



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:28 PM UTC

PDB ID : 5TA3 / pdb_00005ta3
EMDB ID : EMD-8377
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

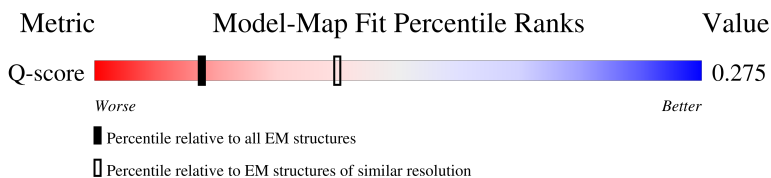
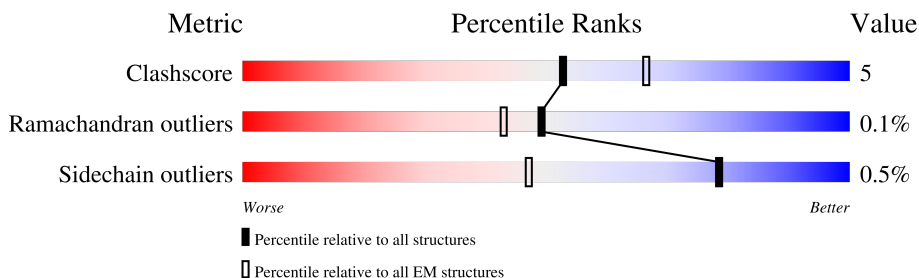
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	108	69% 76% 23% .
1	F	108	69% 72% 27% .
1	H	108	69% 73% 26% .
1	J	108	69% 71% 28% .

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Mol	Chain	Length	Quality of chain
2	B	4416	64% 83% 11% 5%
2	E	4416	63% 83% 12% 5%
2	G	4416	63% 83% 11% 5%
2	I	4416	63% 83% 12% 5%

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

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

2 Entry composition

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

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

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

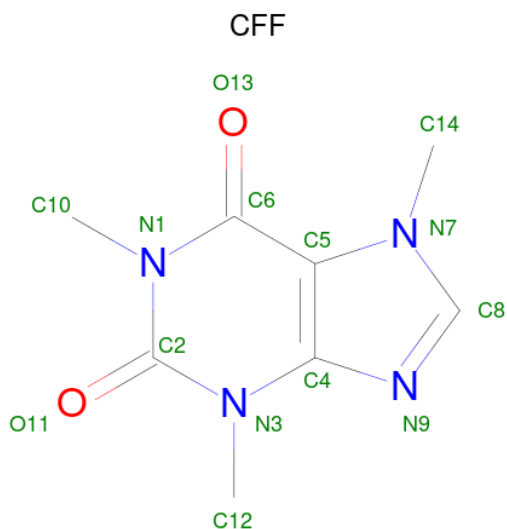
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



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

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



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

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

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

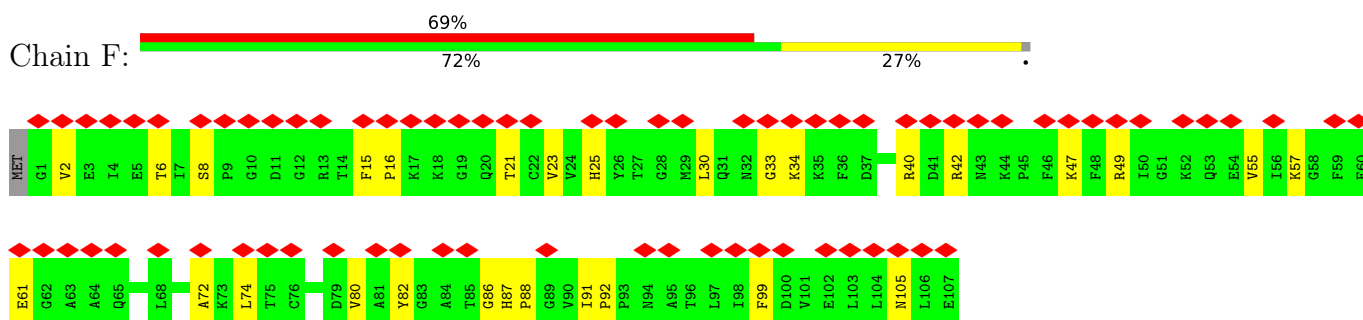
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

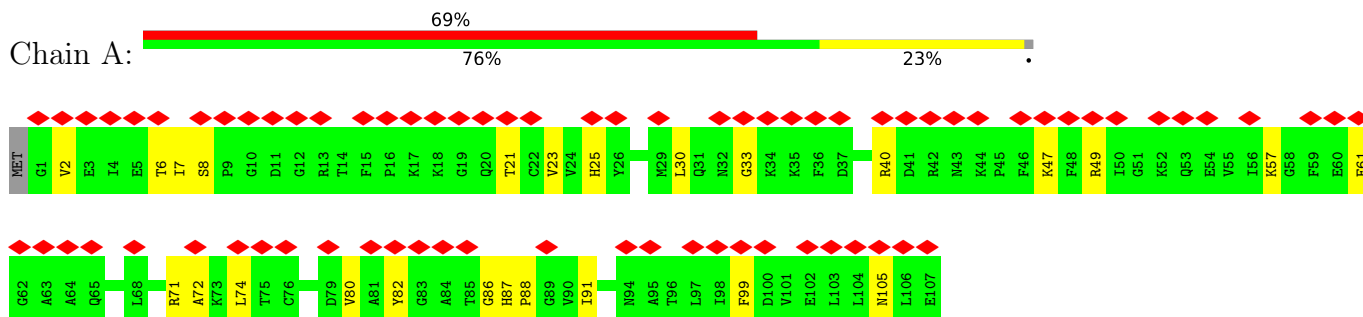
3 Residue-property plots [i](#)

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

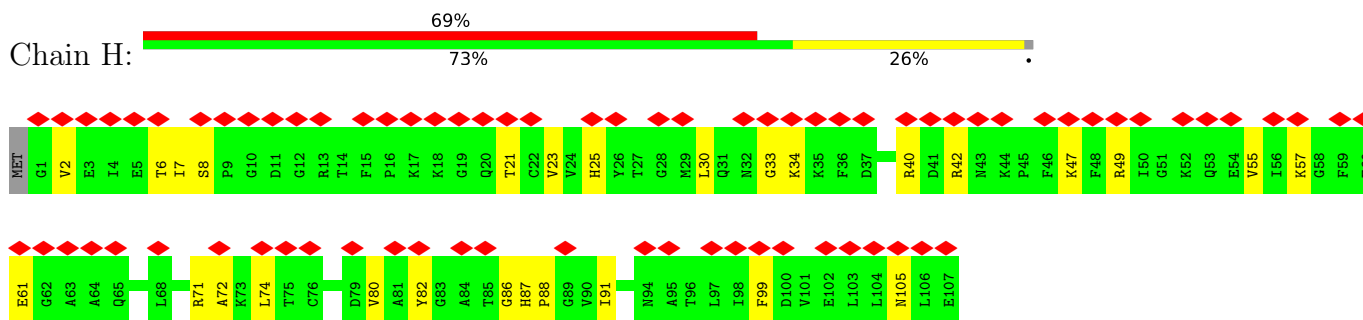
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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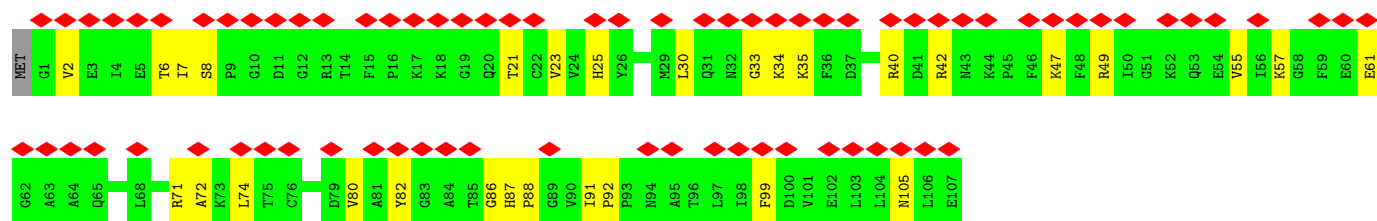


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

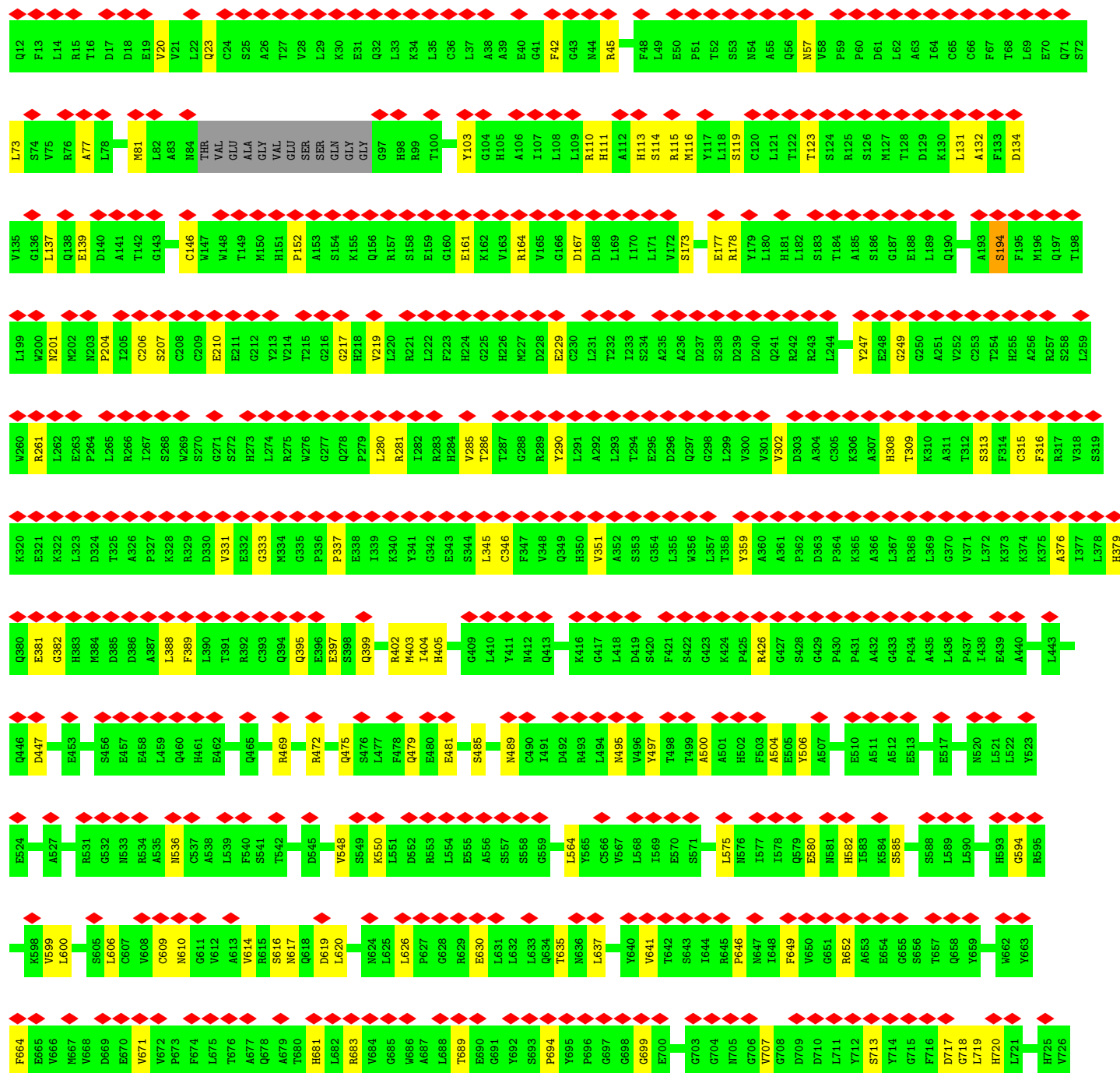
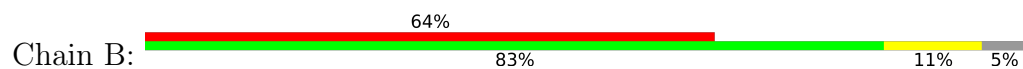


