



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:16 pm GMT

PDB ID : 5TAV
EMDB ID: : EMD-8386
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

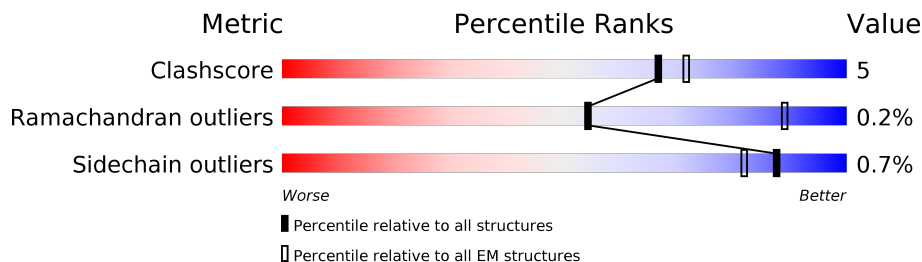
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	108	92% 7% .
1	F	108	91% 8% .
1	H	108	92% 7% .
1	J	108	93% 6% .
2	B	4416	84% 10% 5%
2	E	4416	84% 10% 5%
2	G	4416	85% 10% 5%
2	I	4416	84% 10% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

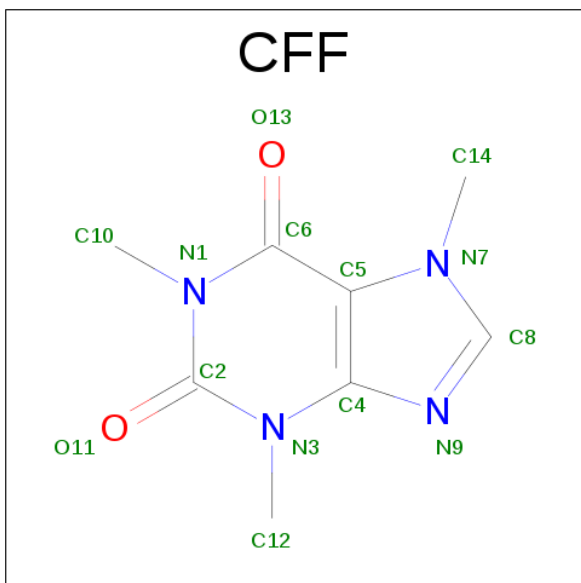
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	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
3	I	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

- Molecule 4 is CAFFEINE (three-letter code: 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	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	
5	E	1	Total	Zn	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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

Chain F: 



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

Chain A: 



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

Chain H: 




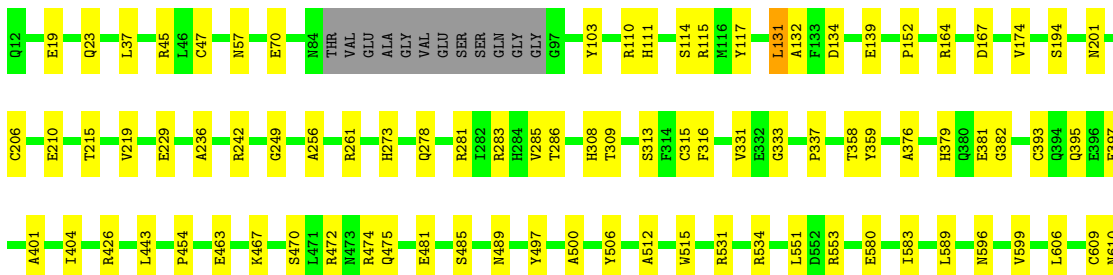
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 




