



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 12:11 AM UTC

PDB ID : 7TDI / pdb_00007tdi
EMDB ID : EMD-25830
Title : Rabbit RyR1 with AMP-PCP and high Ca²⁺ embedded in nanodisc in closed-inactivated conformation class 2 (Dataset-A)
Authors : Nayak, A.R.; Samso, M.
Deposited on : 2021-12-31
Resolution : 3.30 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:

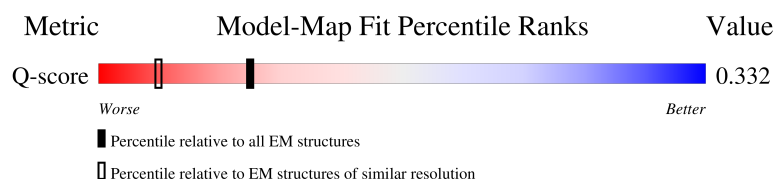
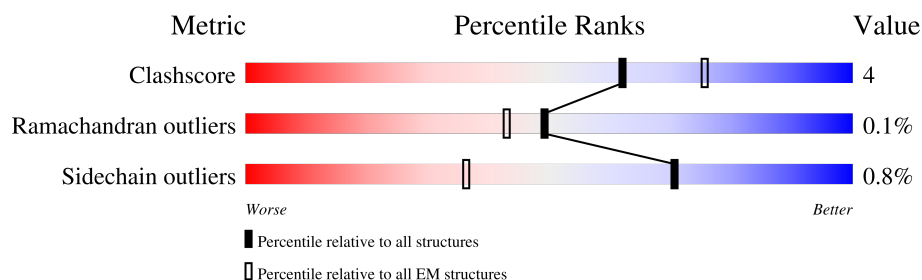
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 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	15087 (2.80 - 3.80)

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	
1	B	5037	
1	C	5037	
1	D	5037	

2 Entry composition [i](#)

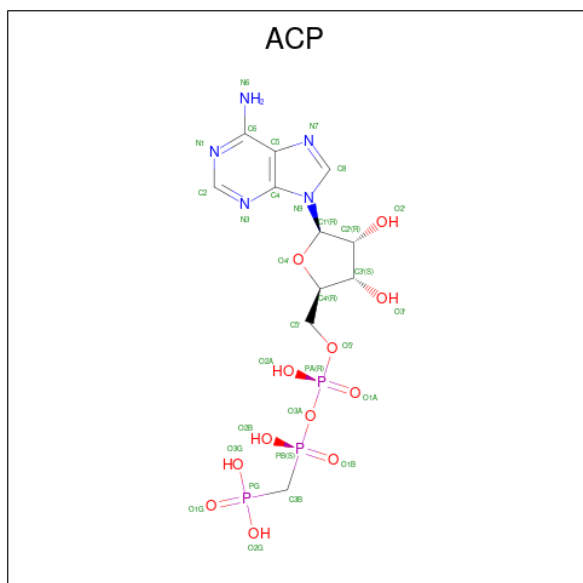
There are 4 unique types of molecules in this entry. The entry contains 117132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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,Ryanodine receptor 1,RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	4134	Total	C	N	O	S	0	0
			29249	18516	5181	5395	157		
1	C	4134	Total	C	N	O	S	0	0
			29249	18516	5181	5395	157		
1	D	4134	Total	C	N	O	S	0	0
			29249	18516	5181	5395	157		
1	A	4134	Total	C	N	O	S	0	0
			29249	18516	5181	5395	157		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

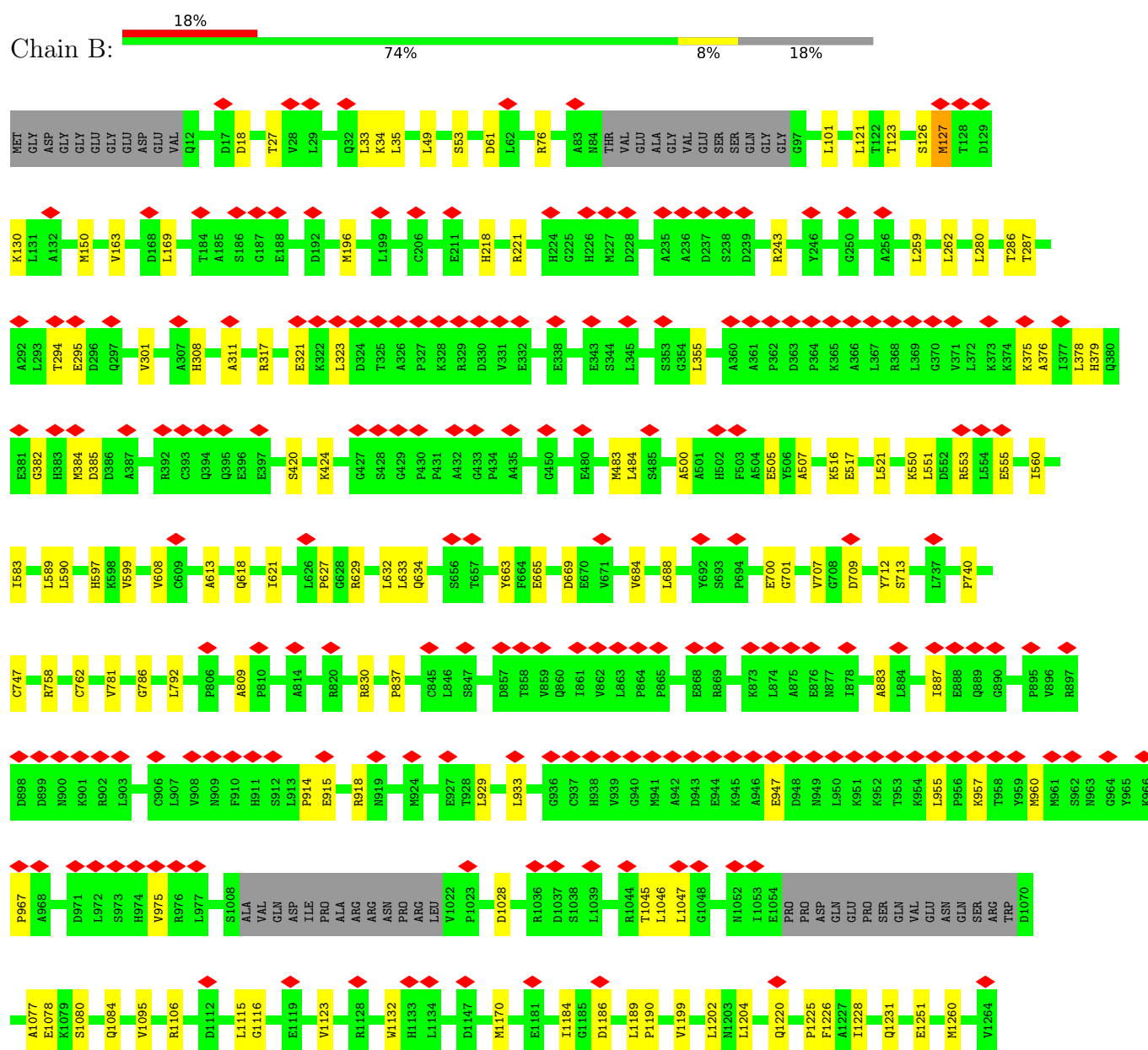
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total	Ca	0
			2	2	
4	C	2	Total	Ca	0
			2	2	
4	D	2	Total	Ca	0
			2	2	
4	A	2	Total	Ca	0
			2	2	

3 Residue-property plots

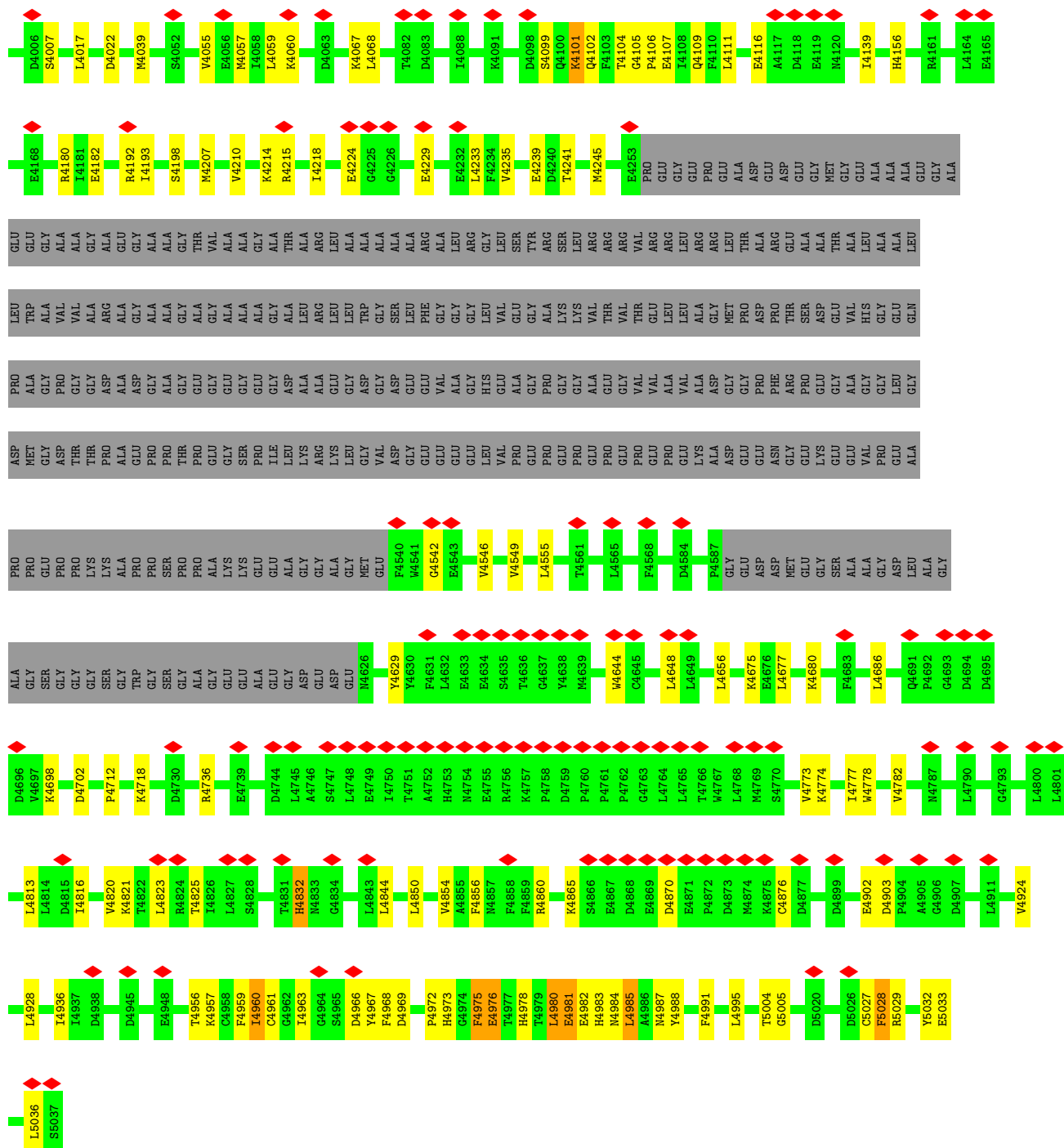
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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,Ryanodine receptor 1,RyR1

