



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 06:37 PM UTC

PDB ID : 7UMZ / pdb_00007umz
EMDB ID : EMD-26610
Title : Cryo-EM structure of rabbit RyR1 in the presence of high Mg²⁺ and AMP-PCP in nanodisc
Authors : Nayak, A.R.; Samso, M.
Deposited on : 2022-04-08
Resolution : 3.09 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:

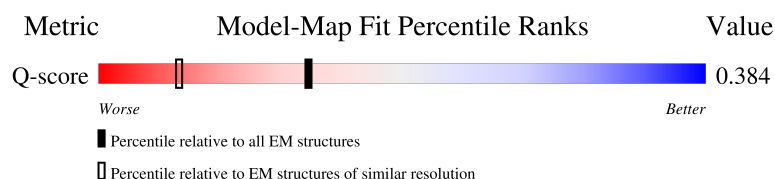
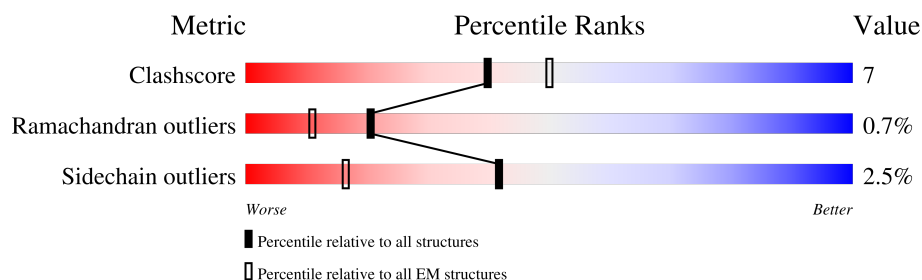
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.09 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	14003 (2.59 - 3.59)

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	5037	9% 67% 10% 22%
1	B	5037	9% 67% 10% 22%
1	C	5037	9% 68% 10% 22%
1	D	5037	9% 67% 10% 22%

2 Entry composition [i](#)

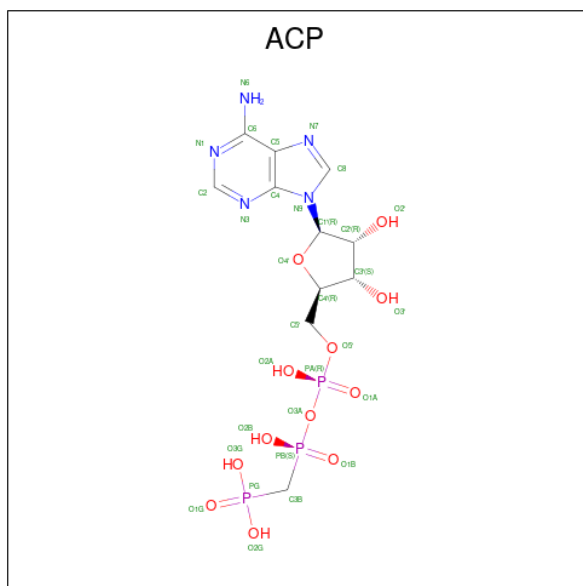
There are 6 unique types of molecules in this entry. The entry contains 111396 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3927	Total	C	N	O	S	0	0
			27759	17494	4909	5192	164		
1	B	3927	Total	C	N	O	S	0	0
			27785	17506	4915	5202	162		
1	C	3927	Total	C	N	O	S	0	0
			27661	17427	4896	5175	163		
1	D	3927	Total	C	N	O	S	0	0
			27670	17436	4891	5180	163		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	B	1	Total	C	N	O	P	0
			31	11	5	12	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	D	1	Total	C	N	O	P	0
			31	11	5	12	3	

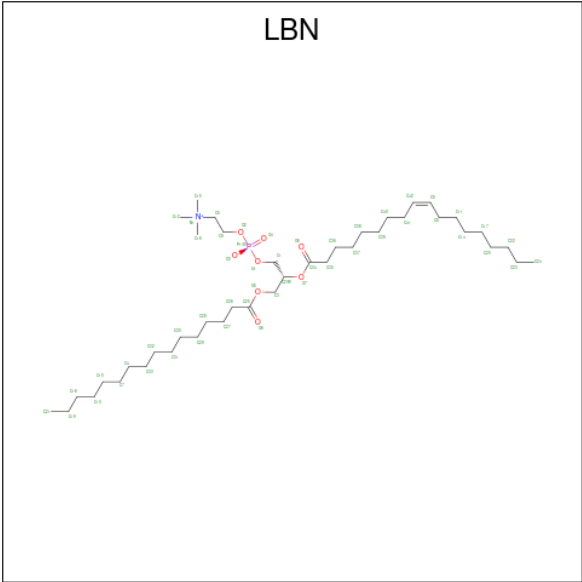
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	4	Total	Mg	0
			4	4	
4	B	3	Total	Mg	0
			3	3	
4	C	3	Total	Mg	0
			3	3	
4	D	3	Total	Mg	0
			3	3	

- Molecule 5 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
5	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
5	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
5	B	1	Total	C	N	O	P	0
			47	37	1	8	1	
5	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
5	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
5	D	1	Total	C	N	O	P	0
			47	37	1	8	1	
5	D	1	Total	C	N	O	P	0
			46	36	1	8	1	

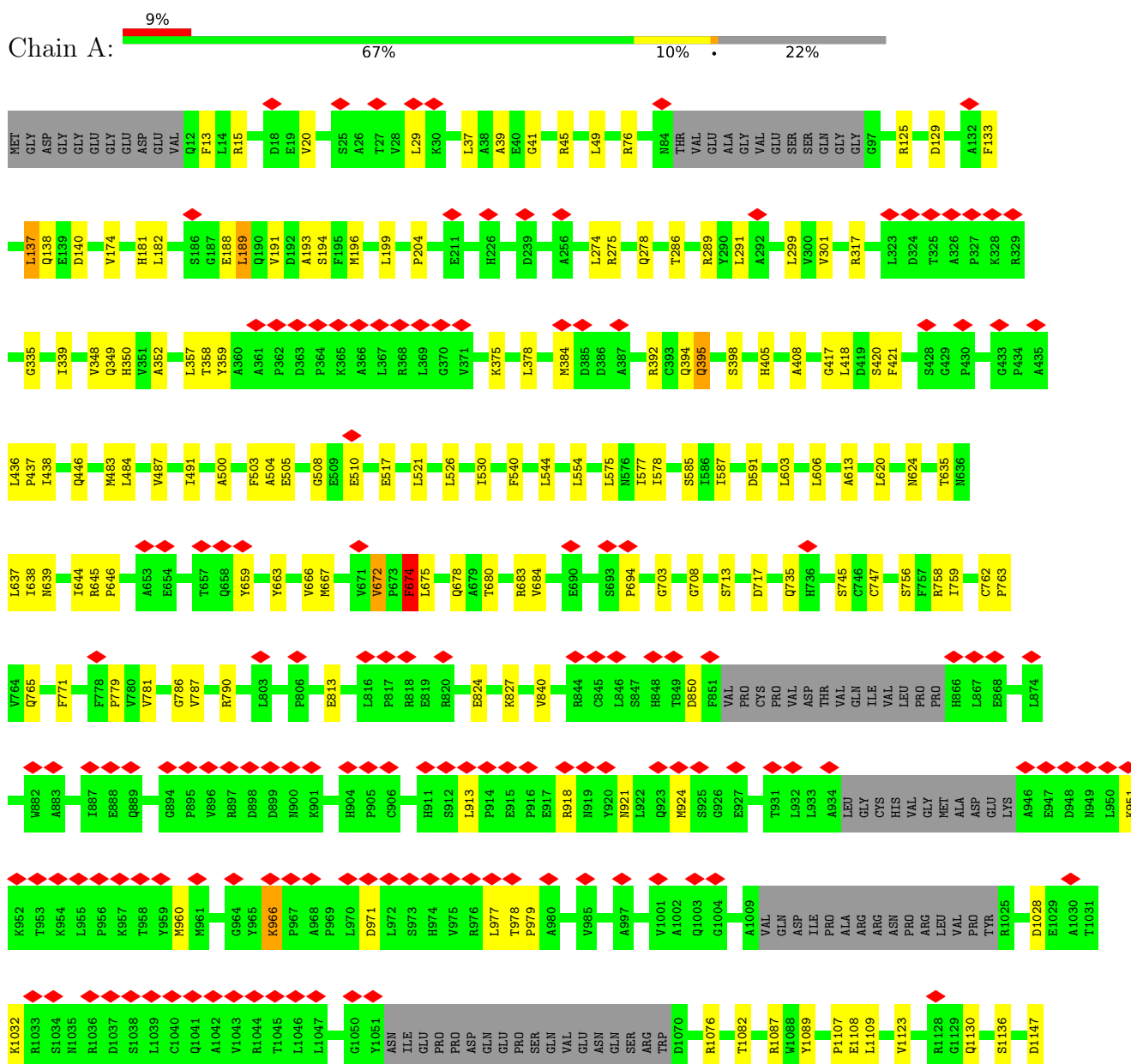
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	O	0
			2	2	
6	B	2	Total	O	0
			2	2	
6	C	2	Total	O	0
			2	2	
6	D	2	Total	O	0
			2	2	

3 Residue-property plots

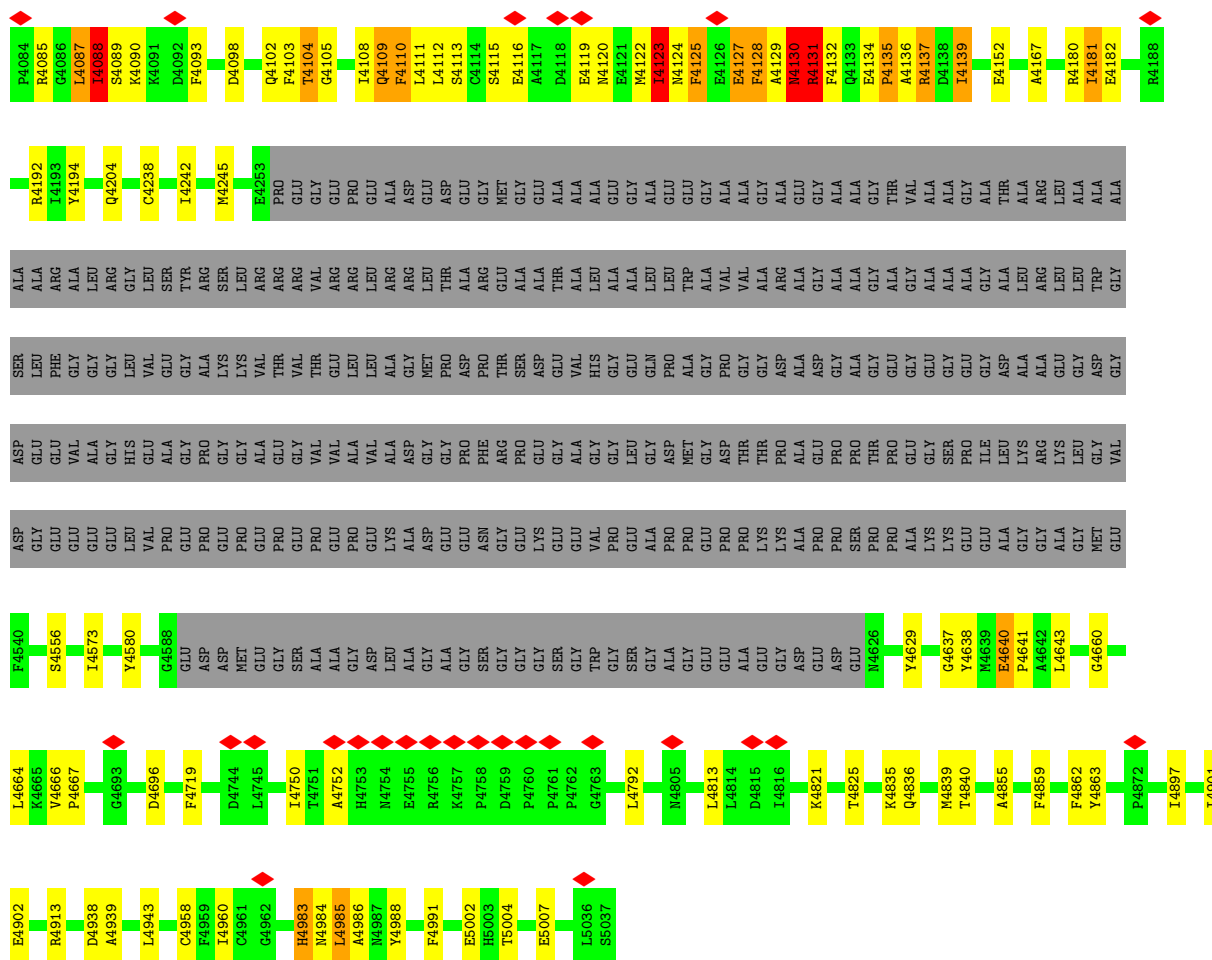
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 1

