



wwPDB EM Validation Summary Report ⓘ

Mar 13, 2026 – 11:50 PM UTC

PDB ID : 7M6L / pdb_00007m6l
EMDB ID : EMD-23699
Title : High resolution structure of the membrane embedded skeletal muscle ryanodine receptor
Authors : Melville, Z.; Kim, K.; Clarke, O.B.; Marks, A.R.
Deposited on : 2021-03-25
Resolution : 3.98 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

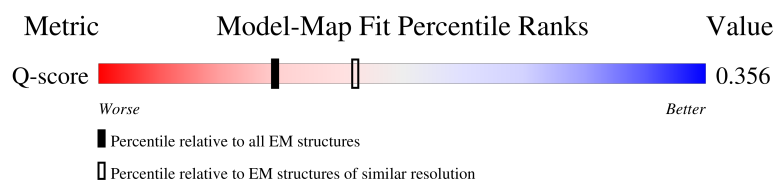
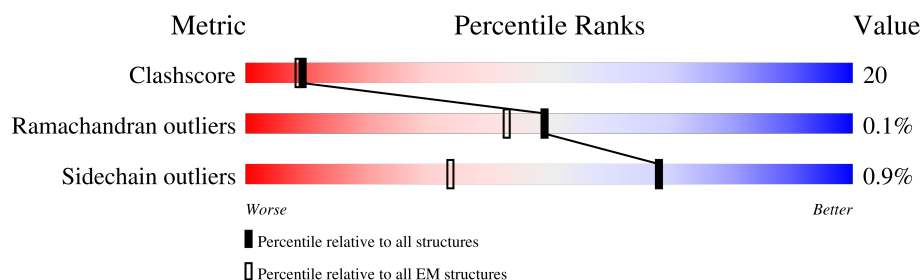
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.98 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.



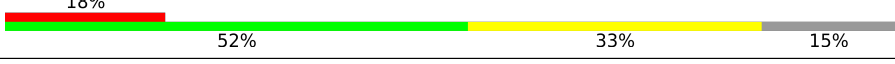
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7512 (3.48 - 4.48)

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	F	108	 63% 30% 5% ..
1	H	108	 64% 29% 5% ..
1	J	108	 65% 28% 5% ..
1	O	108	 65% 28% 5% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	A	5037	
2	B	5037	
2	G	5037	
2	I	5037	

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
6	CFF	A	5304	-	X	-	-
6	CFF	B	5304	-	X	-	-
6	CFF	G	5304	-	X	-	-
6	CFF	I	5304	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 140412 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	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		
1	O	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	A	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		
2	G	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		
2	B	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		
2	I	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		

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



Mol	Chain	Residues	Atoms					AltConf
3	A	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	B	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

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

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0

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

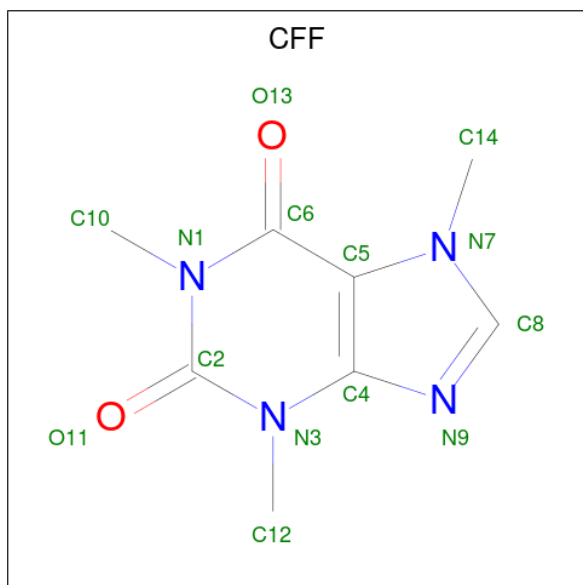
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

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

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).

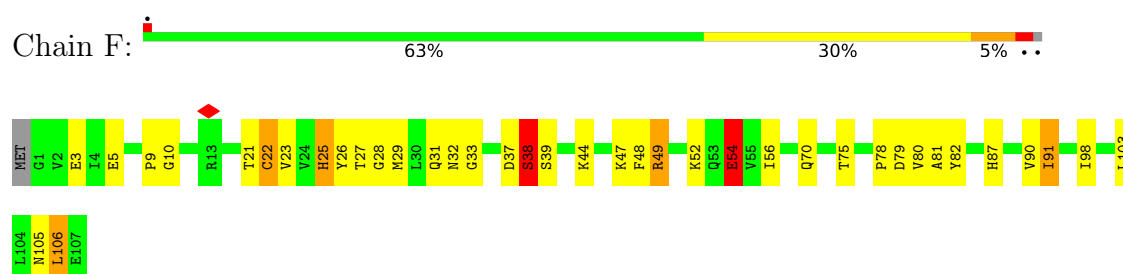


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	I	1	Total	C	N	O	0
			14	8	4	2	

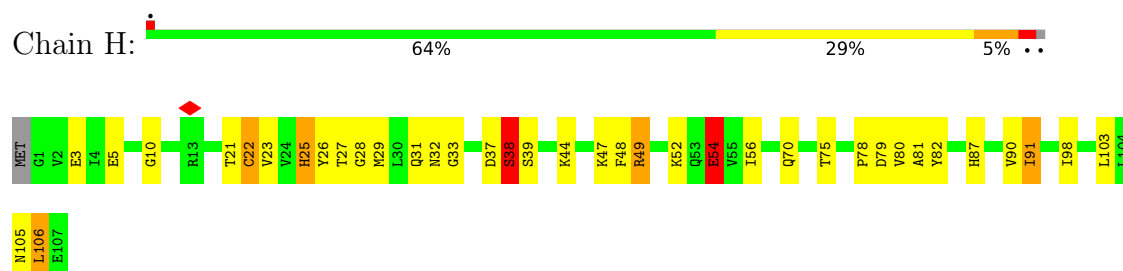
3 Residue-property plots [i](#)

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.

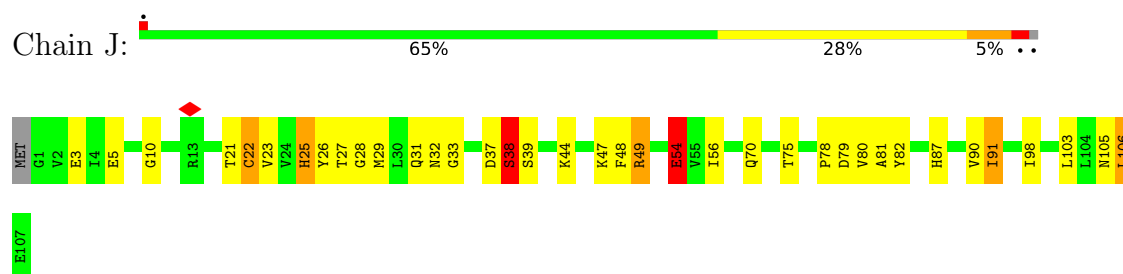
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



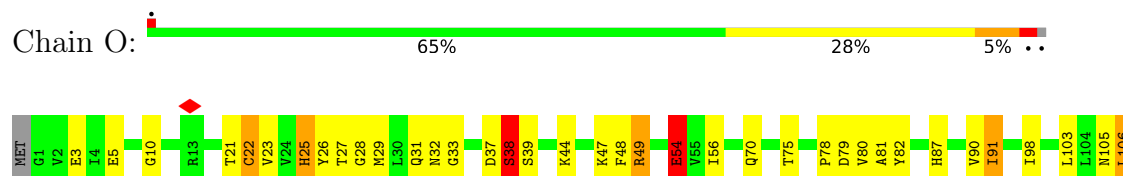
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

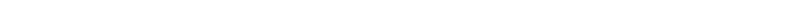


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



Chain A: 







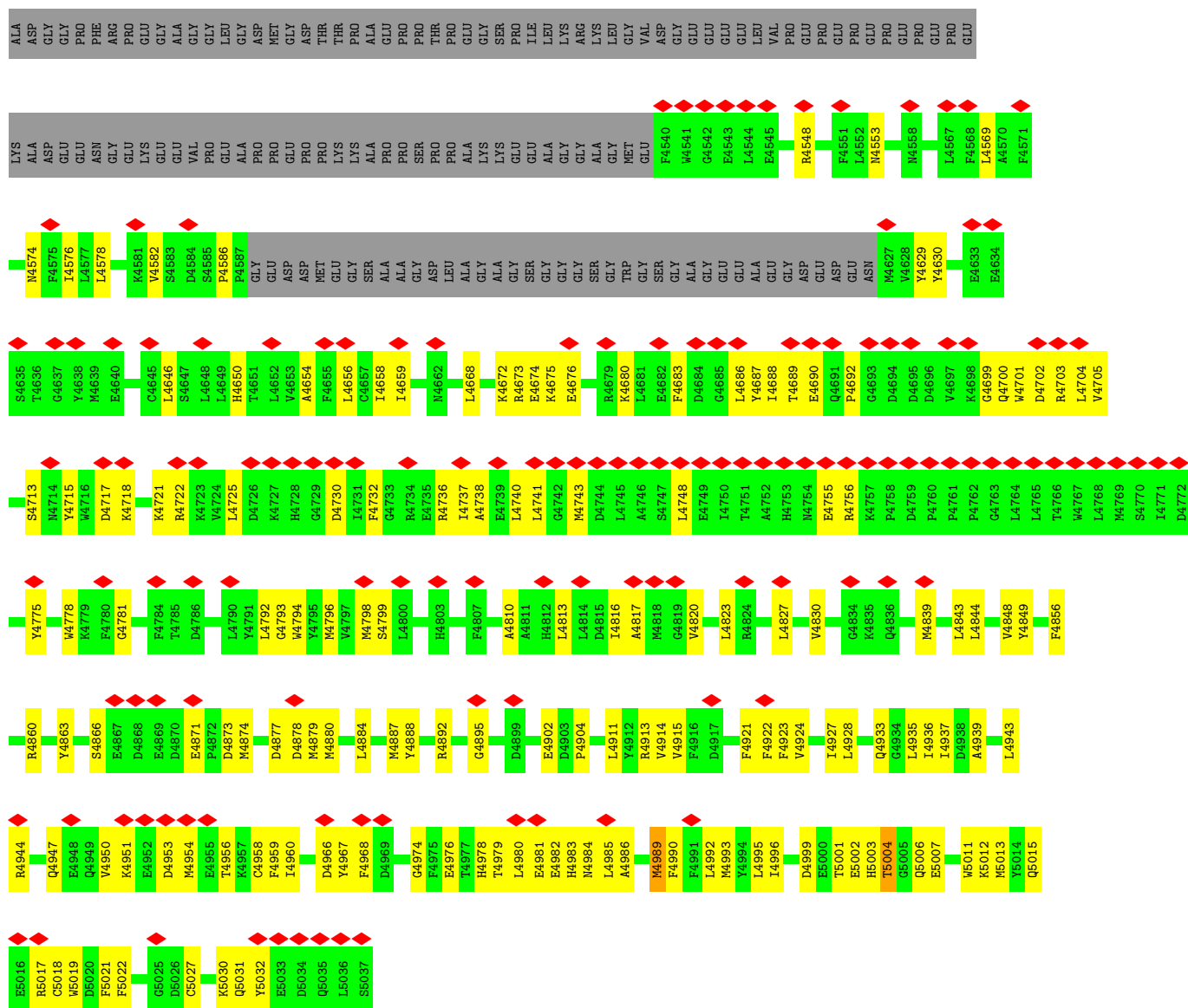
R4188	R4189	T4190	R4191	R4192	T4197	S4198	E4199	T4200	M4201	Q4204	W4205	E4206	M4207	P4208	Q4209	V4210	K4211	K4214	R4215	Q4216	F4217	T4218	F4219	D4220	L4221	V4222	M4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	L4233	F4234	V4235	S4236	F4237	C4238	E4239	D4240	T4241	T4242	F4243	E4244	M4245	Q4246	T4247	A4248	T4251	S4252	E4253	
F4125	E4126	E4127	F4128	A4129	M4130	K4131	F4132	Q4133	A4136	R4137	D4138	I4139	M4142	V4143	A4144	V4145	T4148	M4149	L4150	S4151	E4152	H4153	V4154	P4155	H4156	D4157	P4158	R4159	L4160	R4161	M4162	F4163	M4164	E4165	L4166	A4167	E4168	S4169	I4170	L4171	E4172	Y4173	F4174	R4175	P4176	Y4177	L4178	G4179	R4180	E4181	E4182	I4183	M4184	G4185	A4186	S4187
F3996	A3997	M3998	M4000	M4001	F4002	L4003	A4004	Q4005	D4006	Q4009	E4010	E4011	L4012	L4013	D4018	L4019	Q4020	K4021	D4022	M4023	M4026	L4030	L4031	L4032	G4033	M4034	V4035	V4036	M4037	C4038	M4039	L4040	A4041	R4042	V4045	D4046	M4047	L4048	V4049	E4050	S4051	S4052	S4053	M4054	M4055	E4056	M4057	L4058	M4059	K4060	F4061	F4062	D4063			
M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	A4072	G4073	S4074	A4075	A4076	F4077	Q4078	Y4080	V4081	T4082	D4083	P4084	R4085	A4086	L4087	L4088	S4089	K4090	F4093	Q4094	K4095	A4096	M4097	D4098	S4099	Q4100	K4101	Q4102	F4103	T4104	G4105	P4106	E4107	L4108	Q4109	F4110	L4111	L4112	S4113	E4116	A4117	D4118	E4119	M4120	E4121	M4122	I4123	M4124	
L3842	D3843	L3844	M3845	A3846	F3847	E3848	R3849	A3853	E3854	G3855	L3856	K3857	M3858	V3859	M3860	E3861	D3862	G3863	T3864	V3865	I3866	ASN	ARG	GLN	ASN	GLY	E3872	K3873	V3874	M3875	A3876	D3877	E3878	E3879	F3880	R3886	F3887	L3888	Q3889	L3890	L3891	M3896	K3897	D3898	V3899	Q3900	N3901	V3902	L3903	R3904	M3909	N3914	I3915	I3916		
V3920	L3923	L3924	S3929	Y3934	V3935	V3936	Y3937	S3938	D3941	V3942	I3943	E3944	E3945	Q3946	K3948	R3949	N3950	F3951	S3952	K3953	A3954	A3958	K3959	Q3960	V3961	F3962	L3965	E3967	V3968	Y3969	Q3970	G3971	G3975	L3980	S3983	R3984	L3985	S4052	S4053	D3987	V3988	V3989	V3990	G3991	F3992	L3993	H3994	V3995								
F3996	A3997	M3998	M4000	M4001	F4002	L4003	A4004	Q4005	D4006	Q4009	E4010	E4011	L4012	L4013	D4018	L4019	Q4020	K4021	D4022	M4023	M4026	L4030	L4031	L4032	G4033	M4034	V4035	V4036	M4037	C4038	M4039	L4040	A4041	R4042	V4045	D4046	M4047	L4048	V4049	E4050	S4051	S4052	S4053	M4054	M4055	E4056	M4057	L4058	M4059	K4060	F4061	F4062	D4063			
M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	A4072	G4073	S4074	A4075	A4076	F4077	Q4078	Y4080	V4081	T4082	D4083	P4084	R4085	A4086	L4087	L4088	S4089	K4090	F4093	Q4094	K4095	A4096	M4097	D4098	S4099	Q4100	K4101	Q4102	F4103	T4104	G4105	P4106	E4107	L4108	Q4109	F4110	L4111	L4112	S4113	E4116	A4117	D4118	E4119	M4120	E4121	M4122	I4123	M4124	
F4125	E4126	E4127	F4128	A4129	M4130	K4131	F4132	Q4133	A4136	R4137	D4138	I4139	M4142	V4143	A4144	V4145	T4148	M4149	L4150	S4151	E4152	H4153	V4154	P4155	H4156	D4157	P4158	R4159	L4160	R4161	M4162	F4163	M4164	E4165	L4166	A4167	E4168	S4169	I4170	L4171	E4172	Y4173	F4174	R4175	P4176	Y4177	L4178	G4179	R4180	E4181	E4182	I4183	M4184	G4185	A4186	S4187
R4188	R4189	T4190	R4191	R4192	T4197	S4198	E4199	T4200	M4201	Q4204	W4205	E4206	M4207	P4208	Q4209	V4210	K4211	K4214	R4215	Q4216	F4217	T4218	F4219	D4220	L4221	V4222	M4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	L4233	F4234	V4235	S4236	F4237	C4238	E4239	D4240	T4241	T4242	F4243	E4244	M4245	Q4246	T4247	A4248	T4251	S4252	E4253	
L3353	L3354	H3355	L3356	H3357	F3358	I3359	G3363	R3364	L3365	R3366	K3367	R3368	V3372	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	K3393	L3394	R3395	G3396	E3397	F3398	S3399	V3400	L3401	G3402	R3403	L3404	L3405	L3408	Y3409	P3410	L3411	L3412	I3413	V3416	N3419		
H3422	W3423	L3424	T3425	E3432	E3433	L3434	R3435	R3436	G3439	E3440	F3441	T3442	I3443	Y3444	W3445	N3450	F3451	K3452	R3453	F3454	E3455	Q3461	N3462	E3463	I3464	N3465	N3466	M3467	S3468	F3469	L3470	T3471	ALA	ASP	SER	LYS	LYS	SER	LYS	MET	ALA	LYS	LYS	GLY	GLY	SER	ASP	GLN	GLN	ARG						
THR	LYS	LYS	ARG	ARG	GLY	ASP	ARG	Y3503	S3504	V3505	Q3506	T3507	S3508	L3509	T3510	V3511	L3514	K3515	K3516	K3517	G3525	A3526	P3527	T3528	D3529	Q3530	D3531	L3532	T3533	T3534	L3535	A3536	K3537	T3538	R3539	Y3540	A3541	L3542	K3543	D3544	T3545	E3548	V3549	ARG	ARG	ARG	ARG	ARG	GLN	GLN	ASP	GLY	SER	ASP	GLN	ARG
E3564	L3569	R3570	P3580	G3581	R3582	E3583	E3584	R3585	A3586	D3587	K3591	I3592	V3593	R3595	V3596	Q3597	E3598	V3602	H3611	P3612	Y3613	K3614	S3615	LYS	LYS	ALA	VAL	TRP	HIS	L3642	K3643	LEU	LEU	SER	LYS	GLN	ARG	ARG	ALA	V3632	V3633	A3634	C3635	F3636	R3637	M3638	T3639	P3640								
L3641	Y3642	K3643	L3644	A3649	M3652	Y3657	L3663	F3669	R3672	M3673	I3674	D3675	L3676	L3677	E3682	GLN	GLU	GLU	GLU	GLU	A3693	P3694	Y3695	D3696	L3701	R3707	L3710	T3711	E3712	K3713	S3714	K3715	E3718	D3719	Y3725	I3728	M3729	C3733	H3734	L3735	GLU	F3736	R3737	M3738	T3739	P3740										
GLU	GLY	GLY	ASN	GLY	GLU	ALA	GLU	GLU	GLU	VAL	V3751	S3752	K3756	Q3767	S3768	H3771	T3772	R3773	I3774	ASN	ARG	GLN	ASN	GLY	E3772	K3773	V3774	M3775	A3776	L3780	Q3781	S3784	G3788	M3793	I3802	S3803	L3804	L3805	N3806	V3812	M3816	D3822	K3823	E3825	V3826	G3827	R3828	F3829	Q3830	S3831	L3835					
L3842	D3843	L3844	M3845	A3846	F3847	E3848	R3849	A3853	E3854	G3855	L3856	K3857	M3858	V3859	M3860	E3861	D3862	G3863	T3864	V3865	I3866	ASN	ARG	GLN	ASN	GLY	E3872	K3873	V3874	M3875	A3876	D3877	E3878	E3879	F3880	R3886	F3887	L3888	Q3889	L3890	L3891	M3896	K3897	D3898	V3899	Q3900	N3901	V3902	L3903	R3904	M3909	N3914	I3915	I3916		
V3920	L3923	L3924	S3929	Y3934	V3935	V3936	Y3937	S3938	D3941	V3942	I3943	E3944	E3945	Q3946	K3948	R3949	N3950	F3951	S3952	K3953	A3954	A3958	K3959	Q3960	V3961	F3962	L3965	E3967	V3968	Y3969	Q3970	G3971	G3975	L3980	S3983	R3984	L3985	S4052	S4053	D3987	V3988	V3989	V3990	G3991	F3992	L3993	H3994	V3995								
F3996	A3997	M3998	M4000	M4001	F4002	L4003	A4004	Q4005	D4006	Q4009	E4010	E4011	L4012	L4013	D4018	L4019	Q4020	K4021	D4022	M4023	M4026	L4030	L4031	L4032	G4033	M4034	V4035	V4036	M4037	C4038	M4039	L4040	A4041	R4042	V4045	D4046	M4047	L4048	V4049	E4050	S4051	S4052	S4053	M4054	M4055	E4056	M4057	L4058	M4059	K4060	F4061	F4062	D4063			
M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	A4072	G4073	S4074	A4075	A4076	F4077	Q4078	Y4080	V4081	T4082	D4083	P4084	R4085	A4086	L4087	L4088	S4089	K4090	F4093	Q4094	K4095	A4096	M4097	D4098	S4099	Q4100	K4101	Q4102	F4103	T4104	G4105	P4106	E4107	L4108	Q4109	F4110	L4111	L4112	S4113	E4116	A4117	D4118	E4119	M4120	E4121	M4122	I4123	M4124	
F4125	E4126	E4127	F4128	A4129	M4130	K4131	F4132	Q4133	A4136	R4137	D4138	I4139	M4142	V4143	A4144	V4145	T4148	M4149	L4150	S4151	E4152	H4153	V4154	P4155	H4156	D4157	P4158	R4159	L4160	R4161	M4162	F4163	M4164	E4165	L4166	A4167	E4168	S4169	I4170	L4171	E4172	Y4173	F4174	R4175	P4176	Y4177	L4178	G4179	R4180	E4181	E4182	I4183	M4184	G4185	A4186	S4187
R4188	R4189	T4190	R4191	R4192	T4197	S4198	E4199	T4200	M4201	Q4204	W4205	E4206	M4207	P4208	Q4209	V4210	K4211	K4214	R4215	Q4216	F4217	T4218	F4219	D4220	L4221	V4222	M4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	L4233	F4234	V4235	S4236	F4237	C4238	E4239	D4240	T4241	T4242	F4243	E4244	M4245	Q4246	T4247	A4248	T4251	S4252	E4253	