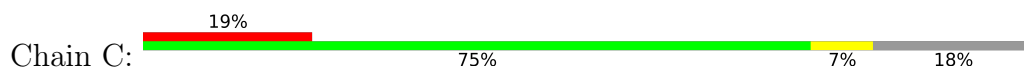


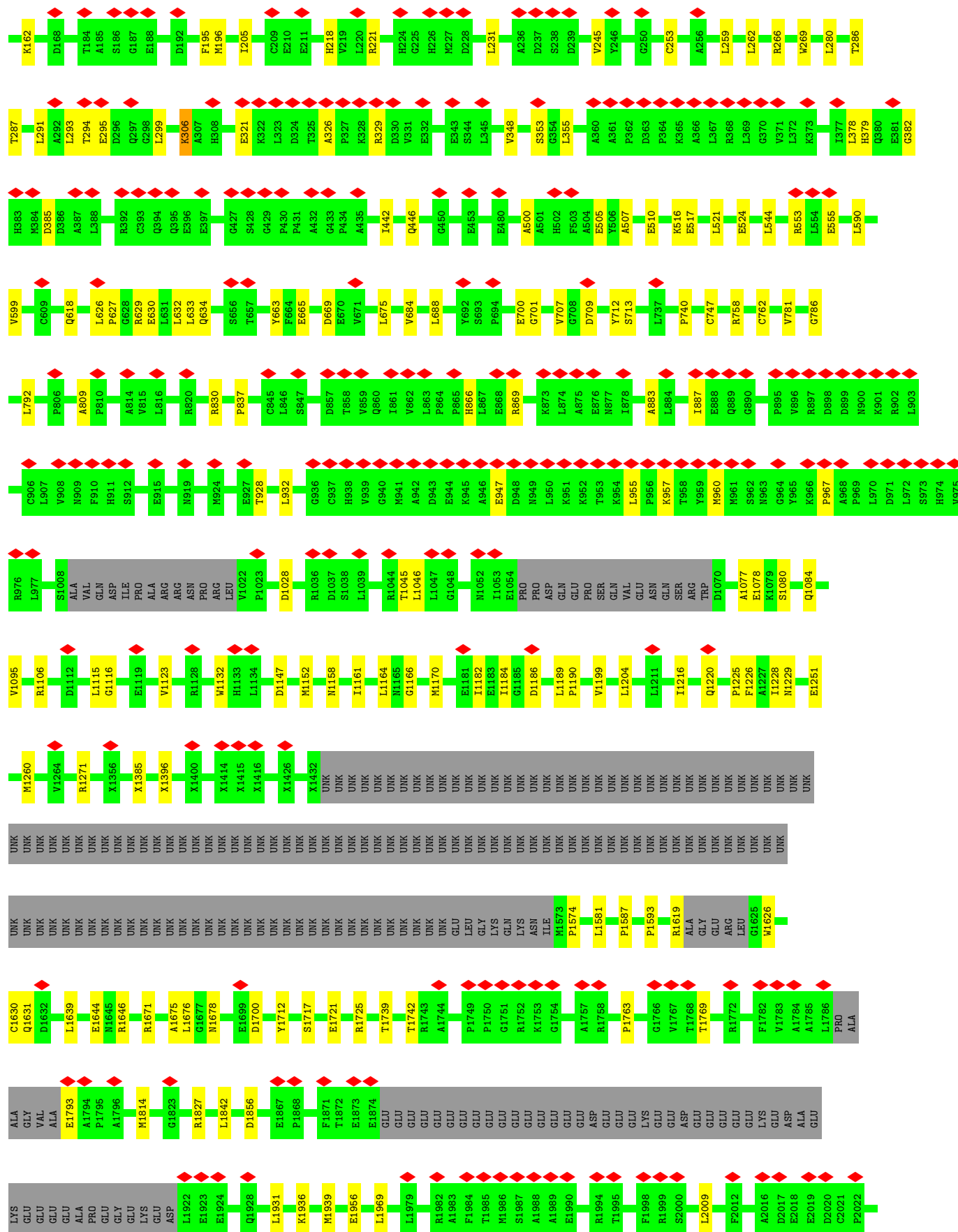


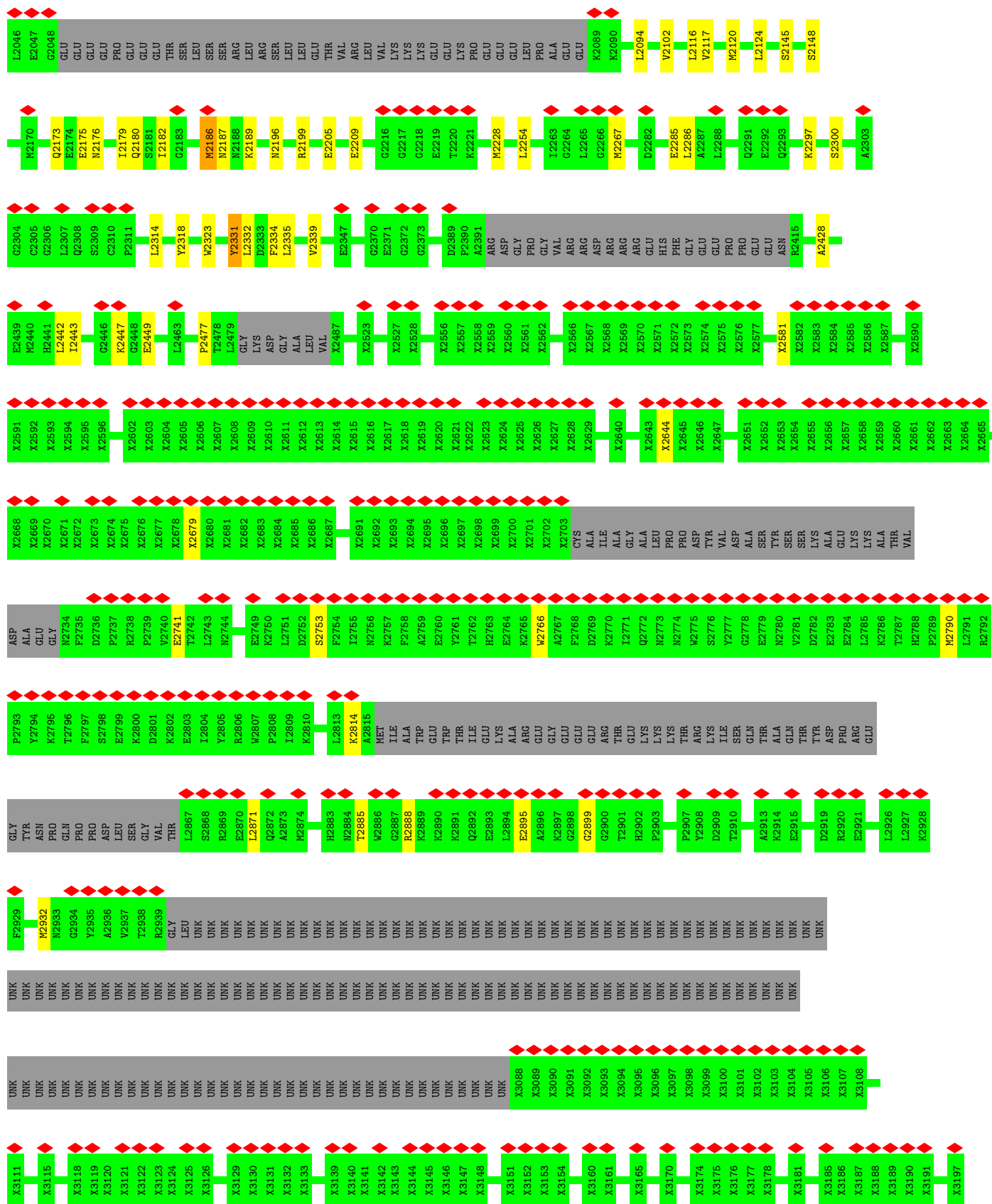




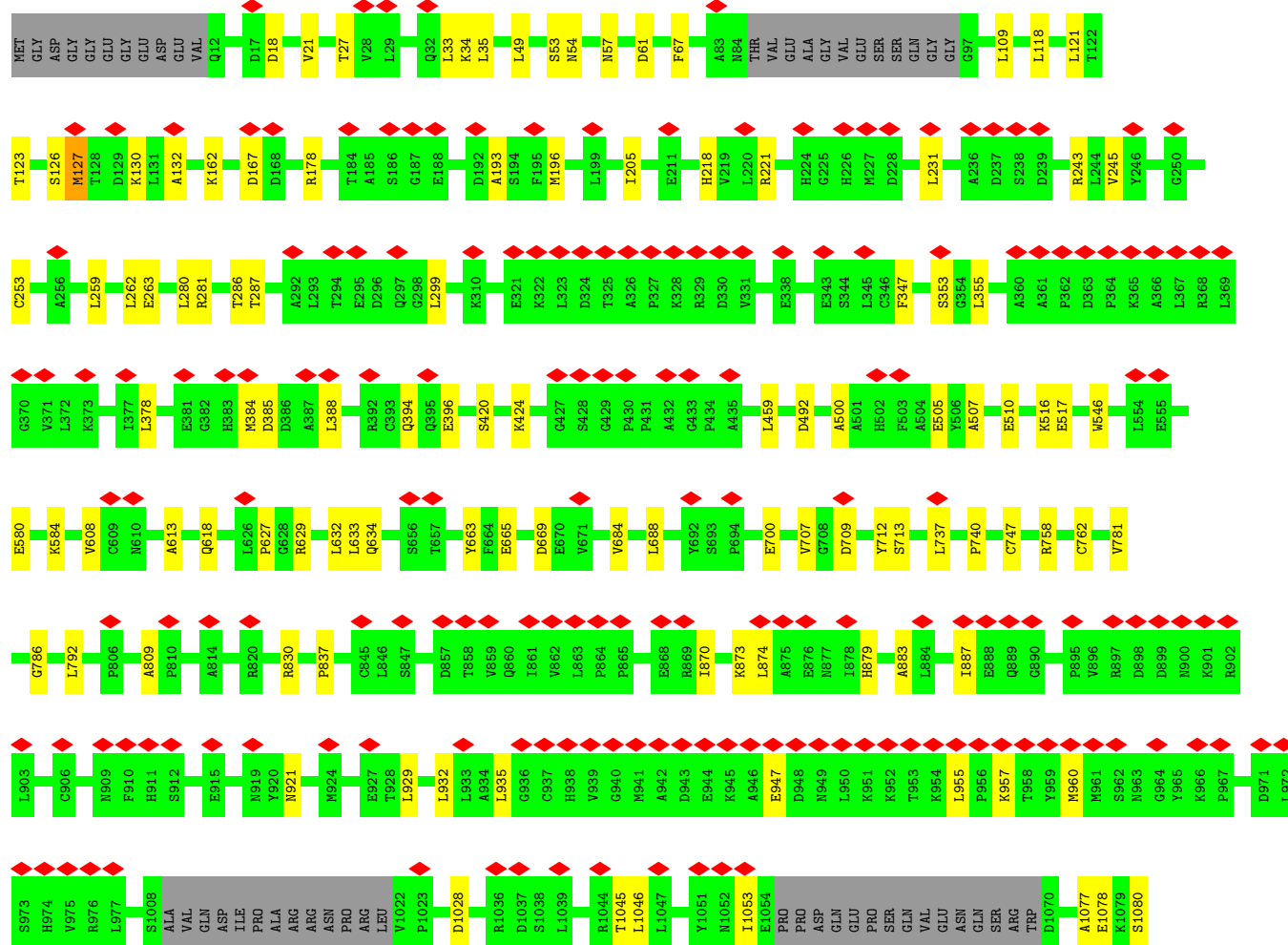
● Molecule 1: Ryanodine receptor 1, Ryanodine receptor 1, RyR1







PRO	GLU	ALA	TRP	GLU	R4192	M4064	E3861	H3734	SER	X3548	X3435	X3317	
PRO	GLY	GLY	ALA	GLY	I4193		D3862	L3735	LYS	X3549	X3436	X3318	
ASP	PRO	PRO	VAL	ALA	Y4194	K4067	E3863	E3736	GLN	X3550	X3437	X3319	
PRO	THR	GLY	VAL	ALA	L4068	L4068	T3864	E3737	ARG	X3551	X3438		
LYS	THR	GLY	ALA	GLY	I4197	D4079	V3865	G3738	ARG	X3552	X3439	X3330	
LYS	ALA	ASP	ARG	ALA	S4198		I3866	G3739	ALA	X3553	X3440		
PRO	GLU	ASP	ALA	GLU	M4207		I3866		VAL	X3556	X3441	X3335	
PRO	GLY	ASP	GLY	ALA	V4210	T4082	R3867	E3740	ASN	X3560	X3442	X3340	
PRO	ALA	ALA	ALA	ALA	D4083	D4083	R3868	GLY	ALA	X3561	X3443	X3341	
PRO	THR	GLY	GLY	THR	P4084	P4084	Q3869	GLY	PHE	X3562	X3444		
PRO	THR	GLY	ALA	THR	R4085	R4085	N3870	ALA	ARG	X3563		X3352	
ALA	VAL	GLY	GLY	VAL	S4089	S4089	G3871	GLU	MET	X3564	X3447	X3353	
ALA	ALA	ALA	ALA	ALA	K4090	K4090	E3872	GLU		X3565	X3448		
LYS	GLY	GLY	ALA	GLY	D4092	D4092	R3873	E3747		X3566	X3449	X3357	
LYS	ALA	ASP	ALA	THR	V4222	V4222	A3876	E3748	A3559	X3567	X3456	X3356	
GLY	ALA	ALA	LEU	ALA	M4223	M4223	D3877	V3749	A3560	X3568	X3457	X3357	
GLY	ALA	ALA	ARG	ARG	E4224	E4224	F3880	E3750	A3561	X3569	X3458	X3358	
ALA	GLY	GLY	LEU	LEU	G4225	G4225	D3877	V3751	A3562	X3570	X3459	X3360	
GLY	LEU	GLY	LEU	ALA	G4226	G4226	F3880	E3755	A3563	X3570		X3361	
GLY	ALA	ASP	TRP	ALA	D4098	D4098	Q3889	E3755	A3564	X3570			
GLU	ALA	ASP	GLY	ALA	S4099	S4099	E3889	E3759	A3565	X3570			
F4540	ASP	ASP	SER	ALA	Q4100	Q4100	N3896	E3759	A3566	X3580			
W4541	GLY	GLY	LEU	ALA	K4101	K4101	E3896	S3768	A3567	X3580			
E4542	GLU	GLU	PHE	ARG	F4103	F4103	N3897	H3771	A3568	X3583	X3470	X3373	
E4543	GLU	VAL	GLY	GLY	T4104	T4104	D3998	T3772	A3569	X3584	X3471		
	GLU	ALA	GLY	LEU	E4107	E4107	I3915	R3773	A3570	X3585		X3378	
W4546	GLY	ALA	GLY	ARG	D4239	D4239	I3916	G3774	A3571	X3586	X3476	X3379	
Q4547	LEU	HIS	LEU	GLY	D4240	D4240	I3917	A3775	A3572	X3587		X3380	
R4548	VAL	GLU	VAL	LEU	L4111	L4111	C3918	A3776	A3573	X3587			
W4549	ALA	ALA	GLY	SER	M4245	M4245	E3918	A3777	A3574	X3588	X3484		
	GLY	PRO	GLY	TYR	E4116	E4116	D3921	K3778	A3575	X3588		X3386	
L4555	PRO	PRO	LYS	ALA	A4117	A4117	E3921	E3779	A3576	X3589	X3488		
	GLY	GLY	LYS	SER	D4118	D4118	I3915	T3772	A3577	X3590	X3488	X3396	
M4558	GLY	ALA	VAL	ARG	E4119	E4119	I3916	R3773	A3578	X3591	X3492	X3397	
	PRO	GLU	THR	ARG	N4120	N4120	C3918	A3776	A3579	X3591	X3495	X3398	
T4561	PRO	GLU	VAL	ARG	S4252	S4252	E3918	G3788	A3580	X3592	X3501	X3399	
	GLU	VAL	THR	VAL	E4253	E4253	I3969	E3788	A3581	X3593	X3502	X3400	
L4565	PRO	VAL	GLY	VAL	PRO	PRO	E3969	Q3781	A3582	X3597	X3501	X3401	
	ALA	ALA	ARG	ARG	T4139	T4139	L3980	E3788	A3583	X3598	X3506	X3402	
	ALA	ALA	LEU	ARG	GLY	GLY	E3969	Q3781	A3584	X3599	X3506	X3407	
D4584	GLY	ALA	LEU	LEU	GLU	GLU	M3999	Q3814	A3585	X3600	X3506	X3408	
E4587	ASP	ASP	ALA	ALA	GLU	GLU	D4006	D3822	A3586	X3603	X3506		
GLY	ASP	ASP	GLY	ASP	ASP	ASP	S4007	K3823	A3587	X3604	X3506	X3407	
GLY	GLU	GLU	GLY	GLY	ASP	ASP	L4013	A3834	A3588	X3605	X3506	X3411	
ASP	GLU	GLU	GLY	GLY	GLU	GLU	L4017	T3838	A3589	X3606	X3506	X3412	
ASP	GLY	GLY	GLY	GLY	GLY	GLY	L4017	T3838	A3590	X3607	X3506	X3413	
GLY	GLY	GLY	GLY	GLY	GLY	GLY	V4024	D3843	A3591	X3609	X3506		
SER	GLY	ALA	VAL	ALA	GLY	GLY	L4027	D3843	A3592	X3610	X3506	X3418	
ALA	VAL	GLY	HIS	LEU	GLY	GLY	L4027	D3843	A3593	X3611	X3506		
ALA	GLY	GLY	GLY	ALA	ALA	ALA	L4027	D3843	A3594	X3612	X3506	X3422	
ALA	LEU	LEU	GLY	ALA	ALA	ALA	M4039	E3854	A3595	X3613	X3506	X3423	
GLY	GLY	GLY	GLY	GLY	ALA	ALA	M4039	E3854	A3596	X3614	X3506	X3424	
ASP	GLY	GLY	GLY	GLY	ALA	ALA	E4056	G3855	A3597	X3615	X3506	X3425	
LEU	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3598	X3616	X3506		
ALA	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3599	X3617	X3506	X3428	
GLY	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3600	X3618	X3506	X3429	
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3601	X3619	X3506	X3431	
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3602	X3620	X3506	X3432	
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3603	X3621	X3506	X3433	
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3604	X3622	X3506	X3434	
