



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jul 12, 2018 – 12:57 AM EDT

PDB ID : 5L1D
EMDB ID: : EMD-8303
Title : Structure of rabbit RyR2 in complex with FKBP12.6 in a closed state (conformation C1)
Authors : Dhindwal, S.; Lobo, J.J.; Samso, M.
Deposited on : 2016-07-29
Resolution : 10.50 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

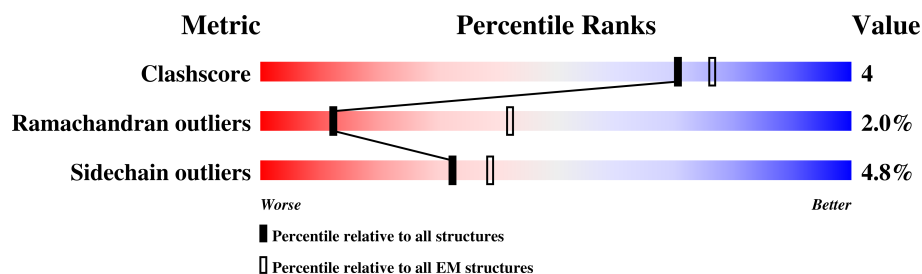
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY









The reported resolution of this entry is 10.50 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	4387	 71% 10% • 19%
1	C	4387	 70% 11% • 19%
1	E	4387	 70% 11% • 19%
1	G	4387	 70% 10% • 19%
2	B	158	 58% 10% 32%
2	D	158	 60% 8% 32%
2	F	158	 56% 12% 32%
2	H	158	 63% • 32%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 112936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	C	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	E	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	G	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-50	MET	-	expression tag	UNP P68106
B	-49	ASN	-	expression tag	UNP P68106
B	-48	HIS	-	expression tag	UNP P68106
B	-47	LYS	-	expression tag	UNP P68106
B	-46	VAL	-	expression tag	UNP P68106
B	-45	HIS	-	expression tag	UNP P68106
B	-44	HIS	-	expression tag	UNP P68106
B	-43	HIS	-	expression tag	UNP P68106
B	-42	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-41	HIS	-	expression tag	UNP P68106
B	-40	HIS	-	expression tag	UNP P68106
B	-39	MET	-	expression tag	UNP P68106
B	-38	ASP	-	expression tag	UNP P68106
B	-37	GLU	-	expression tag	UNP P68106
B	-36	LYS	-	expression tag	UNP P68106
B	-35	THR	-	expression tag	UNP P68106
B	-34	THR	-	expression tag	UNP P68106
B	-33	GLY	-	expression tag	UNP P68106
B	-32	TRP	-	expression tag	UNP P68106
B	-31	ARG	-	expression tag	UNP P68106
B	-30	GLY	-	expression tag	UNP P68106
B	-29	GLY	-	expression tag	UNP P68106
B	-28	HIS	-	expression tag	UNP P68106
B	-27	VAL	-	expression tag	UNP P68106
B	-26	VAL	-	expression tag	UNP P68106
B	-25	GLU	-	expression tag	UNP P68106
B	-24	GLY	-	expression tag	UNP P68106
B	-23	LEU	-	expression tag	UNP P68106
B	-22	ALA	-	expression tag	UNP P68106
B	-21	GLY	-	expression tag	UNP P68106
B	-20	GLU	-	expression tag	UNP P68106
B	-19	LEU	-	expression tag	UNP P68106
B	-18	GLU	-	expression tag	UNP P68106
B	-17	GLN	-	expression tag	UNP P68106
B	-16	LEU	-	expression tag	UNP P68106
B	-15	ARG	-	expression tag	UNP P68106
B	-14	ALA	-	expression tag	UNP P68106
B	-13	ARG	-	expression tag	UNP P68106
B	-12	LEU	-	expression tag	UNP P68106
B	-11	GLU	-	expression tag	UNP P68106
B	-10	HIS	-	expression tag	UNP P68106
B	-9	HIS	-	expression tag	UNP P68106
B	-8	PRO	-	expression tag	UNP P68106
B	-7	GLN	-	expression tag	UNP P68106
B	-6	GLY	-	expression tag	UNP P68106
B	-5	GLN	-	expression tag	UNP P68106
B	-4	ARG	-	expression tag	UNP P68106
B	-3	GLU	-	expression tag	UNP P68106
B	-2	PRO	-	expression tag	UNP P68106
B	-1	GLU	-	expression tag	UNP P68106
B	0	LEU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-50	MET	-	expression tag	UNP P68106
D	-49	ASN	-	expression tag	UNP P68106
D	-48	HIS	-	expression tag	UNP P68106