- Molecule 2: Ryanodine receptor 1

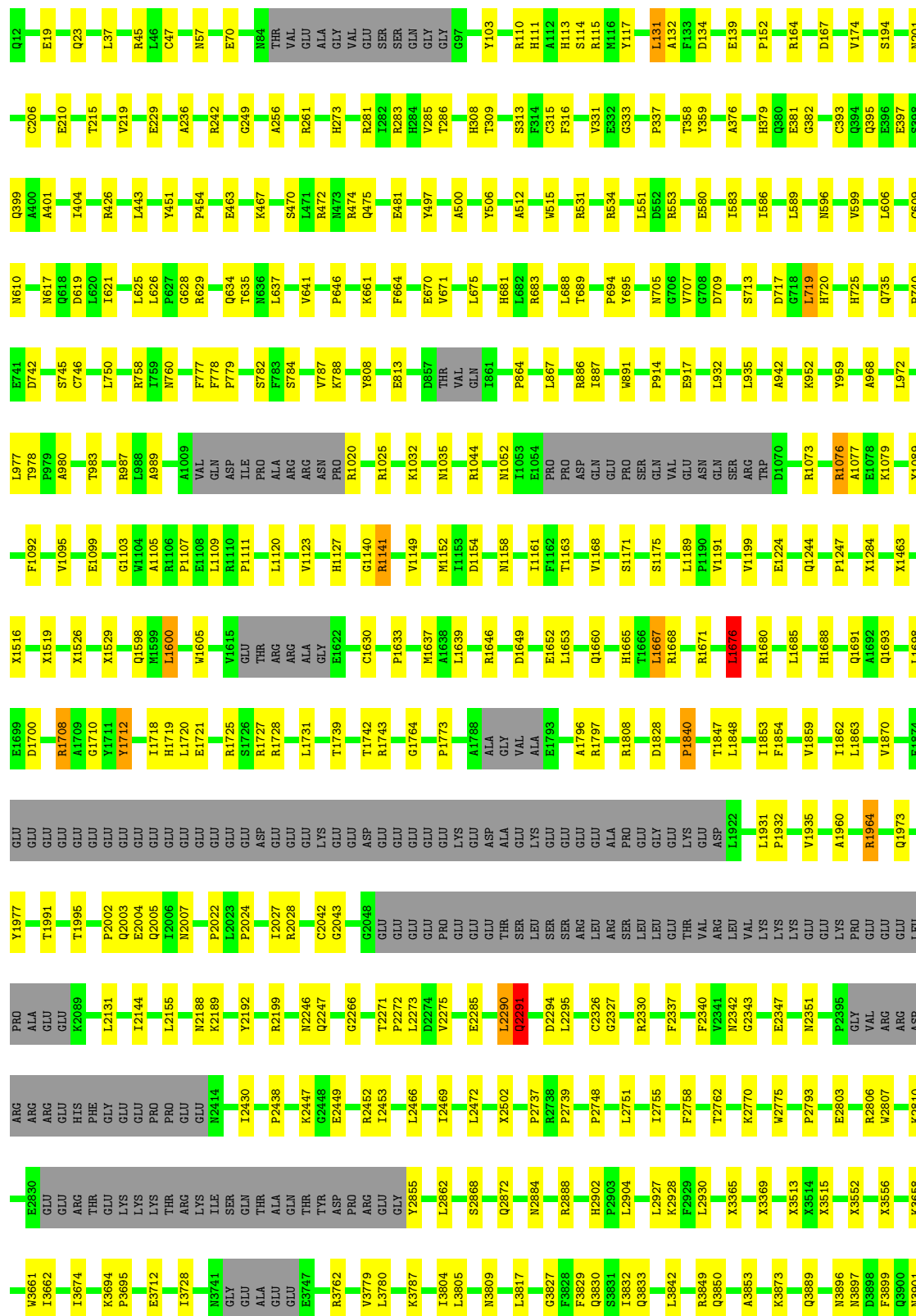
Chain B: 



[illegible]