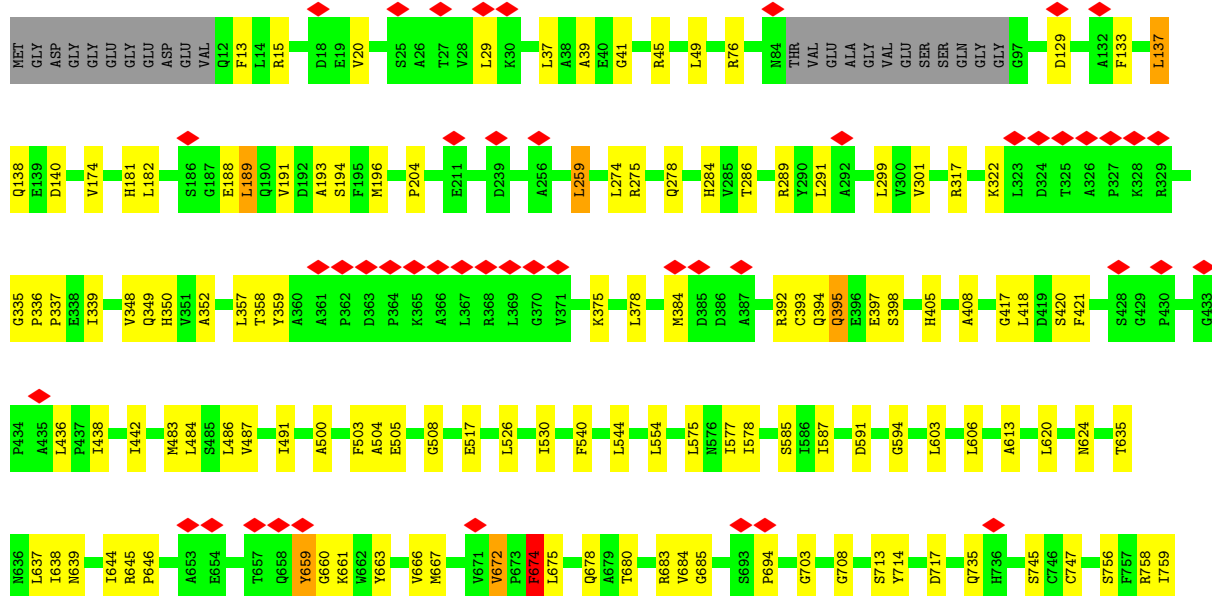




D3932	E3748	A3649	X3561	X3385	X3273	X3015	LYS	SER	PRO
E3944	V3749	M3652	X3562	X3386	X3274	X3016	PHE	ARG	ILE
E3945	E3750	K3658	X3563	X3387	X3275	X3017	LEU	GLU	LYS
E3946	E3751	K3658	X3564	X3388	X3276		GLN	LEU	GLN
E3947	E3752	K3658	X3565	X3389	X3277		MET	ALA	SER
E3948	E3753	M3661	X3566	X3390	X3278		ASN	ALA	LEU
E3949	E3754	L3662	X3567	X3391	X3279		GLY	MET	LYS
E3950	E3755	L3663	X3568	X3392	X3280		TYR	ALA	ALA
E3951	E3756			X3393	X3281		ALA	LEU	ILE
E3952	E3757			X3394	X3282		THR	THR	ALA
E3953	E3758			X3395	X3283		VAL	ALA	TRP
E3954	E3759			X3396	X3284		GLY	ASN	GLU
E3955	E3760			X3397	X3285		LEU	GLY	TRP
E3956	E3761			X3398	X3286			ASN	THR
E3957	E3762			X3399	X3287			HIS	ILE
E3958	E3763			X3400	X3288			ASN	GLU
E3959	E3764			X3401	X3289			THR	LYS
E3960	E3765			X3402	X3290			TRP	ALA
E3961	E3766			X3403	X3291			GLY	ARG
E3962	E3767			X3404	X3292			VAL	GLU
E3963	E3768			X3405	X3293			GLY	ARG
E3964	E3769			X3406	X3294			GLY	GLY
E3965	E3770			X3407	X3295			VAL	GLU
E3966	E3771			X3408	X3296			ASN	GLU
E3967	E3772			X3409	X3297			GLY	ARG
E3968	E3773			X3410	X3298			LEU	THR
E3969	E3774			X3411	X3299			THR	LYS
E3970	E3775			X3412	X3300			GLY	ALA
E3971	E3776			X3413	X3301			GLY	GLY
E3972	E3777			X3414	X3302			ASN	GLU
E3973	E3778			X3415	X3303			GLY	ARG
E3974	E3779			X3416	X3304			LEU	THR
E3975	E3780			X3417	X3305			THR	GLN
E3976	E3781			X3418	X3306			GLY	THR
E3977	E3782			X3419	X3307			VAL	ALA
E3978	E3783			X3420	X3308			GLY	ARG
E3979	E3784			X3421	X3309			GLY	GLY
E3980	E3785			X3422	X3310			GLY	GLY
E3981	E3786			X3423	X3311			GLY	GLY
E3982	E3787			X3424	X3312			GLY	GLY
E3983	E3788			X3425	X3313			GLY	GLY
E3984	E3789			X3426	X3314			GLY	GLY
E3985	E3790			X3427	X3315			GLY	GLY
E3986	E3791			X3428	X3316			GLY	GLY
E3987	E3792			X3429	X3317			GLY	GLY
E3988	E3793			X3430	X3318			GLY	GLY
E3989	E3794			X3431	X3319			GLY	GLY
E3990	E3795			X3432	X3320			GLY	GLY
E3991	E3796			X3433	X3321			GLY	GLY
E3992	E3797			X3434	X3322			GLY	GLY
E3993	E3798			X3435	X3323			GLY	GLY
E3994	E3799			X3436	X3324			GLY	GLY
E3995	E3800			X3437	X3325			GLY	GLY
E3996	E3801			X3438	X3326			GLY	GLY
E3997	E3802			X3439	X3327			GLY	GLY
E3998	E3803			X3440	X3328			GLY	GLY
E3999	E3804			X3441	X3329			GLY	GLY
E4000	E3805			X3442	X3330			GLY	GLY
E4001	E3806			X3443	X3331			GLY	GLY
E4002	E3807			X3444	X3332			GLY	GLY
E4003	E3808			X3445	X3333			GLY	GLY
E4004	E3809			X3446	X3334			GLY	GLY
E4005	E3810			X3447	X3335			GLY	GLY
E4006	E3811			X3448	X3336			GLY	GLY
E4007	E3812			X3449	X3337			GLY	GLY
E4008	E3813			X3450	X3338			GLY	GLY
E4009	E3814			X3451	X3339			GLY	GLY
E4010	E3815			X3452	X3340			GLY	GLY
E4011	E3816			X3453	X3341			GLY	GLY
E4012	E3817			X3454	X3342			GLY	GLY
E4013	E3818			X3455	X3343			GLY	GLY
E4014	E3819			X3456	X3344			GLY	GLY
E4015	E3820			X3457	X3345			GLY	GLY
E4016	E3821			X3458	X3346			GLY	GLY
E4017	E3822			X3459	X3347			GLY	GLY
E4018	E3823			X3460	X3348			GLY	GLY
E4019	E3824			X3461	X3349			GLY	GLY
E4020	E3825			X3462	X3350			GLY	GLY
E4021	E3826			X3463	X3351			GLY	GLY
E4022	E3827			X3464	X3352			GLY	GLY
E4023	E3828			X3465	X3353			GLY	GLY
E4024	E3829			X3466	X3354			GLY	GLY
E4025	E3830			X3467	X3355			GLY	GLY
E4026	E3831			X3468	X3356			GLY	GLY
E4027	E3832			X3469	X3357			GLY	GLY
E4028	E3833			X3470	X3358			GLY	GLY
E4029	E3834			X3471	X3359			GLY	GLY
E4030	E3835			X3472	X3360			GLY	GLY
E4031	E3836			X3473	X3361			GLY	GLY
E4032	E3837			X3474	X3362			GLY	GLY
E4033	E3838			X3475	X3363			GLY	GLY
E4034	E3839			X3476	X3364			GLY	GLY
E4035	E3840			X3477	X3365			GLY	GLY
E4036	E3841			X3478	X3366			GLY	GLY
E4037	E3842			X3479	X3367			GLY	GLY
E4038	E3843			X3480	X3368			GLY	GLY
E4039	E3844			X3481	X3369			GLY	GLY
E4040	E3845			X3482	X3370			GLY	GLY
E4041	E3846			X3483	X3371			GLY	GLY
E4042	E3847			X3484	X3372			GLY	GLY
E4043	E3848			X3485	X3373			GLY	GLY
E4044	E3849			X3486	X3374			GLY	GLY
E4045	E3850			X3487	X3375			GLY	GLY
E4046	E3851			X3488	X3376			GLY	GLY
E4047	E3852			X3489	X3377			GLY	GLY
E4048	E3853			X3490	X3378			GLY	GLY
E4049	E3854			X3491	X3379			GLY	GLY
E4050	E3855			X3492	X3380			GLY	GLY
E4051	E3856			X3493	X3381			GLY	GLY
E4052	E3857			X3494	X3382			GLY	GLY
E4053	E3858			X3495	X3383			GLY	GLY
E4054	E3859			X3496	X3384			GLY	GLY
E4055	E3860			X3497	X3385			GLY	GLY
E4056	E3861			X3498	X3386			GLY	GLY
E4057	E3862			X3499	X3387			GLY	GLY
E4058	E3863			X3500	X3388			GLY	GLY
E4059	E3864			X3501	X3389			GLY	GLY
E4060	E3865			X3502	X3390			GLY	GLY
E4061	E3866			X3503	X3391			GLY	GLY
E4062	E3867			X3504	X3392			GLY	GLY
E4063	E3868			X3505	X3393			GLY	GLY
E4064	E3869			X3506	X3394			GLY	GLY
E4065	E3870			X3507	X3395			GLY	GLY
E4066	E3871			X3508	X3396			GLY	GLY
E4067	E3872			X3509	X3397			GLY	GLY
E4068	E3873			X3510	X3398			GLY	GLY
E4069	E3874			X3511	X3399			GLY	GLY
E4070	E3875			X3512	X3400			GLY	GLY
E4071	E3876			X3513	X3401			GLY	GLY
E4072	E3877			X3514	X3402			GLY	GLY
E4073	E3878			X3515	X3403			GLY	GLY
E4074	E3879			X3516	X3404			GLY	GLY
E4075	E3880			X3517	X3405			GLY	GLY
E4076	E3881			X3518	X3406			GLY	GLY
E4077	E3882			X3519	X3407			GLY	GLY
E4078	E3883			X3520	X3408			GLY	GLY
E4079	E3884			X3521	X3409			GLY	GLY
E4080	E3885			X3522	X3410			GLY	GLY
E4081	E3886			X3523	X3411			GLY	GLY
E4082	E3887			X3524	X3412			GLY	GLY
E4083	E3888			X3525	X3413			GLY	GLY
E4084	E3889			X3526	X3414			GLY	GLY
E4085	E3890			X3527	X3415			GLY	GLY
E4086	E3891			X3528	X3416			GLY	GLY
E4087	E3892			X3529	X3417			GLY	GLY
E4088	E3893			X3530	X3418			GLY	GLY
E4089	E3894			X3531	X3419			GLY	GLY
E4090	E3895			X3532	X3420			GLY	GLY
E4091	E3896			X3533	X3421			GLY	GLY
E4092	E3897			X3534	X3422			GLY	GLY
E4093	E3898			X3535	X3423			GLY	GLY
E4094	E3899			X3536	X3424			GLY	GLY
E4095	E3900			X3537	X3425			GLY	GLY
E4096	E3901			X3538	X3426			GLY	GLY
E4097	E3902			X3539	X3427			GLY	GLY
E4098	E3903			X3540	X3428			GLY	GLY
E4099	E3904			X3541	X3429			GLY	GLY
E4100	E3905			X3542	X3430			GLY	GLY
E4101	E3906			X3543	X3431			GLY	GLY
E4102	E3907			X3544	X3432			GLY	GLY
E4103	E3908			X3545	X3433			GLY	GLY
E4104	E3909			X3546	X3434			GLY	GLY
E4105	E3910			X3547	X3435			GLY	GLY
E4106	E3911			X3548	X3436			GLY	GLY
E4107	E3912			X3549	X3437			GLY	GLY
E4108	E3913			X3550	X3438			GLY	GLY
E4109	E3914			X3551	X3439			GLY	GLY
E4110	E3915			X3552	X3440			GLY	GLY
E4111	E3916			X3553	X3441			GLY	GLY
E4112	E3917			X3554	X3442			GLY	GLY
E4113	E3918			X3555	X3443			GLY	GLY
E4114	E3919			X3556	X3444			GLY	GLY
E4115	E3920			X3557	X3445			GLY	GLY
E4116	E3921			X3558	X3446				



