



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:10 PM UTC

PDB ID : 8XLF / pdb_00008xlf
EMDB ID : EMD-38447
Title : Structure of chimeric RyR
Authors : Lin, L.; Wang, C.; Wang, W.; Jiang, H.; Yuchi, Z.
Deposited on : 2023-12-25
Resolution : 3.62 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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

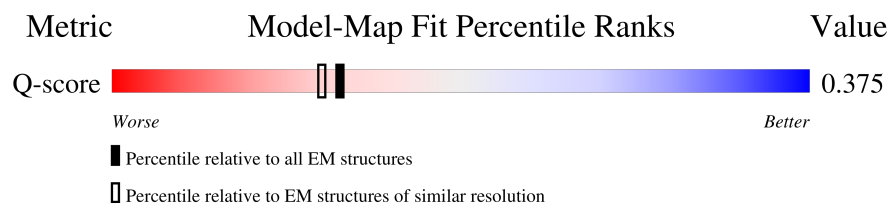
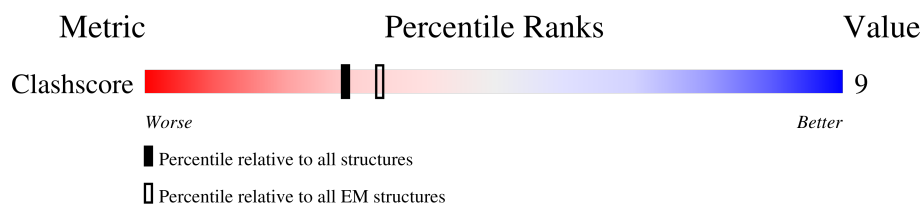
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

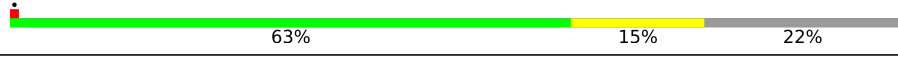
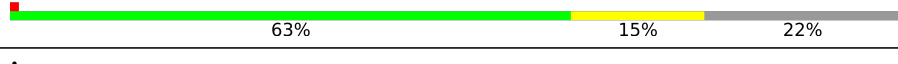
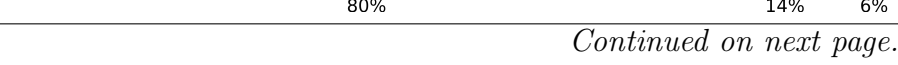
The reported resolution of this entry is 3.62 Å.

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	-
Q-score	-	25397	11773 (3.12 - 4.12)

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	I	148	
2	J	148	

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Mol	Chain	Length	Quality of chain
2	K	148	
2	L	148	
3	E	107	
3	F	107	
3	G	107	
3	H	107	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CFF	A	5104	-	X	-	-
7	CFF	B	5104	-	X	-	-
7	CFF	C	5104	-	X	-	-
7	CFF	D	5104	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 118944 atoms, of which 88 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	3916	Total	C	N	O	S	0	0
			27821	17738	4950	4957	176		
1	B	3916	Total	C	N	O	S	0	0
			27821	17738	4950	4957	176		
1	C	3916	Total	C	N	O	S	0	0
			27821	17738	4950	4957	176		
1	D	3916	Total	C	N	O	S	0	0
			27821	17738	4950	4957	176		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- 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	I	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	K	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
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
J	32	ALA	GLU	engineered mutation	UNP P0DP23
J	68	ALA	GLU	engineered mutation	UNP P0DP23
J	105	ALA	GLU	engineered mutation	UNP P0DP23
J	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

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

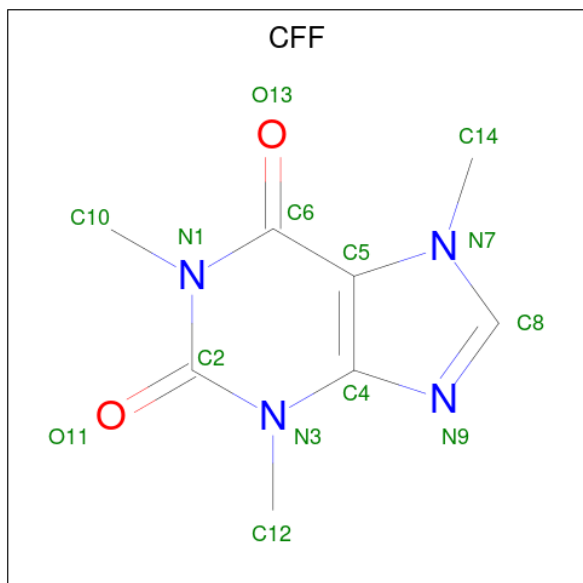
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
3	E	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
3	F	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
3	G	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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Mol	Chain	Residues	Atoms						AltConf
6	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 7 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).

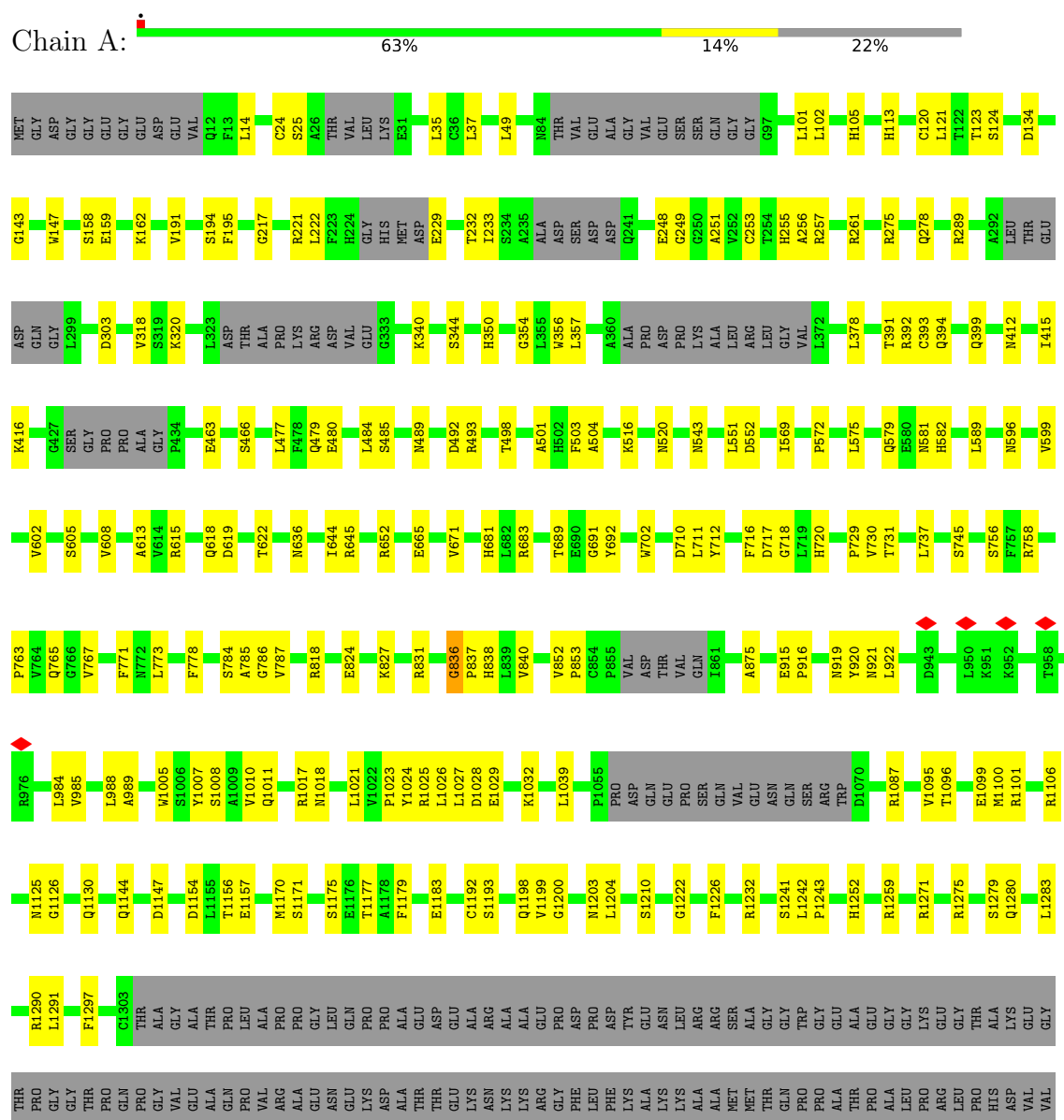


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	N	O	0
			24	8	10	4	2	
7	B	1	Total	C	H	N	O	0
			24	8	10	4	2	
7	C	1	Total	C	H	N	O	0
			24	8	10	4	2	
7	D	1	Total	C	H	N	O	0
			24	8	10	4	2	

3 Residue-property plots

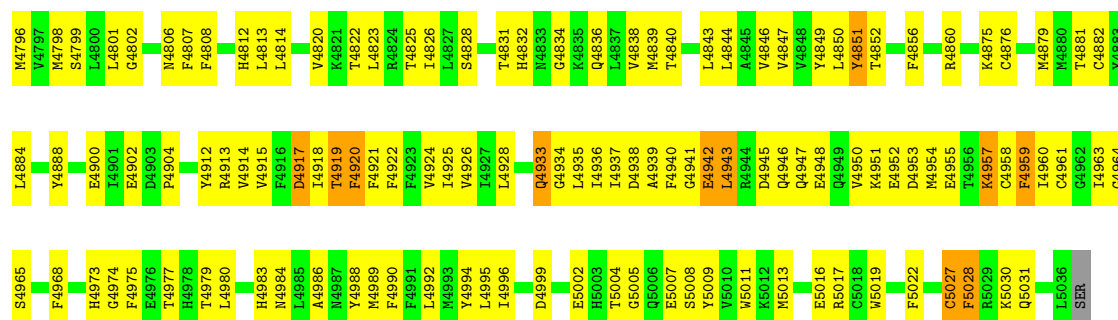
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

