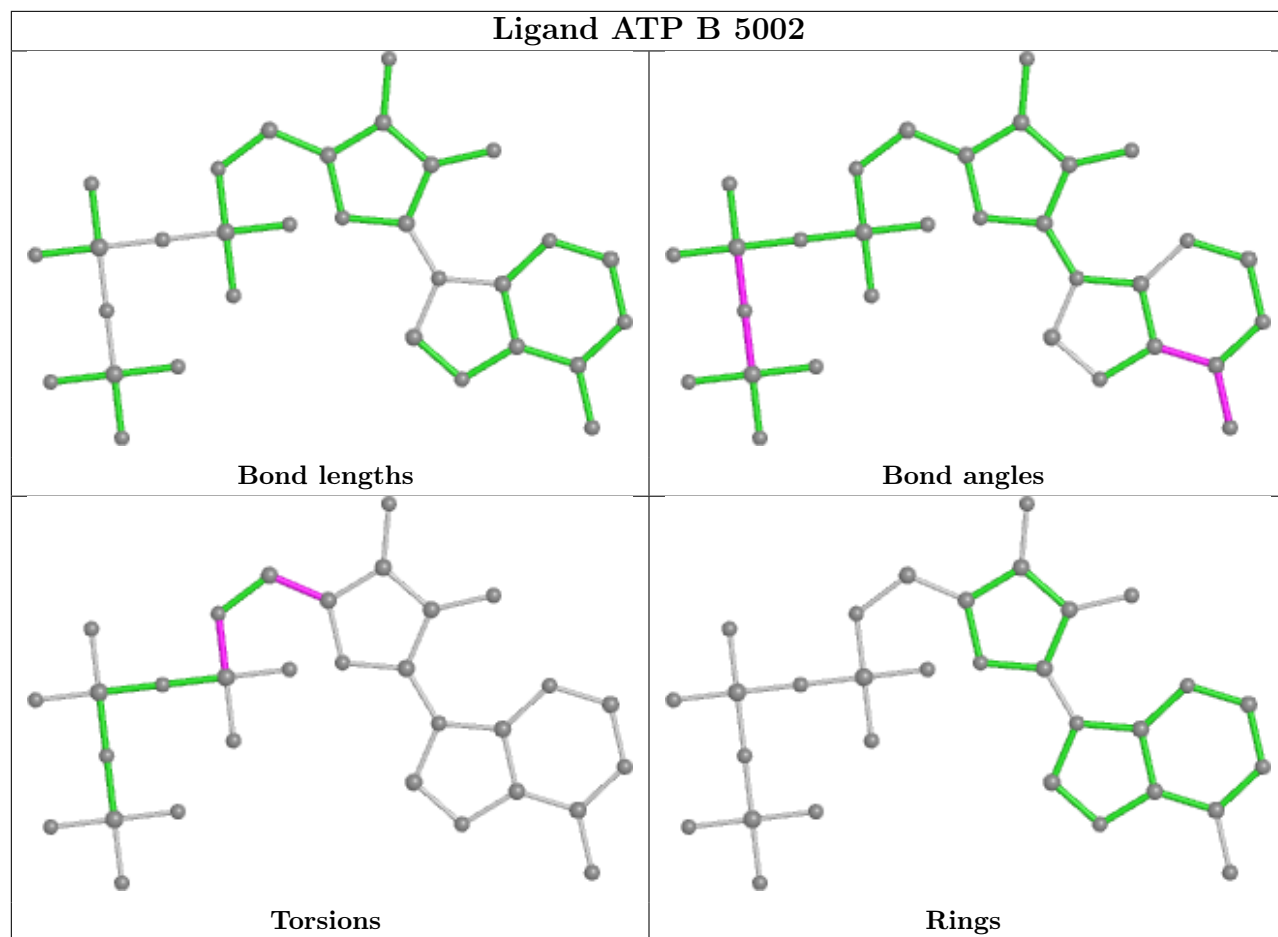
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