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3605	X3623	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3606	X3624	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3607	X3625	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3608	X3626	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3609	X3627	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3610	X3628	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3611	X3629	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3612	X3630	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3613	X3631	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3614	X3632	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3615	X3633	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3616	X3634	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3617	X3635	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3618	X3636	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3619	X3637	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3620	X3638	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3621	X3639	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3622	X3640	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3623	X3641	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3624	X3642	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3625	X3643	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3626	X3644	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3627	X3645	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3628	X3646	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3629	X3647	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3630	X3648	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3631	X3649	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3632	X3650	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3633	X3651	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3634	X3652	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3635	X3653	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3636	X3654	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3637	X3655	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3638	X3656	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3639	X3657	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3640	X3658	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3641	X3659	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3642	X3660	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3643	X3661	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3644	X3662	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3645	X3663	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3646	X3664	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3647	X3665	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3648	X3666	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3649	X3667	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3650	X3668	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3651	X3669	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3652	X3670	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3653	X3671	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3654	X3672	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3655	X3673	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3656	X3674	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3657	X3675	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3658	X3676	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3659	X3677	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3660	X3678	X3506		
	GLY	GLY	GLY	GLY	GLY	GLY	E4056	L3856	A3661	X3679	X3506		
	GLY	GLY	GLY	GLY	GLY								















4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	159444	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	477.36002, 477.36002, 477.36002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.105, 1.105, 1.105	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, ACP, 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	0.19	0/25301	0.47	9/34345 (0.0%)
1	B	0.20	0/25301	0.47	6/34345 (0.0%)
1	C	0.19	0/25301	0.46	8/34345 (0.0%)
1	D	0.22	2/25301 (0.0%)	0.48	10/34345 (0.0%)
All	All	0.20	2/101204 (0.0%)	0.47	33/137380 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4709	PRO	CG-CD	-15.66	0.97	1.50
1	D	4709	PRO	N-CD	7.58	1.58	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4709	PRO	N-CD-CG	-15.58	79.83	103.20
1	D	4709	PRO	CA-N-CD	-10.97	96.65	112.00
1	A	2462	PRO	CA-N-CD	-10.36	97.50	112.00
1	B	967	PRO	CA-N-CD	-10.14	97.80	112.00
1	C	967	PRO	CA-N-CD	-9.85	98.20	112.00

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	A	29249	0	24792	248	0
1	B	29249	0	24790	236	0
1	C	29249	0	24795	224	0
1	D	29249	0	24791	230	0
2	A	31	0	13	0	0
2	B	31	0	13	4	0
2	C	31	0	13	0	0
2	D	31	0	13	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	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	117132	0	99220	923	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 4.