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

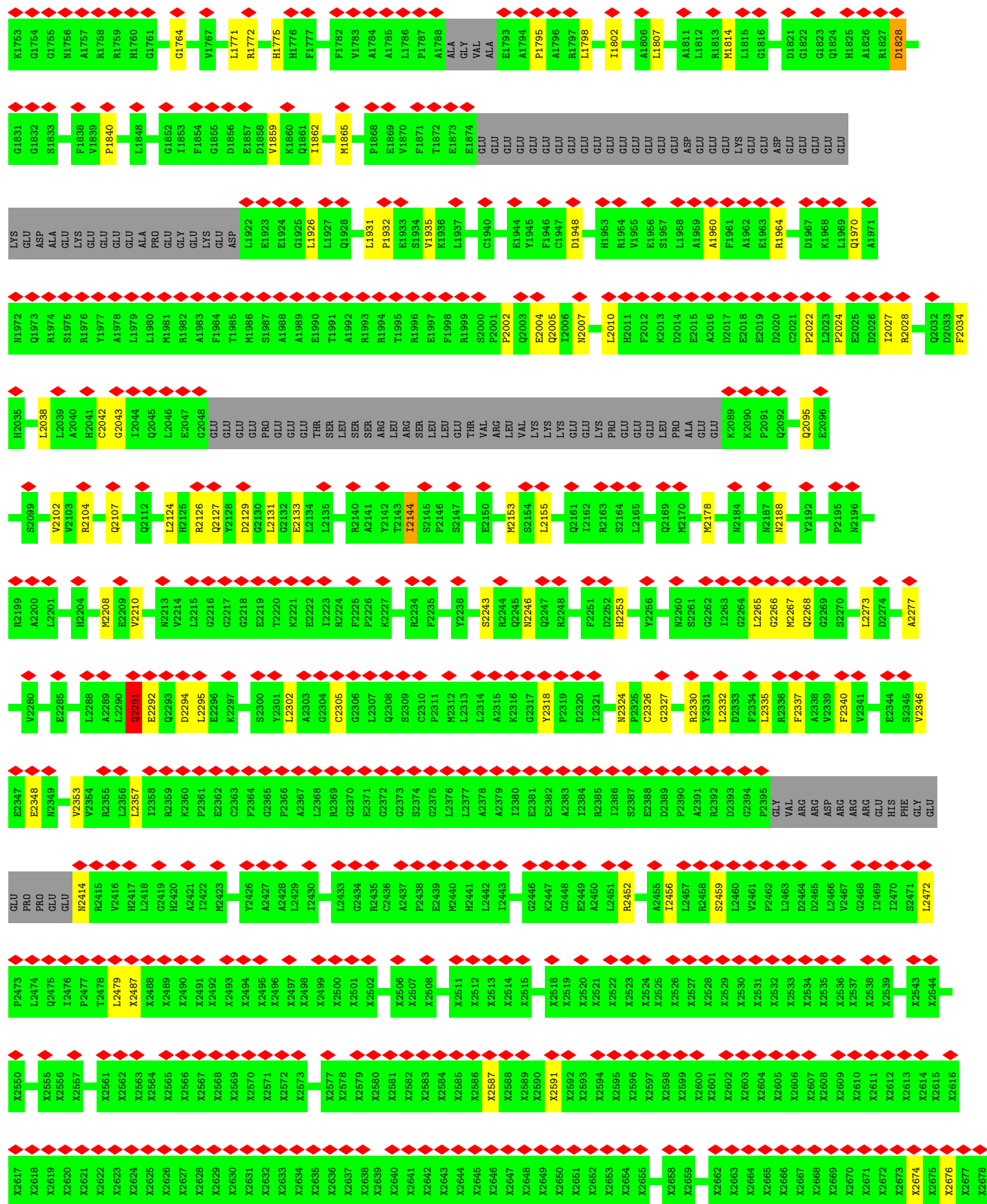




• Molecule 2: Ryanodine receptor 1

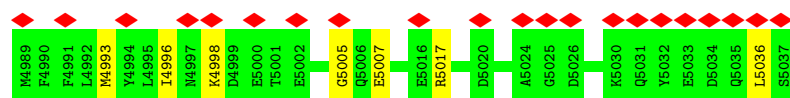


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X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1537	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1554	X1555	X1558	M1573	P1574	L1575	S1576	A1577	A1578	M1579	F1580	E1583	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	E1596	V1597	Q1598	M1599	L1600	V1603	S1604	W1605								
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T1163	L1164	M1165	G1166	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	I1184	G1185	D1186	G1187	F1188	V1191	C1192	S1193	L1194	G1195	Q1198	V1199	G1200	H1201	L1202	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	A1215	L1216	C1217	G1218	L1219	Q1220	E1221	G1222	F1223	A1227						
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Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	
H974	V975	R976	L977	T978	P979	Q980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	E990	R991	G992	A997	R998	D999	R1000	V1001	A1002	Q1003	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040			
C954	P955	V956	D957	THR	VAL	GLN	I961	V962	L963	P964	P965	H966	L967	R968	R969	I970	R971	E972	K973	L974	A975	R976	N977	I978	H979	E980	L981	W982	A983	L984	T985	R986	I987	E988	Q989	G990	W991	T992	Y993	G994	P995	V996	R997	G998	D999	N990	K991	R992	L993	H994	C995	L996	S997	H998	T999	D999	F999	L999	
P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	N961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973
V789	R790	F791	L792	G793	G795	R796	H797	G798	E799	F800	K801	F802	P804	P805	P806	G807	Y808	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	S843	R844	C845	L846	S847	H848	T849	D850	F851	V852	P853					
A727	R728	P729	V730	T731	S732	P733	Q735	H736	L737	L738	A739	P740	E741	L803	D742	S745	C746	C747	L748	D749	L750	S751	V752	P753	S754	F757	R758	I759	N760	G761	C762	P763	V764	Q765	G766	V767	F768	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780	V781	S782	F783	S784	A785	G786	V787	K788			

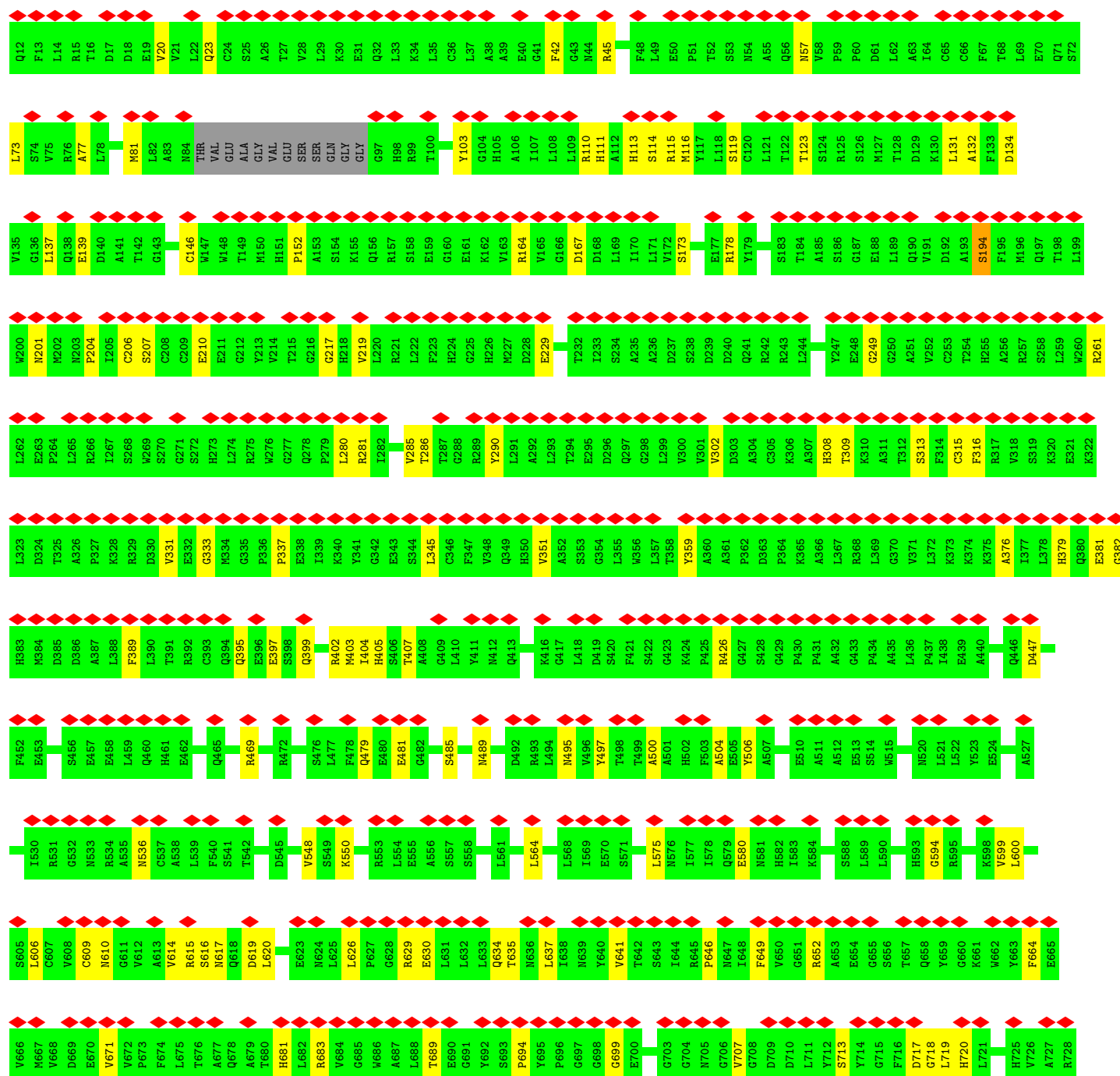
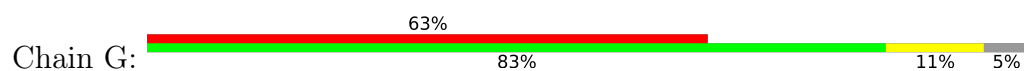


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X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444											X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518									
X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414																		
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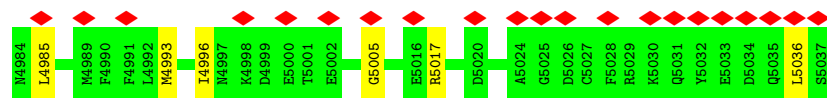