• Molecule 1: Ryanodine receptor 1





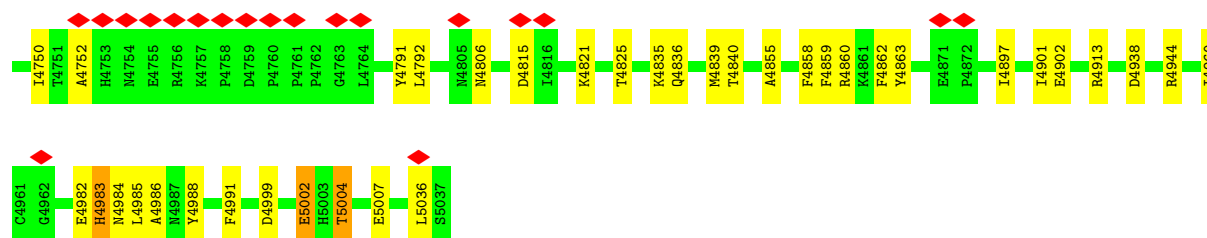




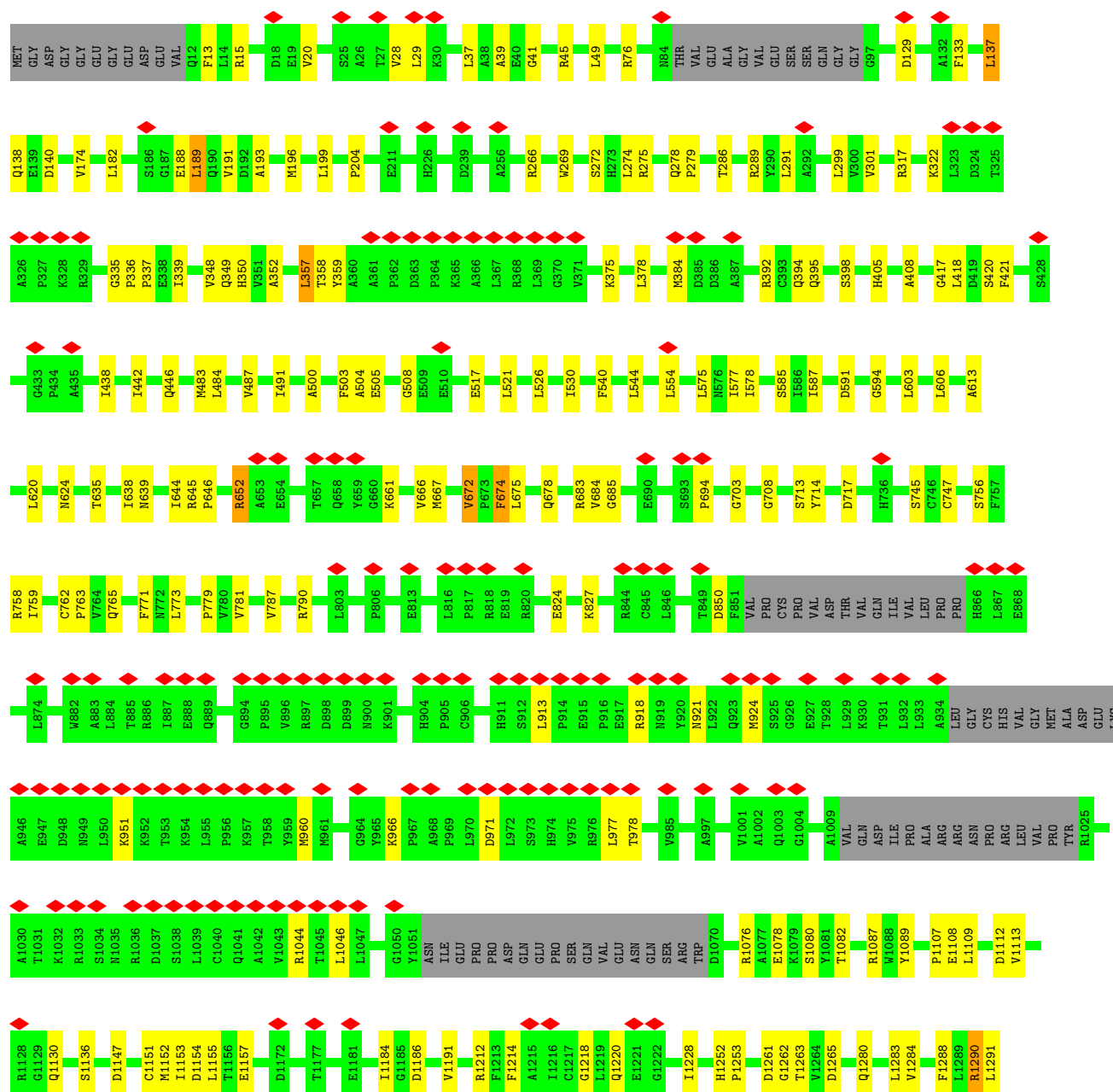








• Molecule 1: Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	167778	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.171	Depositor
Minimum map value	-0.700	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	474.72, 474.72, 474.72	wwPDB
Map dimensions	552, 552, 552	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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: ACP, LBN, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	2/24263 (0.0%)	0.63	34/32920 (0.1%)
1	B	0.29	0/24291	0.59	27/32959 (0.1%)
1	C	0.29	0/24161	0.56	12/32790 (0.0%)
1	D	0.29	0/24170	0.59	24/32806 (0.1%)
All	All	0.30	2/96885 (0.0%)	0.59	97/131475 (0.1%)

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	B	0	1
1	D	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4139	ILE	N-CA	6.91	1.54	1.46
1	A	4135	PRO	C-O	-5.58	1.17	1.24

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4123	ILE	N-CA-C	-14.80	95.77	110.72
1	A	4088	ILE	N-CA-C	-14.16	89.81	108.93
1	D	4123	ILE	N-CA-C	-11.82	98.78	110.72
1	A	4128	PHE	N-CA-C	-10.18	98.30	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4137	ARG	CB-CA-C	-9.81	94.00	110.68

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4131	ARG	Sidechain
1	A	4137	ARG	Sidechain
1	B	4131	ARG	Sidechain
1	D	4131	ARG	Sidechain

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	27759	0	23609	391	0
1	B	27785	0	23649	372	0
1	C	27661	0	23456	332	0
1	D	27670	0	23480	373	0
2	A	31	0	14	1	0
2	B	31	0	14	2	0
2	C	31	0	14	1	0
2	D	31	0	14	0	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	4	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	93	0	0	0	0
5	B	93	0	0	0	0
5	C	93	0	0	3	0
5	D	93	0	0	1	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	2	0	0	0	0
6	D	2	0	0	0	0
All	All	111396	0	94250	1459	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 7.

The worst 5 of 1459 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2128:TYR:HB3	1:D:3669:PHE:CZ	1.61	1.35
1:C:2128:TYR:CD2	1:C:3673:MET:HE3	1.62	1.35
1:B:2128:TYR:CD2	1:B:3673:MET:HE3	1.63	1.33
1:A:2128:TYR:HB3	1:A:3669:PHE:CZ	1.63	1.33
1:D:2128:TYR:CD2	1:D:3673:MET:HE3	1.64	1.30

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	3095/5037 (61%)	2890 (93%)	188 (6%)	17 (0%)	24	57
1	B	3095/5037 (61%)	2880 (93%)	188 (6%)	27 (1%)	14	44
1	C	3095/5037 (61%)	2898 (94%)	178 (6%)	19 (1%)	21	52
1	D	3095/5037 (61%)	2895 (94%)	182 (6%)	18 (1%)	21	52
All	All	12380/20148 (61%)	11563 (93%)	736 (6%)	81 (1%)	20	49

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	674	PHE
1	A	1440	PHE
1	A	1489	CYS
1	A	2476	ILE
1	A	3970	GLN

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	2435/3579 (68%)	2363 (97%)	72 (3%)	36	65
1	B	2444/3579 (68%)	2379 (97%)	65 (3%)	39	67
1	C	2412/3579 (67%)	2365 (98%)	47 (2%)	50	73
1	D	2418/3579 (68%)	2361 (98%)	57 (2%)	43	69
All	All	9709/14316 (68%)	9468 (98%)	241 (2%)	42	69

5 of 241 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3873	LYS
1	D	3897	ASN
1	C	672	VAL
1	D	3875	MET
1	D	4181	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	308	HIS
1	D	5015	GLN
1	D	624	ASN
1	D	3814	GLN
1	B	866	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 17 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
5	LBN	C	5106	-	46,46,51	0.33	0	52,54,59	0.34	0
2	ACP	A	5101	4	31,33,33	1.99	9 (29%)	47,52,52	2.16	11 (23%)
5	LBN	C	5107	-	45,45,51	0.33	0	51,53,59	0.31	0
5	LBN	B	5107	-	46,46,51	0.33	0	52,54,59	0.33	0
2	ACP	C	5101	4	31,33,33	0.75	1 (3%)	47,52,52	0.57	1 (2%)
5	LBN	D	5107	-	45,45,51	0.33	0	51,53,59	0.31	0
5	LBN	B	5106	-	45,45,51	0.33	0	51,53,59	0.31	0
5	LBN	D	5106	-	46,46,51	0.33	0	52,54,59	0.35	0
2	ACP	B	5101	4	31,33,33	2.01	8 (25%)	47,52,52	2.29	12 (25%)
5	LBN	A	5108	-	45,45,51	0.32	0	51,53,59	0.31	0
5	LBN	A	5107	-	46,46,51	0.32	0	52,54,59	0.34	0
2	ACP	D	5101	4	31,33,33	0.76	1 (3%)	47,52,52	0.58	1 (2%)

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
5	LBN	C	5106	-	-	31/50/50/55	-
2	ACP	A	5101	4	-	6/19/38/38	0/3/3/3
5	LBN	C	5107	-	-	29/49/49/55	-
5	LBN	B	5107	-	-	31/50/50/55	-
2	ACP	C	5101	4	-	3/19/38/38	0/3/3/3
5	LBN	D	5107	-	-	18/49/49/55	-
5	LBN	B	5106	-	-	18/49/49/55	-
5	LBN	D	5106	-	-	22/50/50/55	-
2	ACP	B	5101	4	-	8/19/38/38	0/3/3/3
5	LBN	A	5108	-	-	23/49/49/55	-
5	LBN	A	5107	-	-	35/50/50/55	-
2	ACP	D	5101	4	-	5/19/38/38	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5101	ACP	C4-N9	-4.41	1.28	1.37
2	A	5101	ACP	PB-O3A	4.23	1.63	1.58
2	A	5101	ACP	C4-N9	-4.18	1.29	1.37
2	B	5101	ACP	C5-C4	4.08	1.46	1.39
2	B	5101	ACP	PB-O3A	4.00	1.62	1.58

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5101	ACP	C2-N1-C6	8.46	132.62	118.73
2	A	5101	ACP	C2-N1-C6	7.71	131.39	118.73
2	B	5101	ACP	N3-C2-N1	-6.98	118.02	128.58
2	A	5101	ACP	N3-C2-N1	-6.66	118.50	128.58
2	B	5101	ACP	C4-N9-C1'	-4.53	116.04	126.63

There are no chirality outliers.

5 of 229 torsion outliers are listed below:

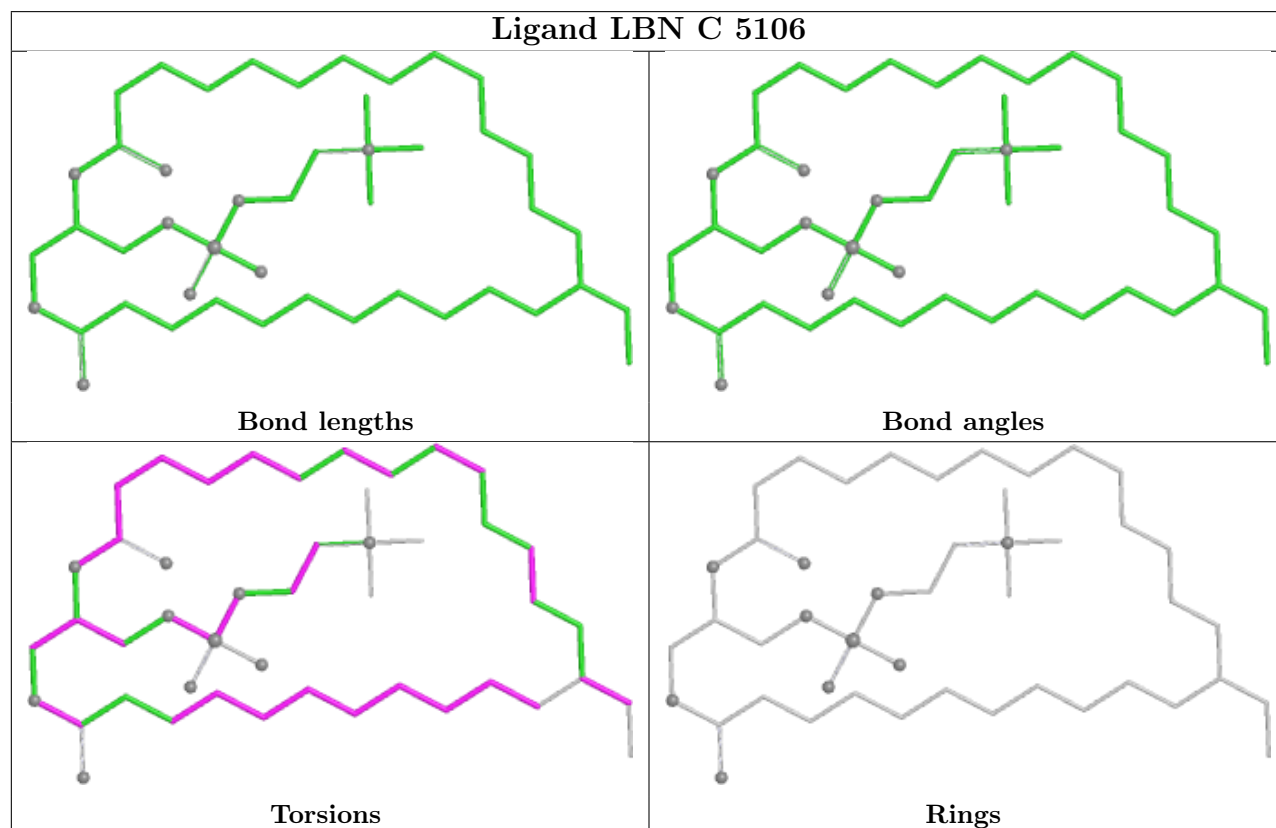
Mol	Chain	Res	Type	Atoms
2	A	5101	ACP	C5'-O5'-PA-O3A
2	A	5101	ACP	O4'-C4'-C5'-O5'
2	A	5101	ACP	C3'-C4'-C5'-O5'
2	B	5101	ACP	PB-C3B-PG-O2G
2	B	5101	ACP	C5'-O5'-PA-O3A