PRO GLY	G1222	F1124	G964	R902	R683	R553	L418	K329	A251	G160	L82	◆
LEU	F1223	N1125	Y965	L903	T689	L554	R426	R328	V252	E161	A83	◆
GLN	F1126	G1126	K966	H904	E697	E555	G427	D330	C253	K162	N84	◆
PRO		R1131	P967	P905	E697	L568	S428	V331	H255	G166	THR	◆
PRO	M1230	W1132	A969	C906	W702	L569	S429	E332	A256	L169	VAL	◆
ALA	G1231	H1133	P969	C906	W702	E570	G429	E332	R257	G166	GLU	◆
GLU	R1232	L1134	P969	L907	V707	E573	P430	M334	S268	L169	ALA	◆
ASP		M1052	L970	Y908	V707	E573	P431	G335	L259		GLY	◆
GLU	T1236	I1053	D971	N909	G708	V574	A432	T339	R261	S173	GLY	◆
ALA	P1247	E1054	S973	P910	D710	L575	A432	K340	W260	S174	GLY	◆
ALA	V1248	P1055	H974	H911	L711	H582	G433	Y341	R261	S175	GLY	◆
ALA		P1056	V975	S912	L711	H582	G433	G342	R261	S175	GLY	◆
GLU		D1057	R976	L913	L719	H582	G433	Y341	R261	S175	GLY	◆
PRO		Q1058	T977	P914	H720	L590	G450	E343	R261	S175	GLY	◆
ASP		E1059	T978	P914	H720	L590	G450	E343	R261	S175	GLY	◆
ASP		P1060	P979	P916	L721	V599	Y451	S344	R261	S175	GLY	◆
TYR		S1061	A980	P916	H725	V599	Y451	L345	R261	S175	GLY	◆
ASN		Q1062	T982	E917	H725	V599	Y451	C346	R261	S175	GLY	◆
LEU		V1063	T983	R918	H725	V599	Y451	C346	R261	S175	GLY	◆
ARG		E1064	L984	N919	H725	V599	Y451	C346	R261	S175	GLY	◆
ARG		M1065	N985	Y920	L748	A613	E462	S353	R261	S175	GLY	◆
SER		E1157	D986	N921	D749	R615	E463	G354	R261	S175	GLY	◆
ALA		N1158	R987	L922	L750	R615	K464	L355	R261	S175	GLY	◆
GLY		T1163	L988	Q923	S751	Q618	Q465	W356	R261	S175	GLY	◆
GLY		L1164	A989	N924	V752	Q618	Q465	T358	R261	S175	GLY	◆
TRP		L1165	E990	S925	V754	L633	Q465	T358	R261	S175	GLY	◆
GLY		N1165	E991	G926	I755	N636	Q465	T358	R261	S175	GLY	◆
ALA		L1169	R1000	E927	I755	N636	Q465	T358	R261	S175	GLY	◆
GLY		D1172	W1005	T928	L773	Y640	Q465	T358	R261	S175	GLY	◆
GLY		S1173	S1007	L929	D774	Y640	Q465	T358	R261	S175	GLY	◆
LYS		G1174	Y1007	R930	G775	F649	Q465	T358	R261	S175	GLY	◆
GLY		I1182	S1008	T931	L776	V650	Q465	T358	R261	S175	GLY	◆
THR		I1183	D1012	L932	P779	R653	Q465	T358	R261	S175	GLY	◆
ALA		E1183	A1015	L935	S782	A653	Q465	T358	R261	S175	GLY	◆
LYS		G1185	R1016	H938	F783	E654	Q465	T358	R261	S175	GLY	◆
GLY		D1186	R1017	V939	S784	T657	Q465	T358	R261	S175	GLY	◆
THR		L1194	N1018	G940	V787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1195	P1019	N941	S787	Y659	Q465	T358	R261	S175	GLY	◆
GLY		P1196	R1020	A942	S787	Y659	Q465	T358	R261	S175	GLY	◆
GLY		G1197	L1021	D943	S787	Y659	Q465	T358	R261	S175	GLY	◆
THR		Q1198	Y1024	F944	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		V1199	L1027	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
GLN		G1200	D1028	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		H1201	D1028	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
GLY		L1202	D1028	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		N1203	K1032	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
GLU		V1208	N1035	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
GLN		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	N949	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	K945	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	L950	S787	Y659	Q465	T358	R261	S175	GLY	◆
ARG		G1218	R1036	A946	S787	Y659	Q465	T358	R261	S175	GLY	◆
PRO		G1218	R1036	E947	S787	Y659	Q465	T358	R261	S175	GLY	◆
VAL		G1218	R1036	D948	S787	Y659	Q465	T358	R261	S175	GLY	◆
ALA		G1218	R1036	N949	S787	Y659						

L2485	D2333	V2168	A1992	ASP	ALA	T1454	T1572	T1454	ALA
V2486	F2334	Q2247	R1993	GLU	GLU	P1455	M1573	P1455	GLU
Q2487	L2335	M2170	R1994	GLU	GLU	D1456	P1574	D1456	ASN
P2488	R2336	E2175	T1995	VAL	VAL	L1575	L1575	L1575	GLU
K2489	F2337	E2174	R1996	ARG	ARG	F1464	S1576	F1464	ASP
M2490	F2340	E2176	E1997	LEU	LEU	V1469	A1577	V1469	LYS
S2493	V2346	E2177	S2000	LYS	LYS	M1476	A1578	M1476	ALA
F2494	E2347	L2177	P2001	GLU	GLU	G1477	M1579	G1477	THR
V2495	E2348	T2182	P2002	LYS	LYS	D1478	R1584	D1478	THR
P2496	N2349	T2185	Q2005	GLU	GLU	E1479	K1585	E1479	LYS
D2497	R2355	M2186	L2006	LYS	LYS	Q1480	N1586	Q1480	ASN
H2498	L2356	K2189	L2009	PRO	PRO	G1481	Q1590	G1481	LYS
K2499	L2357	V2190	F2012	GLU	GLU	N1482	C1591	N1482	ARG
A2500	L2358	F2191	A2016	GLU	GLU	H1483	L1595	H1483	GLY
S2501	R2359	P2195	D2017	ALA	ALA	P1484	L1827	P1484	PHE
M2502	E2362	M2198	E2018	GLU	GLU	D1828	D1828	D1828	LEU
V2503	P2366	L2273	E2019	LEU	LEU	P1829	E1596	P1829	LEU
L2504	P2369	A2277	C2021	PRO	PRO	S1722	V1597	S1722	PHE
R2508	G2370	N2284	L2022	GLY	GLY	E1733	Q1598	E1733	LYS
V2509	G2375	E2285	G1924	LYS	LYS	Y1734	M1599	Y1734	LYS
Y2510	L2376	L2286	L1926	ASP	ASP	T1738	R1607	T1738	LYS
G2511	A2287	A2287	E2025	LEU	LEU	T1739	M1608	T1739	ALA
E2513	G2376	E2287	L2023	GLU	GLU	G1611	M1609	G1611	ALA
N2514	L2377	L2288	G1925	GLU	GLU	F1612	M1610	F1612	ALA
Q2515	L2377	E2289	L1926	LYS	LYS	SER	V1501	SER	MET
D2516	A2377	L2290	L1927	GLU	GLU	PRO	GLN	PRO	THR
F2517	A2378	L2290	M2101	GLU	GLU	GLN	GLN	GLN	GLN
L2518	A2379	D2294	Q1928	LYS	LYS	GLY	GLY	GLY	PRO
R2519	A2380	L2295	M1929	GLY	GLY	R1508	Q1631	R1508	ALA
L2520	E2381	L2296	V1935	GLY	GLY	ASN	T1634	ASN	THR
R2521	A2382	K2287	L2031	ALA	ALA	S1510	T1635	S1510	PRO
V2522	L2384	V2298	Q2032	GLU	GLU	C1518	M1636	C1518	LEU
L2523	R2385	V2299	Q2036	GLU	GLU	G1525	L1639	G1525	PRO
S2459	R2386	S2300	L2044	GLU	GLU	E1543	P1642	E1543	ARG
L2460	I2386	Y2301	GLN	GLU	GLU	T1546	D1649	T1546	VAL
V2461	L2302	L2302	LEU	GLU	GLU	K1547	E1652	K1547	VAL
F2462	A2303	A2303	GLY	GLU	GLU	L1548	E1655	L1548	ASP
L2463	G2304	G2304	GLU	GLU	GLU	F1549	R1656	F1549	ALA
D2464	L2307	L2307	PRO	GLU	GLU	V1552	L1657	V1552	ASP
D2465	Q2308	Q2308	L1978	GLU	GLU	V1554	D1658	V1554	ALA
L2466	S2309	S2309	L1979	GLU	GLU	T1557	L1659	T1557	ALA
V2467	L2312	L2312	L1980	GLU	GLU	Y1433	A1672	Y1433	ALA
G2468	L2313	L2313	M1981	GLU	GLU	V1561	L1676	V1561	ALA
I2470	L2314	L2314	R1982	THR	THR	I1562	G1677	I1562	ALA
L2474	Q2232	Q2232	A1983	SER	SER	Q1563	N1678	Q1563	ALA
Q2475	R2233	R2233	F1984	LEU	LEU	K1568	M1679	K1568	ALA
T2476	F2234	F2234	T1985	SER	SER	Q1569	S1687	Q1569	ALA
P2477	L2236	L2236	M1986	ARG	ARG	K1570	V1448	K1570	ALA
T2478	G2237	G2237	A1988	LEU	LEU	V1448	V1448	V1448	ALA
L2479	Y2238	Y2238	T1988	GLU	GLU	V1448	V1448	V1448	ALA
G2480	N2324	N2324	M1988	GLU	GLU	V1448	V1448	V1448	ALA
K2481	P2328	P2328	A1988	GLU	GLU	V1448	V1448	V1448	ALA
D2482	G2328	G2328	A1988	GLU	GLU	V1448	V1448	V1448	ALA
Q2483	Y2331	Y2331	A1988	GLU	GLU	V1448	V1448	V1448	ALA
L2484	L2332	L2332	A1989	LEU	LEU	V1448	V1448	V1448	ALA
A2557			T1991	LEU	LEU	V1448	V1448	V1448	ALA