D	-47	LYS	-	expression tag	UNP P68106
D	-46	VAL	-	expression tag	UNP P68106
D	-45	HIS	-	expression tag	UNP P68106
D	-44	HIS	-	expression tag	UNP P68106
D	-43	HIS	-	expression tag	UNP P68106
D	-42	HIS	-	expression tag	UNP P68106
D	-41	HIS	-	expression tag	UNP P68106
D	-40	HIS	-	expression tag	UNP P68106
D	-39	MET	-	expression tag	UNP P68106
D	-38	ASP	-	expression tag	UNP P68106
D	-37	GLU	-	expression tag	UNP P68106
D	-36	LYS	-	expression tag	UNP P68106
D	-35	THR	-	expression tag	UNP P68106
D	-34	THR	-	expression tag	UNP P68106
D	-33	GLY	-	expression tag	UNP P68106
D	-32	TRP	-	expression tag	UNP P68106
D	-31	ARG	-	expression tag	UNP P68106
D	-30	GLY	-	expression tag	UNP P68106
D	-29	GLY	-	expression tag	UNP P68106
D	-28	HIS	-	expression tag	UNP P68106
D	-27	VAL	-	expression tag	UNP P68106
D	-26	VAL	-	expression tag	UNP P68106
D	-25	GLU	-	expression tag	UNP P68106
D	-24	GLY	-	expression tag	UNP P68106
D	-23	LEU	-	expression tag	UNP P68106
D	-22	ALA	-	expression tag	UNP P68106
D	-21	GLY	-	expression tag	UNP P68106
D	-20	GLU	-	expression tag	UNP P68106
D	-19	LEU	-	expression tag	UNP P68106
D	-18	GLU	-	expression tag	UNP P68106
D	-17	GLN	-	expression tag	UNP P68106
D	-16	LEU	-	expression tag	UNP P68106
D	-15	ARG	-	expression tag	UNP P68106
D	-14	ALA	-	expression tag	UNP P68106
D	-13	ARG	-	expression tag	UNP P68106
D	-12	LEU	-	expression tag	UNP P68106
D	-11	GLU	-	expression tag	UNP P68106
D	-10	HIS	-	expression tag	UNP P68106
D	-9	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	PRO	-	expression tag	UNP P68106
D	-7	GLN	-	expression tag	UNP P68106
D	-6	GLY	-	expression tag	UNP P68106
D	-5	GLN	-	expression tag	UNP P68106
D	-4	ARG	-	expression tag	UNP P68106
D	-3	GLU	-	expression tag	UNP P68106
D	-2	PRO	-	expression tag	UNP P68106
D	-1	GLU	-	expression tag	UNP P68106
D	0	LEU	-	expression tag	UNP P68106
F	-50	MET	-	expression tag	UNP P68106
F	-49	ASN	-	expression tag	UNP P68106
F	-48	HIS	-	expression tag	UNP P68106
F	-47	LYS	-	expression tag	UNP P68106
F	-46	VAL	-	expression tag	UNP P68106
F	-45	HIS	-	expression tag	UNP P68106
F	-44	HIS	-	expression tag	UNP P68106
F	-43	HIS	-	expression tag	UNP P68106
F	-42	HIS	-	expression tag	UNP P68106
F	-41	HIS	-	expression tag	UNP P68106
F	-40	HIS	-	expression tag	UNP P68106
F	-39	MET	-	expression tag	UNP P68106
F	-38	ASP	-	expression tag	UNP P68106
F	-37	GLU	-	expression tag	UNP P68106
F	-36	LYS	-	expression tag	UNP P68106
F	-35	THR	-	expression tag	UNP P68106
F	-34	THR	-	expression tag	UNP P68106
F	-33	GLY	-	expression tag	UNP P68106
F	-32	TRP	-	expression tag	UNP P68106
F	-31	ARG	-	expression tag	UNP P68106
F	-30	GLY	-	expression tag	UNP P68106
F	-29	GLY	-	expression tag	UNP P68106
F	-28	HIS	-	expression tag	UNP P68106
F	-27	VAL	-	expression tag	UNP P68106
F	-26	VAL	-	expression tag	UNP P68106
F	-25	GLU	-	expression tag	UNP P68106
F	-24	GLY	-	expression tag	UNP P68106
F	-23	LEU	-	expression tag	UNP P68106
F	-22	ALA	-	expression tag	UNP P68106
F	-21	GLY	-	expression tag	UNP P68106
F	-20	GLU	-	expression tag	UNP P68106
F	-19	LEU	-	expression tag	UNP P68106
F	-18	GLU	-	expression tag	UNP P68106