● Molecule 2: Ryanodine receptor 1


Chain E:  84% 10% 5%



T3910	T3911	L3923	S3929	Y3937	Q3946	N3950	M3955	Q3960	V3961	F3962	N3963	G3971	L3980	L3985	F3992	F3996	K4002	L4019	N4034	V4049	R4085	T4104	G4105	P4106	M4120	E4126	M4130	E4152	H4156	R4159	P4176	R4192
I4193	Y4194	I4197	R4202	E4227	A4228	E4232	S4236	E4239	T4561	L4565	L4566	L4567	P4587	GLY	ASP	MET	GLY	SER	ALA	GLY	ASP	LEU	ALA	GLY	SER	GLY	TRP	SER	GLY	ALA	GLY	ASP

I4963	Y4967	F4976	E4976	T4977	H4978	E4982	H4983	W4984	L4995	I4996	Y5014	R5017	C5018	W5019	P5023	D5026	C5027	F5028	Y5032	L5036	S5037															
GLU	M4626	P4641	V4666	P4667	R4673	K4674	K4675	Y4687	K4698	G4699	M4714	Y4715	M4743	A4746	K4757	W4767	S4770	F4807	I4816	R4860	M4864	E4871	R4892	P4904	R4913	I4925	L4928	L4929	A4930	I4931	R4944	C4958	F4959	I4960	C4961	G4962


• Molecule 2: Ryanodine receptor 1

Chain I:  84% 10% 5%

P2024	I2027	R2028	C2042	G2043	G2048	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
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R2199	P2438	GLN	Y4560	Y4687	T4977	H4978	Y4687	Y4560	GLU	GLN	P2438	R2199
N2246	K2447	THR	T4561	K4698	H4978	T4979	K4698	T4561	E3747	THR	K2447	N2246
Q2247	G2448	TYR	F4564	G4699	T4979	T4979	G4699	F4564	R3762	ASP	G2448	Q2247
G2266	E2449	PRO	F4564	G4699	H4982	E4982	G4699	F4564	L4565	ASP	E2449	G2266
T2271	I2453	ARG	S4713	S4713	E4982	H4983	S4713	S4713	V3779	ARG	I2453	T2271
P2272	L2466	GLY	M4714	M4714	E4982	H4983	M4714	M4714	L3780	GLY	L2466	P2272
D2274	L2469	GLY	Y4715	Y4715	E4982	H4983	Y4715	Y4715	K3787	GLY	L2469	D2274
V2275	L2472	GLY	M4743	M4743	E4982	H4983	M4743	M4743	T3804	GLY	L2472	V2275
E2285	L2472	GLY	A4746	A4746	E4982	H4983	A4746	A4746	L3805	GLY	L2472	E2285
L2290	X2502	ASP	K4757	K4757	E4982	H4983	K4757	K4757	N3809	ASP	X2502	L2290
Q2291	P2737	MET	G4763	G4763	E4982	H4983	G4763	G4763	L3817	MET	P2737	Q2291
D2294	P2738	GLY	T4766	T4766	E4982	H4983	T4766	T4766	H2883	GLY	P2738	D2294