The worst 5 of 923 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:A:4961:CYS:SG	1:A:4963:ILE:HG22	1.54	1.48
1:A:4961:CYS:SG	1:A:4963:ILE:CG2	2.16	1.33
1:D:4980:LEU:HA	1:D:4984:ASN:HD21	1.34	0.92
1:A:5029:ARG:O	1:A:5033:GLU:HB3	1.73	0.88
1:B:4960:ILE:HG13	1:B:4983:HIS:HB3	1.60	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3203/5037 (64%)	3060 (96%)	140 (4%)	3 (0%)	48	75
1	B	3203/5037 (64%)	3055 (95%)	143 (4%)	5 (0%)	43	71
1	C	3203/5037 (64%)	3056 (95%)	145 (4%)	2 (0%)	48	75
1	D	3203/5037 (64%)	3059 (96%)	141 (4%)	3 (0%)	48	75
All	All	12812/20148 (64%)	12230 (96%)	569 (4%)	13 (0%)	49	75

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3915	ILE
1	D	3915	ILE
1	B	3788	GLY
1	B	4198	SER
1	C	3788	GLY

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	2513/3264 (77%)	2495 (99%)	18 (1%)	76	80
1	B	2513/3264 (77%)	2483 (99%)	30 (1%)	63	75
1	C	2513/3264 (77%)	2500 (100%)	13 (0%)	81	83
1	D	2513/3264 (77%)	2489 (99%)	24 (1%)	68	76
All	All	10052/13056 (77%)	9967 (99%)	85 (1%)	70	79

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4726	ASP
1	A	3826	VAL
1	D	4731	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4981	GLU
1	A	4101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4997	ASN
1	A	2734	ASN
1	D	1775	HIS
1	A	2260	ASN
1	A	4209	GLN

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, 12 are monoatomic - leaving 4 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	$\# Z > 2$
2	ACP	C	5101	-	31,33,33	3.18	12 (38%)	47,52,52	1.96	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACP	A	5101	-	31,33,33	3.18	12 (38%)	47,52,52	1.96	11 (23%)
2	ACP	D	5101	-	31,33,33	3.18	12 (38%)	47,52,52	1.96	11 (23%)
2	ACP	B	5101	-	31,33,33	3.18	11 (35%)	47,52,52	1.96	11 (23%)

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
2	ACP	C	5101	-	-	6/19/38/38	0/3/3/3
2	ACP	A	5101	-	-	6/19/38/38	0/3/3/3
2	ACP	D	5101	-	-	6/19/38/38	0/3/3/3
2	ACP	B	5101	-	-	6/19/38/38	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5101	ACP	O4'-C1'	8.67	1.62	1.42
2	D	5101	ACP	O4'-C1'	8.66	1.62	1.42
2	C	5101	ACP	O4'-C1'	8.66	1.62	1.42
2	A	5101	ACP	O4'-C1'	8.66	1.62	1.42
2	D	5101	ACP	C2'-C1'	-7.22	1.30	1.53

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5101	ACP	N3-C2-N1	-5.74	119.89	128.58
2	A	5101	ACP	N3-C2-N1	-5.73	119.90	128.58
2	C	5101	ACP	N3-C2-N1	-5.73	119.91	128.58
2	B	5101	ACP	N3-C2-N1	-5.71	119.94	128.58
2	C	5101	ACP	C5-C4-N3	-4.92	119.94	126.72

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5101	ACP	C5'-O5'-PA-O2A
2	B	5101	ACP	C5'-O5'-PA-O3A
2	B	5101	ACP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

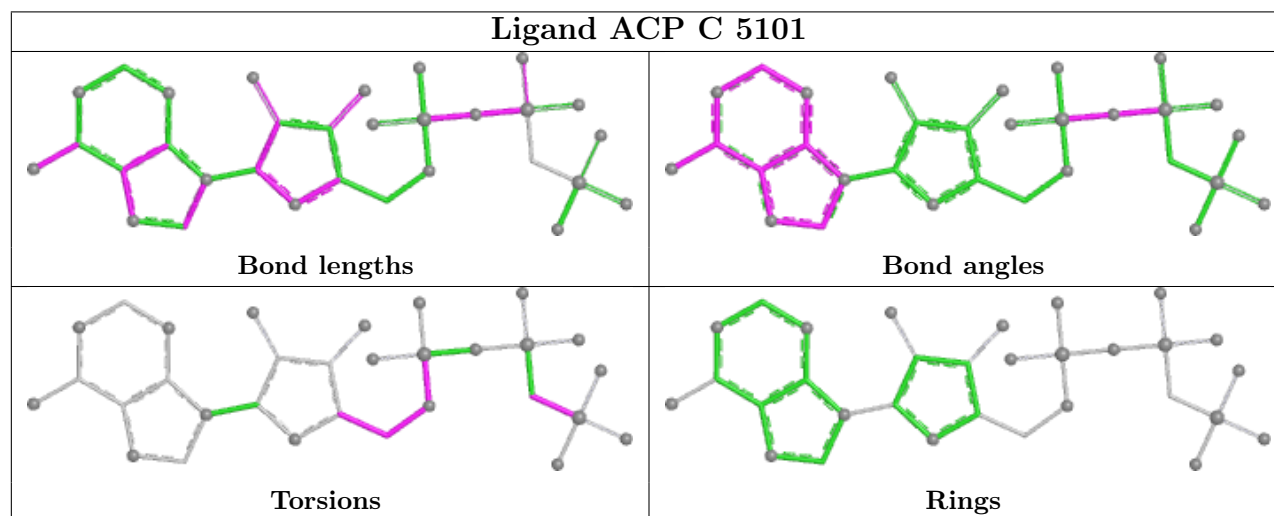
Mol	Chain	Res	Type	Atoms
2	C	5101	ACP	C5'-O5'-PA-O2A
2	C	5101	ACP	C5'-O5'-PA-O3A

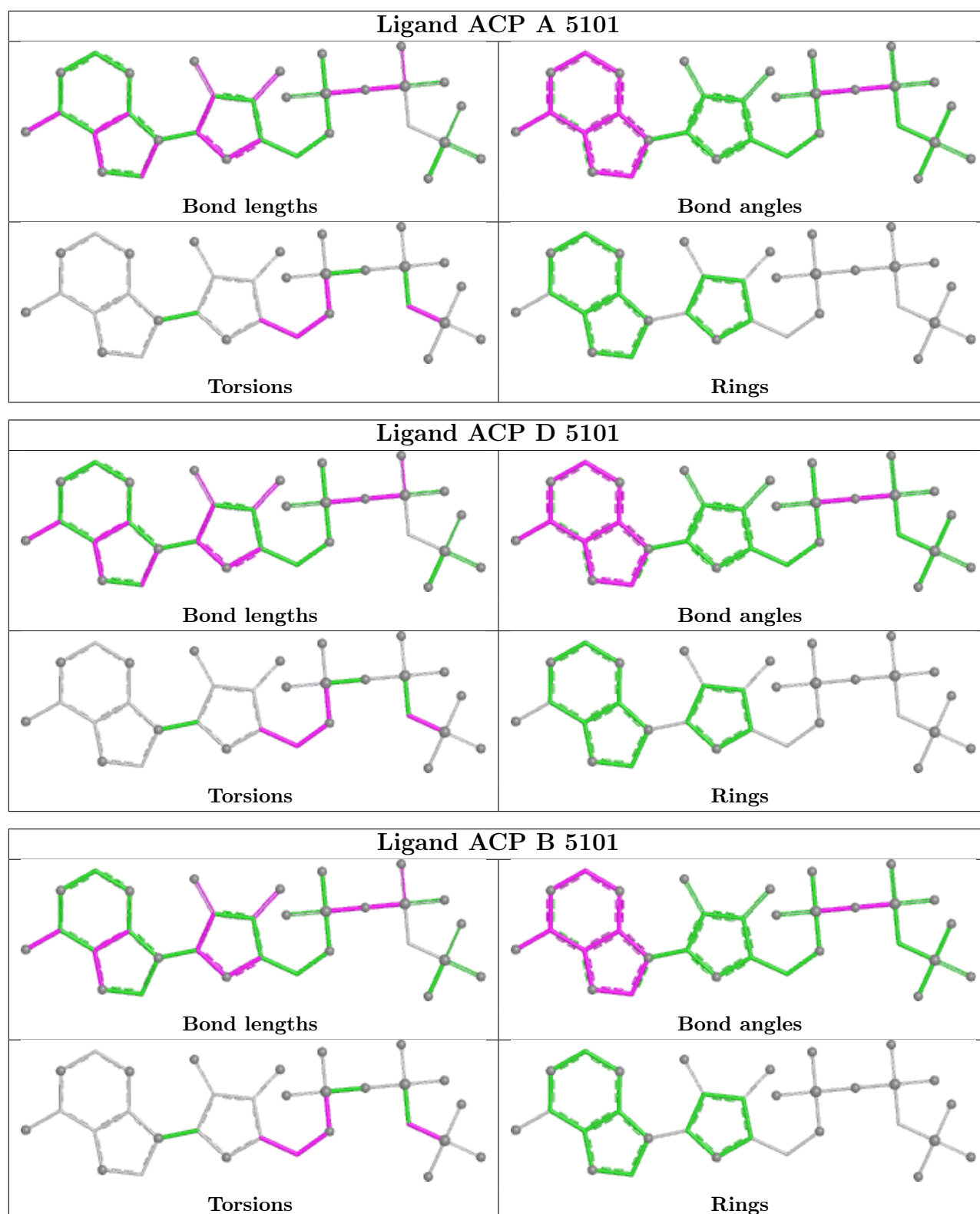
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5101	ACP	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	7
1	B	7
1	C	7
1	A	7