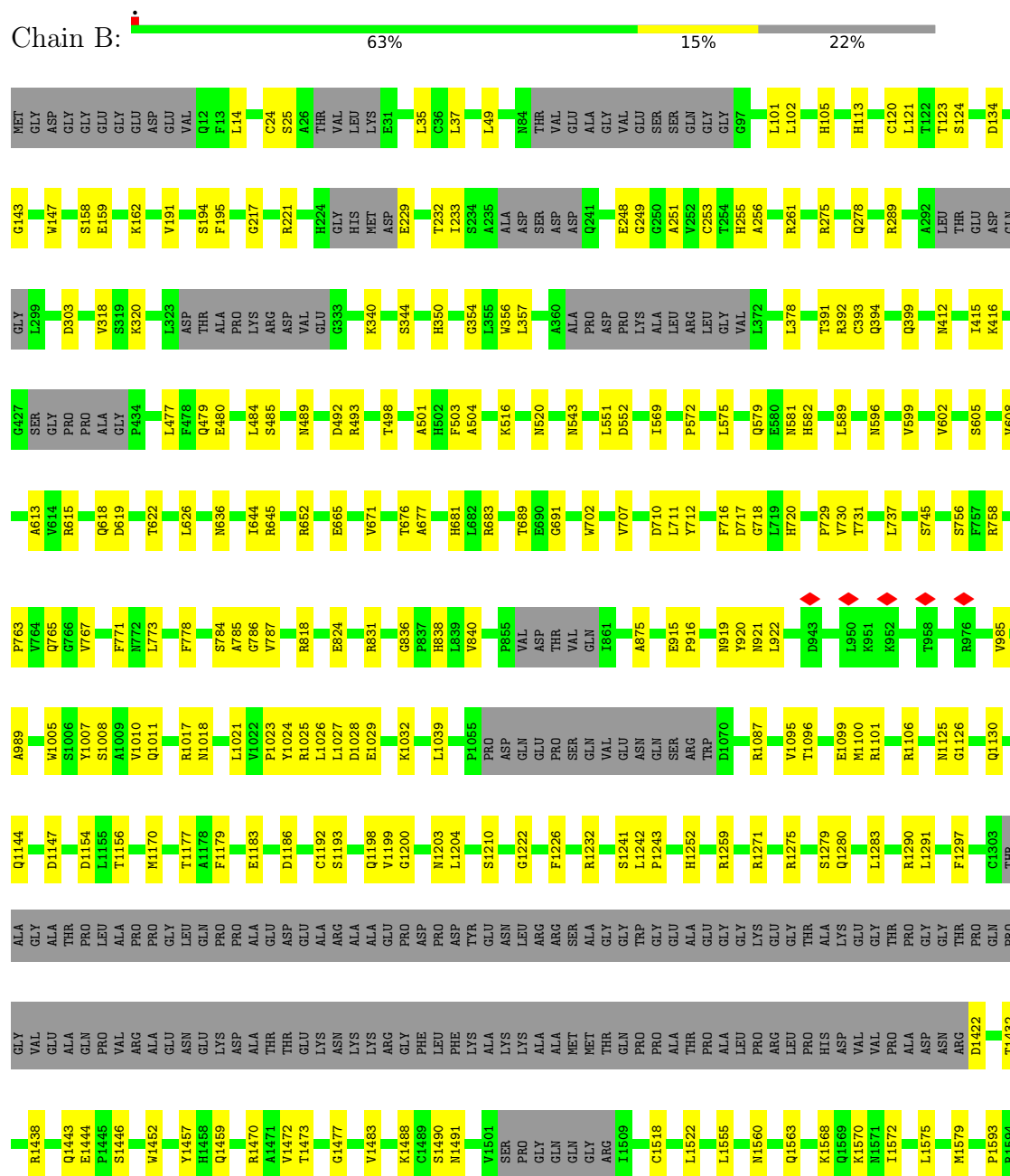








● Molecule 1: Ryanodine receptor 1

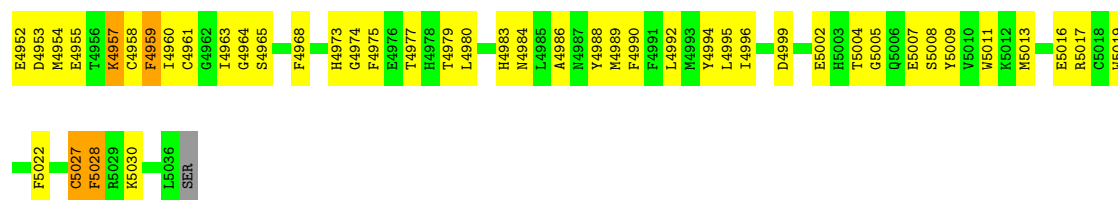




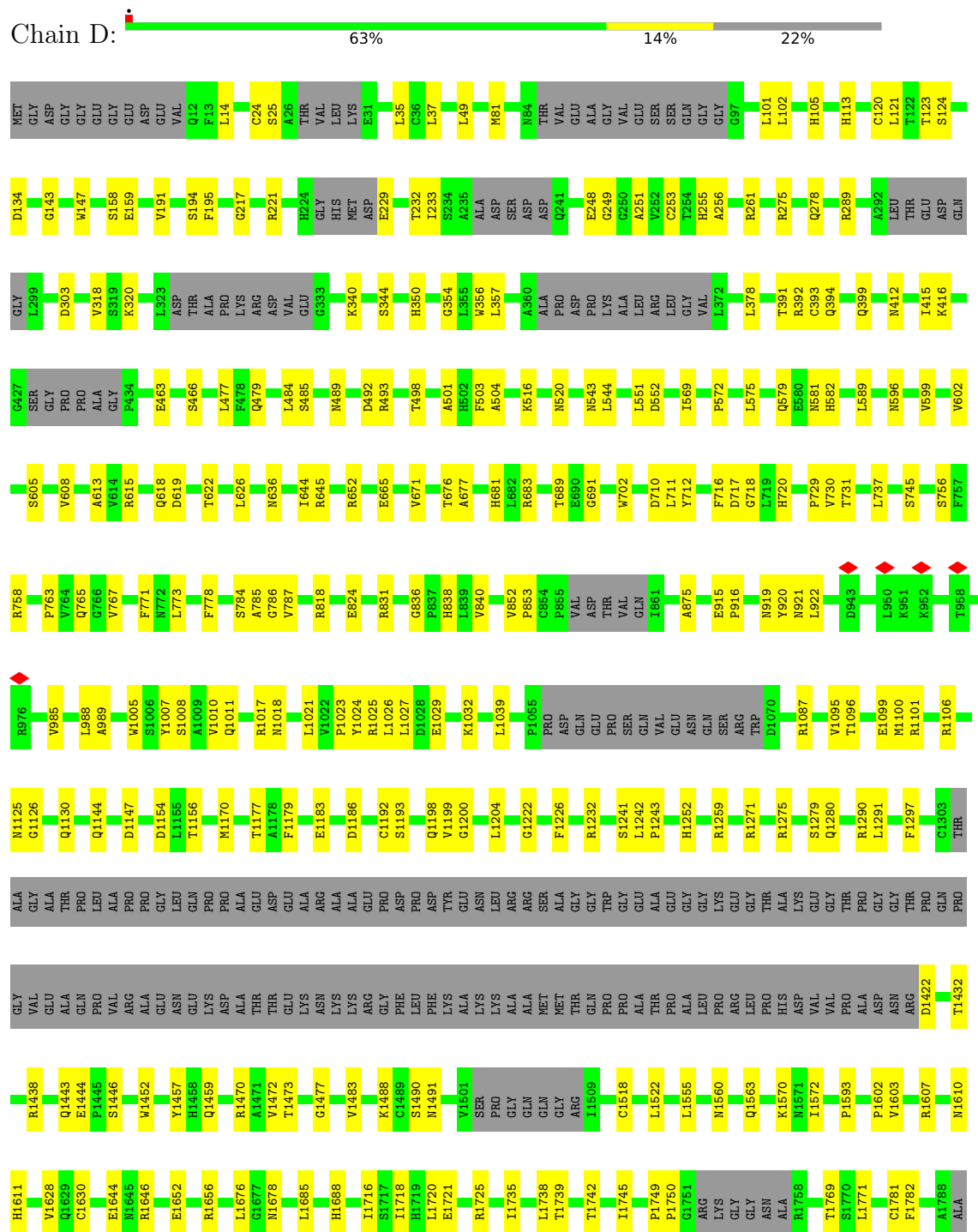
Y4849	K4774	R4703	GLU	S4556	LEU	HIS	LEU	V4245	I4058	V3841	P3697	L3579	GLN	P3344
L4850	Y4775	L4704	N4626	R4557	VAL	GLU	VAL	Q4246	L4059	D3877	L3698	PRO	SER	P3351
T4851	Q4776	V4705	M4627	N4558	PRO	ALA	PRO	T4247	R4085	D3878	D3717	GLY	GLY	
T4852	L4777	L4706	V4628	F4559	PRO	ALA	ALA	A4248	R4086	D3879	D3718	GLU	SER	H3356
F4856	Y4778	N4707	F4631	Y4560	GLU	GLY	GLU	Q4249	E4116	C3892	D3719	GLU	ASP	SER
G4781	Y4782	P4709		L4561	PRO	GLY	LEU	A4250				ASP	GLN	HIS
Y4782	F4710	S4710	Y4638	L4562	GLU	ALA	ARG	D4138	D4139	D3898	S3732	ALA	GLU	PHE
T4785	F4711	P4712	M4639	K4563	PRO	GLY	ARG	I4139		F3899	E3737	ASP	ARG	
			P4641	A4566	PRO	VAL	VAL	D4157	D4158	Q3900	GLY	ASP	THR	P3360
F4789	Y4715	Y4716	A4642	L4567	GLU	VAL	GLU	R4159	R4159	R3904	GLY	E3590	LYS	V3372
Y4790	N4716	D4717	L4643	L4568	PRO	ALA	LEU				GLU		LYS	
Y4791	D4718		L4646	F4571	LEU	LEU	LEU				ASN	HIS	ARG	E3376
S4792	F4719	V4720		N4574	LYS	ALA	ALA	M4162		T3913	GLY		ARG	
	F4719		H4649	F4575	ASP	GLY	ASP	GLY			GLY	PRO	GLY	E3388
Y4796	V4725		H4650	L4577	GLU	PRO	PRO	E4182	E4183	T3917	ALA	TYR	ASP	GLY
M4798			V4653	L4578	GLU	PRO	ASP	I4183		L3926	GLU	SER	TYR	GLU
S4799			A4654		ASN	ARG	ARG	I4190		E3944	GLU	LYS	SER	LEU
L4800	Q4729		F4654	P4586	GLY	ARG	THR	GLY			GLU	LYS	VAL	LEU
L4801	L4730	L4731	F4655	P4587	GLU	PRO	SER	I4193	E3945	Q3946	VAL	ALA	GLN	VAL
G4802	L4731	F4732	L4656	GLY	LYS	GLU	ASP	Y4194	F4195		E3750	VAL	THR	R3395
	F4732	G4733	I4657	P4588	GLU	GLY	GLU	ALA		A3958	S3752	TRP	SER	
N4806	R4734		I4658	ASP	GLU	ALA	VAL	ALA			F3753	HIS	LEU	P3410
F4807	G4690	E4735	I4659	ASP	VAL	GLY	LEU	ALA	T4200			LYS	ILE	
F4808	Y4661	L4737	Y4661	MET	PRO	GLY	ALA	GLU	W4205	V3961	E3757	L3623	VAL	P3427
				GLY	GLU	LEU	GLY	ALA	E4206	T3969		L3624	ALA	
H4812	L4664	L4740	L4664	GLY	PRO	GLY	GLN	ALA	M4207		Q3761	S3625	T3513	N3430
L4813	K4665	L4741	K4665	GLY	PRO	ASP	ALA	ALA	P4208	T3974	Y3765	R3629	P3519	ALA
L4814	L4666	G4742	L4666	ALA	PRO	GLY	ALA	ALA	Q4209	Q3977	Q3766	V3632	P3527	GLU
	P4667	N4743	L4668	GLY	PRO	GLY	VAL	ALA	K4211	R3984	R3769	C3635	D3528	LEU
Y4820	V4669	ASP	V4669	ASP	LYS	THR	GLY	ALA	E4212		L3770	M3638	D3529	F3435
K4821		LEU		LEU	LYS	PRO	ASP	ALA	S4213	D3987	H3771		GLN	K3482
L4823	R4673	ALA		ALA	ALA	ALA	ALA	GLY	K4214		T3772		ASP	ARG
R4824	E4676	SER		GLY	PRO	GLU	ASP	GLY	R4215	K3997	R3773	Y3642	LEU	GLU
L4825		LEU		ALA	PRO	PRO	GLY	ALA	Q4216	H3998	M3793		ILE	GLU
I4826	GLY	LEU		ALA	PRO	THR	ALA	ALA	F4217	M3999	V3794	H3647		
S4828	SER	GLU		SER	PRO	GLY	GLY	GLY	I4218		S3795	R3648	GLU	MET
	K4680	THR		GLY	PRO	GLU	ALA	VAL	F4219		S3796	D3676	VAL	SER
T4831	E4682	ALA		GLY	LYS	GLY	GLY	ALA	D4220	L4003	R3796	L3677	ARG	PHE
H4832	F4683	ASN		SER	LYS	SER	ALA	ALA	V4221	S4007	T3797	S3678	LEU	THR
N4833	D4684	GLU		GLY	GLY	PRO	GLY	GLY	N4222		L3798	K3679	PHE	
G4834	L4686	ARG		TRP	GLU	ILE	GLY	ALA	N4223	L4017	K3799		L3553	ALA
Q4836	Y4687	LYS		GLY	ALA	LEU	ASP	THR	E4224			E3684	ASP	ALA
L4837	I4688	PRO		SER	GLY	LYS	ALA	ALA	M4231	M4039	I3604		SER	SER
M4838	T4689	ASP		GLY	GLY	ARG	ALA	ALA	E4232	Q4043		GLU	LYS	
V4839		PRO		ALA	ALA	LYS	GLY	LEU	L4233		N3809	GLU	GLY	
T4840	P4692	PRO		GLY	ALA	LEU	GLY	ALA	F4234	D4046	A3810	GLU	VAL	SER
V4841	GLY	PRO		GLU	MET	GLY	TRP	ALA	P4235	M4047	Q3813	GLU	VAL	LYS
G4842	ASP	GLY		GLU	GLY	VAL	GLY	ALA	S4236	L4048	Q3814	VAL	GLY	ALA
L4843	ASP	LEU		ALA	F4540	ASP	ASP	ALA	D4240	V4049	K3815	GLU	SER	LYS
L4844	D4696	LEU		GLY		GLY	LEU	ALA	T4241			GLU	PRO	ALA
A4845	V4697			GLY	E4543	GLU	PHE	ARG	I4242	M4054	F3829	F3693	GLY	ASP
V4846	K4698			ASP		GLU	GLY	ALA	I4243				SER	GLY
V4847		D4772		GLU	V4546	GLU	ALA	LEU	E4244	M4057		D3696	L3569	ALA
V4848	D4702	V4773		ASP		GLU	GLY	ARG						



F4856	G4781	T4708	F4631	L4562	PRO	GLY	ALA	GLY	VAL	LYS	LEU	E4283	D4138	N3901	E3737	PRO	E3590	LYS	V3372
R4860	V4782	F4709	Y4638	K4563	GLU	GLU	GLU	GLU	THR	VAL	ARG	PRO	I4139	R3904	GLY	PRO	E3610	ARG	E3376
C4875	T4785	F4710	M4639	A4566	GLU	GLU	VAL	VAL	THR	VAL	ARG	GLU	T4148	I3913	GLY	GLY	HIS	ARG	E3368
C4876		P4712	E4640	L4569	GLU	VAL	ALA	ALA	GLU	GLU	ARG	PRO	S4151	I3917	GLY	ASN	PRO	GLY	GLY
M4879	F4789	Y4715	A4642	A4570	PRO	ALA	VAL	VAL	LEU	LEU	ARG	GLU	P4158	I3926	GLY	GLY	TYR	ASP	GLY
M4880	Y4790	D4716	A4643	A4571	GLU	ALA	ALA	ALA	LEU	LEU	ARG	GLU	R4159	I3926	GLY	GLY	LYS	ARG	GLY
T4881	S4792	K4718	L4646	A4572	LYS	ASP	ASP	ASP	ALA	ALA	ARG	GLU	E3944	E3944	GLY	GLY	LYS	TYR	GLY
C4882	F4719	F4719	L4649	N4574	ASP	GLY	GLY	GLY	MET	MET	LEU	GLU	E3945	E3945	GLY	GLY	LYS	VAL	LEU
Y4883	W4796	V4720	L4650	F4575	GLU	PRO	PRO	THR	THR	THR	ALA	ASP	N4162	E3946	GLY	GLY	ALA	GLN	VAL
L4884	Y4797	V4725	H4650	L4576	GLU	ASP	PHE	GLY	GLY	GLY	ARG	GLY	E4182	Q3946	VAL	TRP	VAL	THR	R3395
Y4888	M4798	L4725	V4653	L4577	ASN	GLY	GLY	ARG	THR	THR	GLU	MET	I4183	N3950	VAL	HIS	LYS	LEU	P3410
E4900	S4799	C4729	A4654	L4578	GLY	GLY	PRO	ARG	THR	THR	ALA	GLY	I4190	A3958	VAL	LYS	VAL	ILE	P2427
L4901	L4800	D4730	F4655	P4586	LYS	GLY	GLY	GLY	GLY	GLY	ALA	GLY	T4190	A3958	ALA	ASP	ALA	ALA	T3513
L4901	G4801	T4731	L4656	P4587	GLU	ALA	ALA	ALA	VAL	VAL	THR	ALA	I4193	V3961	GLY	GLY	L3624	THR	R3430
E4902	F4732	D4732	I4657	G4587	VAL	GLY	GLY	GLY	HIS	GLY	LEU	ALA	Y4194	V3961	GLY	GLY	L3625	GLY	ALA
E4903	I4658	G4733	I4658	GLY	PRO	GLY	GLY	GLY	GLY	GLY	ALA	GLY	F4195	I3969	GLY	GLY	R3629	GLY	ALA
P4904	I4659	R4734	I4659	ASP	GLU	LEU	LEU	LEU	GLN	GLY	ALA	GLY	T4200	T3974	GLY	GLY	V3632	LEU	F3435
	F4807	E4735	G4660	MET	PRO	GLU	ASP	GLY	GLY	GLY	TRP	GLY	W4205	Q3977	GLY	GLY	H3647	LEU	R3452
	F4808	R4736	MET	GLY	PRO	GLY	GLY	GLY	GLY	GLY	ALA	GLY	E4206	Q3977	GLY	GLY	R3648	GLY	ALA
	H4812	I4737	GLY	GLY	GLU	GLY	GLY	GLY	GLY	GLY	ALA	GLY	M4207	D3987	GLY	GLY	H3667	GLY	ARG
L4813	L4814	L4740	K4664	SER	GLU	GLY	GLY	GLY	GLY	GLY	VAL	ALA	F4208	A3997	GLY	GLY	S3668	GLY	ARG
		L4741	V4666	ALA	PRO	ASP	THR	THR	THR	THR	VAL	ALA	Q4209	H3998	GLY	GLY	F3669	LEU	GLY
V4915	V4820	G4742	P4667	GLY	PRO	GLY	THR	THR	GLY	GLY	VAL	ALA	Q4210	H3998	GLY	GLY	Y3642	LEU	GLY
V4915	K4821	N4743	L4668	ASP	LYS	PRO	PRO	PRO	GLY	GLY	ARG	ALA	W4211	H3998	GLY	GLY	H3647	LEU	GLY
V4915	T4822	ASP	V4669	LEU	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	K4211	N3999	GLY	GLY	R3647	LEU	GLY
V4915	L4823	LEU	R4673	ALA	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	E4212	K3773	GLY	GLY	R3648	LEU	GLY
V4915	E4824	ALA	E4676	GLY	PRO	GLY	PRO	PRO	GLY	GLY	ALA	ALA	S4213	L4003	GLY	GLY	H3647	LEU	GLY
V4915	T4825	SER	E4676	GLY	PRO	GLY	PRO	PRO	ALA	ALA	ALA	ALA	R4214	L4003	GLY	GLY	H3667	LEU	GLY
V4915	L4826	LEU	E4676	ALA	PRO	GLY	PRO	PRO	ALA	ALA	ALA	ALA	K4215	S4007	GLY	GLY	S3668	LEU	GLY
V4915	L4827	GLU	E4676	GLY	PRO	GLY	THR	THR	GLY	GLY	GLY	GLY	R4216	S4007	GLY	GLY	S3668	LEU	GLY
V4915	S4828	ILE	K4680	SER	PRO	GLY	PRO	PRO	GLY	GLY	GLY	GLY	Q4217	L4017	GLY	GLY	F3669	LEU	GLY
V4915		THR	L4681	GLY	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	I4217	L4017	GLY	GLY	D3676	LEU	GLY
V4915		ALA	E4682	GLY	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	I4218	L4017	GLY	GLY	D3676	LEU	GLY
V4915	T4831	ALA	F4683	GLY	LYS	SER	GLY	SER	GLY	GLY	GLY	GLY	F4219	M4039	GLY	GLY	L3677	LEU	GLY
V4915	H4832	HIS	F4683	GLY	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	D4220	M4039	GLY	GLY	L3677	LEU	GLY
V4915	N4833	ASN	D4684	SER	GLY	PRO	PRO	PRO	GLY	GLY	GLY	GLY	V4221	Q4043	GLY	GLY	S3678	LEU	GLY
V4915	G4834	GLU	G4685	GLY	GLY	GLY	ILE	ILE	GLY	GLY	GLY	GLY	V4222	Q4043	GLY	GLY	K3679	LEU	GLY
V4915	K4835	LYS	L4686	TRP	ALA	ALA	LEU	LEU	ASP	ASP	ALA	ALA	N4223	D4046	GLY	GLY	E3684	LEU	GLY
V4915	L4836	ARG	Y4687	GLY	GLY	GLY	GLY	GLY	ALA	ALA	ARG	ALA	N4224	M4047	GLY	GLY	E3684	LEU	GLY
V4915	V4838	PRO	I4688	SER	GLY	GLY	ARG	ARG	ALA	ALA	GLY	LEU	E4224	M4047	GLY	GLY	E3684	LEU	GLY
V4915	M4839	ASP	T4689	GLY	ALA	LYS	LYS	LYS	GLY	GLY	GLY	LEU		M4047	GLY	GLY	E3684	LEU	GLY
V4915	T4840	PRO		GLY	ALA	LEU	LEU	LEU	GLY	GLY	GLY	LEU		M4047	GLY	GLY	E3684	LEU	GLY
V4915	A4939	PRO		GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	TRP		M4047	GLY	GLY	E3684	LEU	GLY
V4915	G4842	PRO		GLY	GLY	GLY	VAL	VAL	GLY	GLY	GLY	GLY		M4054	GLY	GLY	E3684	LEU	GLY
V4915	L4843	LEU		GLY	ASP	ASP	ASP	ASP	ASP	ASP	SER	ALA	V4235	N4054	GLY	GLY	E3684	LEU	GLY
V4915	L4844	LEU		GLY	ASP	ASP	GLY	GLY	GLY	GLY	LEU	ALA	D4240	M4057	GLY	GLY	E3684	LEU	GLY
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V4915	V4846	LEU		GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ARG	I4242	M4057	GLY	GLY	E3684	LEU	GLY
V4915	V4847	LEU		ASP	GLY	GLY	GLY	GLY	VAL	VAL	GLY	LEU	F4243	M4057	GLY	GLY	E3684	LEU	GLY
V4915	V4848	LEU		GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU	E4244	M4057	GLY	GLY	E3684	LEU	GLY
V4915	Y4849	LEU		GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU	N4245	M4057	GLY	GLY	E3684	LEU	GLY
V4915	Q4947	LEU		GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU	I4246	M4057	GLY	GLY	E3684	LEU	GLY
V4915	E4948	LEU		GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU	I4247	M4057	GLY	GLY	E3684	LEU	GLY
V4915	Y4851	LEU		GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU	A4248	M4057	GLY	GLY	E3684	LEU	GLY
V4915	T4852	LEU		GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU	A4249	M4057	GLY	GLY	E3684	LEU	GLY
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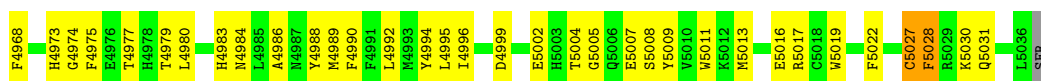