L2295	P2739	SER	W4767	W4767	E4982	H4983	W4767	W4767	N2884	SER	P2739	L2295
C2326	P2749	ALA	S4770	S4770	E4982	H4983	S4770	S4770	R2888	ALA	P2749	C2326
G2327	L2751	GLY	Y4775	Y4775	E4982	H4983	Y4775	Y4775	H2902	GLY	L2751	G2327
N2342	L2755	LEU	F4807	F4807	E4982	H4983	F4807	F4807	P2903	LEU	L2755	N2342
G2343	L2755	ALA	L5032	L5032	E4982	H4983	L5032	L5032	L2904	ALA	L2755	G2343
E2347	F2759	GLY	L5036	L5036	E4982	H4983	L5036	L5036	L2906	GLY	F2759	E2347
N2351	T2762	GLY	S5037	S5037	E4982	H4983	S5037	S5037	L2927	GLY	T2762	N2351
P2395	K2810	GLY	Y4925	Y4925	E4982	H4983	Y4925	Y4925	R3849	GLY	K2810	P2395
GLY	E2803	VAL	L4928	L4928	E4982	H4983	L4928	L4928	Q3850	VAL	E2803	GLY
ARG	R2806	ARG	A4930	A4930	E4982	H4983	A4930	A4930	F2928	ARG	R2806	ARG
ARG	W2807	ARG	I4931	I4931	E4982	H4983	I4931	I4931	F2929	ARG	W2807	ARG
ASP	E2830	ASP	R4944	R4944	E4982	H4983	R4944	R4944	L2930	ASP	E2830	ASP
ARG	GLU	ARG	K4957	K4957	E4982	H4983	K4957	K4957	X3365	ARG	GLU	ARG
ARG	GLU	ARG	C4958	C4958	E4982	H4983	C4958	C4958	X3365	ARG	GLU	ARG
ARG	THR	ARG	F4959	F4959	E4982	H4983	F4959	F4959	X3369	ARG	THR	ARG
HIS	GLY	HIS	I4960	I4960	E4982	H4983	I4960	I4960	X3513	HIS	GLY	HIS
PHE	LYS	PHE	C4961	C4961	E4982	H4983	C4961	C4961	X3514	PHE	LYS	PHE
GLY	LYS	GLY	G4962	G4962	E4982	H4983	G4962	G4962	X3515	GLY	LYS	GLY
GLU	LYS	GLU	I4963	I4963	E4982	H4983	I4963	I4963	X3552	GLU	LYS	GLU
PRO	LYS	PRO	C4964	C4964	E4982	H4983	C4964	C4964	X3556	PRO	LYS	PRO
GLU	ILE	GLU	Y4967	Y4967	E4982	H4983	Y4967	Y4967	K3658	GLU	ILE	GLU
N2414	SER	N2414	F4975	F4975	E4982	H4983	F4975	F4975	W3661	N2414	SER	N2414
I2430	THR	I2430	E4976	E4976	E4982	H4983	E4976	E4976	I3662	I2430	THR	I2430
	ALA				E4982	H4983			I3674		ALA	
					E4982	H4983			E3712			
					E4982	H4983			I3728			
					E4982	H4983			M3955			
					E4982	H4983			Q3946			
					E4982	H4983			N3950			
					E4982	H4983			M3961			
					E4982	H4983			Q3960			
					E4982	H4983			F3962			
					E4982	H4983			N3963			