The worst 5 of 28 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	3288:UNK	C	3289:UNK	N	13.33
1	B	3288:UNK	C	3289:UNK	N	13.32
1	C	3288:UNK	C	3289:UNK	N	13.32
1	A	3288:UNK	C	3289:UNK	N	13.25
1	A	3510:UNK	C	3511:UNK	N	13.22

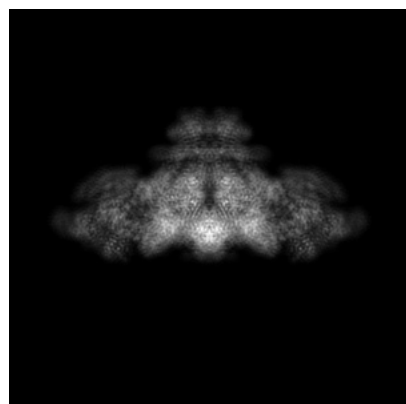
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25830. These allow visual inspection of the internal detail of the map and identification of artifacts.

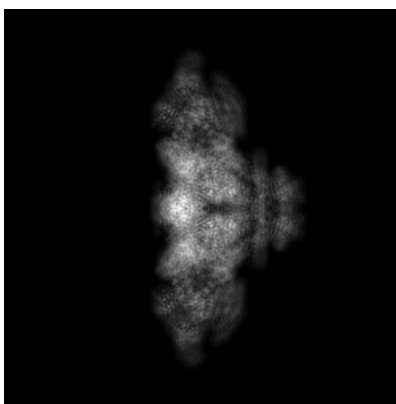
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

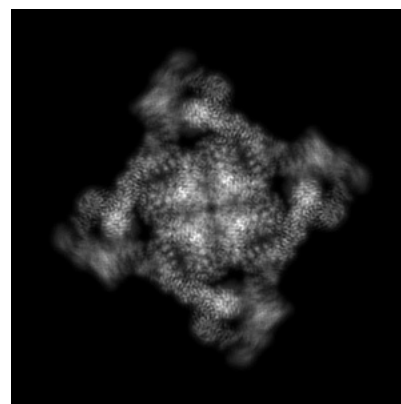
6.1.1 Primary map



X

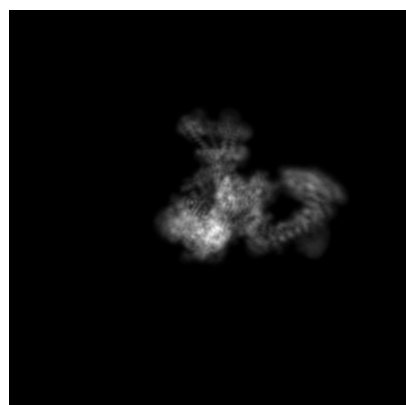


Y

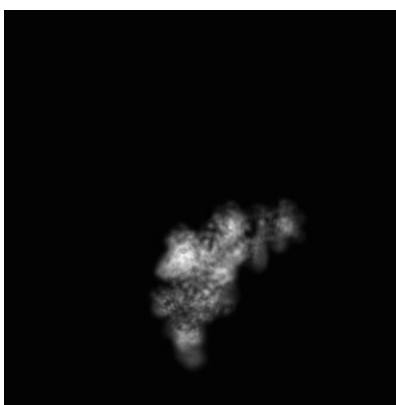


Z

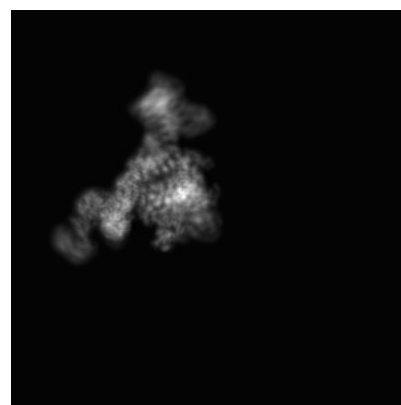
6.1.2 Raw map



X



Y



Z

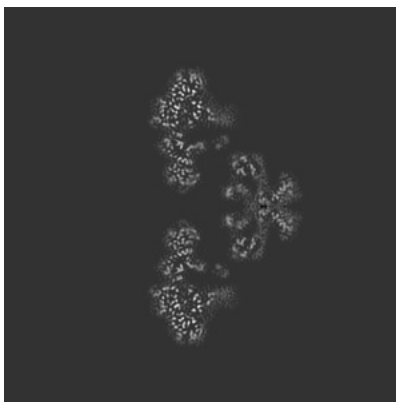
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

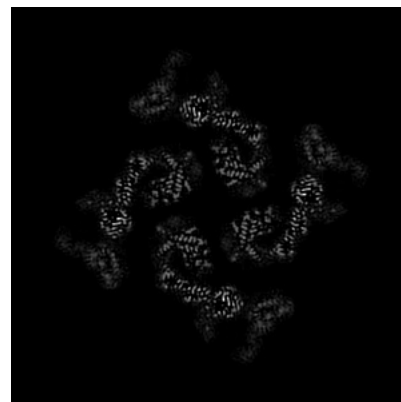
6.2.1 Primary map



X Index: 216



Y Index: 216

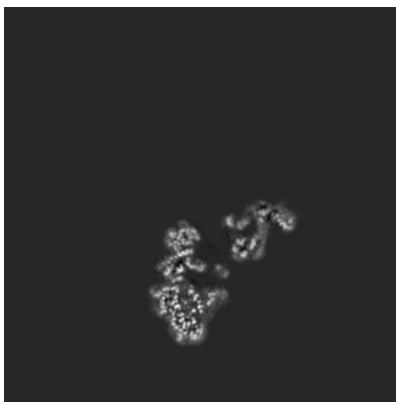


Z Index: 216

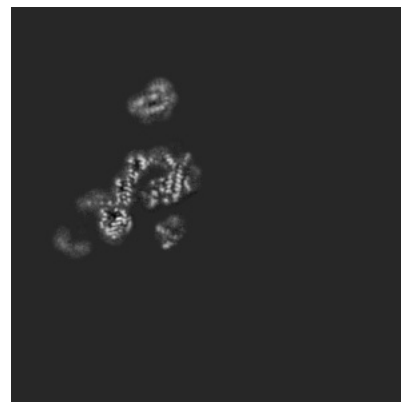
6.2.2 Raw map



X Index: 216



Y Index: 216

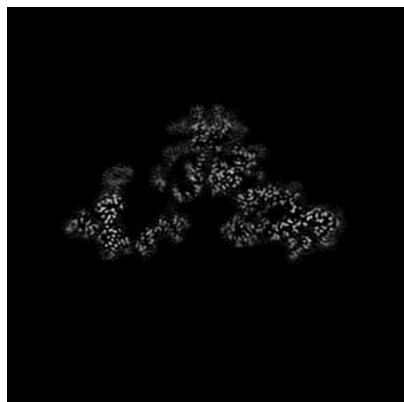


Z Index: 216

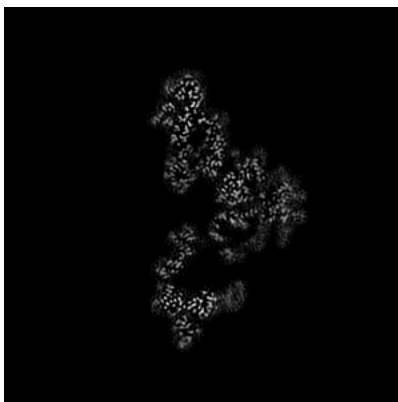
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

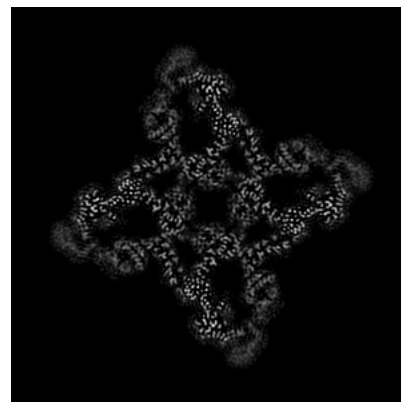
6.3.1 Primary map



X Index: 226



Y Index: 206

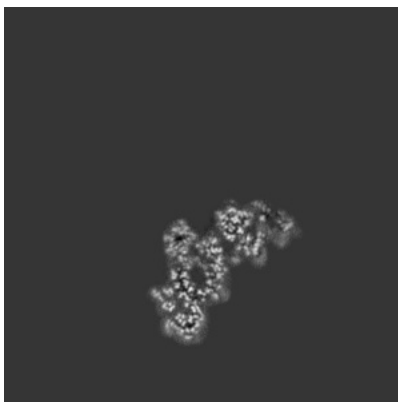


Z Index: 198

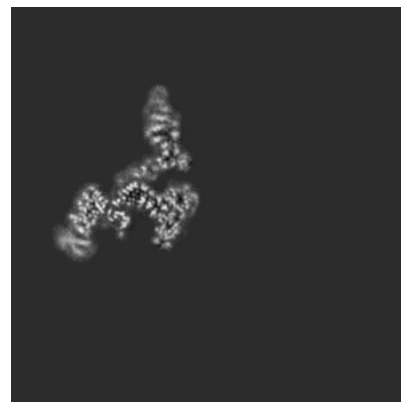
6.3.2 Raw map



X Index: 167



Y Index: 226

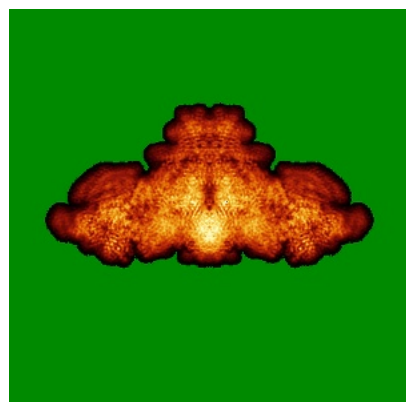


Z Index: 192

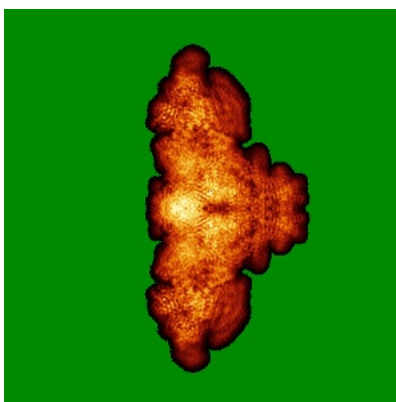
The images above show the largest variance slices of the map in three orthogonal directions.

