



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:44 AM UTC

PDB ID : 5TAQ / pdb_00005taq
EMDB ID : EMD-8382
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 3&4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.10 Å(reported)

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:

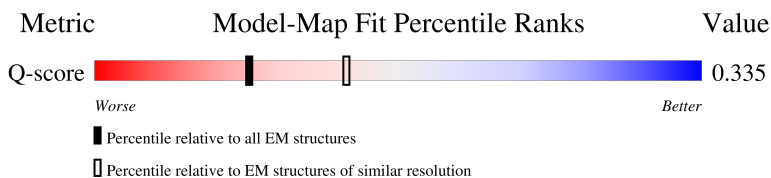
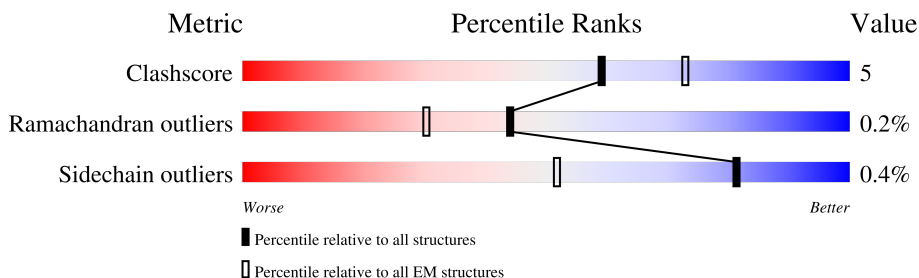
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.10 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.



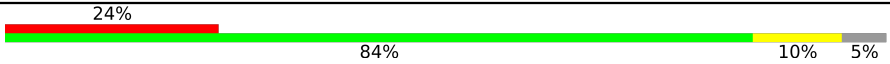
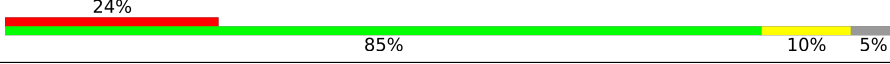
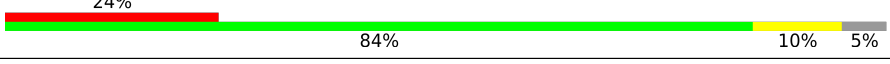
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	108	20% 80% 19% ..
1	F	108	19% 80% 19% ..
1	H	108	21% 80% 19% ..
1	J	108	19% 78% 20% ..

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Mol	Chain	Length	Quality of chain
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	B	5102	-	X	-	-
4	CFF	E	5102	-	X	-	-
4	CFF	G	5102	-	X	-	-
4	CFF	I	5102	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

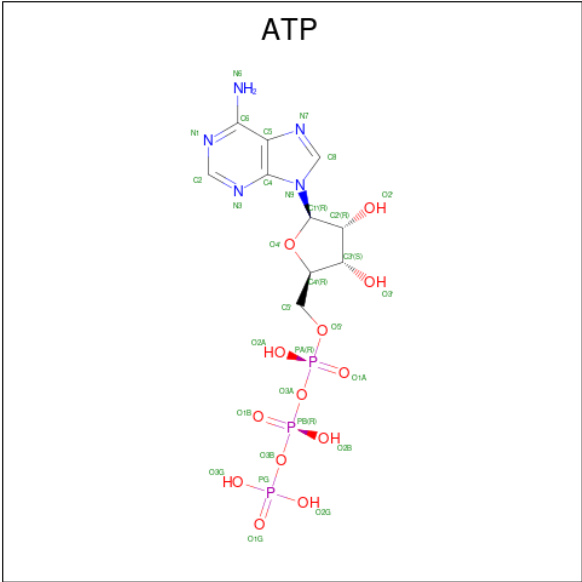
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

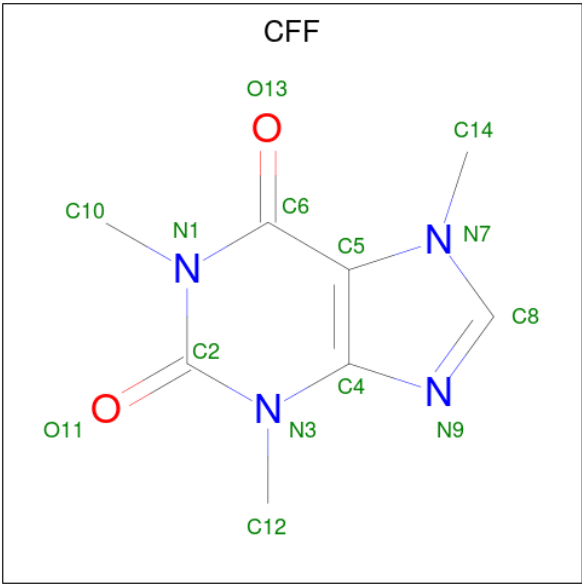
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	

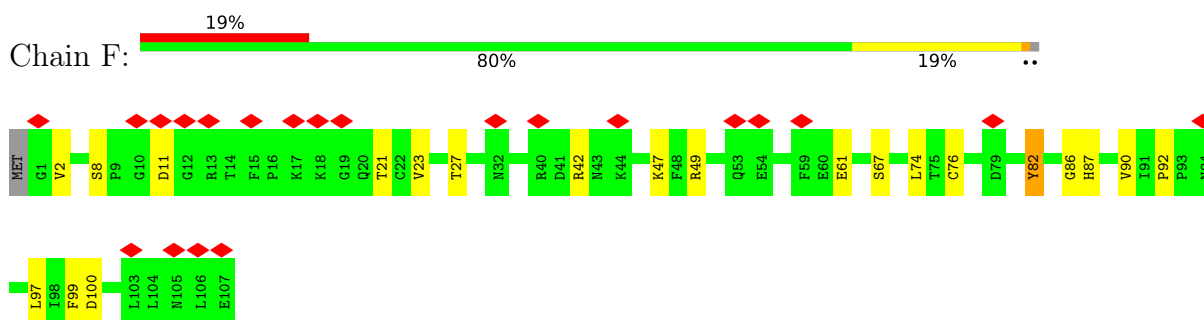
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	G	1	Total	Ca	0
			1	1	

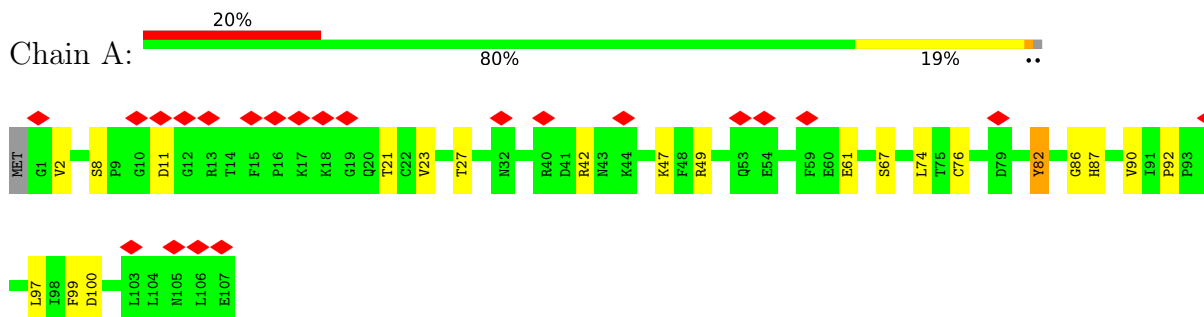
3 Residue-property plots [i](#)

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

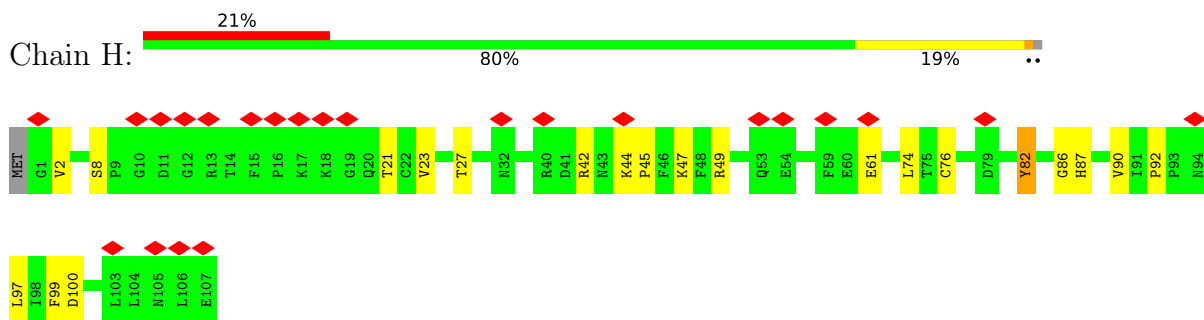
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



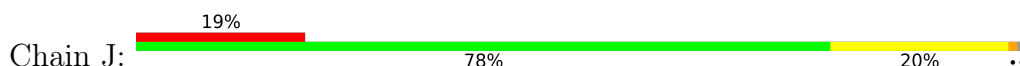
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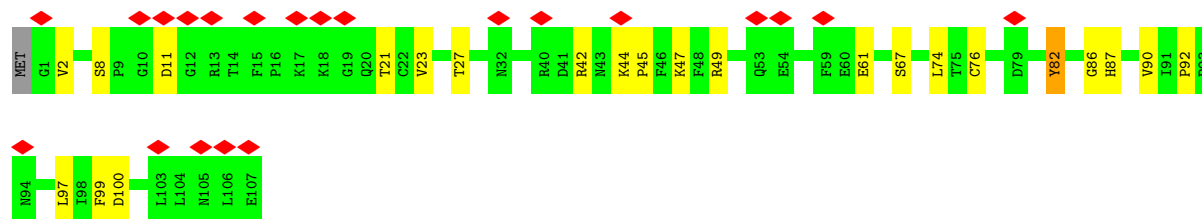


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

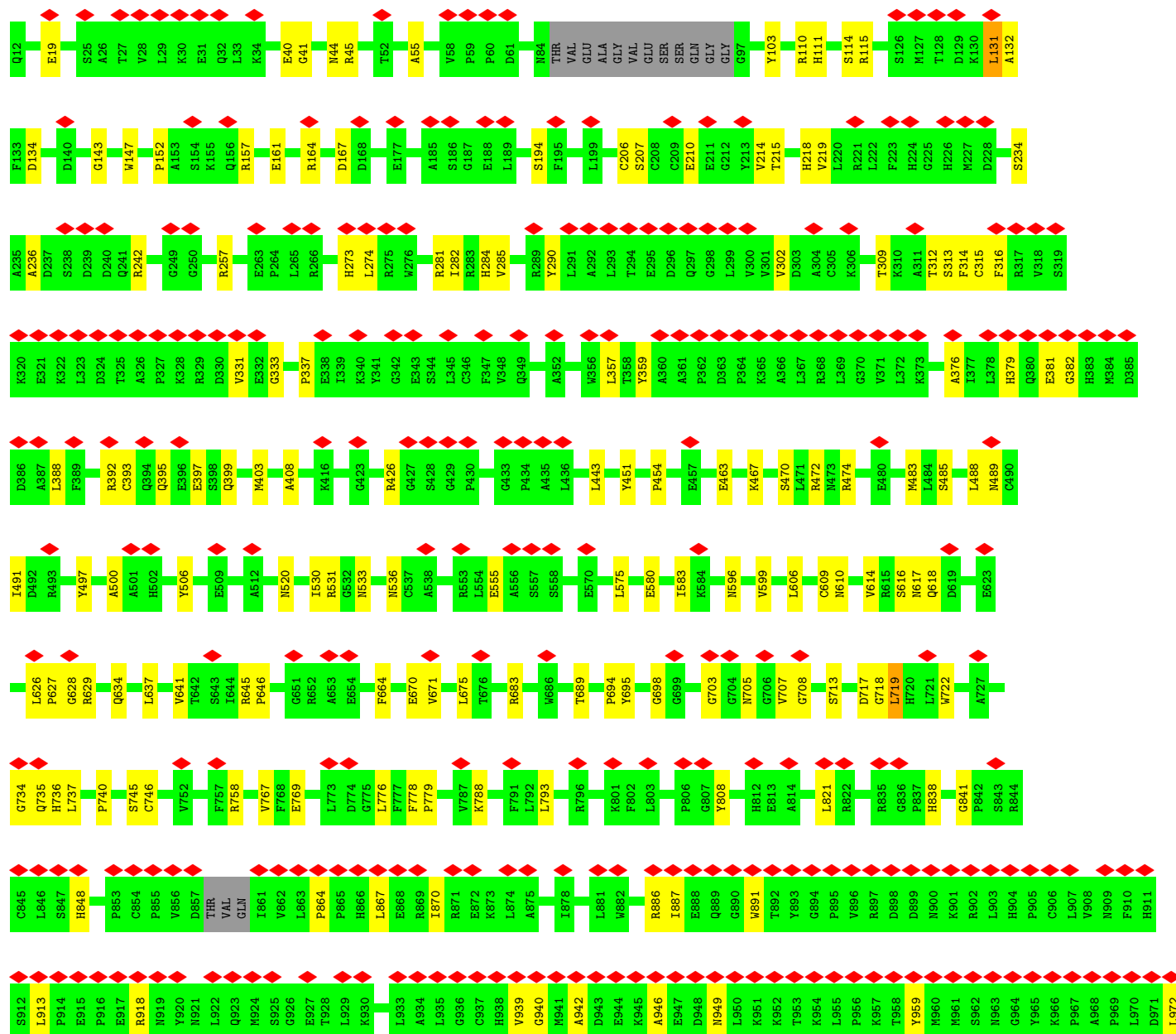
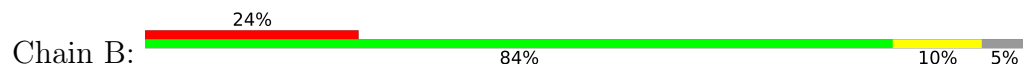