● Molecule 1: Ryanodine receptor 1

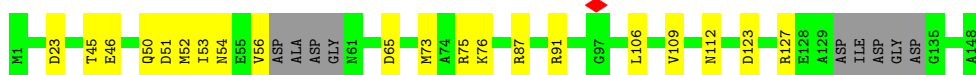
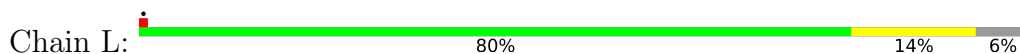


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S3279	A3198	T2822	R2600	GLY	C2305	M2153	PRO	L1926	E1793
P3282	P3202	I2823	R2615	ASP	N2324	S2154	GLU	L1927	D1828
R3283	P3208	K2825	R2616	GLY	N2324	L2165	GLU	Q1928	D1856
W3284	P3208	A2826	S2617	ALA	G2327	G2171	THR	K1930	D1856
W3285	E3212	R2827	M2618	ALA	Y2331	E2174	SER	L1931	K1860
GLU	TYR	R2827	L2619	W2486	Y2331	E2174	SER	C1947	E1873
ASN	GLY	E2830	L2623	F2494	L2332	M2178	SER	E1956	GLU
LEU	VAL	GLU	L2626	V2503	D2333	R2189	ARG	E1966	GLU
ARG	ASP	ARG	L2626	V2510	R2336	W2190	LEU	F1961	GLU
CYS	ALA	THR	N2634	Y2510	N2342	F2191	SER	A1962	GLU
E2915	K2914	GLU	GLU	D2516	Q2193	L2192	LEU	R1964	GLU
E2915	E2915	GLU	ASN	Q2516	Q2193	Q2193	LEU	Y1965	GLU
K2916	K2916	GLU	PHE	R2516	K2360	F2617	THR	V1966	GLU
L2919	D2919	GLU	ALA	L2517	C2363	F2195	THR		GLU
D2919	D2919	THR	K2638	L2518	C2363	F2195	VAL	Q1970	GLU
M2932	M2932	ARG	P2639	L2519	R2369	M2196	ARG	A1971	GLU
N2933	N2933	GLU	P2640	L2519	GLY	L2197	LEU	N1972	GLU
C2934	C2934	SER	E2741	L2522	GLY	R2199	VAL	Q1973	GLU
R2939	R2939	THR	C2655	D2529	GLY	M2211	LYS	R1974	GLU
GLY	GLY	THR	LEU	W2530	C2373	M2211	LYS	S1975	GLU
GLN	ALA	ALA	PRO	R2531	E2381	G2216	GLU	R1976	GLU
GLN	CYS	GLN	THR	A2532	E2381	G2216	GLU	A1992	ASP
THR	LYS	THR	GLY	A2533	I2384	GLY	PRO	GLU	GLU
LYS	LYS	TYR	TRP	A2533	I2384	GLY	PRO	GLU	GLU
ASP	ASP	ASP	A2662	L2536	P2395	THR	GLU	R1996	GLU
PRO	PRO	PRO	A2662	D2537	P2395	THR	GLU	R1996	GLU
E2749	E2749	GLU	L2678	THR	GLY	LYS	GLU	S2000	LYS
K2750	K2750	ASP	PHE	ALA	VAL	E2722	LEU	Q2005	GLU
L2751	L2751	GLY	TRP	THR	ARG	E2722	LEU	Q2005	GLU
D2752	D2752	GLY	GLY	PHE	ARG	C2232	ALA	D2014	ASP
I2755	I2755	ILE	ILE	THR	ASP	C2233	GLU	D2014	GLU
L2755	L2755	PHE	ASP	THR	ARG	R2244	LYS	GLU	GLU
E2760	E2760	SER	SER	T2544	ARG	R2244	LYS	ALA	GLU
Y2761	Y2761	L2686	L2686	L2544	ARG	K2245	ASP	ASP	GLU
L2762	L2762	PRO	M2700	V2558	GLU	M2246	GLU	GLU	GLU
H2763	H2763	CYS	CYS	L2568	PHE	L2254	LYS	C2020	ASP
E2764	E2764	LEU	LEU	L2568	GLY	L2257	GLU	C2021	GLU
F2768	F2768	THR	THR	T2572	GLU	L2257	GLU	P2022	ALA
D2769	D2769	ALA	CYS	T2572	PRO	G2262	LYS	L2023	GLU
K2770	K2770	ILE	ALA	R2575	PRO	ILE	LYS	P2024	LYS
I2771	I2771	ALA	ALA	A2576	GLU	GLY	GLU	I2027	GLU
Q2772	Q2772	GLY	GLY	L2577	GLU	M2120	GLU	R2028	GLU
A2872	A2872	ALA	ALA	W2578	N2414	GLY	GLU	Q2029	GLU
Q2873	Q2873	GLY	LEU	V2578	N2414	W2267	ALA	D2030	ALA
Q2877	Q2877	LYS	LEU	V2578	L2433	W2267	LYS	L2124	PRO
Q2883	Q2883	PRO	PRO	D2580	L2433	A2276	GLU	L2124	PRO
H2886	H2886	THR	ASP	W2582	G2434	A2276	GLU	C2042	GLU
W2886	W2886	GLY	TYR	M2582	R2435	S2279	GLY	G2043	GLY
G2886	G2886	GLN	VAL	V2586	R2457	Y2142	LYS	E2047	LYS
E2794	E2794	THR	ASP	V2586	L2458	D2282	GLU	GLY	GLU
F2797	F2797	GLY	ASP			M2283			ASP
A2815	A2815								
W2819	W2819								

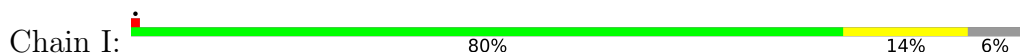
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E4902	M4799	V4653	L4578	ASN	THR	THR	ARG	GLY	I4191	R3395	ALA	TRP	THR	VAL
P4904	L4801	L4656	P4586	GLY	PRO	SER	ALA	GLY	R4192	V3961	GLU	HIS	LEU	P2410
	G4802	I4657	P4587	GLY	ASP	GLY	ALA	GLY	R4193	L3969	GLU	LYS	ILE	P3427
M4806	F4807	I4658	GLY	GLU	ALA	VAL	THR	ALA	Y4194	T3974	GLU	L3623	ALA	P3430
F4808	G4680	I4659	ASP	VAL	GLY	HIS	LEU	ALA	F4195	T3974	GLU	L3624	ALA	A3430
H4812	R4736	Y4661	MET	GLY	LEU	GLY	ALA	GLY	T4200	Q3977	VAL	S3625	ALA	GLU
L4814	I4737	L4664	GLY	ALA	GLY	GLN	LEU	ALA	W4205	L3980	GLY	R3629	GLY	LEU
	L4740	K4665	GLY	PRO	ASP	PRO	LEU	GLY	E4206	S3983	GLY	V3632	LEU	P3435
V4820	L4741	K4666	SER	PRO	MET	ALA	TRP	GLY	M4207	R3984	GLY	C3635	GLY	P3452
T4821	G4742	P4667	ALA	GLY	GLY	GLY	VAL	ALA	V4210	D3987	GLY	M3638	GLY	ARG
T4822	N4743	L4668	GLY	THR	THR	GLY	VAL	ALA	E4211	K4211	GLY	Q3766	ASP	GLY
L4823	ASP	V4669	ASP	PRO	PRO	GLY	ALA	ARG	S4213	S4213	GLY	S3768	LEU	GLY
K4824	LEU	R4673	LEU	ALA	ALA	ALA	ALA	ALA	K4214	K4214	GLY	Y3642	ILE	GLY
T4825	SER	E4676	ALA	PRO	GLY	GLY	ALA	ALA	R4215	R4215	GLY	H3647	GLY	P3456
I4826	LEU	E4676	ALA	PRO	PRO	GLY	ALA	ALA	Q4216	Q4216	ALA	R3648	GLY	M3466
L4827	GLY	K4680	GLY	SER	THR	GLY	ALA	GLY	F4217	F4217	ALA	H3667	GLY	MET
S4828	THR	L4681	SER	PRO	PRO	GLY	ALA	THR	I4218	I4218	GLY	H3668	GLY	GLY
	ALA	E4682	GLY	PRO	GLY	GLY	GLY	VAL	F4219	S4007	GLY	S3669	GLY	P3456
T4831	ALA	F4683	GLY	ALA	GLY	GLY	GLY	ALA	E4220	L4017	GLY	F3669	GLY	P3456
H4832	HIS	D4684	SER	LYS	GLY	GLY	ALA	ALA	V4221	L4017	GLY	D3676	GLY	THR
G4934	ASN	G4685	GLY	LYS	SER	GLY	ALA	ALA	W4222	S3795	GLY	D3676	GLY	THR
L4935	GLY	G4686	GLY	GLY	PRO	GLY	ALA	GLY	N4039	T3797	GLY	L3677	ASP	ASP
K4836	ARG	L4686	TRP	ILE	ILE	GLY	GLY	GLY	L3798	L3798	GLY	Q3560	GLY	LYS
Q4836	LYS	Y4687	GLY	ALA	LEU	ASP	ALA	THR	Q4043	Q4043	GLY	K3679	GLY	LYS
L4837	PRO	I4688	SER	GLY	LYS	ALA	LEU	ALA	M4231	D4046	GLY	E3684	GLY	SER
I4937	ASP	T4689	GLY	GLY	ARG	ALA	ARG	ALA	E4232	M4047	GLY	E3684	GLY	SER
D4938	ASP	P4692	GLY	GLY	LYS	ALA	ARG	ALA	L4233	M4047	GLY	E3684	GLY	LYS
A4939	PRO	GLY	ALA	LEU	LEU	GLY	LEU	LEU	F4234	L4048	GLY	GLU	VAL	LYS
F4940	PRO	GLY	GLY	LEU	LEU	GLY	LEU	LEU	V4235	V4049	GLY	GLU	GLY	ALA
G4941	PRO	GLY	GLY	VAL	VAL	ASP	GLY	GLY	S4236	E4050	GLY	GLU	GLY	LYS
L4843	GLY	GLY	ALA	ASP	ASP	ASP	SER	SER	S4051	S4051	GLY	VAL	ASP	ASP
L4844	LEU	ASP	ALA	GLY	GLY	GLY	LEU	LEU	D4240	M4054	GLY	GLU	ALA	ALA
A4845	LEU	D4696	GLY	GLY	GLY	GLY	PHE	ARG	T4241	M4054	GLY	GLU	GLN	ALA
V4846	ASP	K4698	ASP	GLY	GLY	VAL	GLY	ALA	I4242	M4057	GLY	GLU	PRO	SER
V4847	GLY		GLY	GLY	GLY	ALA	GLY	LEU	F4243	M4057	GLY	GLU	GLY	ALA
V4848	GLY		GLY	GLY	GLY	GLY	GLY	GLY	E4244	M4057	GLY	GLU	GLY	LYS
Y4849	D4702	D4702	ASP	LEU	LEU	HIS	LEU	GLY	M4245	Q4078	GLY	D3696	GLY	LYS
L4850	R4703	R4703	GLY	VAL	VAL	GLY	VAL	LEU	Q4246	Q4246	GLY	F3697	SER	GLY
Y4851	L4704	L4704	M4626	PRO	PRO	ALA	GLY	LEU	I4247	Y4081	GLY	L3698	ASP	GLY
L4852	V4705	V4705	M4558	GLY	GLY	GLY	GLY	SER	A4248	A4248	GLY	L3698	GLN	ALA
F4856	L4706	L4706	F4559	PRO	PRO	PRO	ALA	ALA	R4085	R4085	GLY	D3717	ALA	GLY
	N4707	N4707	Y4560	GLY	GLY	GLY	LYS	SER	A4249	A4249	GLY	E3718	ASP	ARG
	T4708	T4708	T4561	GLY	GLY	GLY	LYS	SER	Q4250	Q4250	GLY	D3719	ASP	THR
	P4709	P4709	L4562	PRO	PRO	GLY	LYS	LEU	E4116	E4116	GLY	D3719	PRO	LYS
	S4710	S4710	K4563	GLY	GLY	ALA	VAL	ARG	E4253	E4253	GLY	D3727	LYS	LYS
	F4711	F4711	A4566	PRO	PRO	GLY	THR	ARG	PRO	PRO	GLY	D3727	LYS	LYS
	P4712	P4712	A4566	GLY	GLY	GLY	VAL	ARG	D4138	D4138	GLY	K3731	ARG	ARG
			E4640	PRO	PRO	VAL	THR	VAL	I4139	I4139	GLY	S3732	ARG	ARG
	Y4715	Y4715	L4569	GLY	GLY	VAL	GLY	ARG	P4158	P4158	GLY	S3732	PRO	GLY
	L4716	L4716	K4570	PRO	PRO	ALA	LEU	ARG	R4159	R4159	GLY	E3737	TYR	ASP
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	F4719	F4719	M4574	ALA	ALA	ASP	GLY	ARG	E3945	E3945	GLY	GLY	SER	ARG
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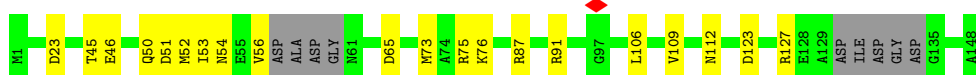
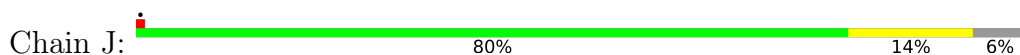
• Molecule 2: Calmodulin-1



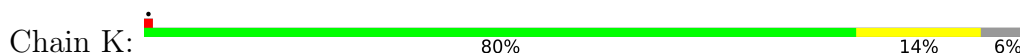
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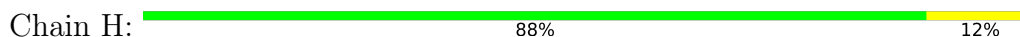
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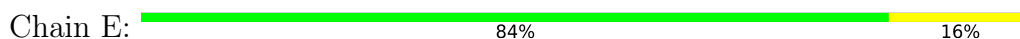
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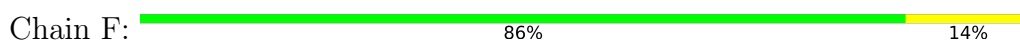
• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