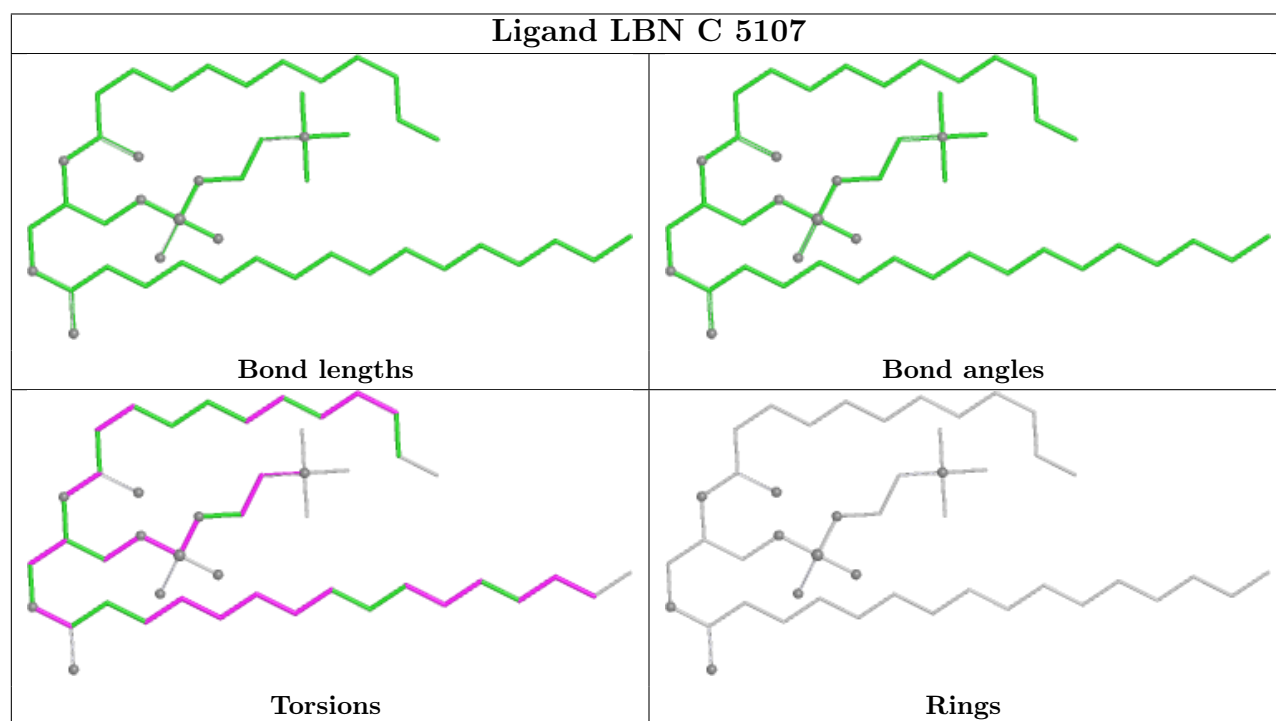
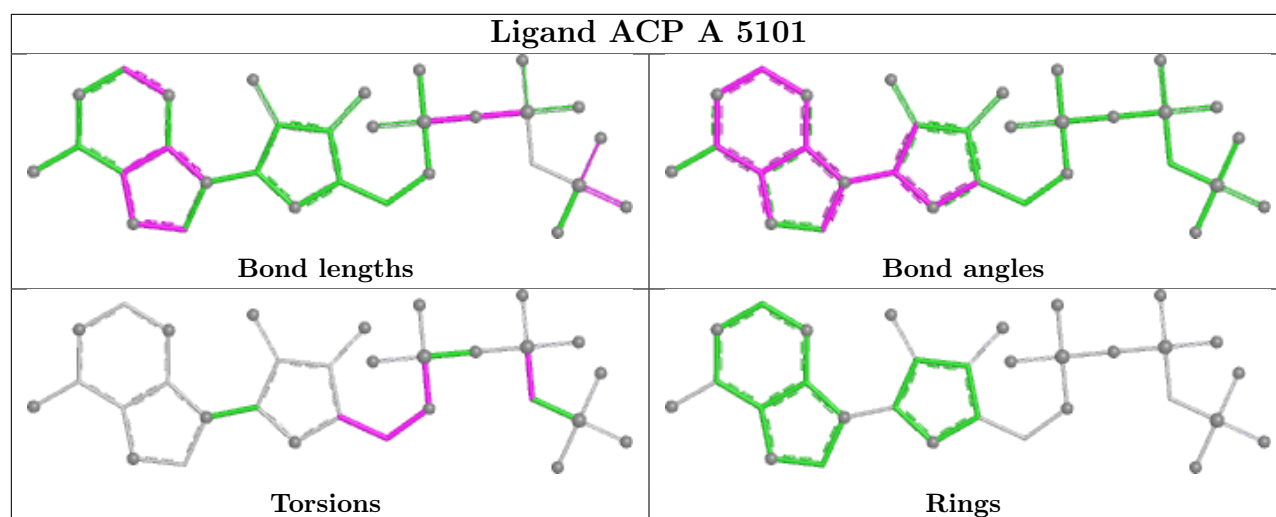
There are no ring outliers.

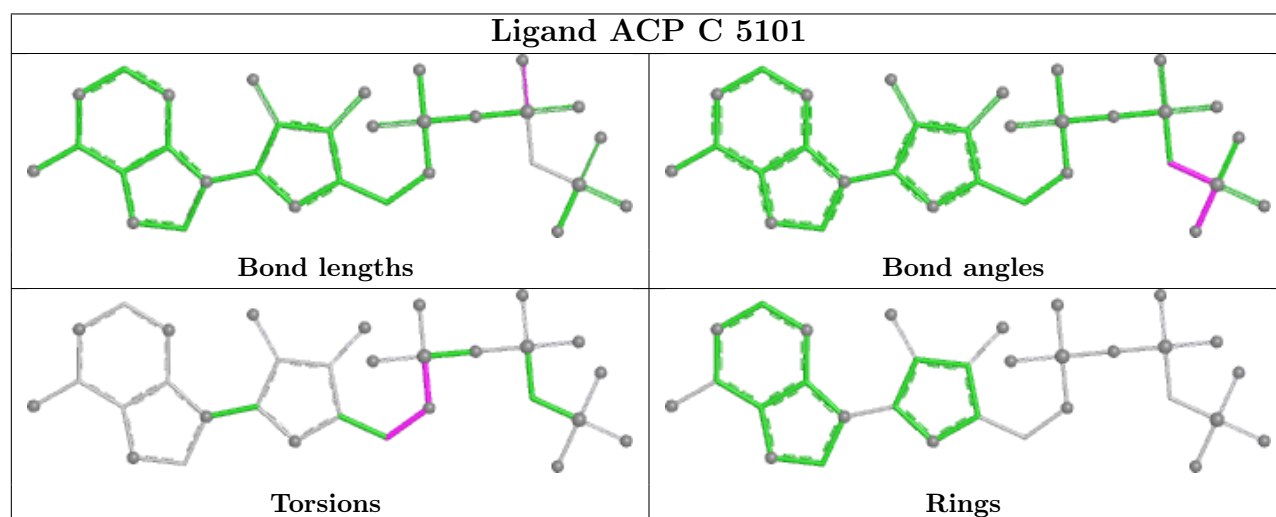
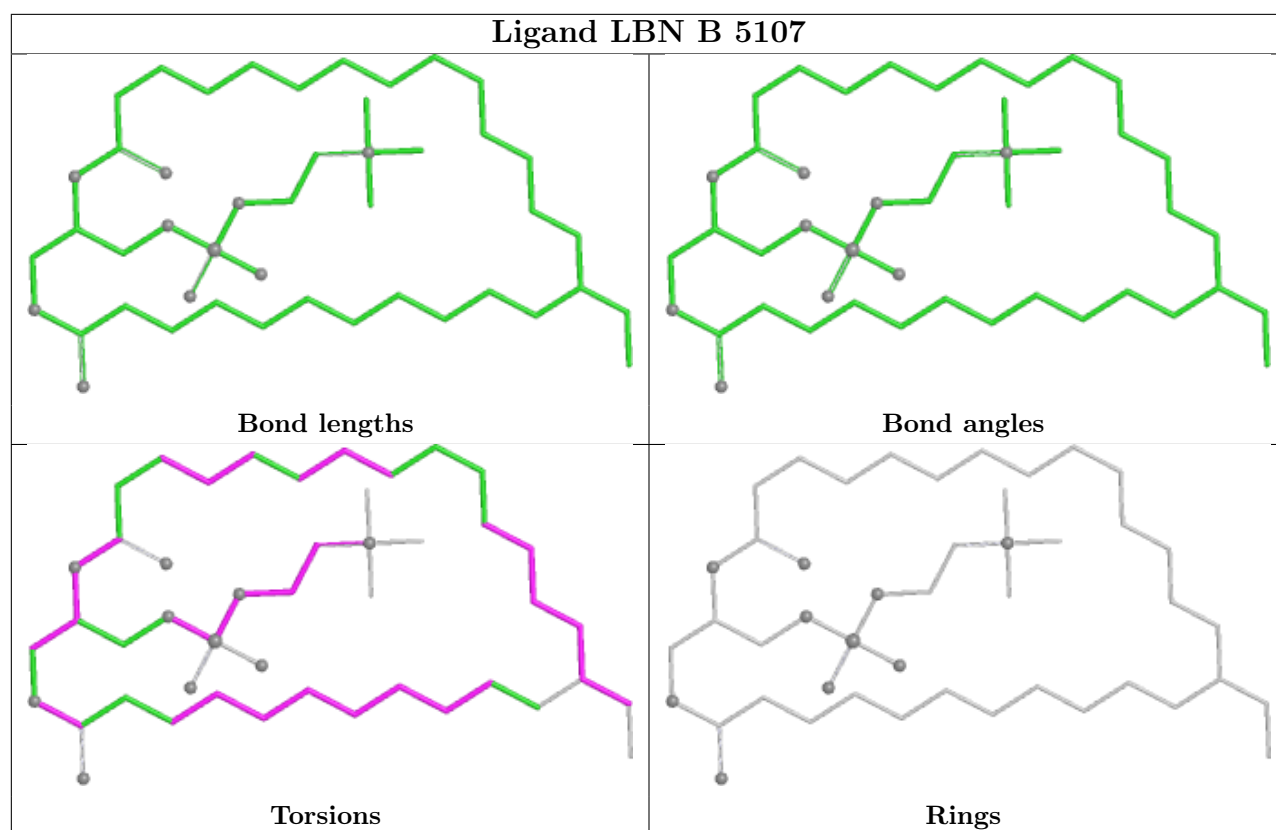
6 monomers are involved in 8 short contacts:

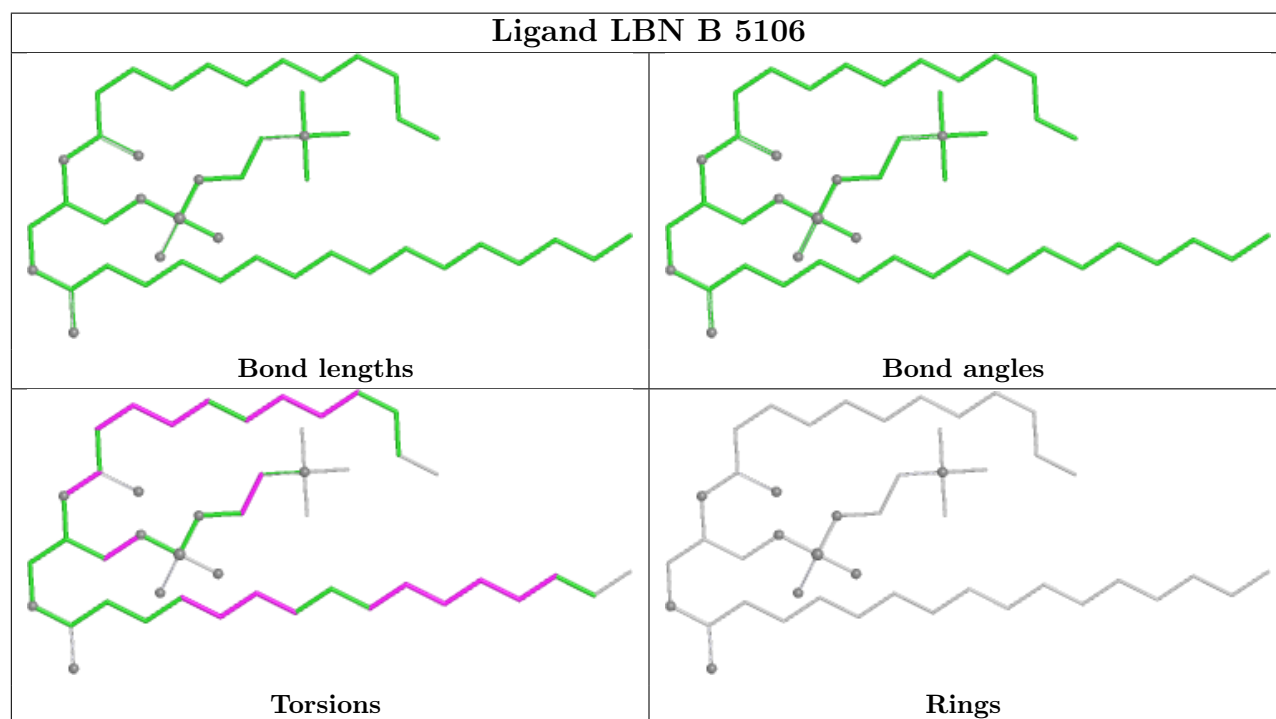
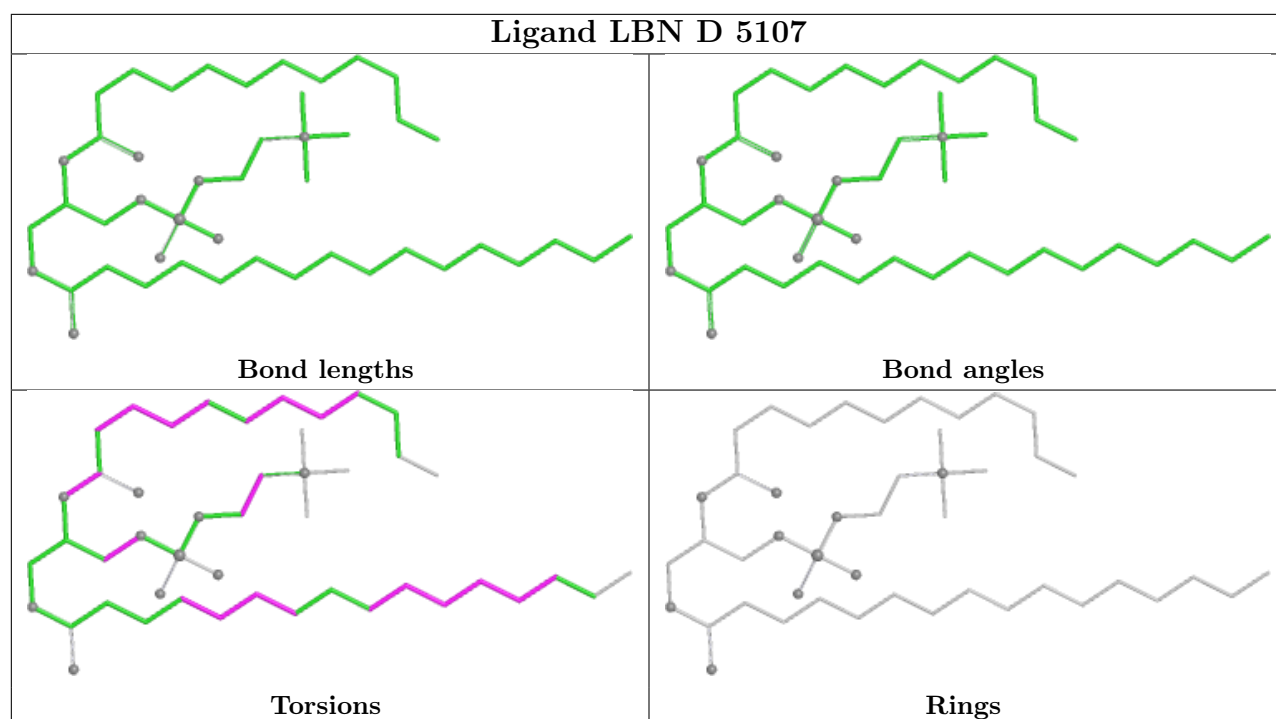
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5106	LBN	1	0
2	A	5101	ACP	1	0
5	C	5107	LBN	2	0
2	C	5101	ACP	1	0
5	D	5106	LBN	1	0
2	B	5101	ACP	2	0