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

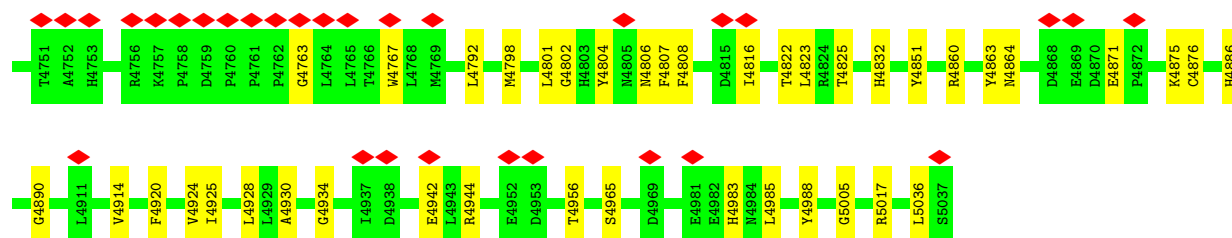




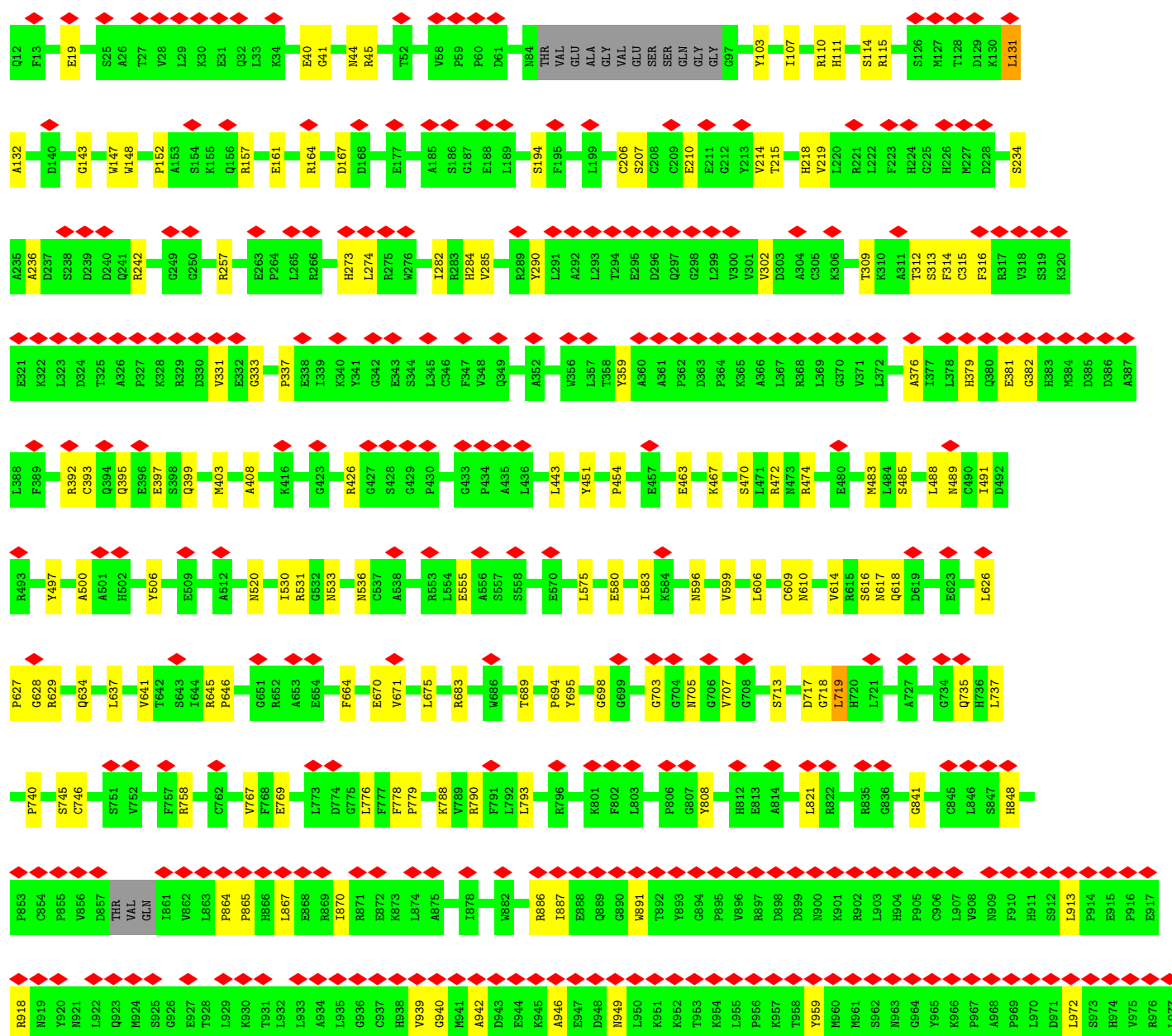
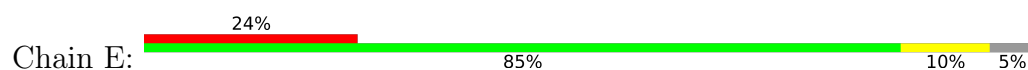
• Molecule 2: Ryanodine receptor 1