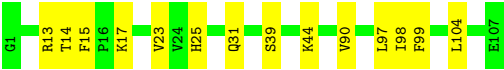
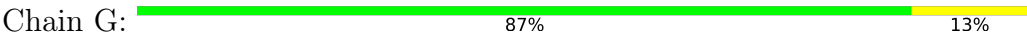


• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B





- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19505	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	1.484	Depositor
Minimum map value	-0.814	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	613.2, 613.2, 613.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2775, 1.2775, 1.2775	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, ZN, ATP, 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	A	0.39	6/28349 (0.0%)	0.67	49/38619 (0.1%)
1	B	0.39	6/28349 (0.0%)	0.66	43/38619 (0.1%)
1	C	0.39	6/28349 (0.0%)	0.67	48/38619 (0.1%)
1	D	0.39	7/28349 (0.0%)	0.67	48/38619 (0.1%)
2	I	0.20	0/1052	0.44	0/1416
2	J	0.20	0/1052	0.44	0/1416
2	K	0.20	0/1052	0.44	0/1416
2	L	0.20	0/1052	0.44	0/1416
3	E	0.23	0/820	0.52	0/1105
3	F	0.23	0/820	0.52	0/1105
3	G	0.23	0/820	0.51	0/1105
3	H	0.23	0/820	0.52	0/1105
All	All	0.38	25/120884 (0.0%)	0.66	188/164560 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4200	THR	C-N	8.97	1.46	1.34
1	B	4200	THR	C-N	8.97	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4200	THR	C-N	8.97	1.46	1.34
1	D	4200	THR	C-N	8.97	1.46	1.34
1	A	4943	LEU	C-O	6.56	1.31	1.24

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	836	GLY	CA-C-N	15.87	139.68	119.84
1	A	836	GLY	C-N-CA	15.87	139.68	119.84
1	B	836	GLY	CA-C-N	15.87	139.68	119.84
1	B	836	GLY	C-N-CA	15.87	139.68	119.84
1	C	836	GLY	CA-C-N	15.87	139.68	119.84

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4231	MET	Peptide
1	A	4957	LYS	Peptide
1	A	4959	PHE	Peptide
1	B	4231	MET	Peptide
1	B	4957	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	27821	0	24966	519	0
1	B	27821	0	24966	522	0
1	C	27821	0	24966	524	0
1	D	27821	0	24966	516	0
2	I	1042	0	972	13	0
2	J	1042	0	972	12	0
2	K	1042	0	972	13	0
2	L	1042	0	972	13	0
3	E	804	0	812	10	0
3	F	804	0	812	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	804	0	812	8	0
3	H	804	0	812	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	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	31	12	12	1	0
6	B	31	12	12	1	0
6	C	31	12	12	1	0
6	D	31	12	12	1	0
7	A	14	10	10	1	0
7	B	14	10	10	1	0
7	C	14	10	10	1	0
7	D	14	10	10	1	0
All	All	118856	88	107088	2134	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 9.

The worst 5 of 2134 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:B:4586:PRO:HG3	1:B:4628:VAL:HG11	1.39	1.04
1:A:4586:PRO:HG3	1:A:4628:VAL:HG11	1.39	1.03
1:C:4586:PRO:HG3	1:C:4628:VAL:HG11	1.39	1.00
1:D:4586:PRO:HG3	1:D:4628:VAL:HG11	1.39	1.00
1:B:4569:LEU:HD21	1:B:4649:LEU:HD23	1.47	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ATP	C	5103	-	32,33,33	3.09	23 (71%)	48,52,52	3.08	20 (41%)
6	ATP	D	5103	-	32,33,33	3.10	22 (68%)	48,52,52	3.08	20 (41%)
6	ATP	B	5103	-	32,33,33	3.10	22 (68%)	48,52,52	3.08	20 (41%)
7	CFF	A	5104	-	15,15,15	4.54	11 (73%)	23,23,23	3.36	12 (52%)
7	CFF	B	5104	-	15,15,15	4.54	11 (73%)	23,23,23	3.36	12 (52%)
6	ATP	A	5103	-	32,33,33	3.10	23 (71%)	48,52,52	3.08	20 (41%)
7	CFF	C	5104	-	15,15,15	4.55	11 (73%)	23,23,23	3.37	12 (52%)
7	CFF	D	5104	-	15,15,15	4.54	11 (73%)	23,23,23	3.36	12 (52%)

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
6	ATP	C	5103	-	-	5/22/38/38	0/3/3/3
6	ATP	D	5103	-	-	5/22/38/38	0/3/3/3
6	ATP	B	5103	-	-	5/22/38/38	0/3/3/3
7	CFF	A	5104	-	-	-	0/2/2/2
7	CFF	B	5104	-	-	-	0/2/2/2
6	ATP	A	5103	-	-	5/22/38/38	0/3/3/3
7	CFF	C	5104	-	-	-	0/2/2/2
7	CFF	D	5104	-	-	-	0/2/2/2

The worst 5 of 134 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	5104	CFF	O11-C2	8.99	1.39	1.22
7	A	5104	CFF	O11-C2	8.98	1.39	1.22
7	C	5104	CFF	O11-C2	8.98	1.39	1.22
7	D	5104	CFF	O11-C2	8.98	1.39	1.22
7	C	5104	CFF	O13-C6	8.68	1.40	1.23

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5103	ATP	C4-N9-C8	10.36	116.62	105.74
6	C	5103	ATP	C4-N9-C8	10.36	116.62	105.74
6	D	5103	ATP	C4-N9-C8	10.35	116.61	105.74
6	B	5103	ATP	C4-N9-C8	10.32	116.57	105.74
6	B	5103	ATP	C4'-O4'-C1'	-9.47	88.56	109.47

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

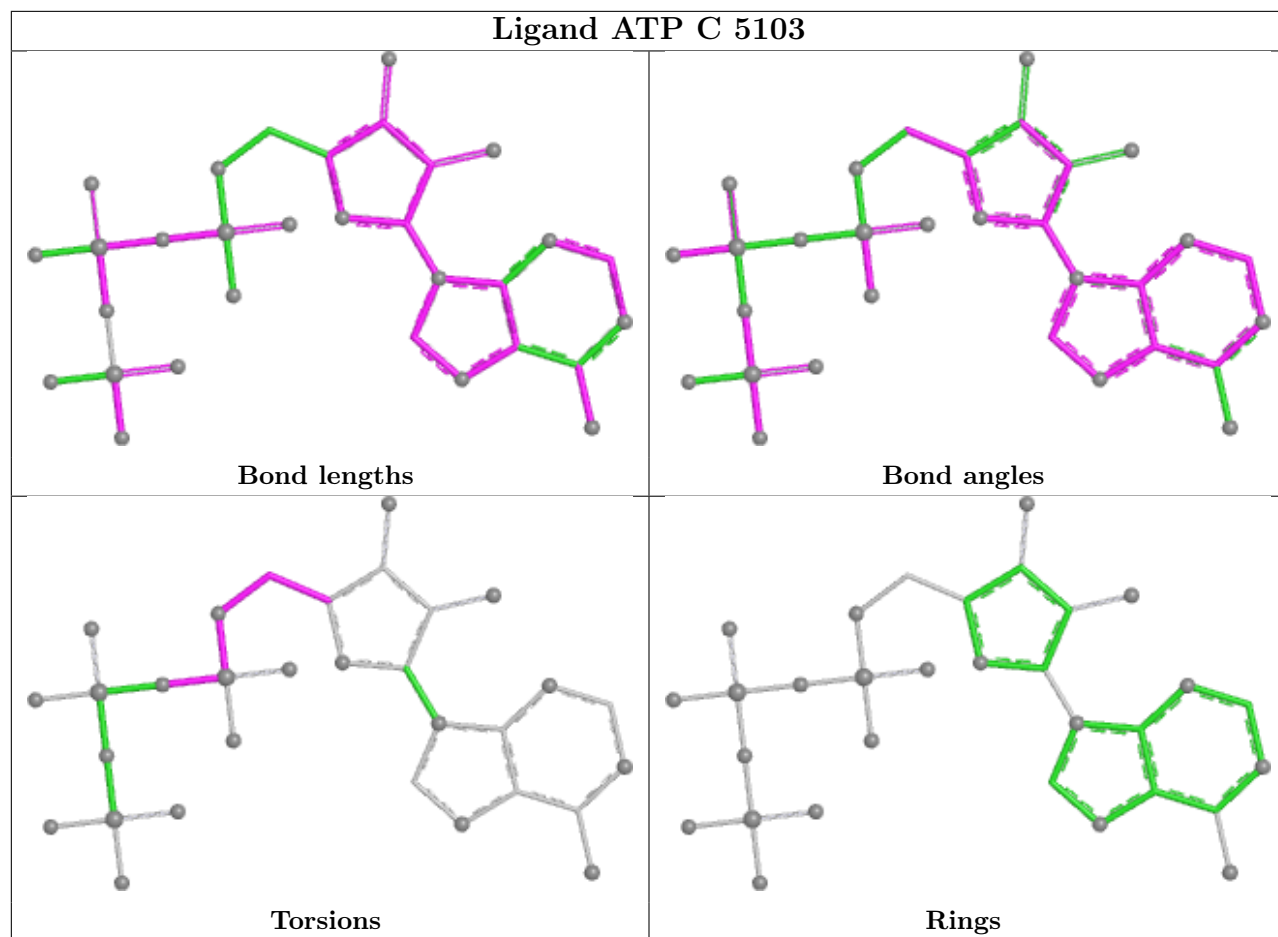
Mol	Chain	Res	Type	Atoms
6	A	5103	ATP	C4'-C5'-O5'-PA
6	B	5103	ATP	C4'-C5'-O5'-PA
6	C	5103	ATP	C4'-C5'-O5'-PA
6	D	5103	ATP	C4'-C5'-O5'-PA
6	A	5103	ATP	PB-O3A-PA-O5'

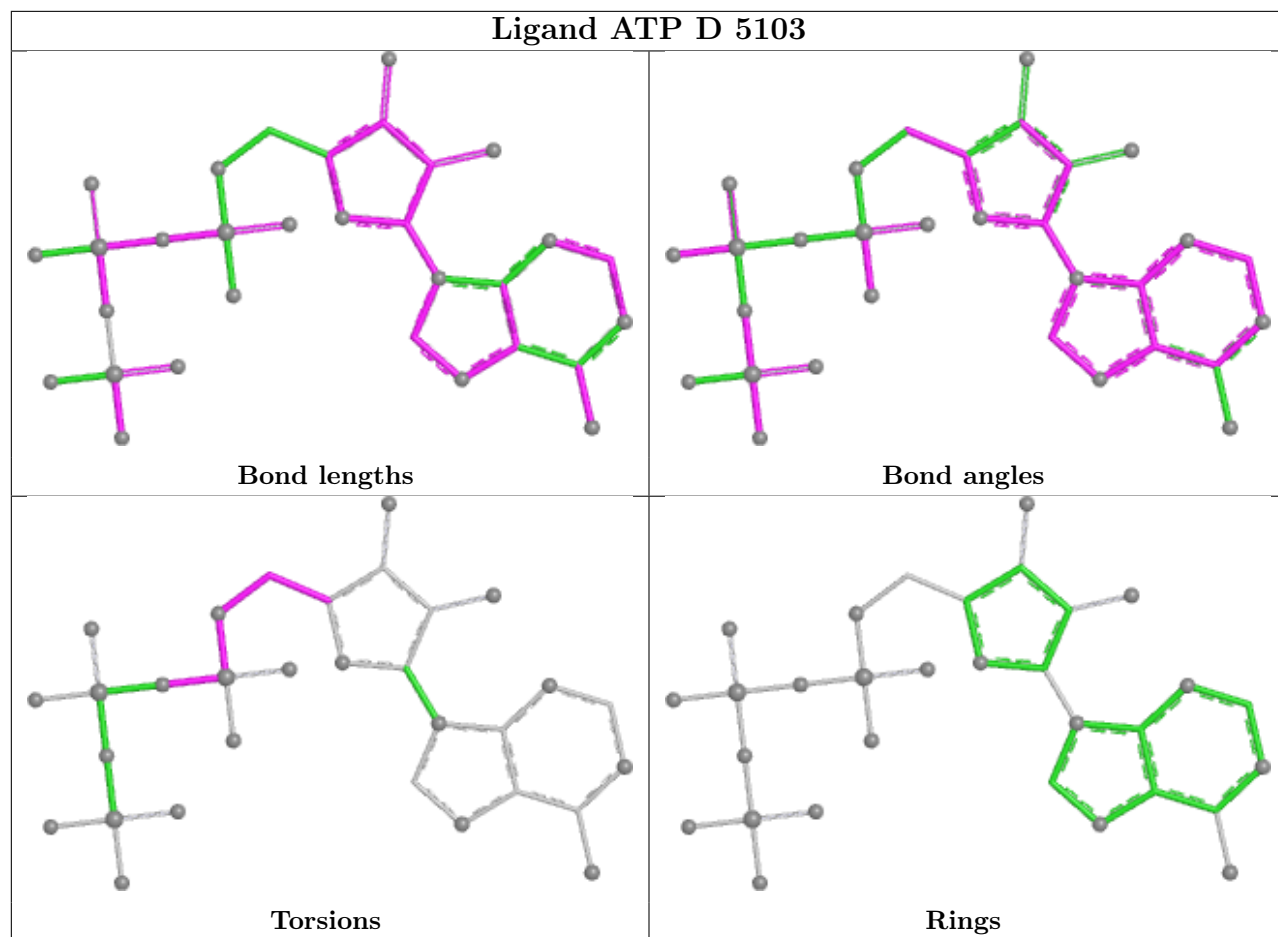
There are no ring outliers.

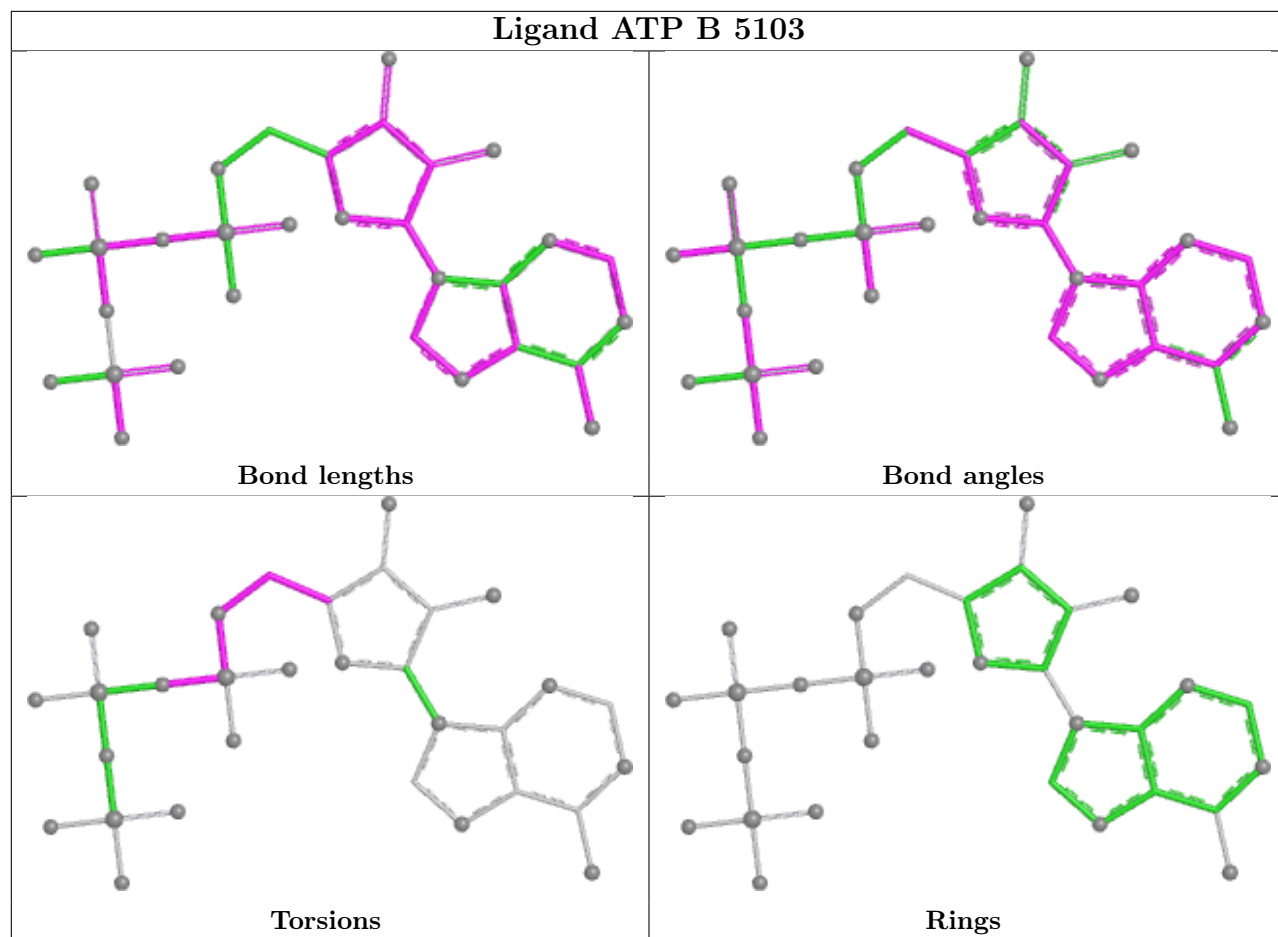
8 monomers are involved in 8 short contacts:

