



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 12:53 AM UTC

PDB ID : 8XJI / pdb_00008xji
EMDB ID : EMD-38398
Title : Structure of chimeric RyR complex with flubendiamide
Authors : Lin, L.; Wang, C.; Wang, W.; Jiang, H.; Yuchi, Z.
Deposited on : 2023-12-21
Resolution : 3.91 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

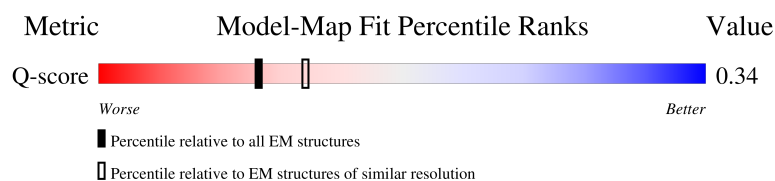
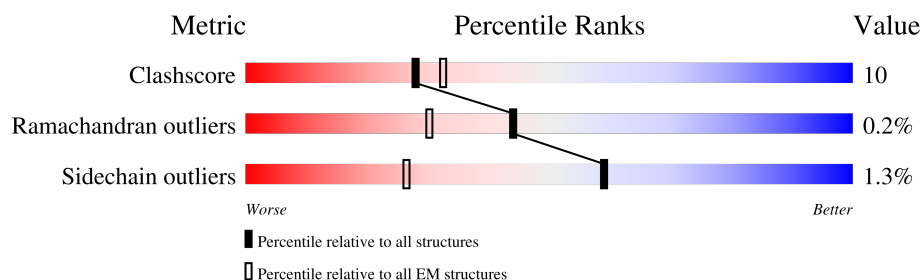
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.91 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	7920 (3.41 - 4.41)

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	107	11% 81% 19%
1	F	107	11% 85% 15%
1	G	107	11% 86% 14%
1	H	107	9% 86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	148	
2	J	148	
2	K	148	
2	L	148	
3	A	5037	
3	B	5037	
3	C	5037	
3	D	5037	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 119704 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	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
1	G	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
1	F	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
1	E	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
2	K	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
2	J	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
2	I	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23
K	32	ALA	GLU	engineered mutation	UNP P0DP23
K	68	ALA	GLU	engineered mutation	UNP P0DP23
K	105	ALA	GLU	engineered mutation	UNP P0DP23
K	141	ALA	GLU	engineered mutation	UNP P0DP23
J	32	ALA	GLU	engineered mutation	UNP P0DP23

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	68	ALA	GLU	engineered mutation	UNP P0DP23
J	105	ALA	GLU	engineered mutation	UNP P0DP23
J	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23

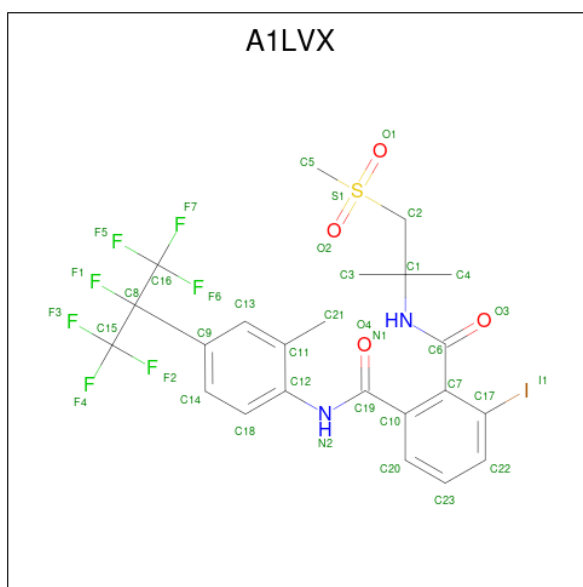
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	3928	Total	C	N	O	S	1	0
			27995	17849	4984	4987	175		
3	A	3928	Total	C	N	O	S	1	0
			27995	17849	4984	4987	175		
3	B	3928	Total	C	N	O	S	1	0
			27995	17849	4984	4987	175		
3	C	3928	Total	C	N	O	S	1	0
			27995	17849	4984	4987	175		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	4563	LYS	ARG	engineered mutation	UNP P11716
D	4564	TYR	PHE	engineered mutation	UNP P11716
D	4657	ILE	CYS	engineered mutation	UNP P11716
D	4792	SER	LEU	engineered mutation	UNP P11716
A	4563	LYS	ARG	engineered mutation	UNP P11716
A	4564	TYR	PHE	engineered mutation	UNP P11716
A	4657	ILE	CYS	engineered mutation	UNP P11716
A	4792	SER	LEU	engineered mutation	UNP P11716
B	4563	LYS	ARG	engineered mutation	UNP P11716
B	4564	TYR	PHE	engineered mutation	UNP P11716
B	4657	ILE	CYS	engineered mutation	UNP P11716
B	4792	SER	LEU	engineered mutation	UNP P11716
C	4563	LYS	ARG	engineered mutation	UNP P11716
C	4564	TYR	PHE	engineered mutation	UNP P11716
C	4657	ILE	CYS	engineered mutation	UNP P11716
C	4792	SER	LEU	engineered mutation	UNP P11716

- Molecule 4 is Flubendiamide (CCD ID: A1LVX) (formula: C₂₃H₂₂F₇IN₂O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
4	D	1	Total	C	F	I	N	O	S	0
			38	23	7	1	2	4	1	
4	A	1	Total	C	F	I	N	O	S	0
			38	23	7	1	2	4	1	
4	B	1	Total	C	F	I	N	O	S	0
			38	23	7	1	2	4	1	
4	C	1	Total	C	F	I	N	O	S	0
			38	23	7	1	2	4	1	

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

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

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

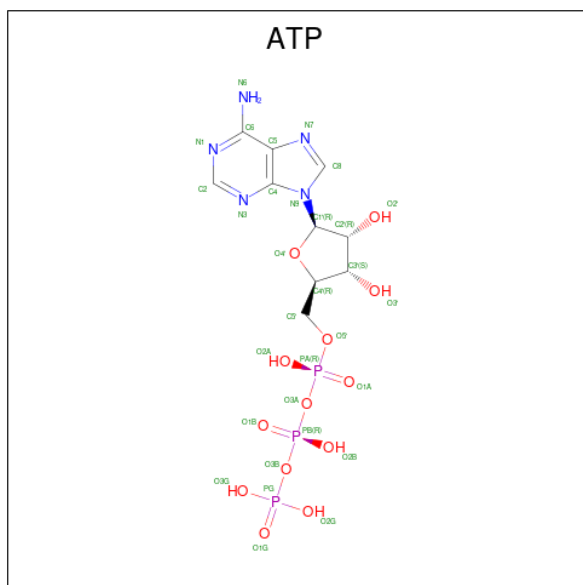
Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	

Continued on next page...

Continued from previous page...

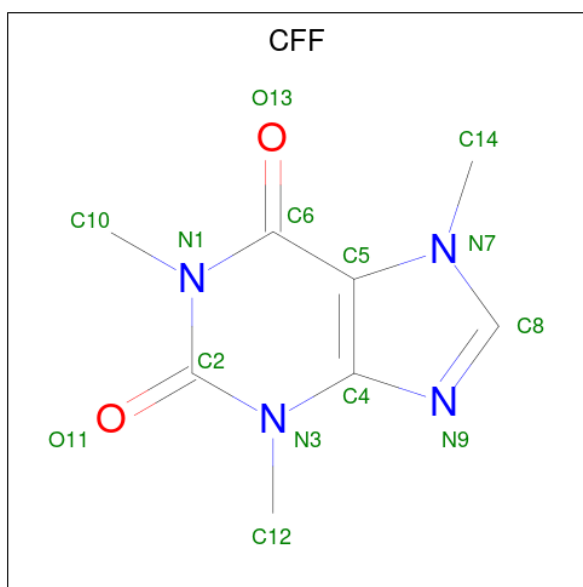
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 8 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).

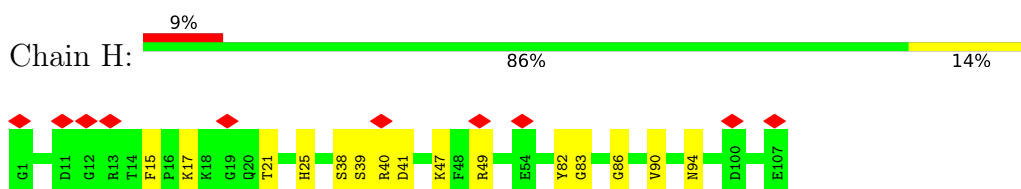


Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	N	O	0
			14	8	4	2	
8	A	1	Total	C	N	O	0
			14	8	4	2	
8	B	1	Total	C	N	O	0
			14	8	4	2	
8	C	1	Total	C	N	O	0
			14	8	4	2	

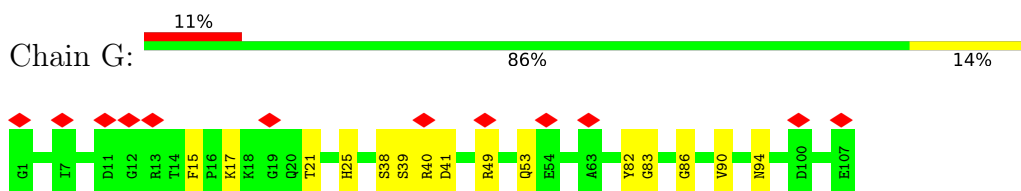
3 Residue-property plots

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

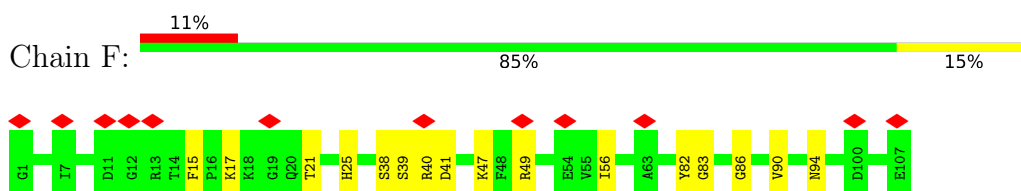
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



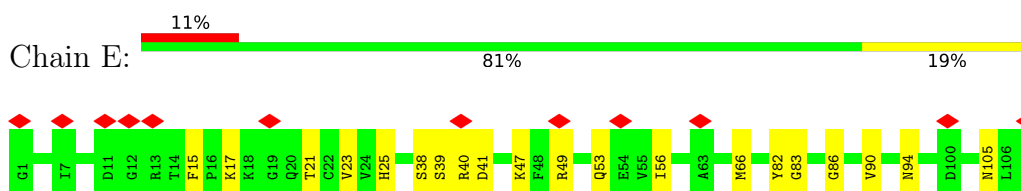
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



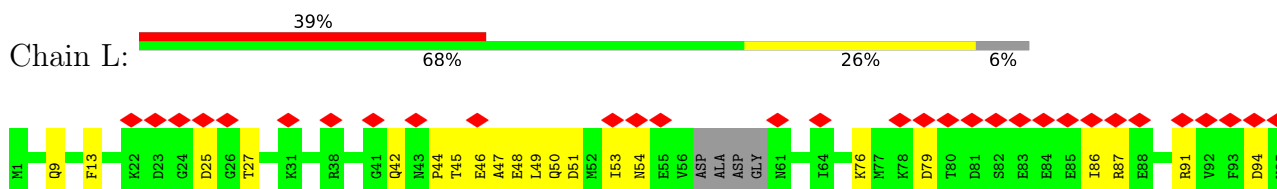
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

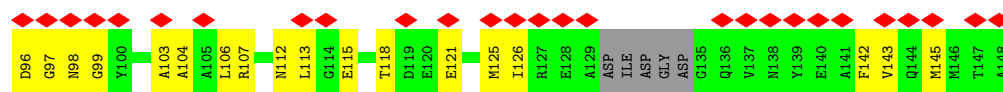


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

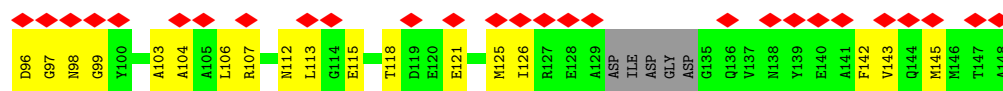
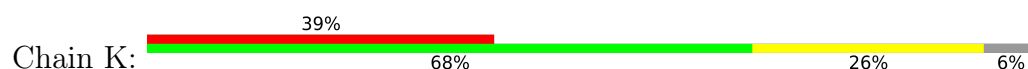


- Molecule 2: Calmodulin-1

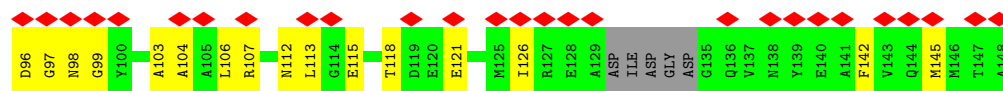
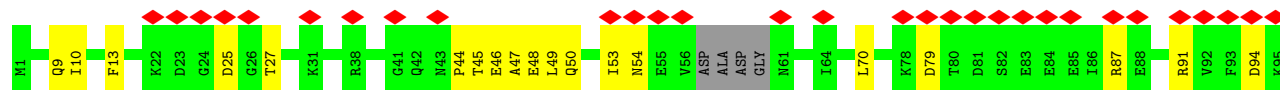
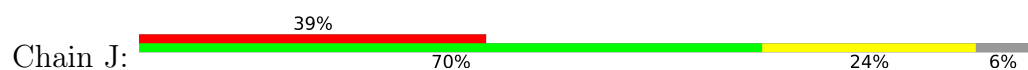




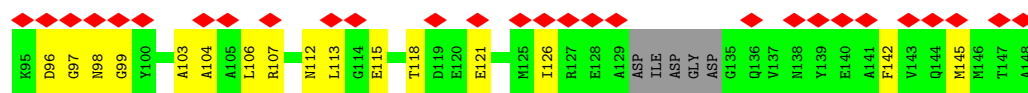
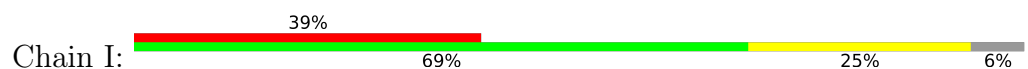
• Molecule 2: Calmodulin-1



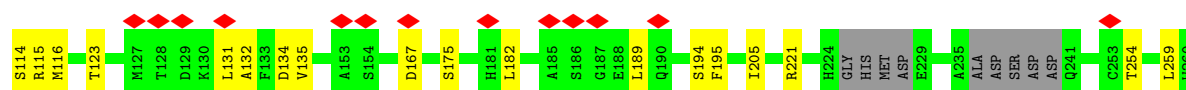
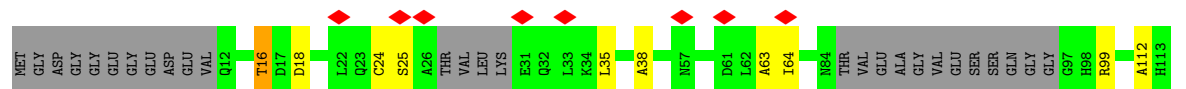
• Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1