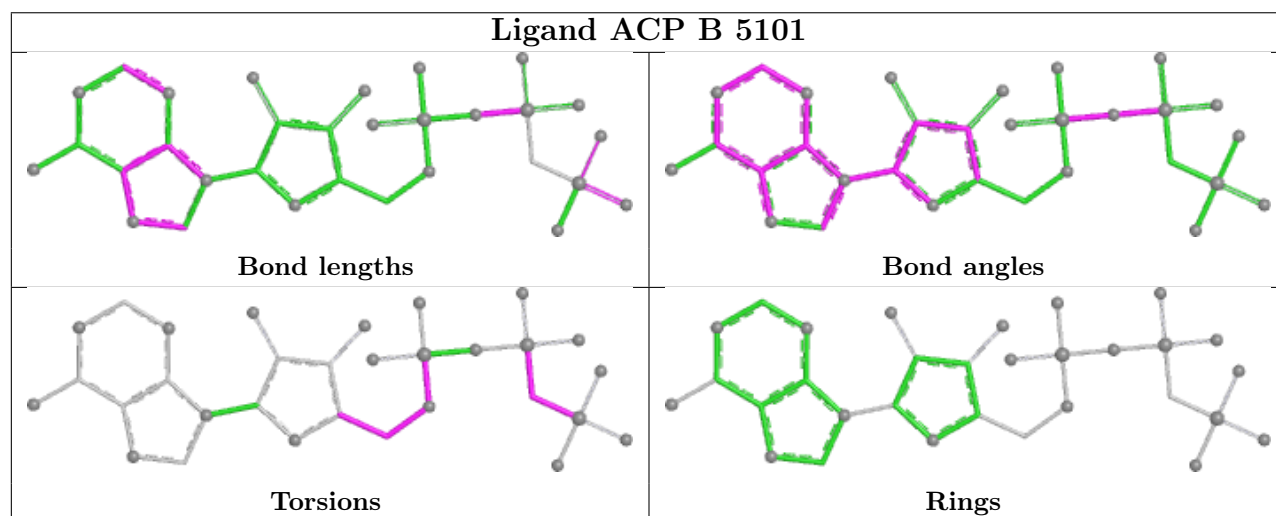
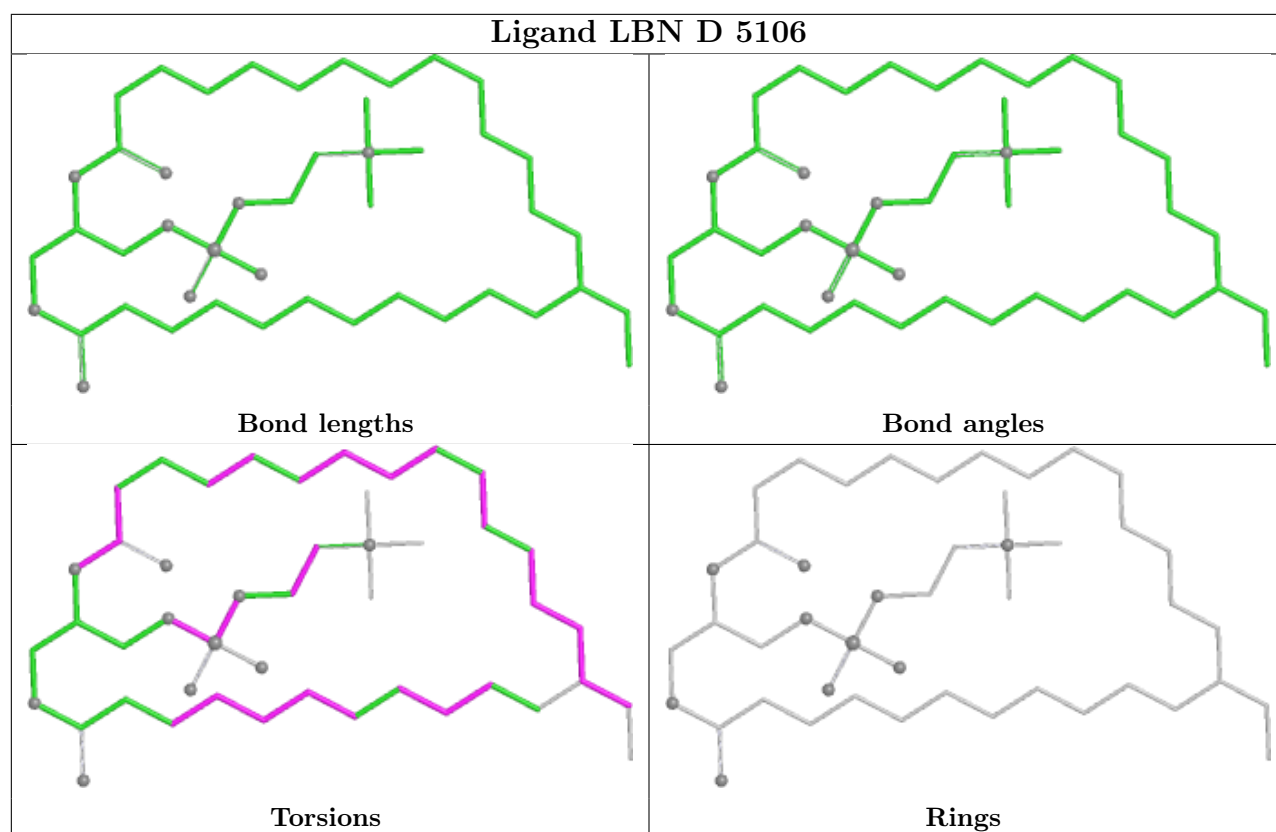
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

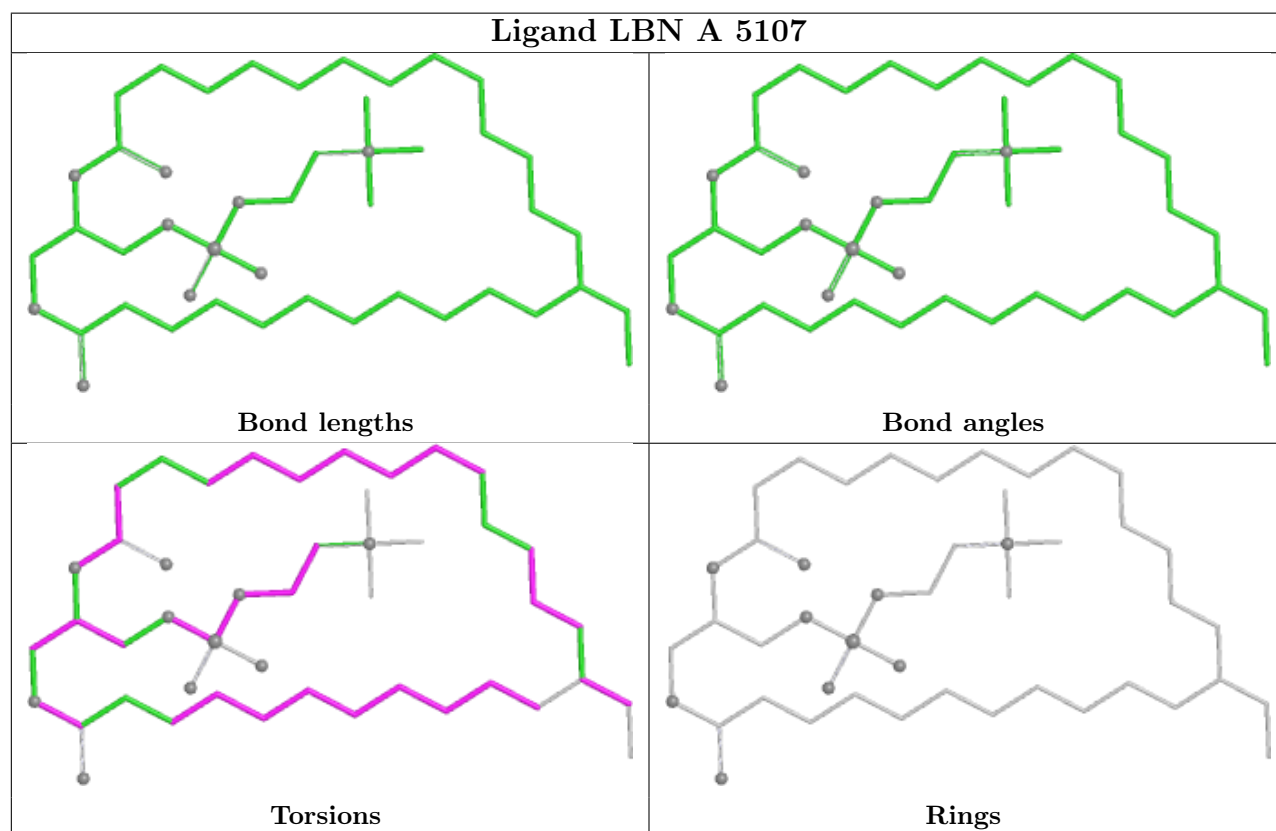
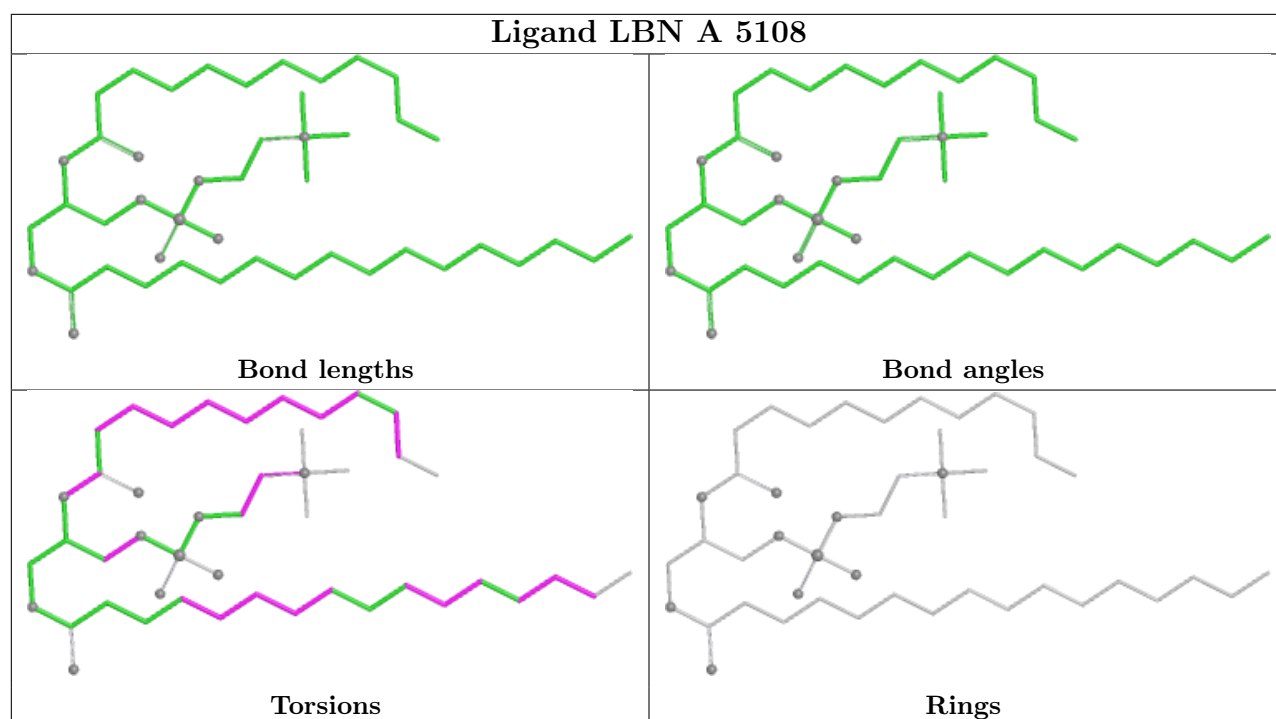


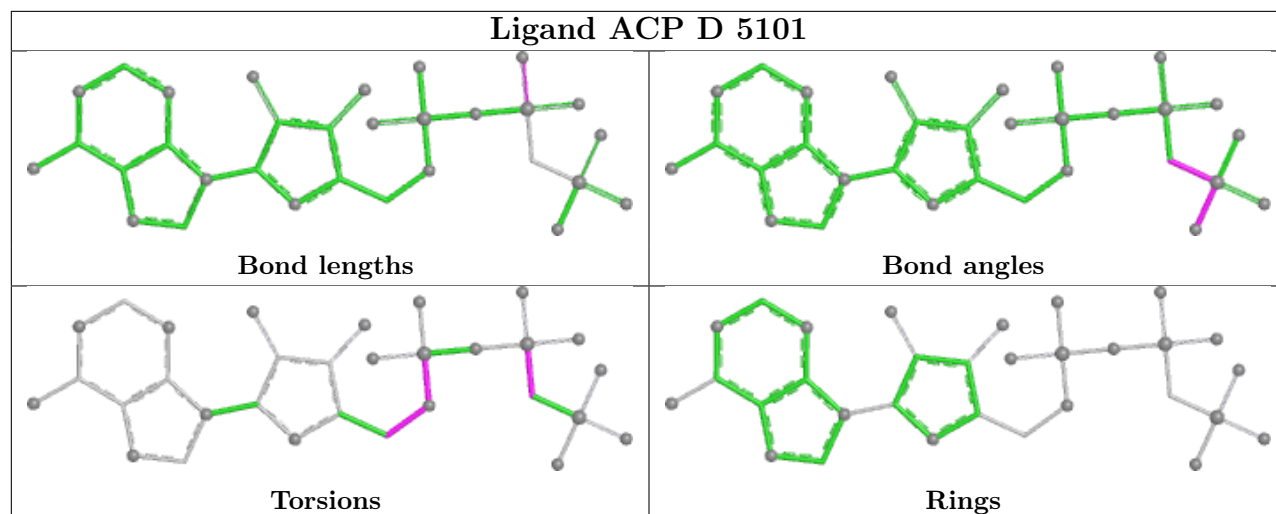












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

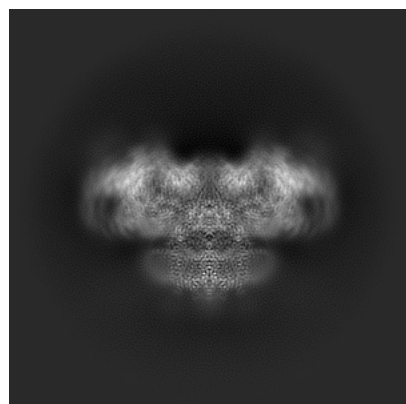
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26610. These allow visual inspection of the internal detail of the map and identification of artifacts.