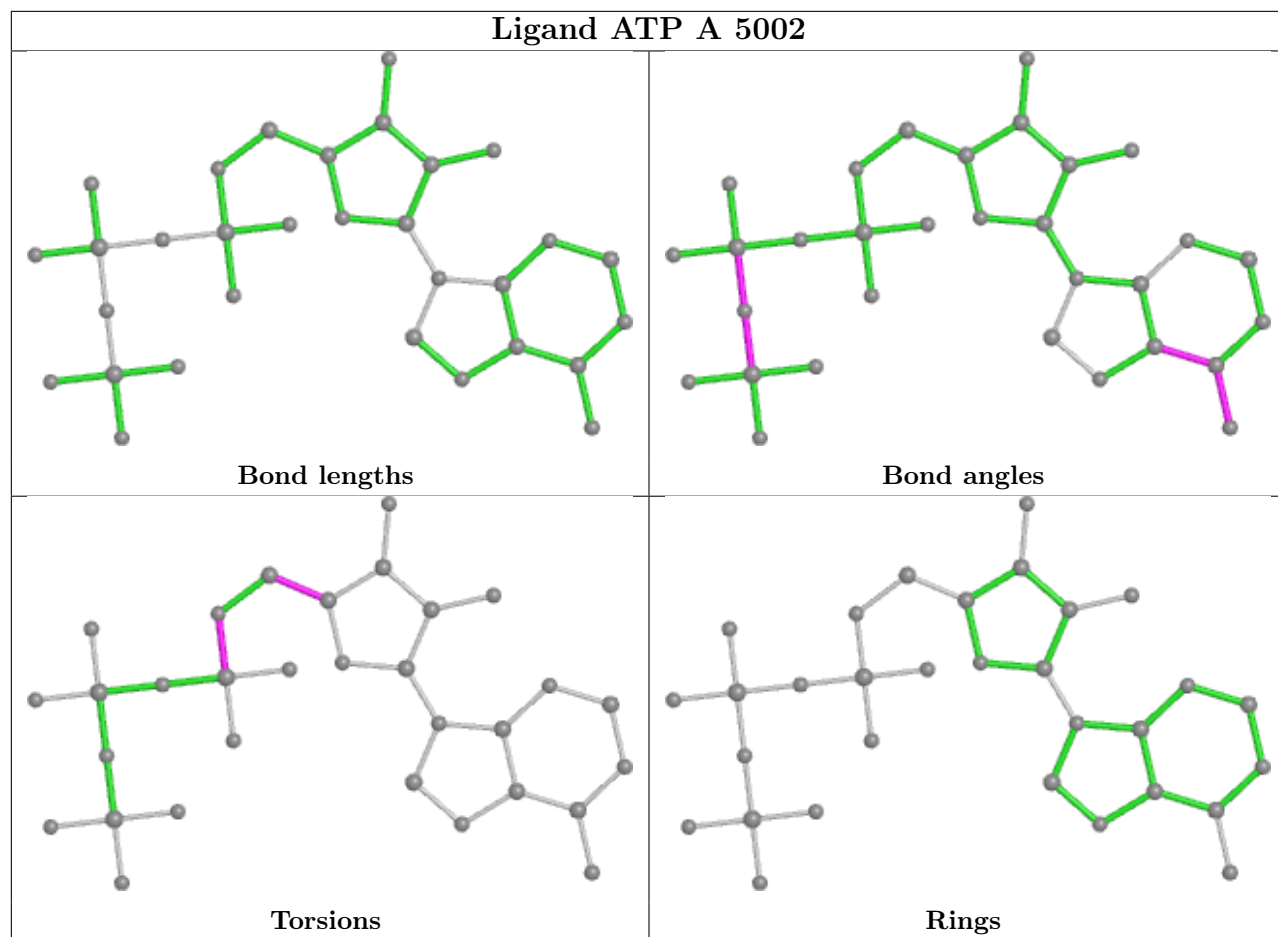


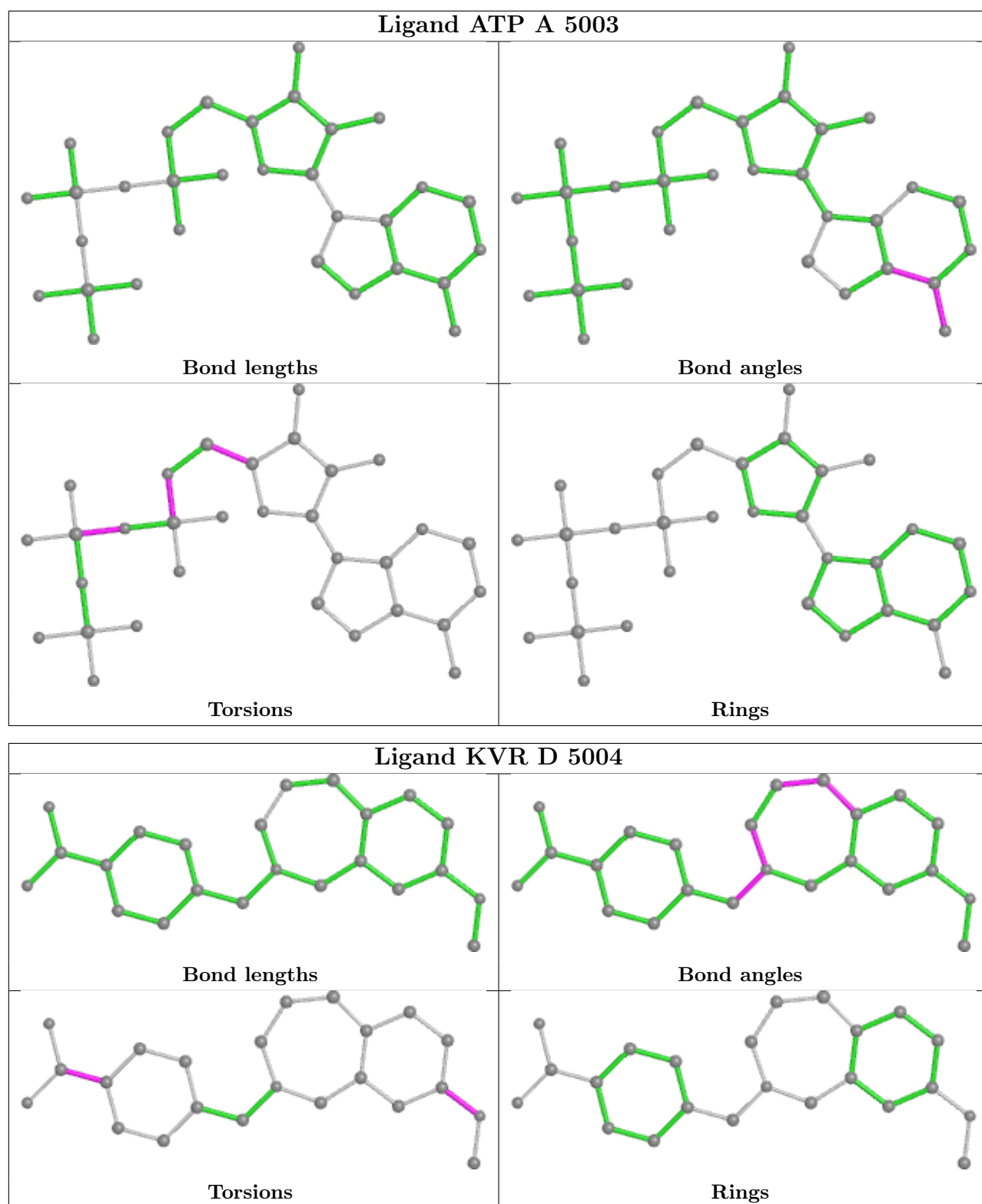


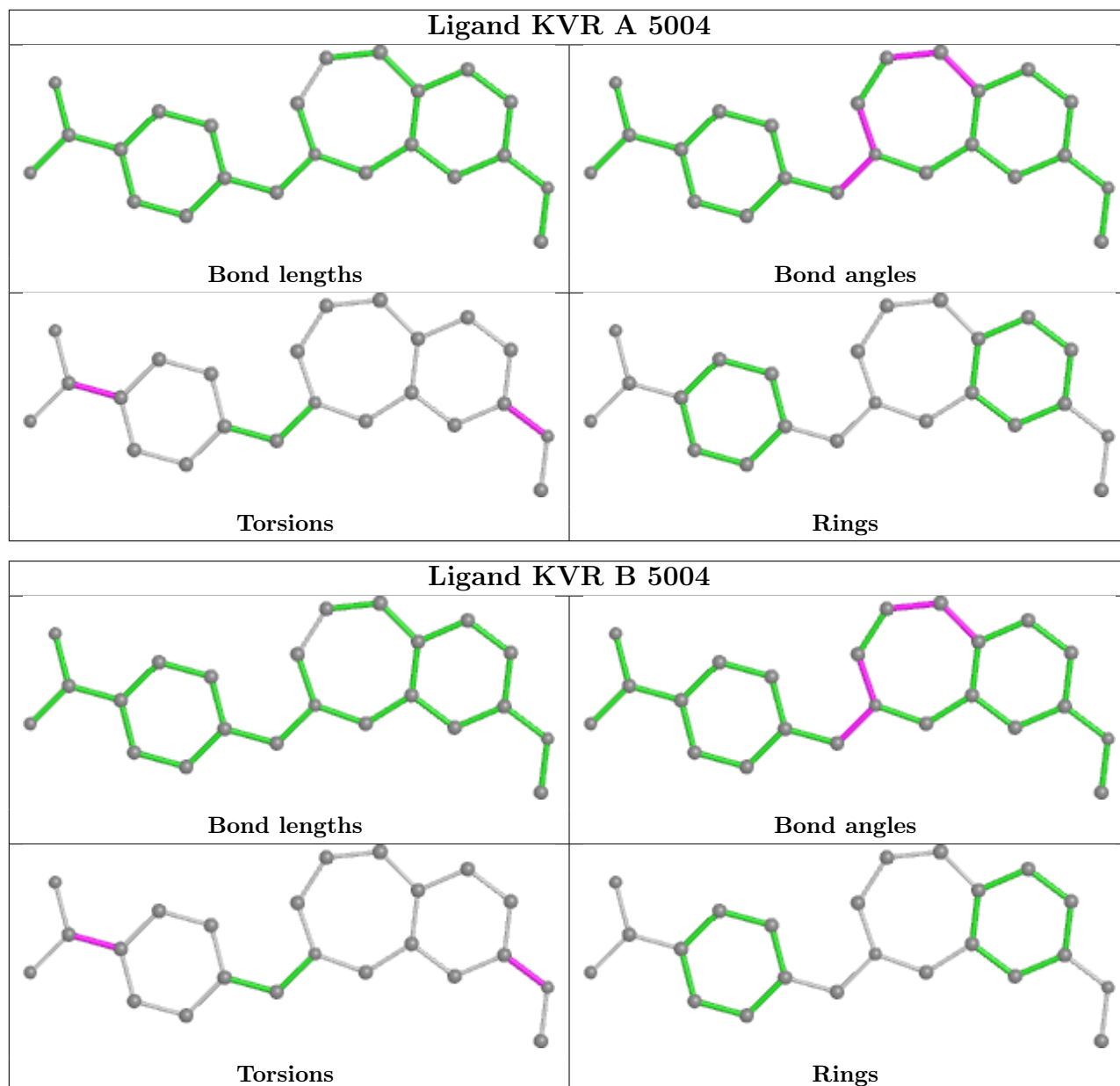


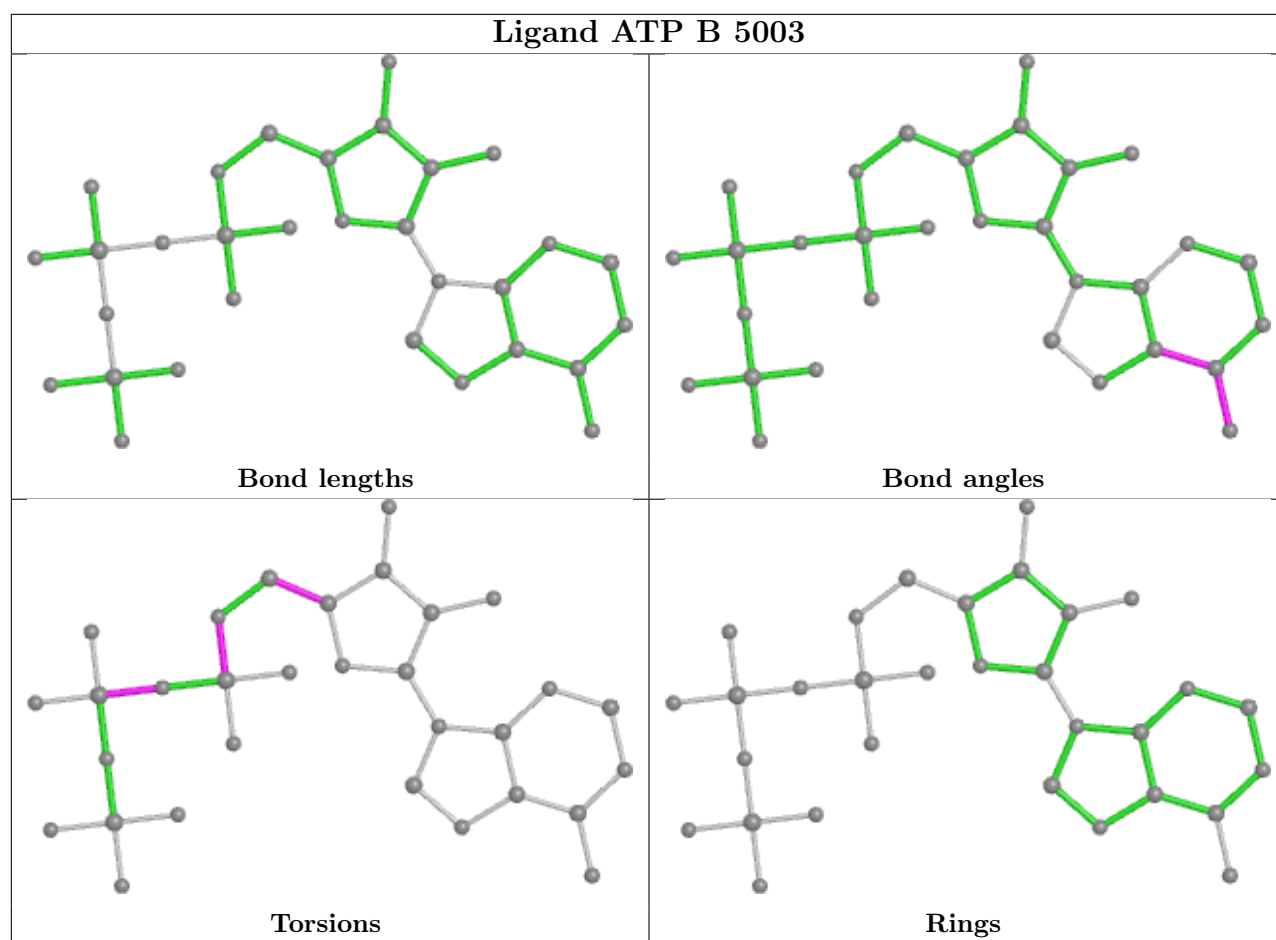












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

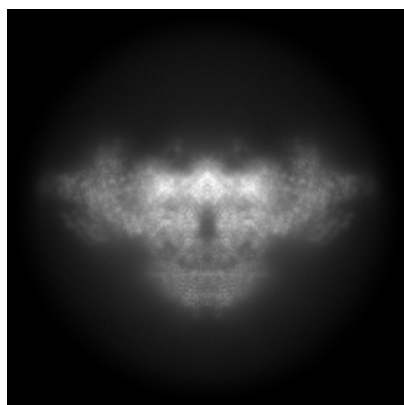
6 Map visualisation [i](#)