• Molecule 3: Ryanodine receptor 1







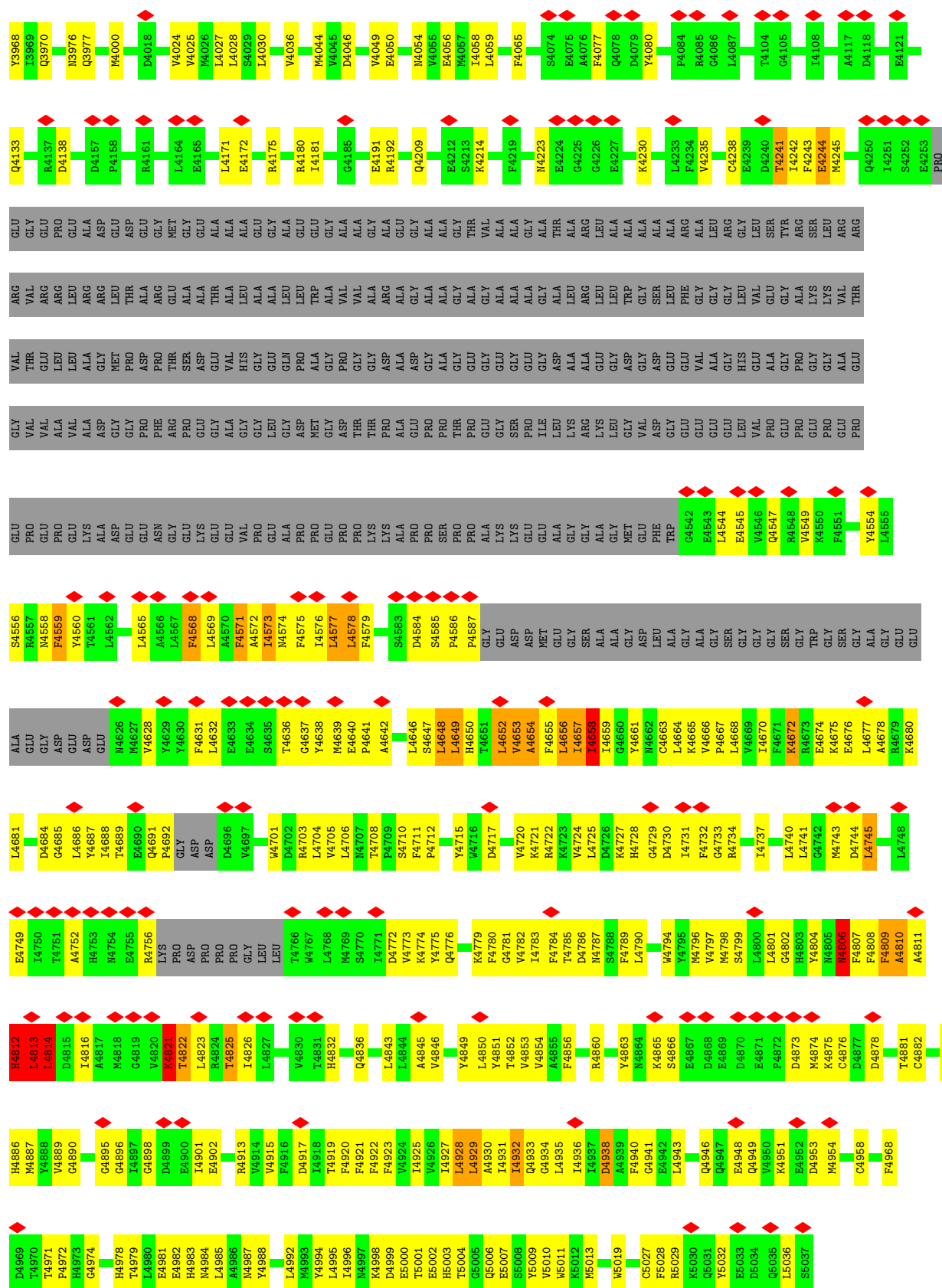
F2955	F2956	F2959	L2960	Q2961	Q2962	Q2966	Q2967	S2970	Q2971	E2972	F2973	T2974	A2975	H2976	LEU	GLU	ALA	VAL	VAL	SER	SER	GLY	ARG	VAL	VAL	GLU	VAL	ASN	LYS	SER	PRO	HIS	ILE	GLU	GLN	GLU	ILE	K2996	F2997	F2998	I3001	L3002	L3003	P3004	L3005	Y3009	H3013	C3014	L3015	TYR	PHE	LEU	THR	PRO	ALA	LYS	
VAL	L3025	A3031	K3034	E3035	M3038	L3042	PHE	CYS	LYS	LEU	ALA	L3049	H3052	R3053	T3059	D3060	A3061	P3062	VAL	VAL	VAL	ASN	ASN	CYS	LEU	THR	TYR	THR	ILE	LEU	ALA	ALA	ARG	SER	LEU	ASP	ALA	ARG	THR	VAL	MET	LYS	GLY	PRO	GLU	ILE	VAL	LYS	ALA	GLY	ARG	VAL	PHE				
GLU	SER	ALA	SER	ASP	ILE	GLU	LYS	VAL	MET	VAL	ASN	GLN	LEU	ARG	THR	GLN	ALA	ALA	GLY	GLN	ASN	ASN	LEU	THR	TYR	THR	THR	VAL	LEU	ALA	LEU	LEU	PRO	VAL	LEU	T3141	T3142	L3143	Q3149	G3153	I3157	D3160	V3161	Q3162	VAL	SER	CYS										
TYR	ARG	THR	L3169	C3170	S3171	T3172	Y3173	S3174	L3175	G3176	T3177	T3178	E3184	P3188	A3189	LEU	GLY	GLU	CYS	LEU	VAL	ALA	ALA	GLY	ARG	PRO	HIS	V3269	I3270	E3271	P3275	M3276	Y3280	L3281	P3282	R3283	W3284	W3285	GLU	ARG	GLY	PRO	GLU	ALA	PRO	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301			
GLU	MET	CYS	PRO	ASP	ILE	PRO	VAL	LEU	ASP	ARG	ASP	ALA	ILE	GLY	LEU	ALA	GLU	SER	GLY	ALA	ALA	GLU	SER	GLY	ALA	TYR	THR	MET	PRO	HIS	V3269	I3270	E3271	P3275	M3276	Y3280	L3281	P3282	R3283	W3284	W3285	GLU	ARG	GLY	PRO	GLU	ALA	PRO	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301
P3302	P3303	A3306	V3307	T3308	S3309	HIS	ASN	SER	LEU	L3316	V3324	L3327	D3330	E3331	A3332	T3333	TRP	MET	LYS	ARG	LEU	ALA	V3340	F3341	A3342	Q3343	P3344	V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	L3354	H3355	SER	HIS	PHE	V3359	P3360	T3361	L3365	A3369	V3373	E3376										
R3380	A3383	K3384	A3385	E3386	A3387	E3388	GLU	GLY	GLU	LEU	VAL	R3395	D3396	E3397	F3398	S3399	V3400	L3401	C3402	R3403	D3404	L3408	Y3409	P3410	L3411	L3412	L3413	R3414	N3418	N3419	R3420	A3421	P3427	N3430	ALA	GLU	GLU	LEU	F3435	V3438	I3441	W3445	S3446	K3452	ARG	GLU	GLU	N3457									
F3458	H3466	MET	SER	PHE	LEU	THR	ALA	ASP	SER	LYS	SER	LYS	MET	ALA	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	ASP	GLN	GLU	ARG	THR	LYS	LYS	ARG	LYS	ARG	GLY	ASP	TYR	SER	VAL	GLN	THR	SER	ILE	VAL	ALA	T3513	L3514	K3515	K3516	P3519	L3522	N3523	A3526					
P3527	T3528	D3529	GLN	ASP	LEU	ILE	M3534	L3535	A3536	A3541	L3542	K3543	E3547	VAL	GLU	ARG	GLU	PHE	L3553	Q3554	N3555	N3556	L3557	H3558	L3559	Q3560	GLY	LYS	VAL	GLU	GLY	SER	PRO	SER	L3569	L3579	PRO	GLY	ARG	GLU	GLU	ASP	ALA	ASP	ASP	PRO	E3590	V3596	V3599	L3606	E3610	HIS					
PRO	TYR	LYS	SER	LYS	ALA	VAL	TRP	HIS	LYS	L3623	K3626	R3629	A3634	R3637	N3643	K3658	F3669	D3675	D3676	L3677	S3678	K3679	A3680	G3681	E3682	Q3683	E3684	GLU	GLU	GLU	GLU	VAL	GLU	GLU	GLU	GLU	VAL	GLU	GLU	K3693	K3694	P3697	L3703	S3706	R3707	S3714	K3715	L3716	D3717								
K3729	S3732	C3733	H3734	L3735	E3736	E3737	GLY	GLY	GLU	ASN	GLU	GLY	ALA	GLU	VAL	E3750	V3751	S3752	F3753	Q3766	Q3767	S3768	R3769	L3770	H3771	R3772	R3773	L3780	Q3781	V3794	T3797	L3800	L3804	L3805	K3816	L3817	D3818	Y3819	G3827	F3828	F3829	L3842	D3843	A3846													
R3849	K3852	N3860	E3861	D3862	R3868	Q3869	N3870	G3871	V3874	D3878	F3885	R3886	F3887	L3888	Q3889	D3898	F3899	Q3900	L3903	R3904	N3914	I3915	I3916	T3919	S3929	K3940	Q3946	R3949	N3950	T3966	E3967	Y3968	I3969	Q3970	N3976	Q3977	D3987	M4000	V4024	V4025																	
V4026	L4027	L4028	L4030	V4036	M4039	D4046	V4049	V4054	V4055	E4056	M4057	L4058	L4059	F4065	S4074	E4075	A4076	F4077	D4078	D4079	Y4080	P4084	R4085	T4104	G4105	T4108	A4117	D4118	E4121	Q4133	D4138	D4157	P4158	E4165	E4172	R4175	R4180	I4181																			







D3818	D3819	D3822	F3829	I3832	L3842	L3843	A3846	R3849	K3852	N3860	E3861	D3862	R3868	Q3869	N3870	G3871	V3874	D3878	Q3882	F3885	L3888	Q3889	D3898	F3899	Q3900	L3903	R3904	N3914	I3915	I3916	T3919	S3929	Q3946	R3949	N3950	T3966	E3967																						
R3707	S3714	K3715	L3716	D3717	M3729	S3732	C3733	H3734	L3735	E3736	E3737	GLY	GLY	GLY	ASN	GLY	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU																					
GLU	GLU	ASP	ALA	ASP	PRO	E3590	V3596	V3599	L3606	E3610	HIS	PRO	GLY	TYR	LYS	GLY	GLY	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU																						
GLN	THR	SER	LEU	ILE	VAL	ALA	T3513	L3514	K3515	K3516	P3519	L3522	N3523	A3526	P3527	T3528	D3529	GLN	ASP	LEU	ILE	M3534	L3535	A3536	E3547	VAL	ARG	GLU	GLY	GLU	LEU	LEU	VAL	R3395	D3396	E3397	F3398	V3400	L3401	C3402	R3403	D3404	A3407	L3408	T3409	P3410	L3411	L3412	L3413	R3414	V3415	N3418	N3419	R3420	A3421	H3422	P3427		
ALA	GLU	GLU	LEU	F3435	V3438	I3441	V3445	S3446	K3452	ARG	GLU	GLU	GLU	Q3456	N3466	MET	SER	PHE	LEU	THR	ALA	ASP	ASP	LYS	SER	GLY	GLY	LEU	LEU	VAL	R3395	D3396	E3397	F3398	V3400	L3401	C3402	R3403	D3404	A3407	L3408	T3409	P3410	L3411	L3412	L3413	R3414	V3415	N3418	N3419	R3420	A3421	H3422	P3427					
SER	HIS	PHE	T3359	F3360	T3361	L3365	A3369	V3373	E3376	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	GLU	GLY	GLU	LEU	LEU	VAL	R3395	D3396	E3397	F3398	V3400	L3401	C3402	R3403	D3404	A3407	L3408	T3409	P3410	L3411	L3412	L3413	R3414	V3415	N3418	N3419	R3420	A3421	H3422	P3427											
ARG	GLY	PRO	ALA	PRO	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	A3306	V3307	T3308	S3309	ASP	HIS	LEU	ASP	ARG	ASN	SER	LEU	L3316	V3324	L3327	D3330	E3331	A3332	T3333	TRP	MET	LYS	ARG	LEU	ALA	V3340	F3341	A3342	Q3343	P3344	I3345	V3346	S3347	R3348	A3349	P3351	E3352	L3353	L3354					
K3222	S3223	P3224	R3225	E3226	R3227	A3228	L3229	L3230	G3231	PRO	ASN	SER	VAL	GLY	MET	CYS	PRO	ASP	ILE	PRO	VAL	LEU	ASP	ARG	ASN	MET	ASP	ILE	GLY	ALA	GLU	SER	GLY	ALA	GLU	SER	GLY	ALA	GLU	PRO	HIS	V3269	I3270	E3271	P3275	N3276	V3280	L3281	P3282	R3283	V3284	V3285							
T3142	L3143	G3149	G3153	I3157	D3160	V3161	Q3162	VAL	CYS	TYR	ARG	THR	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	T3178	E3184	P3188	A3189	LEU	GLY	GLU	ALA	GLU	SER	GLY	ALA	GLU	THR	VAL	CYS	LEU	ALA	ARG	THR	GLN	ASN	PRO	TYR	THR	THR	ALA	LEU	PRO	VAL	TYR	ASN	ALA	CYS	SER	VAL	TYR	T3221
LYS	SER	PRO	GLY	ILE	VAL	LYS	ALA	THR	ALA	SER	GLU	ASP	ILE	GLY	LYS	MET	VAL	ASN	ASN	ARG	LEU	GLY	VAL	SER	GLN	ALA	ARG	THR	VAL	LYS	GLY	VAL	GLY	GLN	ASN	LEU	THR	TYR	THR	THR	ALA	LEU	LEU	PRO	VAL	LEU	ASP	ALA	ARG	THR	VAL	MET	T3141						
H2883	H2884	T2885	H2886	G2887	R2888	H2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	LYS	GLY	GLY	THR	PRO	HIS	PRO	LEU	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	A2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	R2932	H2933	G2934	V2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS
ASP	MET	GLU	LEU	THR	SER	SER	I2951	E2952	K2953	R2954	F2955	A2956	F2959	L2960	Q2961	Q2962	H2966	M2967	S2970	Q2971	E2972	F2973	I2974	A2975	H2976	LEU	GLU	ALA	VAL	VAL	SER	SER	GLY	ARG	VAL	GLU	LYS	SER	PRO	HIS	GLN	GLU	ILE	K2996	F2997	F2998	I3001	L3002	L3003	P3004	L3005	Y3009							