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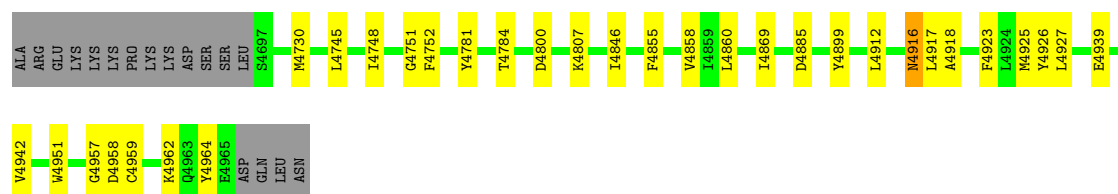
Chain	Residue	Modelled	Actual	Comment	Reference
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F	-13	ARG	-	expression tag	UNP P68106
F	-12	LEU	-	expression tag	UNP P68106
F	-11	GLU	-	expression tag	UNP P68106
F	-10	HIS	-	expression tag	UNP P68106
F	-9	HIS	-	expression tag	UNP P68106
F	-8	PRO	-	expression tag	UNP P68106
F	-7	GLN	-	expression tag	UNP P68106
F	-6	GLY	-	expression tag	UNP P68106
F	-5	GLN	-	expression tag	UNP P68106
F	-4	ARG	-	expression tag	UNP P68106
F	-3	GLU	-	expression tag	UNP P68106
F	-2	PRO	-	expression tag	UNP P68106
F	-1	GLU	-	expression tag	UNP P68106
F	0	LEU	-	expression tag	UNP P68106
H	-50	MET	-	expression tag	UNP P68106
H	-49	ASN	-	expression tag	UNP P68106
H	-48	HIS	-	expression tag	UNP P68106
H	-47	LYS	-	expression tag	UNP P68106
H	-46	VAL	-	expression tag	UNP P68106
H	-45	HIS	-	expression tag	UNP P68106
H	-44	HIS	-	expression tag	UNP P68106
H	-43	HIS	-	expression tag	UNP P68106
H	-42	HIS	-	expression tag	UNP P68106
H	-41	HIS	-	expression tag	UNP P68106
H	-40	HIS	-	expression tag	UNP P68106
H	-39	MET	-	expression tag	UNP P68106
H	-38	ASP	-	expression tag	UNP P68106
H	-37	GLU	-	expression tag	UNP P68106
H	-36	LYS	-	expression tag	UNP P68106
H	-35	THR	-	expression tag	UNP P68106
H	-34	THR	-	expression tag	UNP P68106
H	-33	GLY	-	expression tag	UNP P68106
H	-32	TRP	-	expression tag	UNP P68106
H	-31	ARG	-	expression tag	UNP P68106
H	-30	GLY	-	expression tag	UNP P68106
H	-29	GLY	-	expression tag	UNP P68106
H	-28	HIS	-	expression tag	UNP P68106
H	-27	VAL	-	expression tag	UNP P68106