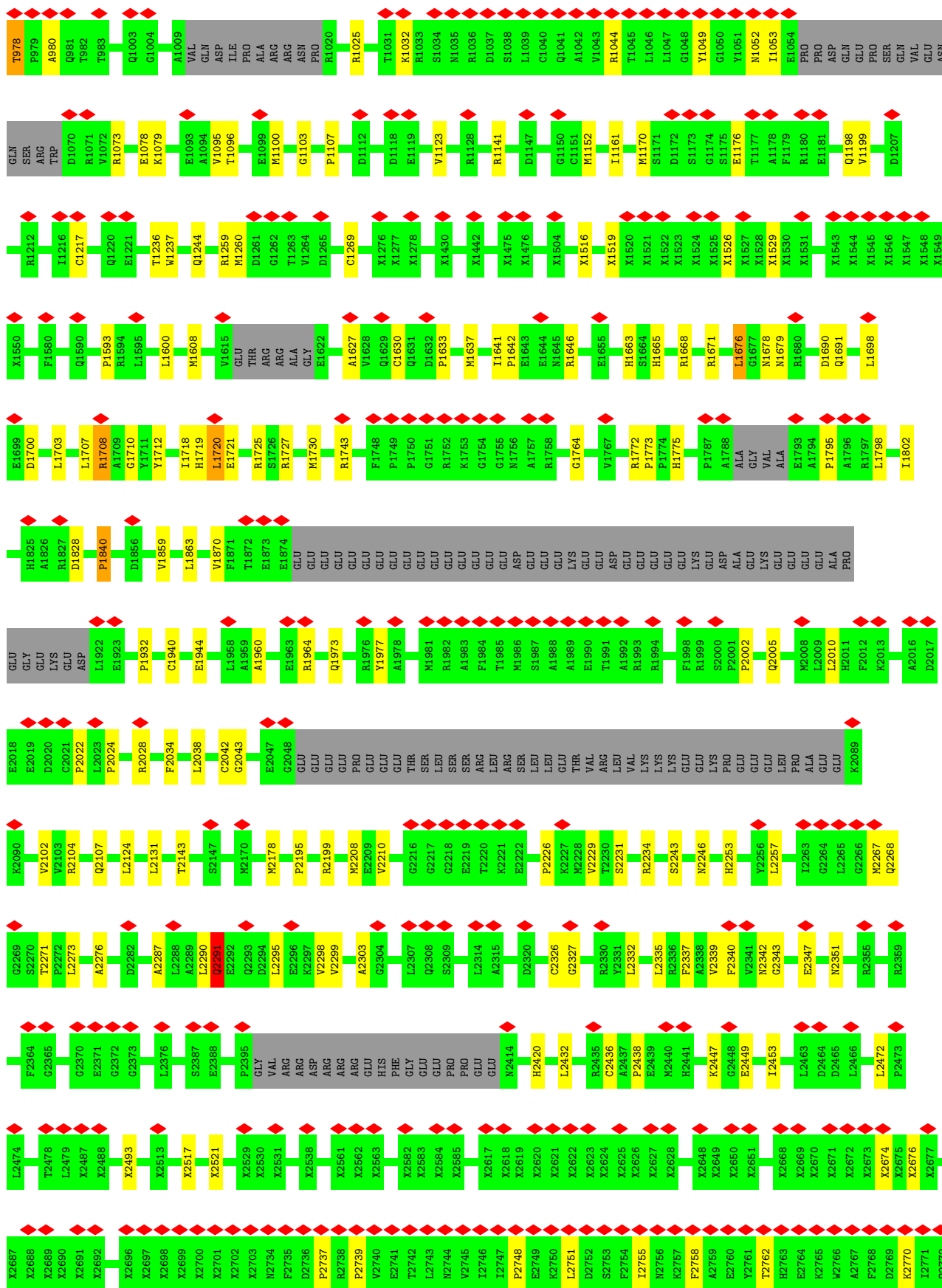




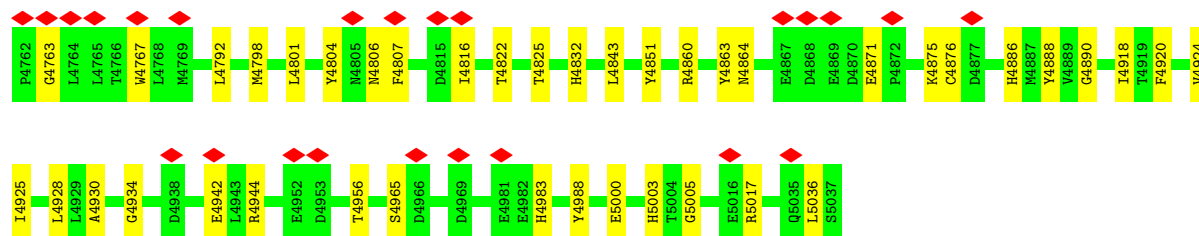


• Molecule 2: Ryanodine receptor 1

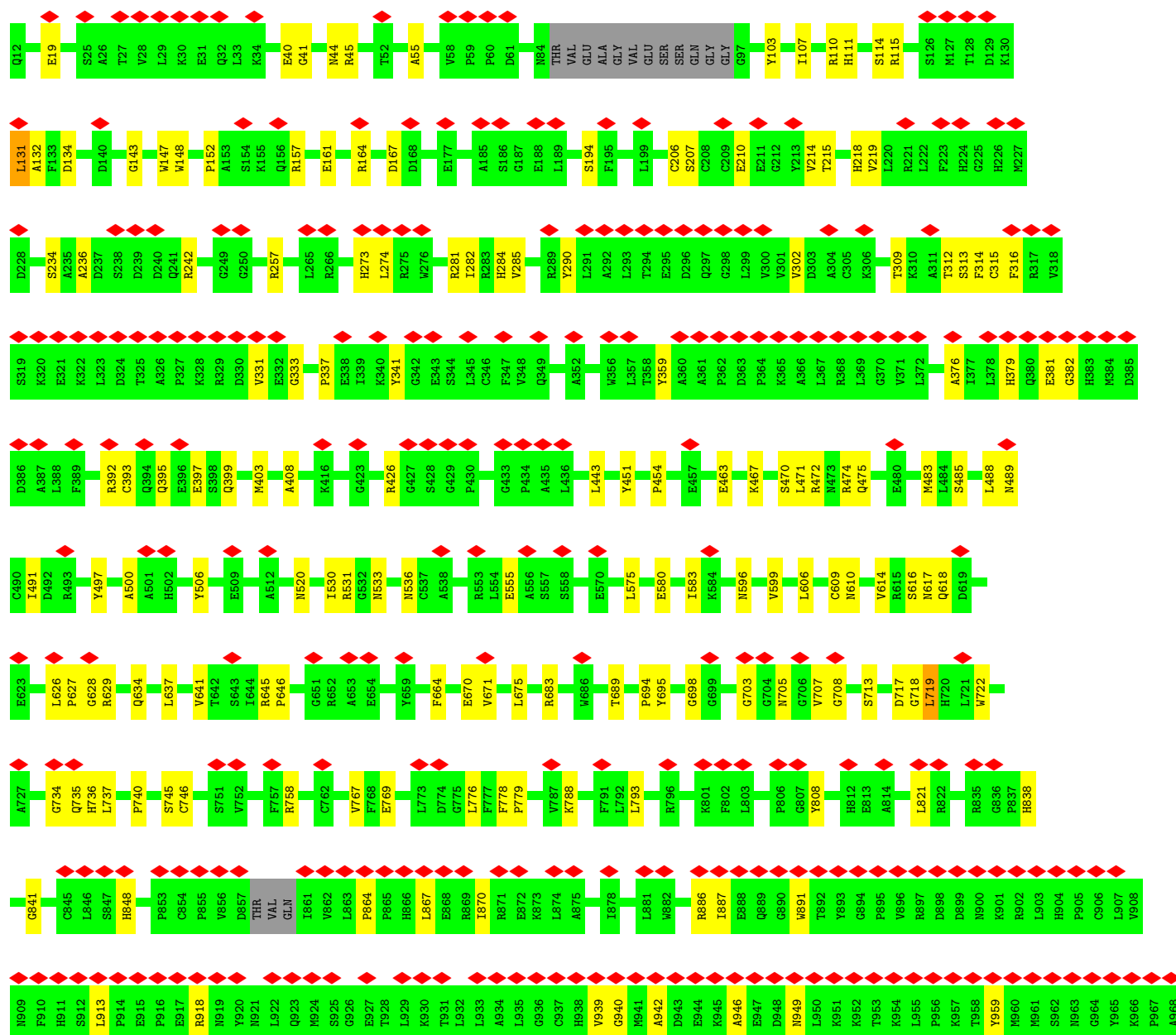
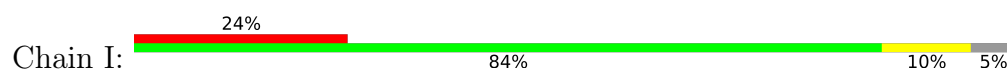


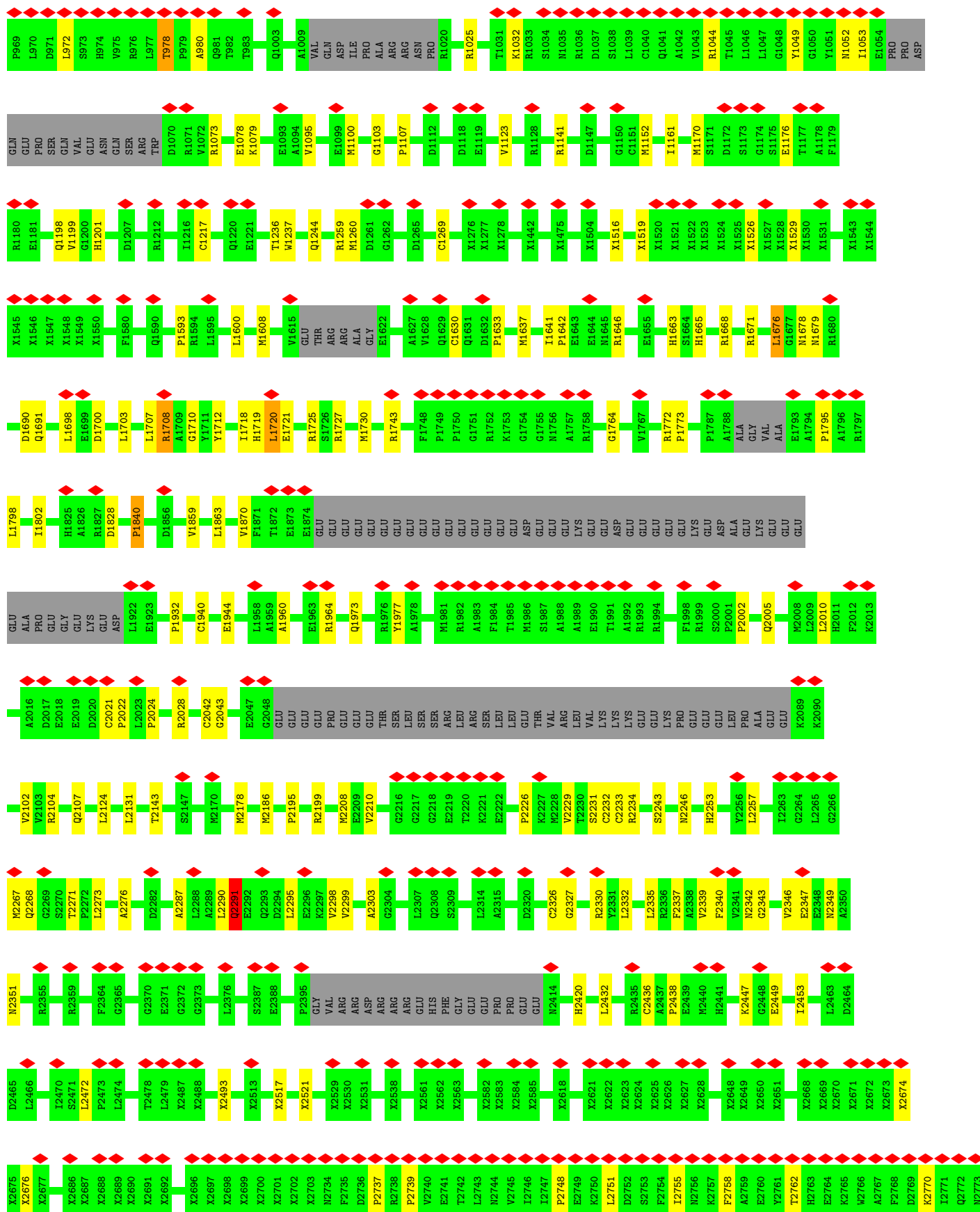




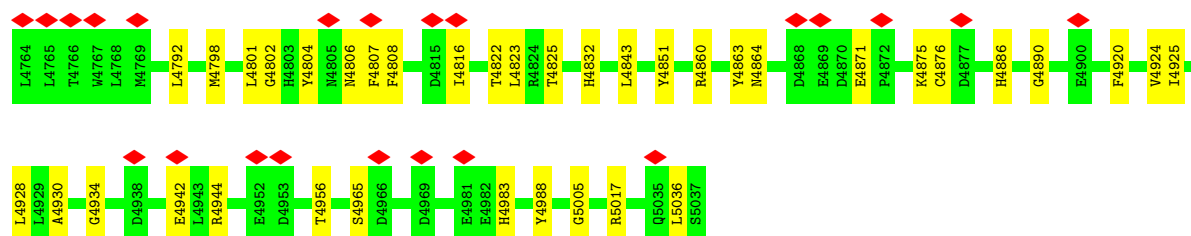


• Molecule 2: Ryanodine receptor 1

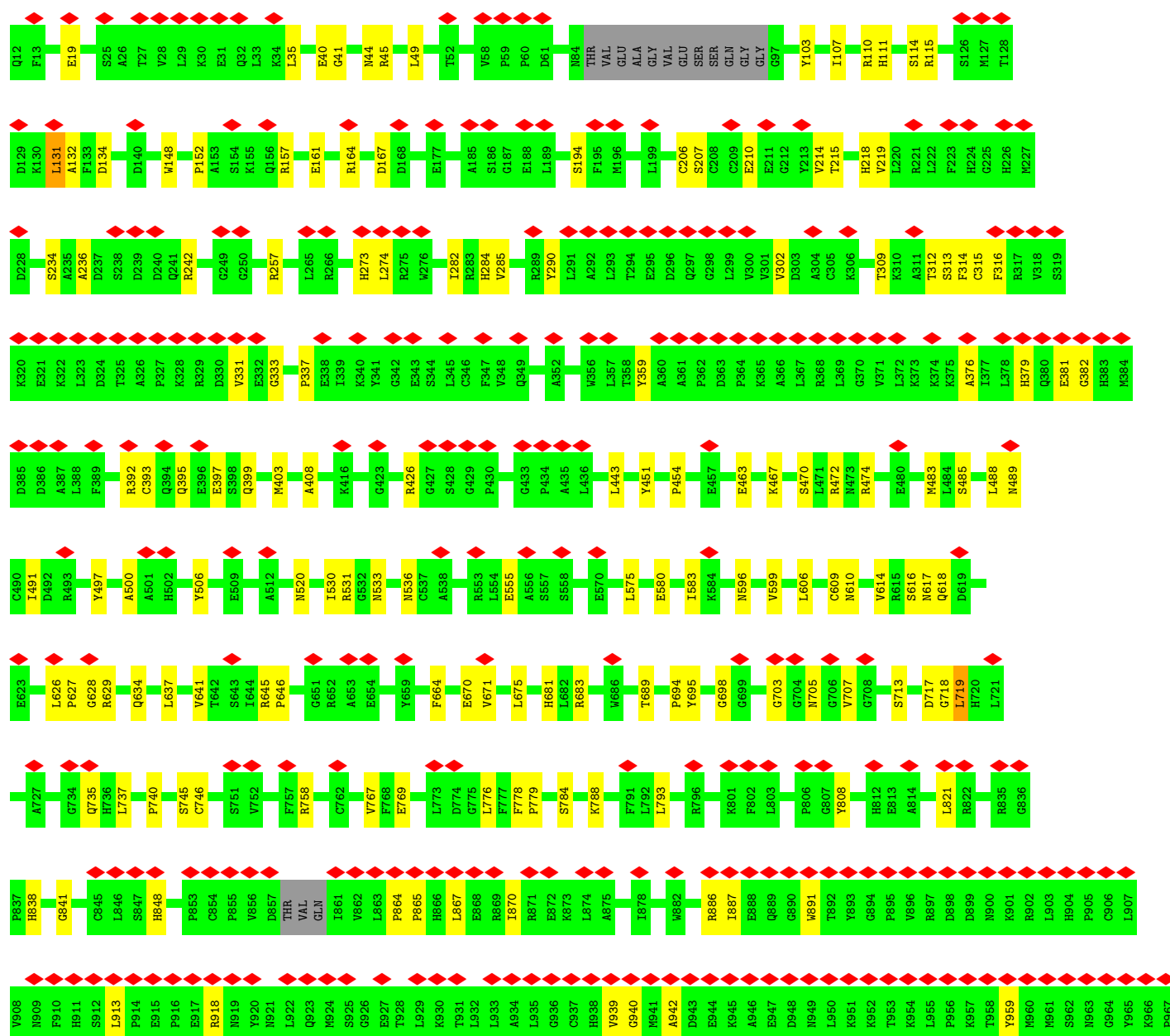
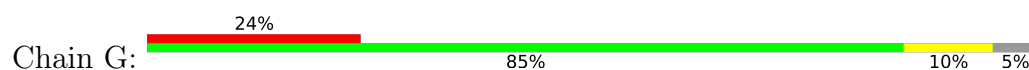