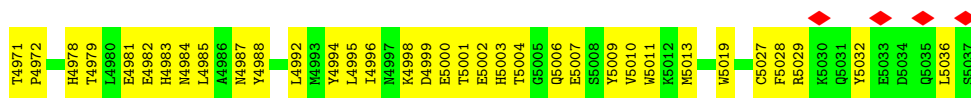
• Molecule 3: Ryanodine receptor 1



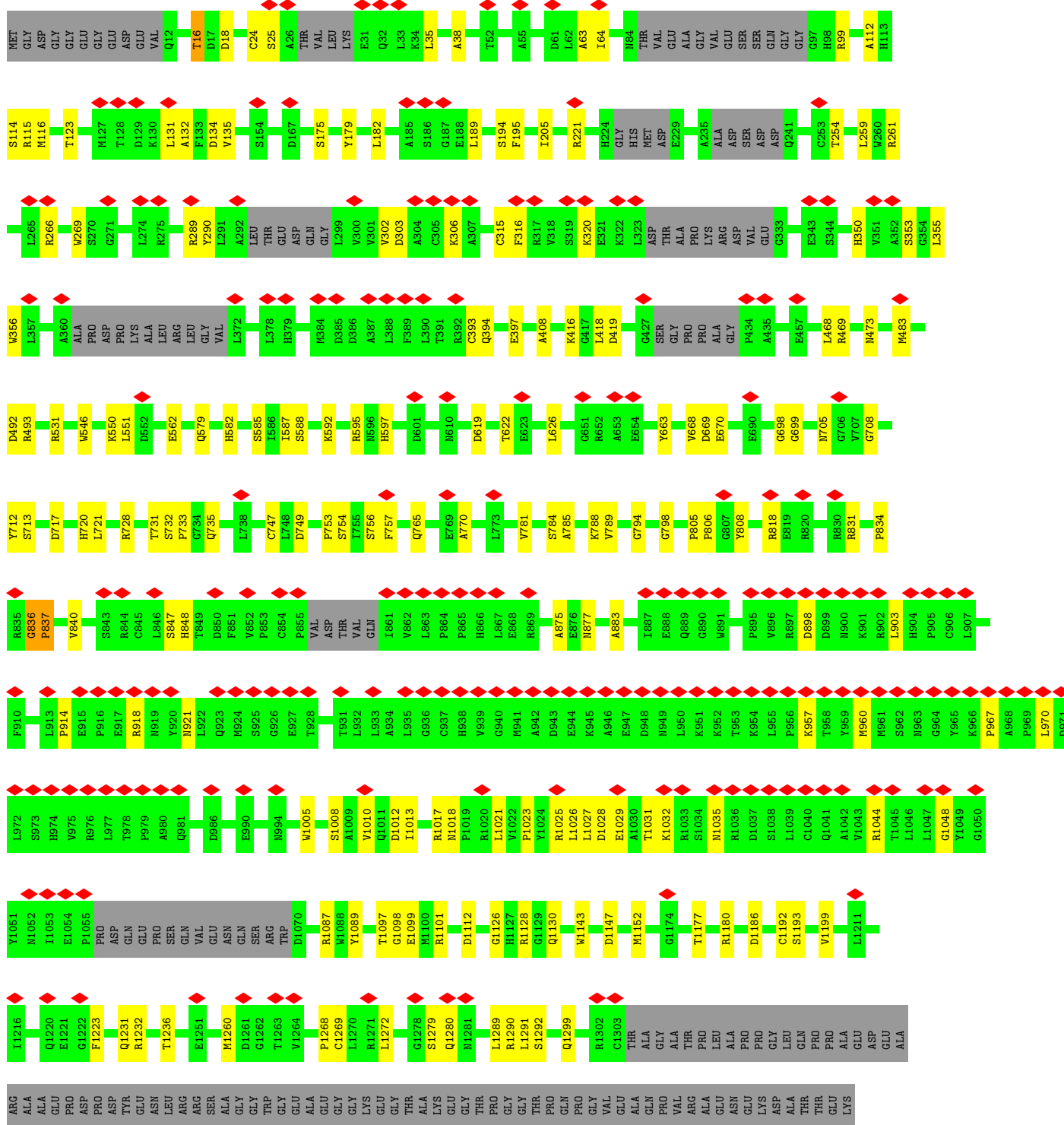








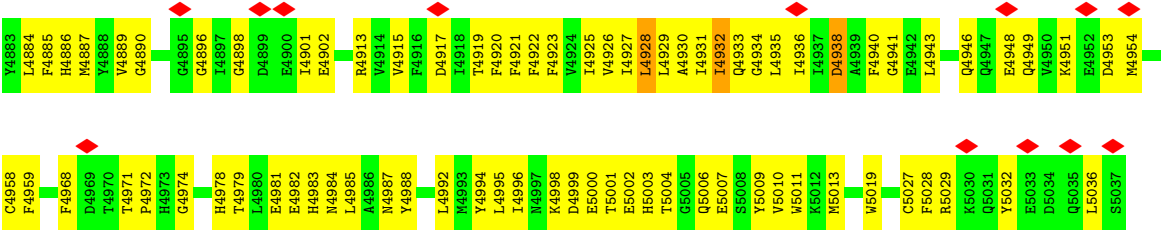
• Molecule 3: Ryanodine receptor 1



ASN	LYS	LYS	ARG	GLY	PHE	LEU	PHE	LYS	ALA	LYS	LYS	ALA	ALA	ALA	MET	THR	GLN	PRO	PRO	ALA	ALA	THR	PRO	ALA	LEU	PRO	ARG	LEU	PRO	HIS	ASP	ASP	ASN	ARG	D1422	T1431	Q1443	G1451	W1452	P1455	D1456	Q1459	H1460	D1461	H1462	M1476	E1479	Q1480	G1481				
N1482	S1486	L1487	K1488	C1489	Y1493	M1494	W1496	G1497	G1498	V1501	SER	PRO	GLY	GLN	GLN	GLY	ARG	I1509	S1510	H1511	T1512	D1513	L1514	H1527	G1533	N1537	N1545	L1548	F1549	P1550	A1551	V1552	T1557	V1561	I1562	E1565	L1566	G1567	K1568	Q1569	I1572	L1575	A1588										
E1596	V1597	Q1598	M1599	M1608	R1618	R1619	W1626	Q1629	C1630	Q1631	D1632	M1636	M1637	E1643	L1653	R1656	L1657	H1665	T1666	L1667	L1676	R1680	Q1691	A1697	D1713	R1727	L1738	T1739	T1742	G1751	ARG	LYS	GLY	ASN	ALA	R1758	P1763	S1770															
H1775	F1782	V1783	A1784	P1787	A1788	ALA	VAL	ALA	E1793	A1794	P1795	A1796	I1802	K1810	M1814	D1828	S1833	V1834	F1838	V1839	V1841	L1849	D1856	E1857	K1860	Q1861	K1864	M1865	P1868	F1871	T1872	E1873	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU									
GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU							
F1998	Q2003	W2007	D2014	ALA	ASP	GLU	GLU	GLU	D2020	L2023	P2024	E2025	I2027	R2028	Q2029	D2030	C2042	Q2045	L2046	E2047	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU						
LYS	PRO	GLU	GLU	LEU	PRO	ALA	GLU	LYS	P2091	L2094	M2101	P2114	R2126	Q2127	Y2128	D2138	P2146	S2147	S2148	T2152	L2165	L2166	I2167	M2170	I2179	M2186	K2189	V2190	F2191	Y2192	Q2193	H2204	M2208	V2214	L2215	G2216	GLY	GLY	GLY	THR	LYS												
E2222	M2228	M2250	H2253	L2258	G2262	ILE	LEU	GLY	M2267	S2270	T2271	D2274	E2285	L2288	G2306	C2310	P2311	M2312	L2313	L2314	A2315	K2316	P2319	D2320	I2321	D2333	R2336	R2355	G2365	P2366	L2368	R2369	GLY	GLY	G2373	S2374	G2375	L2376	L2377	A2378													
A2379	I2380	E2381	I2384	R2385	I2386	S2387	E2388	P2389	P2390	D2393	C2394	P2395	VAL	ARG	ARG	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	PRO	GLU	GLU	W2414	R2415	L2418	G2419	D2431	G2434	A2437	L2442	K2447	R2452	L2457	L2460	V2461	P2462	L2463	D2464	V2467								
G2468	I2469	I2470	S2471	L2472	P2473	L2474	P2477	T2478	L2479	GLY	LYS	ASP	GLY	ALA	LEU	V2486	Q2487	P2488	R2489	S2493	F2494	K2499	A2500	V2503	R2508	V2509	G2511	L2512	E2513	D2516	F2517	L2518	L2519	H2520	V2521	L2522	D2523	V2524	G2525	F2526	L2527	M2530	R2531	A2532	A2533	A2534	S2535	L2536	D2537	THR	ALA		
THR	PHE	SER	THR	T2544	A2547	L2548	N2551	R2552	T2553	L2554	A2557	K2564	L2568	F2569	P2570	A2571	T2572	E2573	A2576	T2577	V2579	D2580	S2581	M2582	L2583	H2584	Y2587	R2588	G2592	R2593	S2594	L2596	T2597	A2598	Q2599	R2600	E2604	D2605	L2607	M2608	Y2611	D2612	P2616	L2619									
Q2620	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	P2631	I2632	L2633	N2634	GLU	PHE	ALA	K2638	M2639	P2640	Y2655	CYS	LEU	PRO	THR	GLY	TRP	A2662	N2663	F2664	S2668	E2669	E2670	E2671	L2674	T2675	L2676	TRP	GLY	ILE	PHE	ASP	SER	L2686	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	R2697	M2698	A2699	
H2700	PRO	CYS	CYS	ALA	ALA	ALA	ALA	PRO	PRO	ASP	TYR	VAL	ASP	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	ALA	GLU	GLY	ASN	PHE	ASP	PRO	ARG	PRO	VAL	E2741	T2742	L2743	N2744	V2745	L2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35721	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.266	Depositor
Minimum map value	-0.185	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, A1LVX, ZN, CFF, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.38	0/820	0.56	0/1105
1	F	0.38	0/820	0.56	0/1105
1	G	0.38	0/820	0.56	0/1105
1	H	0.37	0/820	0.56	0/1105
2	I	0.24	0/1052	0.53	0/1416
2	J	0.25	0/1052	0.53	0/1416
2	K	0.25	0/1052	0.53	0/1416
2	L	0.24	0/1052	0.53	0/1416
3	A	0.38	3/28526 (0.0%)	0.65	41/38845 (0.1%)
3	B	0.38	3/28526 (0.0%)	0.65	41/38845 (0.1%)
3	C	0.38	3/28526 (0.0%)	0.65	41/38845 (0.1%)
3	D	0.38	3/28526 (0.0%)	0.65	41/38845 (0.1%)
All	All	0.37	12/121592 (0.0%)	0.64	164/165464 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1268	PRO	N-CD	-28.10	1.47	2.03
3	B	1268	PRO	N-CD	-28.10	1.47	2.03
3	C	1268	PRO	N-CD	-28.10	1.47	2.03
3	D	1268	PRO	N-CD	-28.10	1.47	2.03
3	D	4813	LEU	CA-C	-5.38	1.45	1.52

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	836	GLY	CA-C-N	12.15	135.02	119.84
3	C	836	GLY	C-N-CA	12.15	135.02	119.84
3	D	836	GLY	CA-C-N	12.14	135.01	119.84
3	D	836	GLY	C-N-CA	12.14	135.01	119.84
3	A	836	GLY	CA-C-N	12.11	134.98	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	804	0	812	13	0
1	F	804	0	812	10	0
1	G	804	0	812	9	0
1	H	804	0	812	9	0
2	I	1042	0	972	25	0
2	J	1042	0	972	25	0
2	K	1042	0	972	25	0
2	L	1042	0	972	25	0
3	A	27995	0	25202	517	0
3	B	27995	0	25202	524	0
3	C	27995	0	25202	532	0
3	D	27995	0	25202	534	0
4	A	38	0	0	0	0
4	B	38	0	0	0	0
4	C	38	0	0	0	0
4	D	38	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	31	0	12	2	0
7	B	31	0	12	2	0
7	C	31	0	12	2	0
7	D	31	0	12	2	0
8	A	14	0	10	0	0
8	B	14	0	10	0	0
8	C	14	0	10	0	0
8	D	14	0	10	0	0
All	All	119704	0	108032	2193	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 10.

The worst 5 of 2193 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)
3:A:4802:GLY:HA2	3:A:4808:PHE:HB2	1.52	0.90
3:D:4578:LEU:CD1	3:A:4849:TYR:HE2	1.84	0.90
3:C:4802:GLY:HA2	3:C:4808:PHE:HB2	1.52	0.90
3:D:4802:GLY:HA2	3:D:4808:PHE:HB2	1.52	0.89
3:B:4802:GLY:HA2	3:B:4808:PHE:HB2	1.52	0.89

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	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	F	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	G	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	I	133/148 (90%)	128 (96%)	5 (4%)	0	100	100
2	J	133/148 (90%)	128 (96%)	5 (4%)	0	100	100
2	K	133/148 (90%)	128 (96%)	5 (4%)	0	100	100
2	L	133/148 (90%)	128 (96%)	5 (4%)	0	100	100
3	A	3813/5037 (76%)	3598 (94%)	205 (5%)	10 (0%)	36	70
3	B	3813/5037 (76%)	3597 (94%)	206 (5%)	10 (0%)	36	70
3	C	3813/5037 (76%)	3597 (94%)	206 (5%)	10 (0%)	36	70
3	D	3813/5037 (76%)	3597 (94%)	206 (5%)	10 (0%)	36	70
All	All	16204/21168 (76%)	15297 (94%)	867 (5%)	40 (0%)	44	75

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	837	PRO
3	D	4653	VAL
3	D	4745	LEU
3	A	837	PRO
3	A	4653	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	84/88 (96%)	84 (100%)	0	100	100
1	F	84/88 (96%)	84 (100%)	0	100	100
1	G	84/88 (96%)	84 (100%)	0	100	100
1	H	84/88 (96%)	84 (100%)	0	100	100
2	I	104/122 (85%)	103 (99%)	1 (1%)	68	76
2	J	104/122 (85%)	103 (99%)	1 (1%)	68	76
2	K	104/122 (85%)	103 (99%)	1 (1%)	68	76
2	L	104/122 (85%)	103 (99%)	1 (1%)	68	76
3	A	2475/4276 (58%)	2442 (99%)	33 (1%)	61	72
3	B	2475/4276 (58%)	2441 (99%)	34 (1%)	59	71
3	C	2475/4276 (58%)	2441 (99%)	34 (1%)	59	71
3	D	2475/4276 (58%)	2441 (99%)	34 (1%)	59	71
All	All	10652/17944 (59%)	10513 (99%)	139 (1%)	59	72

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	4230	LYS
3	C	4573	ILE
3	C	4814	LEU
3	A	4241	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	4230	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 257 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	2007	ASN
3	C	2291	GLN
3	A	1041	GLN
3	A	877	ASN
3	C	3851	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 20 ligands modelled in this entry, 8 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	A1LVX	A	5101	-	38,39,39	1.00	2 (5%)	57,63,63	0.94	3 (5%)
8	CFF	C	5105	-	15,15,15	1.68	4 (26%)	23,23,23	1.71	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ATP	A	5104	-	32,33,33	3.09	12 (37%)	48,52,52	1.74	9 (18%)
8	CFF	A	5105	-	15,15,15	1.67	3 (20%)	23,23,23	1.70	5 (21%)
4	A1LVX	C	5101	-	38,39,39	1.00	2 (5%)	57,63,63	0.93	3 (5%)
7	ATP	B	5104	-	32,33,33	3.10	12 (37%)	48,52,52	1.74	9 (18%)
7	ATP	C	5104	-	32,33,33	3.10	12 (37%)	48,52,52	1.75	9 (18%)
7	ATP	D	5104	-	32,33,33	3.10	12 (37%)	48,52,52	1.74	9 (18%)
8	CFF	B	5105	-	15,15,15	1.68	4 (26%)	23,23,23	1.70	6 (26%)
4	A1LVX	B	5101	-	38,39,39	1.00	2 (5%)	57,63,63	0.93	3 (5%)
4	A1LVX	D	5101	-	38,39,39	1.00	2 (5%)	57,63,63	0.93	3 (5%)
8	CFF	D	5105	-	15,15,15	1.68	4 (26%)	23,23,23	1.70	5 (21%)

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	A1LVX	A	5101	-	-	1/47/47/47	0/2/2/2
8	CFF	C	5105	-	-	-	0/2/2/2
7	ATP	A	5104	-	-	11/22/38/38	0/3/3/3
8	CFF	A	5105	-	-	-	0/2/2/2
4	A1LVX	C	5101	-	-	1/47/47/47	0/2/2/2
7	ATP	B	5104	-	-	12/22/38/38	0/3/3/3
7	ATP	C	5104	-	-	11/22/38/38	0/3/3/3
7	ATP	D	5104	-	-	12/22/38/38	0/3/3/3
8	CFF	B	5105	-	-	-	0/2/2/2
4	A1LVX	B	5101	-	-	1/47/47/47	0/2/2/2
4	A1LVX	D	5101	-	-	1/47/47/47	0/2/2/2
8	CFF	D	5105	-	-	-	0/2/2/2

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5104	ATP	C2'-C3'	-8.66	1.29	1.53
7	C	5104	ATP	C2'-C3'	-8.66	1.29	1.53
7	B	5104	ATP	C2'-C3'	-8.64	1.29	1.53
7	D	5104	ATP	C2'-C3'	-8.64	1.29	1.53
7	B	5104	ATP	C6-N6	6.00	1.49	1.34

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	5104	ATP	C5-C4-N3	-5.14	119.64	126.72
7	C	5104	ATP	C5-C4-N3	-5.13	119.65	126.72
7	D	5104	ATP	C5-C4-N3	-5.13	119.66	126.72
7	A	5104	ATP	C5-C4-N3	-5.11	119.69	126.72
7	B	5104	ATP	N3-C2-N1	-4.69	121.48	128.58

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	5104	ATP	PB-O3B-PG-O3G
7	D	5104	ATP	C5'-O5'-PA-O3A
7	A	5104	ATP	PB-O3B-PG-O3G
7	A	5104	ATP	C5'-O5'-PA-O3A
7	B	5104	ATP	PB-O3B-PG-O3G

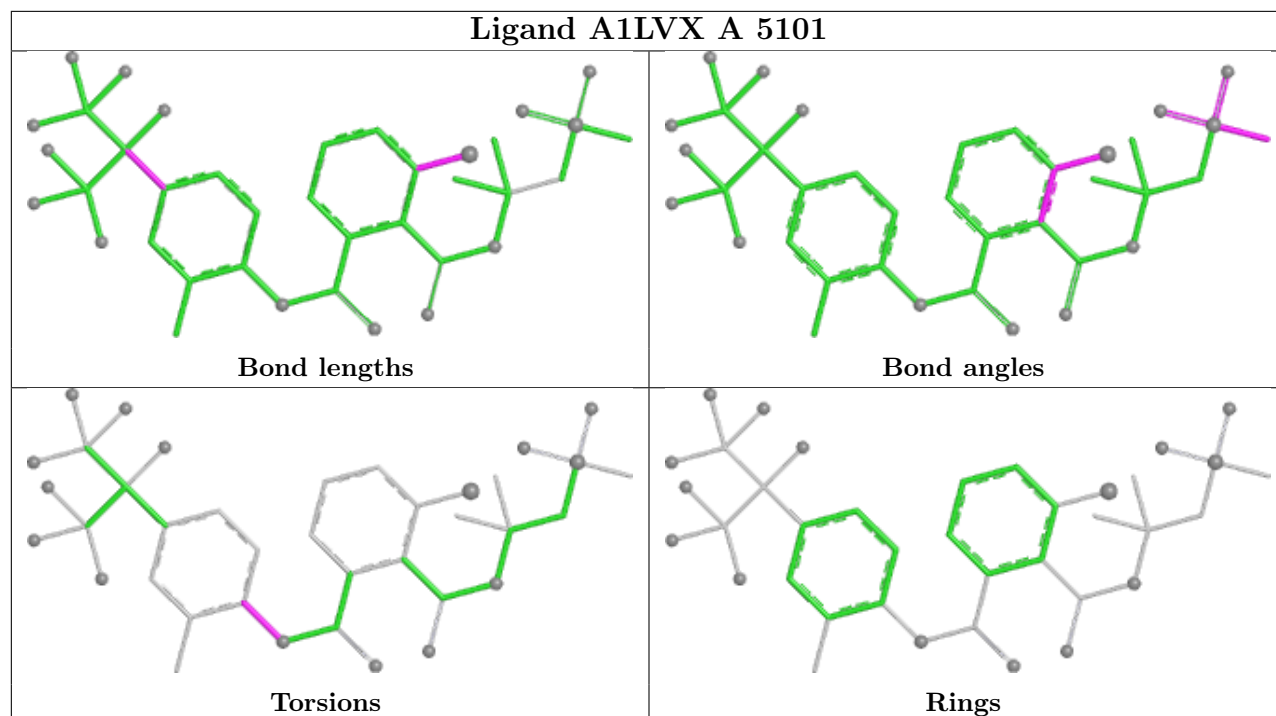
There are no ring outliers.