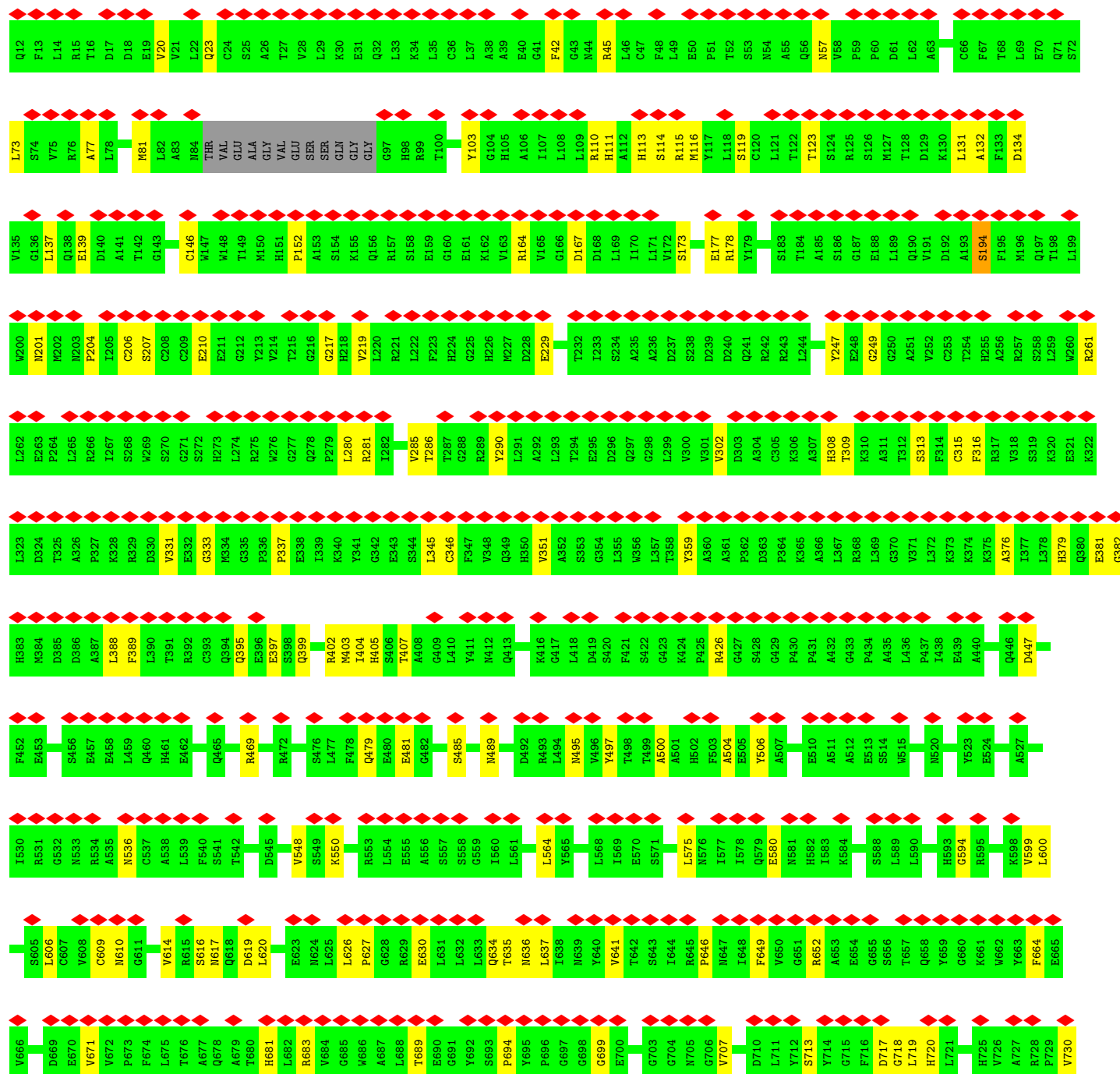
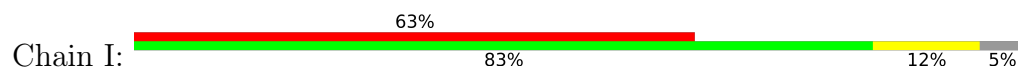


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L4937	E4674	L4740	ALA	M4231	R4159	G4086	K4014	G3939	R3769	R3769	K3694
E4942	K4675	L4741	ASP	E4232	L4160	L4087	E4015	K3940	T3772	T3772	L3698
L4943	K4675	G4742	LEU	E4239	R4161	S4089	D4018	V3942	R3773	R3773	H3699
D4945	E4674	M4743	GLY	D4240	M4162	K4090	L4019	I3943	G3774	G3774	Q3700
Q4946	K4675	D4744	GLY	Q4250	F4163	D4092	D4022	E3944	L3780	L3780	H3704
E4952	R4679	L4745	GLY	T4251	E4165	F4093	D4022	Q3946	Q3781	Q3781	H3707
E4957	K4680	A4746	GLY	E4252	A4167	Q4094	L4031	G3947	S3784	S3784	L3710
L4960	L4681	S4747	GLY	E4253	E4168	K4095	E4032	Q3948	G3788	G3788	E3712
C4961	L4682	E4748	GLY	X4320	S4169	A4096	G4033	R3949	E3789	E3789	K3713
L4963	E4683	E4749	GLY	X4321	I4170	M4097	N4034	N3950	L3804	L3804	S3714
S4965	F4684	L4751	TRP	X4322	L4171	D4098	N4037	K3953	N3805	N3805	K3715
D4966	G4685	A4752	GLY	X4322	L4171	Q4100	G4038	A3954	L3806	L3806	L3716
D4969	L4686	H4753	ALA	X4330	E4172	Q4102	A4041	M3955	G3807	G3807	D3717
T4970	Y4687	N4754	GLY	X4330	F4174	K4101	A4041	F3962	G3808	G3808	D3718
D4974	L4688	E4755	GLY	X4340	R4175	Q4102	A4041	N3963	V3812	V3812	D3719
F4975	T4689	R4756	GLY	X4341	L4178	F4103	R4042	T3881	Q3813	Q3813	A3726
L4983	E4690	K4757	GLU	X4342	G4179	T4104	Q4043	F3881	Q3814	Q3814	D3727
S4985	Q4691	P4758	ALA	X4343	E4181	G4105	M4044	Q3982	M3816	M3816	L3728
D4986	P4692	D4759	GLY	X4344	E4182	G4105	V4045	D3877	L3817	L3817	D3720
A4855	G4693	P4760	ASP	X4345	I4181	P4106	D4046	F3880	V3812	V3812	A3726
R4860	D4694	P4761	ASP	X4345	E4182	E4107	M4047	T3881	Q3813	Q3813	A3726
K4861	D4695	P4762	GLU	W4541	L4108	I4108	M4047	Q3882	Q3814	Q3814	D3727
K4865	D4696	G4763	GLY	G4542	Q4109	F4110	V4049	D3883	M3816	M3816	L3728
S4866	D4697	L4764	ASP	E4543	F4110	L4111	E4050	L3884	K3821	K3821	K3731
E4867	K4697	L4765	GLY	E4544	L4112	L4112	S4053	F3885	D3822	D3822	S3732
D4868	C4699	T4766	GLY	E4545	S4113	E4113	E4056	R3886	H3734	H3734	C3733
E4869	R4703	K4767	ASP	V4546	E4116	E4116	E4056	Q3889	L3735	L3735	L3736
D4870	L4704	L4768	GLY	Q4547	A4117	A4117	E4056	L3890	E3825	E3825	E3736
	F4711	M4769	GLY	F4551	R4192	D4118	L4059	N3997	V3826	V3826	E3737
	Y4715	S4770	GLY	Y4554	I4193	E4119	K4060	F3898	G3827	G3827	C3738
	W4716	D4771	GLY	Y4554	F4195	F4061	F4062	Q3900	F3829	F3829	G3739
		D4772	GLY	R4557	E4196	E4121	D4063	N3901			E3740
		Y4775	GLY		I4197	I4122		R3904			N3741
		Q4776	GLY			I4123					GLY
		I4777	GLY								



Molecule 2: Ryanodine receptor 1

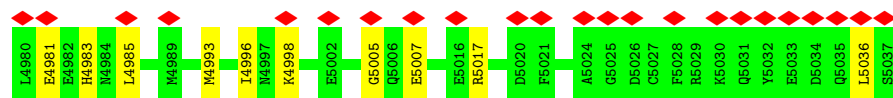




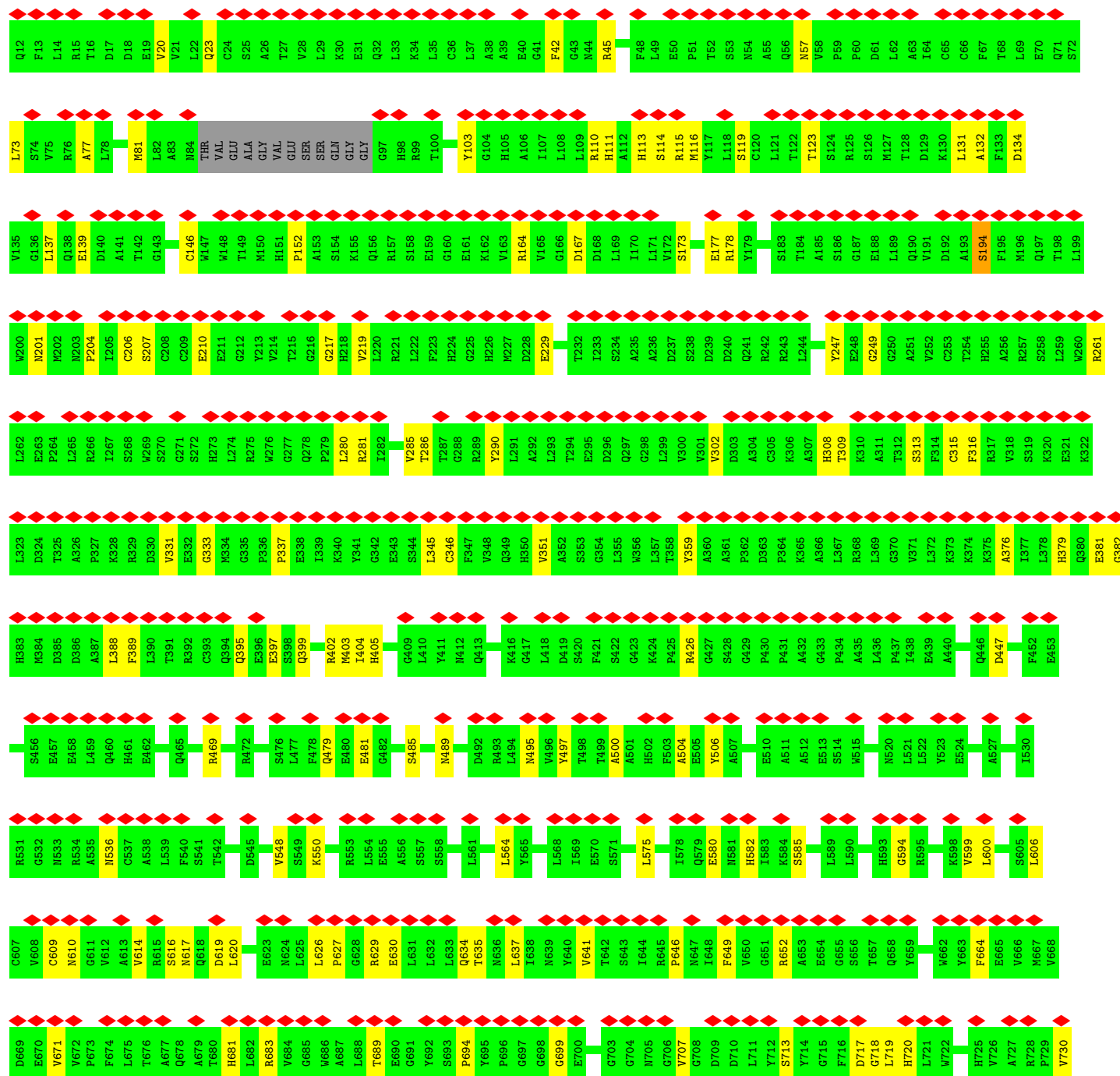
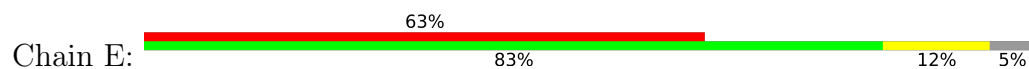