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

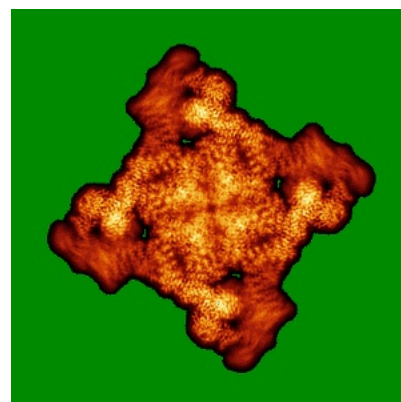
6.4.1 Primary map



X

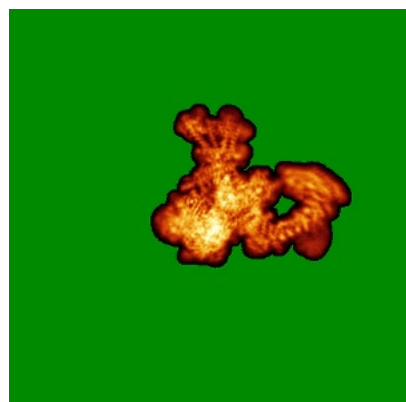


Y

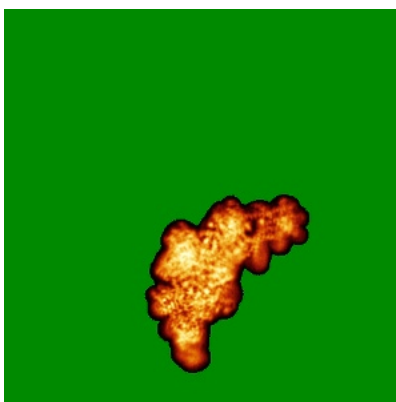


Z

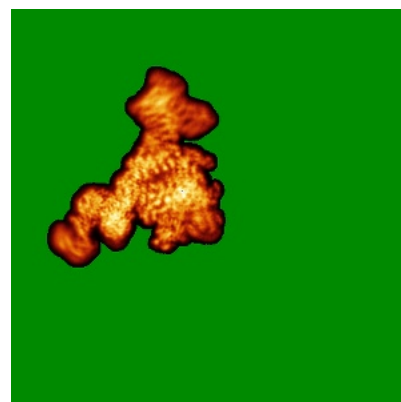
6.4.2 Raw map



X



Y

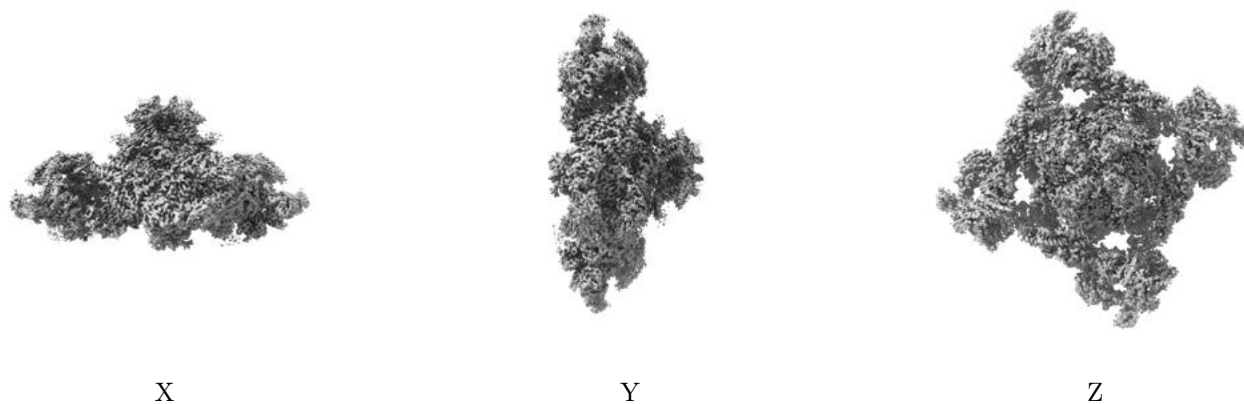


Z

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.

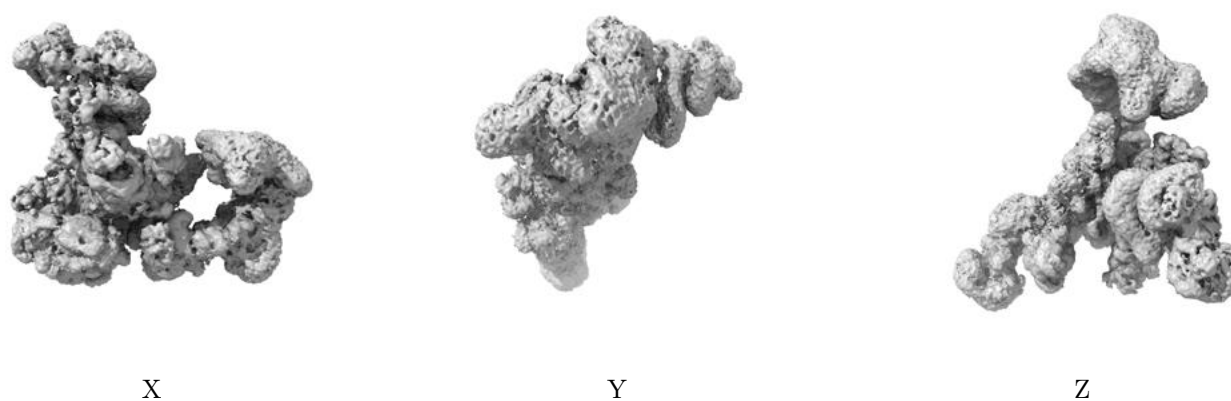
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

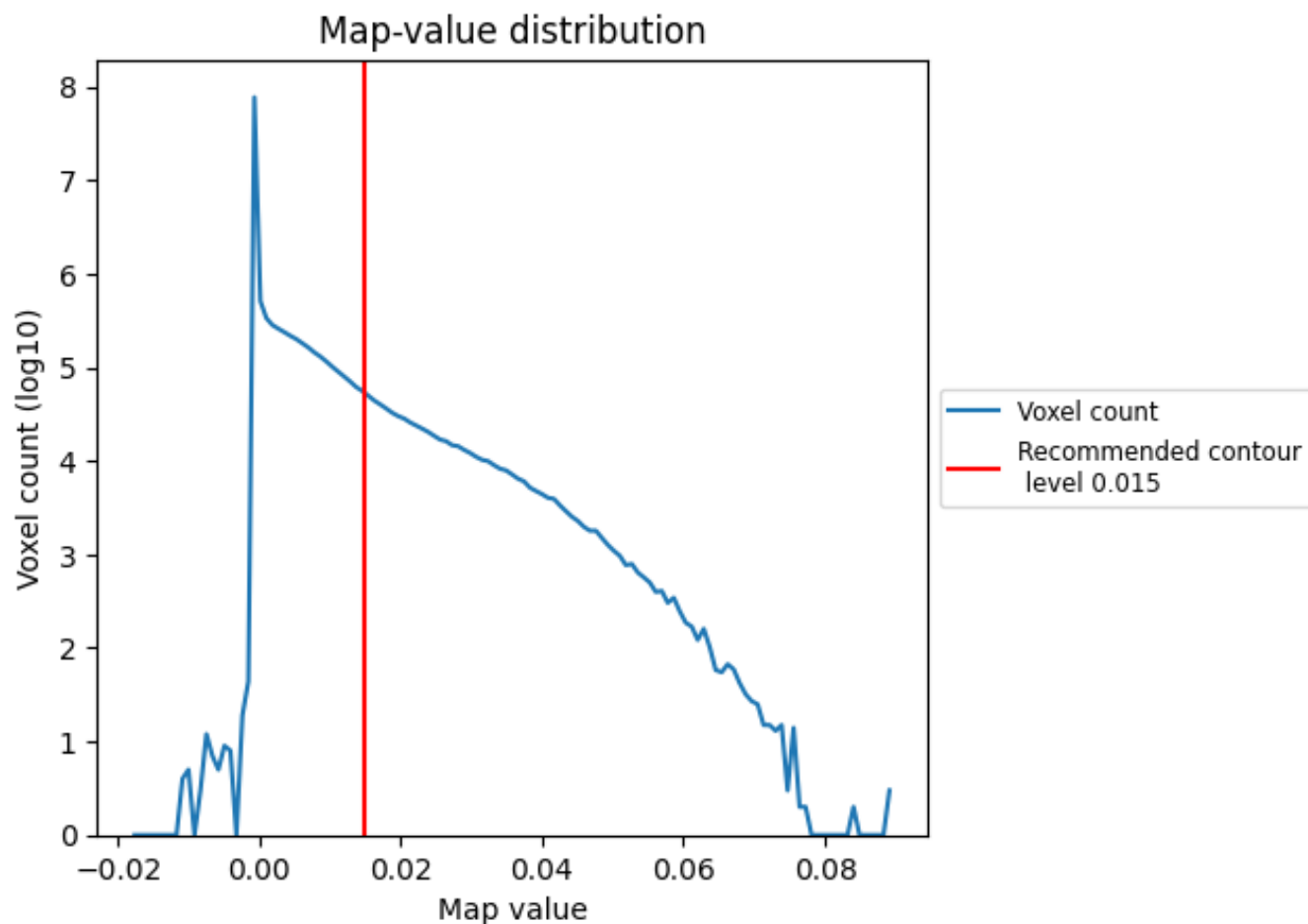
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