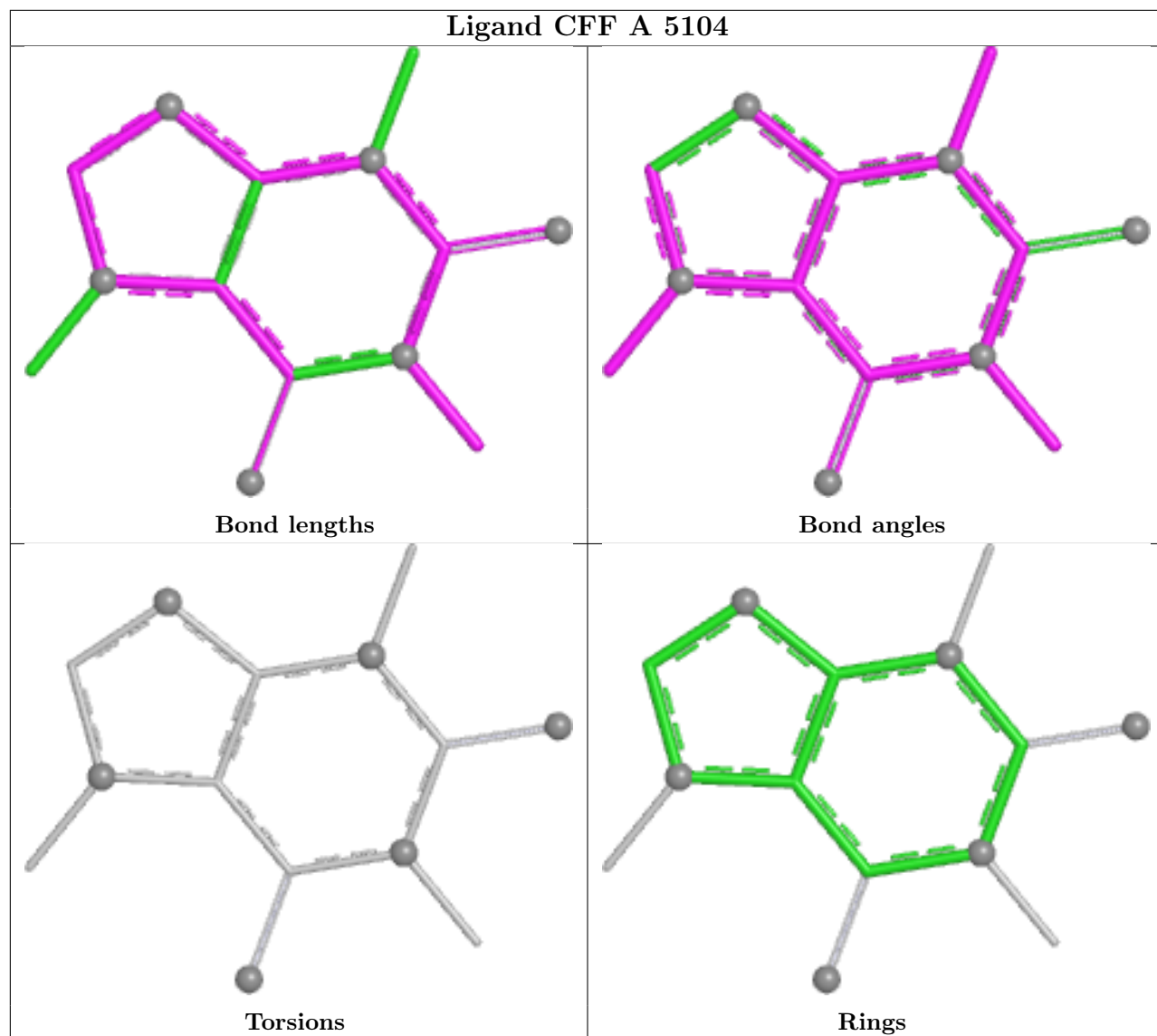
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	5103	ATP	1	0
6	D	5103	ATP	1	0
6	B	5103	ATP	1	0
7	A	5104	CFF	1	0
7	B	5104	CFF	1	0
6	A	5103	ATP	1	0
7	C	5104	CFF	1	0
7	D	5104	CFF	1	0

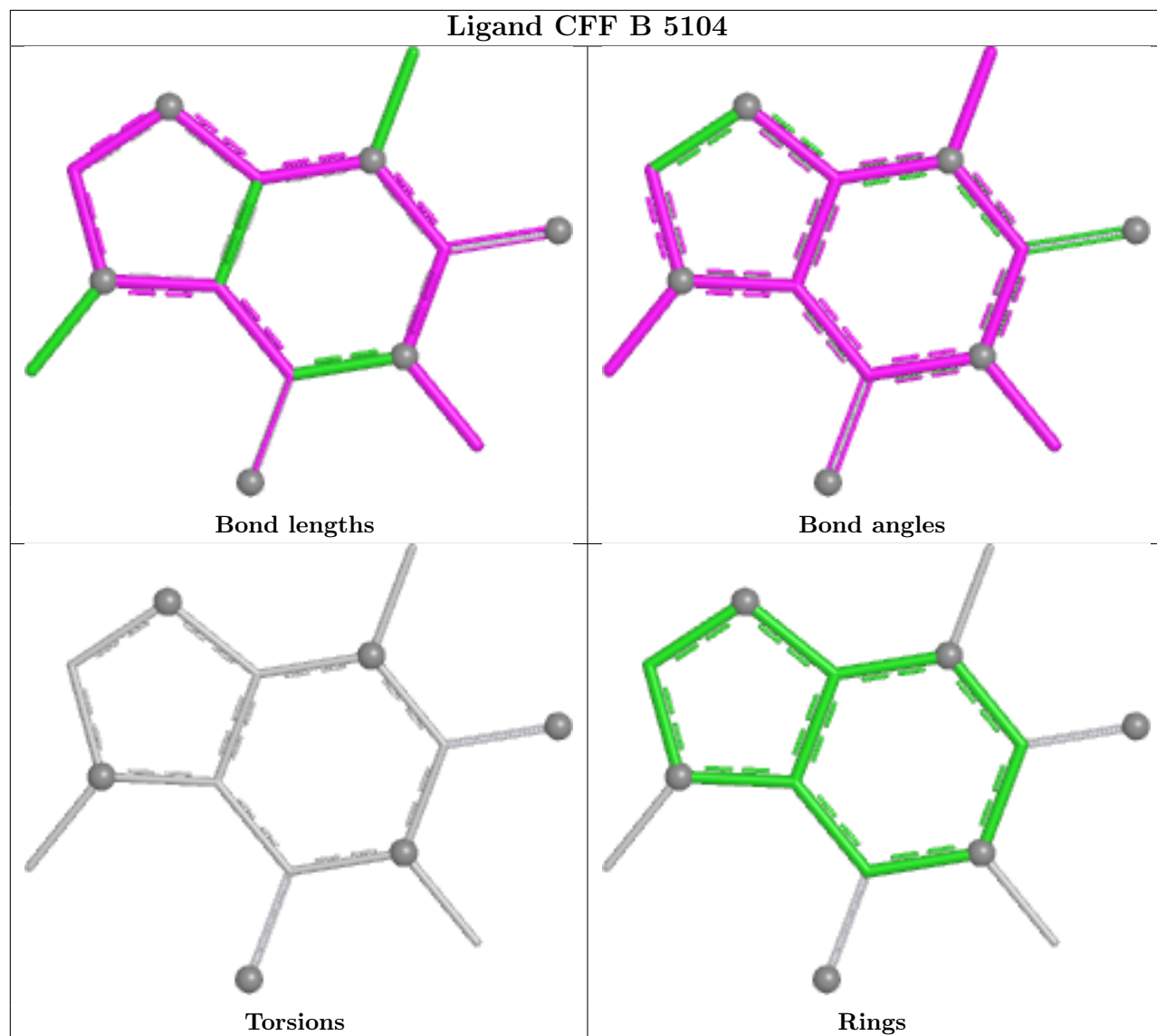
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