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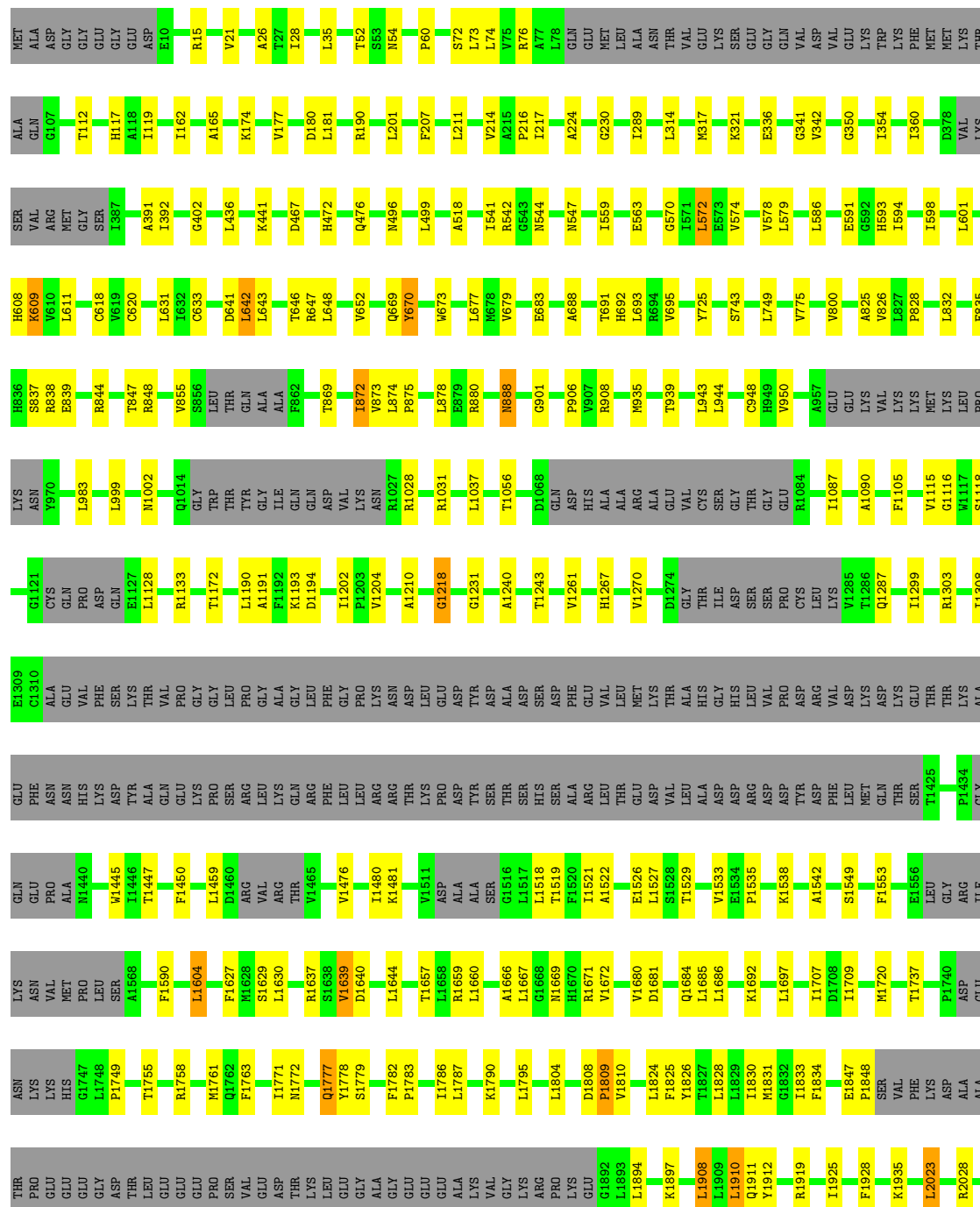
Chain	Residue	Modelled	Actual	Comment	Reference
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H	-23	LEU	-	expression tag	UNP P68106
H	-22	ALA	-	expression tag	UNP P68106
H	-21	GLY	-	expression tag	UNP P68106
H	-20	GLU	-	expression tag	UNP P68106
H	-19	LEU	-	expression tag	UNP P68106
H	-18	GLU	-	expression tag	UNP P68106
H	-17	GLN	-	expression tag	UNP P68106
H	-16	LEU	-	expression tag	UNP P68106
H	-15	ARG	-	expression tag	UNP P68106
H	-14	ALA	-	expression tag	UNP P68106
H	-13	ARG	-	expression tag	UNP P68106
H	-12	LEU	-	expression tag	UNP P68106
H	-11	GLU	-	expression tag	UNP P68106
H	-10	HIS	-	expression tag	UNP P68106
H	-9	HIS	-	expression tag	UNP P68106
H	-8	PRO	-	expression tag	UNP P68106
H	-7	GLN	-	expression tag	UNP P68106
H	-6	GLY	-	expression tag	UNP P68106
H	-5	GLN	-	expression tag	UNP P68106
H	-4	ARG	-	expression tag	UNP P68106
H	-3	GLU	-	expression tag	UNP P68106
H	-2	PRO	-	expression tag	UNP P68106
H	-1	GLU	-	expression tag	UNP P68106
H	0	LEU	-	expression tag	UNP P68106