G3363	L2703	H2763	I2823	H2883	N3012	M3081	I3157	R3225	P3292	G3363	V3372	G3309	L3312	N3318	L3249	L3256	G3325	N3326	G3328	D3329	W3334	M3335	L3400	G3342	I3345	R3348	A3348	R3350	P3351	L3352	L3353	L3354	H3355	S3356	F3357	F3358	I3359		
L3364	C2704	E2764	E2824	N2884	H3013	K3082	L3158	E3226	P3293	L3364	V3373	G3374	L3313	N3319	M3250	L3257	L3258	N3327	G3329	D3330	R3331	M3332	L3401	C3402	P3403	L3404	Y3406	L3408	P3409	P3410	L3411	L3412	L3413	Y3416	N3419	H3422	L3423	T3425	E3432
L3365	A2705	K2765	K2825	T2885	C3014	S3083	D3159	R3227	P3294	L3365	V3374	A3374	L3314	N3320	A3251	A3252	A3253	N3325	G3327	L3329	W3335	M3336	L3402	C3403	P3404	L3405	L3408	P3409	P3410	L3411	L3412	L3413	Y3416	N3419	H3422	L3423	T3425	E3432	
L3366	I2706	K2766	A2826	W2886	L3015	G3084	V3161	A3228	A3295	L3366	V3375	A3375	L3315	N3321	A3252	A3253	A3254	N3326	G3328	L3330	W3336	M3337	L3403	C3404	P3405	L3406	L3409	P3410	P3411	L3412	L3413	Y3417	N3420	H3423	L3424	T3426	E3433		
L3367	I2707	K2767	E2827	G2887	Y3016	K3089	Q3162	I3229	A3296	L3367	V3376	A3376	L3316	N3322	A3253	A3254	A3255	N3327	G3329	L3331	W3337	M3338	L3404	C3405	P3406	L3407	L3410	P3411	P3412	L3413	L3414	Y3418	N3421	H3424	L3425	T3427	E3434		
L3368	I2708	K2768	E2828	F2887	F3017	K3090	Q3163	L3230	A3297	L3368	V3377	A3377	L3317	N3323	A3254	A3255	A3256	N3328	G3330	L3332	W3338	M3339	L3405	C3406	P3407	L3408	L3411	P3412	P3413	L3414	L3415	Y3419	N3422	H3425	L3426	T3428	E3435		
L3369	I2709	K2769	E2829	G2888	L3018	A3090	Q3164	L3231	A3298	L3369	V3378	A3378	L3318	N3324	A3255	A3256	A3257	N3329	G3331	L3333	W3339	M3340	L3406	C3407	P3408	L3409	L3412	P3413	P3414	L3415	L3416	Y3420	N3423	H3426	L3427	T3429	E3436		
L3370	I2710	K2770	E2952	K2889	L3019	R3093	T3165	L3232	A3299	L3370	V3379	A3379	L3319	N3325	A3256	A3257	A3258	N3330	G3332	L3334	W3340	M3341	L3407	C3408	P3409	L3410	L3413	P3414	P3415	L3416	L3417	Y3421	N3424	H3427	L3428	T3430	E3437		
L3371	I2711	K2771	E2953	K2890	L3020	R3094	T3166	L3233	A3300	L3371	V3380	A3380	L3320	N3326	A3257	A3258	A3259	N3331	G3333	L3335	W3341	M3342	L3408	C3409	P3410	L3411	L3414	P3415	P3416	L3417	L3418	Y3422	N3425	H3428	L3429	T3431	E3438		
L3372	I2712	K2772	E2954	K2891	L3021	F3096	T3167	L3234	A3301	L3372	V3381	A3381	L3321	N3327	A3258	A3259	A3260	N3332	G3334	L3336	W3342	M3343	L3409	C3410	P3411	L3412	L3415	P3416	P3417	L3418	L3419	Y3423	N3426	H3429	L3430	T3432	E3439		
L3373	I2713	K2773	E2955	K2892	L3022	F3097	T3168	L3235	A3302	L3373	V3382	A3382	L3322	N3328	A3259	A3260	A3261	N3333	G3335	L3337	W3343	M3344	L3410	C3411	P3412	L3413	L3416	P3417	P3418	L3419	L3420	Y3424	N3427	H3430	L3431	T3433	E3440		
L3374	I2714	K2774	E2956	K2893	L3023	S3098	T3169	L3236	A3303	L3374	V3383	A3383	L3323	N3329	A3260	A3261	A3262	N3334	G3336	L3338	W3344	M3345	L3411	C3412	P3413	L3414	L3417	P3418	P3419	L3420	L3421	Y3425	N3428	H3431	L3432	T3434	E3441		
L3375	I2715	K2775	E2957	K2894	L3024	E3101	T3170	L3237	A3304	L3375	V3384	A3384	L3324	N3330	A3261	A3262	A3263	N3335	G3337	L3339	W3345	M3346	L3412	C3413	P3414	L3415	L3418	P3419	P3420	L3421	L3422	Y3426	N3429	H3432	L3433	T3435	E3442		
L3376	I2716	K2776	E2958	K2895	L3025	E3102	T3171	L3238	A3305	L3376	V3385	A3385	L3325	N3331	A3262	A3263	A3264	N3336	G3338	L3340	W3346	M3347	L3413	C3414	P3415	L3416	L3419	P3420	P3421	L3422	L3423	Y3427	N3430	H3433	L3434	T3436	E3443		
L3377	I2717	K2777	E2959	K2896	L3026	E3103	T3172	L3239	A3306	L3377	V3386	A3386	L3326	N3332	A3263	A3264	A3265	N3337	G3339	L3341	W3347	M3348	L3414	C3415	P3416	L3417	L3420	P3421	P3422	L3423	L3424	Y3428	N3431	H3434	L3435	T3437	E3444		
L3378	I2718	K2778	E2960	K2897	L3027	E3104	T3173	L3240	A3307	L3378	V3387	A3387	L3327	N3333	A3264	A3265	A3266	N3338	G3340	L3342	W3348	M3349	L3415	C3416	P3417	L3418	L3421	P3422	P3423	L3424	L3425	Y3429	N3432	H3435	L3436	T3438	E3445		
L3379	I2719	K2779	E2961	K2898	L3028	E3105	T3174	L3241	A3308	L3379	V3388	A3388	L3328	N3334	A3265	A3266	A3267	N3339	G3341	L3343	W3349	M3350	L3416	C3417	P3418	L3419	L3422	P3423	P3424	L3425	L3426	Y3430	N3433	H3436	L3437	T3439	E3446		
L3380	I2720	K2780	E2962	K2899	L3029	E3106	T3175	L3242	A3309	L3380	V3389	A3389	L3329	N3335	A3266	A3267	A3268	N3340	G3342	L3344	W3350	M3351	L3417	C3418	P3419	L3420	L3423	P3424	P3425	L3426	L3427	Y3431	N3434	H3437	L3438	T3440	E3447		
L3381	I2721	K2781	E2963	K2900	L3030	E3107	T3176	L3243	A3310	L3381	V3390	A3390	L3330	N3336	A3267	A3268	A3269	N3341	G3343	L3345	W3351	M3352	L3418	C3419	P3420	L3421	L3424	P3425	P3426	L3427	L3428	Y3432	N3435	H3438	L3439	T3441	E3448		
L3382	I2722	K2782	E2964	K2901	L3031	E3108	T3177	L3244	A3311	L3382	V3391	A3391	L3331	N3337	A3268	A3269	A3270	N3342	G3344	L3346	W3352	M3353	L3419	C3420	P3421	L3422	L3425	P3426	P3427	L3428	L3429	Y3433	N3436	H3439	L3440	T3442	E3449		
L3383	I2723	K2783	E2965	K2902	L3032	E3109	T3178	L3245	A3312	L3383	V3392	A3392	L3332	N3338	A3269	A3270	A3271	N3343	G3345	L3347	W3353	M3354	L3420	C3421	P3422	L3423	L3426	P3427	P3428	L3429	L3430	Y3434	N3437	H3440	L3441	T3443	E3450		
L3384	I2724	K2784	E2966	K2903	L3033	E3110	T3179	L3246	A3313	L3384	V3393	A3393	L3333	N3339	A3270	A3271	A3272	N3344	G3346	L3348	W3354	M3355	L3421	C3422	P3423	L3424	L3427	P3428	P3429	L3430	L3431	Y3435	N3438	H3441	L3442	T3444	E3451		
L3385	I2725	K2785	E2967	K2904	L3034	E3111	T3180	L3247	A3314	L3385	V3394	A3394	L3334	N3340	A3271	A3272	A3273	N3345	G3347	L3349	W3355	M3356	L3422	C3423	P3424	L3425	L3428	P3429	P3430	L3431	L3432	Y3436	N3439	H3442	L3443	T3445	E3452		
L3386	I2726	K2786	E2968	K2905	L3035	E3112	T3181	L3248	A3315	L3386	V3395	A3395	L3335	N3341	A3272	A3273	A3274	N3346	G3348	L3350	W3356	M3357	L3423	C3424	P3425	L3426	L3429	P3430	P3431	L3432	L3433	Y3437	N3440	H3443	L3444	T3446	E3453		
L3387	I2727	K2787	E2969	K2906	L3036	E3113	T3182	L3249	A3316	L3387	V3396	A3396	L3336	N3342	A3273	A3274	A3275	N3347	G3349	L3351	W3357	M3358	L3424	C3425	P3426	L3427	L3430	P3431	P3432	L3433	L3434	Y3438	N3441	H3444	L3445	T3447	E3454		
L3388	I2728	K2788	E2970	K2907	L3037	E3114	T3183	L3250	A3317	L3388	V3397	A3397	L3337	N3343	A3274	A3275	A3276	N3348	G3350	L3352	W3358	M3359	L3425	C3426	P3427	L3428	L3431	P3432	P3433	L3434	L3435	Y3439	N3442	H3445	L3446	T3448	E3455		
L3389	I2729	K2789	E2971	K2908	L3038	E3115	T3184	L3251	A3318	L3389	V3398	A3398	L3338	N3344	A3275	A3276	A3277	N3349	G3351	L3353	W3359	M3360	L3426	C3427	P3428	L3429	L3432	P3433	P3434	L3435	L3436	Y3440	N3443	H3446	L3447	T3449	E3456		
L3390	I2730	K2790	E2972	K2909	L3039	E3116	T3185	L3252	A3319	L3390	V3399	A3399	L3339	N3345	A3276	A3277	A3278	N3350	G3352	L3354	W3360	M3361	L3427	C3428	P3429	L3430	L3433	P3434	P3435	L3436	L3437	Y3441	N3444	H3447	L3448	T3450	E3457		
L3391	I2731	K2791	E2973	K2910	L3040	E3117	T3186	L3253	A3320	L3391	V3400	A3400	L3340	N3346	A3277	A3278	A3279	N3351	G3353	L3355	W3361	M3362	L3428	C3429	P3430	L3431	L3434	P3435	P3436	L3437	L3438	Y3442	N3445	H3448	L3449	T3451	E3458		
L3392	I2732	K2792	E2974	K2911	L3041	E3118	T3187	L3254	A3321	L3392	V3401	A3401	L3341	N3347	A3278	A3279	A3280	N3352	G3354	L3356	W3362	M3363	L3429	C3430	P3431	L3432	L3435	P3436	P3437	L3438	L3439	Y3443	N3446	H3449	L3450	T3452	E3459		
L3393	I2733	K2793	E2975	K2912	L3042	E3119	T3188	L3255	A3322	L3393	V3402	A3402	L3342	N3348	A3279	A3280	A3281	N3353	G3355	L3357	W3363	M3364	L3430	C3431	P3432	L3433	L3436	P3437	P3438	L3439	L3440	Y3444	N3447	H3450	L3451	T3453	E3460		
L3394	I2734	K2794	E2976	K2913	L3043	E3120	T3189	L3256	A3323	L3394	V3403	A3403	L3343	N3349	A3280	A3281	A3282	N3354	G3356	L3358	W3364	M3365	L3431	C3432	P3433	L3434	L3437	P3438	P3439	L3440	L3441	Y3445	N3448	H3451	L3452	T3454	E3461		
L3395	I2735	K2795	E2977	K2914	L3044	E3121	T3190	L3257	A3324	L3395	V3404	A3404	L3344	N3350	A3281	A3282	A3283	N3355	G3357	L3359	W3365	M3366	L3432	C3433	P3434	L3435	L3438	P3439	P3440	L3441	L3442	Y3446	N3449	H3452	L3453	T3455	E3462		
L3396	I2736	K2796	E2978	K2915	L3045	E3122	T3191	L3258	A3325	L3396	V3405	A3405	L3345	N3351	A3282	A3283	A3284	N3356	G3358	L3360	W3366	M3367	L3433	C3434	P3435	L3436	L3439	P3440	P3441	L3442	L3443	Y3447	N3450	H3453	L3454	T3456	E3463		
L3397	I2737	K2797	E2979	K2916	L3046	E3123	T3192	L3259	A3326	L3397	V3406	A3406	L3346	N3352	A3283	A3284	A3285	N3357	G3359	L3361	W3367	M3368	L3434	C3435	P3436	L3437	L3440	P3441	P3442	L3443	L3444	Y3448	N3451	H3454	L3455	T3457	E3464		
L3398	I2738	K2798	E2980</																																				