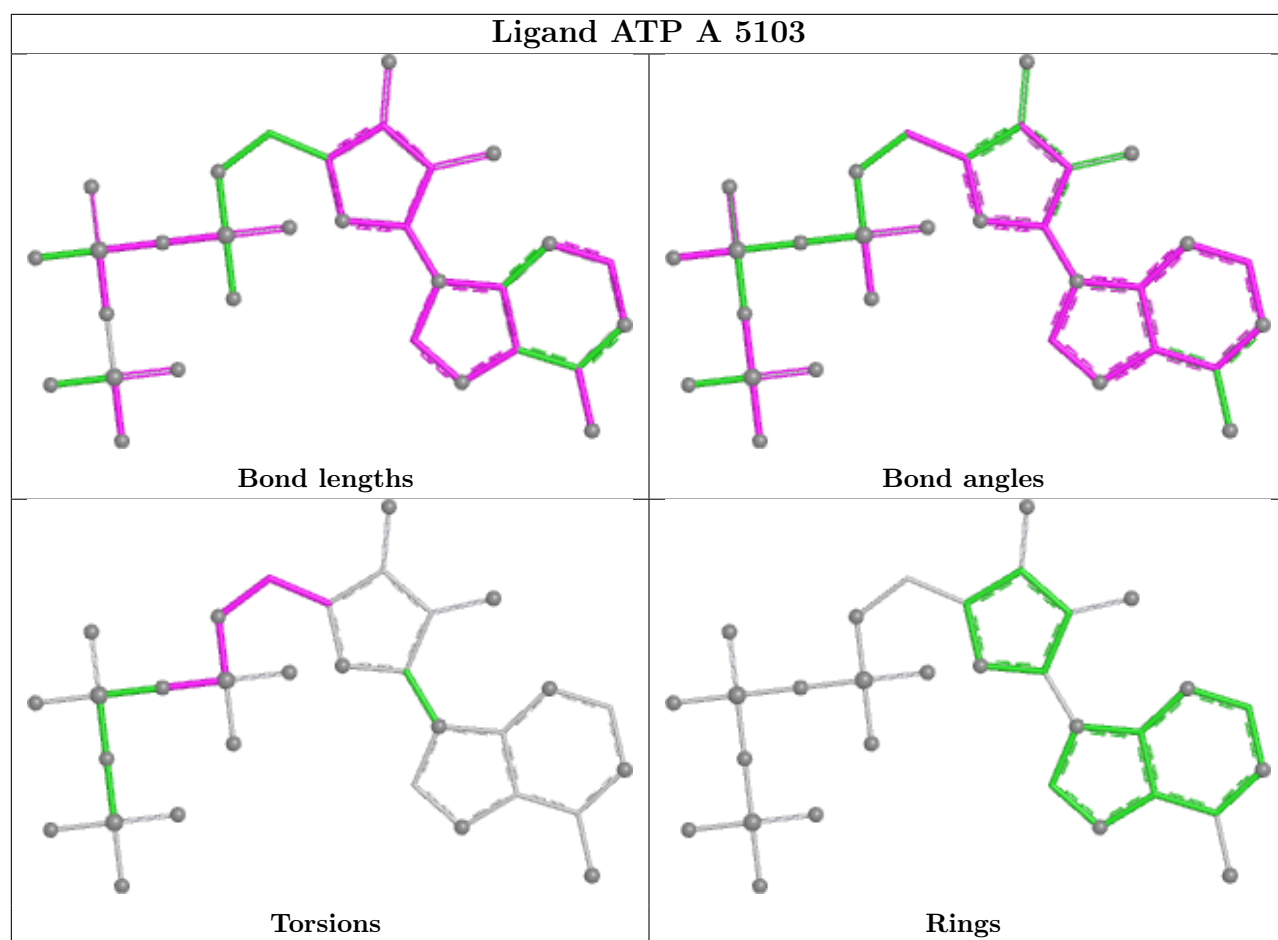


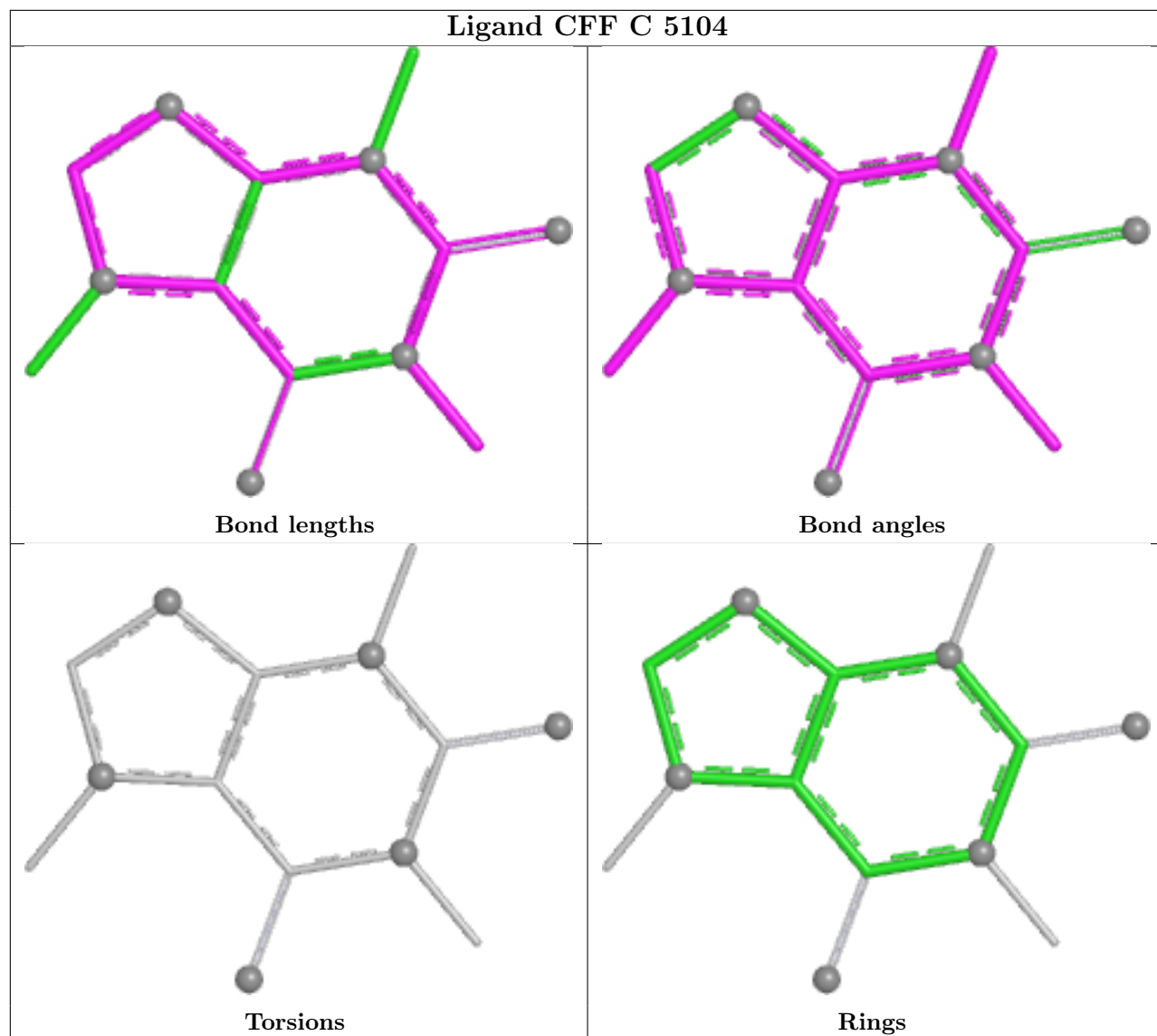


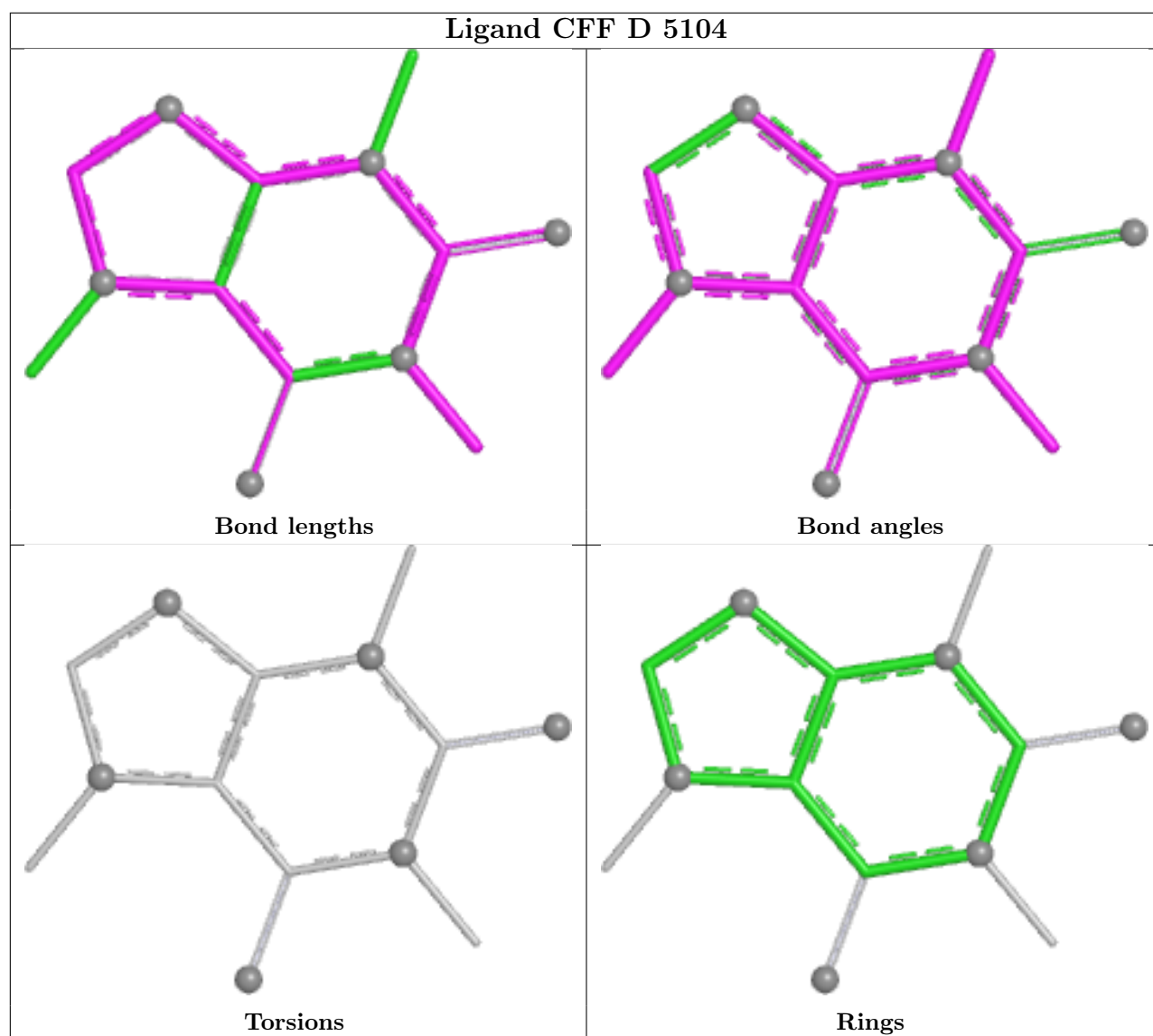












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

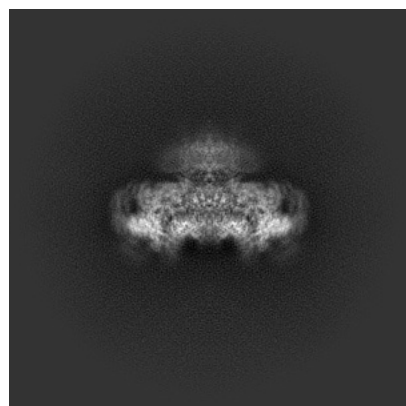
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38447. These allow visual inspection of the internal detail of the map and identification of artifacts.

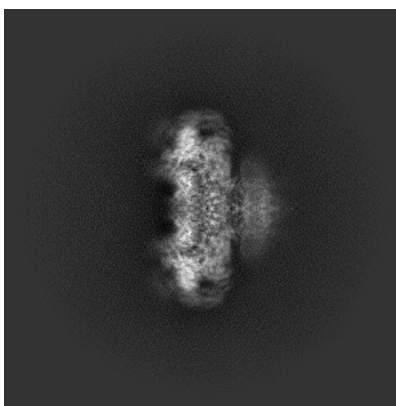
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

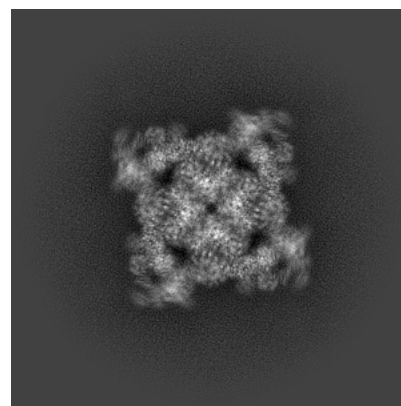
6.1.1 Primary map



X

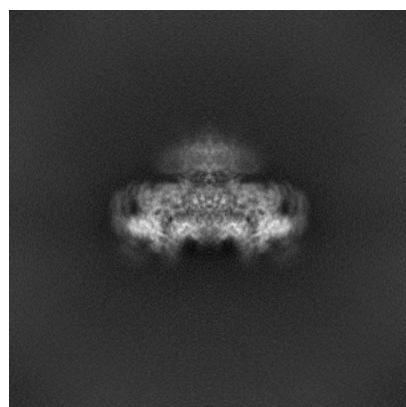


Y

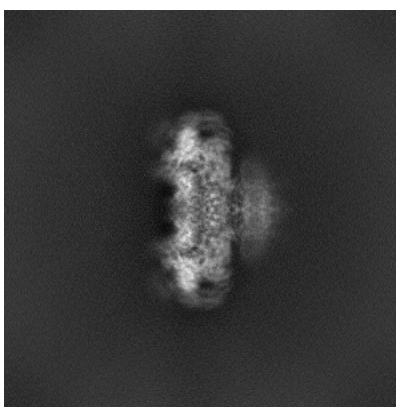


Z

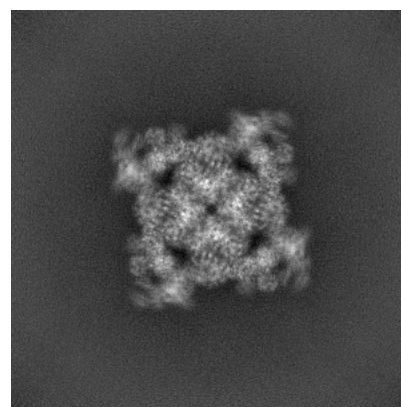
6.1.2 Raw map



X



Y

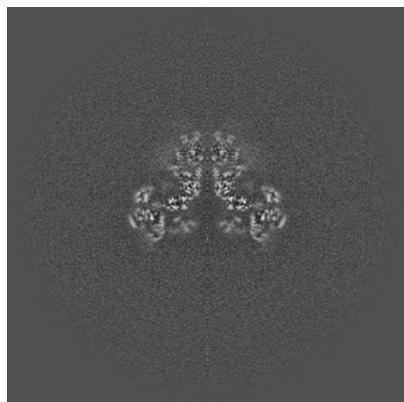


Z

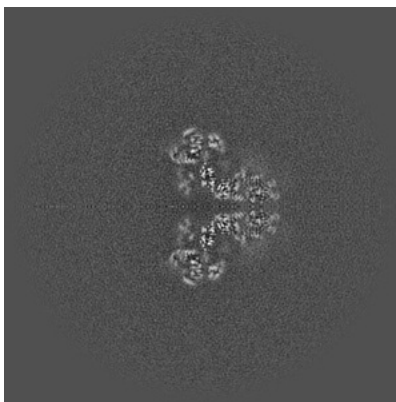
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

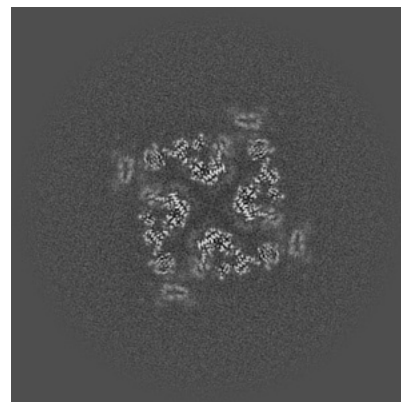
6.2.1 Primary map



X Index: 240

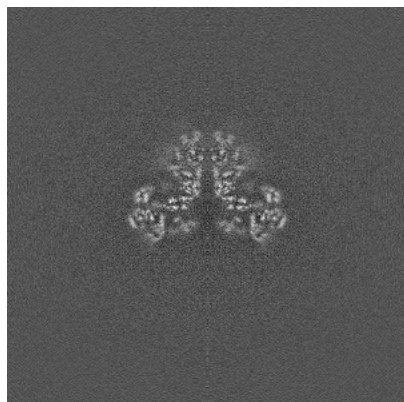


Y Index: 240

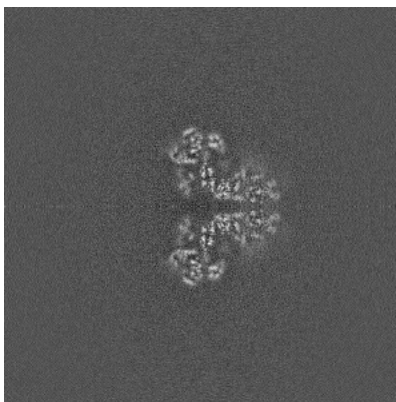


Z Index: 240

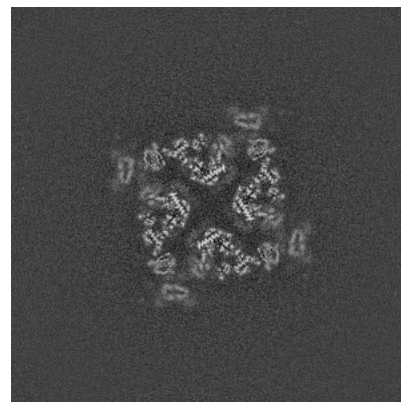
6.2.2 Raw map



X Index: 240



Y Index: 240

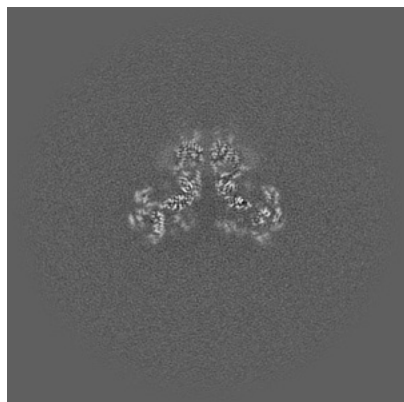


Z Index: 240

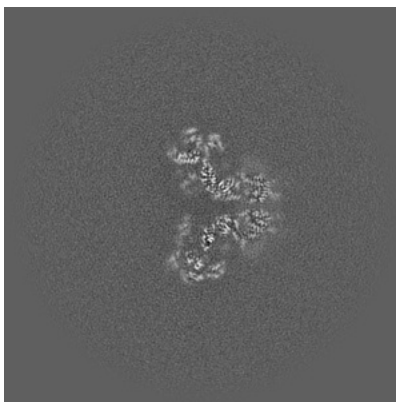
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

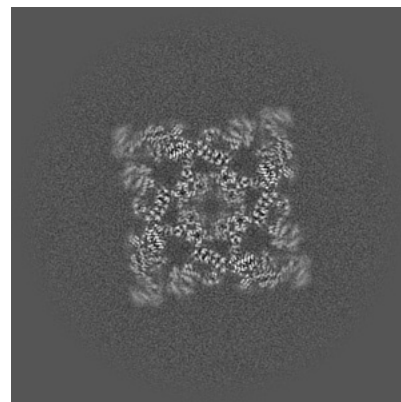
6.3.1 Primary map



X Index: 238

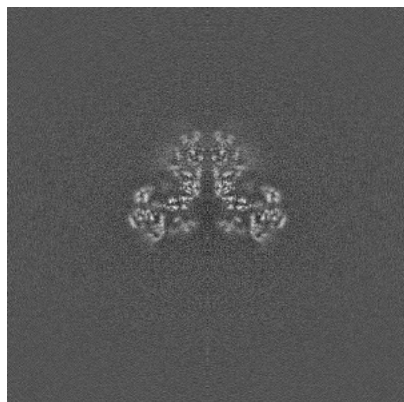


Y Index: 238

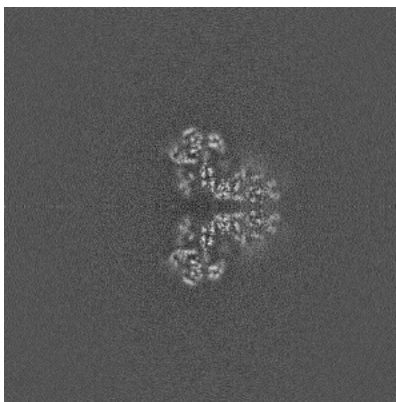


Z Index: 223

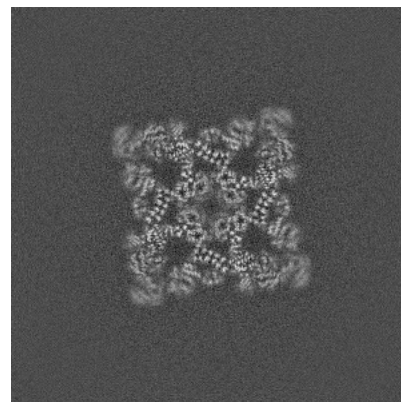
6.3.2 Raw map



X Index: 240



Y Index: 240

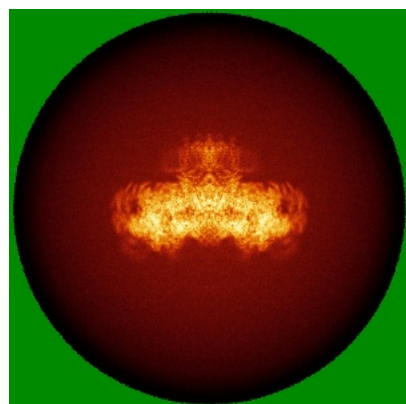


Z Index: 222

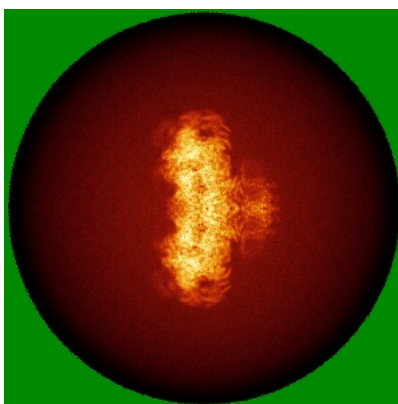
The images above show the largest variance slices of the map in three orthogonal directions.