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.

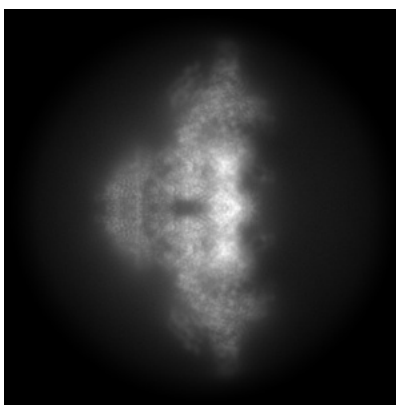
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

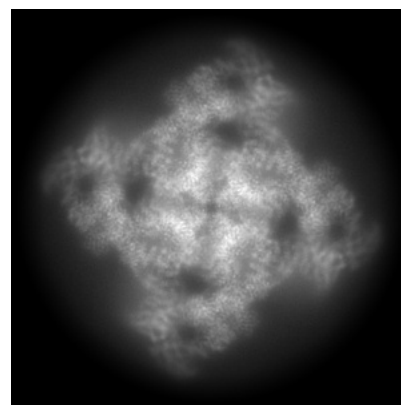
6.1.1 Primary map



X



Y

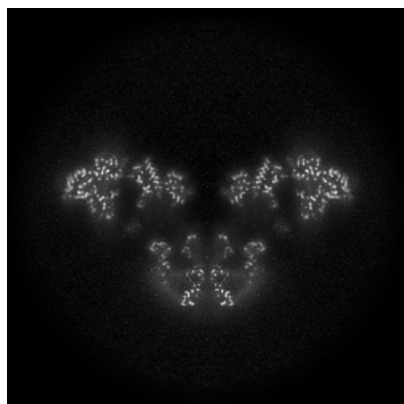


Z

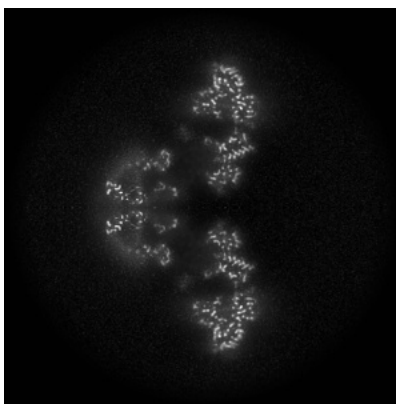