• Molecule 2: Ryanodine receptor 1

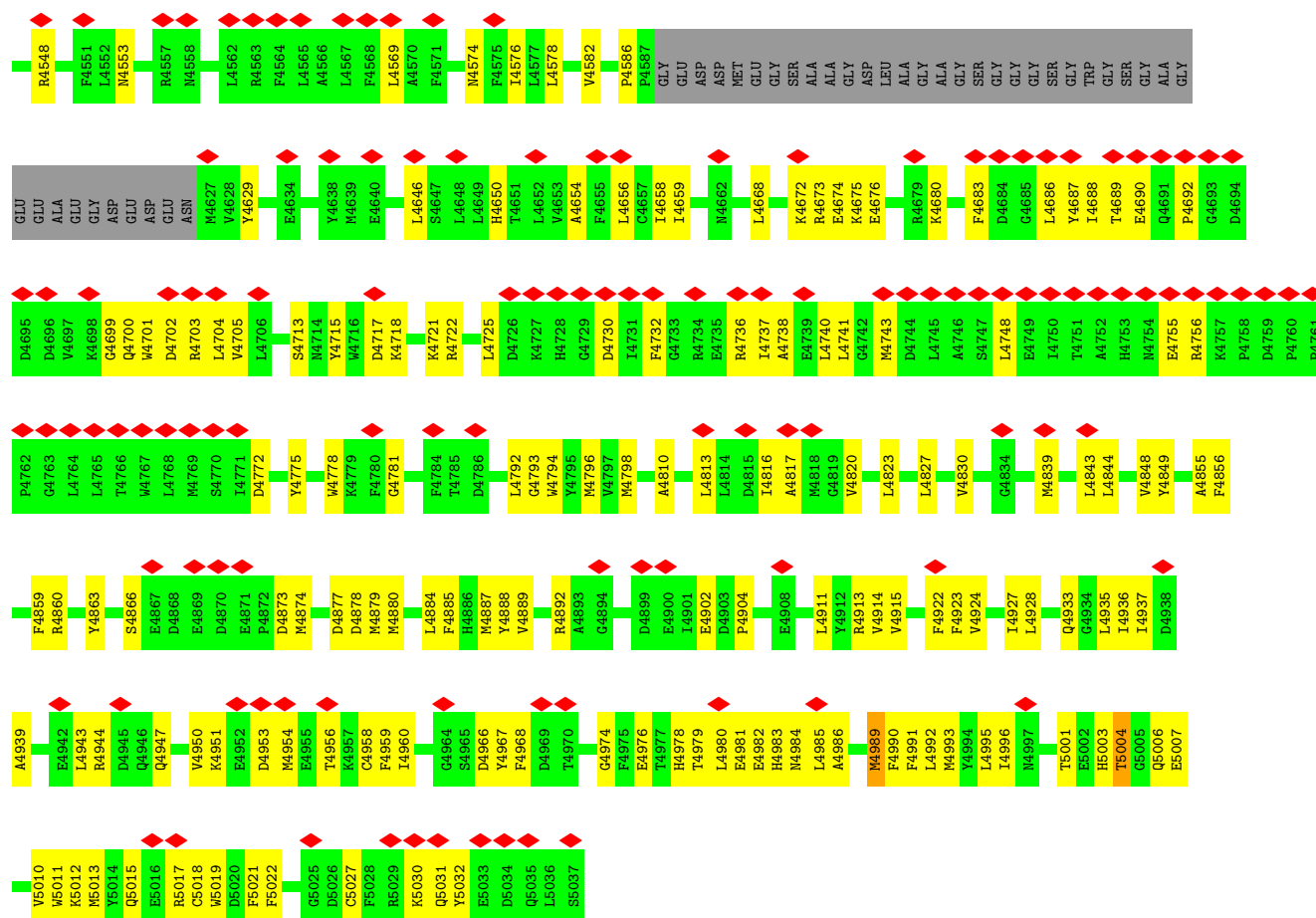




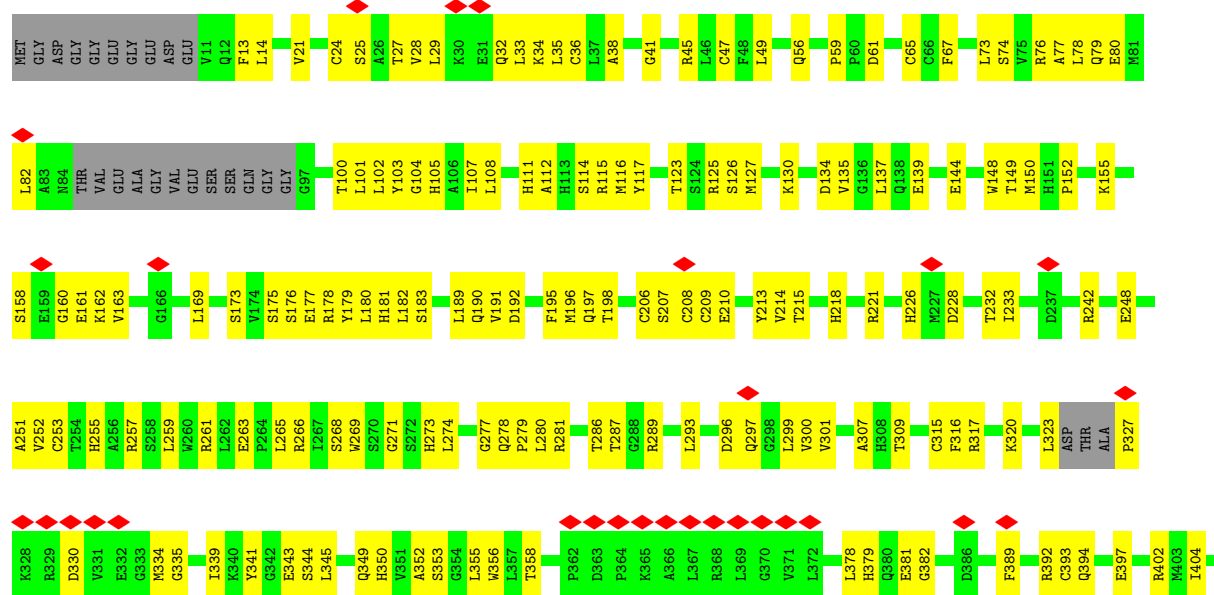








• Molecule 2: Ryanodine receptor 1

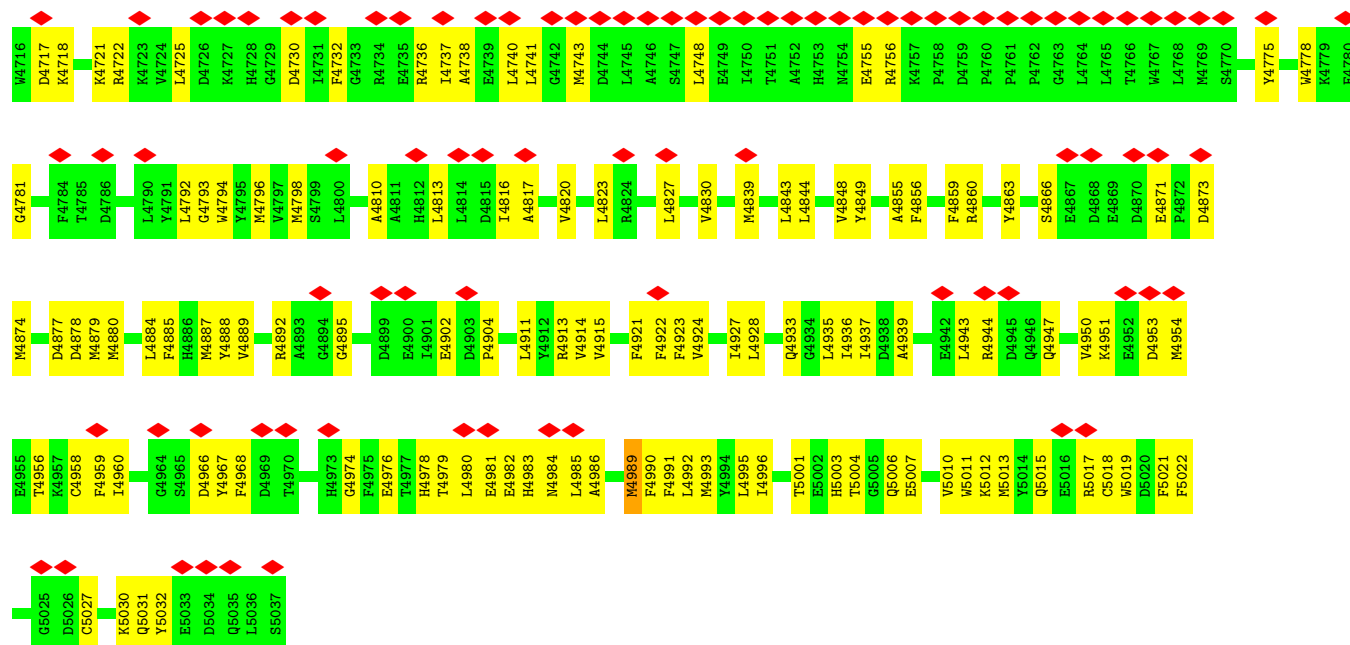




D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	W2781	Z2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	R2792	F2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	L2822	L2823	E2824	K2825	A2826	R2827	E2828
A2709	L2710	P2711	D2712	D2713	Y2714	W2715	A2717	S2718	Y2719	S2720	K2721	K2722	A2723	E2724	K2725	L2726	ALA	THR	VAL	ASP	ALA	GLY	N2734	F2735	D2736	T2737	K2738	P2739	V2740	E2741	T2742	L2743	N2744	W2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	
F2636	A2637	M2638	P2639	L2640	L2641	K2642	L2643	L2644	T2645	N2646	H2647	Y2648	E2649	R2650	C2651	W2652	K2653	Y2654	L2657	W2661	S2668	E2669	E2670	E2671	H2672	H2673	L2674	T2675	K2676	K2677	L2678	D2684	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	Y2696	R2697	M2698	A2699	M2700	P2701	C2702	L2703	C2704	A2705	L2706	A2707	G2708				
F2569	A2570	R2575	A2576	T2577	M2578	V2579	D2580	S2581	M2582	L2583	W2584	T2585	K2588	L2589	S2590	K2591	Q2592	R2593	S2594	L2595	T2596	Q2599	R2600	D2601	L2602	E2604	D2605	C2606	L2607	M2608	A2609	L2610	C2611	R2612	Y2613	L2614	R2615	P2616	S2617	M2618	L2619	Q2620	H2621	L2622	L2623	R2624	R2625	L2626	W2627	F2628	D2629	W2630	N2634	E2635				
P2496	D2497	H2498	K2499	A2500	S2501	M2502	V2503	L2504	F2505	R2508	V2509	Y2510	G2511	E2513	N2514	Q2515	D2516	F2517	L2518	L2519	H2520	V2521	L2522	W2523	V2524	G2525	L2527	P2528	L2529	M2530	R2531	A2534	S2535	L2536	D2537	T2538	F2541	S2542	E2545	Y2553	L2554	A2557	V2558	L2559	P2560	L2561	L2562	K2564	C2565									
L2422	M2423	L2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	T2443	K2447	G2448	E2449	A2450	L2451	R2452	L2453	R2454	L2457	R2458	S2459	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	L2469	T2470	L2474	Q2475	L2476	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	P2488	K2489	M2490	S2493	F2494	V2495							
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	F2340									
K2169	M2170	E2174	M2175	N2176	L2177	L2182	L2185	M2186	K2189	V2190	F2191	P2195	M2198	L2201	G2202	M2203	H2204	E2205	L2206	V2207	M2211	V2212	N2213	V2214	L2215	G2216	GLY	GLY	GLY	THR	L2238	GLU	K2227	M2228	C2232	C2233	R2234	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245										
N2246	Q2247	M2250	Y2256	S2261	GLY	ILE	GLY	LEU	GLY	Q2268	G2269	S2270	L2273	A2277	N2284	E2285	H2286	A2287	L2288	D2294	L2295	E2296	K2297	V2298	V2299	S2300	Y2301	L2302	A2303	G2304	S2309	M2312	P2319	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245									
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245			
L2422	M2423	L2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	T2443	K2447	G2448	E2449	A2450	L2451	R2452	L2453	R2454	L2457	R2458	S2459	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	L2469	T2470	L2474	Q2475	L2476	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	P2488	K2489	M2490	S2493	F2494	V2495							
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245			
N2246	Q2247	M2250	Y2256	S2261	GLY	ILE	GLY	LEU	GLY	Q2268	G2269	S2270	L2273	A2277	N2284	E2285	H2286	A2287	L2288	D2294	L2295	E2296	K2297	V2298	V2299	S2300	Y2301	L2302	A2303	G2304	S2309	M2312	P2319	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245									
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245			
L2422	M2423	L2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	T2443	K2447	G2448	E2449	A2450	L2451	R2452	L2453	R2454	L2457	R2458	S2459	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	L2469	T2470	L2474	Q2475	L2476	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	P2488	K2489	M2490	S2493	F2494	V2495							
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245			
N2246	Q2247	M2250	Y2256	S2261	GLY	ILE	GLY	LEU	GLY	Q2268	G2269	S2270	L2273	A2277	N2284	E2285	H2286	A2287	L2288	D2294	L2295	E2296	K2297	V2298	V2299	S2300	Y2301	L2302	A2303	G2304	S2309	M2312	P2319	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245									
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245			
L2422	M2423	L2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	T2443	K2447	G2448	E2449	A2450	L2451	R2452	L2453	R2454	L2457	R2458	S2459	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	L2469	T2470	L2474	Q2475	L2476	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	P2488	K2489	M2490	S2493	F2494	V2495							
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245			
N2246	Q2247	M2250	Y2256	S2261	GLY	ILE	GLY	LEU	GLY	Q2268	G2269	S2270	L2273	A2277	N2284	E2285	H2286	A2287	L2288	D2294	L2295	E2296	K2297	V2298	V2299	S2300	Y2301	L2302	A2303	G2304	S2309	M2312	P2319	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245									
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245			
L2422	M2423	L2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	T2443	K2447	G2448	E2449	A2450	L2451	R2452	L2453	R2454	L2457	R2458	S2459	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	L2469	T2470	L2474	Q2475	L2476	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	P2488	K2489	M2490	S2493	F2494	V2495							
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245			
N2246	Q2247	M2250	Y2256	S2261	GLY	ILE	GLY	LEU	GLY	Q2268	G2269	S2270	L2273	A2277	N2284	E2285	H2286	A2287	L2288	D2294	L2295	E2296	K2297	V2298	V2299	S2300	Y2301	L2302	A2303	G2304	S2309	M2312	P2319	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245									
V2346	E2347	N2349	M2349	R2355	L2356	L2357	R2358	R2359	E2362	P2366	R2369	Q2375	L2376	L2377	A2378	A2379	E2380	E2381	E2382	A2383	L2384	R2385	L2386	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	N2324	G2328	Y2331	L2332	D2333	F2235	L2236	C2237	Y2238	F2239	G2240	R2241	L2242	S2243	R2244	Q2245			
L2422	M2423	L2430	D2431	L2432	L2433	G2434</																																																				

A3649	G3581	V3505	R3366	A3295	V3160	F3017	S2949	K2889	G2829
R3652	R3582	Q3506	K3567	L3296	V3161	L3018	S2950	K2890	E2830
Y3657	E3507	T3507	R3368	P3297	Q3162	S3019	E2952	K2891	GLU
D3584	S3508	S3508	V3372	A3298	V3166	V3024	K2953	Q2892	GLU
A3586	L3509	L3509	V3373	G3231	R3167	L3025	R2954	E2893	THR
D3587	L3510	L3510	E3374	L3232	L3168	G3026	F2955	E2894	GLU
D3588	V3511	V3511	E3375	P3233	C3170	S3027	A2956	L2896	LYS
			E3376	E3237	S3171	G3028	F2957	A2897	LYS
			E3377	E3238	T3172	G3029	R2958	K2898	THR
			Q3378	C3240	T3173		L2960	G2899	ARG
			L3379	P3241	S3174	N3033		E2899	LYS
			R3380	D3242	L3175	K3034	L2963	G2900	ILE
			L3381	L3243	G3176	E3035	L2964	T2901	SER
			E3382	P3244	T3177	K3036	R2965	G2902	GLN
			A3383	V3245	T3178	E3037	W2966	H2902	THR
			A3384	L3246	K3179	M3038	D2968	P2903	ALA
			A3385	G3317	N3180	I3039	D2969	L2904	GLN
			E3386	L3249	T3181	L3042	S2970	L2905	THR
			A3387	M3250	Y3182	F3043	Q2971	V2906	ASP
			E3388	A3251	V3183	C3044	E2972	V2907	PRO
			E3389	D3252	E3184	K3045	F2973	Y2908	ARG
			G3390	I3263	K3185	L3046	T2974	GLU	GLY
			E3391	L3266	L3186	A3047	A2975	D2909	Y2865
			L3392	A3257	R3187	A3048	H2976	T2910	N2856
			L3393	E3258	L3190	L3049	L2977	L2911	P2857
			V3394		G3191	V3050	V2980	T2912	Q2858
			R3395		E3192	R3053	S2982	A2913	F2859
			D3396		C3193	V3054	S2983	K2914	P2860
			E3397		L3194	S3055	G2984	E2915	L2862
			F3398		A3195	L3056	R2985	K2916	L2863
			S3399		R3196	F3057	V2986	A2917	G2864
			V3400		L3197	G3058	E2987	D2918	Q2865
			L3401		A3198	T3059	K2988	R2920	T2866
			C3402		A3199	S3060	P2990	E2921	L2867
			R3403		A3200	L3136	P2991	K2922	S2868
			D3404		E3271	L3137	E2992	Q2924	R2869
			L3405		L3338	P3138	E2993	E2925	E2870
					F3341	T3141	E2994	L2871	L2871
			L3408		A3342	L3142	E2995	Q2872	Q2872
			Y3409		I3345	L3143	L2995	A2873	A2873
			P3410		T3346	H3069	K2996	A2875	A2875
			L3412		Q3145	T3070		E2877	E2877
			I3413		H3146	L3071	A2999	Q2877	Q2877
			V3416		N3211	A3072	K3000	E2879	E2879
			N3419		E3212	S3073	N3007	E2880	E2880
			H3422		V3213	S3074	Q3008	N2881	N2881
			V3423		N3214	L3075	Q3009	N2932	N2882
			T3425		A3215	D3076	F3010	N2933	H2883
			E3432		V3218	A3077	N3012	Y2935	N2884
			E3433		T3219	R3078	N3013	A2936	T2885
			F3435		T3220	V3080	C3014	Y2937	W2886
			R3436		T3221	M3081	L3015	T2938	G2887
					R3226	K3082	Y3016	R2939	R2888
					R3227	S3083		GLY	
						G3084		LEU	
								LYS	
								ASP	
								MET	
								GLU	
								LEU	
								ASP	
								THR	





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	31599	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 ($e^-/\text{\AA}^2$)	58.34	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.771	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.106	Depositor
Map size (Å)	425.472, 425.472, 425.472	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, CFF, CA, 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	F	0.94	3/834 (0.4%)	0.87	4/1123 (0.4%)
1	H	0.94	4/834 (0.5%)	0.87	4/1123 (0.4%)
1	J	0.94	4/834 (0.5%)	0.87	4/1123 (0.4%)
1	O	0.94	3/834 (0.4%)	0.87	4/1123 (0.4%)
2	A	0.38	6/35023 (0.0%)	0.56	13/47448 (0.0%)
2	B	0.38	7/35023 (0.0%)	0.56	13/47448 (0.0%)
2	G	0.38	7/35023 (0.0%)	0.56	13/47448 (0.0%)
2	I	0.38	6/35023 (0.0%)	0.56	13/47448 (0.0%)
All	All	0.40	40/143428 (0.0%)	0.57	68/194284 (0.0%)

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	752	VAL	CA-C	-11.00	1.43	1.52
2	G	752	VAL	CA-C	-11.00	1.43	1.52
2	I	752	VAL	CA-C	-10.92	1.43	1.52
2	B	752	VAL	CA-C	-10.91	1.43	1.52
2	G	755	ILE	CA-C	-8.30	1.42	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	752	VAL	CA-C-N	-28.03	82.41	120.25
2	A	752	VAL	C-N-CA	-28.03	82.41	120.25
2	G	752	VAL	CA-C-N	-28.02	82.42	120.25
2	G	752	VAL	C-N-CA	-28.02	82.42	120.25
2	B	752	VAL	CA-C-N	-28.02	82.42	120.25

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	F	818	0	824	27	0
1	H	818	0	824	25	0
1	J	818	0	824	24	0
1	O	818	0	824	24	0
2	A	34238	0	33844	1399	0
2	B	34238	0	33844	1416	0
2	G	34238	0	33844	1400	0
2	I	34238	0	33844	1410	0
3	A	31	0	12	5	0
3	B	31	0	12	5	0
3	G	31	0	12	6	0
3	I	31	0	12	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	A	14	0	10	2	0
6	B	14	0	10	2	0
6	G	14	0	10	2	0
6	I	14	0	10	2	0
All	All	140412	0	138760	5626	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 20.