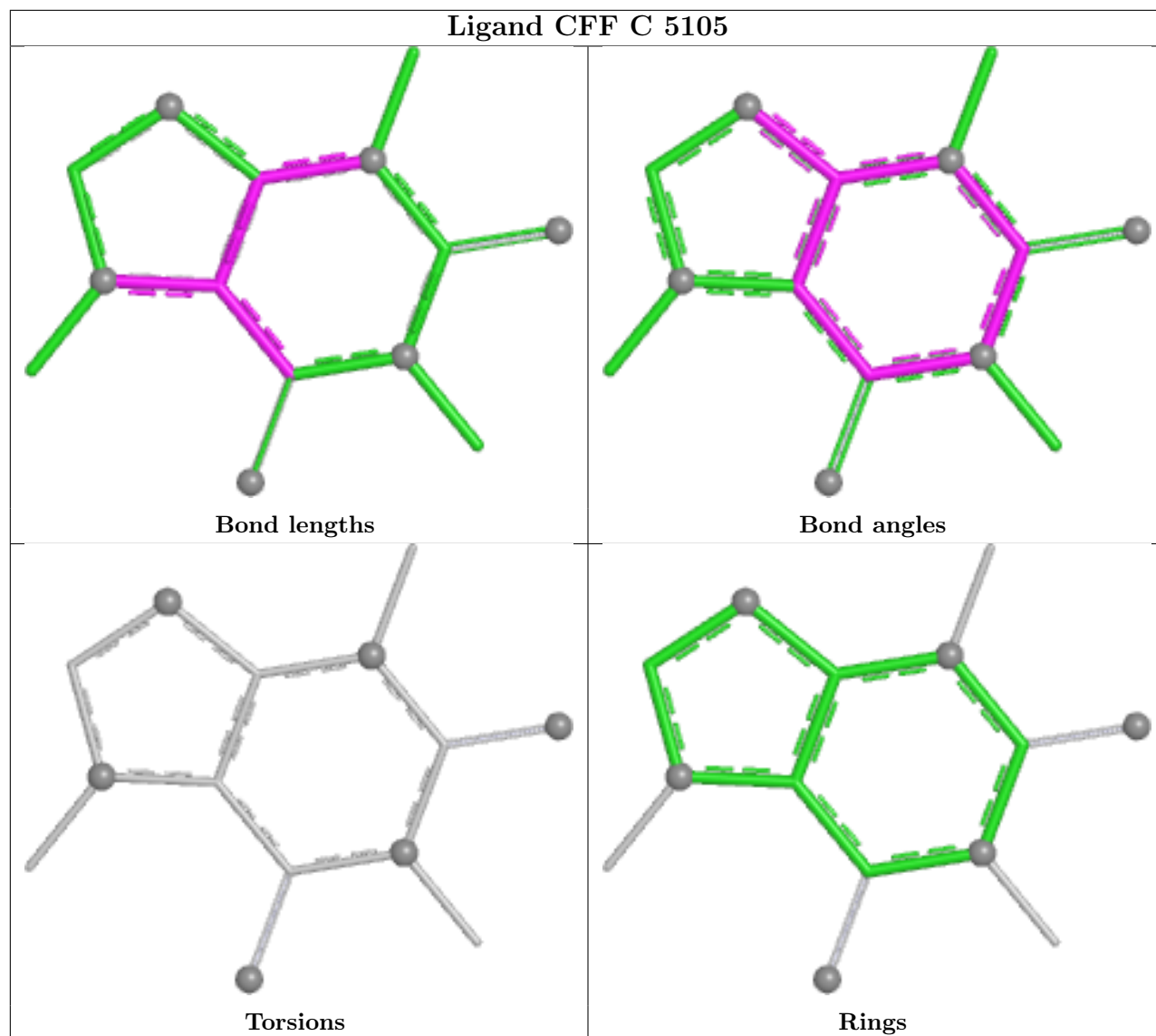
4 monomers are involved in 8 short contacts:

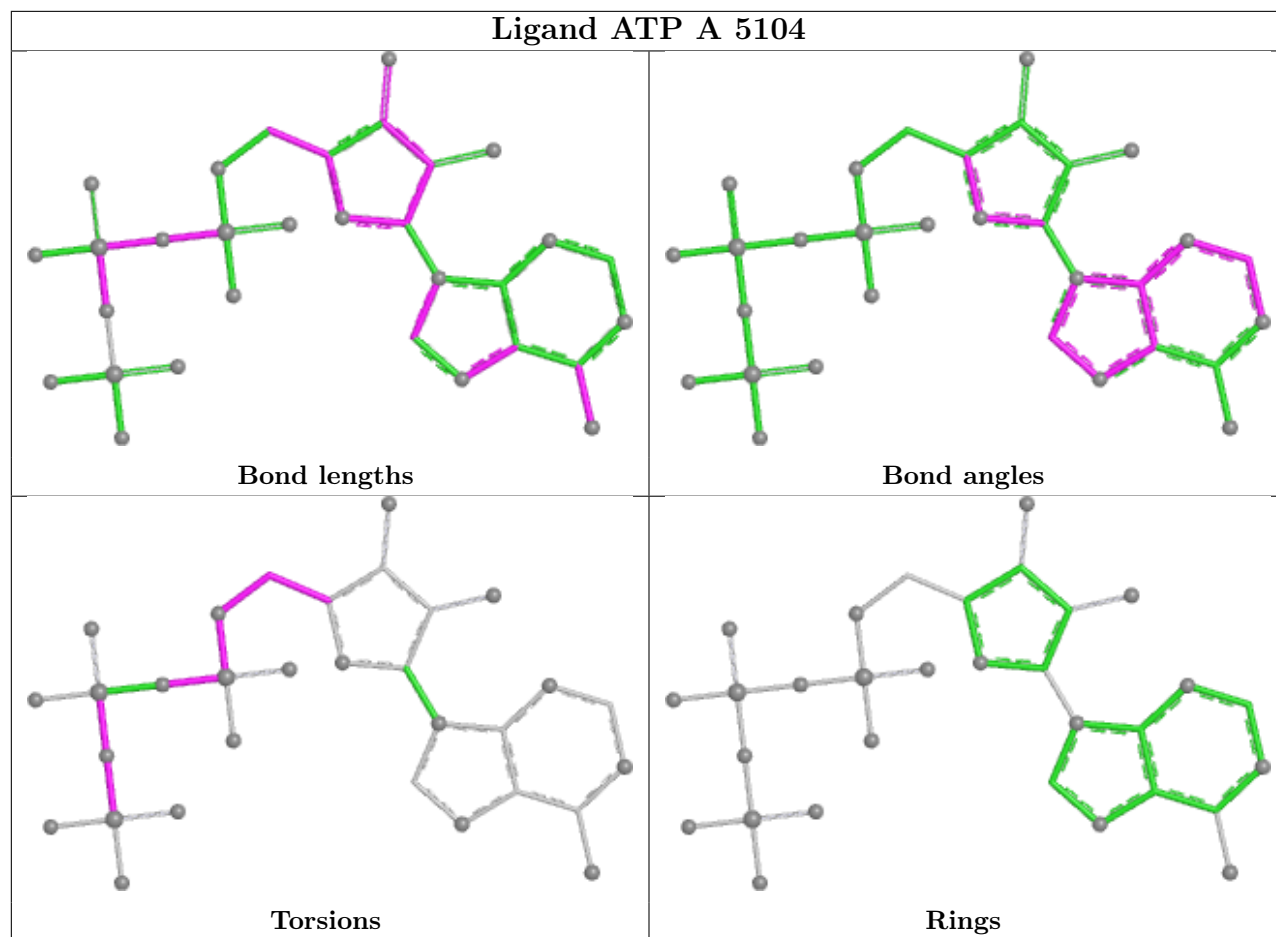
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	5104	ATP	2	0
7	B	5104	ATP	2	0
7	C	5104	ATP	2	0
7	D	5104	ATP	2	0

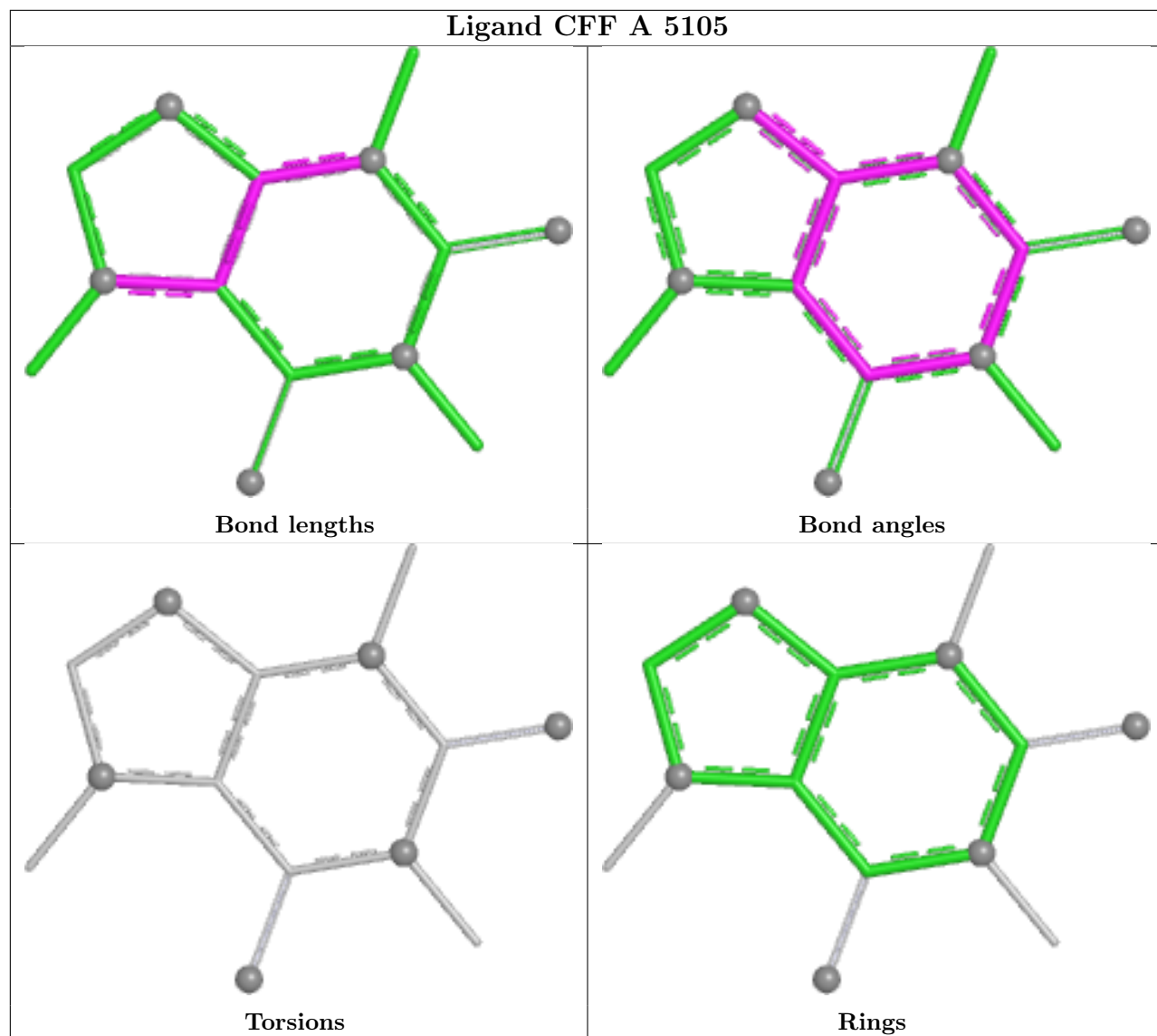
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand A1LVX A 5101