[illegible]

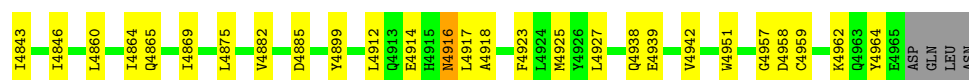


• Molecule 1: Ryanodine Receptor

Chain C: 70% 11% 19%

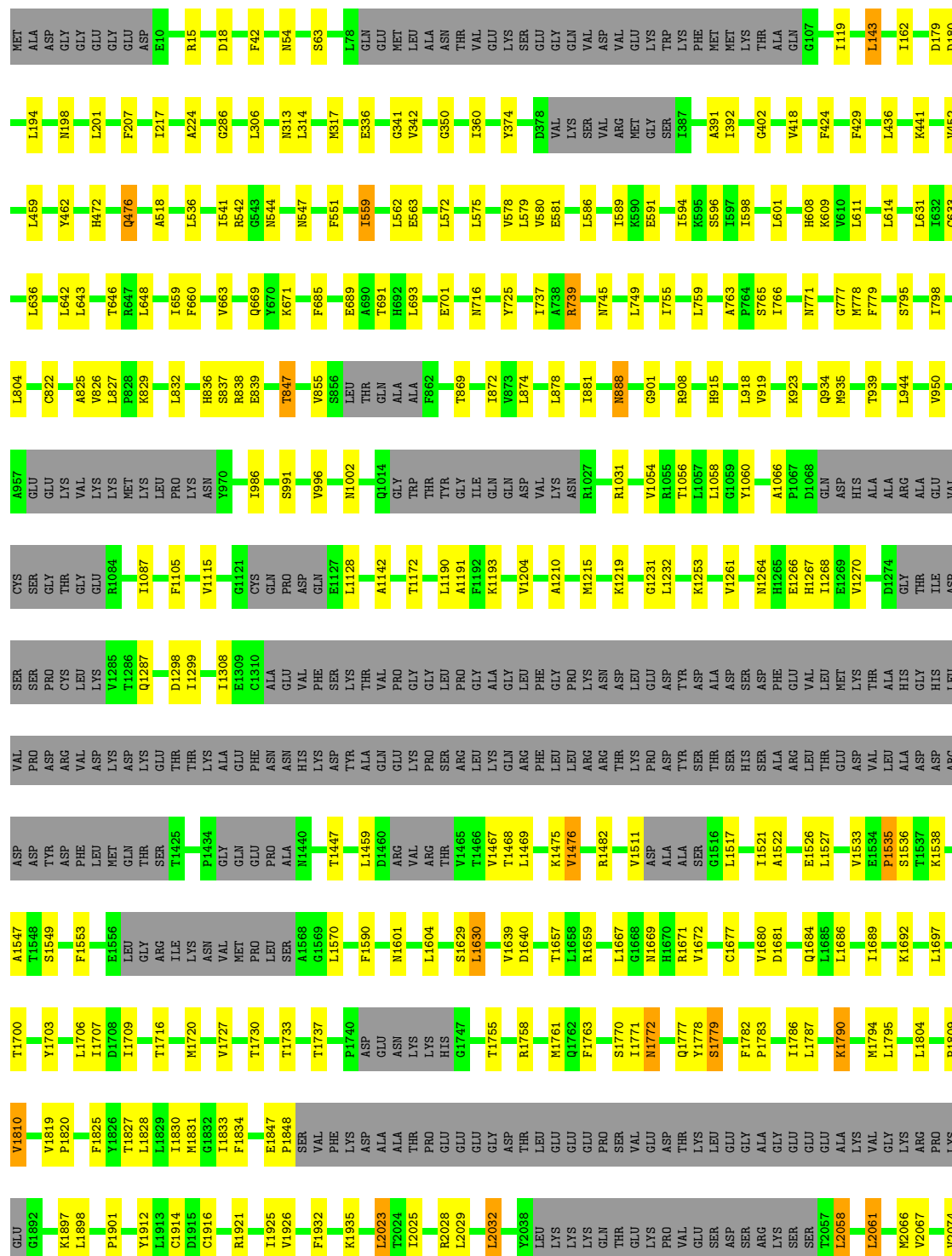




• Molecule 1: Ryanodine Receptor

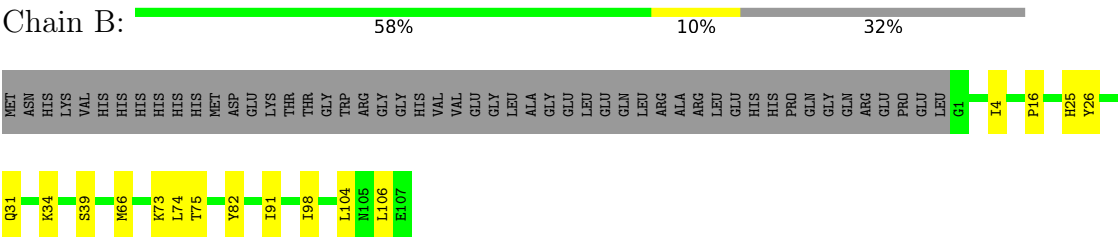
Chain E: 70% 11% 19%



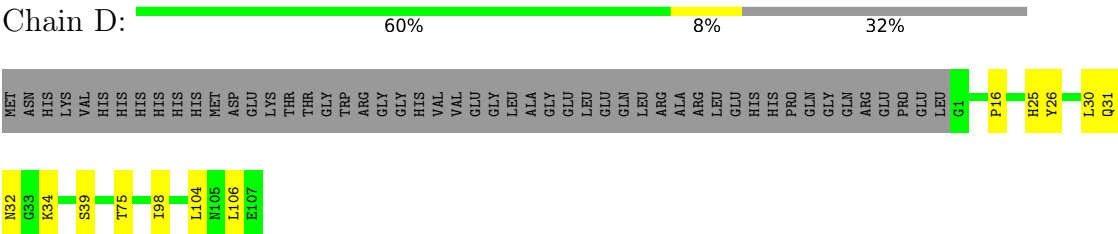




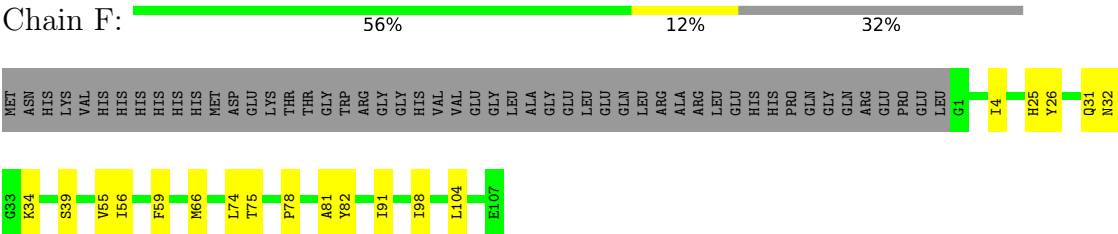

T4911	T4912	I4037	SER	SER	THR	LEU	LEU	GLY	LEU	N4192	F4018	L3847	GLU	GLN	V2481	ASP	PRO	ASP	SER	SER	T2107
H4915	H4916	Q4940	VAL	VAL	GLU	SER	ASP	LEU	ASP	D4019	PHE	T3860	ASP	THR	L2489	GLU	GLU	GLU	GLU	GLU	G2110
L4917	L4918	K4652	GLY	GLY	GLY	LEU	LEU	VAL	LEU	T4197	LEU	T3863	GLY	VAL	G2492	ASP	ASP	ASP	GLY	GLY	V2113
A4918	F4922	I4068	LYS	LYS	LYS	LEU	LEU	ALA	LEU	I4198	LYS	G3864	GLU	VAL	F2493	PRO	PRO	PRO	PRO	PRO	I2117
M4925	L4927	L4672	LEU	LEU	GLY	LEU	LEU	LYS	ASP	F4199	LYS	N3866	GLU	ASP	L2497	SER	SER	SER	SER	SER	L2120
E4939	V4942	G4673	ARG	ARG	GLY	GLY	GLY	VAL	GLY	L4027	ASP	L3879	GLU	L2838	R2498	THR	THR	THR	THR	THR	L2123
D4958	C4959	M4926	THR	THR	GLY	GLY	GLY	ALA	GLY	H4050	GLY	V3882	GLY	L3861	L2503	ASP	ASP	ASP	ASP	ASP	I2126
K4962	F4965	ASP	THR	THR	GLY	GLY	GLY	VAL	GLY	H4056	GLY	K3896	GLY	G2866	D2512	GLN	GLN	GLN	GLN	GLN	R2127
ASP	GLN	LEU	SER	SER	GLY	GLY	GLY	ALA	GLY	E4065	LEU	D3897	GLY	G2866	M2513	SER	SER	SER	SER	SER	S2128