• Molecule 2: Ryanodine receptor 1

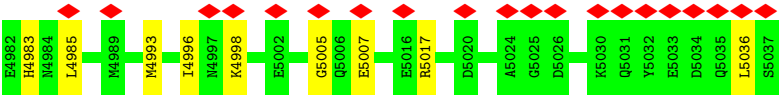












4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.029	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.47	0/1123
1	J	0.20	0/834	0.46	0/1123
2	B	0.21	0/25428	0.53	8/34534 (0.0%)
2	E	0.21	0/25428	0.53	6/34534 (0.0%)
2	G	0.21	0/25428	0.53	6/34534 (0.0%)
2	I	0.21	0/25428	0.53	6/34534 (0.0%)
All	All	0.21	0/105048	0.53	26/142628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2807	TRP	CA-C-N	-7.95	111.88	120.94
2	G	2807	TRP	C-N-CA	-7.95	111.88	120.94
2	B	2807	TRP	CA-C-N	-7.93	111.90	120.94
2	B	2807	TRP	C-N-CA	-7.93	111.90	120.94
2	I	2807	TRP	CA-C-N	-7.92	111.91	120.94

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	18	0
1	H	818	0	824	17	0
1	J	818	0	824	19	0
2	B	29499	0	24746	288	0
2	E	29499	0	24745	291	0
2	G	29499	0	24745	281	0
2	I	29499	0	24745	290	0
3	B	31	0	12	2	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102365	1191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1191 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.52	0.74
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.73
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.71	0.73
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.52	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	43	77
2	G	3235/4416 (73%)	2881 (89%)	349 (11%)	5 (0%)	43	77
2	I	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	43	77
All	All	13360/18096 (74%)	11903 (89%)	1437 (11%)	20 (0%)	49	83

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	B	4641	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	E	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	G	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	I	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
All	All	10324/12444 (83%)	10268 (100%)	56 (0%)	78	81

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	131	LEU

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Mol	Chain	Res	Type
2	E	4792	LEU
2	I	2144	ILE
2	E	4166	LEU
2	E	2144	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 216 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	395	GLN
2	I	3850	GLN
2	E	3900	GLN
2	I	520	ASN
2	I	1775	HIS

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
4	CFF	I	5102	-	15,15,15	1.95	7 (46%)	23,23,23	2.78	11 (47%)
4	CFF	E	5102	-	15,15,15	1.94	7 (46%)	23,23,23	2.78	11 (47%)
3	ATP	B	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.74	12 (25%)
4	CFF	B	5102	-	15,15,15	1.92	7 (46%)	23,23,23	2.78	11 (47%)
3	ATP	I	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.73	12 (25%)
4	CFF	G	5102	-	15,15,15	1.94	7 (46%)	23,23,23	2.78	11 (47%)
3	ATP	G	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.73	12 (25%)
3	ATP	E	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.74	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	E	5101	-	-	5/22/38/38	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5101	ATP	C5-C4	4.45	1.47	1.39
3	I	5101	ATP	C5-C4	4.43	1.47	1.39
3	B	5101	ATP	C5-C4	4.42	1.47	1.39
3	G	5101	ATP	C5-C4	4.42	1.47	1.39
4	I	5102	CFF	C6-N1	-3.92	1.32	1.40

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-7.87	111.56	126.28
4	I	5102	CFF	C14-N7-C8	-7.86	111.57	126.28
4	E	5102	CFF	C14-N7-C8	-7.84	111.61	126.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5102	CFF	C14-N7-C8	-7.83	111.62	126.28
3	E	5101	ATP	C5-C4-N3	-5.28	119.45	126.72

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

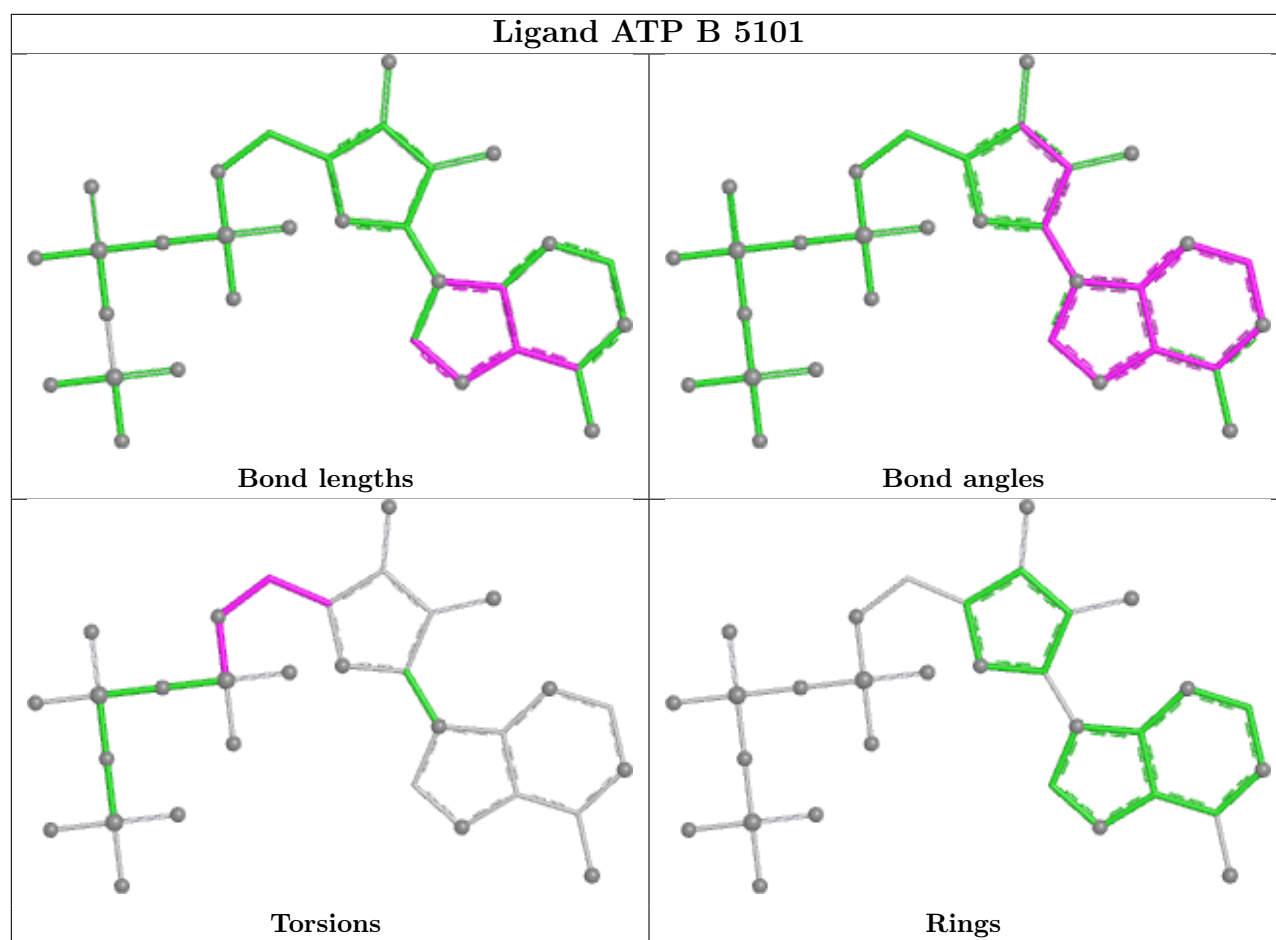
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A

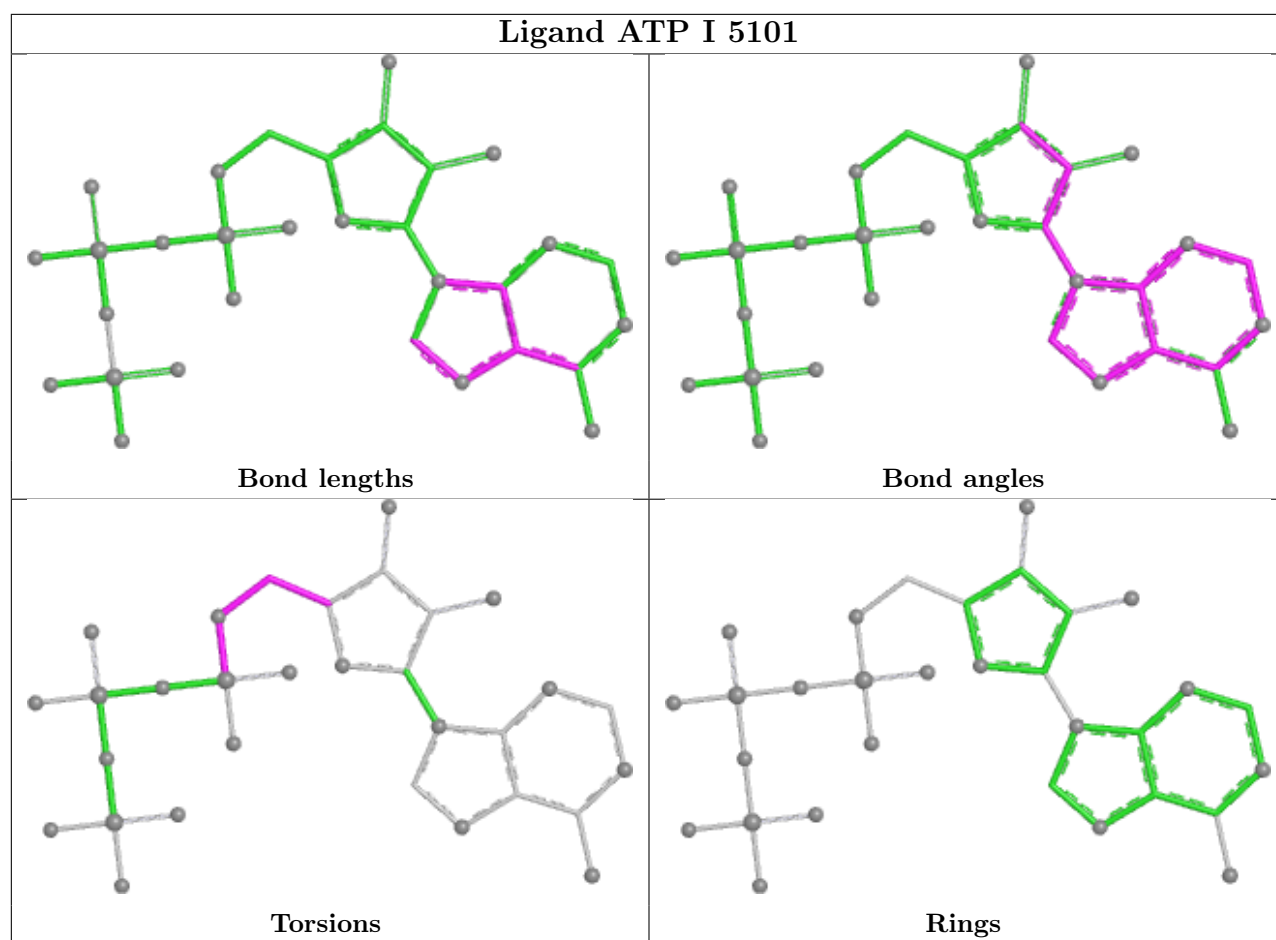
There are no ring outliers.