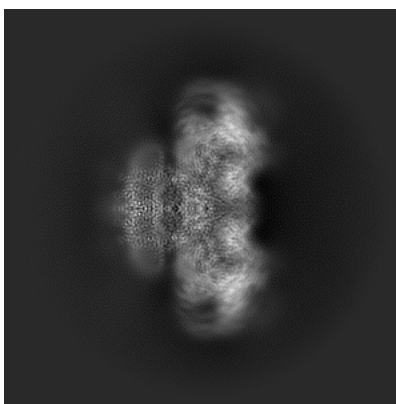
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

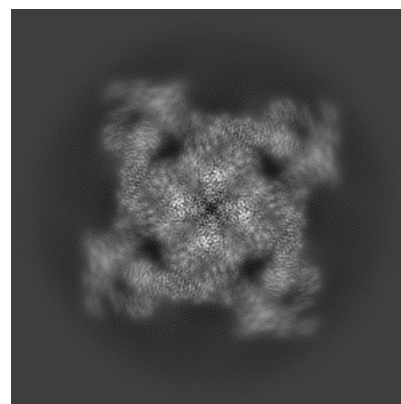
6.1.1 Primary map



X

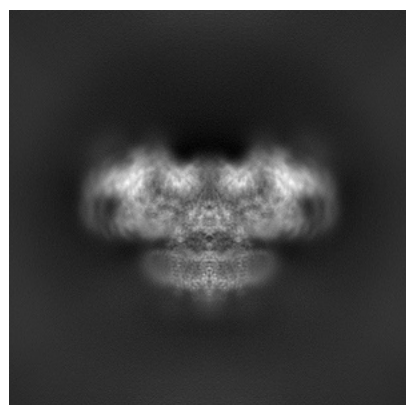


Y

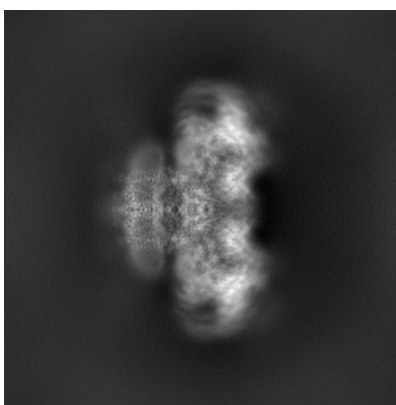


Z

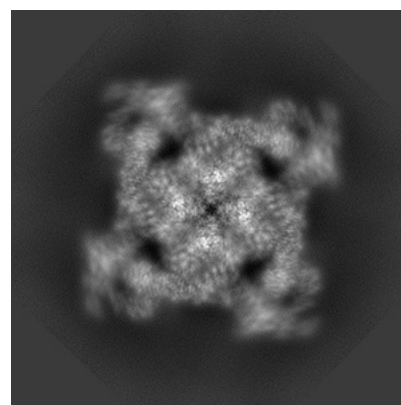
6.1.2 Raw map



X



Y

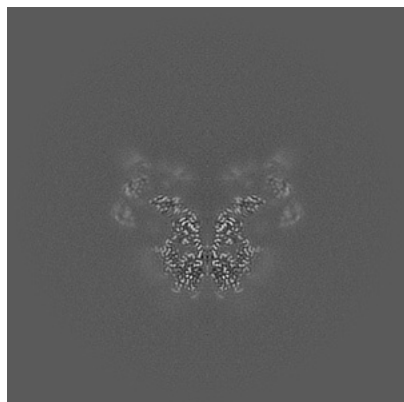


Z

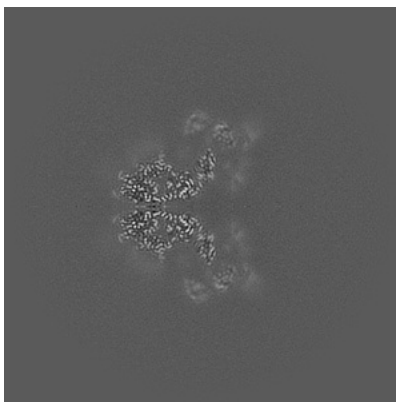
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

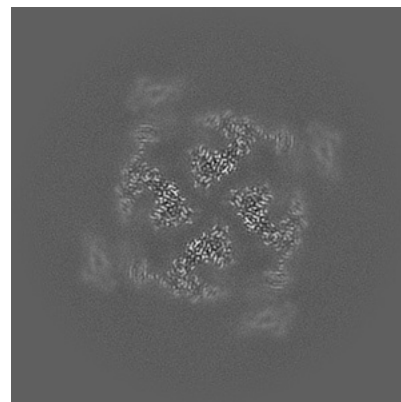
6.2.1 Primary map



X Index: 276

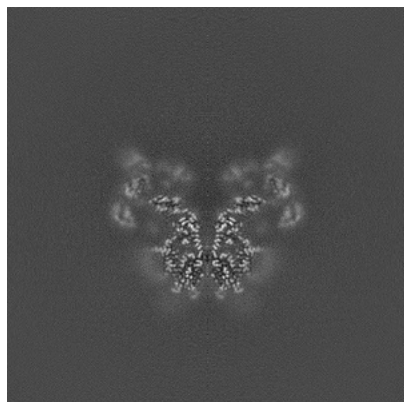


Y Index: 276

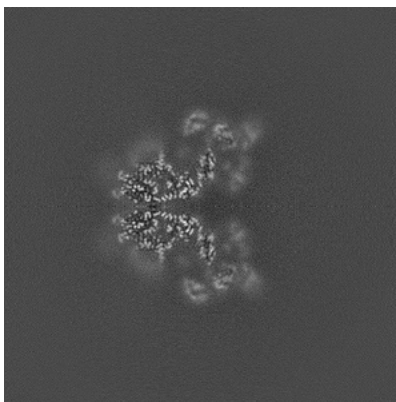


Z Index: 276

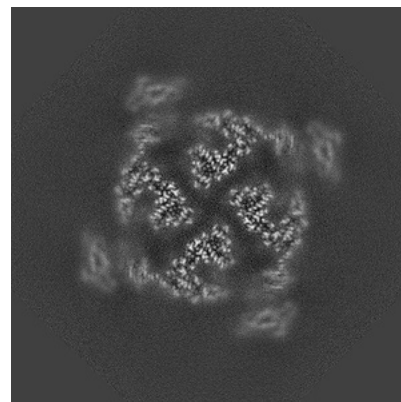
6.2.2 Raw map



X Index: 276



Y Index: 276

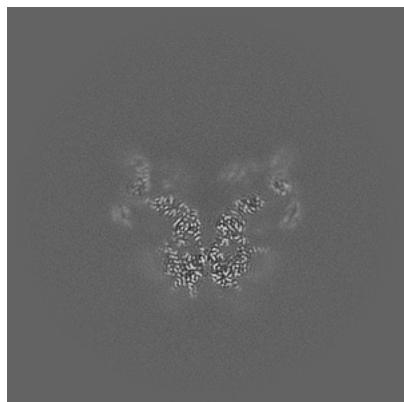


Z Index: 276

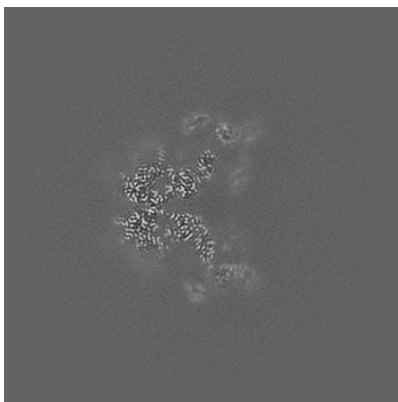
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

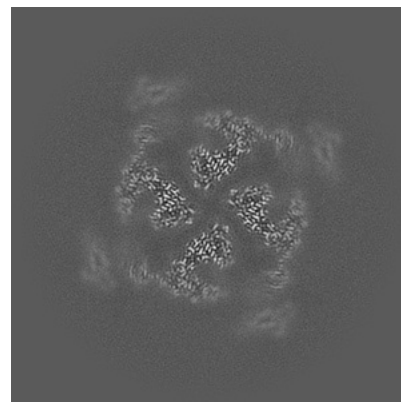
6.3.1 Primary map



X Index: 280

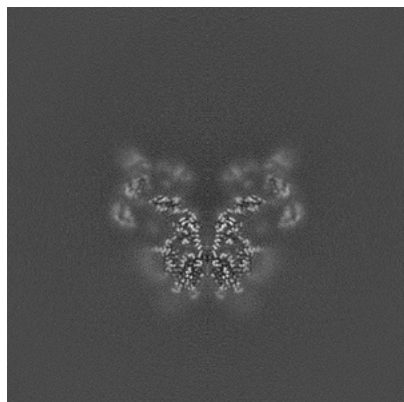


Y Index: 272

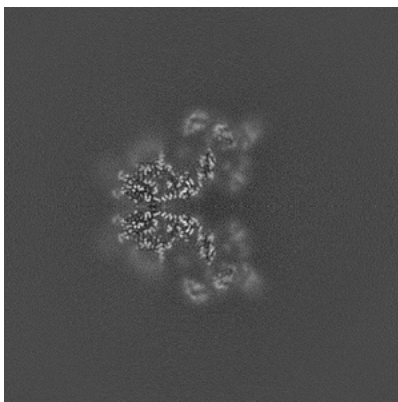


Z Index: 275

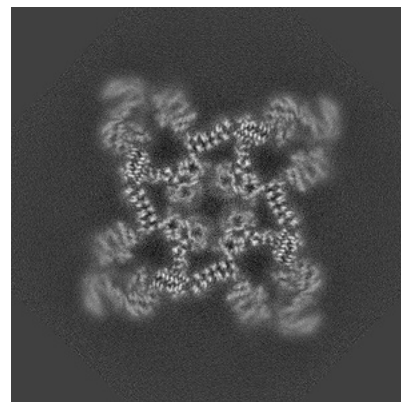
6.3.2 Raw map



X Index: 276



Y Index: 276

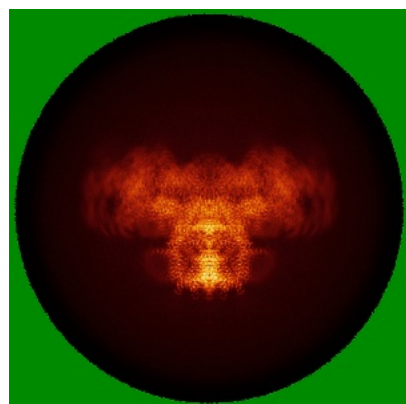


Z Index: 311

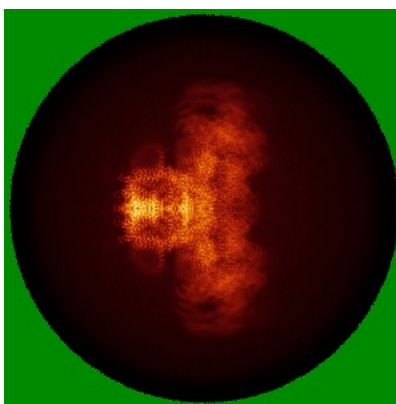
The images above show the largest variance slices of the map in three orthogonal directions.