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

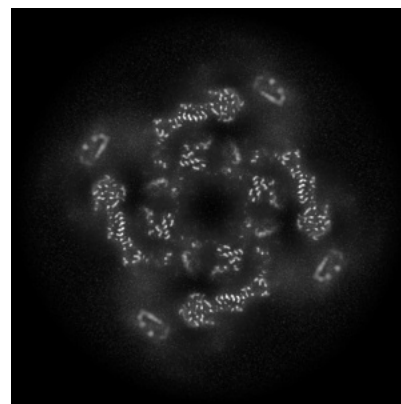
6.2.1 Primary map



X Index: 256



Y Index: 256

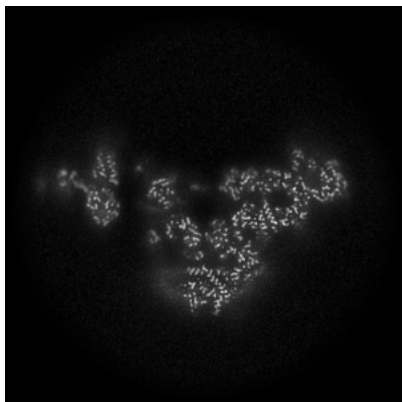


Z Index: 256

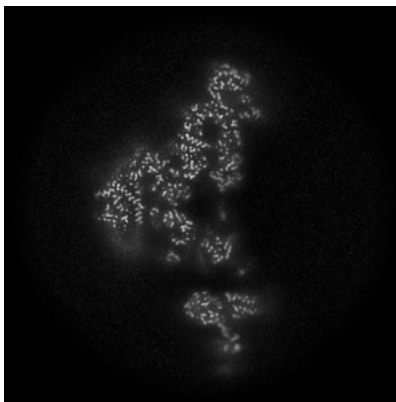
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

