



wwPDB EM Map/Model Validation Report ⓘ

Sep 14, 2016 – 12:09 PM EDT

PDB ID : 5GKY
EMDB ID: : EMD-9518
Title : Structure of RyR1 in a closed state (C1 conformer)
Authors : Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-07
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

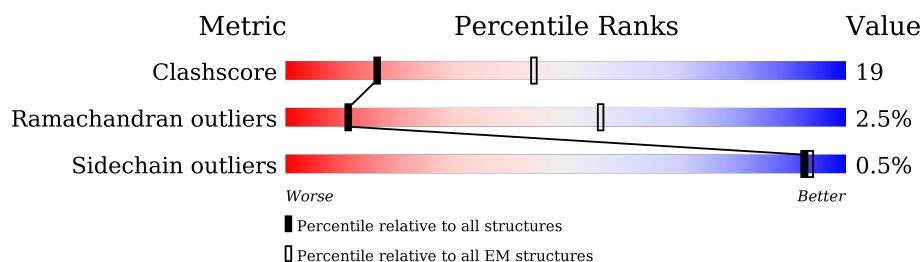
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	5037	
1	C	5037	
1	E	5037	
1	G	5037	
2	B	108	
2	D	108	
2	F	108	
2	H	108	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 111036 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		
1	C	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		
1	E	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		
1	G	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	D	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	F	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	H	107	Total	C	N	O	S	0	0
			832	527	146	155	4		

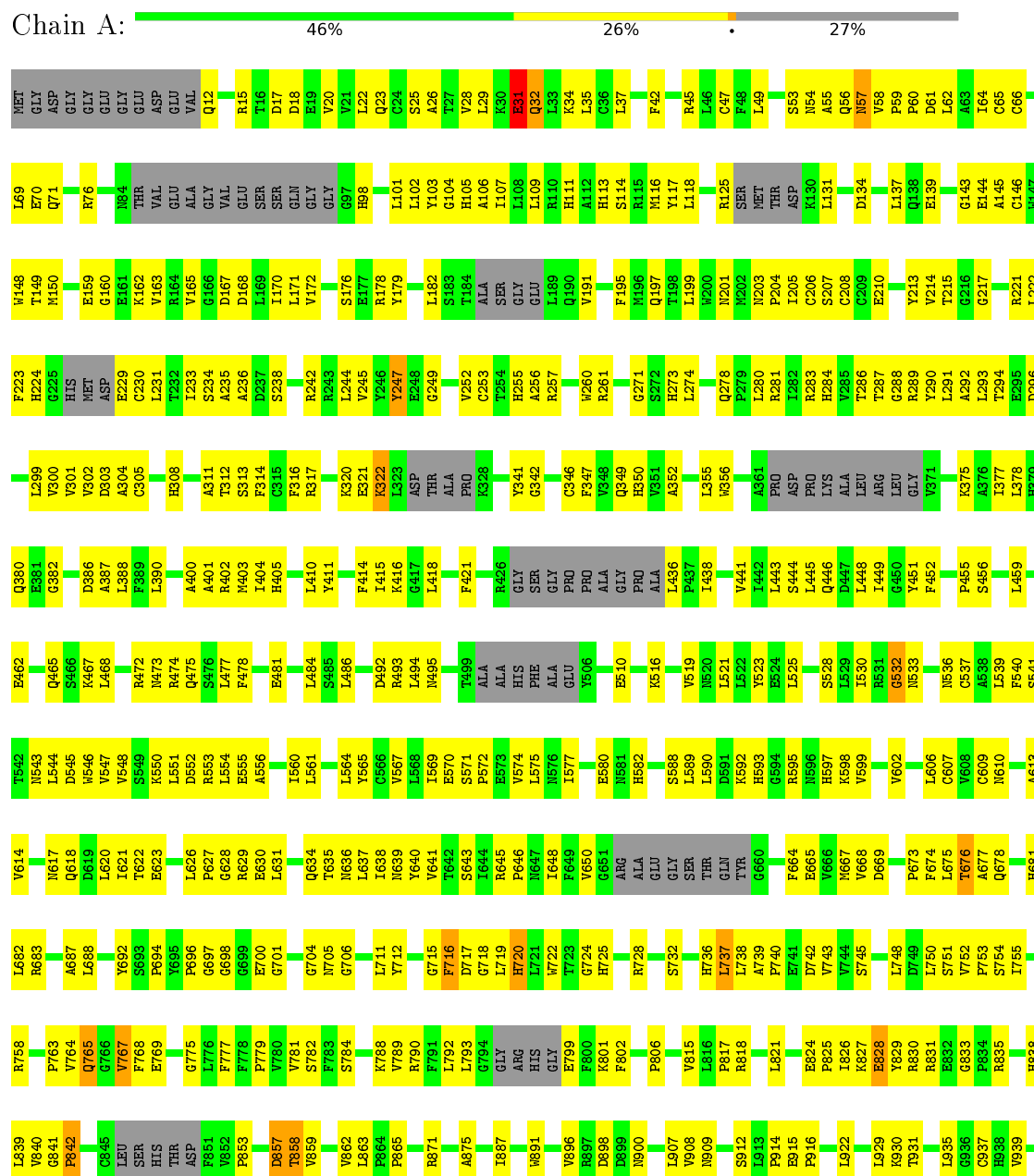
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	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 errors 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: Ryanodine receptor 1