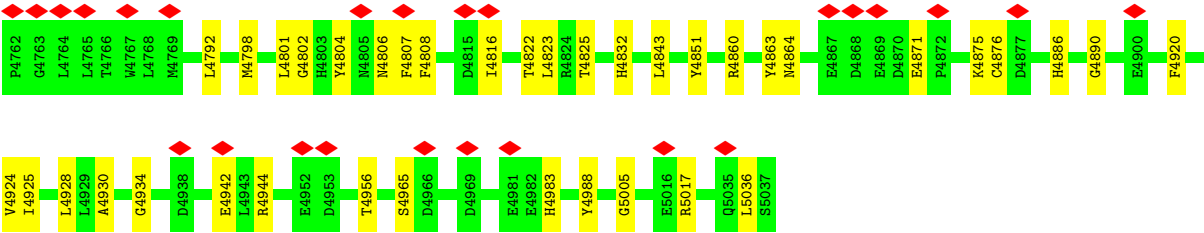


• Molecule 2: Ryanodine receptor 1





GLU ASP GLU	S4635 T4636 Q4637 V4638 M4639 E4640 P4641 A4642 C4645 V4666 P4667 L4668 V4669 R4673 E4674 K4680 G4685 L4686 Y4687 I4688 D4694 D4695 D4696 V4697 K4698 G4699 Y4715 H4728 G4729 A4738 H4743 D4744 L4745 A4746 T4751 S4187 R4188 Q4209 R4215 G4226 E4227 R4756 K4757 P4758 D4759 P4760 P4761	A4228 E4232 L4233 S4236 X4321 X4322 F4540 R4548 Y4560 L4567 A4570 M4574 V4582 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA GLY ASP LEU ALA GLY GLY SER GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU ALA GLU GLY GLY R4756 K4757 P4758 D4759 P4760 P4761	E3748 V3749 E3750 E3754 T3772 R3773 E3777 M3778 V3779 L3780 Q3781 S3784 I3804 L3805 M3809 V3812 K3815 L3842 D3843 Q3850 G3857 M3858 V3859 M3860 E3861 D3862 G3863 T3864 V3865 I3866 M3867 R3868 Q3870 M3871 R4180 A4186 S4187 R4188 Q4209 R4215 G4226 E4227 Q3889 I3915 T3919 S3929 Y3937	X3436 X3441 X3452 X3453 X3454 X3455 X3456 X3464 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3520 X3530 X3533 X3534 X3540 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3553 X3554 X3559 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3576 X3580 X3581 X3582 X3583 X3584	X3342 X3348 X3349 X3350 X3351 X3352 X3358 X3359 X3360 X3361 X3362 X3365 X3366 X3369 X3370 X3373 X3374 X3378 X3381 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3409 X3410 X3411 X3412 X3413 X3414 X3421 X3433	X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3267 X3268 X3269 X3270 X3271 X3274 X3275 X3276 X3277 X3278 X3281 X3284 X3285 X3286 X3287 X3290 X3291 X3292 X3295 X3296 X3313 X3314 X3318 X3330 X3331 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341	X3142 X3143 X3144 X3153 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3177 X3178 X3179 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3207 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3226 X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241	X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2995 X2996 X2997 X3003 X3004 X3005 X3006 X3010 X3019 X3020 X3021 X3022 X3023 X3027 X3037 X3038 X3039 X3040 X3041 X3042 X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3053 X3054 X3055 X3060 X3061 X3062 X3063 X3134 X3135 X3136 X3137 X3138	E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 GLN L2905 THR V2906 ASP P2907 D2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 D2918 D2919 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 Q2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2952 X2957	Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 L2872 P2808 L2809 K2810 E2811 S2812 L2813 L2814 A2815 M2816 L2817 A2818 W2819 T2885 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894	GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY N2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 L2872 P2808 L2809 K2810 E2811 S2812 L2813 L2814 A2815 M2816 L2817 A2818 W2819 T2885 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894	GLU GLU ARG THR
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.070	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.22	0/834	0.51	0/1123
1	F	0.22	0/834	0.51	0/1123
1	H	0.22	0/834	0.51	0/1123
1	J	0.22	0/834	0.51	0/1123
2	B	0.26	0/25428	0.57	9/34534 (0.0%)
2	E	0.26	0/25428	0.57	8/34534 (0.0%)
2	G	0.26	0/25428	0.57	8/34534 (0.0%)
2	I	0.25	0/25428	0.57	8/34534 (0.0%)
All	All	0.25	0/105048	0.57	33/142628 (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	2
1	F	0	2
1	H	0	2
1	J	0	2
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	80

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4666	VAL	CA-C-N	-9.47	109.58	121.04
2	G	4666	VAL	C-N-CA	-9.47	109.58	121.04
2	B	4666	VAL	CA-C-N	-9.46	109.59	121.04
2	B	4666	VAL	C-N-CA	-9.46	109.59	121.04
2	E	4666	VAL	CA-C-N	-9.46	109.60	121.04

There are no chirality outliers.

5 of 80 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
1	A	82	TYR	Peptide
1	F	8	SER	Peptide
1	F	82	TYR	Peptide
1	H	8	SER	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	818	0	824	11	0
1	F	818	0	824	11	0
1	H	818	0	824	11	0
1	J	818	0	824	12	0
2	B	29499	0	24752	256	0
2	E	29499	0	24752	251	0
2	G	29499	0	24752	251	0
2	I	29499	0	24752	255	0
3	B	31	0	12	1	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102392	1034	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 5.

The worst 5 of 1034 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:G:646:PRO:HD2	2:G:779:PRO:HB2	1.73	0.70
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.69
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.73	0.69
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.75	0.69

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	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	43	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	43	76
2	G	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	43	76
2	I	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	43	76
All	All	13360/18096 (74%)	11884 (89%)	1452 (11%)	24 (0%)	44	76

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1840	PRO
2	B	1932	PRO
2	B	4641	PRO
2	E	1708	ARG

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2482 (100%)	11 (0%)	84	83
2	E	2493/3022 (82%)	2482 (100%)	11 (0%)	84	83
2	G	2493/3022 (82%)	2482 (100%)	11 (0%)	84	83
2	I	2493/3022 (82%)	2482 (100%)	11 (0%)	84	83
All	All	10324/12444 (83%)	10280 (100%)	44 (0%)	81	83

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	2339	VAL

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Mol	Chain	Res	Type
2	G	978	THR
2	I	3663	LEU
2	I	4792	LEU
2	G	1676	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 224 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	57	ASN
2	G	4933	GLN
2	I	2005	GLN
2	G	4776	GLN
2	G	2260	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 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
3	ATP	B	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.70	10 (20%)
4	CFF	E	5102	-	15,15,15	1.99	6 (40%)	23,23,23	2.74	10 (43%)
4	CFF	B	5102	-	15,15,15	1.98	6 (40%)	23,23,23	2.74	10 (43%)
4	CFF	I	5102	-	15,15,15	1.98	6 (40%)	23,23,23	2.74	10 (43%)
3	ATP	I	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.71	9 (18%)
3	ATP	E	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.71	9 (18%)
3	ATP	G	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.71	9 (18%)
4	CFF	G	5102	-	15,15,15	1.98	7 (46%)	23,23,23	2.74	10 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	3/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	3/22/38/38	0/3/3/3
3	ATP	E	5101	-	-	3/22/38/38	0/3/3/3
3	ATP	G	5101	-	-	3/22/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	C5-C4	4.30	1.46	1.39
3	E	5101	ATP	C5-C4	4.29	1.46	1.39
3	G	5101	ATP	C5-C4	4.28	1.46	1.39
3	B	5101	ATP	C5-C4	4.28	1.46	1.39
4	E	5102	CFF	C6-N1	-4.14	1.31	1.40

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5102	CFF	C14-N7-C8	-7.69	111.89	126.28
4	G	5102	CFF	C14-N7-C8	-7.68	111.91	126.28
4	E	5102	CFF	C14-N7-C8	-7.67	111.93	126.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	5102	CFF	C14-N7-C8	-7.66	111.94	126.28
3	E	5101	ATP	C5-C4-N3	-5.31	119.41	126.72

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

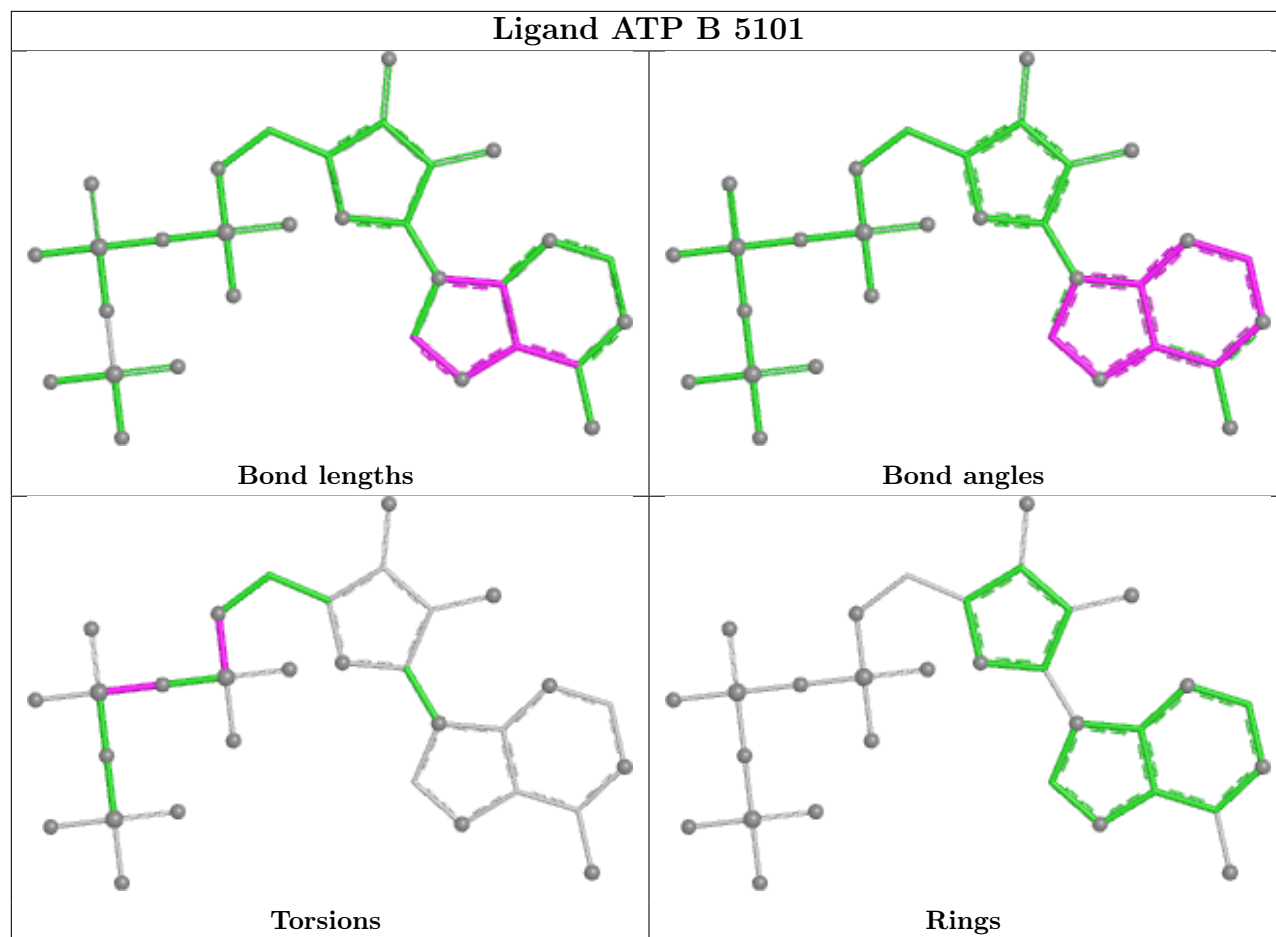
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	PA-O3A-PB-O1B