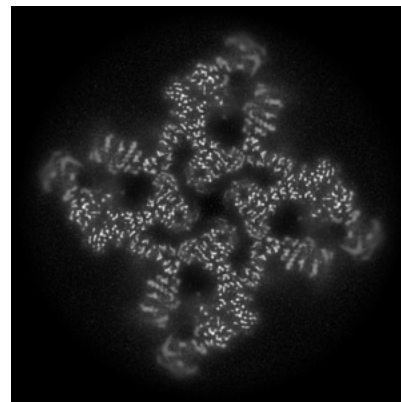
6.3.1 Primary map



X Index: 238



Y Index: 274

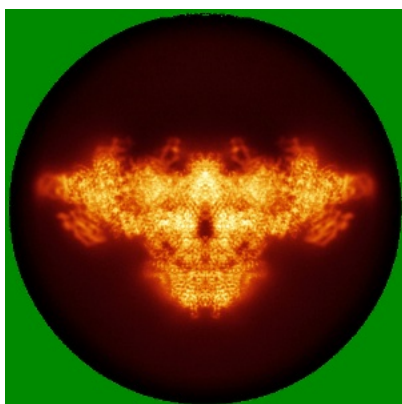


Z Index: 282

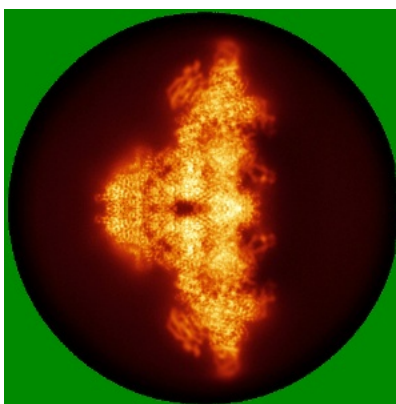
The images above show the largest variance slices of the map in three orthogonal directions.

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

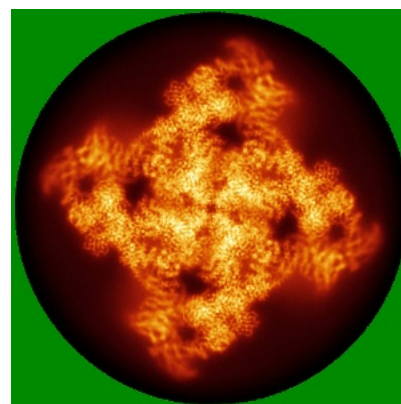
6.4.1 Primary map



X



Y

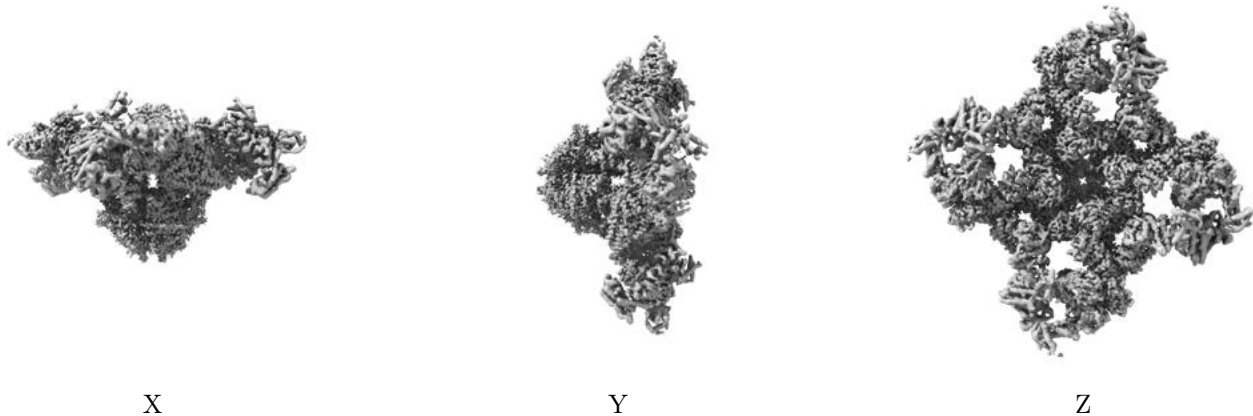


Z

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.

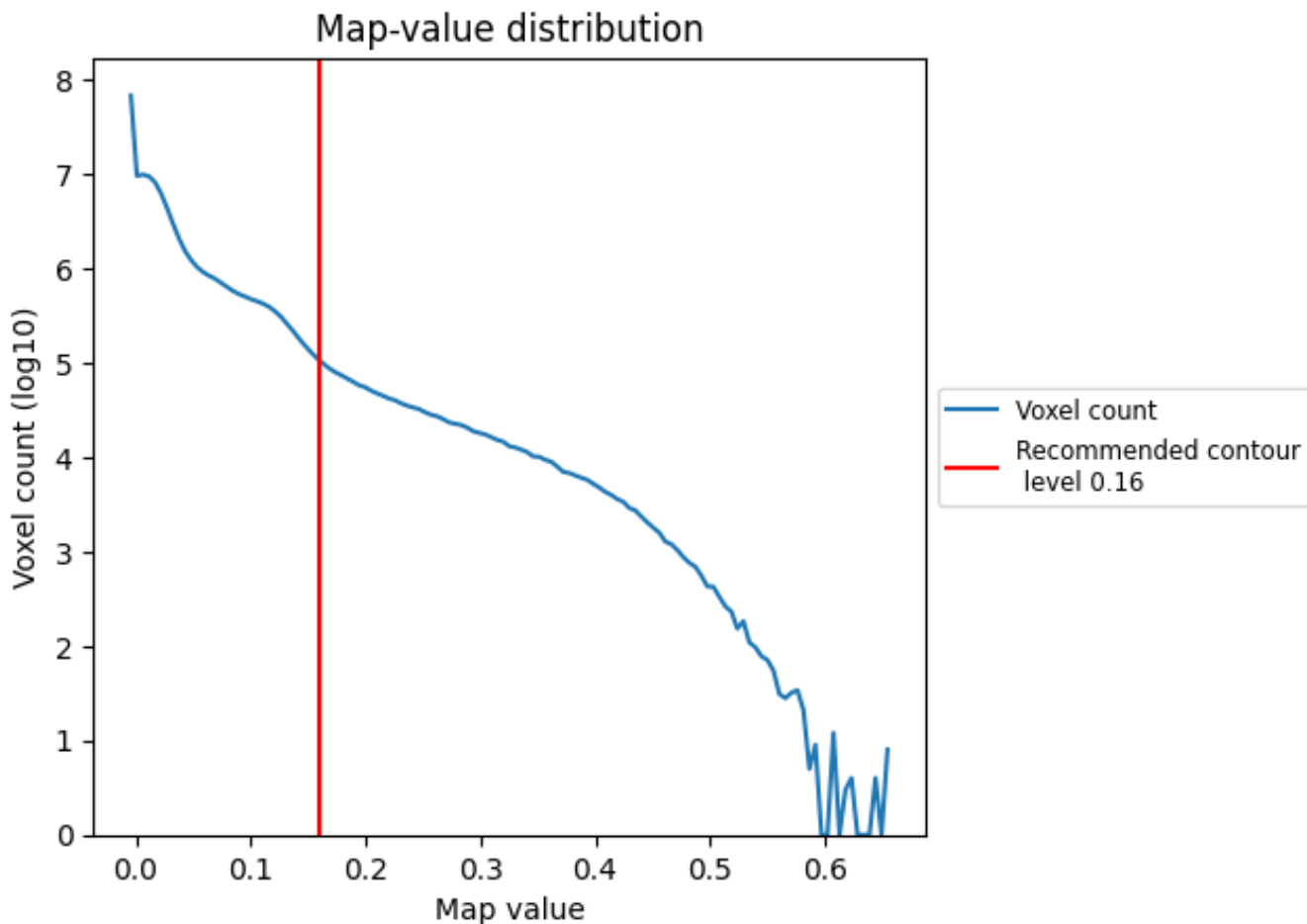
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