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

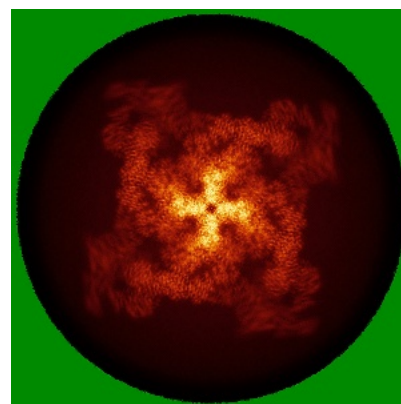
6.4.1 Primary map



X

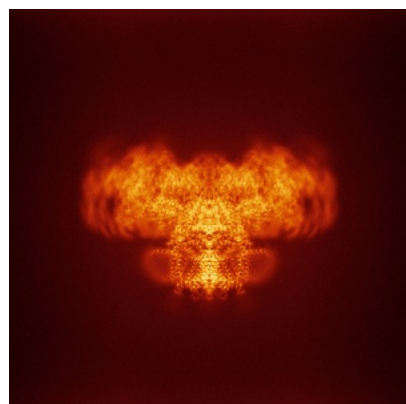


Y

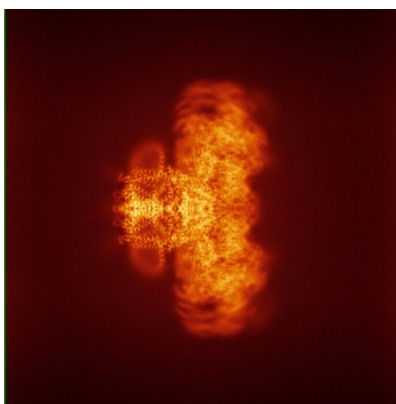


Z

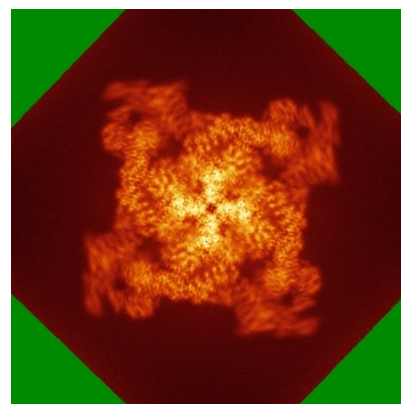
6.4.2 Raw map



X



Y

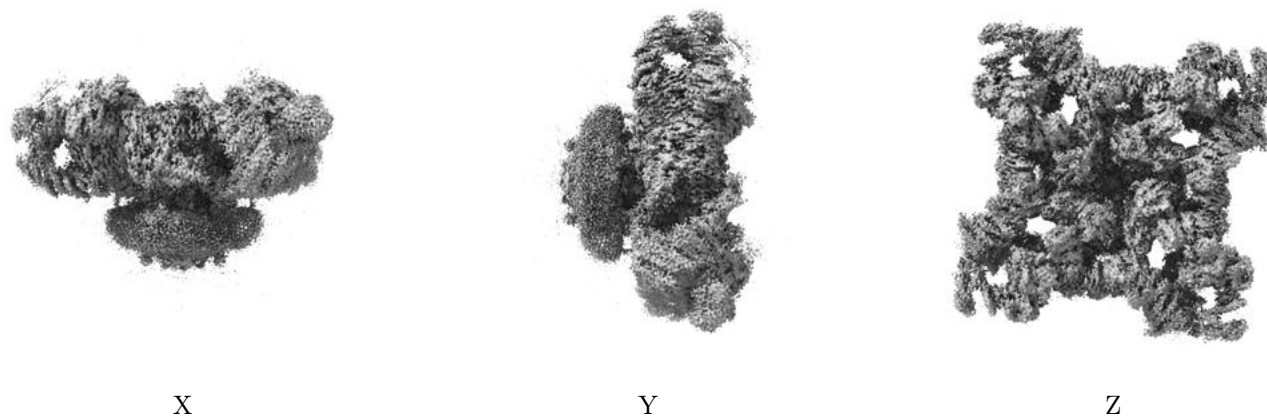


Z

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.

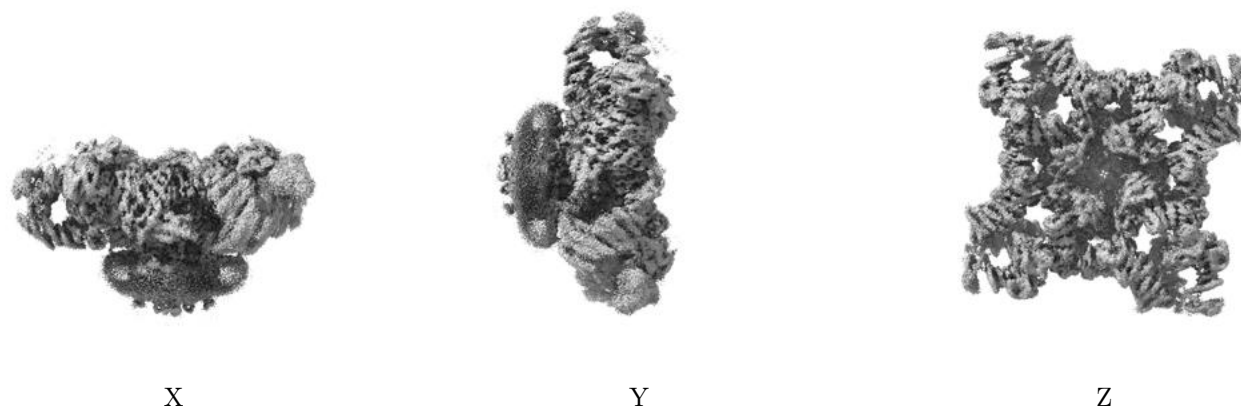
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

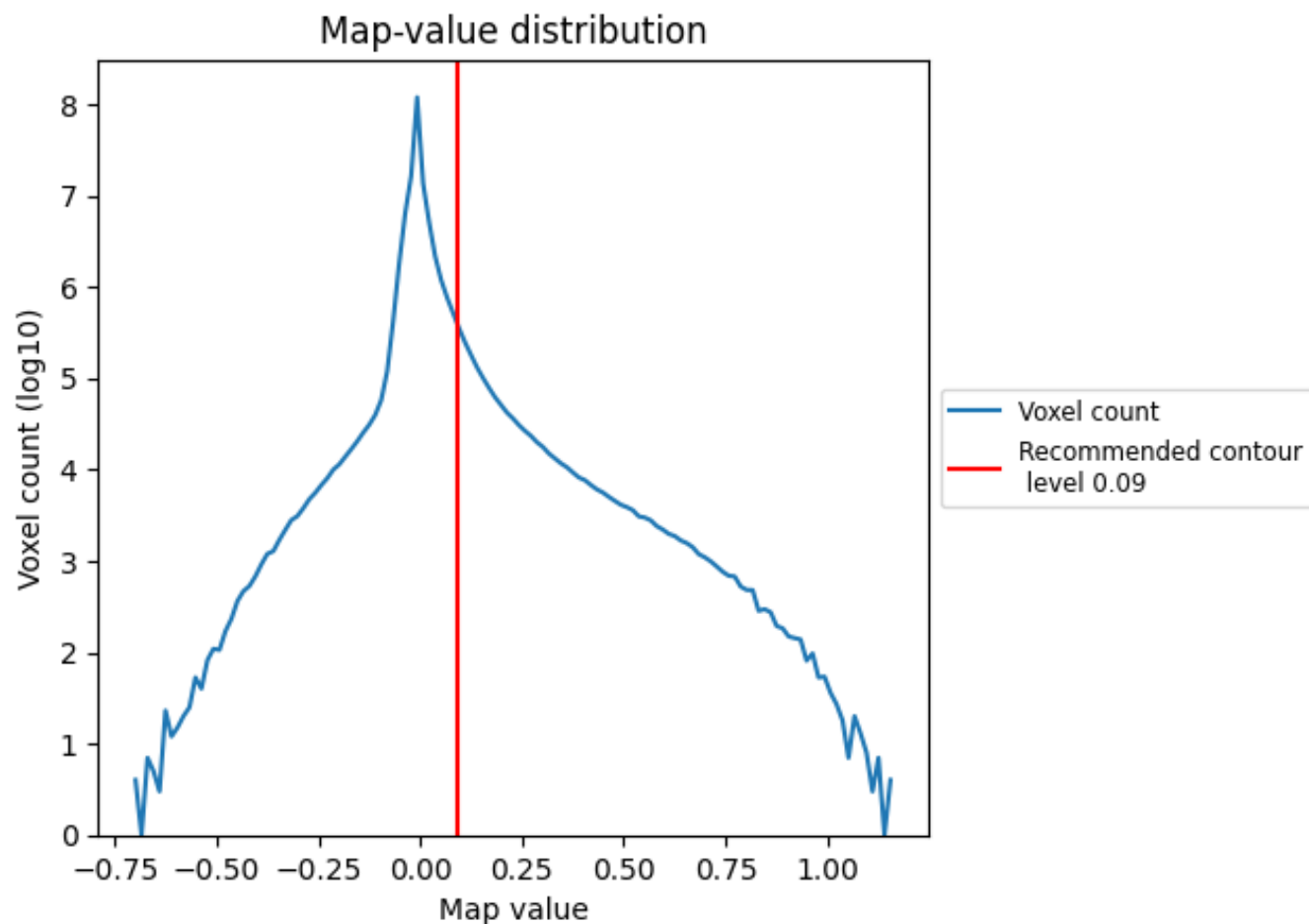
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

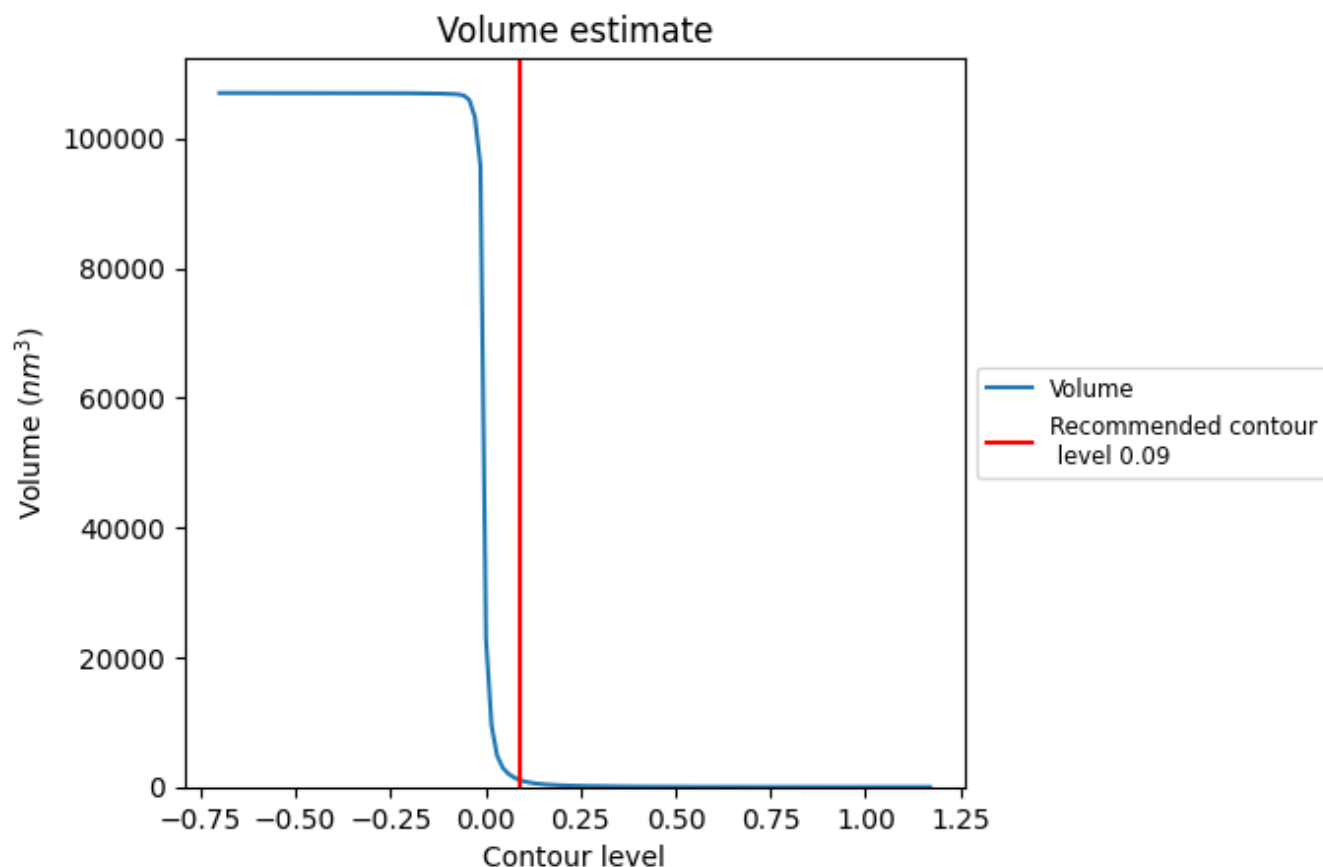
This section contains the results of statistical analysis of the map.

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.

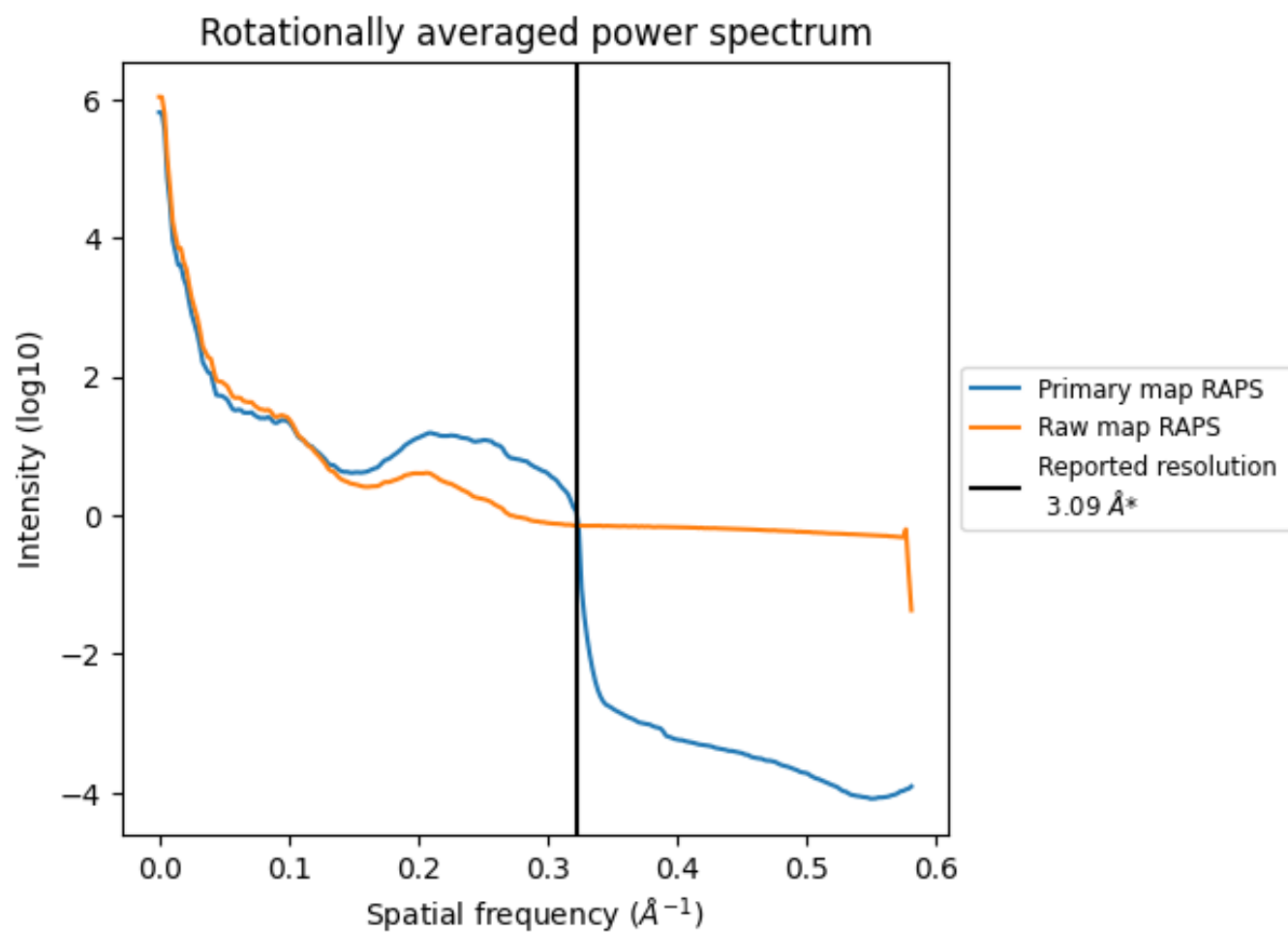
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1086 nm^3 ; this corresponds to an approximate mass of 981 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 ⓘ