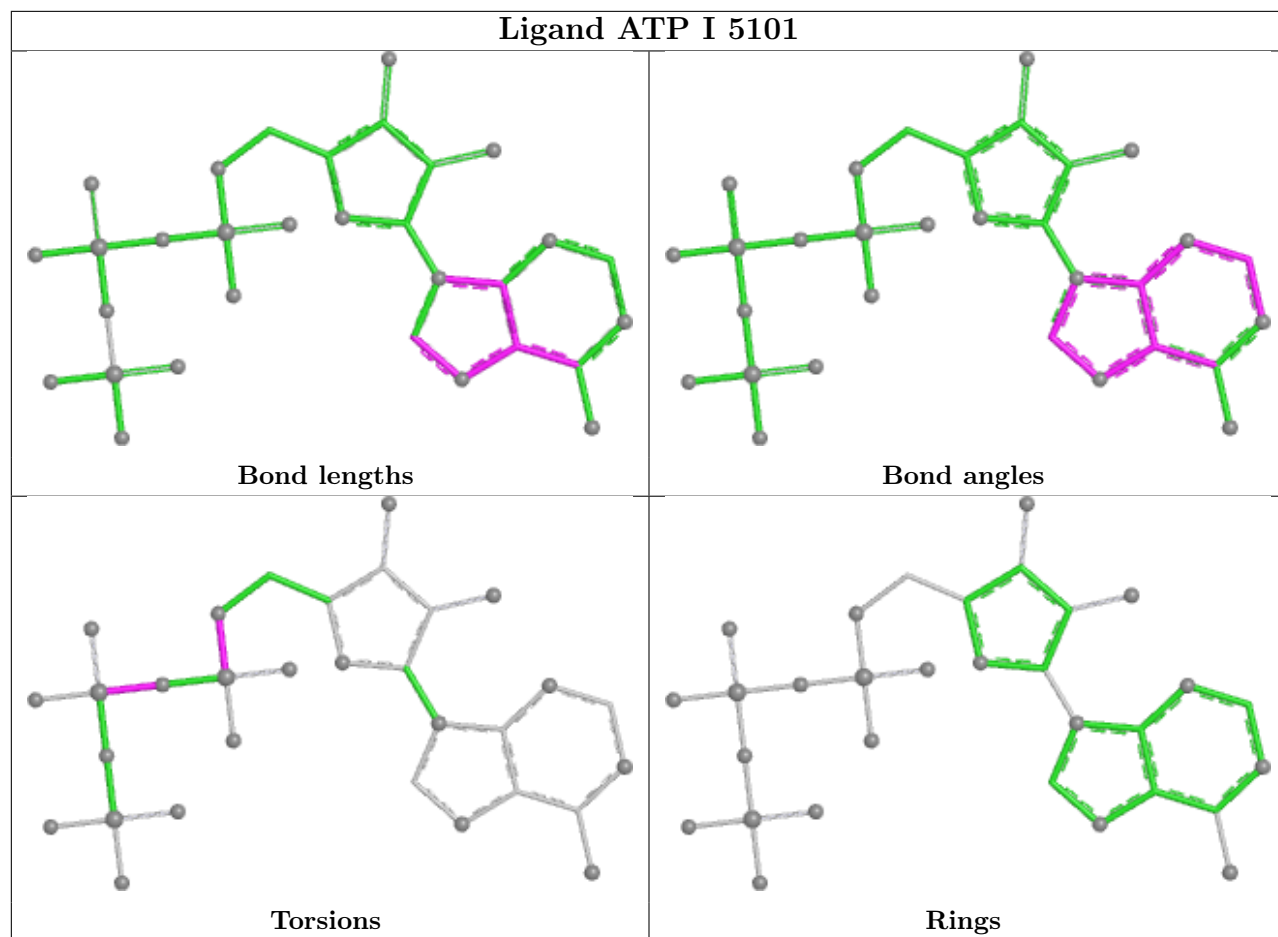
There are no ring outliers.

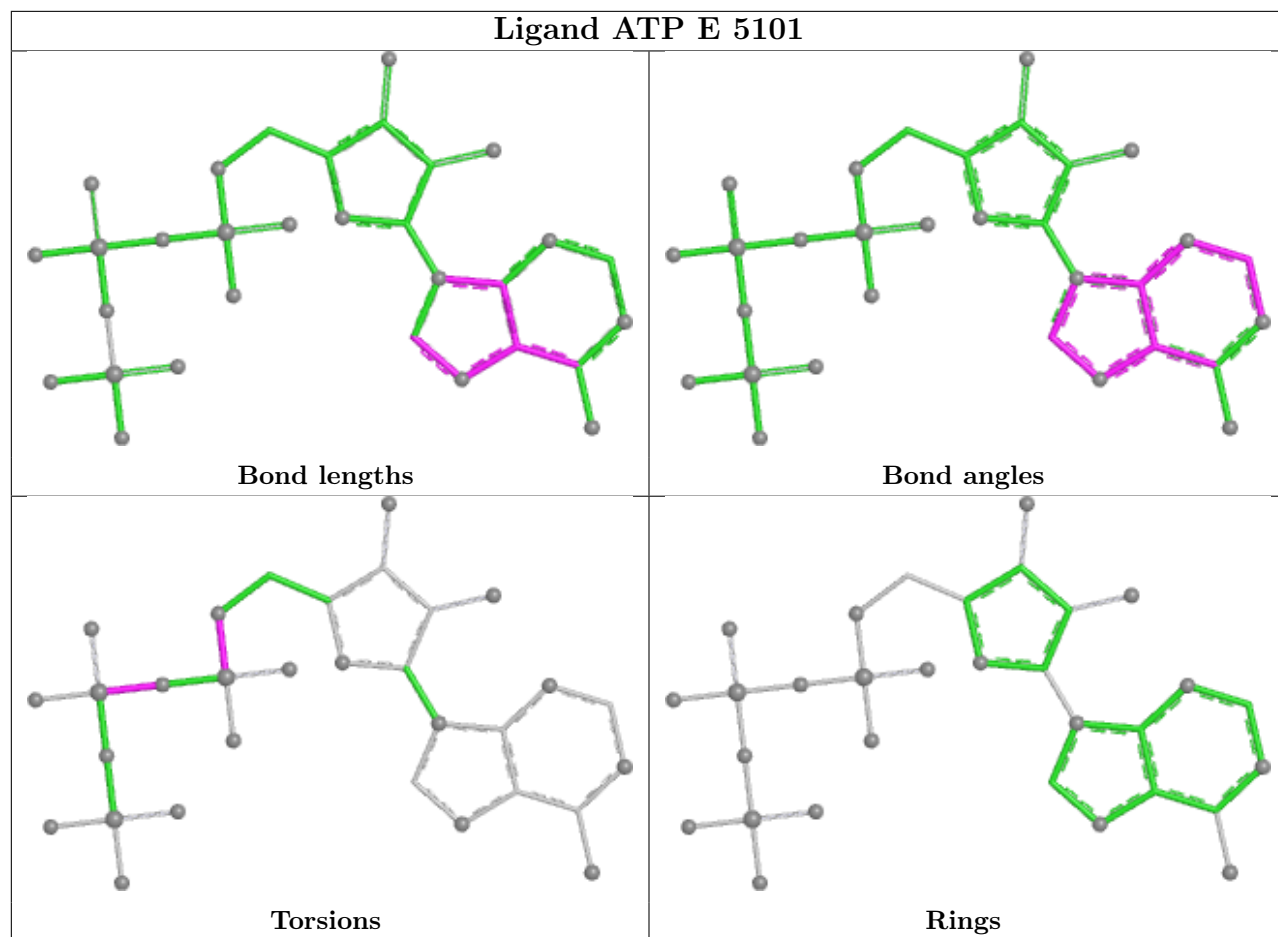
1 monomer is involved in 1 short contact:

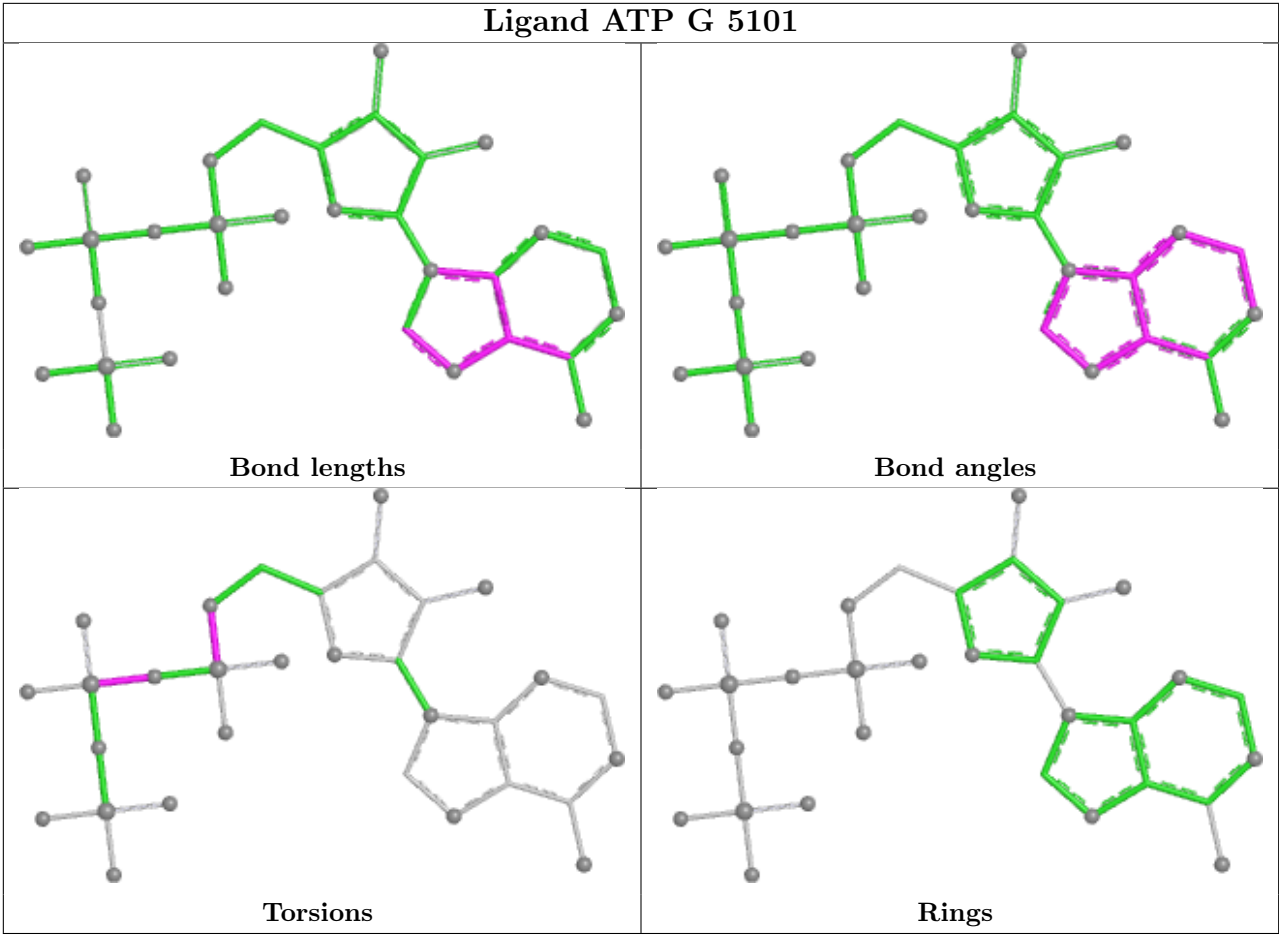
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	14
2	B	14
2	I	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	72.62
1	B	4345:UNK	C	4540:PHE	N	72.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.60
1	G	4345:UNK	C	4540:PHE	N	72.60
1	E	3613:UNK	C	3639:THR	N	43.07

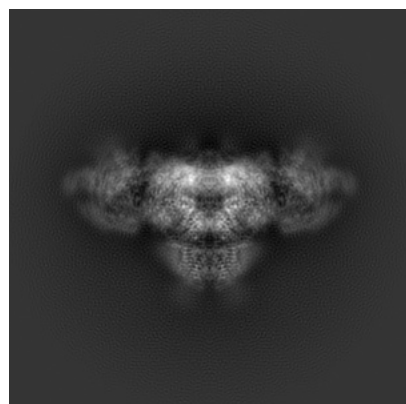
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8382. These allow visual inspection of the internal detail of the map and identification of artifacts.