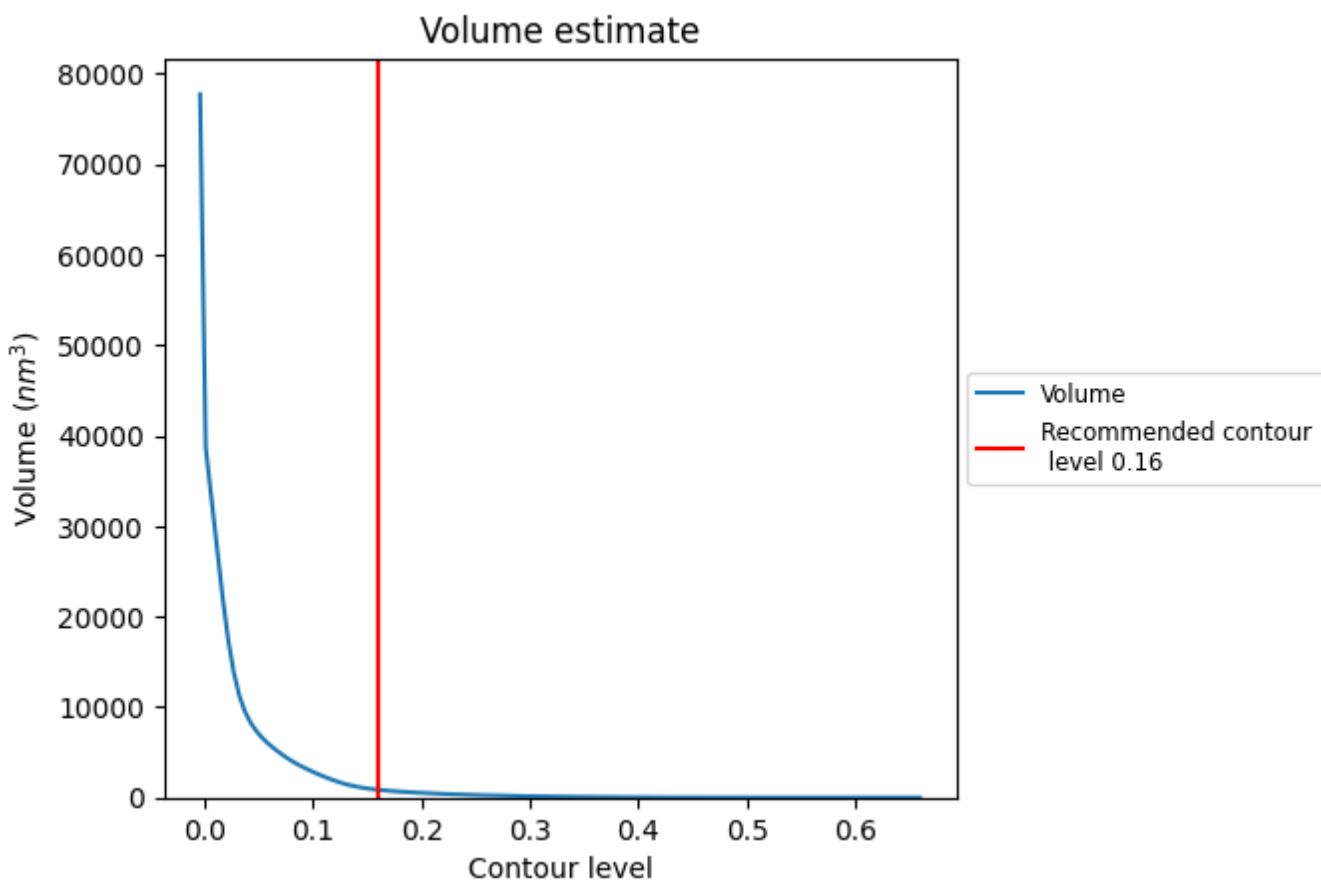
This section contains the results of statistical analysis of the map.

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.