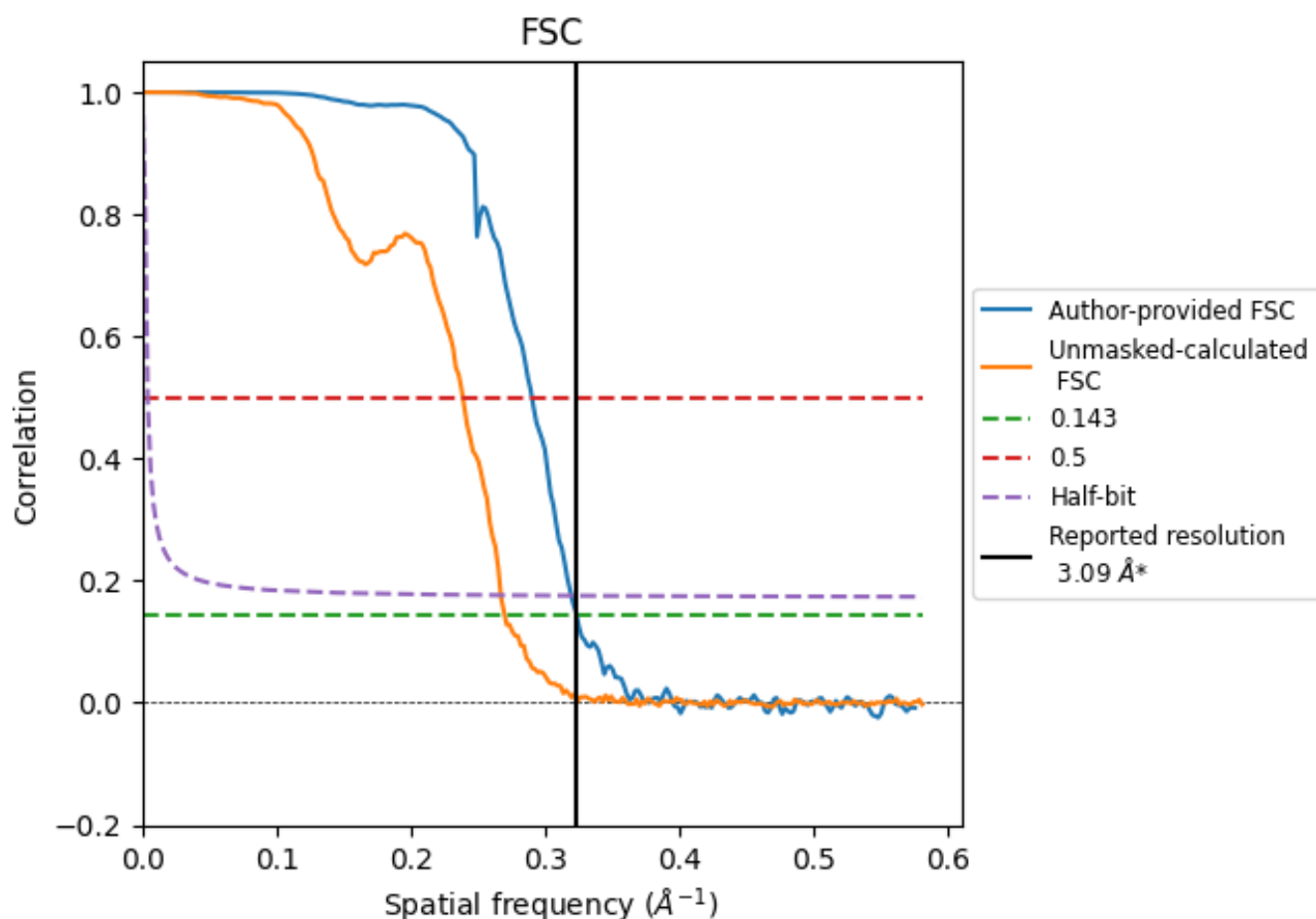


*Reported resolution corresponds to spatial frequency of 0.324 $\text{\AA}^{-1}$

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 0.324 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

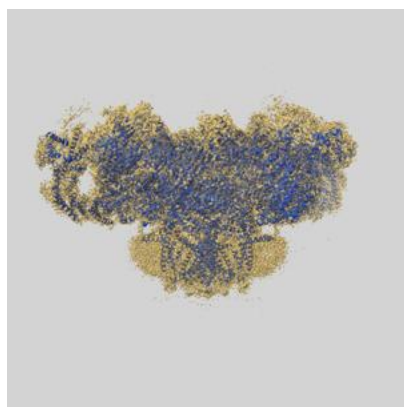
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.44	3.13
Unmasked-calculated*	3.70	4.18	3.74

*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 3.70 differs from the reported value 3.09 by more than 10 %

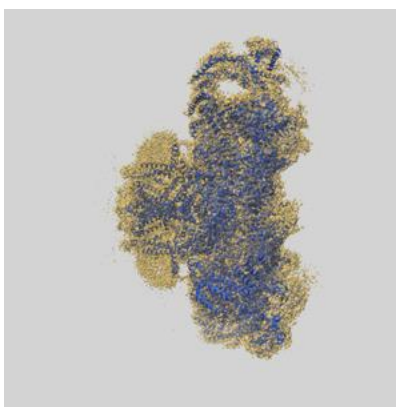
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26610 and PDB model 7UMZ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

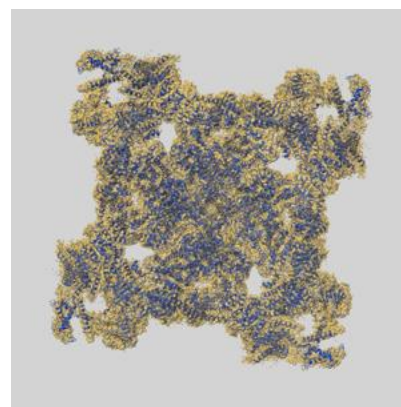
9.1 Map-model overlay [i](#)



X



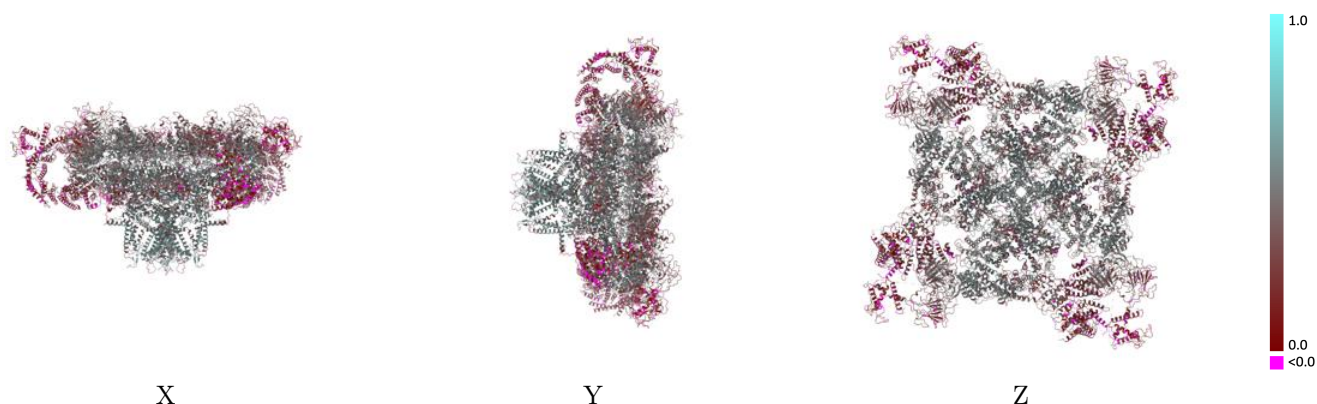
Y



Z

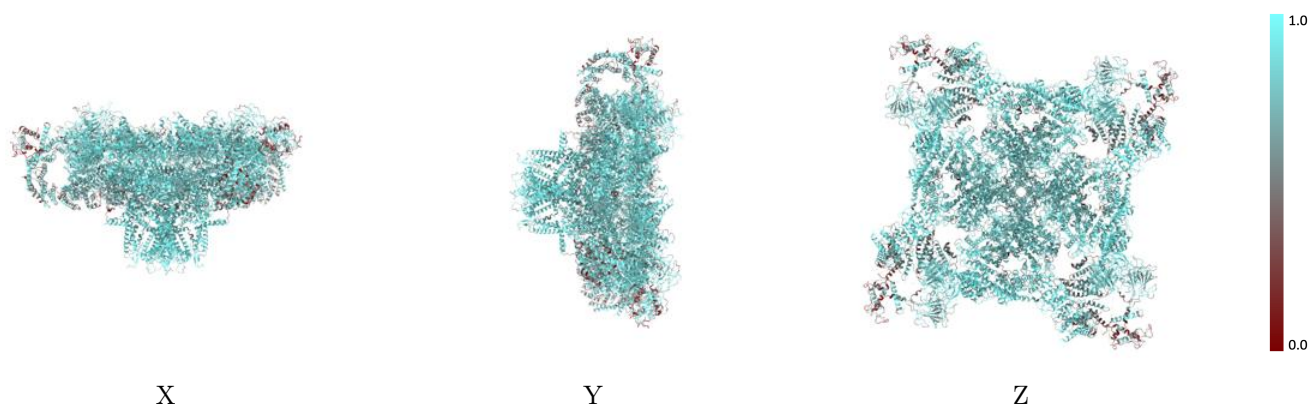
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



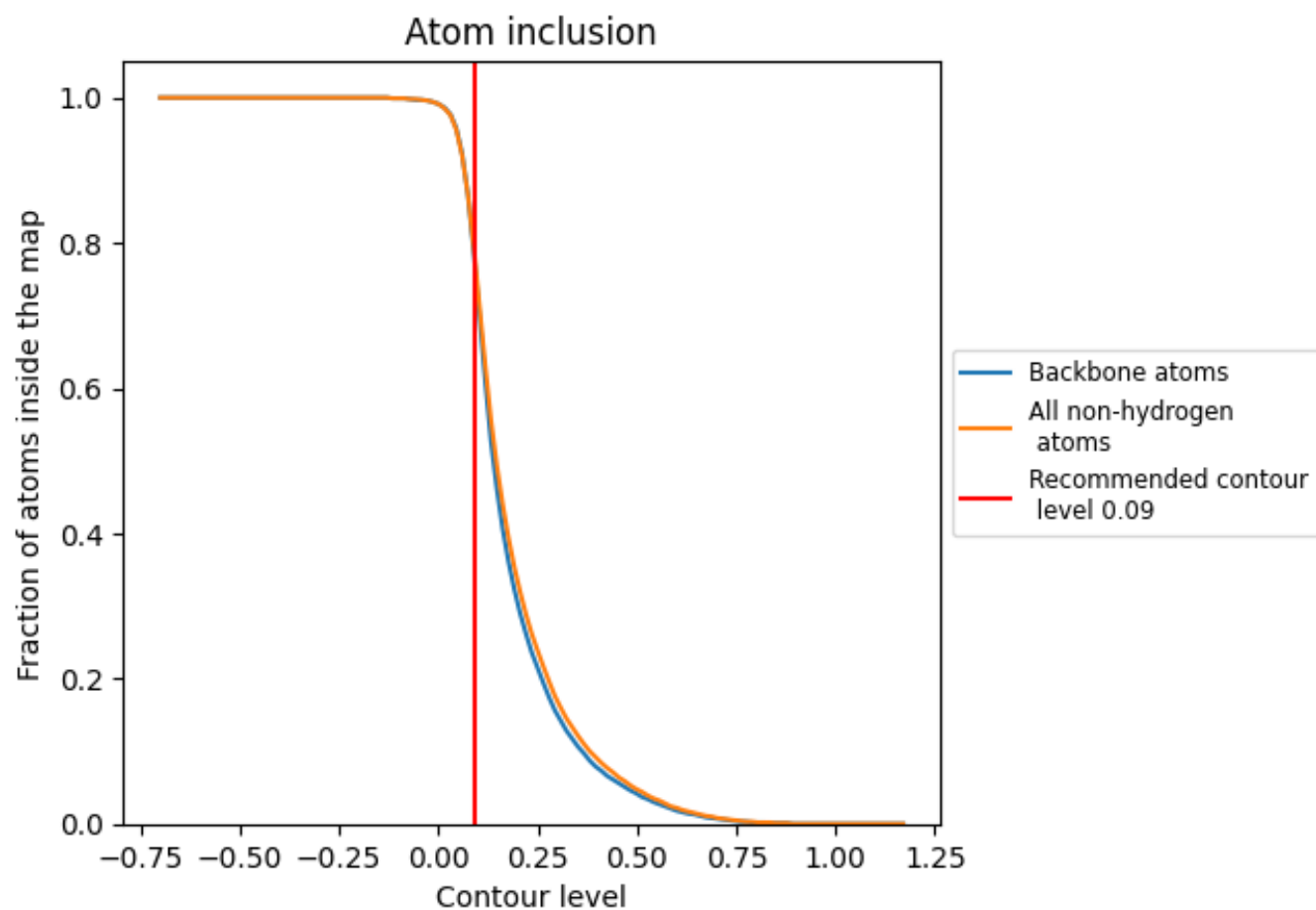
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 79% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.3840
A	0.7930	0.3840
B	0.7910	0.3840
C	0.7920	0.3830
D	0.7940	0.3840