GLU L3694	ASP G3572	PRO H3313	GLY P3021	GLN T2751	LEU L2518	ALA I2453	LEU G2375	L2290	L2197
L3695	GLY G3572	LEU H3313	L3039	D2752	L2522	GLY I2456	ARG E2381	E2296	T2206
D3696	LEU G3572	GLN H3313	THR I3039	I2755	ASP V2524	THR I2460	GLY E2381	L2207	V2207
P3697	THR P3567	LEU H3313	LEU P3043	K2757	A2532	ALA I2460	GLY E2381	S2300	V2210
L3698	GLY Q3572	LEU H3313	THR P3043	F2758	L2536	VAL I2460	SER G2375	Y2301	V2211
H3699	THR Q3572	LEU H3313	ASP P3062	H2763	ASP L2536	PRO I2460	GLN E2381	L2307	V2212
L3701	LEU Q3572	LEU H3313	VAL P3062	K2765	THR L2536	THR I2460	SER E2381	GLN E2381	V2214
F3705	THR P3567	LEU H3313	VAL P3062	D2769	ALA L2536	THR I2460	CYS E2381	CYS E2381	L2215
A3709	GLY Q3572	LEU H3313	THR P3062	K2770	THR L2536	THR I2460	PRO E2381	PRO E2381	L2216
L3710	THR Q3572	LEU H3313	THR P3062	I2771	PHE L2536	THR I2460	SER E2381	MET E2381	GLY E2381
L3711	LEU Q3572	LEU H3313	THR P3062	Q2772	SER L2536	THR I2460	GLY E2381	LEU E2381	GLY E2381
E3712	THR P3567	LEU H3313	THR P3062	N2773	THR L2536	THR I2460	ASP E2381	ALA E2381	THR E2381
K3713	GLY Q3572	LEU H3313	THR P3062	N2774	THR L2536	THR I2460	PRO E2381	LYS E2381	LYS E2381
S3714	THR P3567	LEU H3313	THR P3062	V2775	A2547	THR I2460	ALA E2381	GLY E2381	GLU E2381
K3715	GLY Q3572	LEU H3313	THR P3062	H2788	L2550	THR I2460	ARG E2381	THR E2381	ILE E2381
L3721	THR Q3572	LEU H3313	THR P3062	P2789	N2551	THR I2460	ASP E2381	PRO E2381	ARG E2381
Y3722	GLY Q3572	LEU H3313	THR P3062	K2792	R2552	THR I2460	GLY E2381	ASP E2381	PHE E2381
M3723	THR P3567	LEU H3313	THR P3062	R2792	Y2553	THR I2460	GLY E2381	ILE E2381	ILE E2381
A3724	GLY Q3572	LEU H3313	THR P3062	E2799	L2554	THR I2460	VAL E2381	TRP E2381	C2233
Y3725	THR P3567	LEU H3313	THR P3062	P2701	A2557	THR I2460	ARG E2381	ASN E2381	R2234
I3728	GLY Q3572	LEU H3313	THR P3062	K2802	V2558	THR I2460	ARG E2381	C2325	F2235