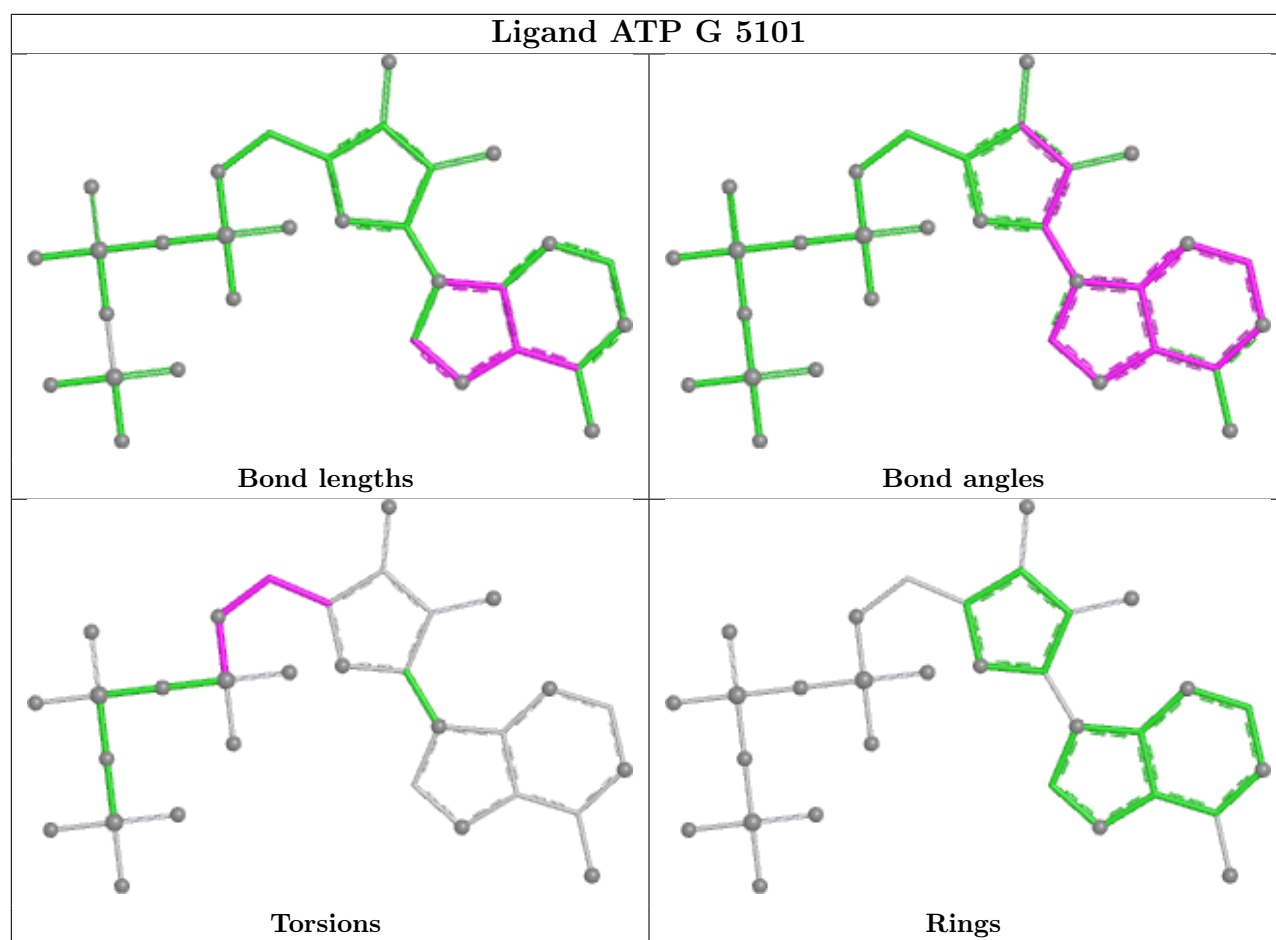
4 monomers are involved in 5 short contacts:

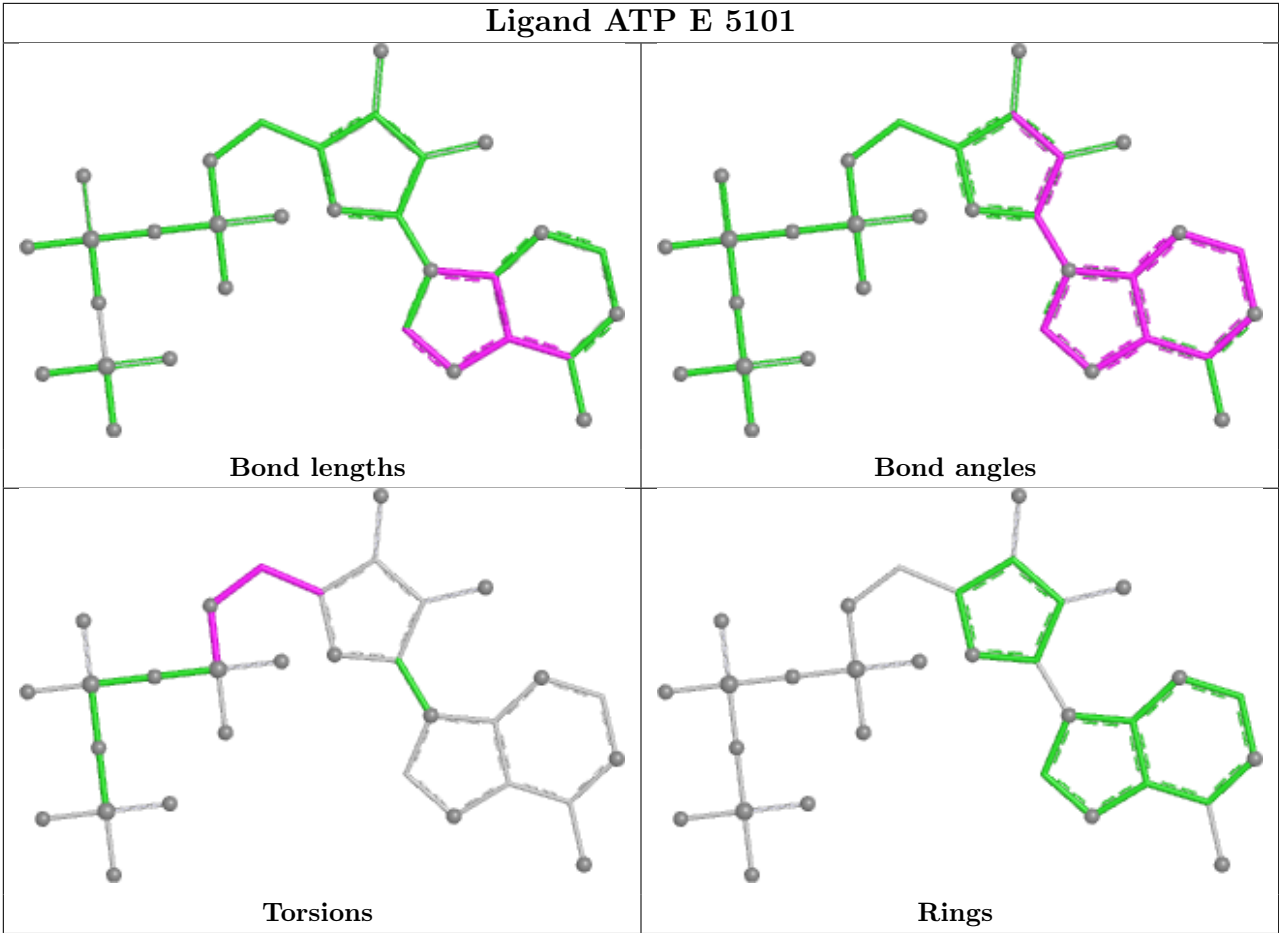
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
3	I	5101	ATP	1	0
3	G	5101	ATP	1	0
3	E	5101	ATP	1	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	73.04
1	B	4345:UNK	C	4540:PHE	N	73.02

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	73.01
1	G	4345:UNK	C	4540:PHE	N	73.00
1	E	3613:UNK	C	3639:THR	N	45.97

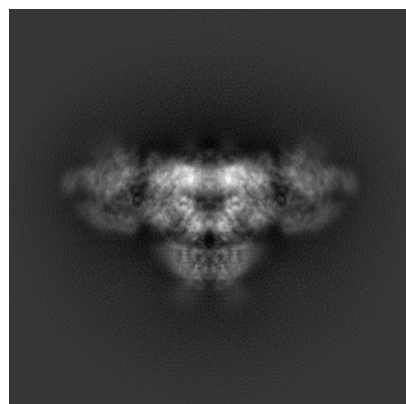
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8377. These allow visual inspection of the internal detail of the map and identification of artifacts.

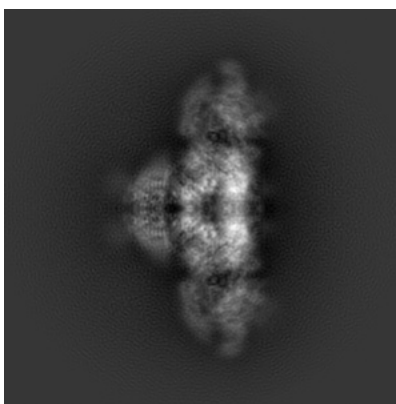
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