LEU	ASN	LEU	THR	THR	GLY	GLY	GLY	VAL	GLY	F4066	LEU	V3898	GLY	G2866	L2517	CYS	CYS	CYS	CYS	CYS	L2129
ASN	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4067	LEU	I3899	GLY	G2866	T2511	LEU	LEU	LEU	LEU	LEU	L2130
ASP	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	R4097	LEU	S3908	GLY	G2866	A2818	THR	THR	THR	THR	THR	S2131
LEU	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	P4091	LEU	N3932	GLY	G2866	L2517	VAL	VAL	VAL	VAL	VAL	V2132
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4097	LEU	Y3924	GLY	G2866	D2511	GLU	GLU	GLU	GLU	GLU	ARG
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	V4101	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	MET
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	T4104	LEU	Q3926	GLY	G2866	D2511	GLU	GLU	GLU	GLU	GLU	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	N4112	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	Q4117	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	V4126	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4130	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4134	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	G4135	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	R4136	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	I4137	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	I4146	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	Y4150	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4151	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	E4152	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	P4164	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	Q4165	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	V4166	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	Y4166	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	K4170	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	K4186	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	M4187	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	E4188	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	M4013	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	E4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	M4013	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	F4012	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
THR	THR	THR	GLY	GLY	GLY	GLY	GLY	VAL	GLY	L4014	LEU	Q3926	GLY	G2866	T2511	SER	SER	SER	SER	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	F4012	LEU	Q3926	GLY	G2866							