C3733	THR P3567	LEU H3313	THR P3062	E2803	L2559	THR I2460	ARG E2381	C2326	Y2238
H3734	GLY Q3572	LEU H3313	THR P3062	R2806	P2560	THR I2460	ARG E2381	E2329	L2242
LEU	THR P3567	LEU H3313	THR P3062	V2807	L2561	THR I2460	GLU E2381	R2330	N2246
GLU	GLY Q3572	LEU H3313	THR P3062	P2808	I2562	THR I2460	HIS E2381	Y2331	Q2247
GLY	THR P3567	LEU H3313	THR P3062	K2809	CYS L2562	THR I2460	PHE E2381	L2332	R2248
GLU	GLY Q3572	LEU H3313	THR P3062	K2810	ALA L2562	THR I2460	GLY E2381	F2333	S2249
ASN	THR P3567	LEU H3313	THR P3062	E2811	ALA L2562	THR I2460	GLY E2381	L2335	M2250
GLY	GLY Q3572	LEU H3313	THR P3062	A2818	P2567	THR I2460	GLU E2381	R2336	F2251
GLU	THR P3567	LEU H3313	THR P3062	L2821	V2586	THR I2460	PRO E2381	V2339	Y2256
ALA	GLY Q3572	LEU H3313	THR P3062	A2826	TRP L2586	THR I2460	GLU E2381	F2340	L2257
GLU	THR P3567	LEU H3313	THR P3062	E2830	LEU L2586	THR I2460	ASN E2381	N2342	L2258
THR	GLY Q3572	LEU H3313	THR P3062	GLU	R2591	THR I2460	ARG E2381	V2346	I2263
ASP	THR P3567	LEU H3313	THR P3062	LYS	D2601	THR I2460	HIS E2381	E2347	GLY E2381
GLY	GLY Q3572	LEU H3313	THR P3062	LEU	A2609	THR I2460	LEU E2381	N2351	LEU E2381
GLN	THR P3567	LEU H3313	THR P3062	THR	LEU	THR I2460	GLY E2381	V2354	GLY E2381
LEU	GLY Q3572	LEU H3313	THR P3062	LYS	ANG	THR I2460	GLY E2381	R2355	GLY E2381
THR	THR P3567	LEU H3313	THR P3062	LYS	TRP	THR I2460	GLY E2381	L2356	SER
GLY	GLY Q3572	LEU H3313	THR P3062	LYS	TRP	THR I2460	GLY E2381	L2357	T2271
GLN	THR P3567	LEU H3313	THR P3062	LYS	ILE	THR I2460	GLY E2381	P2272	P2272
LEU	GLY Q3572	LEU H3313	THR P3062	LYS	P2616	THR I2460	GLY E2381	E2362	V2275
THR	THR P3567	LEU H3313	THR P3062	LYS	R2625	THR I2460	GLY E2381	CYS	GLY E2381
ASP	GLY Q3572	LEU H3313	THR P3062	LYS	P2745	THR I2460	HIS E2381	PHE	N2283
GLY	THR P3567	LEU H3313	THR P3062	LYS	P2748	THR I2460	ILE E2381	PRO	L2286
GLN	GLY Q3572	LEU H3313	THR P3062	ALA	P2748	THR I2460	GLN E2381	ALA	