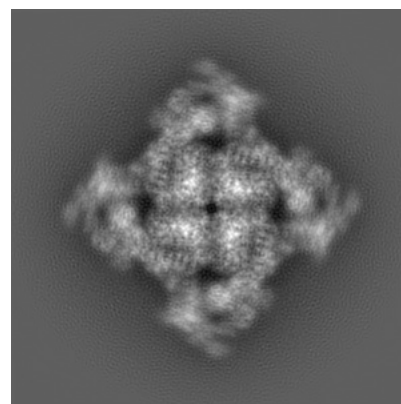
6.1.1 Primary map



X

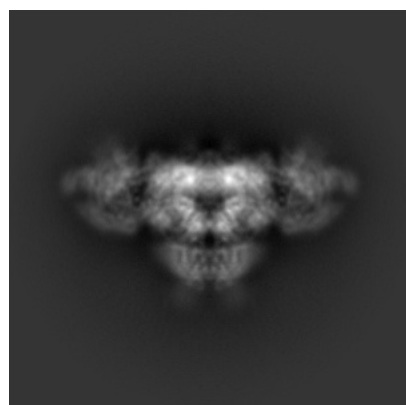


Y

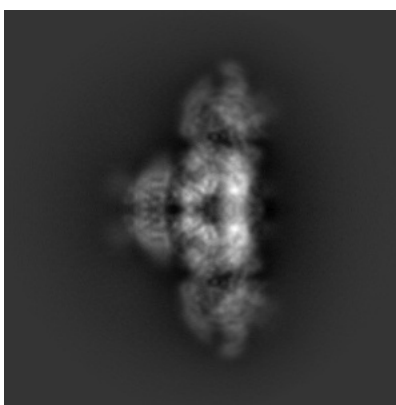


Z

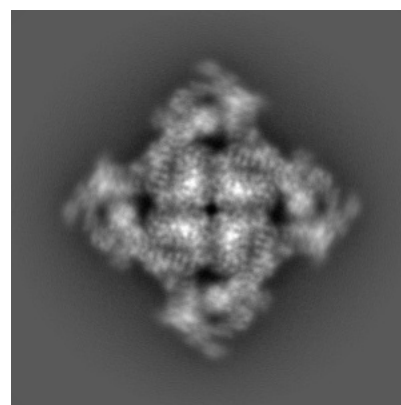
6.1.2 Raw map



X



Y

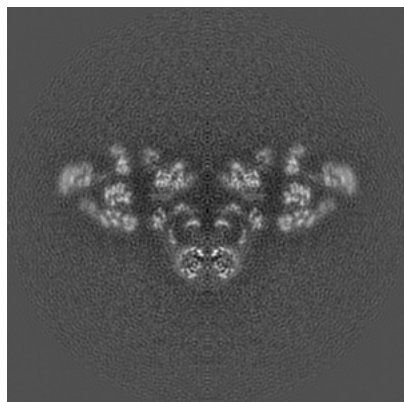


Z

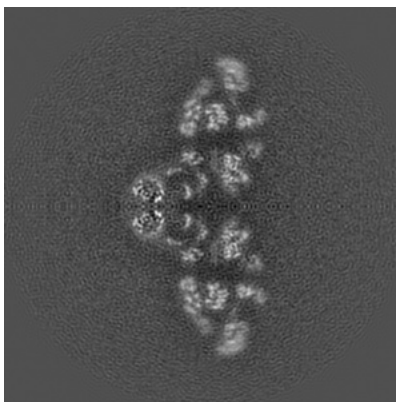
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

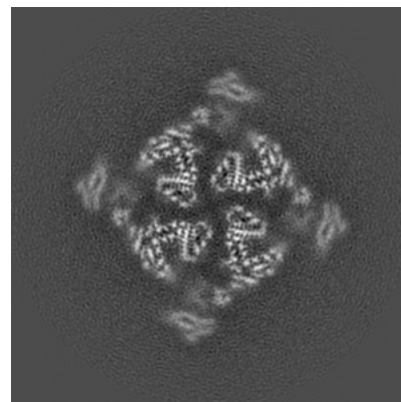
6.2.1 Primary map



X Index: 200

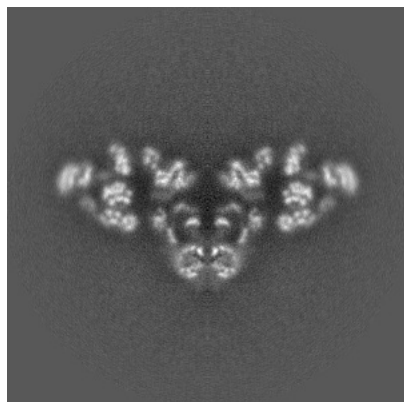


Y Index: 200

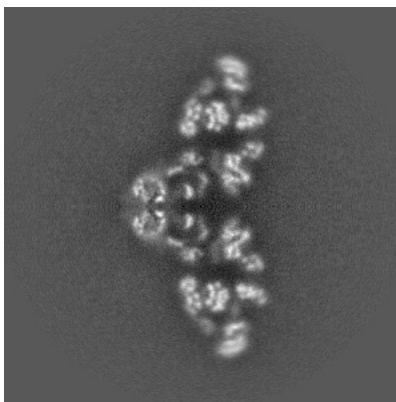


Z Index: 200

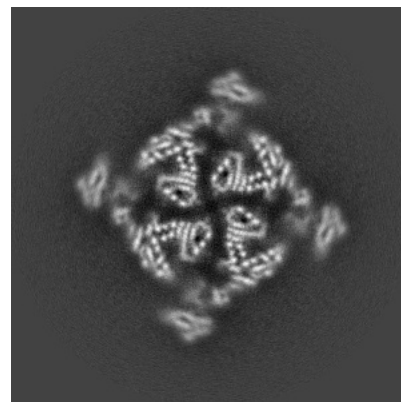
6.2.2 Raw map



X Index: 200



Y Index: 200

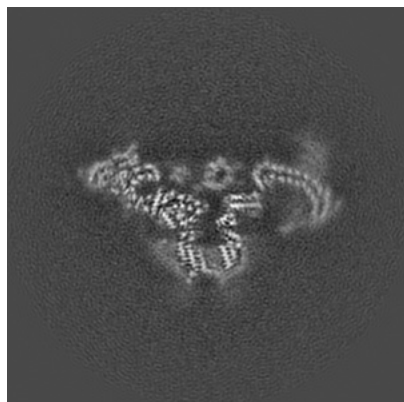


Z Index: 200

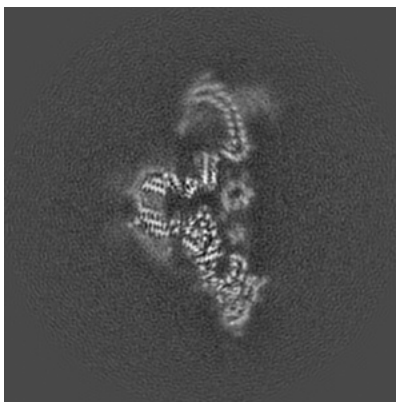
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

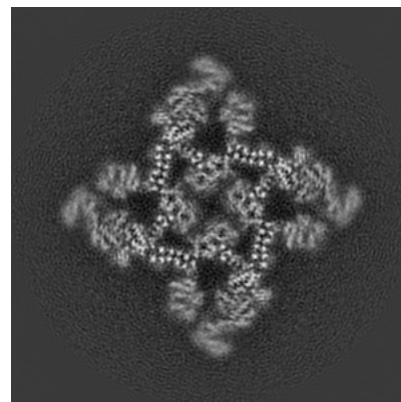
6.3.1 Primary map



X Index: 225

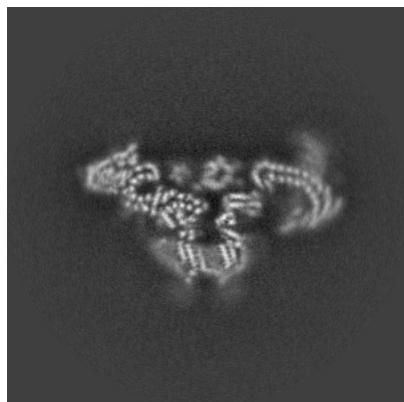


Y Index: 175

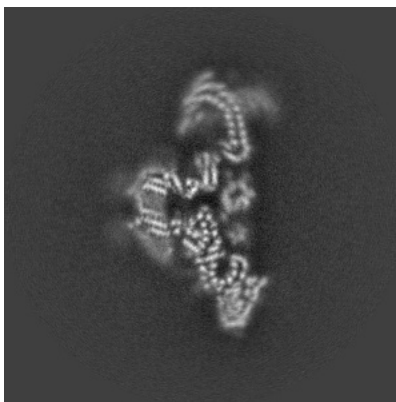


Z Index: 226

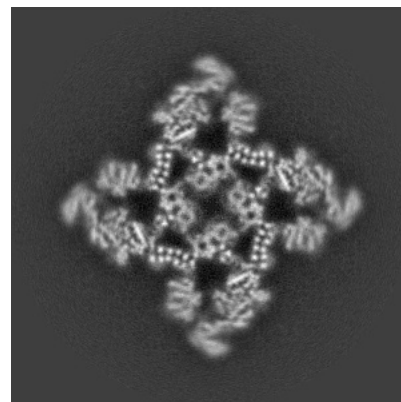
6.3.2 Raw map



X Index: 225



Y Index: 175

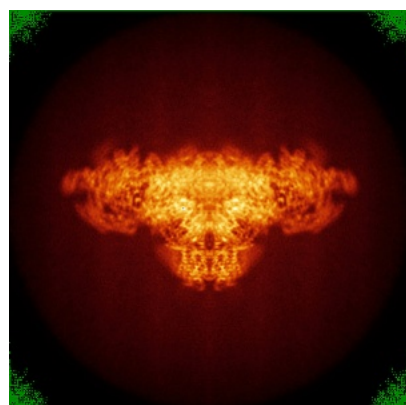


Z Index: 226

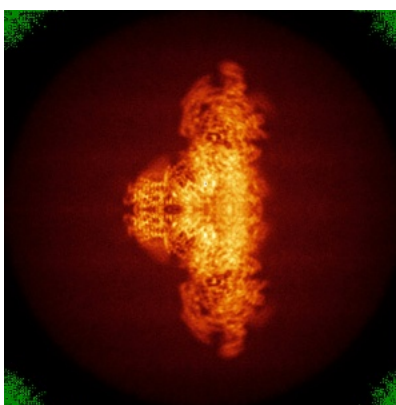
The images above show the largest variance slices of the map in three orthogonal directions.

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

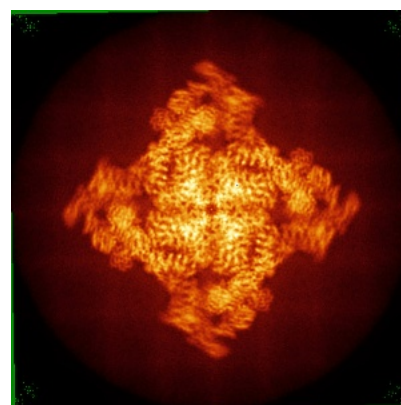
6.4.1 Primary map



X

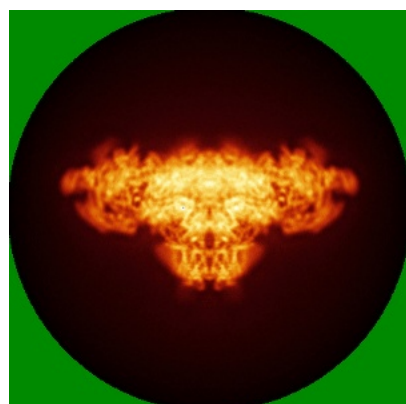


Y

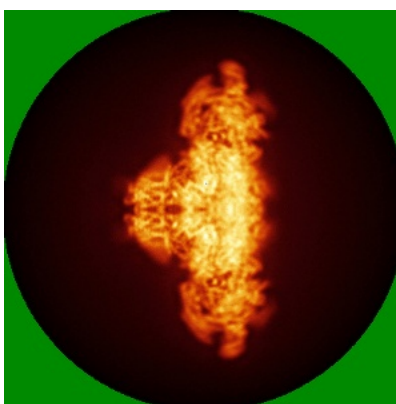


Z

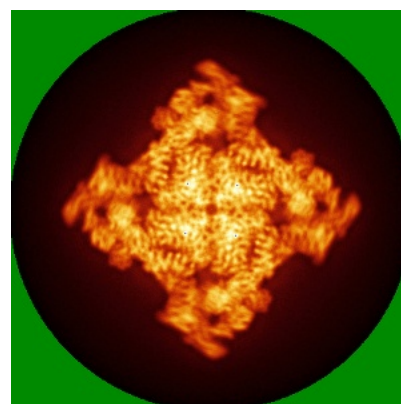
6.4.2 Raw map



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](#)

This section was not generated.