• Molecule 2: Ryanodine receptor 1

Chain G:  85% 10% 5%

Q12	E210	E463	T635	R1141	ALA	Q12	E210	E463	T635	R1141	ALA
E19	T215	K467	H636	V1149	ARG	E19	T215	K467	H636	V1149	ARG
Q23	V219	S470	L637	M1152	ASN	Q23	V219	S470	L637	M1152	ASN
L37	A236	L471	V641	D1154	PRO	L37	A236	L471	V641	D1154	PRO
R45	R242	R472	P646	T1158	N1035	R45	R242	R472	P646	T1158	N1035
C47	A256	R474	F664	I1161	R1044	C47	A256	R474	F664	I1161	R1044
N57	R261	E481	V671	F1162	T1045	N57	R261	E481	V671	F1162	T1045
E70	H273	Y497	L675	T1163	N1052	E70	H273	Y497	L675	T1163	N1052
N84	R283	A500	H681	V1168	I1053	N84	R283	A500	H681	V1168	I1053
THR	R284	Y506	L682	L1189	PRO	THR	R284	Y506	L682	L1189	PRO
VAL	V285	Y506	R683	V1199	ASP	VAL	V285	Y506	R683	V1199	ASP
GLU	T286	A512	L688	E1224	GLN	GLU	T286	A512	L688	E1224	GLN
GLY	H308	W515	T689	Q1244	PRO	GLY	H308	W515	T689	Q1244	PRO
VAL	T309	W515	P694	Q1244	GLN	VAL	T309	W515	P694	Q1244	GLN
GLU	S313	R531	Y695	P1247	VAL	GLU	S313	R531	Y695	P1247	VAL
SER	F314	R534	N705	X1247	ASN	SER	F314	R534	N705	X1247	ASN
GLN	C315	G706	G706	X1284	GLN	GLN	C315	G706	G706	X1284	GLN
GLY	F316	W707	V707	X1463	SER	GLY	F316	W707	V707	X1463	SER
GLY	V331	L551	G708	X1516	ARG	GLY	V331	L551	G708	X1516	ARG
G97	F332	D552	D709	X1516	TRP	G97	F332	D552	D709	X1516	TRP
Y103	C333	R553	S713	X1519	D1070	Y103	C333	R553	S713	X1519	D1070
R110	P337	E580	D717	X1519	R1073	R110	P337	E580	D717	X1519	R1073
H111	T358	I583	G718	X1526	R1076	H111	T358	I583	G718	X1526	R1076
S114	Y359	L589	L719	X1529	A1077	S114	Y359	L589	L719	X1529	A1077
R115	Y359	L589	H720	X1529	E1078	R115	Y359	L589	H720	X1529	E1078
H116	A376	N596	H725	L1595	K1079	H116	A376	N596	H725	L1595	K1079
Y117	H379	V599	Q735	Q1598	Y1089	Y117	H379	V599	Q735	Q1598	Y1089
L131	Q380	L606	P740	M1599	F1092	L131	Q380	L606	P740	M1599	F1092
A132	E381	L606	E741	L1600	F1092	A132	E381	L606	E741	L1600	F1092
F133	C382	C609	D742	W1605	V1095	F133	C382	C609	D742	W1605	V1095
D134	C393	N610	S745	V1615	G1103	D134	C393	N610	S745	V1615	G1103
E139	Q394	N617	C746	W1615	A1104	E139	Q394	N617	C746	W1615	A1104
P152	E395	Q618	L750	W1615	R1106	P152	E395	Q618	L750	W1615	R1106
R164	E397	D619	L750	W1615	P1107	R164	E397	D619	L750	W1615	P1107
D167	A401	L620	R758	W1615	E1108	D167	A401	L620	R758	W1615	E1108
S194	I404	L621	I759	W1615	L1109	S194	I404	L621	I759	W1615	L1109
N201	L625	L626	N760	E1622	P1111	N201	L625	L626	N760	E1622	P1111
C206	R426	P627	F777	C1630	L1120	C206	R426	P627	F777	C1630	L1120
	L443	G628	F778	P1633	V1123		L443	G628	F778	P1633	V1123
	P454	R629	F779	M1637	G1140		P454	R629	F779	M1637	G1140
		PRO	S782					PRO	S782		

Y5032	S5037	L4816	LEU	L4019	L3817	N2884	P2737	Q2291	GLU	GLU	A1788	A1838
		R4860	GLY	N4034	G3827	R2388	R2738	D2294	THR	GLU	ALA	L1839
		N4864	GLY	V4049	F3828	R2388	P2739	L2295	LEU	LYS	GLY	L1839
		E4871	SER	R4085	F3829	R2903	P2748	C2326	SER	ASP	VAL	R1846
		P4904	GLY	G4105	G3830	G2903	P2748	G2327	SER	ALA	ALA	D1849
		R4913	GLY	P4106	G3833	L2904	L2751	R2330	ARG	GLU	E1793	E1852
		L4925	SER	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4928	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4929	ALA	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4930	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y4963	Y4964	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y4967	Y4968	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y4971	Y4972	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y4975	Y4976	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y4978	Y4979	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y4982	Y4983	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y4984	Y4985	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y5007	Y5017	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y5018	Y5019	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y5023	Y5026	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
Y5027	Y5028	L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860
		L4931	GLY	E4126	F3829	L2927	L2755	F2337	LEU	GLU	L1802	Q1860