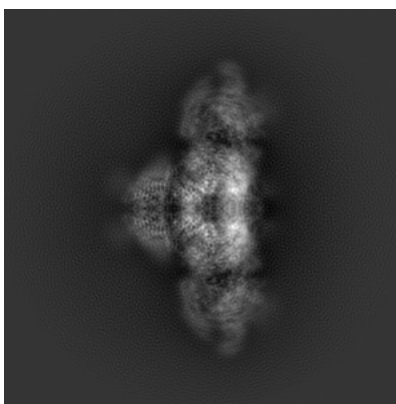
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

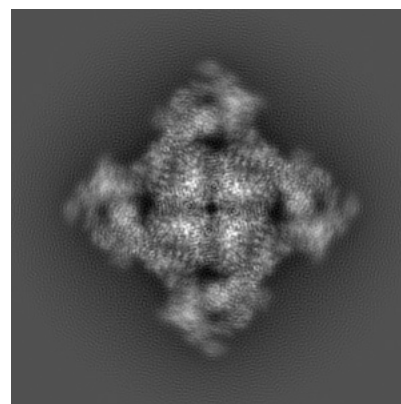
6.1.1 Primary map



X

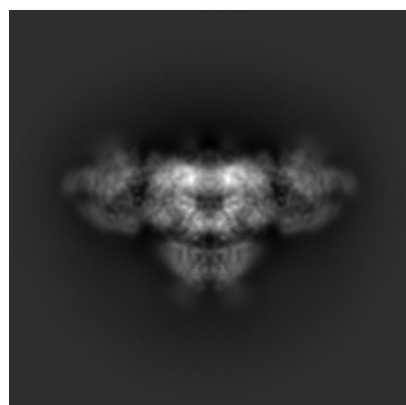


Y

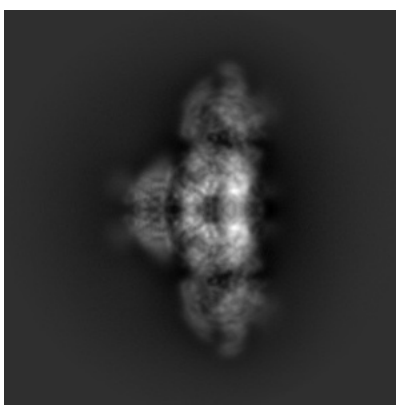


Z

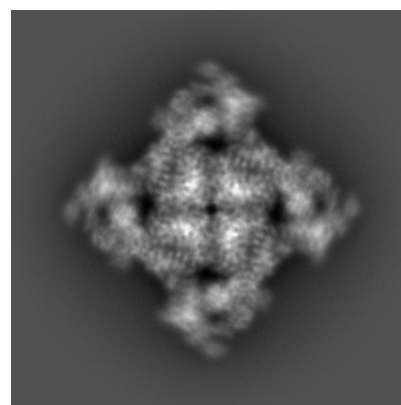
6.1.2 Raw map



X



Y

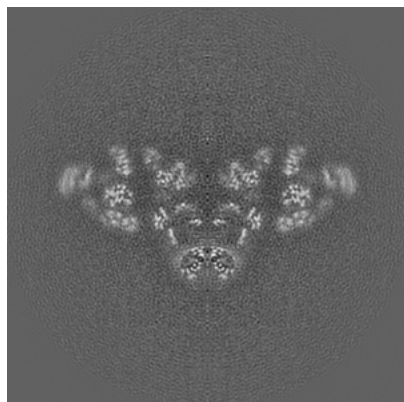


Z

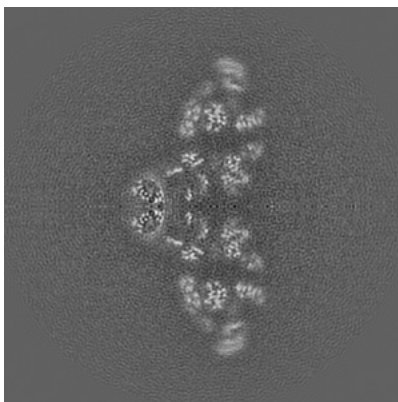
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

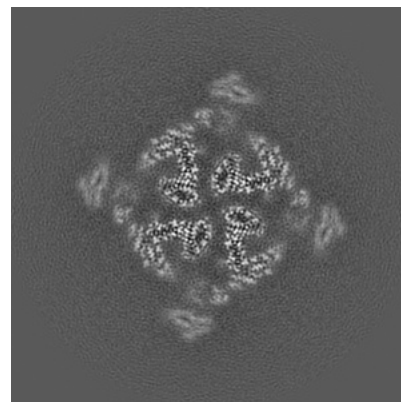
6.2.1 Primary map



X Index: 200

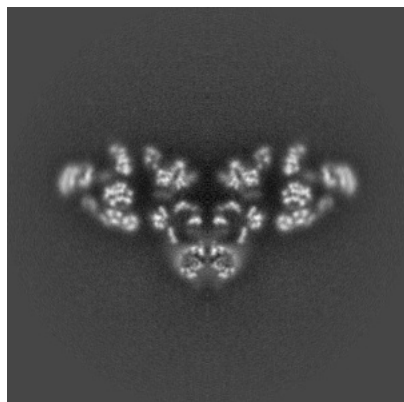


Y Index: 200

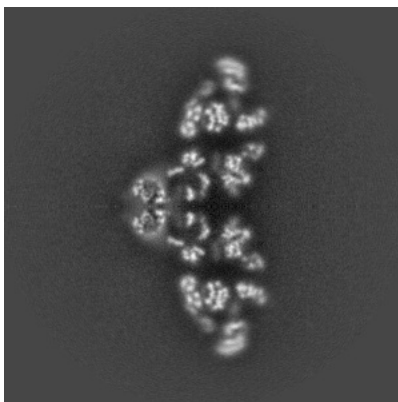


Z Index: 200

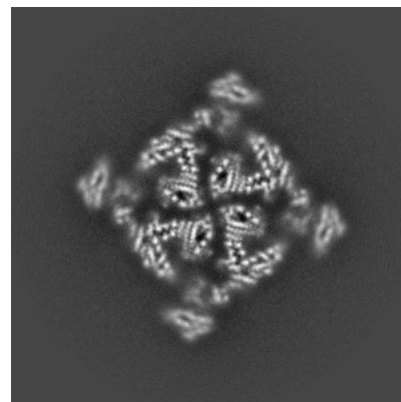
6.2.2 Raw map



X Index: 200



Y Index: 200

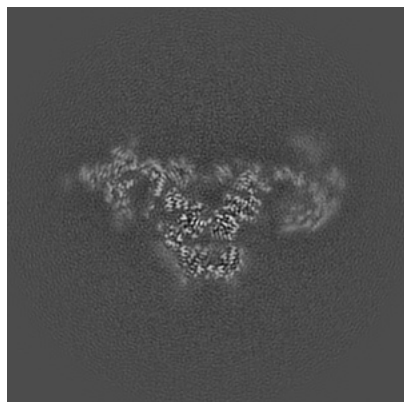


Z Index: 200

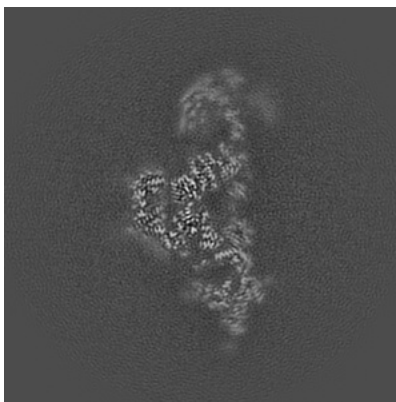
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

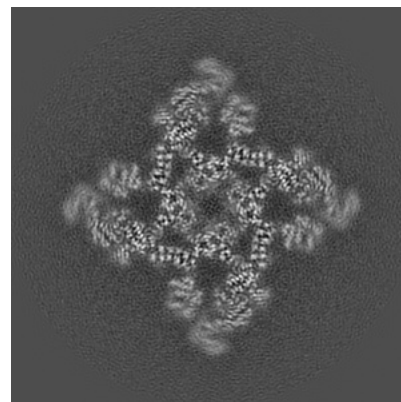
6.3.1 Primary map



X Index: 216

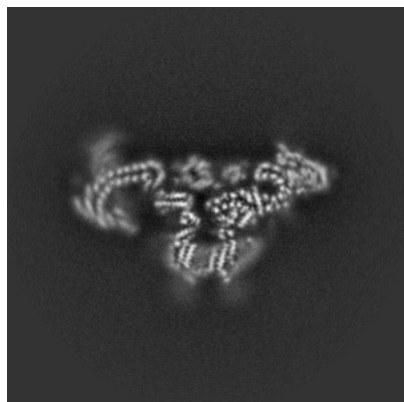


Y Index: 184

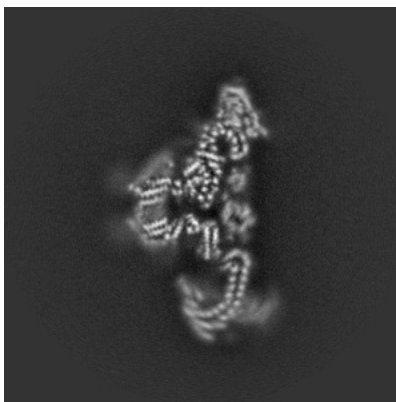


Z Index: 226

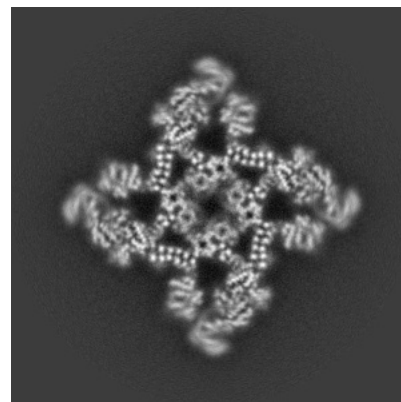
6.3.2 Raw map



X Index: 176



Y Index: 224

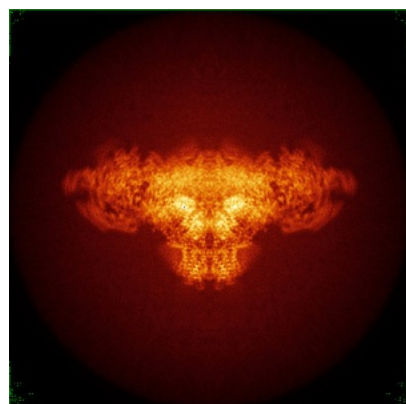


Z Index: 227

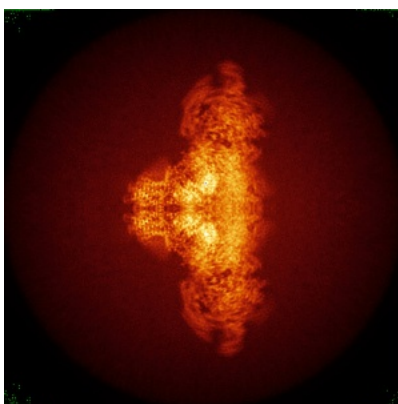
The images above show the largest variance slices of the map in three orthogonal directions.

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

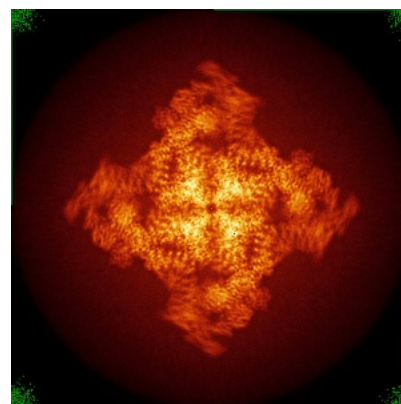
6.4.1 Primary map



X

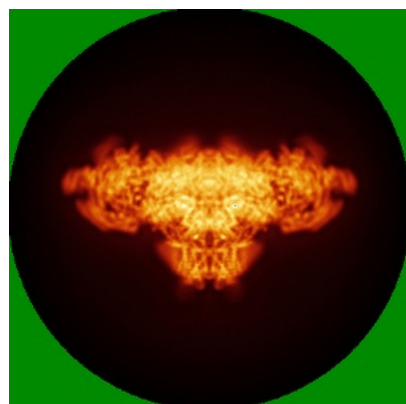


Y

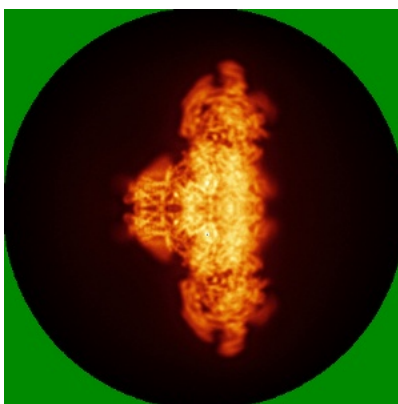


Z

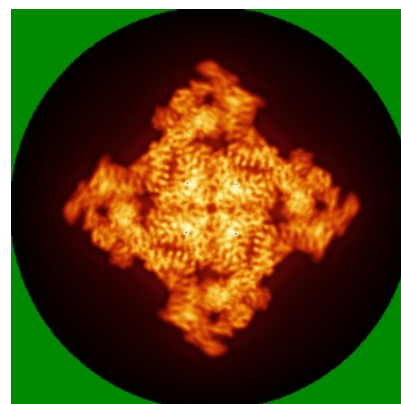
6.4.2 Raw map



X



Y

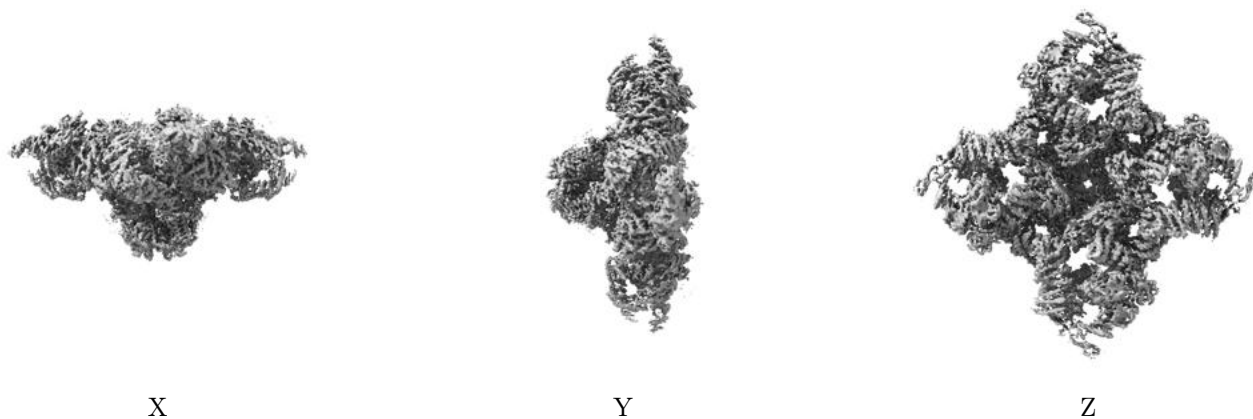


Z

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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