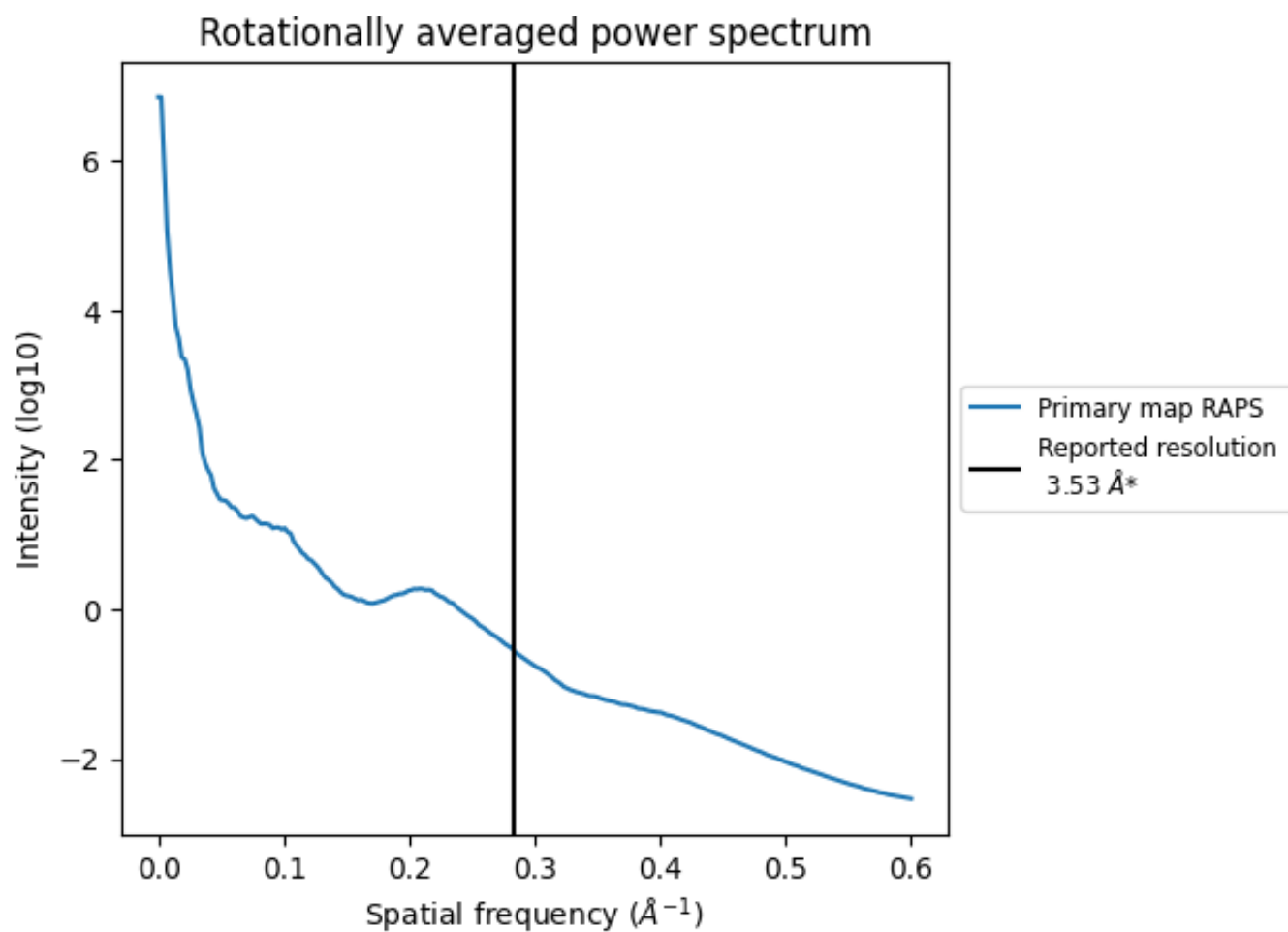
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 858 nm³; 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.283 Å⁻¹

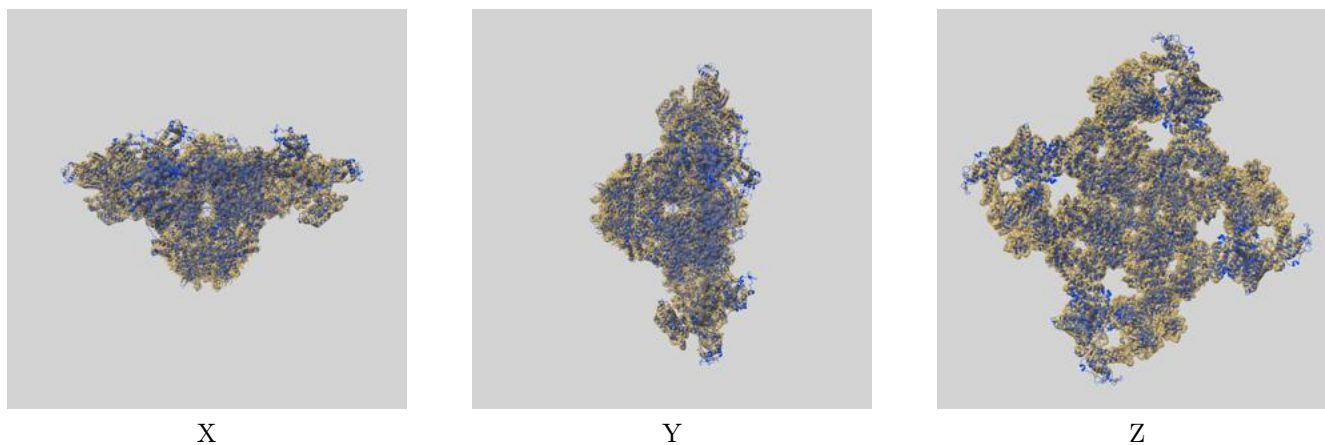
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

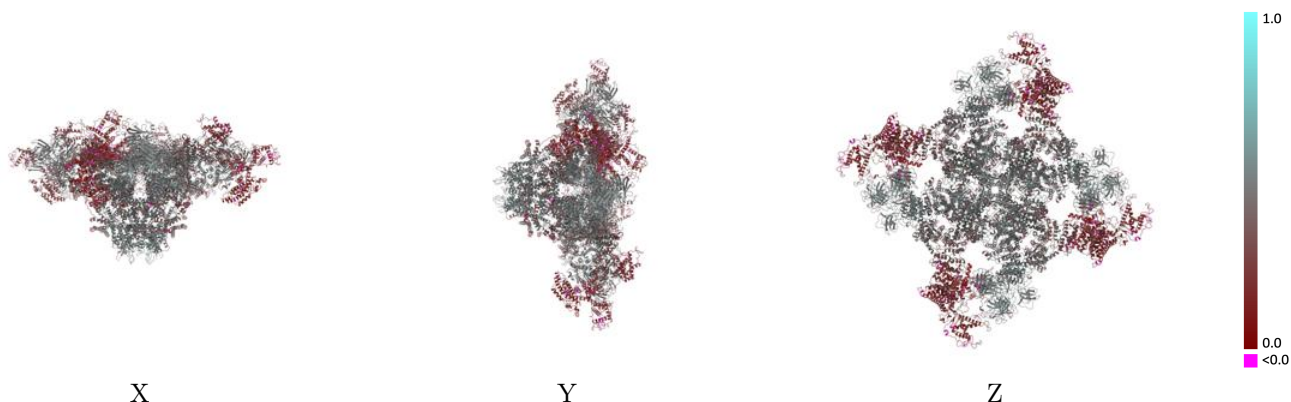
This section contains information regarding the fit between EMDB map EMD-42761 and PDB model 8UXE. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