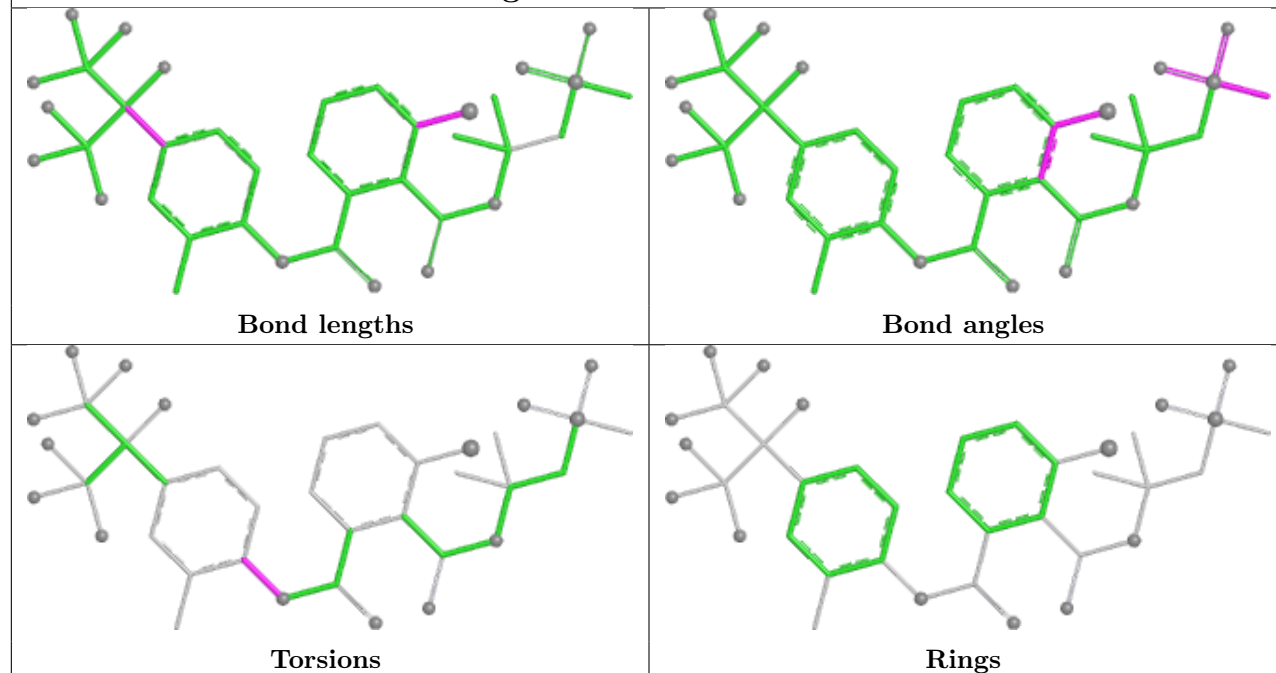




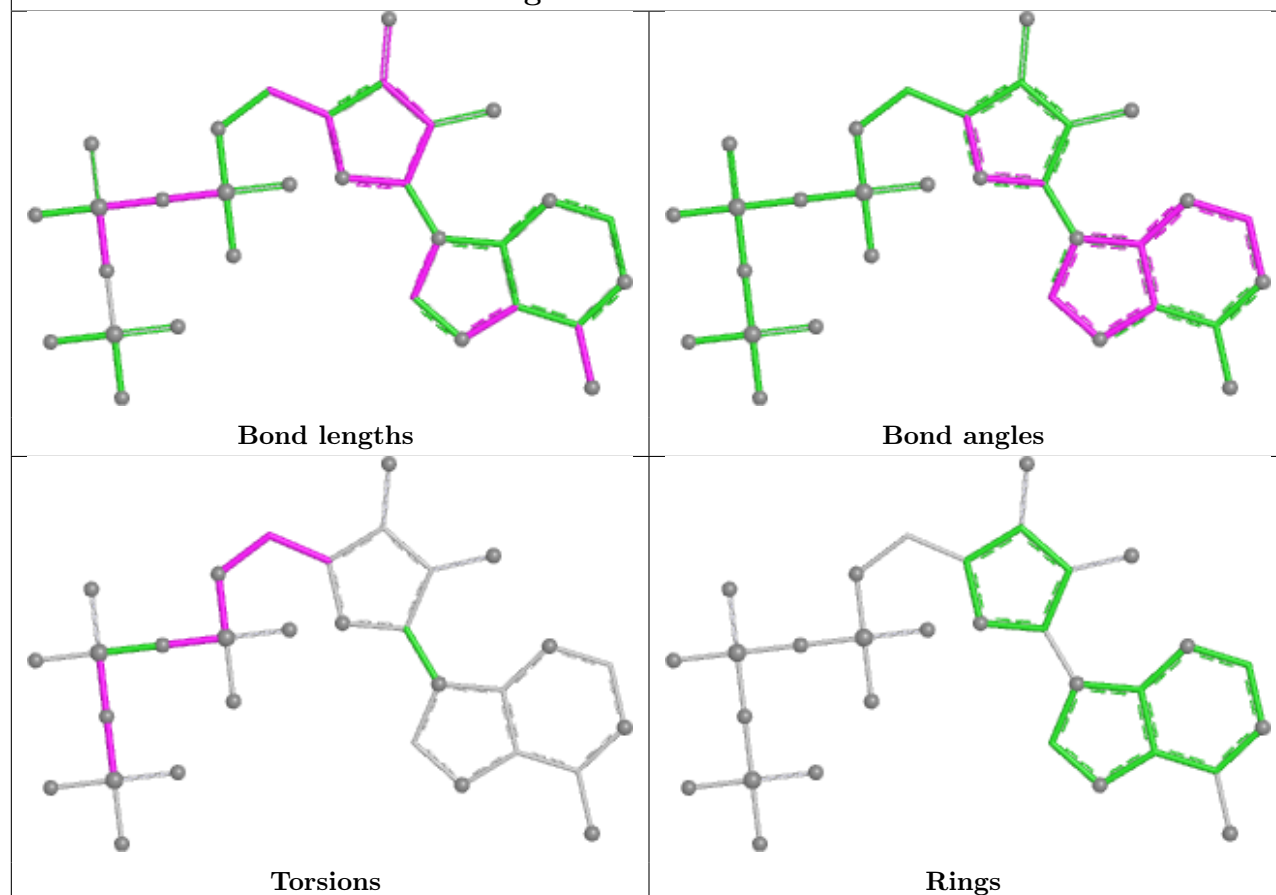


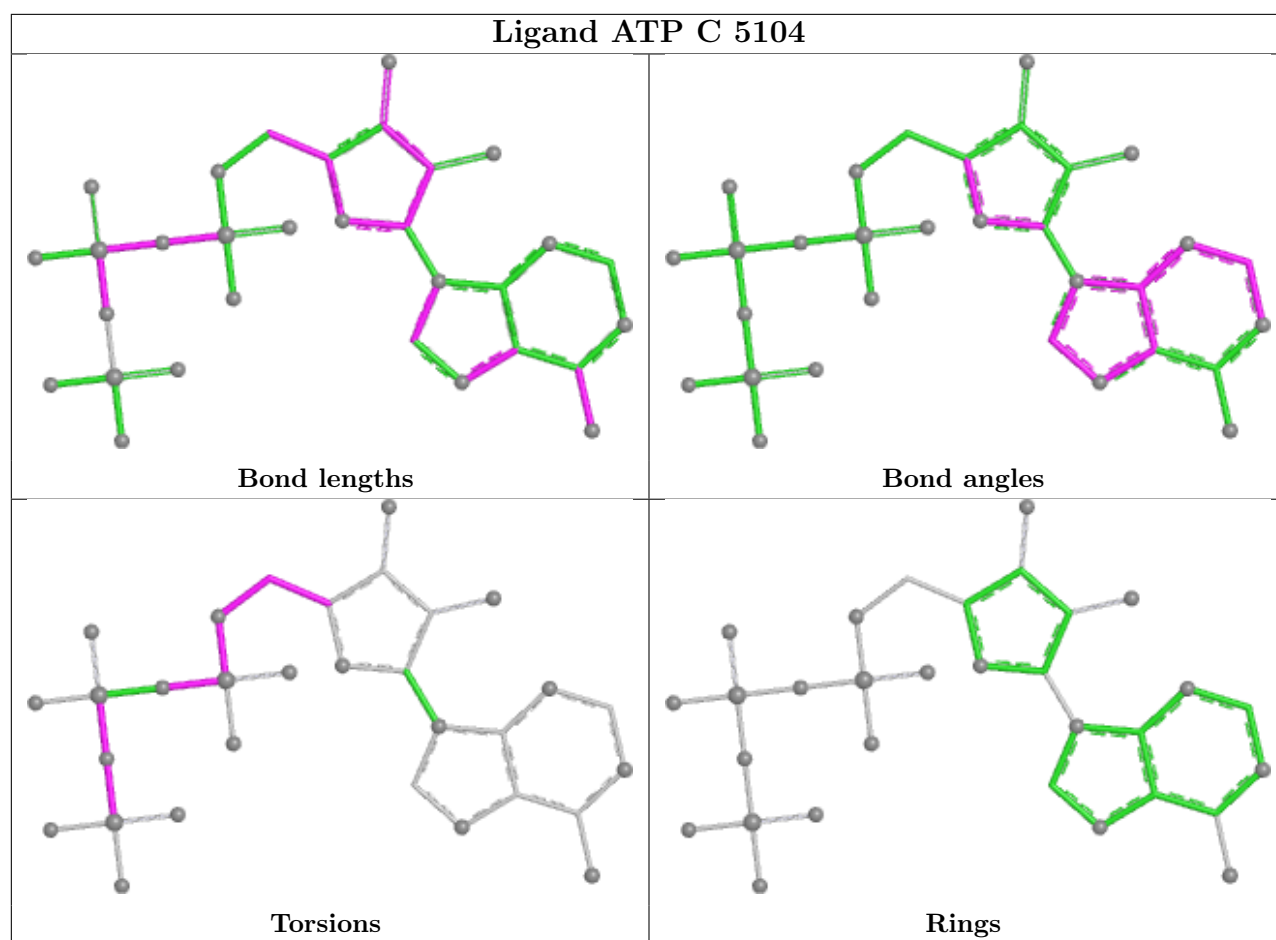


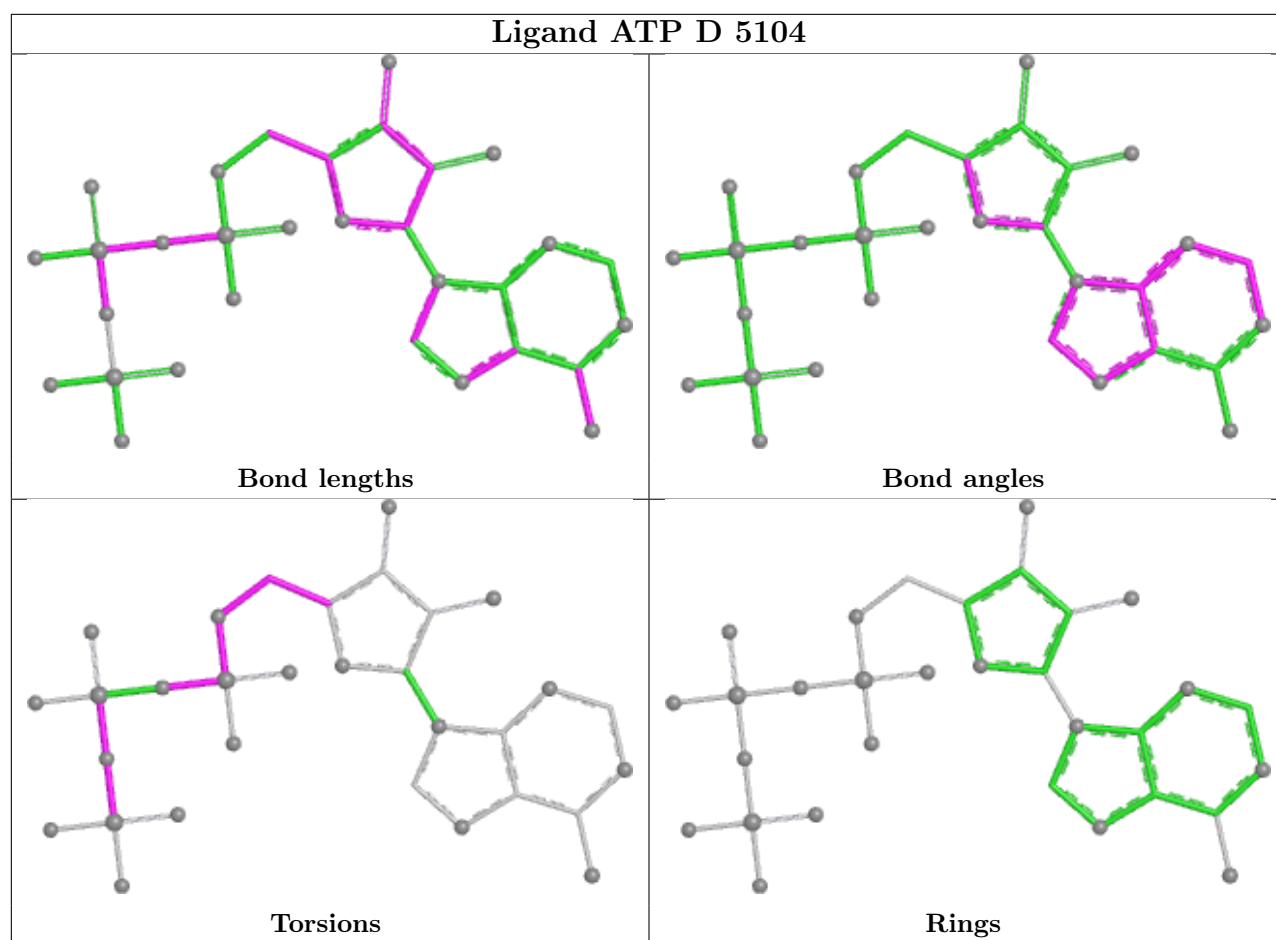
Ligand A1LVX C 5101

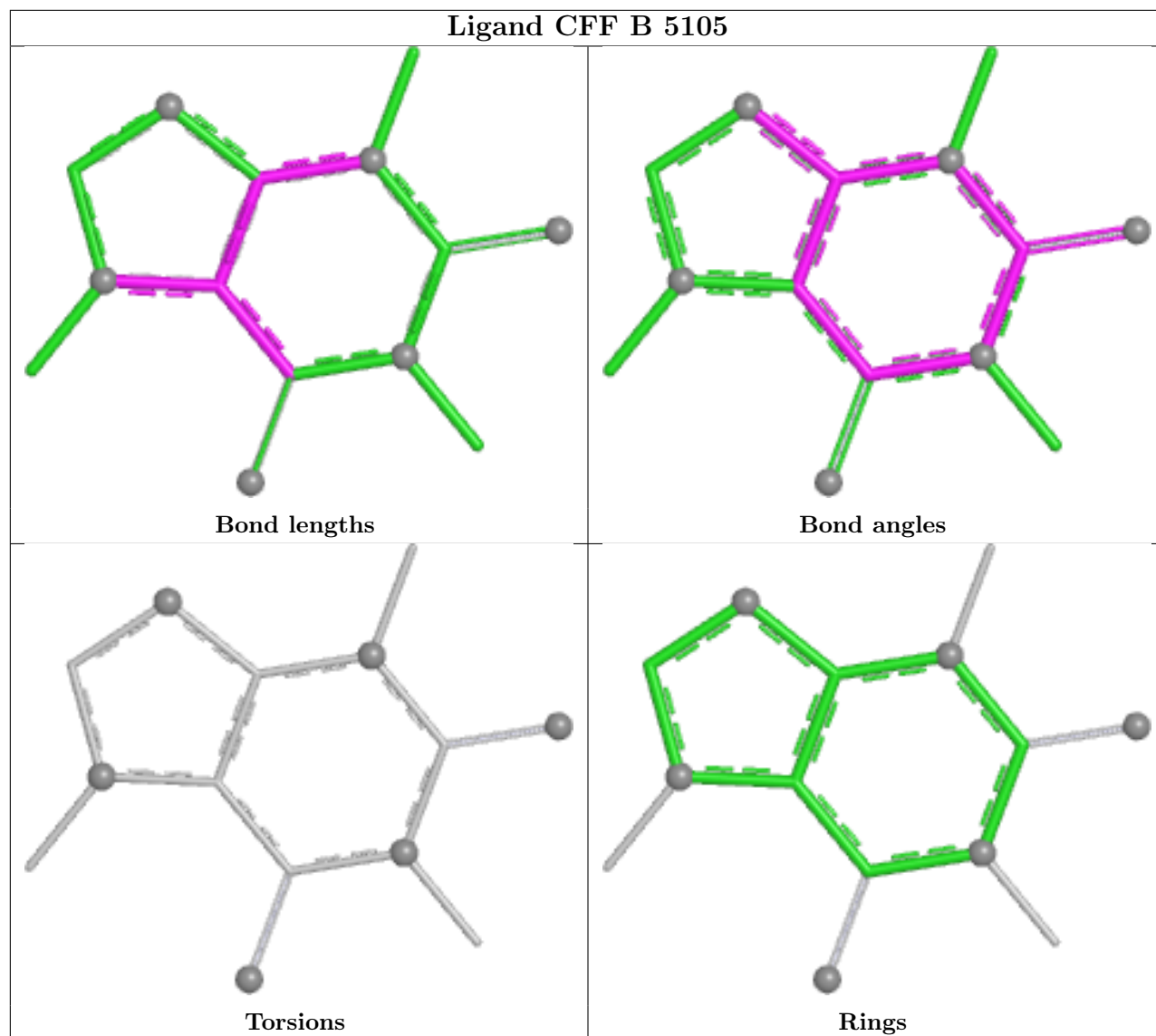


Ligand ATP B 5104

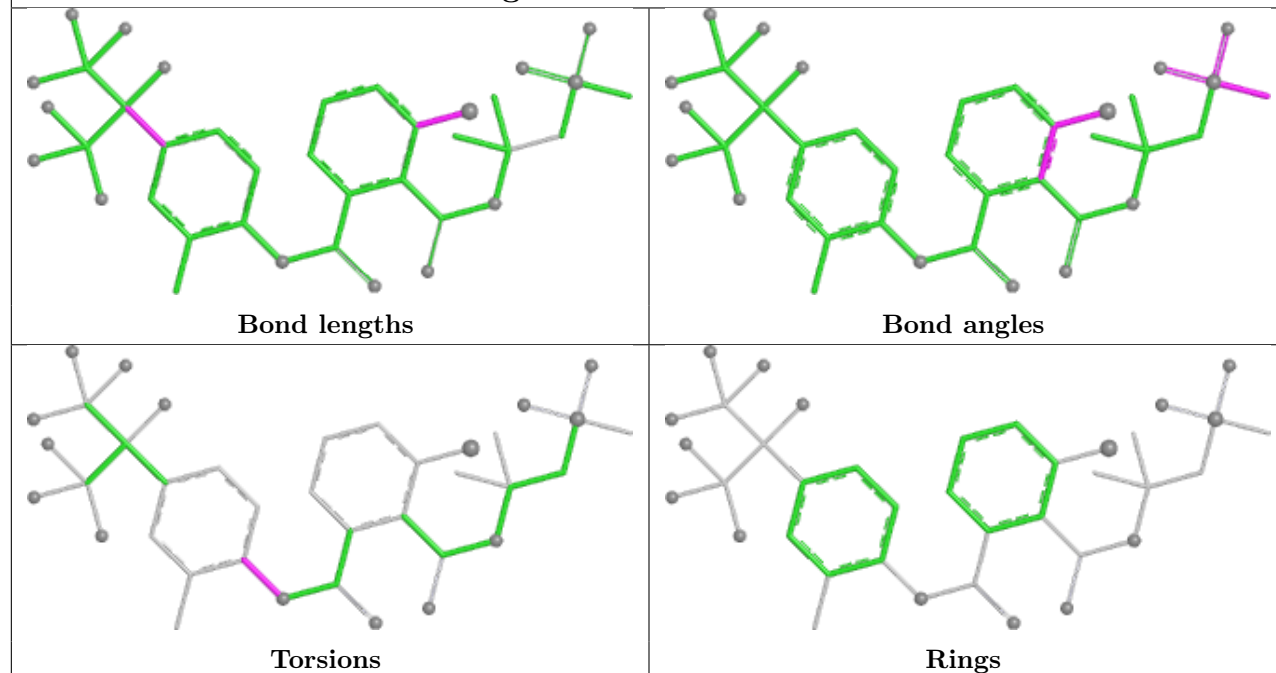




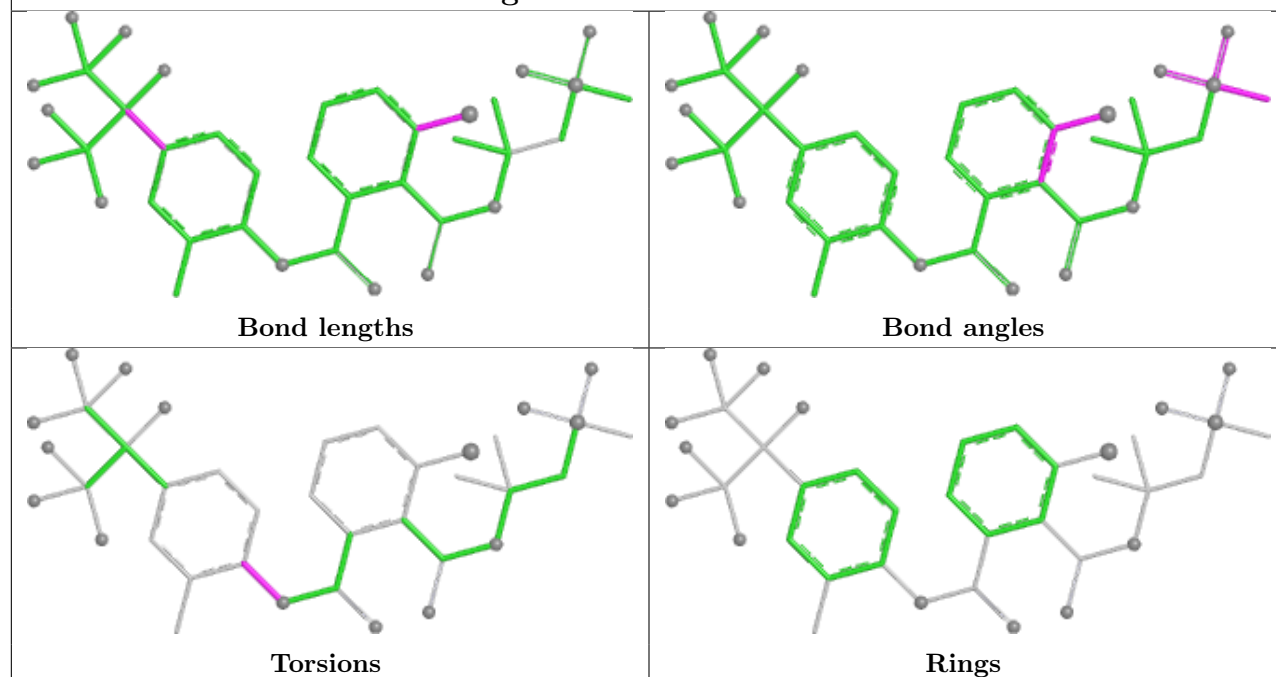


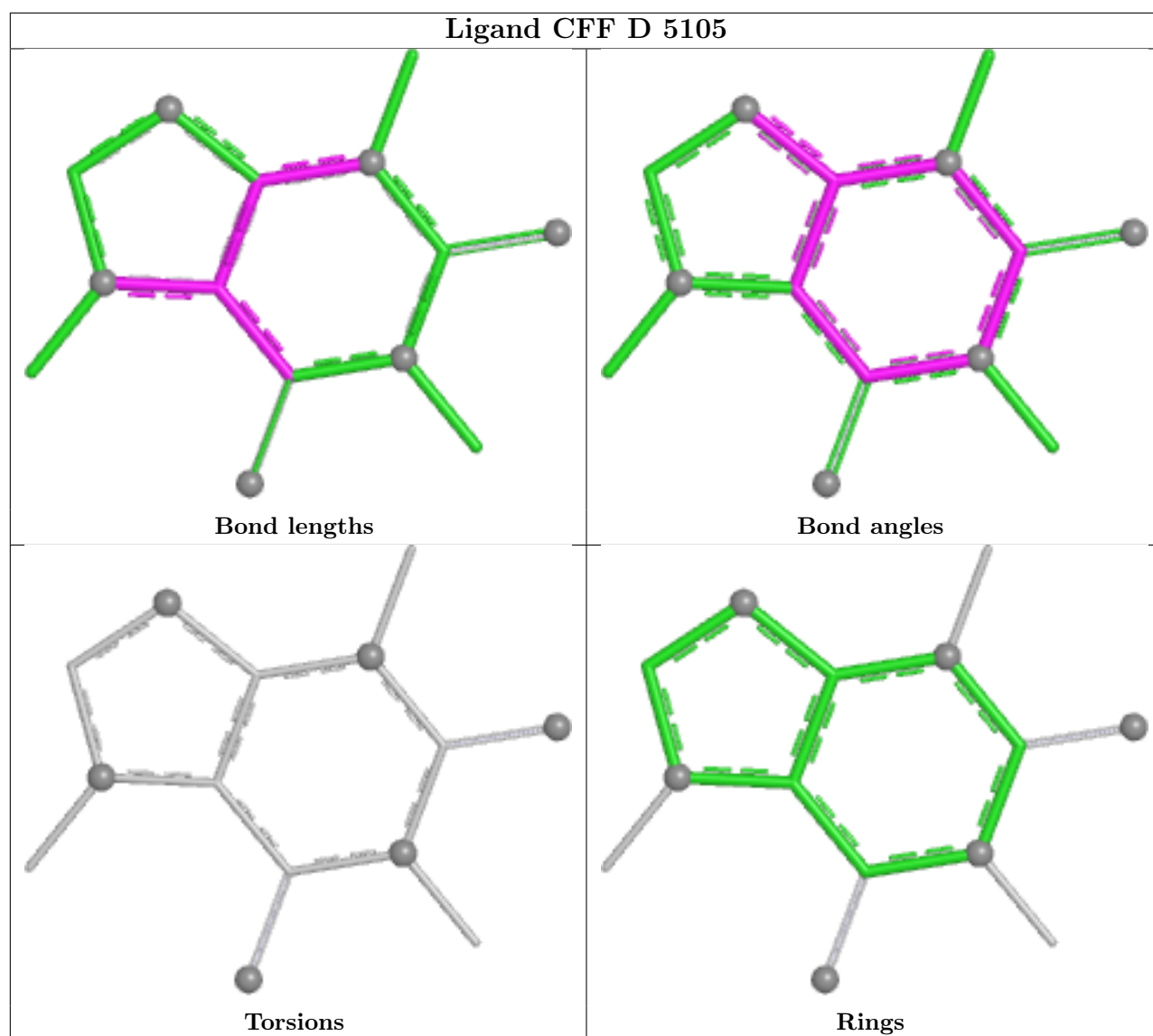


Ligand A1LVX B 5101



Ligand A1LVX D 5101





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.

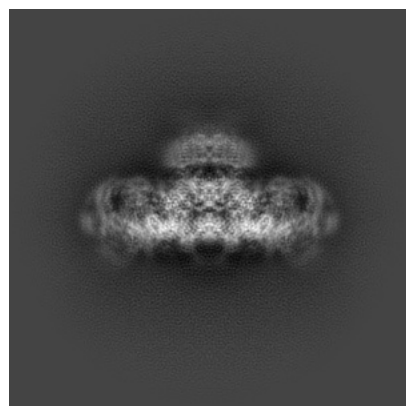
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38398. These allow visual inspection of the internal detail of the map and identification of artifacts.

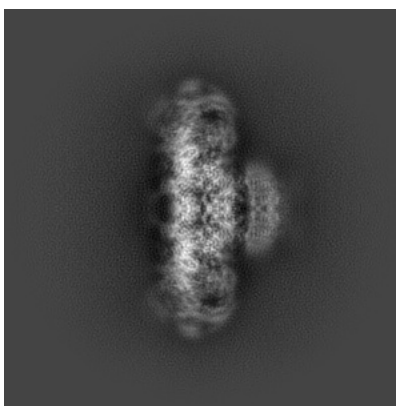
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