The worst 5 of 5626 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:G:4658:ILE:HD13	2:G:4796:MET:HE3	1.35	1.09
2:I:4658:ILE:HD13	2:I:4796:MET:HE3	1.35	1.08
2:A:4658:ILE:HD13	2:A:4796:MET:HE3	1.35	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4658:ILE:HD13	2:B:4796:MET:HE3	1.35	1.06
2:G:4983:HIS:HB2	3:G:5301:ATP:HN62	1.25	1.01

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	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	O	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	A	4256/5037 (84%)	3938 (92%)	314 (7%)	4 (0%)	48	80
2	B	4256/5037 (84%)	3936 (92%)	316 (7%)	4 (0%)	48	80
2	G	4256/5037 (84%)	3939 (93%)	313 (7%)	4 (0%)	48	80
2	I	4256/5037 (84%)	3940 (93%)	312 (7%)	4 (0%)	48	80
All	All	17444/20580 (85%)	16137 (92%)	1291 (7%)	16 (0%)	49	80

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3876	ALA
2	G	3876	ALA
2	B	3876	ALA
2	I	3876	ALA
2	A	1783	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	88/89 (99%)	77 (88%)	11 (12%)	4	20
1	H	88/89 (99%)	77 (88%)	11 (12%)	4	20
1	J	88/89 (99%)	77 (88%)	11 (12%)	4	20
1	O	88/89 (99%)	77 (88%)	11 (12%)	4	20
2	A	3732/4276 (87%)	3708 (99%)	24 (1%)	78	81
2	B	3732/4276 (87%)	3708 (99%)	24 (1%)	78	81
2	G	3732/4276 (87%)	3708 (99%)	24 (1%)	78	81
2	I	3732/4276 (87%)	3708 (99%)	24 (1%)	78	81
All	All	15280/17460 (88%)	15140 (99%)	140 (1%)	68	76

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	5004	THR
2	I	754	SER
2	I	3875	MET
1	J	22	CYS
1	J	21	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 161 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	4754	ASN
2	I	3150	HIS
2	I	241	GLN
2	I	1660	GLN
2	I	3900	GLN

5.3.3 RNA ⓘ

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$
3	ATP	G	5301	-	32,33,33	1.27	5 (15%)	48,52,52	1.74	10 (20%)
6	CFF	I	5304	-	15,15,15	1.95	8 (53%)	23,23,23	3.02	12 (52%)
3	ATP	I	5301	-	32,33,33	1.26	5 (15%)	48,52,52	1.75	10 (20%)
6	CFF	A	5304	-	15,15,15	1.94	8 (53%)	23,23,23	3.02	12 (52%)
3	ATP	B	5301	-	32,33,33	1.27	5 (15%)	48,52,52	1.75	10 (20%)
6	CFF	G	5304	-	15,15,15	1.94	8 (53%)	23,23,23	3.02	12 (52%)
6	CFF	B	5304	-	15,15,15	1.95	8 (53%)	23,23,23	3.02	12 (52%)
3	ATP	A	5301	-	32,33,33	1.27	5 (15%)	48,52,52	1.74	10 (20%)

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
3	ATP	G	5301	-	-	7/22/38/38	0/3/3/3
6	CFF	I	5304	-	-	-	0/2/2/2
3	ATP	I	5301	-	-	7/22/38/38	0/3/3/3
6	CFF	A	5304	-	-	-	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5301	-	-	7/22/38/38	0/3/3/3
6	CFF	G	5304	-	-	-	0/2/2/2
6	CFF	B	5304	-	-	-	0/2/2/2
3	ATP	A	5301	-	-	7/22/38/38	0/3/3/3

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5304	CFF	C6-N1	-3.99	1.32	1.40
6	I	5304	CFF	C6-N1	-3.97	1.32	1.40
3	B	5301	ATP	C5-C4	3.97	1.46	1.39
3	I	5301	ATP	C5-C4	3.97	1.46	1.39
3	A	5301	ATP	C5-C4	3.96	1.46	1.39

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5304	CFF	C14-N7-C8	-8.64	110.12	126.28
6	I	5304	CFF	C14-N7-C8	-8.61	110.18	126.28
6	G	5304	CFF	C14-N7-C8	-8.59	110.20	126.28
6	A	5304	CFF	C14-N7-C8	-8.59	110.20	126.28
6	B	5304	CFF	C14-N7-C5	5.99	142.03	127.77

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O3A
3	G	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O3A
3	I	5301	ATP	C5'-O5'-PA-O3A
3	A	5301	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 30 short contacts:

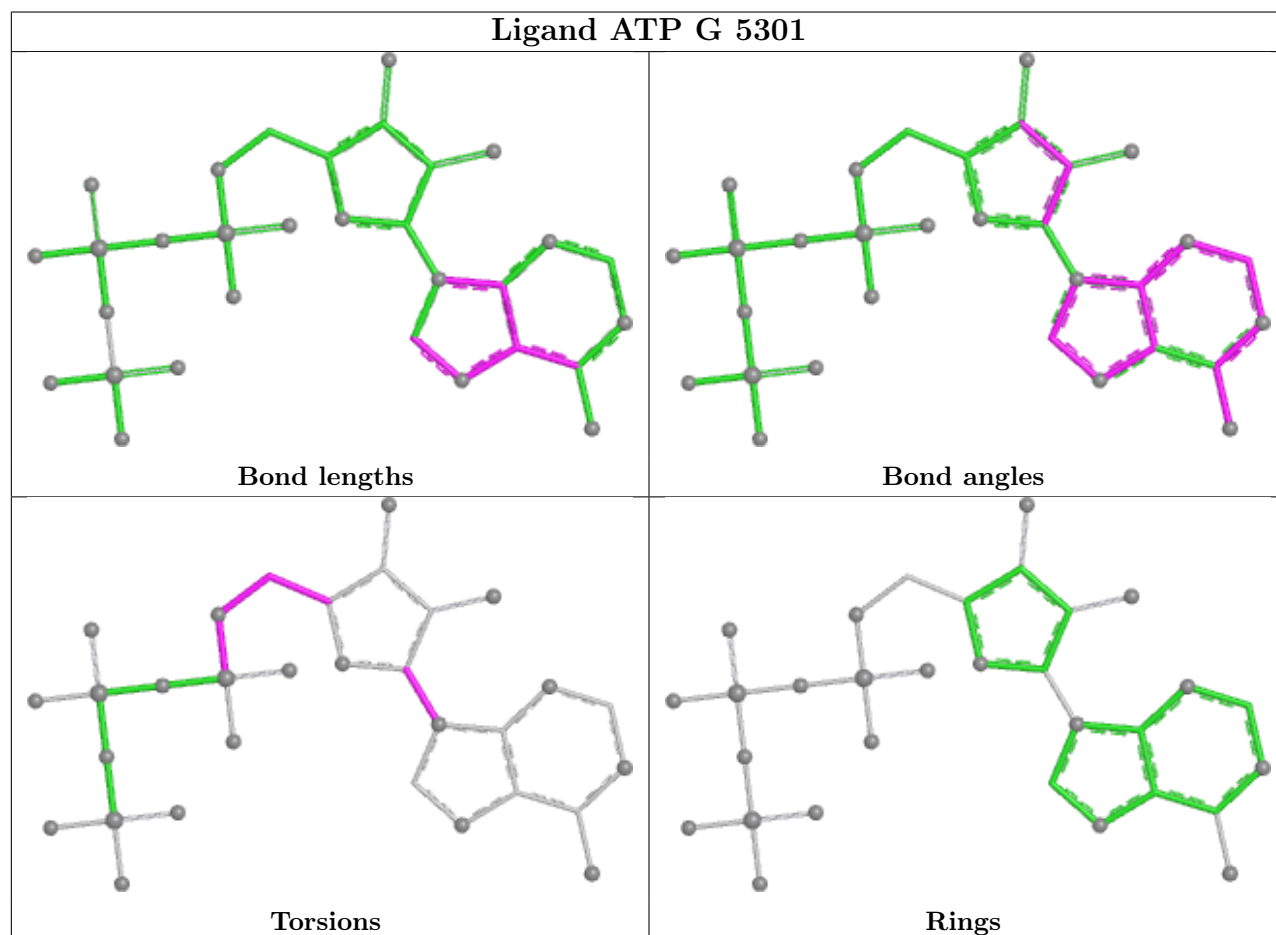
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5301	ATP	6	0
6	I	5304	CFF	2	0
3	I	5301	ATP	6	0

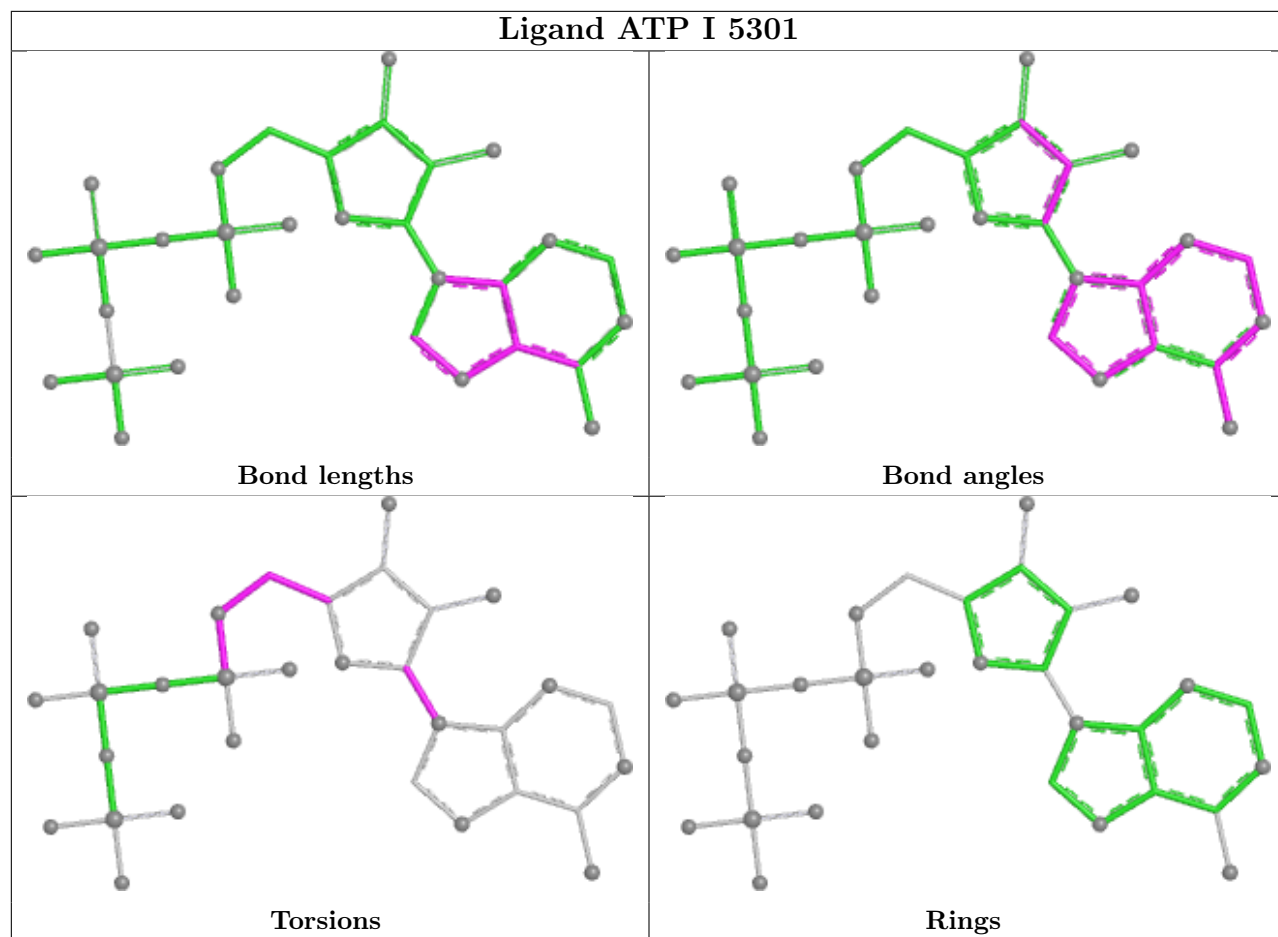
Continued on next page...