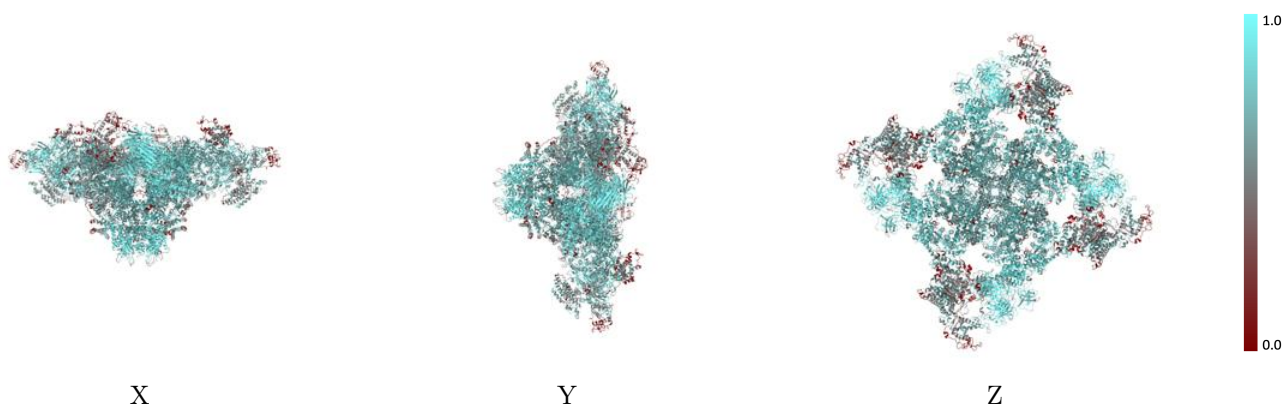
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



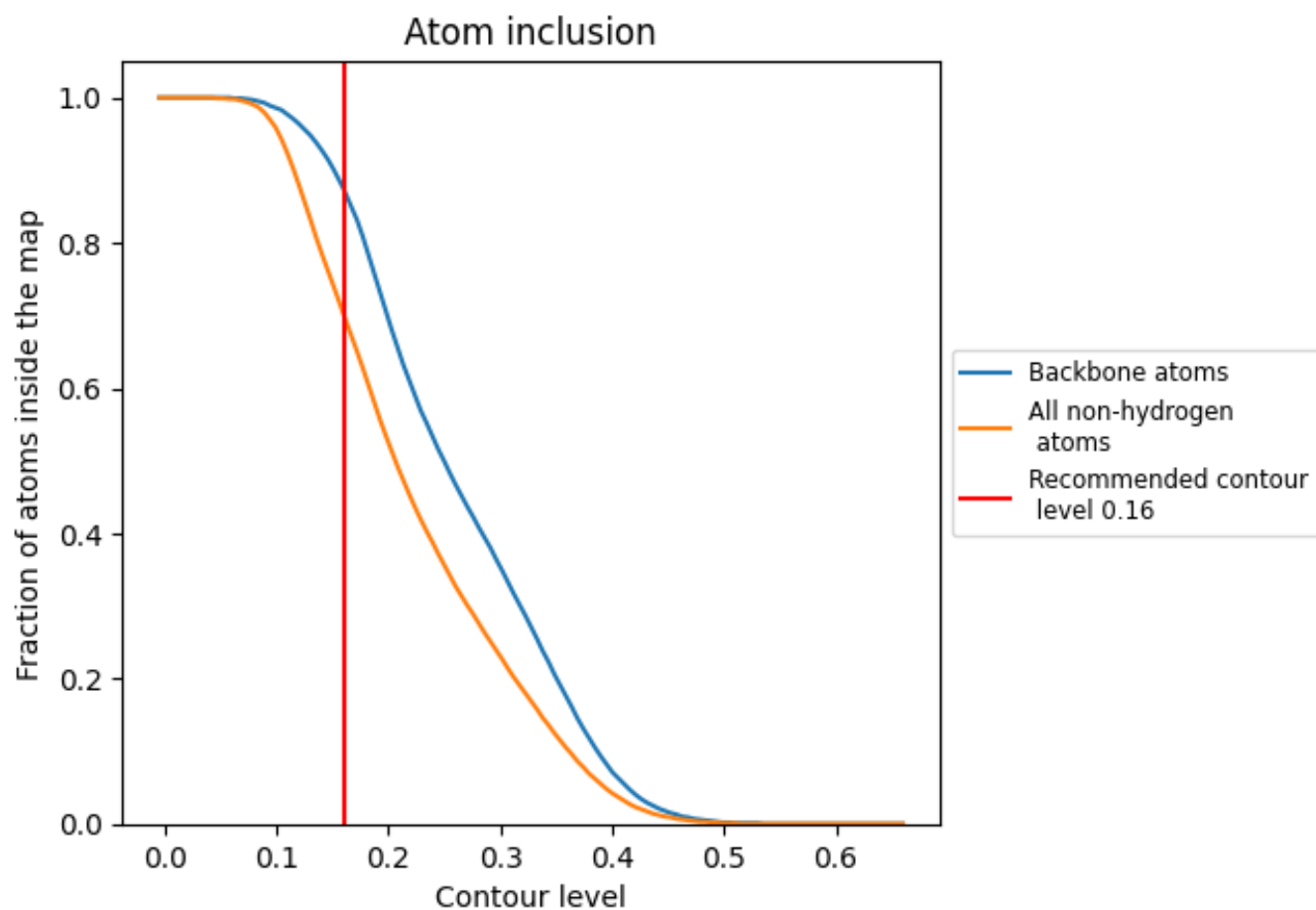
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.7020	 0.3910
A	 0.6990	 0.3870
B	 0.7000	 0.3900
C	 0.7000	 0.3900
D	 0.7000	 0.3900
E	 0.8190	 0.4810
F	 0.8090	 0.4800
G	 0.8180	 0.4790
H	 0.8230	 0.4800