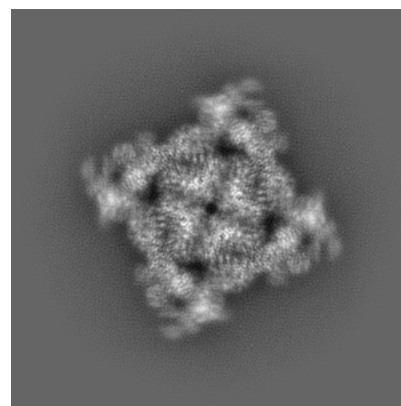
6.1.1 Primary map



X

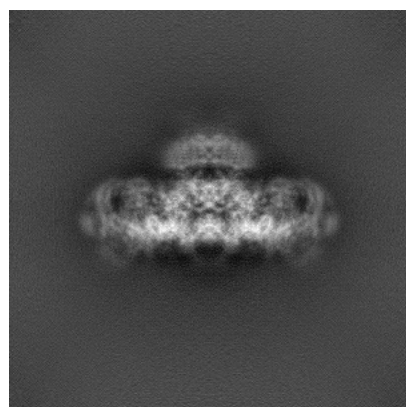


Y

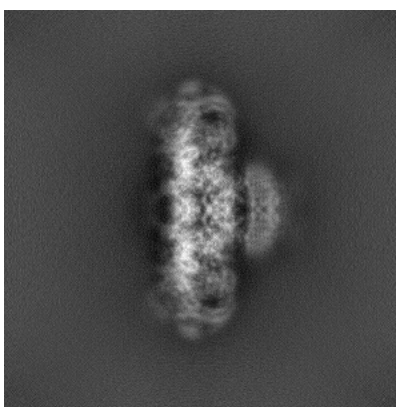


Z

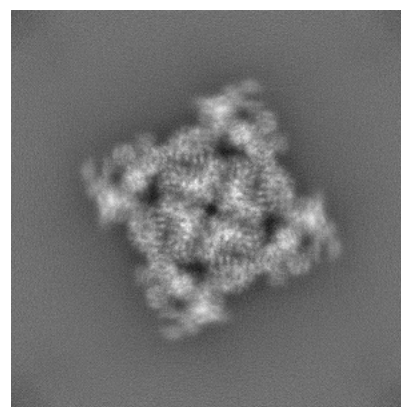
6.1.2 Raw map



X



Y

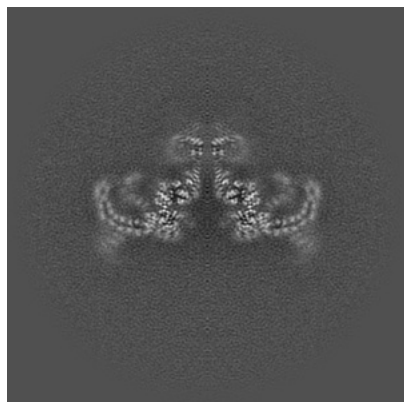


Z

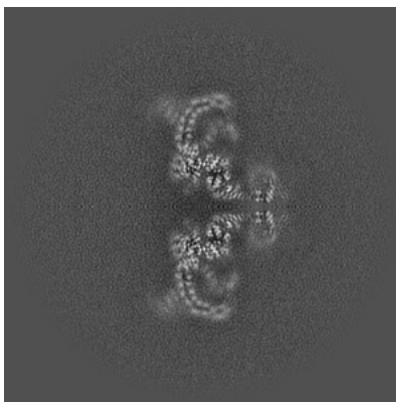
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

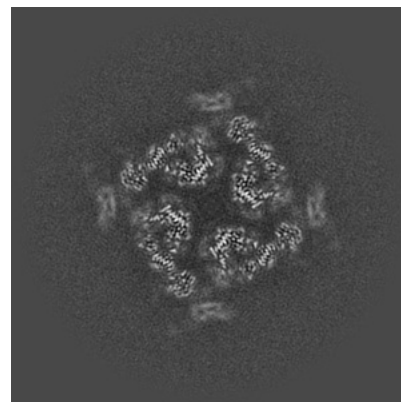
6.2.1 Primary map



X Index: 256

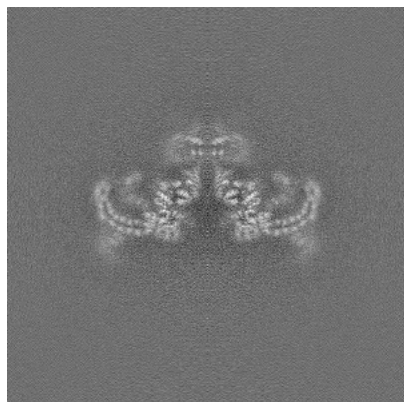


Y Index: 256

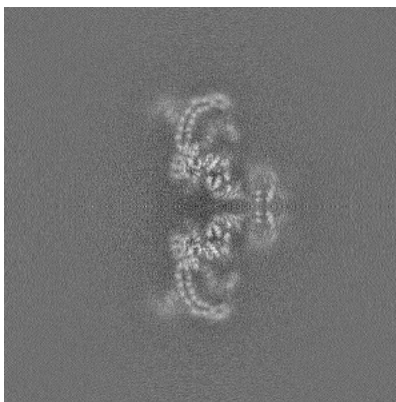


Z Index: 256

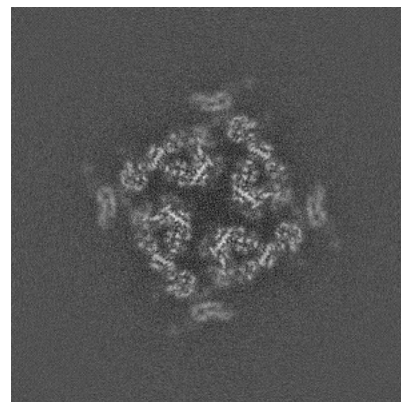
6.2.2 Raw map



X Index: 256



Y Index: 256

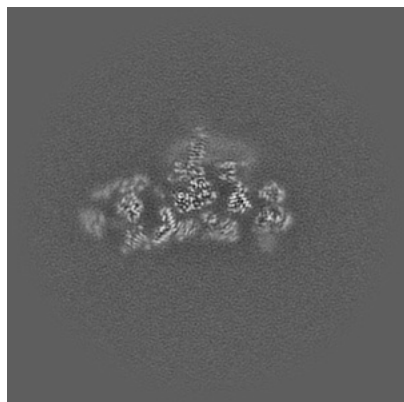


Z Index: 256

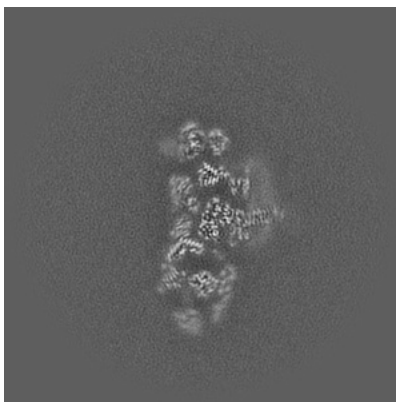
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