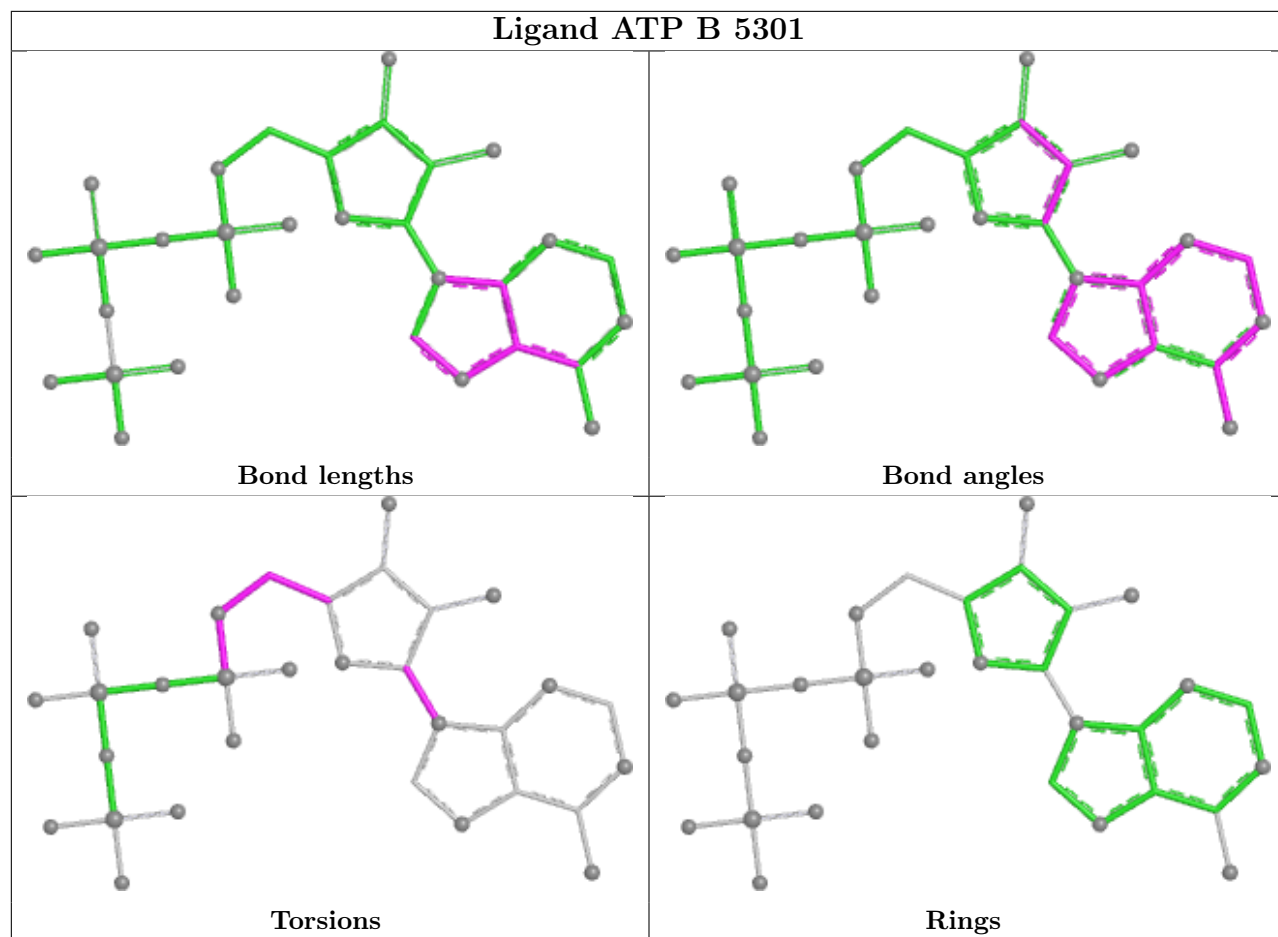
Continued from previous page...

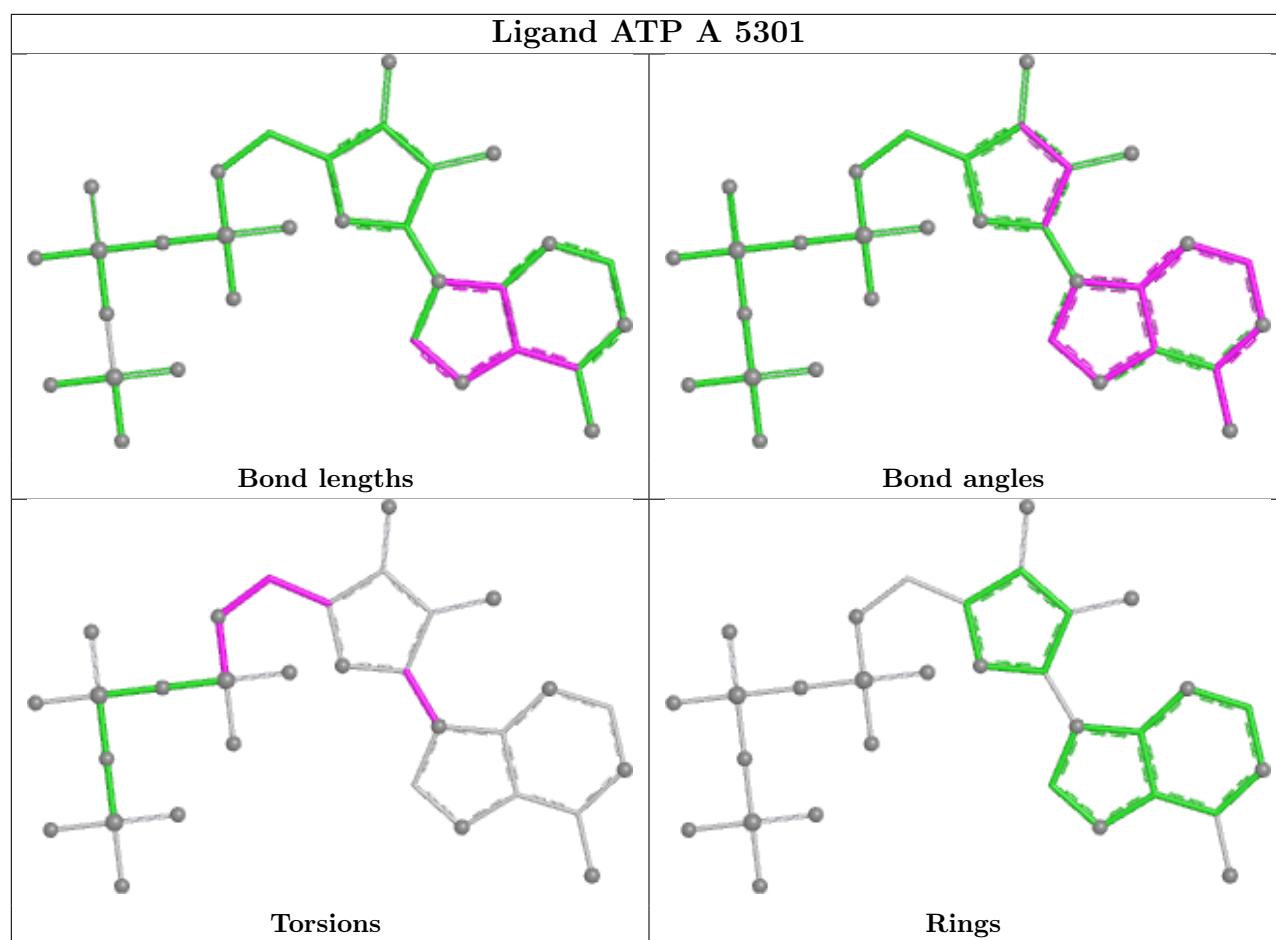
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5304	CFF	2	0
3	B	5301	ATP	5	0
6	G	5304	CFF	2	0
6	B	5304	CFF	2	0
3	A	5301	ATP	5	0

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.

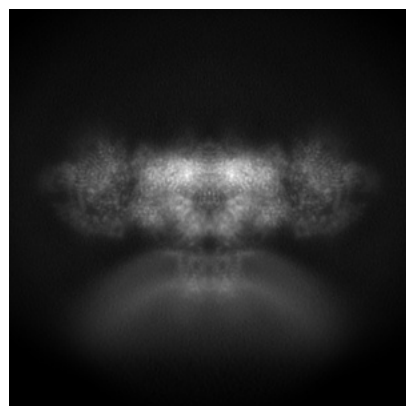
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23699. These allow visual inspection of the internal detail of the map and identification of artifacts.

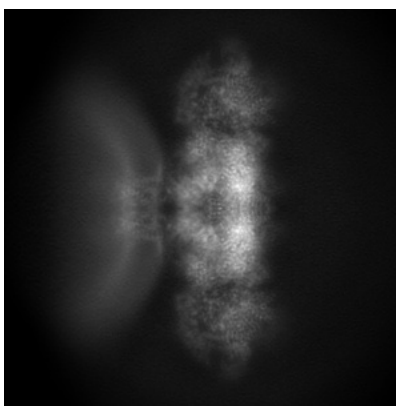
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

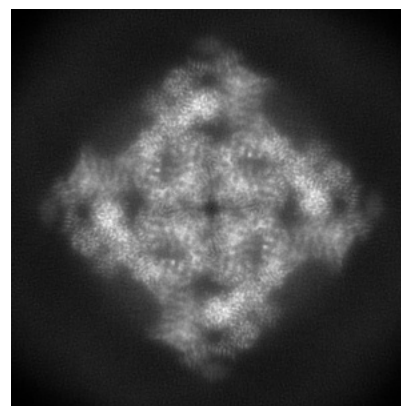
6.1.1 Primary map



X

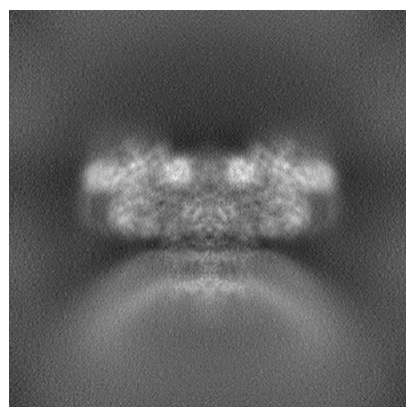


Y

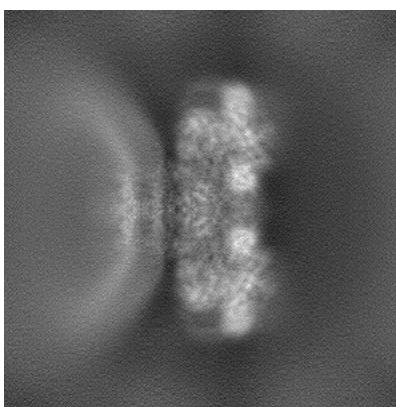


Z

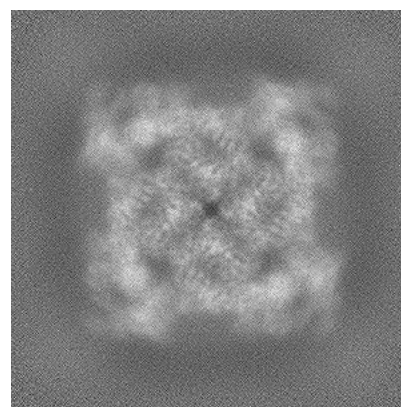
6.1.2 Raw map



X



Y

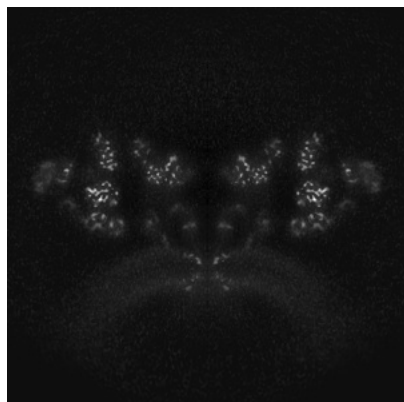


Z

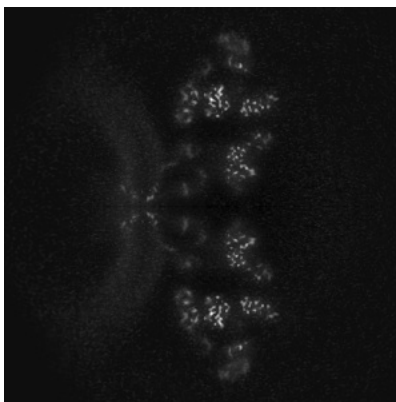
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

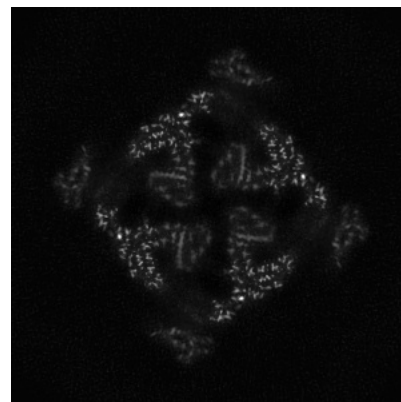
6.2.1 Primary map



X Index: 256



Y Index: 256

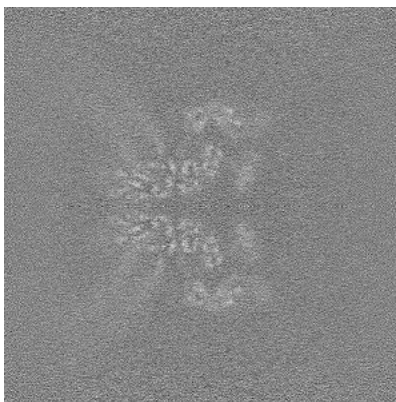


Z Index: 256

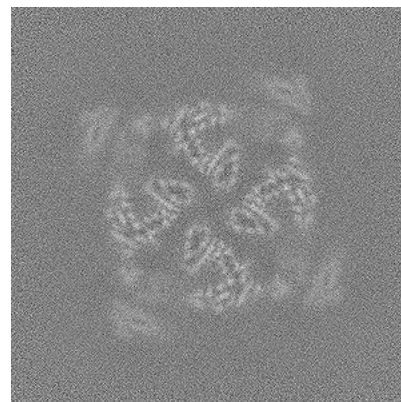
6.2.2 Raw map



X Index: 256



Y Index: 256

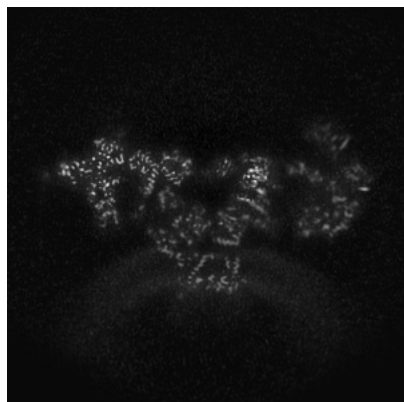


Z Index: 256

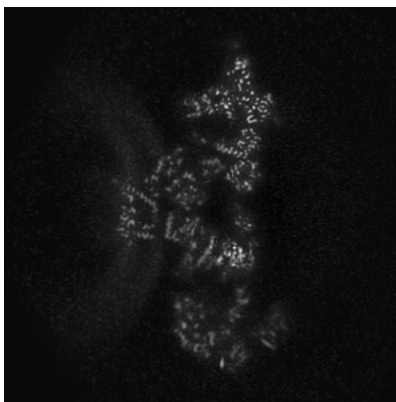
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

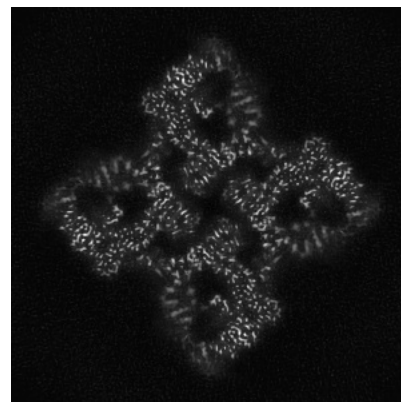
6.3.1 Primary map



X Index: 279

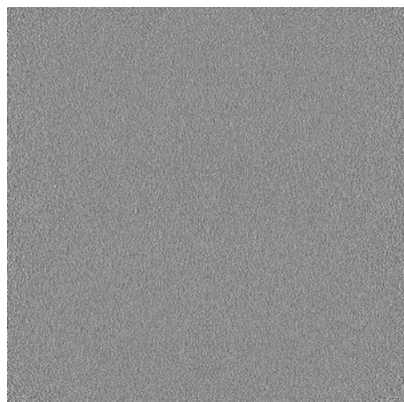


Y Index: 279

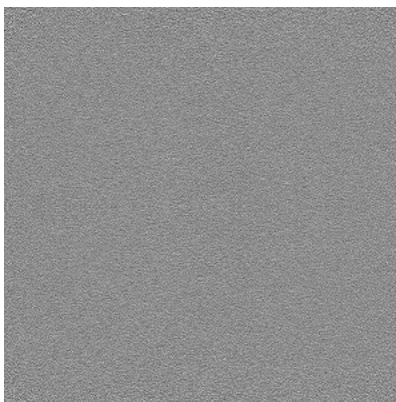


Z Index: 304

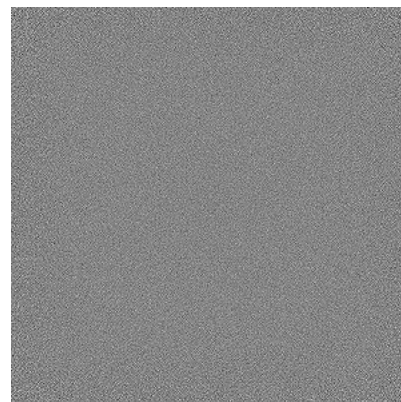
6.3.2 Raw map



X Index: 0



Y Index: 0

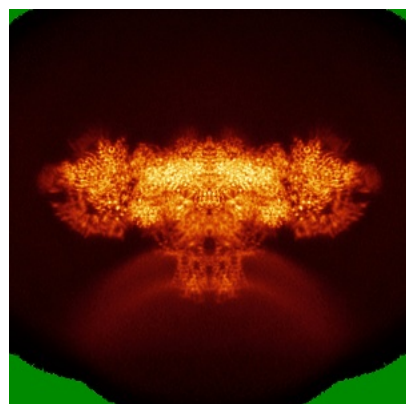


Z Index: 0

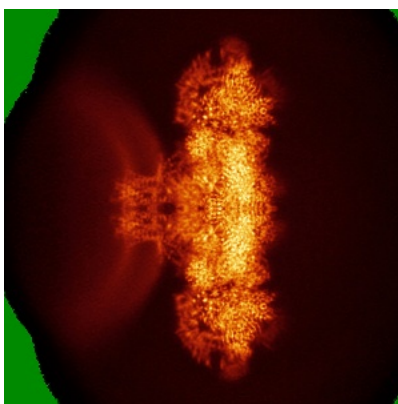
The images above show the largest variance slices of the map in three orthogonal directions.