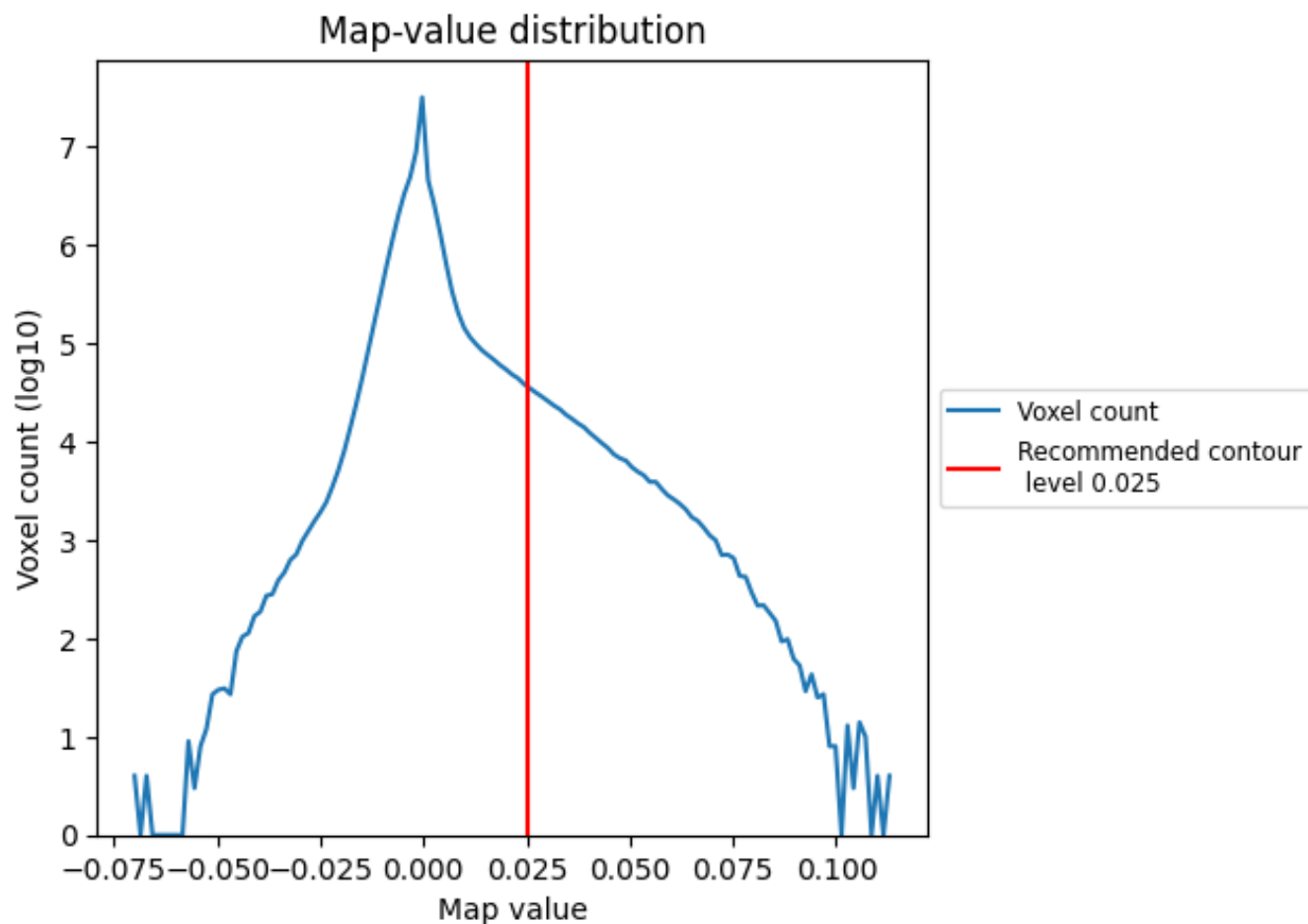
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

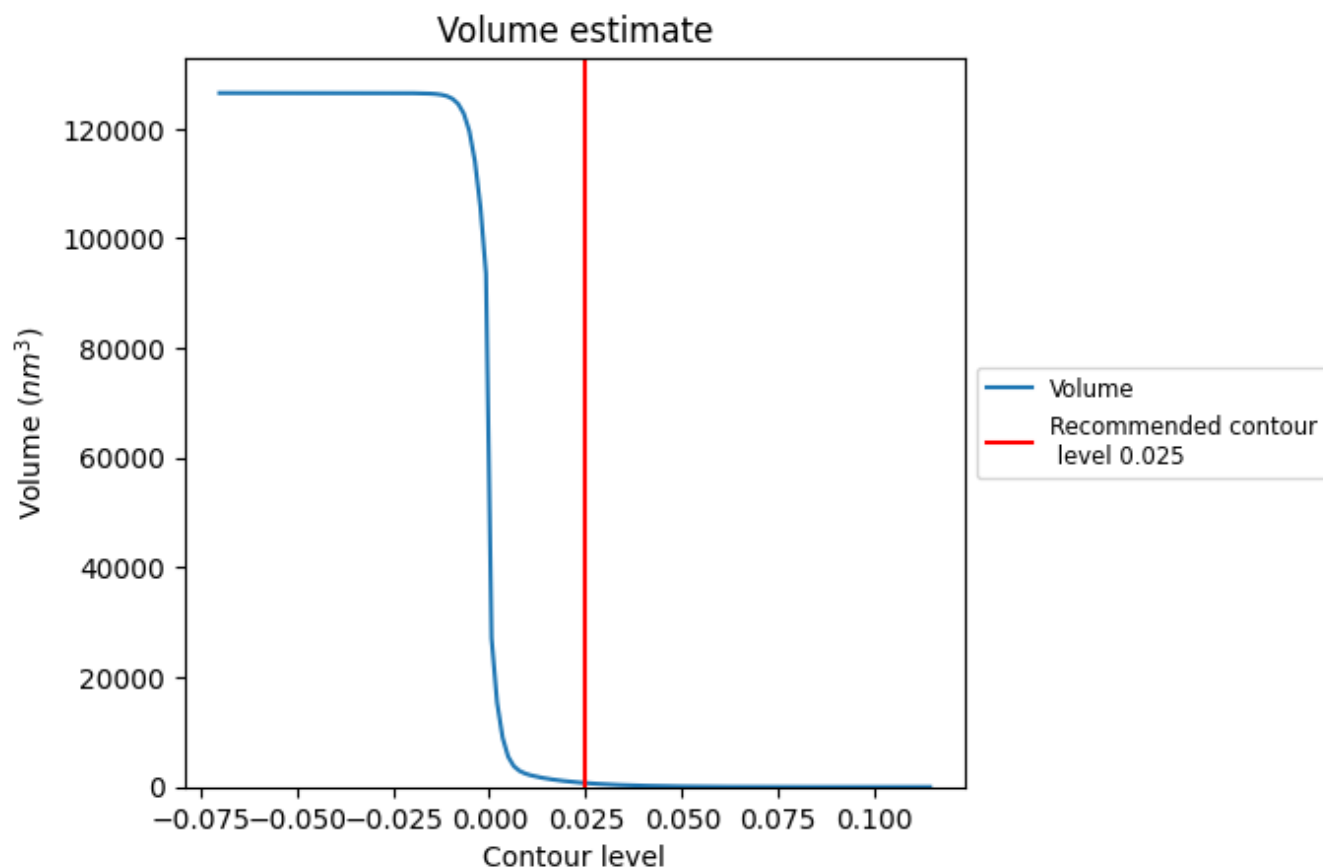
This section contains the results of statistical analysis of the map.

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.

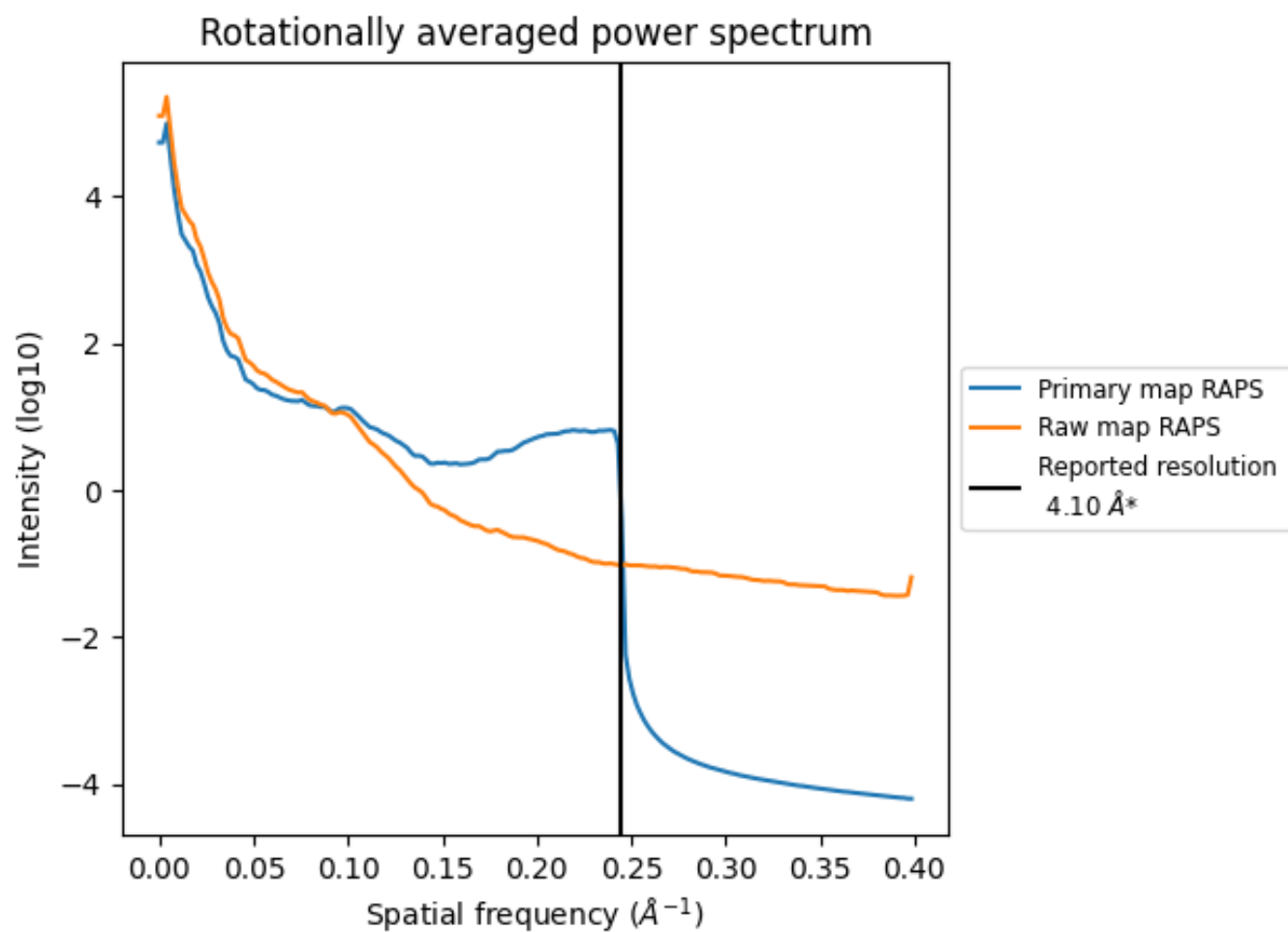
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 713 nm³; this corresponds to an approximate mass of 644 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 ⓘ