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.29	0/834	0.52	0/1123
1	F	0.29	0/834	0.52	0/1123
1	H	0.29	0/834	0.52	0/1123
1	J	0.29	0/834	0.52	0/1123
2	B	0.29	0/25428	0.54	10/34534 (0.0%)
2	E	0.29	0/25428	0.54	10/34534 (0.0%)
2	G	0.29	0/25428	0.54	10/34534 (0.0%)
2	I	0.29	0/25428	0.54	10/34534 (0.0%)
All	All	0.29	0/105048	0.54	40/142628 (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
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.42	134.66	115.30
2	B	131	LEU	CA-CB-CG	8.41	134.65	115.30
2	E	131	LEU	CA-CB-CG	8.41	134.63	115.30
2	I	131	LEU	CA-CB-CG	8.39	134.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1600	LEU	CA-CB-CG	6.97	131.33	115.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	694	PRO	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	5	0
1	F	818	0	824	5	0
1	H	818	0	824	4	0
1	J	818	0	824	4	0
2	B	29499	0	24746	252	0
2	E	29499	0	24746	258	0
2	G	29499	0	24746	248	0
2	I	29499	0	24746	255	0
3	B	31	0	12	0	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102368	1020	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 1020 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:5028:PHE:HE1	2:G:5032:TYR:CD2	1.87	0.93
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.87	0.93
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.87	0.92
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.87	0.92
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.58	0.92

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%)	2916 (90%)	311 (10%)	8 (0%)	51	84
2	E	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	51	84
2	G	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	51	84
2	I	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	51	84
All	All	13360/18096 (74%)	12037 (90%)	1291 (10%)	32 (0%)	54	84

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE

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Mol	Chain	Res	Type
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG

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%)	2476 (99%)	17 (1%)	87	93
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	87	93

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	4944	ARG
2	I	1141	ARG
2	G	4085	ARG
2	E	4983	HIS
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3946	GLN

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Mol	Chain	Res	Type
2	I	395	GLN
2	G	3889	GLN
2	E	3960	GLN
2	E	4806	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	B	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.69	2 (8%)
4	CFF	B	5102	-	7,15,15	1.93	2 (28%)	8,23,23	1.23	1 (12%)
3	ATP	E	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.70	2 (8%)
4	CFF	E	5102	-	7,15,15	1.93	2 (28%)	8,23,23	1.23	1 (12%)
3	ATP	G	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.69	2 (8%)
4	CFF	G	5102	-	7,15,15	1.93	2 (28%)	8,23,23	1.24	1 (12%)
3	ATP	I	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.69	2 (8%)
4	CFF	I	5102	-	7,15,15	1.94	2 (28%)	8,23,23	1.23	1 (12%)

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	B	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	E	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	G	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	I	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	0/0/0/0	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C6-N1	-4.00	1.32	1.38
4	E	5102	CFF	C6-N1	-3.98	1.32	1.38
4	G	5102	CFF	C6-N1	-3.97	1.32	1.38
4	B	5102	CFF	C6-N1	-3.97	1.32	1.38
4	G	5102	CFF	O13-C6	-2.32	1.18	1.24

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-6.53	123.17	128.86
3	I	5101	ATP	N3-C2-N1	-6.48	123.22	128.86
3	B	5101	ATP	N3-C2-N1	-6.47	123.22	128.86
3	G	5101	ATP	N3-C2-N1	-6.47	123.22	128.86
4	G	5102	CFF	C14-N7-C8	-2.83	112.02	125.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5102	CFF	1	0
4	E	5102	CFF	1	0
4	G	5102	CFF	1	0
4	I	5102	CFF	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	72.89
1	E	4345:UNK	C	4540:PHE	N	72.89
1	I	4345:UNK	C	4540:PHE	N	72.89
1	G	4345:UNK	C	4540:PHE	N	72.89
1	B	3613:UNK	C	3639:THR	N	44.63