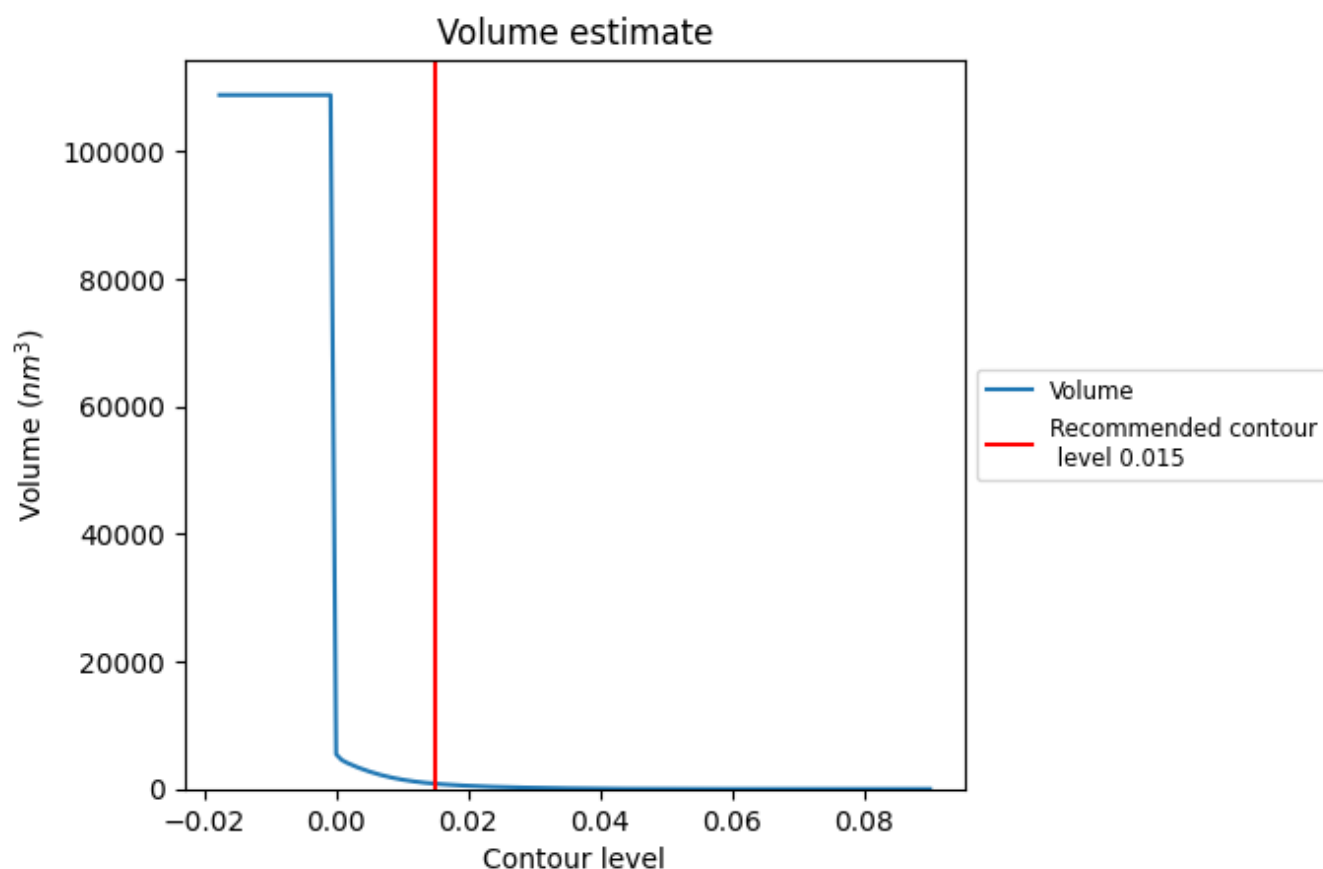
This section contains the results of statistical analysis of the map.

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.

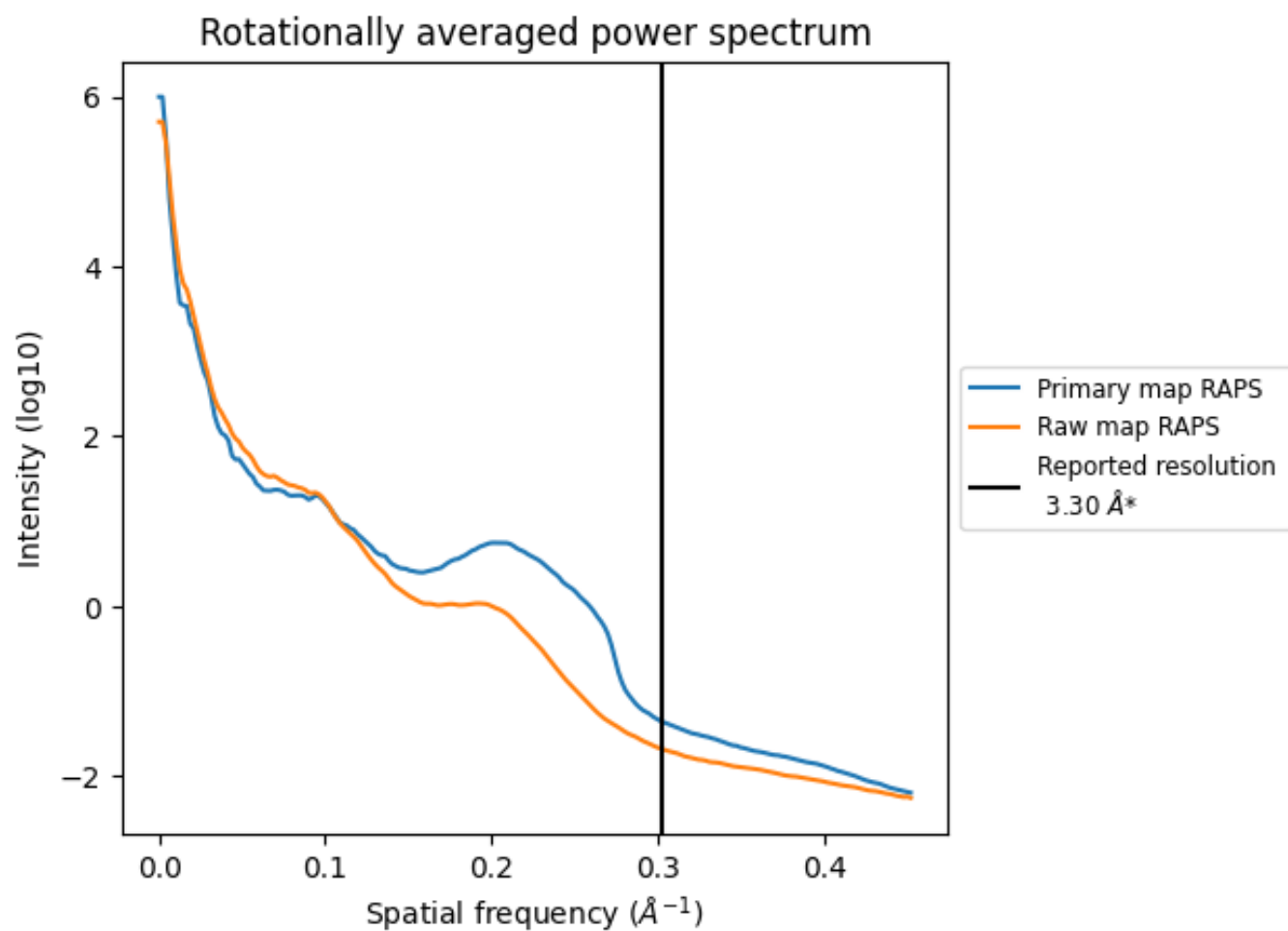
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 826 nm^3 ; this corresponds to an approximate mass of 746 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 ⓘ