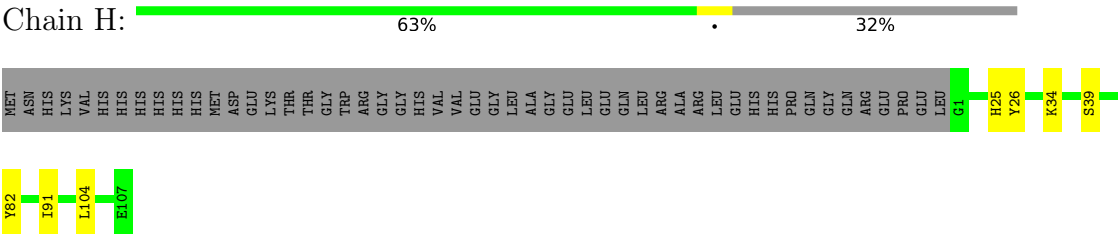
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	13158	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	62000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.78	0/25831	0.64	1/34865 (0.0%)
1	C	0.78	0/25831	0.64	1/34865 (0.0%)
1	E	0.78	0/25831	0.64	1/34865 (0.0%)
1	G	0.78	0/25831	0.64	0/34865
2	B	0.85	0/834	0.64	0/1123
2	D	0.85	0/834	0.63	0/1123
2	F	0.84	0/834	0.64	0/1123
2	H	0.86	0/834	0.65	0/1123
All	All	0.78	0/106660	0.64	3/143952 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1630	LEU	CA-CB-CG	6.09	129.32	115.30
1	A	1630	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	1630	LEU	CA-CB-CG	5.38	127.68	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	604	HIS	Peptide
1	C	3614	ARG	Peptide
1	G	3614	ARG	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	27416	0	25487	197	0
1	C	27416	0	25485	217	0
1	E	27416	0	25489	211	0
1	G	27416	0	25485	206	0
2	B	818	0	824	10	0
2	D	818	0	824	5	0
2	F	818	0	824	9	0
2	H	818	0	824	5	0
All	All	112936	0	105242	843	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 843 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3945:VAL:HG11	1:E:3983:LEU:HD21	1.47	0.94
1:A:874:LEU:HD23	1:A:878:LEU:HD13	1.50	0.94
1:E:1172:THR:HG21	1:E:1190:LEU:HD13	1.58	0.86
1:G:874:LEU:HD23	1:G:878:LEU:HD13	1.60	0.82
1:E:1261:VAL:HG11	1:E:1270:VAL:HG11	1.63	0.78

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	3065/4387 (70%)	2784 (91%)	217 (7%)	64 (2%)	8	43
1	C	3065/4387 (70%)	2773 (90%)	236 (8%)	56 (2%)	9	47
1	E	3065/4387 (70%)	2765 (90%)	238 (8%)	62 (2%)	8	45
1	G	3065/4387 (70%)	2789 (91%)	211 (7%)	65 (2%)	8	43
2	B	105/158 (66%)	97 (92%)	7 (7%)	1 (1%)	17	60
2	D	105/158 (66%)	96 (91%)	8 (8%)	1 (1%)	17	60
2	F	105/158 (66%)	97 (92%)	6 (6%)	2 (2%)	9	45
2	H	105/158 (66%)	97 (92%)	8 (8%)	0	100	100
All	All	12680/18180 (70%)	11498 (91%)	931 (7%)	251 (2%)	12	45

5 of 251 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	HIS
1	A	1476	VAL
1	A	1549	SER
1	A	1779	SER
1	A	3897	ASP

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	2774/3480 (80%)	2648 (96%)	126 (4%)	30	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	2774/3480 (80%)	2639 (95%)	135 (5%)	27	58
1	E	2774/3480 (80%)	2624 (95%)	150 (5%)	24	55
1	G	2774/3480 (80%)	2642 (95%)	132 (5%)	28	58
2	B	88/131 (67%)	87 (99%)	1 (1%)	76	88
2	D	88/131 (67%)	87 (99%)	1 (1%)	76	88
2	F	88/131 (67%)	87 (99%)	1 (1%)	76	88
2	H	88/131 (67%)	87 (99%)	1 (1%)	76	88
All	All	11448/14444 (79%)	10901 (95%)	547 (5%)	32	58

5 of 547 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4200	GLU
1	E	1287	GLN
1	G	2747	ILE
1	C	4752	PHE
1	E	441	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4010	ASN
1	E	1147	GLN
1	G	3926	GLN
1	C	4644	ASN
1	E	476	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

There are no ligands in this entry.

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
1	G	27
1	A	27
1	C	27
1	E	27

The worst 5 of 108 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3612:UNK	C	3613:PRO	N	76.52
1	G	3612:UNK	C	3613:PRO	N	75.29
1	E	3612:UNK	C	3613:PRO	N	74.52
1	A	3612:UNK	C	3613:PRO	N	74.10
1	E	2701:UNK	C	2702:PHE	N	43.29