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

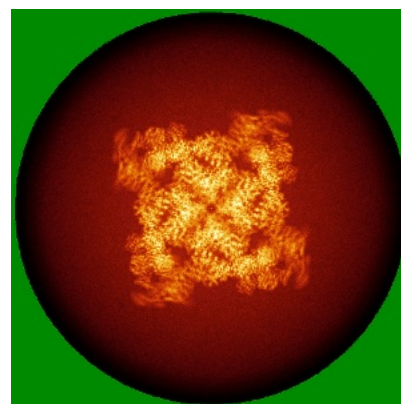
6.4.1 Primary map



X

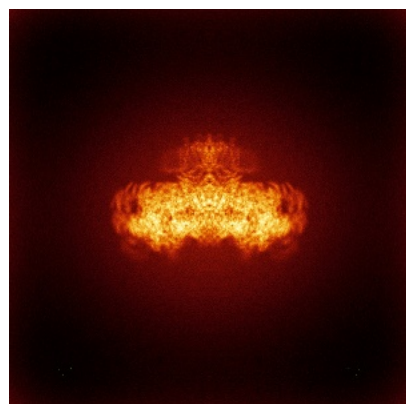


Y

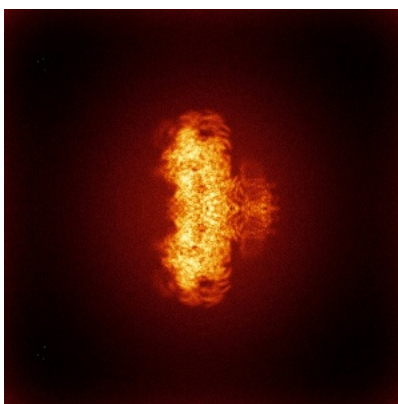


Z

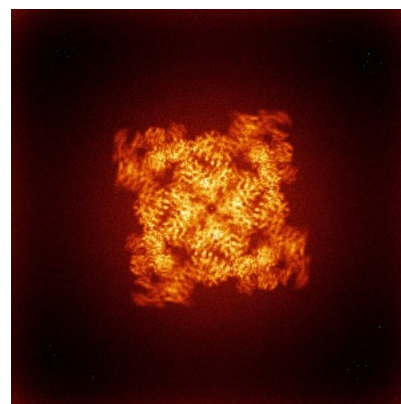
6.4.2 Raw map



X



Y

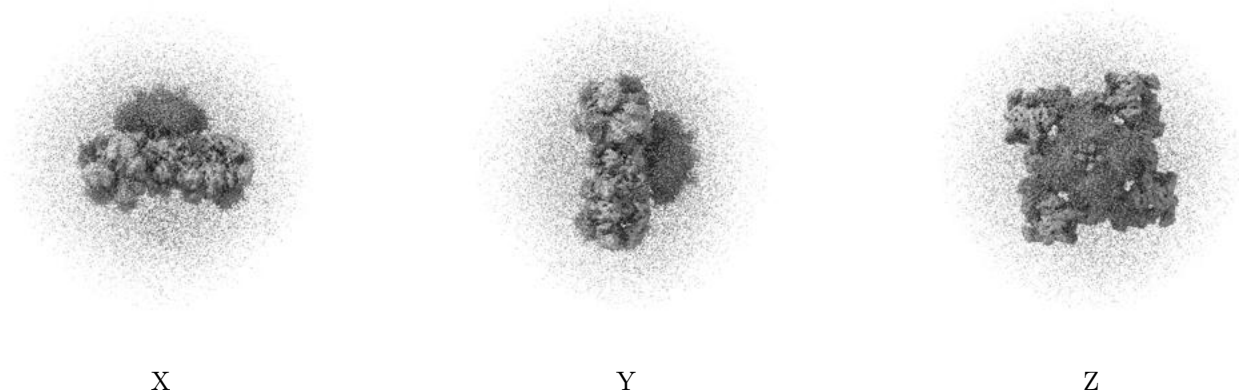


Z

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.

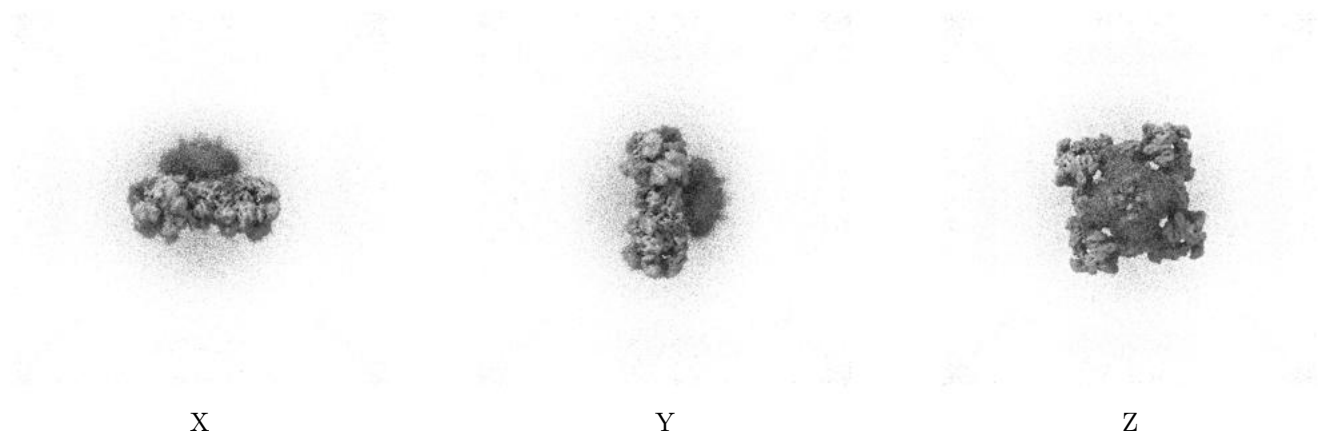
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

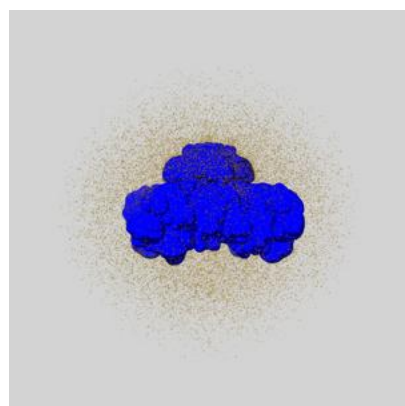
6.6 Mask visualisation [i](#)

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

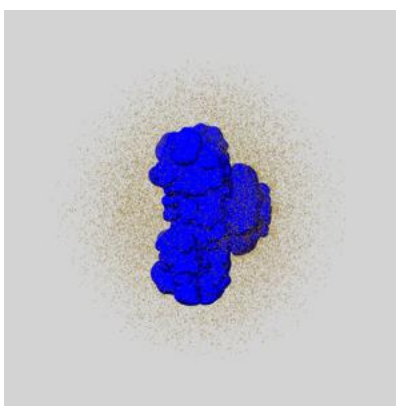
A mask typically either:

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

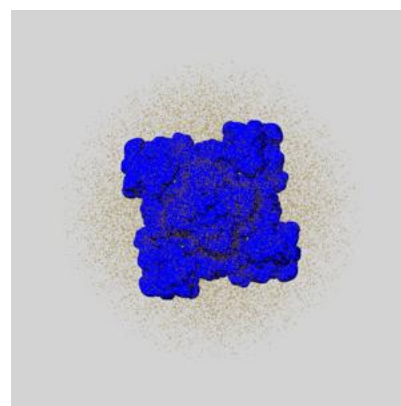
6.6.1 emd_38447_msk_1.map [i](#)



X



Y

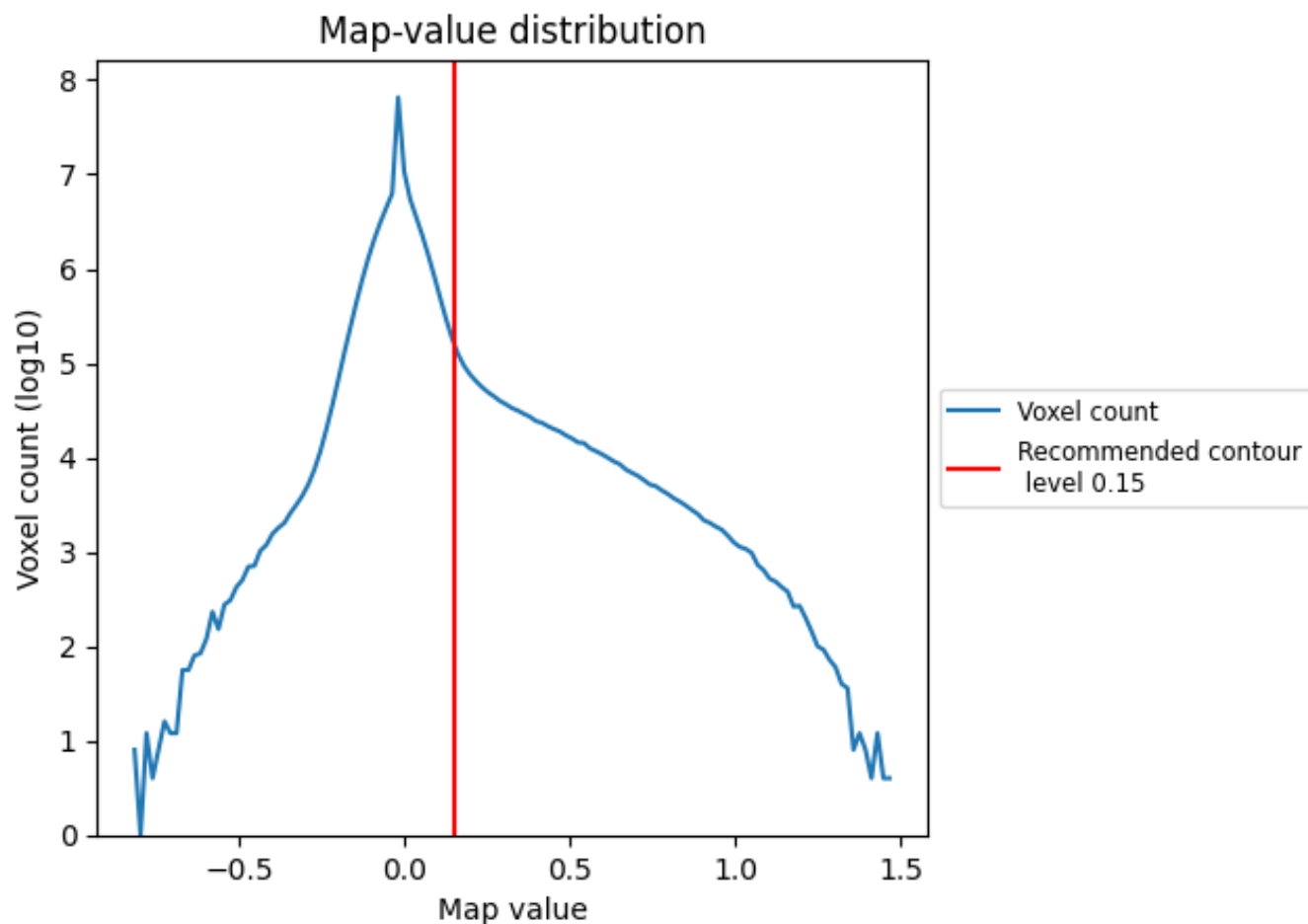


Z

7 Map analysis [i](#)

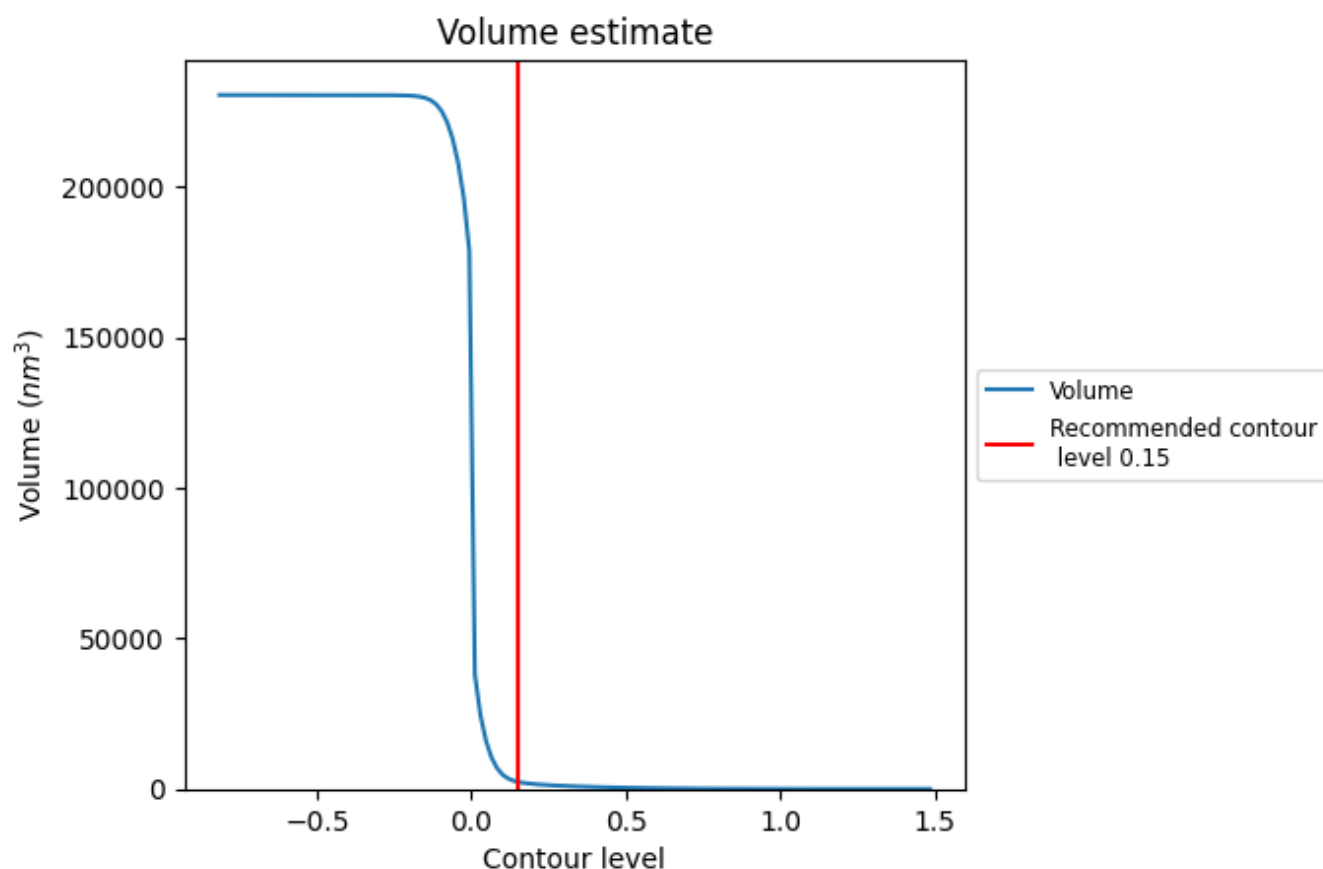
This section contains the results of statistical analysis of the map.

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.