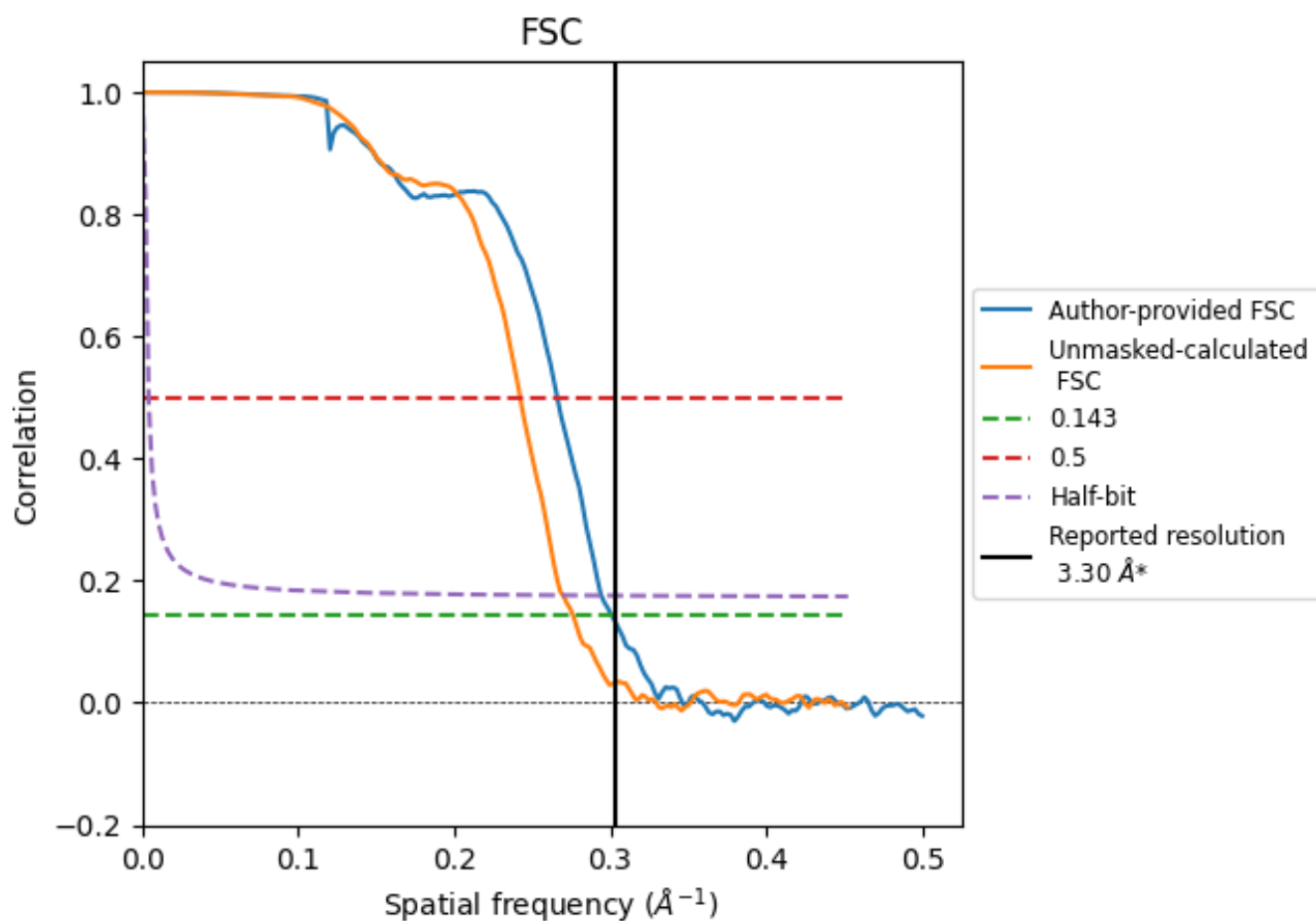


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

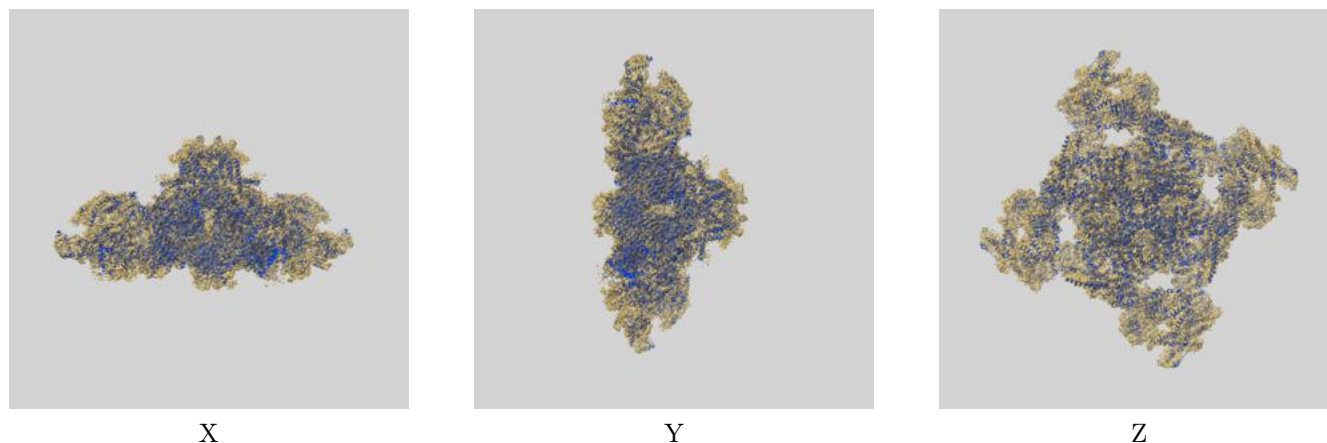
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.76	3.40
Unmasked-calculated*	3.62	4.13	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

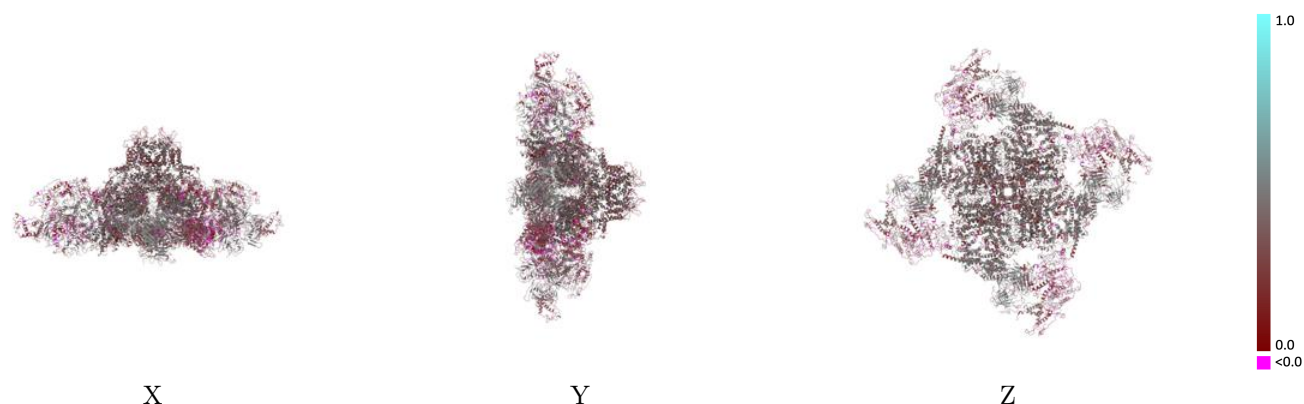
This section contains information regarding the fit between EMDB map EMD-25830 and PDB model 7TDI. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



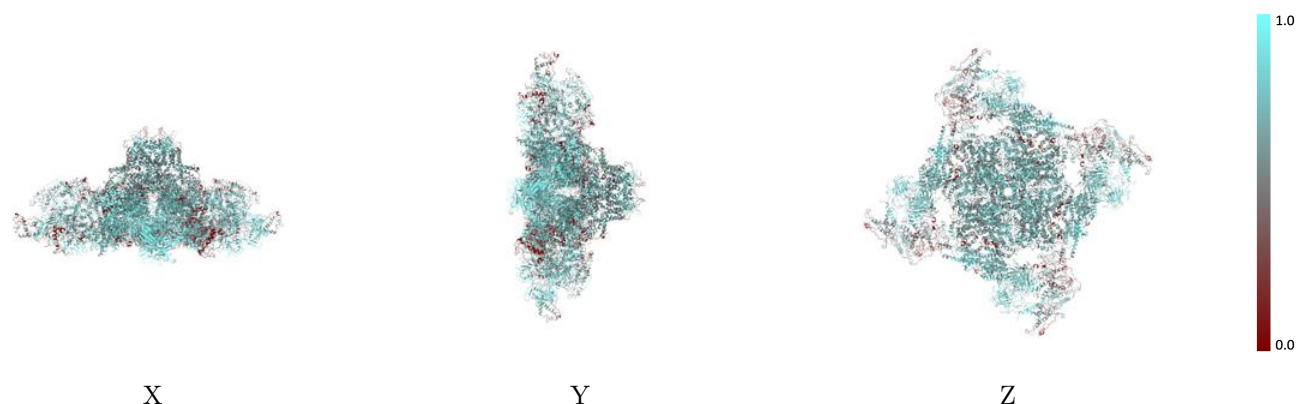
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



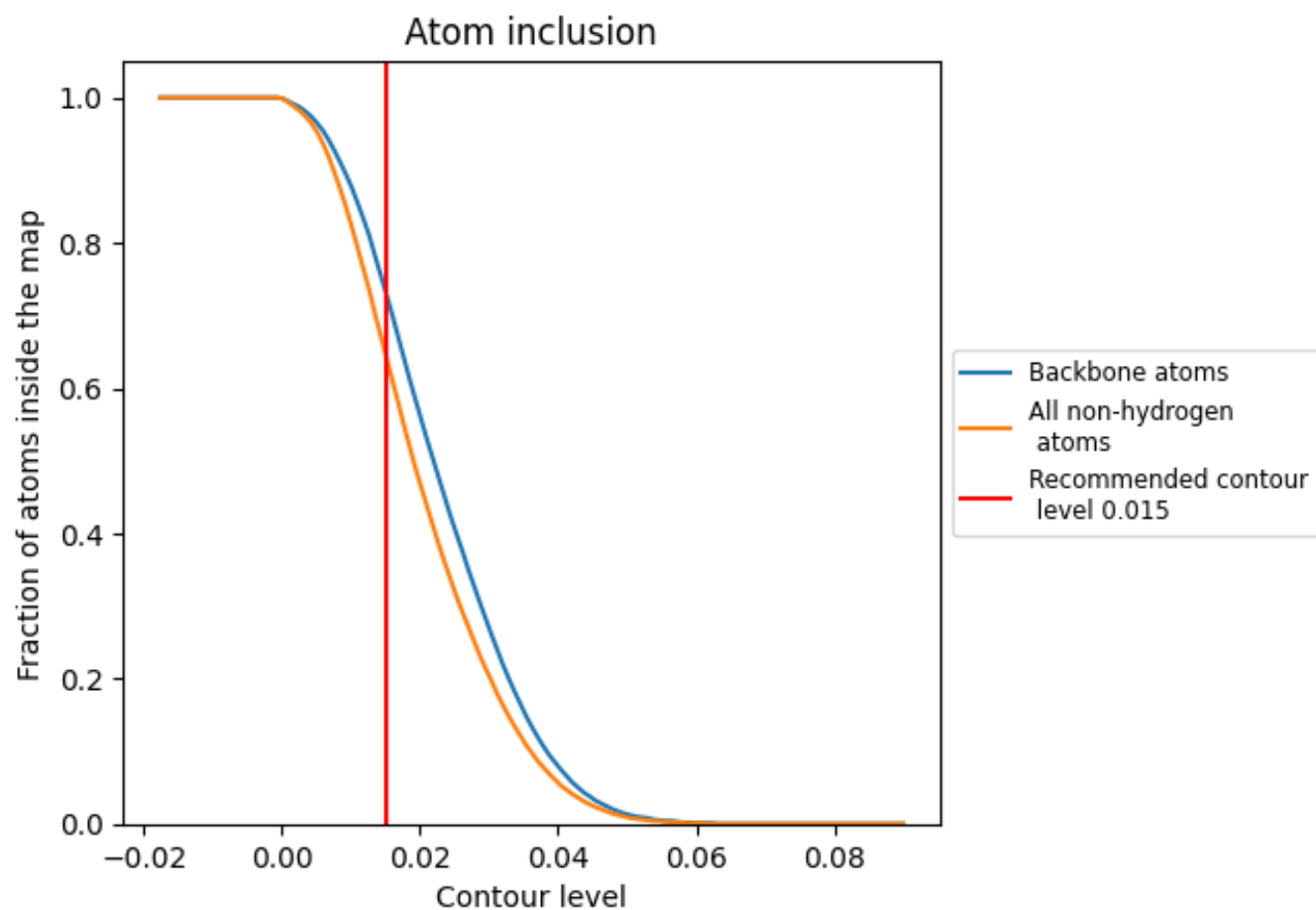
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 65% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.3320
A	0.6390	0.3250
B	0.6490	0.3350
C	0.6510	0.3350
D	0.6520	0.3350