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

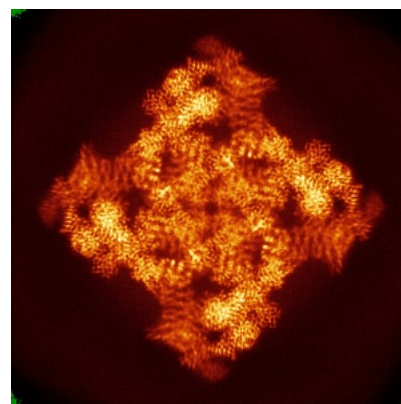
6.4.1 Primary map



X

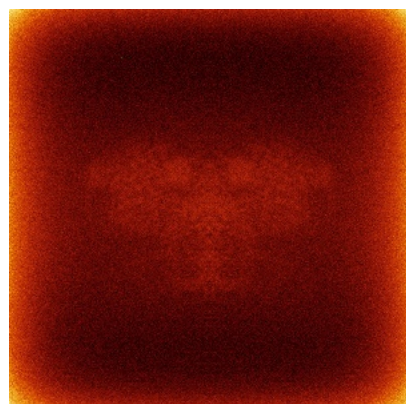


Y

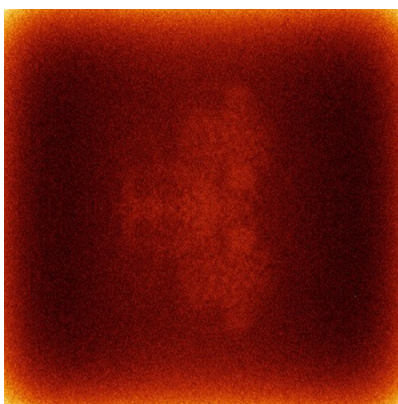


Z

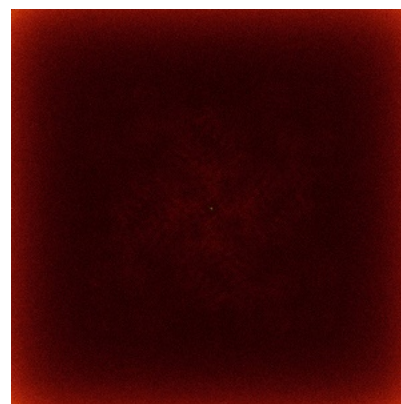
6.4.2 Raw map



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.

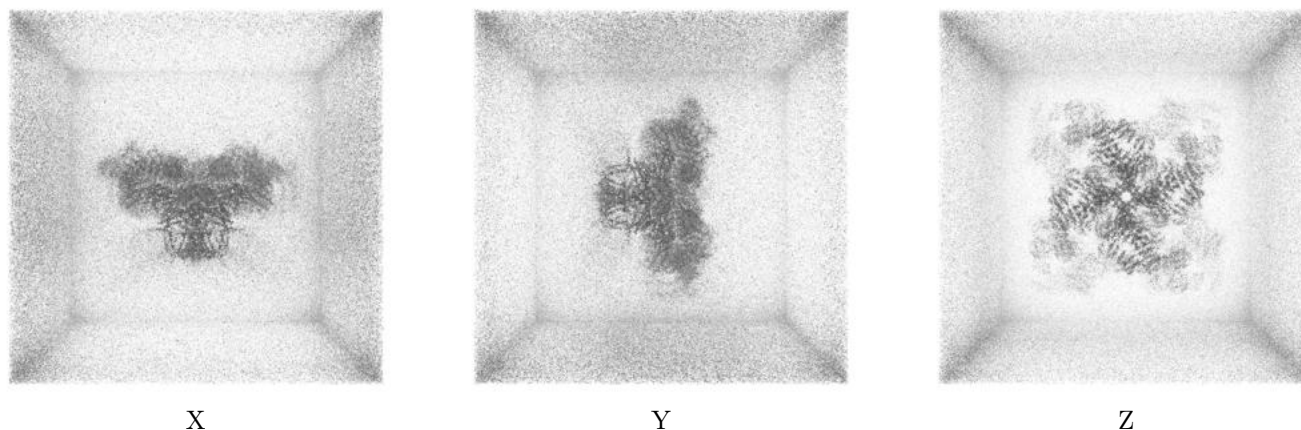
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.106. 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.

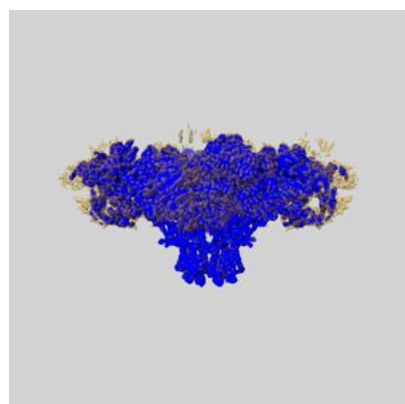
6.6 Mask visualisation [i](#)

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

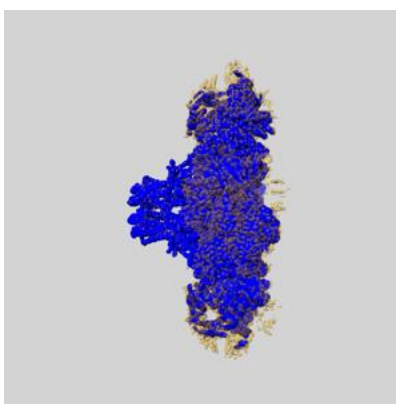
A mask typically either:

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

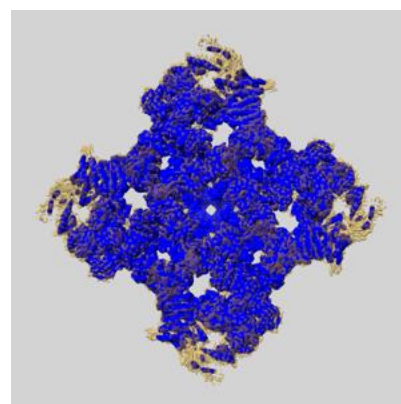
6.6.1 emd_23699_msk_1.map [i](#)



X



Y

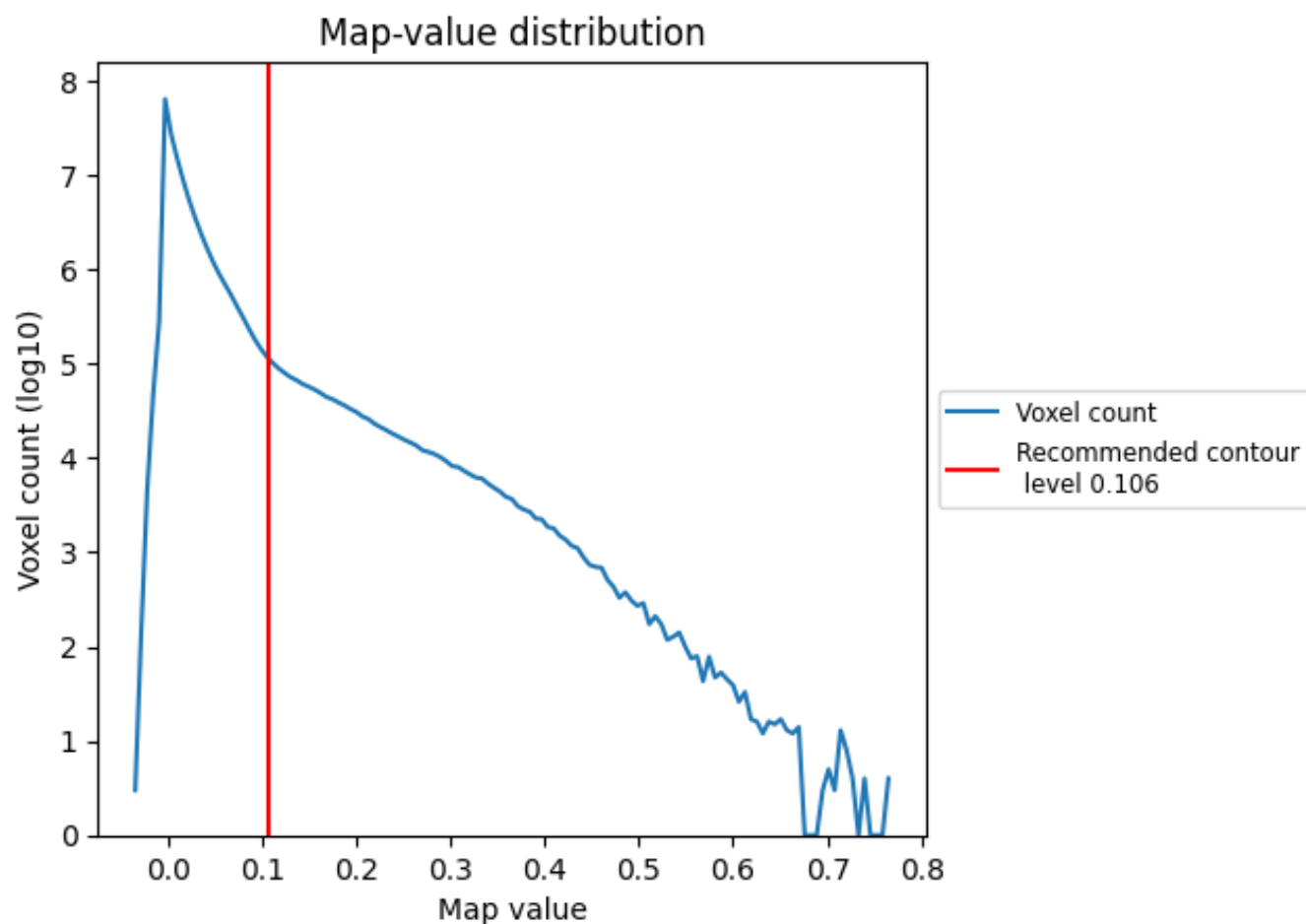


Z

7 Map analysis [i](#)

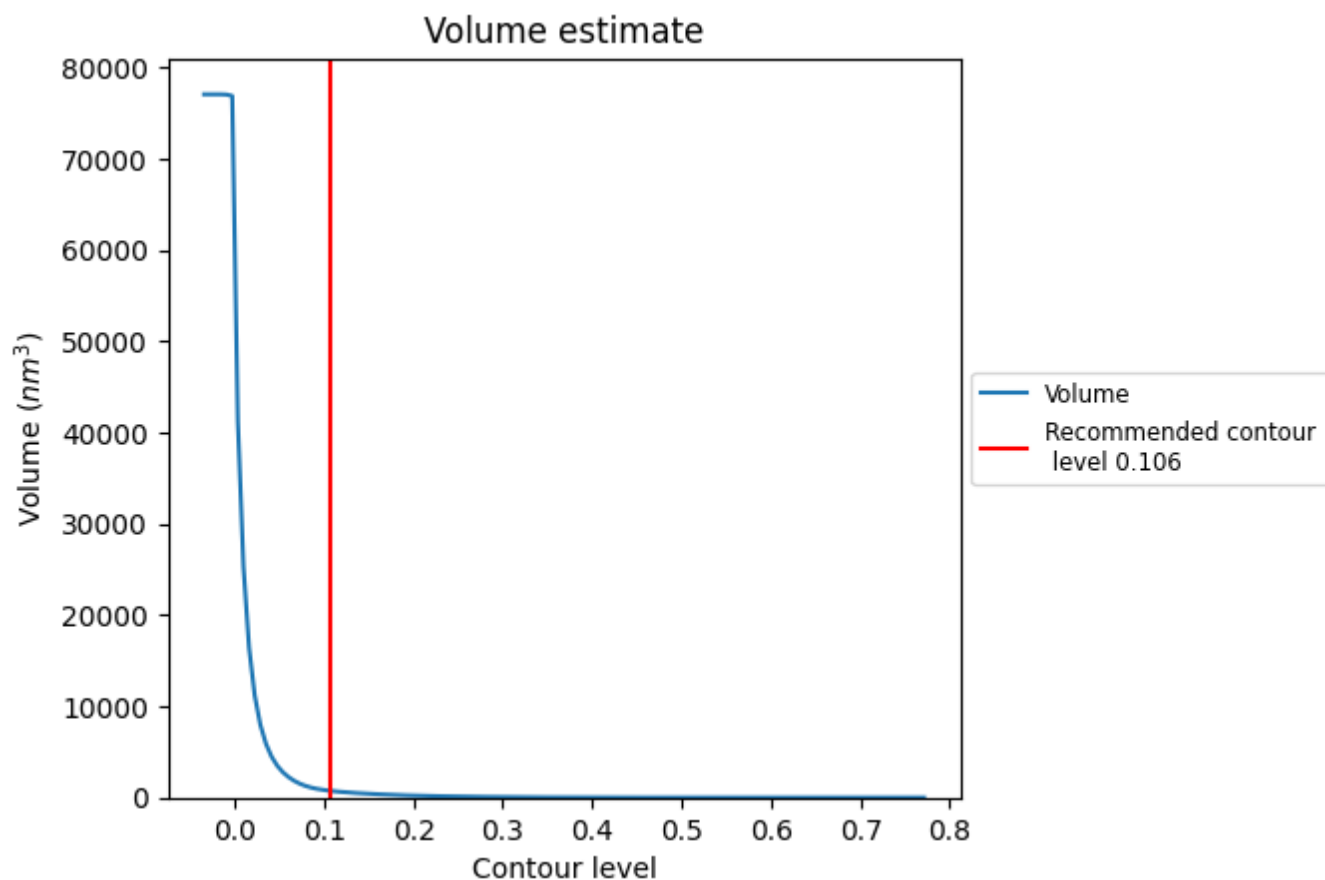
This section contains the results of statistical analysis of the map.

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.