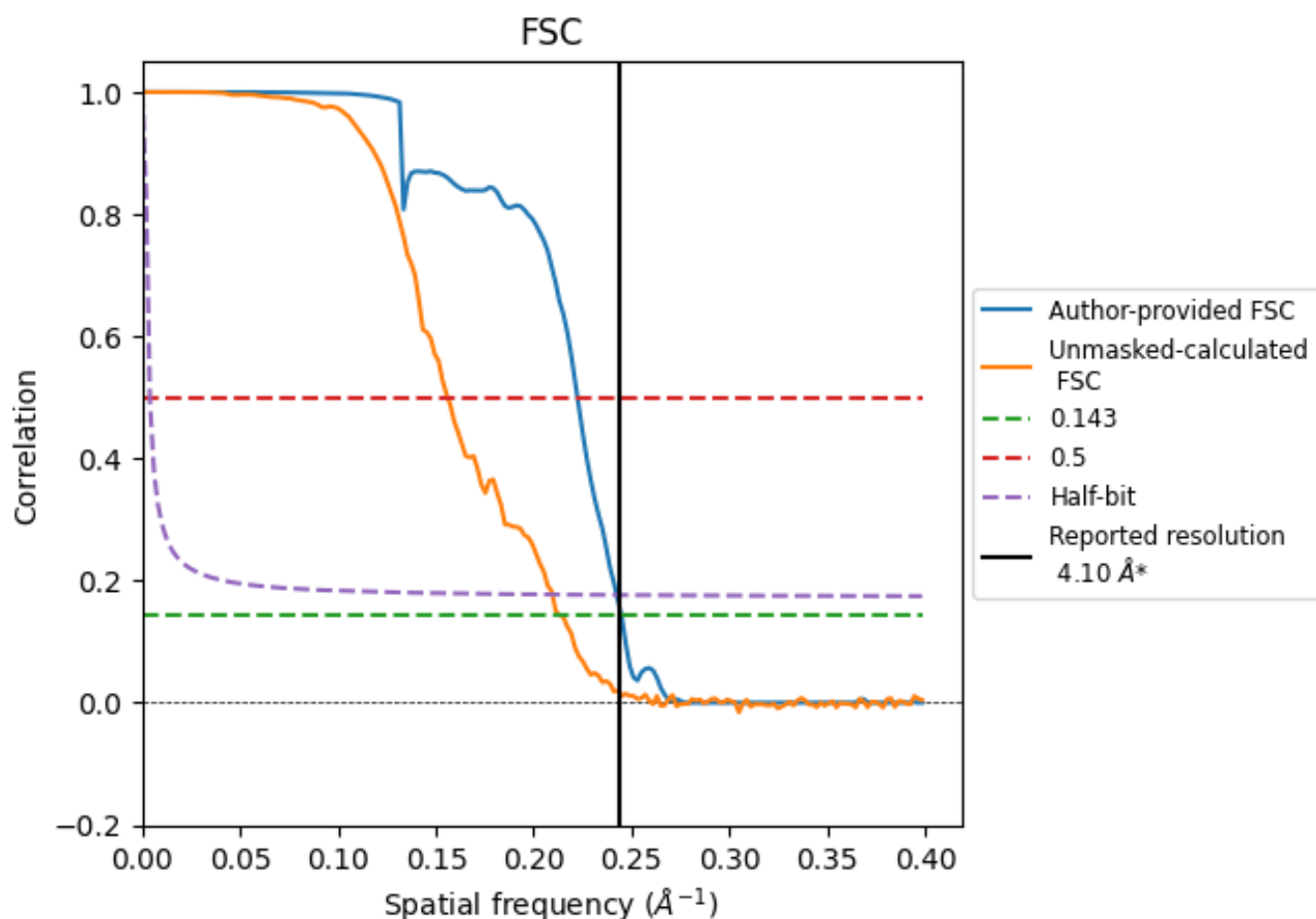


*Reported resolution corresponds to spatial frequency of $0.244 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	4.50	4.13
Unmasked-calculated*	4.69	6.41	4.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.69 differs from the reported value 4.1 by more than 10 %

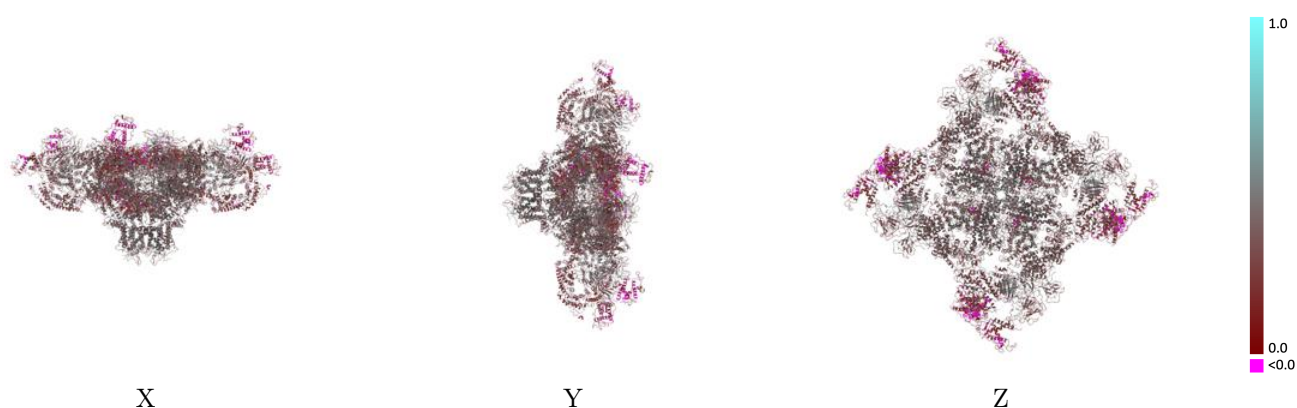
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8382 and PDB model 5TAQ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

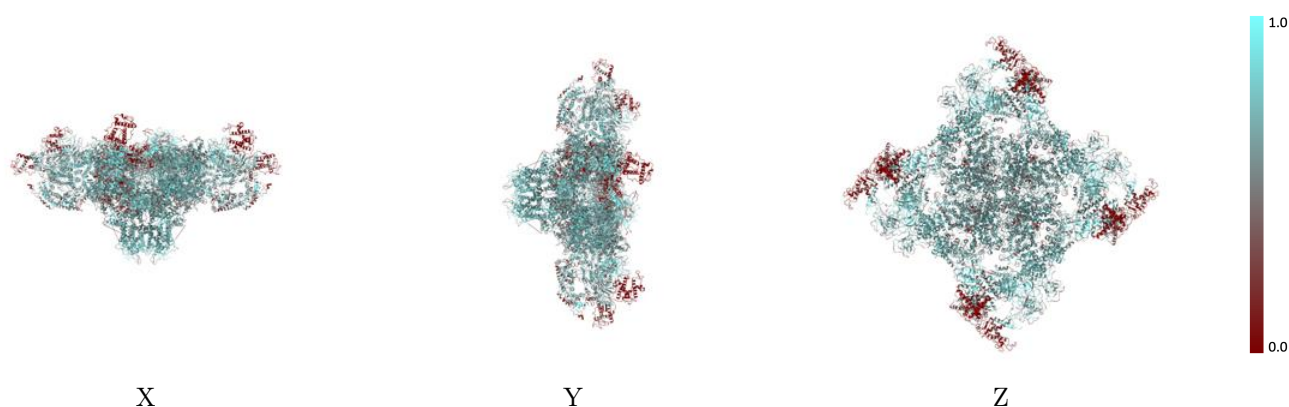
This section was not generated.

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



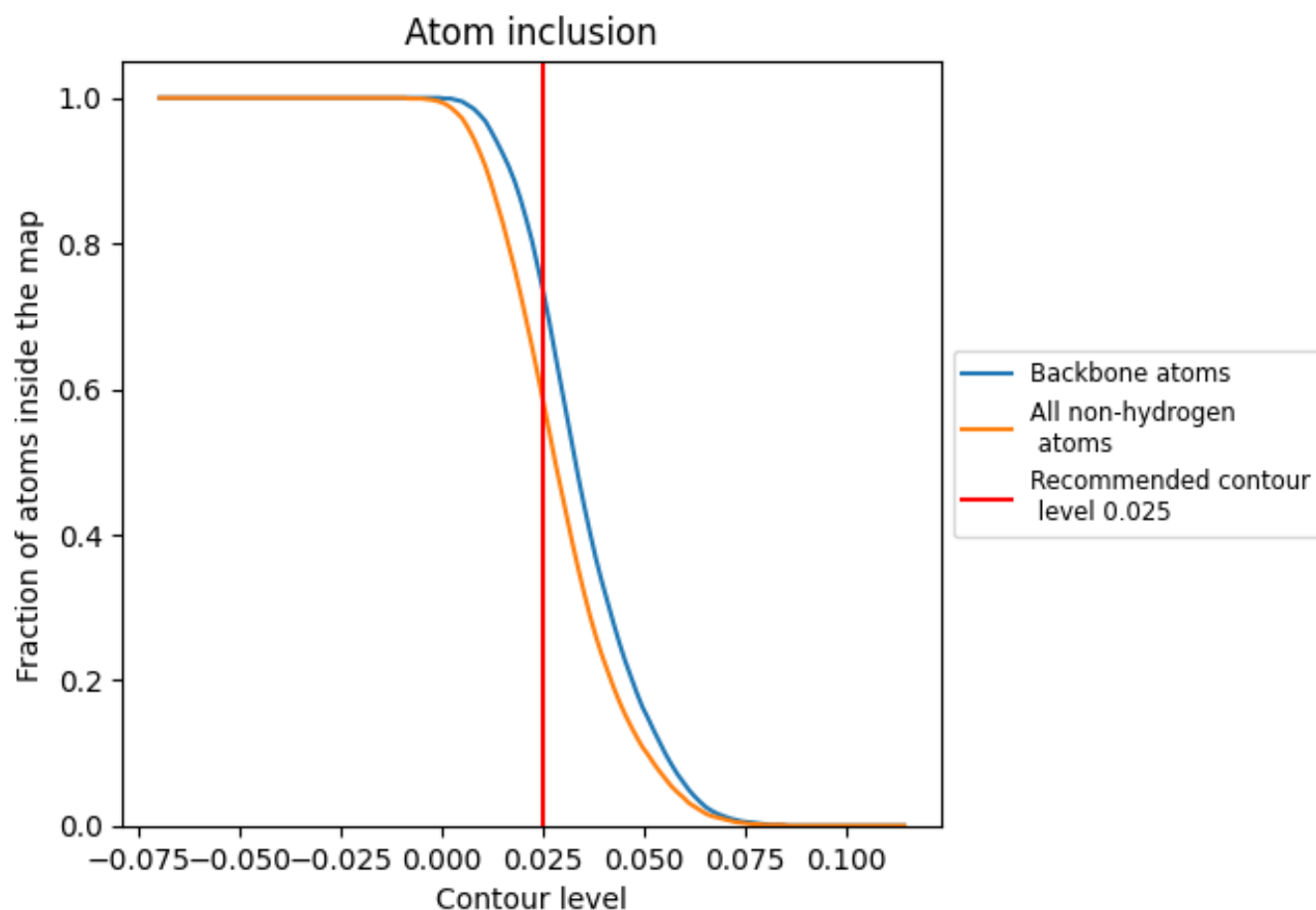
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 58% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5830	0.3350
A	0.5570	0.3500
B	0.5830	0.3340
E	0.5840	0.3340
F	0.5600	0.3560
G	0.5840	0.3350
H	0.5560	0.3530
I	0.5840	0.3350
J	0.5620	0.3490

1.0

0.0

<0.0