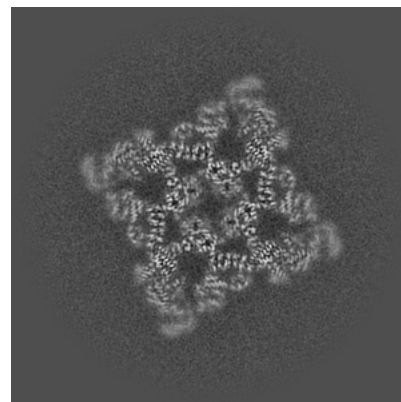
6.3.1 Primary map



X Index: 221

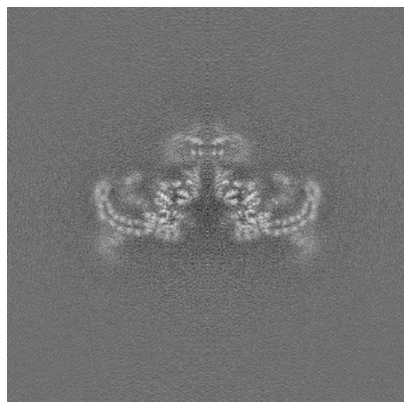


Y Index: 291

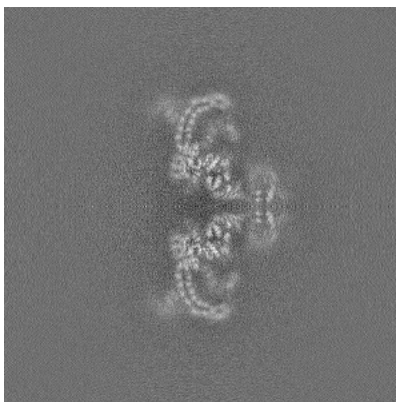


Z Index: 236

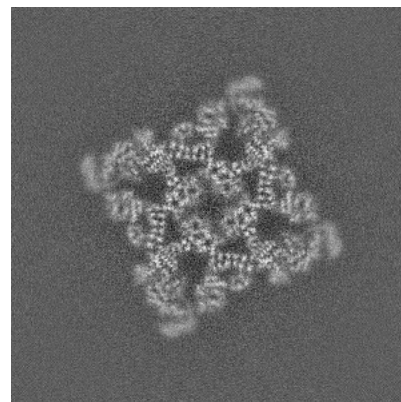
6.3.2 Raw map



X Index: 256



Y Index: 256

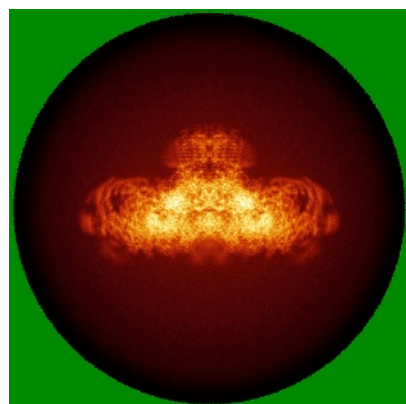


Z Index: 236

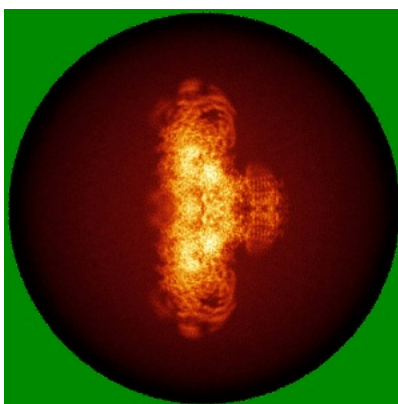
The images above show the largest variance slices of the map in three orthogonal directions.

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

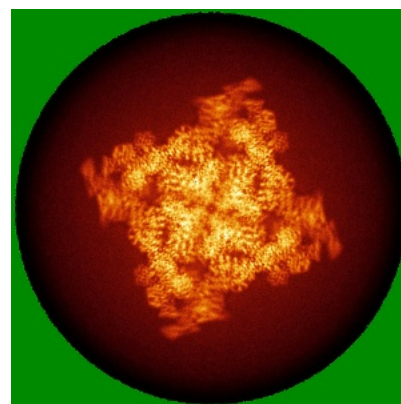
6.4.1 Primary map



X

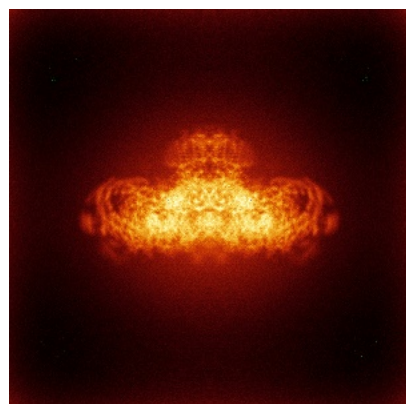


Y

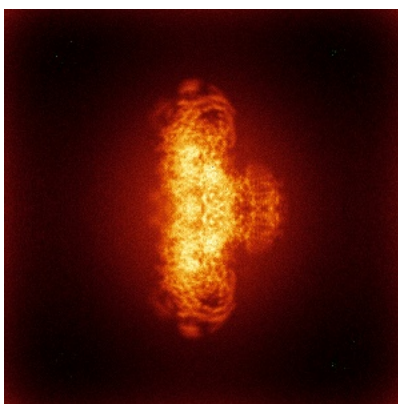


Z

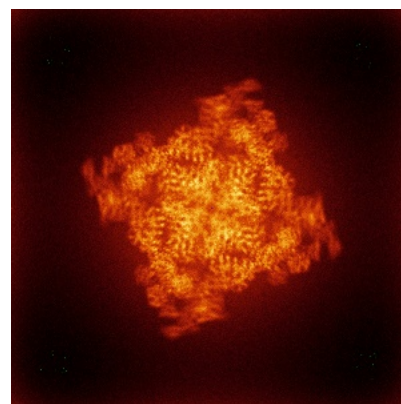
6.4.2 Raw map



X



Y

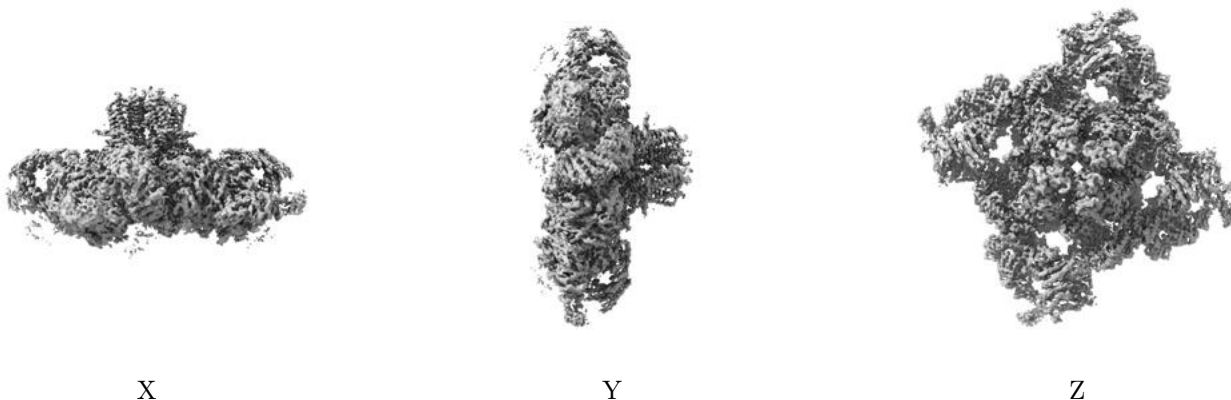


Z

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 0.06. 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.

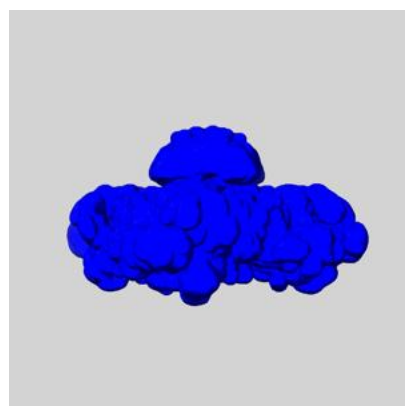
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

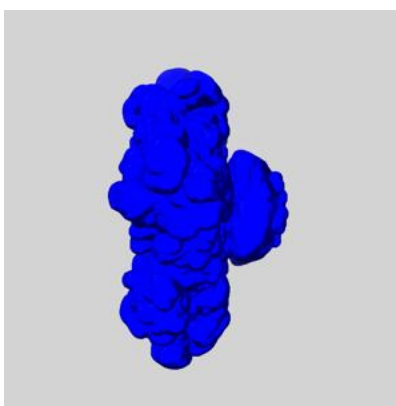
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

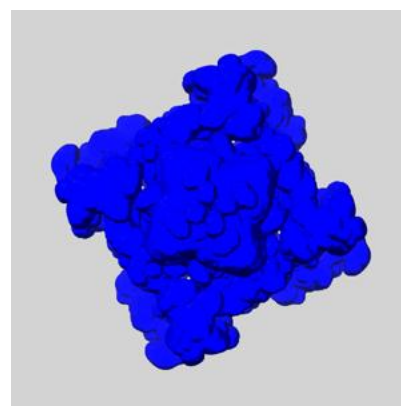
6.6.1 emd_38398_msk_1.map [i](#)



X



Y

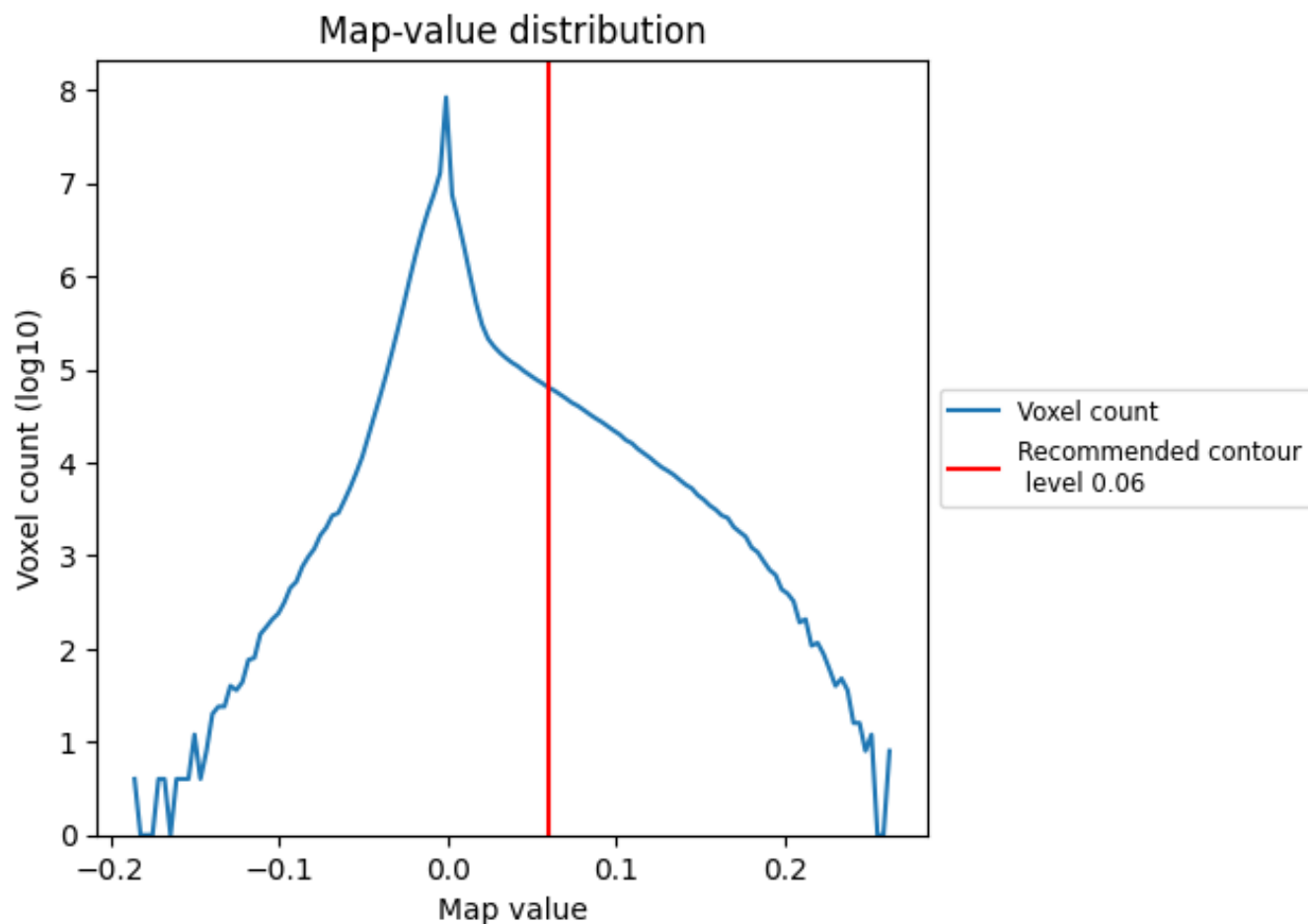


Z

7 Map analysis [i](#)

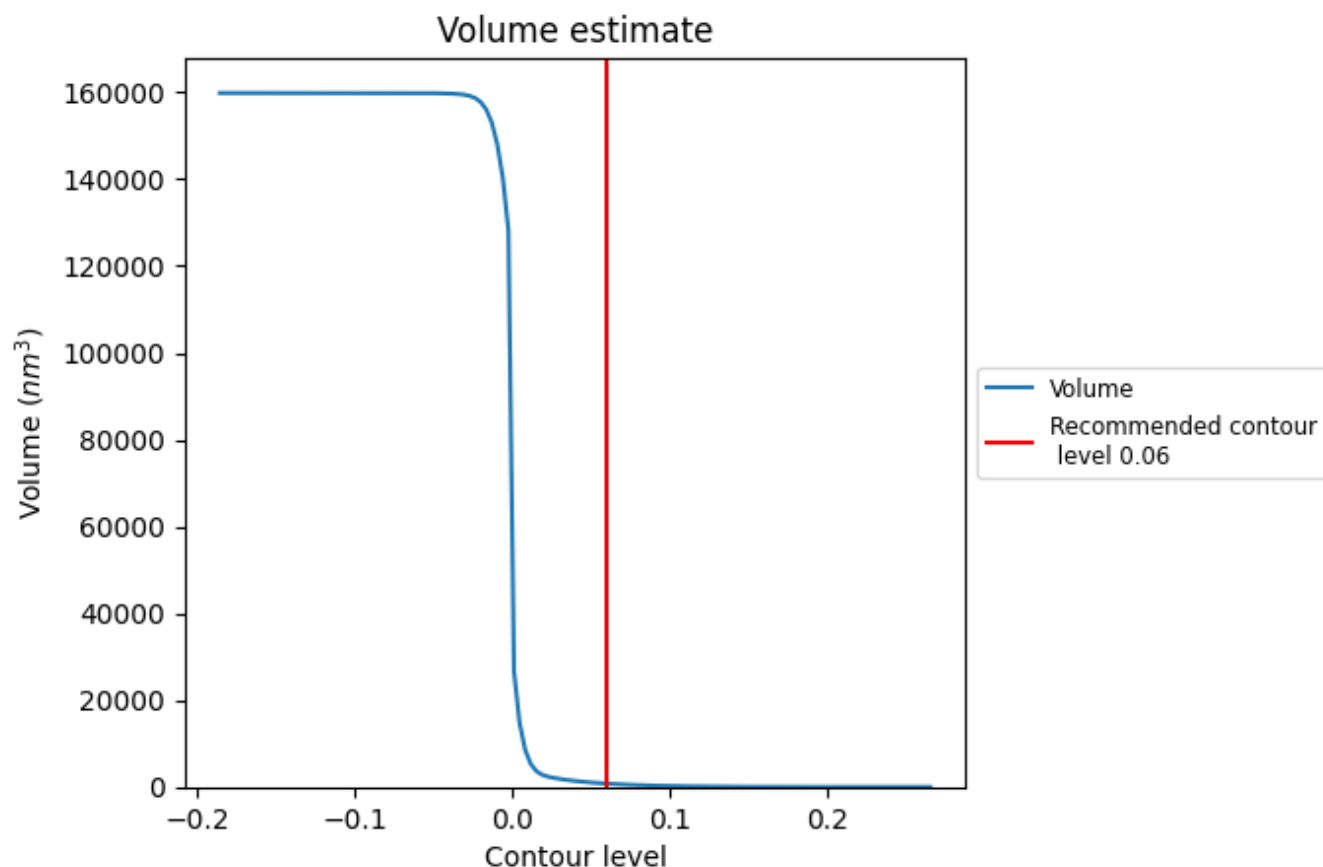
This section contains the results of statistical analysis of the map.

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.