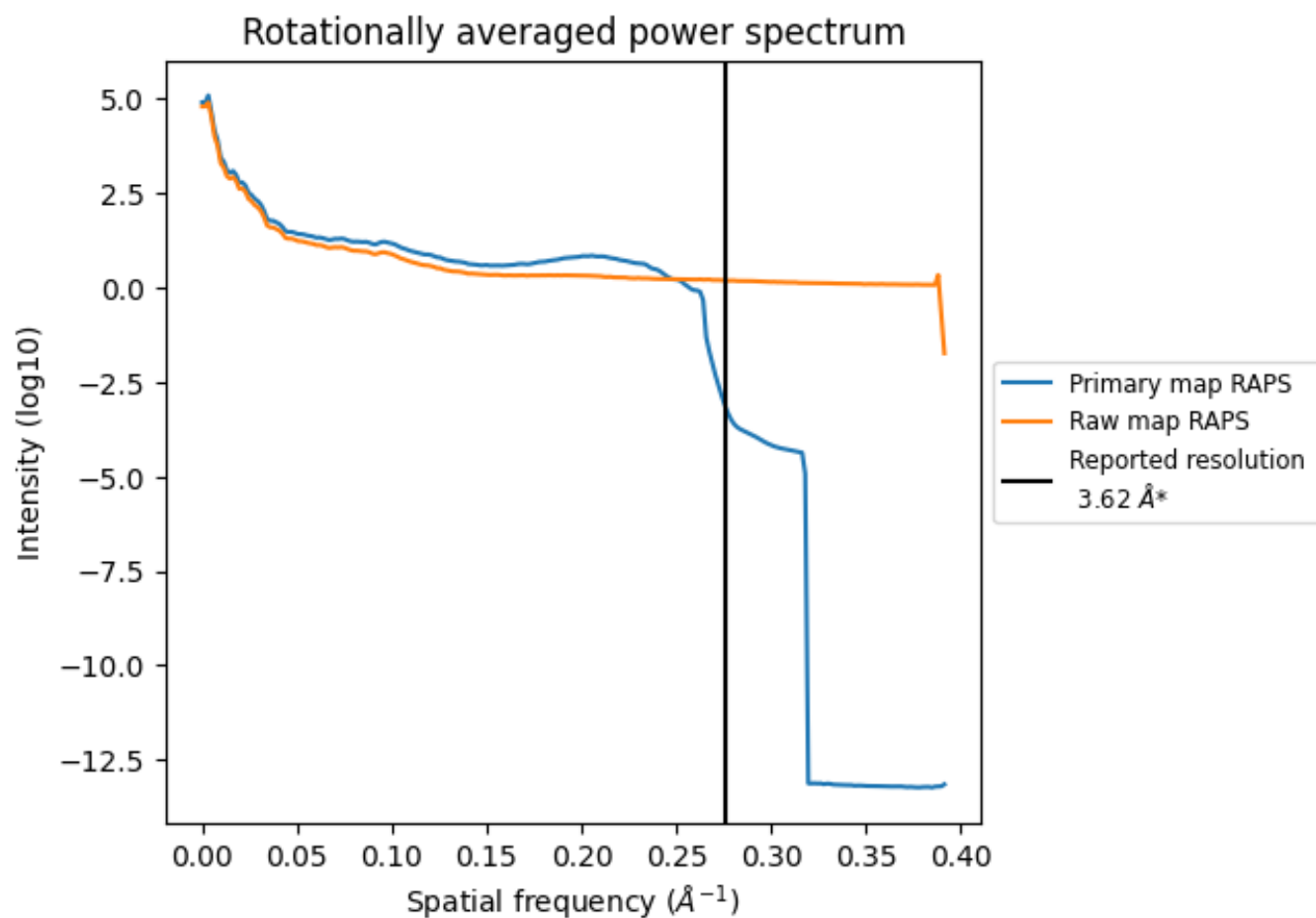
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2397 nm^3 ; this corresponds to an approximate mass of 2166 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 ⓘ

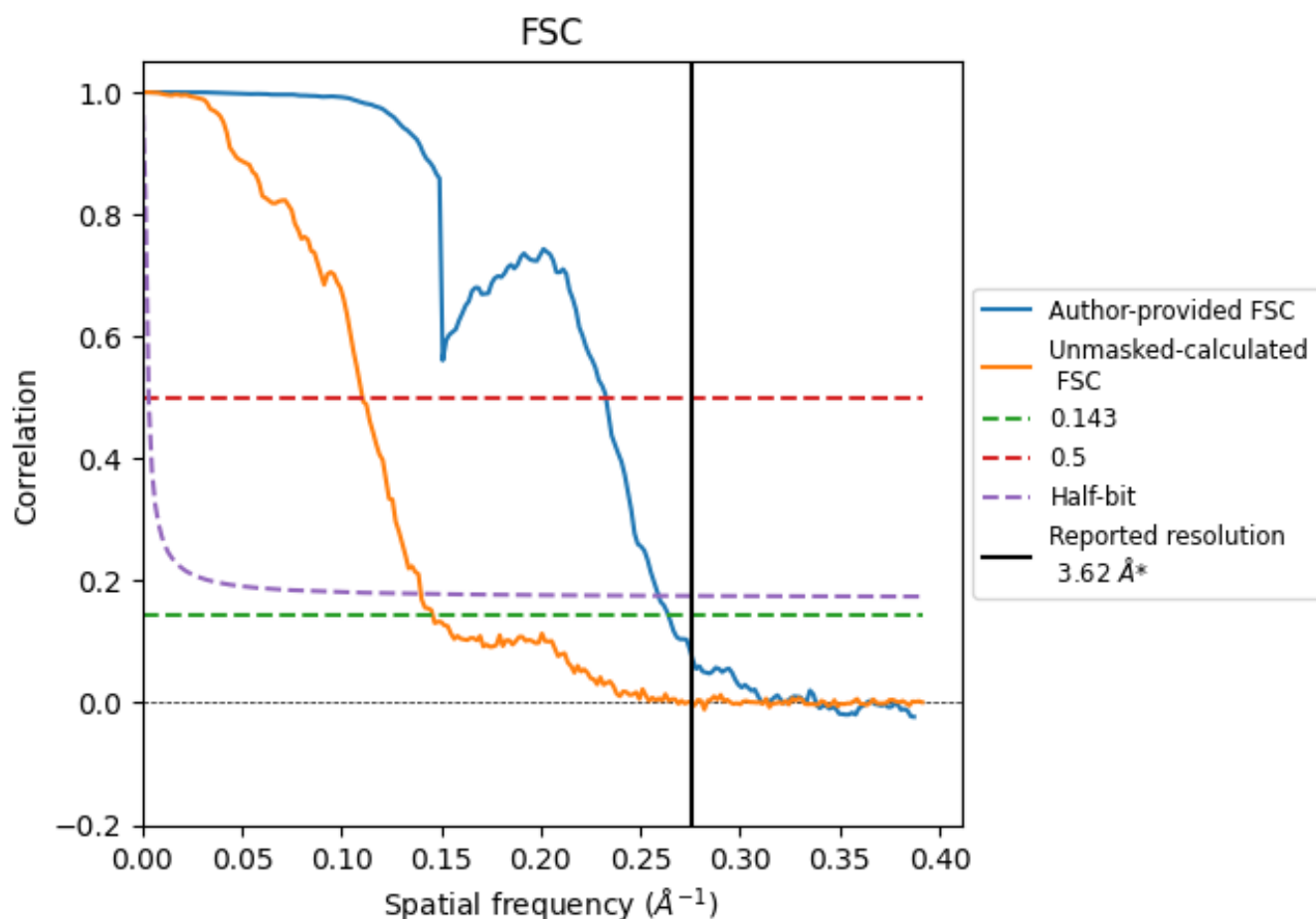


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

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 $0.276 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

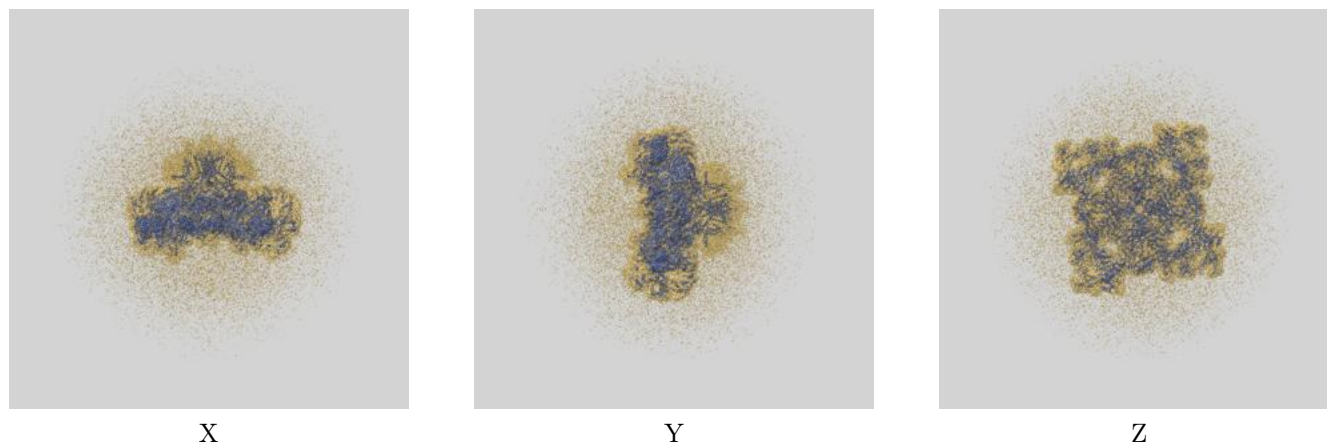
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.79	4.30	3.86
Unmasked-calculated*	6.86	9.05	7.15

*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 6.86 differs from the reported value 3.62 by more than 10 %

9 Map-model fit [i](#)

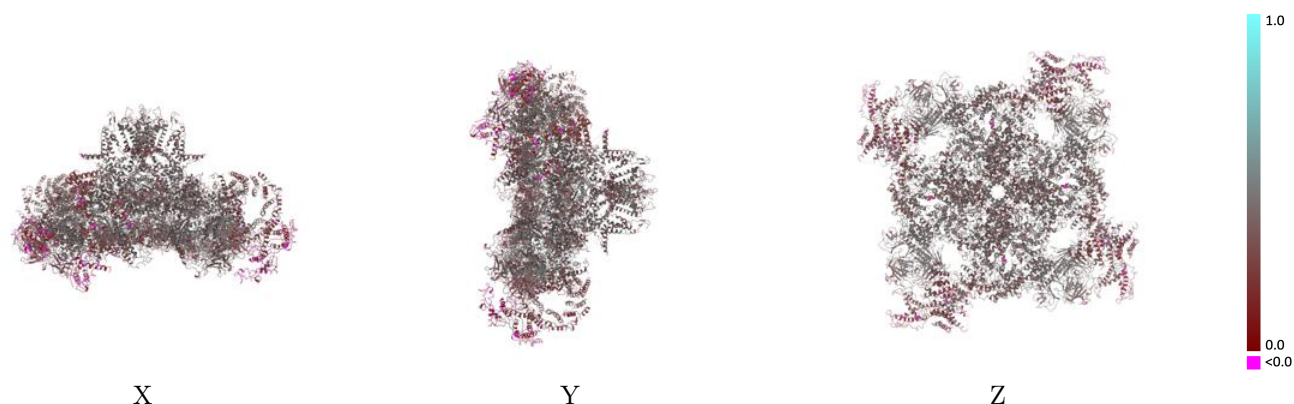
This section contains information regarding the fit between EMDB map EMD-38447 and PDB model 8XLF. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



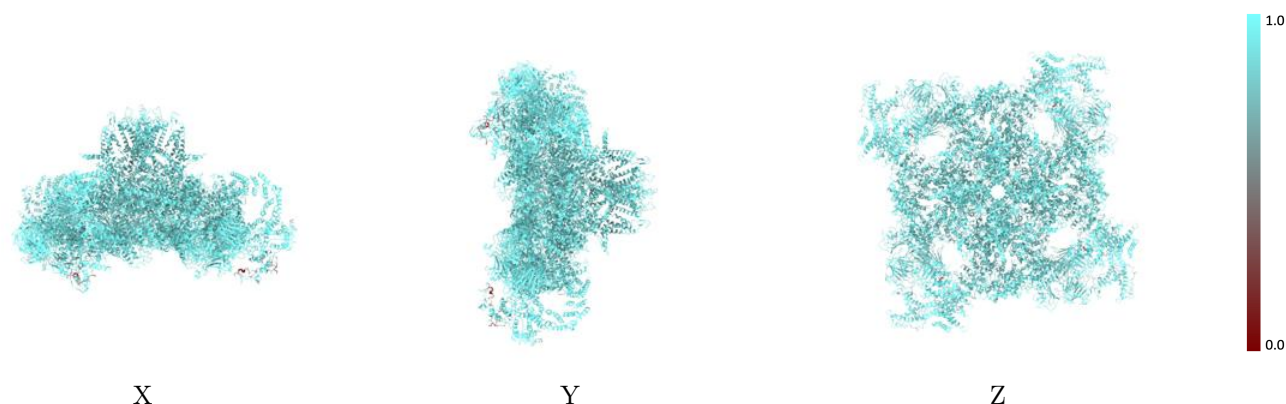
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



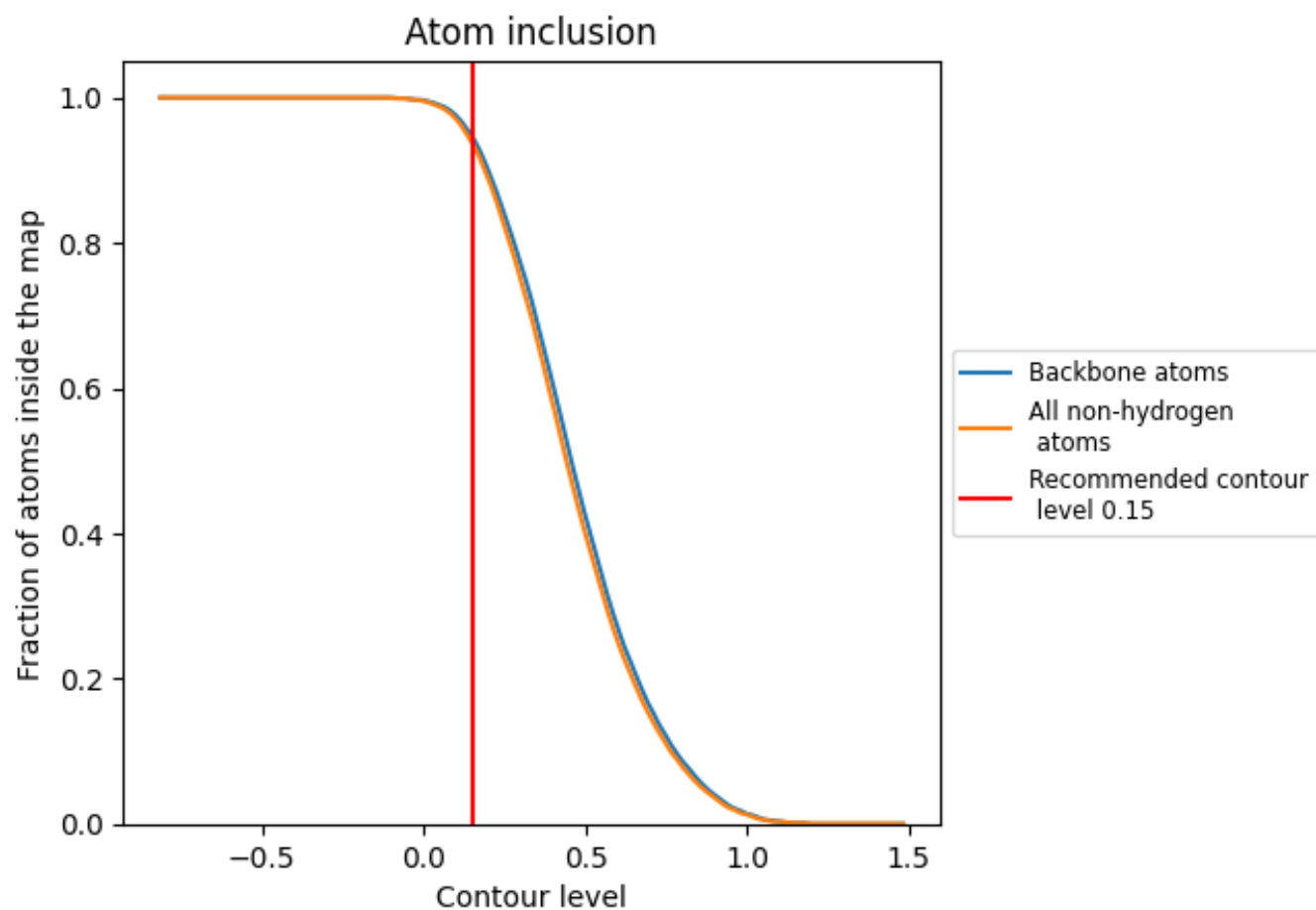
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.3750
A	0.9410	0.3780
B	0.9410	0.3780
C	0.9410	0.3780
D	0.9410	0.3790
E	0.9510	0.3920
F	0.9510	0.3890
G	0.9530	0.3890
H	0.9510	0.3910
I	0.8990	0.2850
J	0.9000	0.2880
K	0.8990	0.2870
L	0.9010	0.2840

1.0

0.0

<0.0