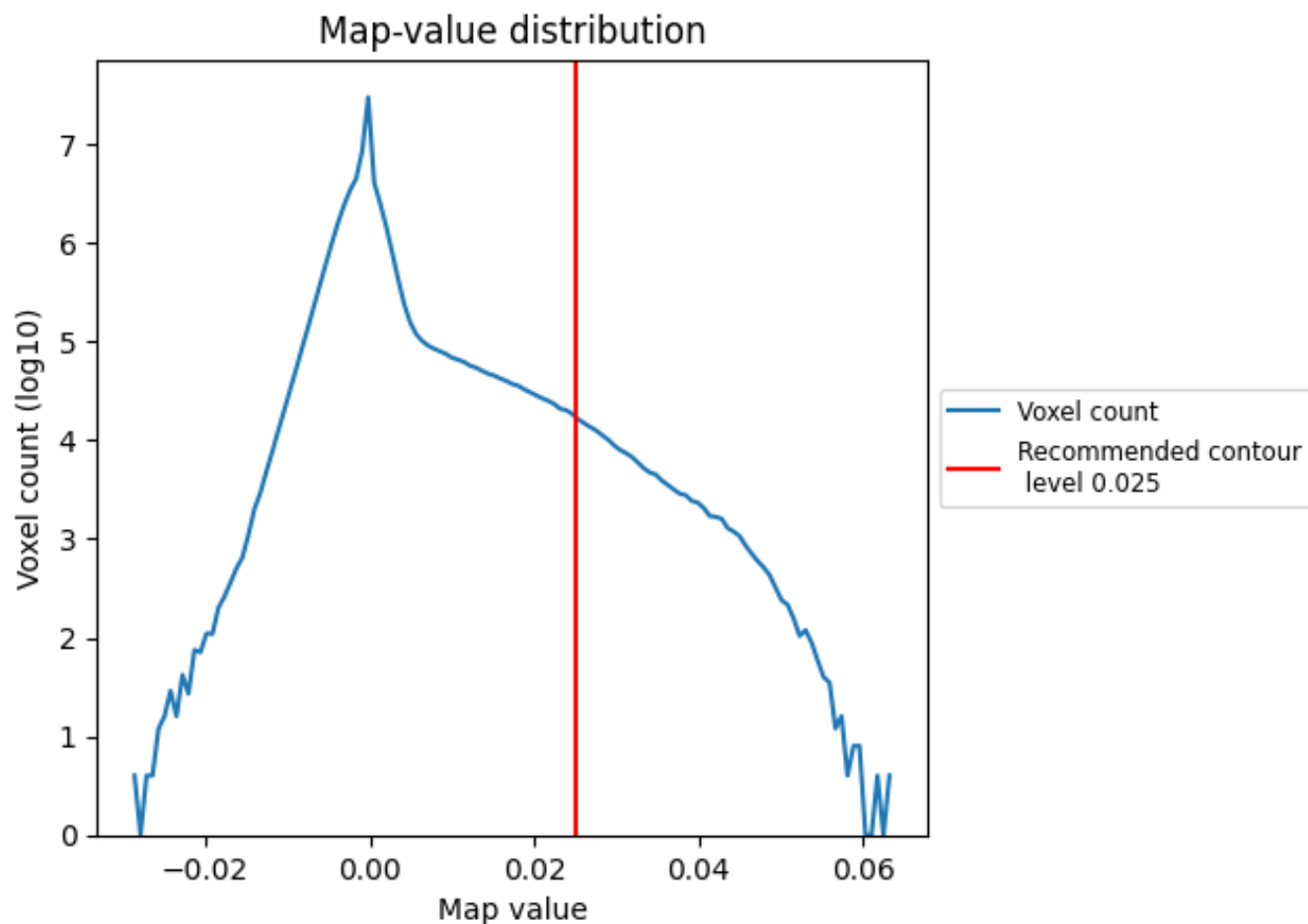
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

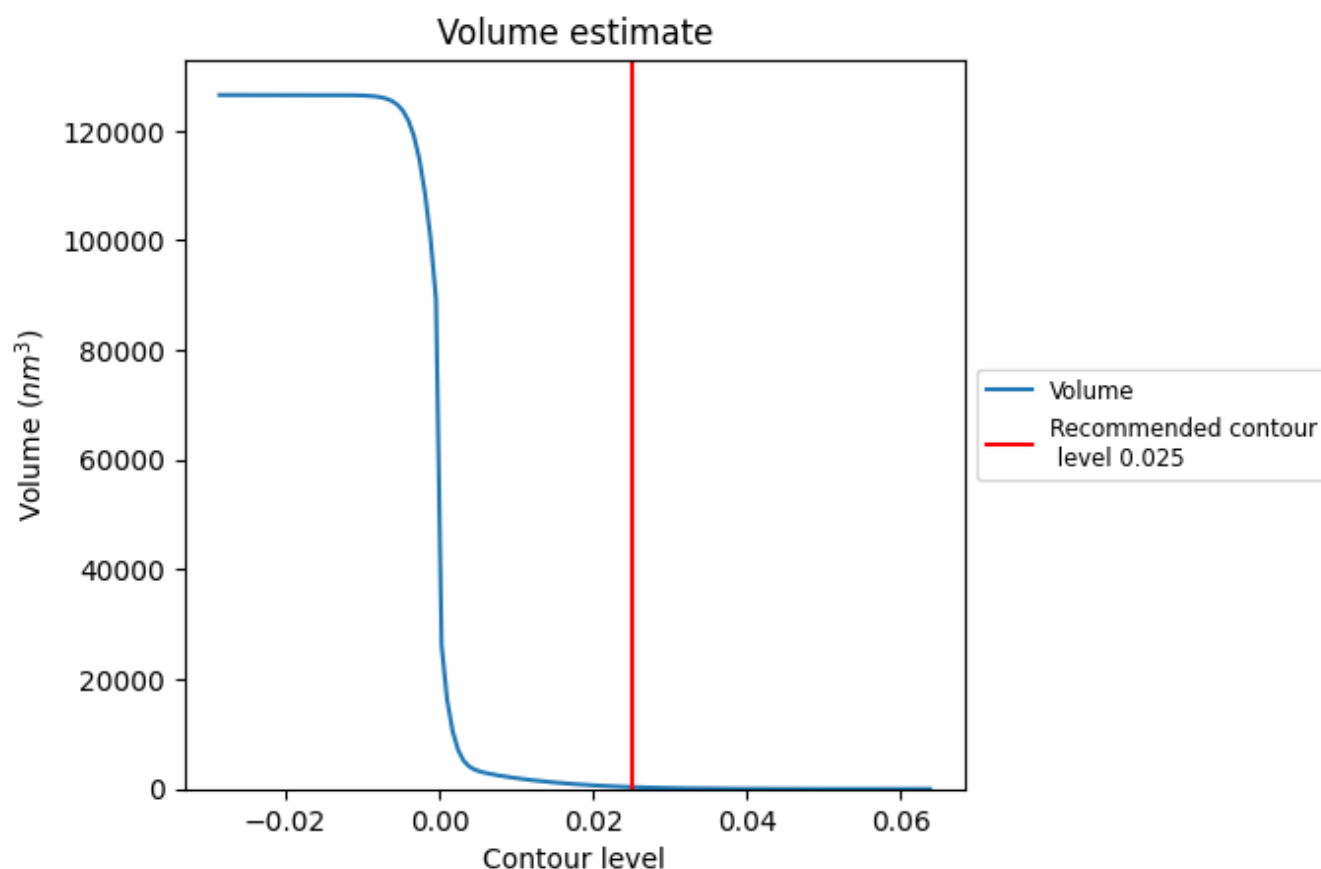
This section contains the results of statistical analysis of the map.

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.

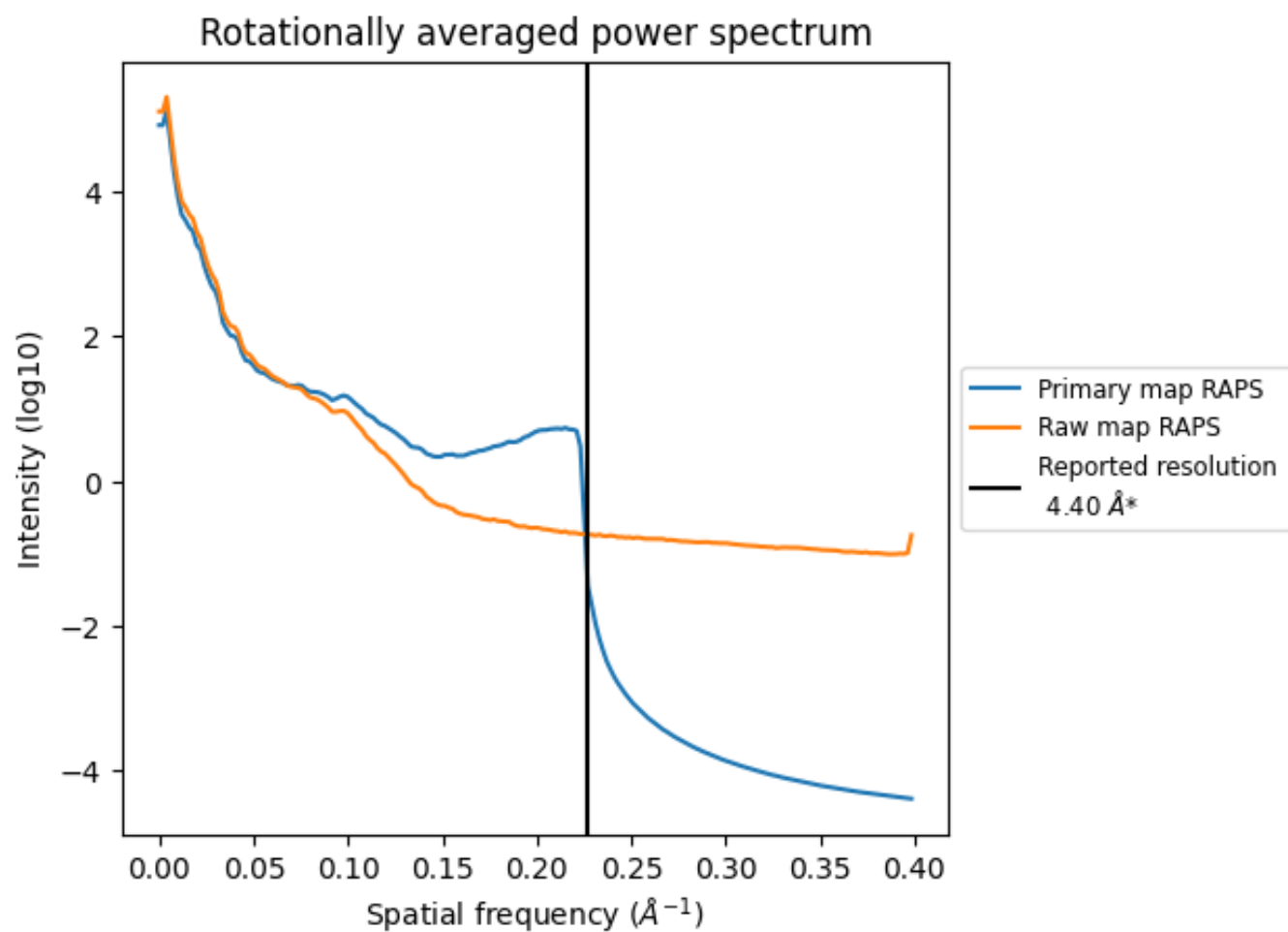
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm³; this corresponds to an approximate mass of 311 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 ⓘ