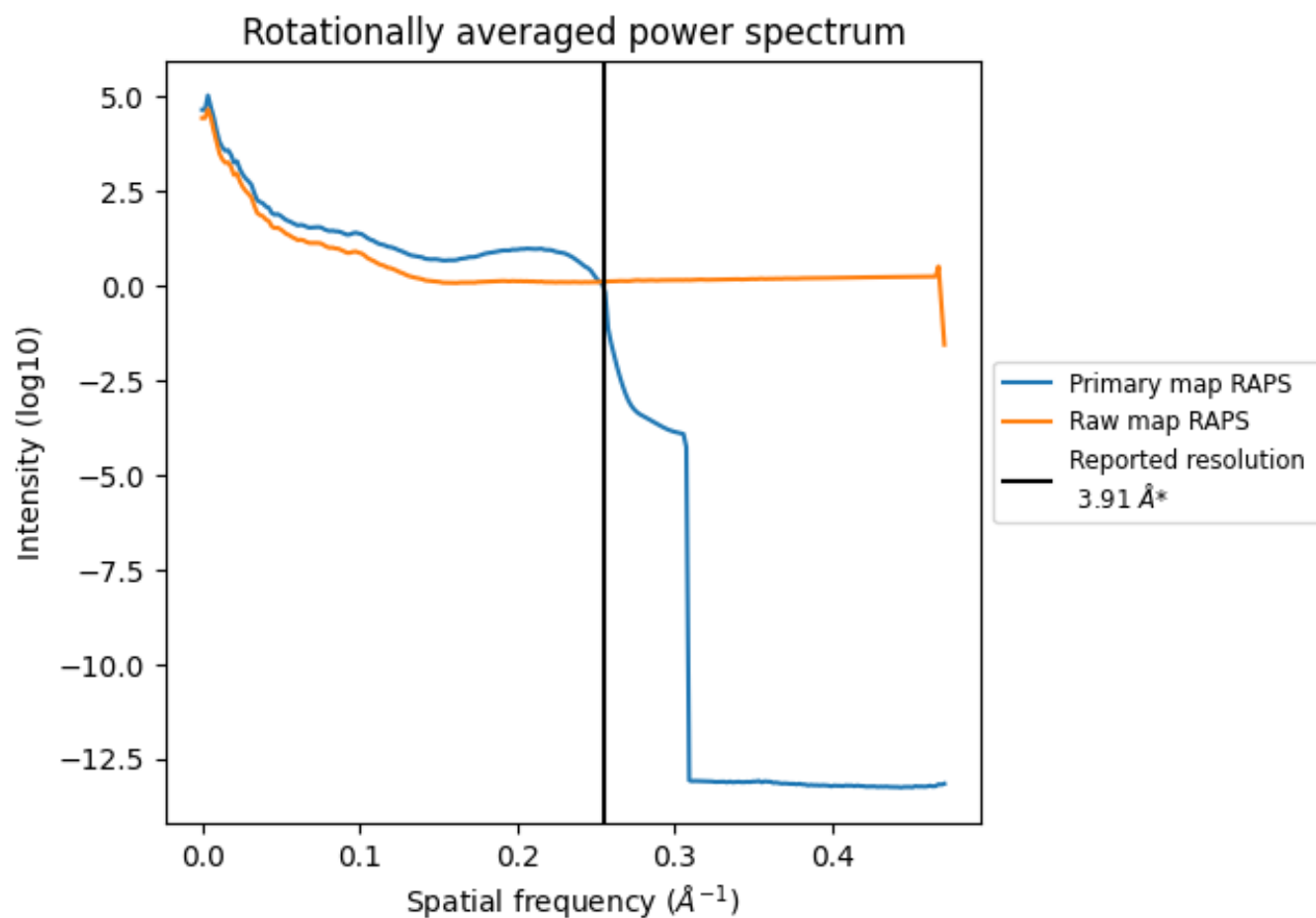
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 783 nm³; this corresponds to an approximate mass of 707 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 ⓘ

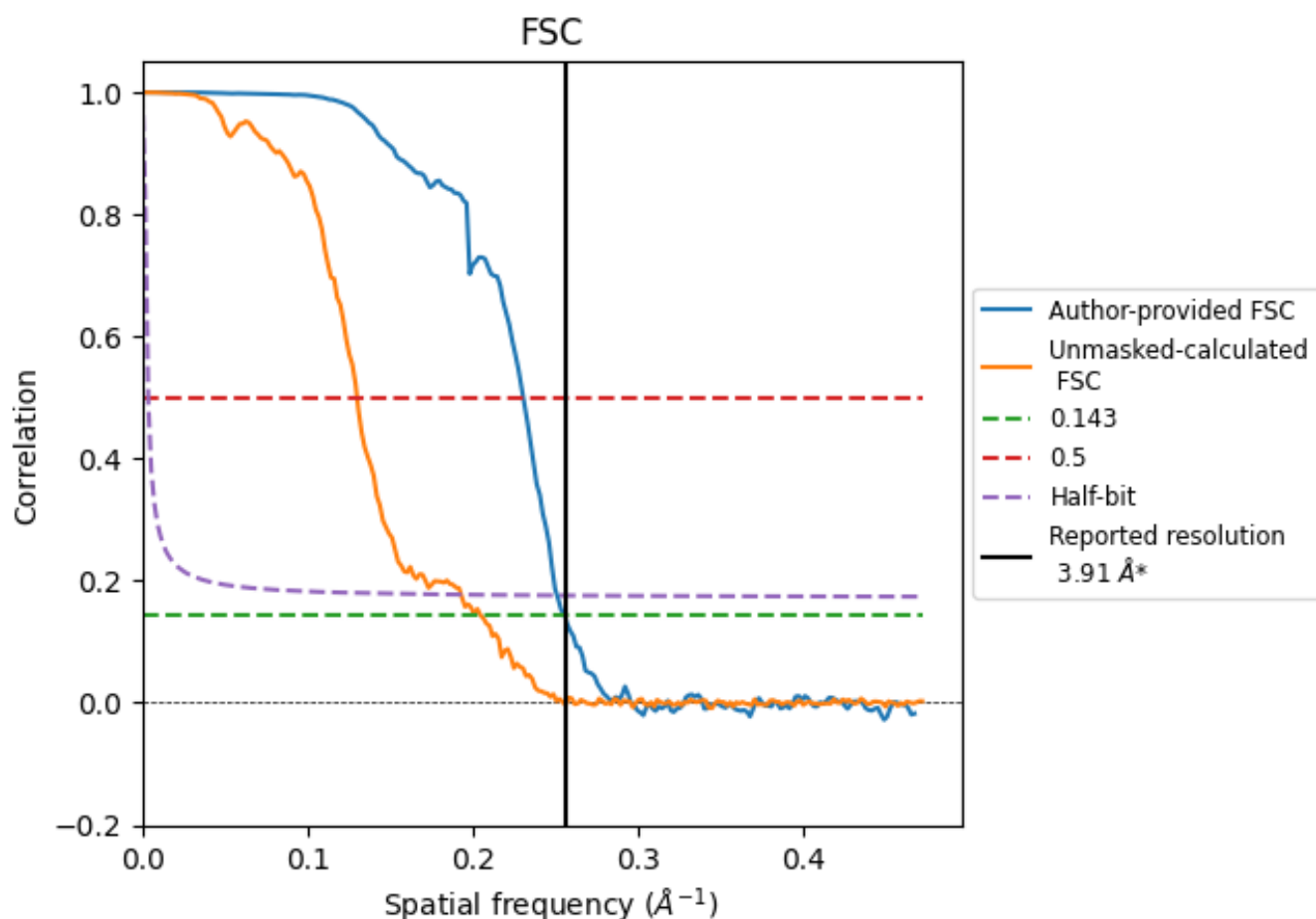


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

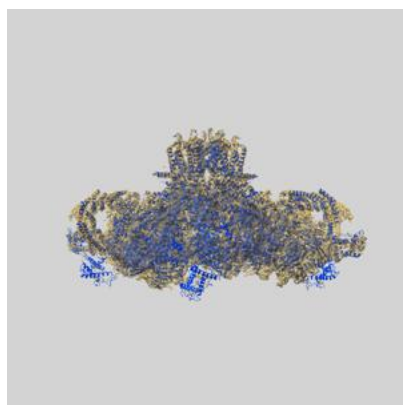
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.91	-	-
Author-provided FSC curve	3.91	4.34	3.99
Unmasked-calculated*	4.89	7.70	5.19

*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 4.89 differs from the reported value 3.91 by more than 10 %

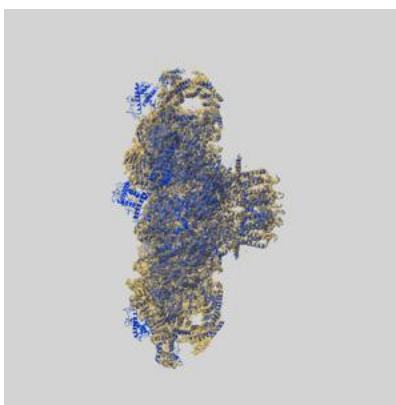
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38398 and PDB model 8XJI. Per-residue inclusion information can be found in section 3 on page 9.

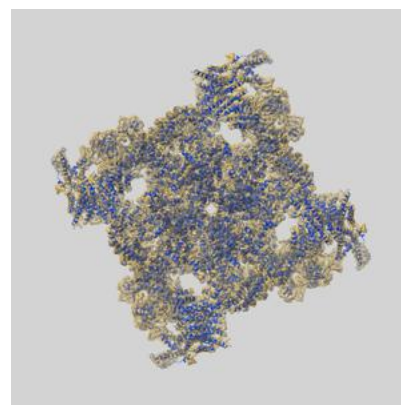
9.1 Map-model overlay [i](#)



X



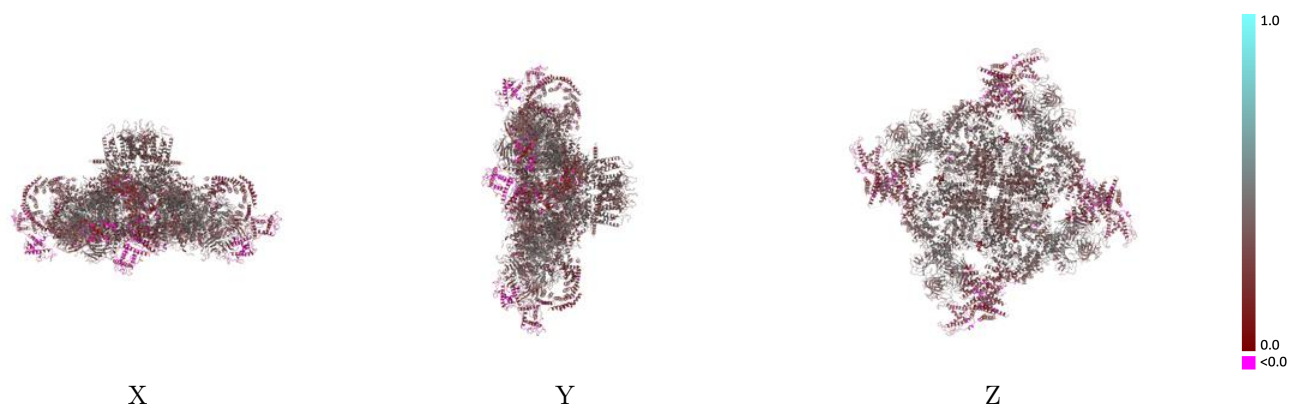
Y



Z

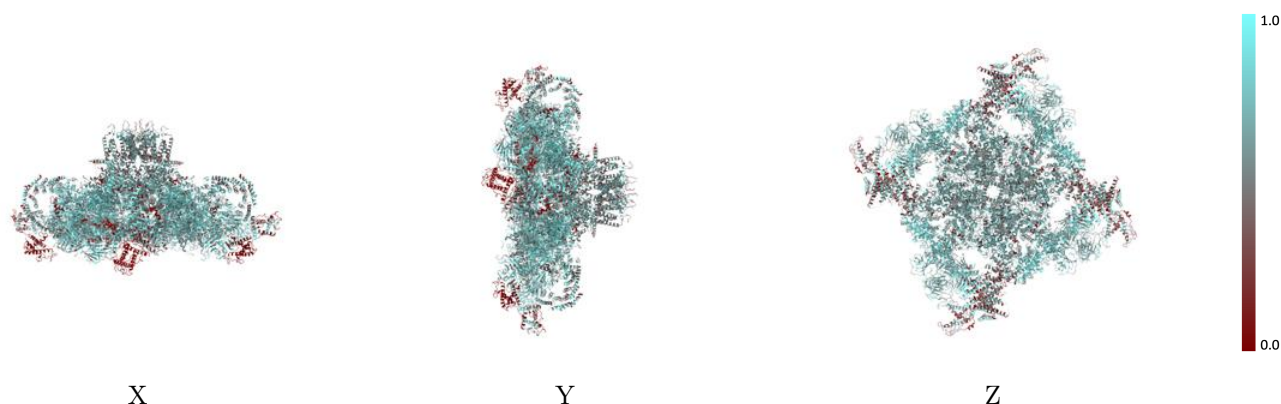
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



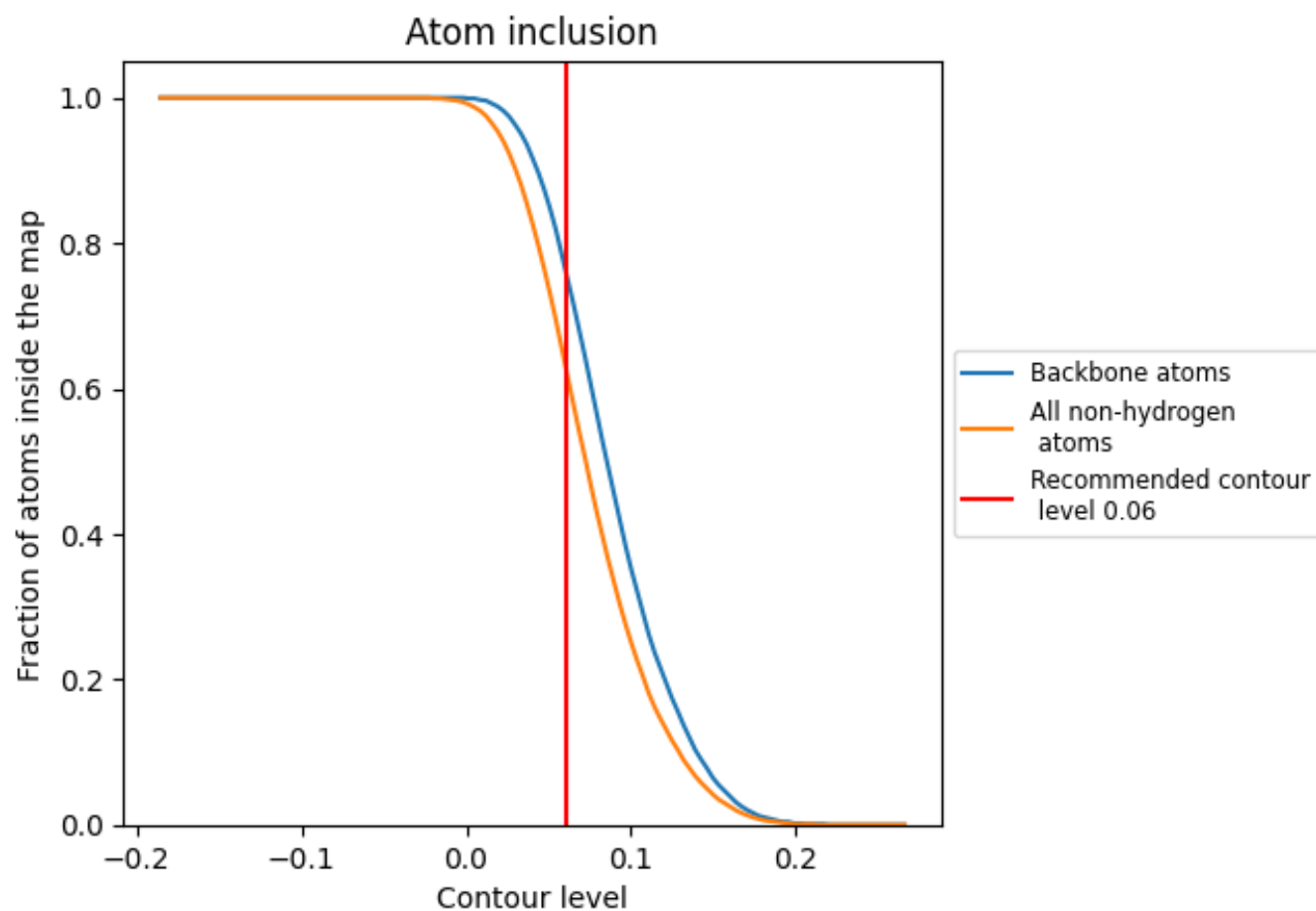
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 63% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6320	0.3400
A	0.6360	0.3410
B	0.6370	0.3410
C	0.6370	0.3410
D	0.6430	0.3490
E	0.6620	0.3580
F	0.6600	0.3580
G	0.6600	0.3630
H	0.6630	0.3690
I	0.4580	0.2340
J	0.4570	0.2330
K	0.4550	0.2350
L	0.4490	0.2300

1.0

0.0

<0.0