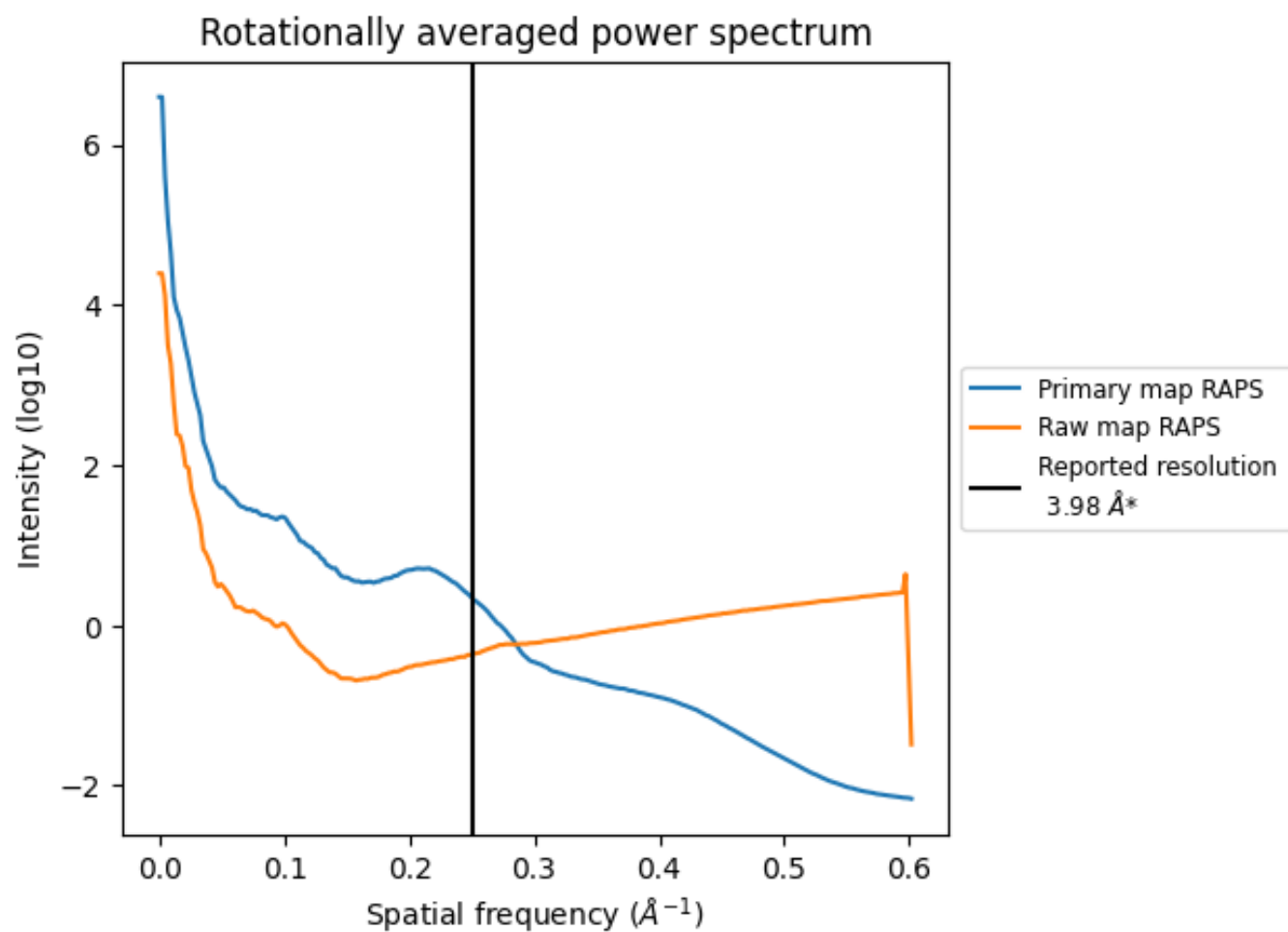
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm³; this corresponds to an approximate mass of 675 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 ⓘ

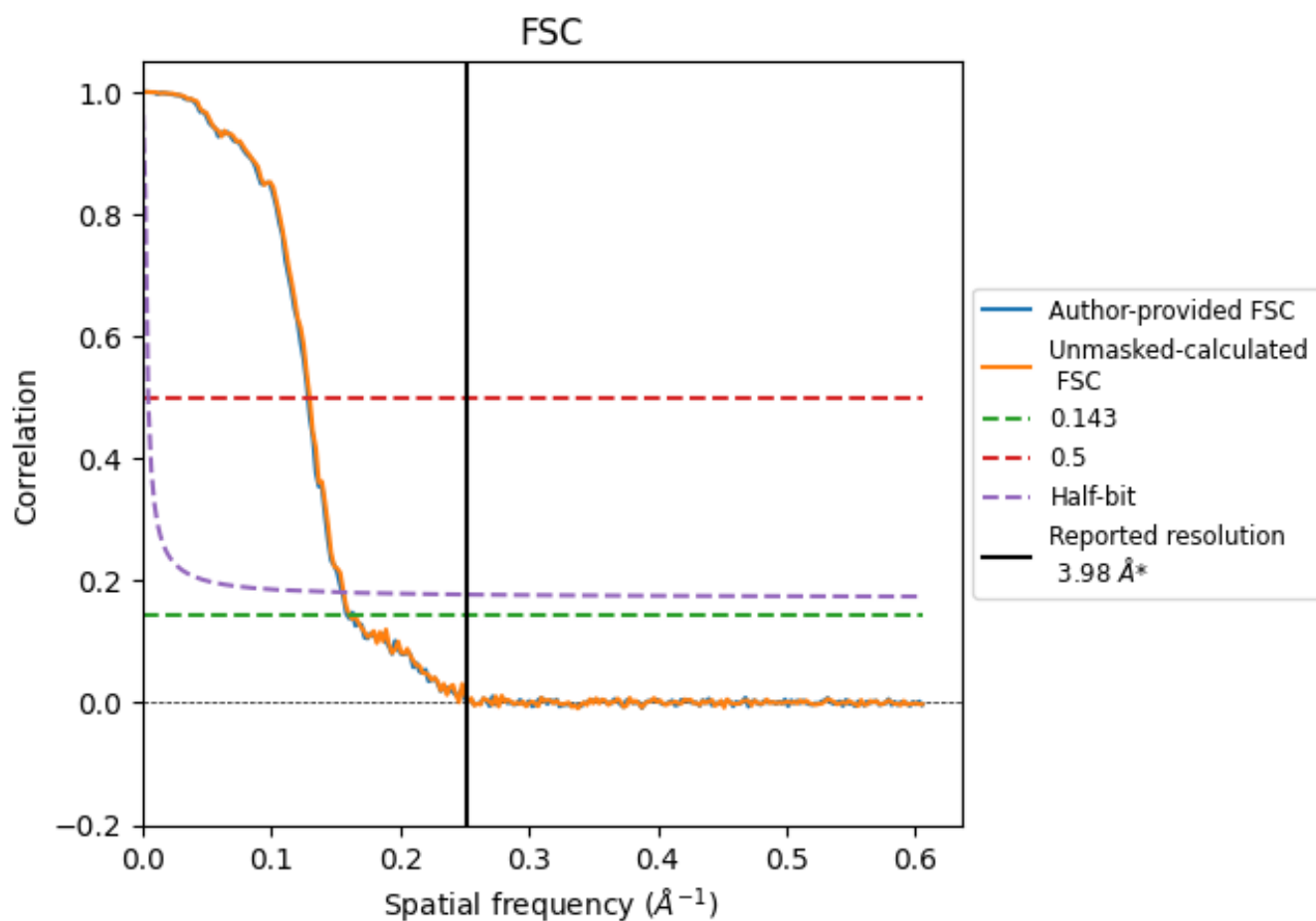


*Reported resolution corresponds to spatial frequency of 0.251 $\text{\AA}^{-1}$

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 0.251 Å⁻¹

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	6.28	7.78	6.44
Unmasked-calculated*	6.22	7.70	6.40

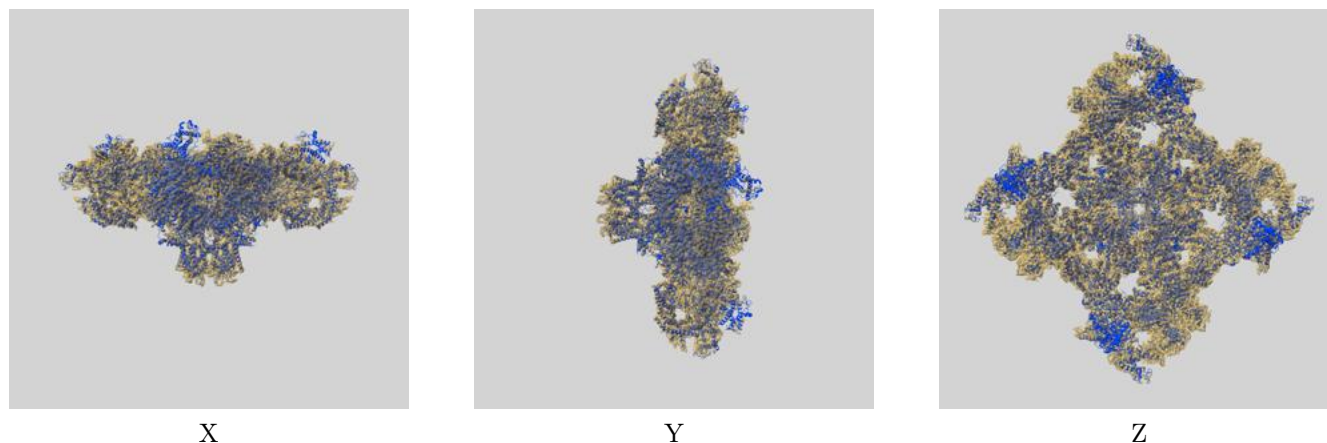
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.28 differs from the reported value 3.98 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.22 differs from the reported value 3.98 by more than 10 %

9 Map-model fit [i](#)

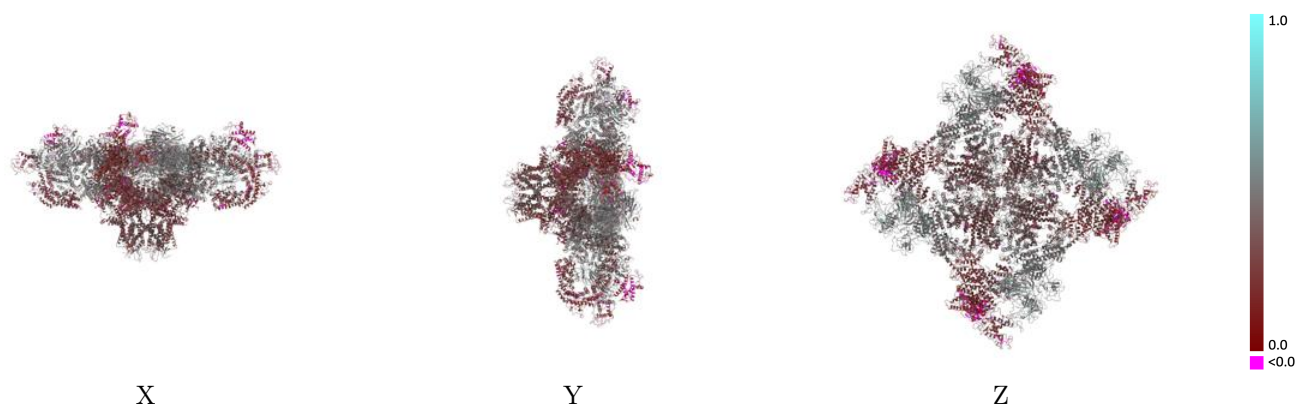
This section contains information regarding the fit between EMDB map EMD-23699 and PDB model 7M6L. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



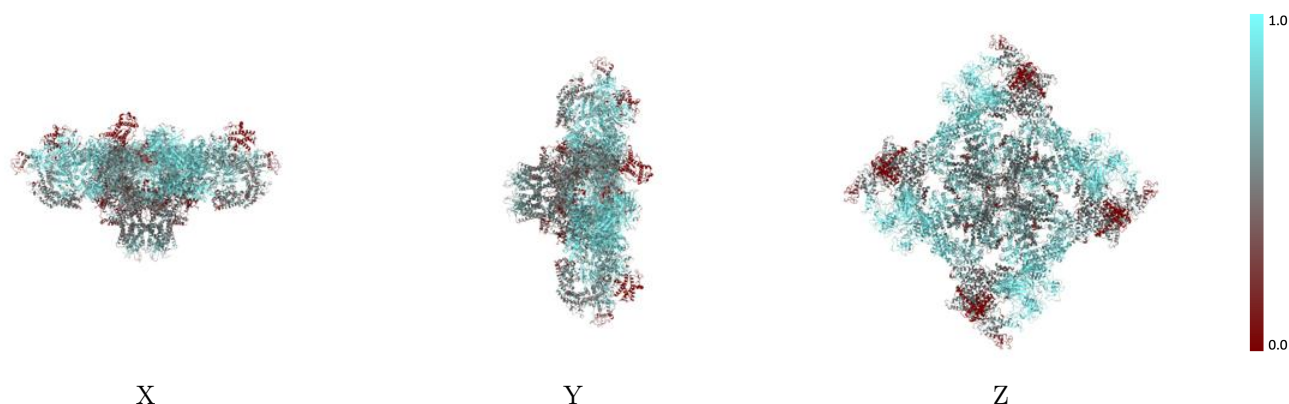
The images above show the 3D surface view of the map at the recommended contour level 0.106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



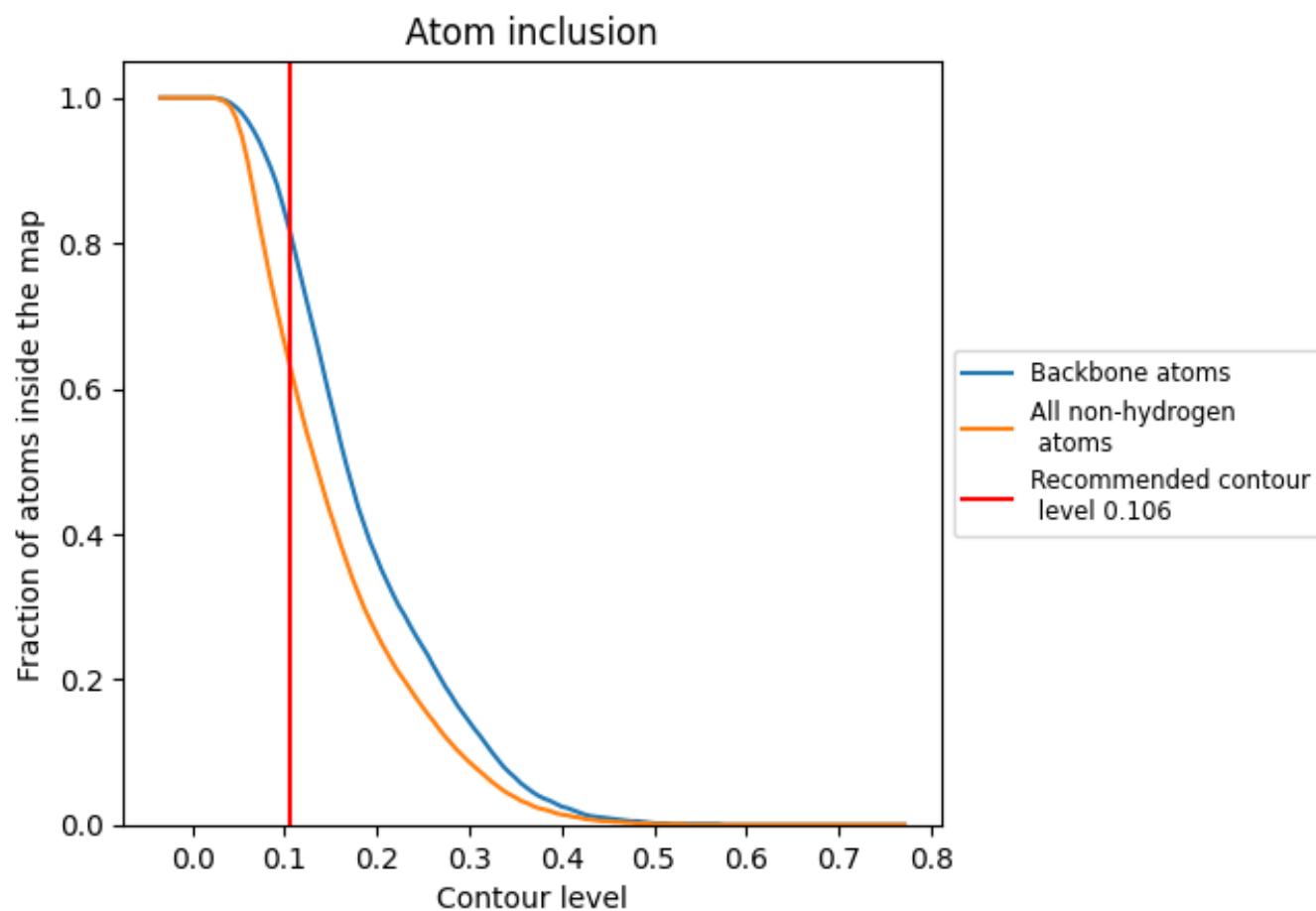
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.106).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6300	0.3560
A	0.6280	0.3600
B	0.6240	0.3500
F	0.8110	0.4790
G	0.6250	0.3500
H	0.8000	0.4790
I	0.6260	0.3500
J	0.8100	0.4780
O	0.8090	0.4800

1.0

0.0

<0.0