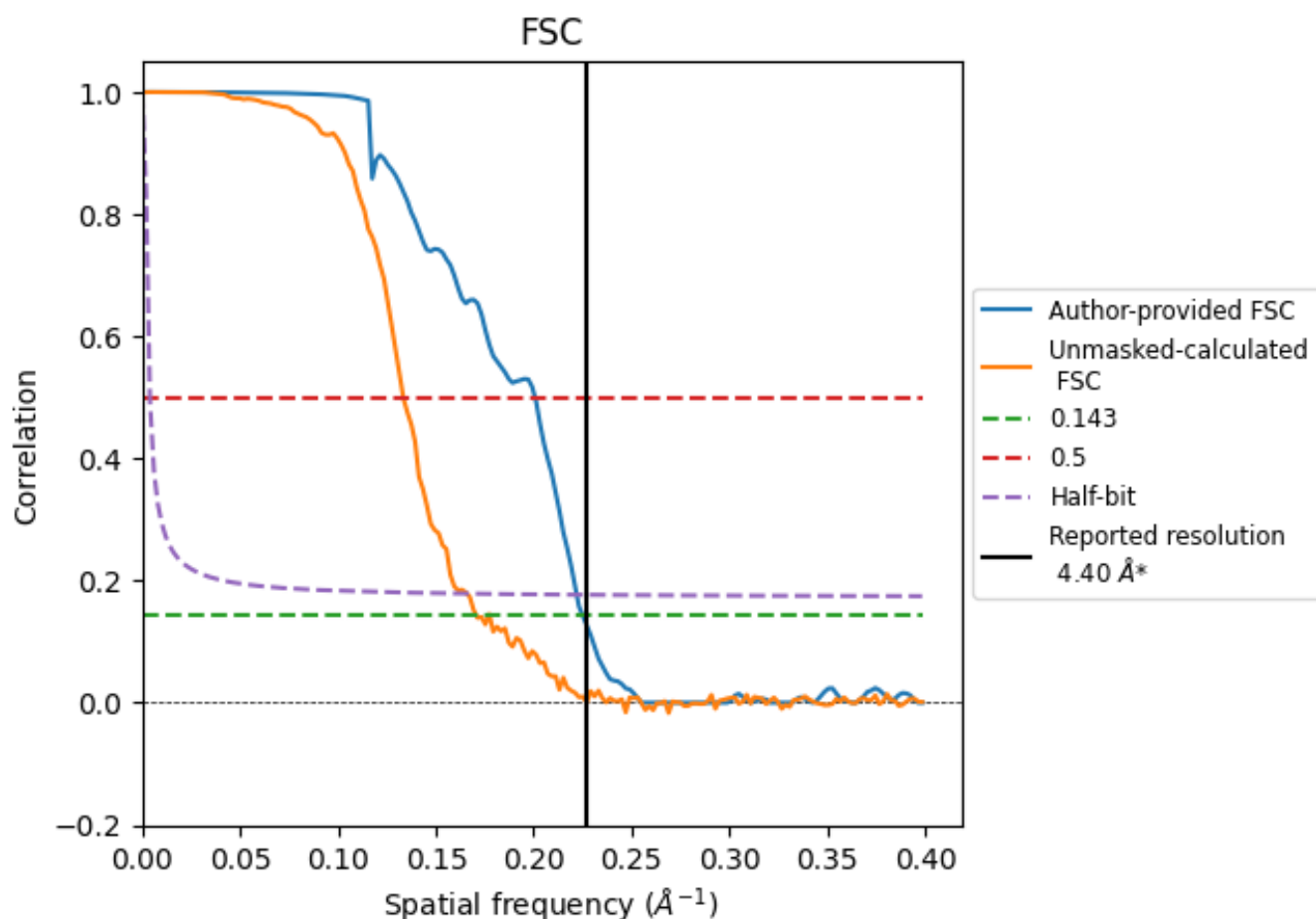


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.45	4.99	4.50
Unmasked-calculated*	5.86	7.50	6.03

*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 5.86 differs from the reported value 4.4 by more than 10 %

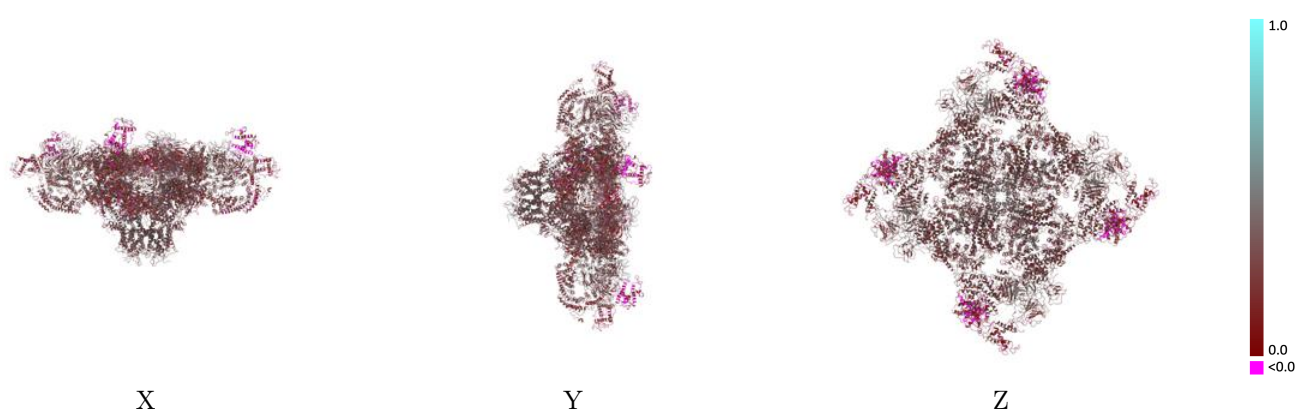
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8377 and PDB model 5TA3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

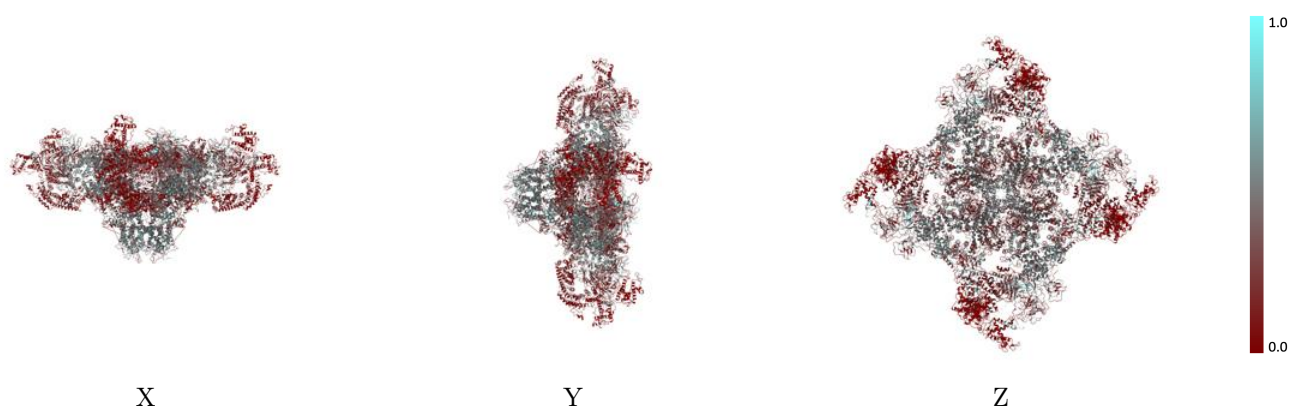
This section was not generated.

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



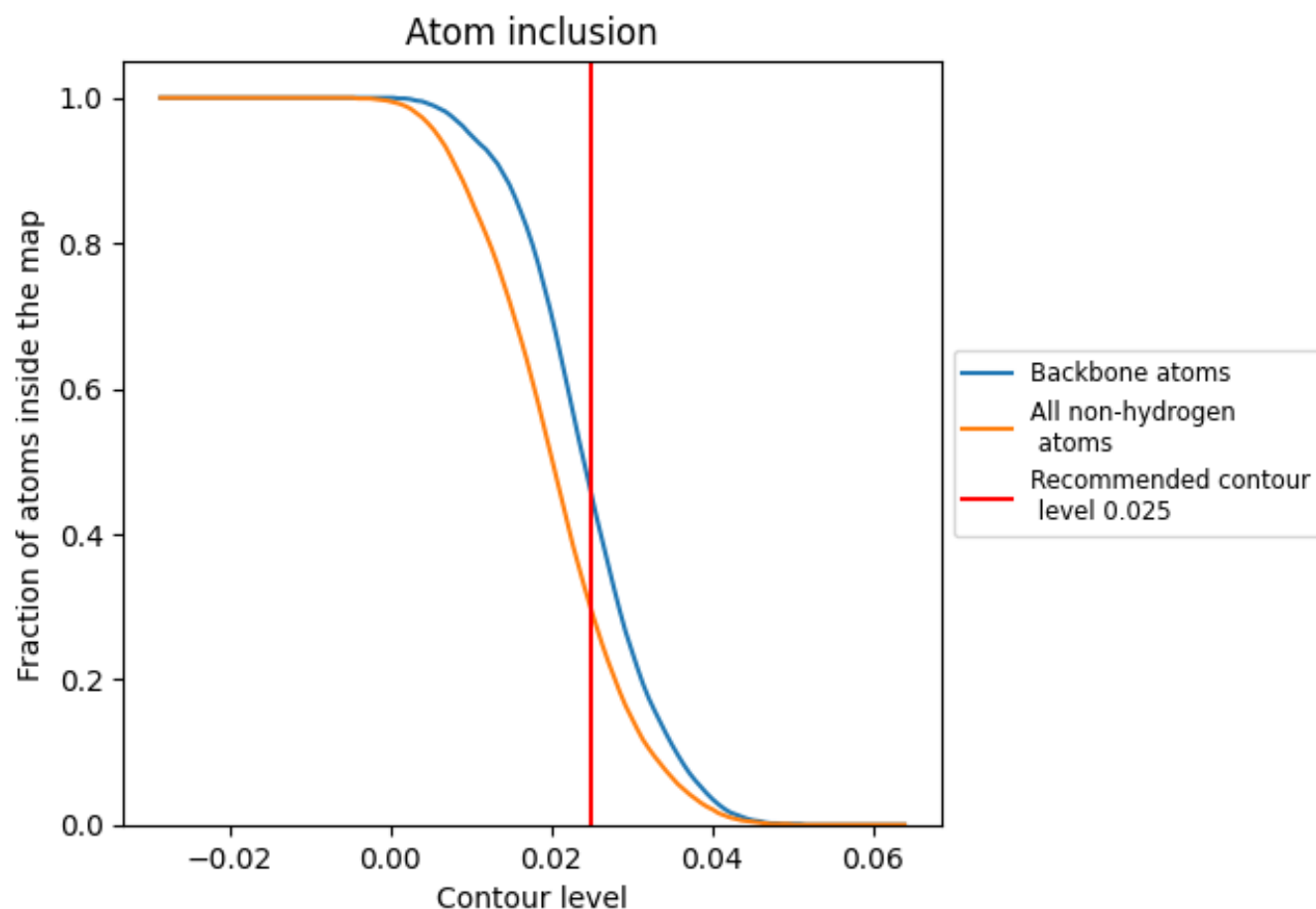
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2940	0.2750
A	0.3000	0.3110
B	0.2950	0.2780
E	0.2940	0.2720
F	0.2960	0.3140
G	0.2940	0.2750
H	0.3010	0.3150
I	0.2930	0.2730
J	0.3030	0.3120

1.0

0.0

<0.0