ILE	L3783	S3784	GLU	L3694	SER	L3410	PRO	P3188	P3021	GLY	R3852	F2758	P2640	A2532	I2453	SER
ASN	S3785	S3786	LYS	P3695	LYS	P3424	VAL	A3200	I3039	PHE	E2853	H2763	P2658	A2536	I2456	G2375
ARG	S3795	S3796	GLN	P3696	ARG	L3424	GLN	MET	THR	LEU	G3854	H2764	T2659	ASP	THR	E2381
ASN	S3797	S3798	ARG	P3697	ARG	THR	GLU	VAL	LEU	LEU	N2855	K2765	G2660	THR	ALA	I2384
GLY	T3797	L3698	ARG	P3697	ALA	P3427	ILE	A3204	F3043	LEU	P2857	D2769	TRP	THR	VAL	R2385
GLU	L3798	H3699	VAL	Q3572	VAL	F3435	T3273	A3204	P3062	ARG	L2862	K2770	ALA	THR	PHE	I2386
LYS	K3799	Q3700	VAL	MET	ALA	ARG	P3274	P3208	VAL	MET	E2870	I2771	ASN	SER	GLU	SER
VAL	I3802	L3701	ALA	LEU	ALA	MET	P3275	S3217	VAL	ASP	A2875	N2773	VAL	THR	ASP	ASP
MET	I3802	L3701	CYS	LEU	CYS	THR	P3282	VAL	VAL	ILE	A2876	N2774	T2667	THR	ALA	PRO
ALA	L3805	A3709	TYR	TYR	TYR	V3438	P3289	THR	ASN	GLN	R2876	N2775	T2667	ALA	ALA	ALA
D3877	L3806	A3710	ARG	ARG	ARG	P3438	E3290	THR	CYS	THR	Y2882	H2788	L2686	I2550	ANG	ANG
D3878	G3807	T3711	ARG	GLY	GLY	Q3456	ALA	THR	L3068	GLU	H2883	K2789	ALA	N2551	ASP	ASP
E3879	G3808	K3712	THR	GLY	THR	N3457	PRO	THR	P3085	PHE	Y2883	P2789	HIS	R2552	GLY	GLY
F3880	N3809	K3713	PRO	PRO	PRO	L3470	GLY	THR	P3085	ILE	K2891	R2792	LYS	L2554	PRO	PRO
T3881	S3714	S3715	LEU	GLY	TYR	THR	P3294	PRO	GLY	ALA	K2891	R2792	LYS	L2554	GLY	GLY
Q3882	D3883	K3715	TYR	ARG	GLU	ALA	P3297	ARG	A3090	HIS	H2902	E2799	LYS	I2557	VAL	VAL
D3883	Q3813	Y3722	ASN	GLU	GLU	ASP	P3297	GLU	GLY	LEU	P2903	E2799	LYS	A2557	LYS	ANG
Q3814	Q3814	Y3722	LEU	GLU	GLU	ASP	P3301	ARG	LEU	GLU	L2904	K2802	VAL	V2558	ASP	ARG
F3885	K3815	N3723	ASP	ALA	ALA	SER	P3302	ALA	ALA	ARG	L2905	E2803	ALA	L2559	GLY	ASP
F3886	M3816	A3724	ALA	VAL	SER	LYS	P3303	ILE	ARG	VAL	V2906	E2803	ALA	P2560	ARG	ARG
F3887	L3817	Y3725	ASP	ASP	ASP	LYS	P3303	GLY	F3095	VAL	P2907	R2806	ASP	L2561	ARG	ARG
L3888	D3818	Y3728	PRO	PRO	PRO	N3478	N3813	LEU	S3116	SER	P2907	R2807	THR	I2562	GLU	GLU
Q3889	Y3819	L3820	GLU	GLY	GLY	VAL	S3116	LEU	GLN	GLY	T2910	R2807	THR	I2562	GLN	GLU
L3890	L3820	L3821	LYS	LYS	ILE	A3484	SER	PRO	GLN	THR	P2910	R2807	THR	I2562	PRO	HIS
L3891	K3821	C3733	ILE	ILE	ILE	Q3491	LEU	ASN	ALA	ARG	T2910	R2807	THR	I2562	GLU	GLU
E3892	K3822	HIS	GLU	VAL	VAL	Q3491	LEU	ASN	ALA	ARG	T2910	R2807	THR	I2562	GLU	GLU
E3893	K3823	LEU	GLY	VAL	VAL	Q3491	LEU	ASN	ALA	ARG	T2910	R2807	THR	I2562	GLU	GLU
N3896	K3824	GLY	GLY	ARG	ARG	ARG	G3317	SER	THR	GLN	K2916	R2807	THR	I2562	GLU	GLU
N3897	E3825	GLY	GLY	ARG	ARG	ARG	G3317	SER	THR	GLN	K2916	R2807	THR	I2562	GLU	GLU
D3898	F3828	GLY	GLY	VAL	VAL	VAL	A3339	MET	LYS	SER	R2920	R2807	THR	I2562	GLU	GLU
F3899	F3829	GLU	GLU	VAL	VAL	VAL	A3339	MET	LYS	SER	R2920	R2807	THR	I2562	GLU	GLU
N3901	L3835	ASN	ASN	VAL	VAL	VAL	A3339	MET	LYS	SER	R2920	R2807	THR	I2562	GLU	GLU
Y3902	L3836	GLY	GLY	SER	SER	S3504	ALA	CYS	GLY	LYS	T2927	R2807	THR	I2562	GLU	GLU
L3903	M3836	GLU	GLY	SER	GLN	VAL	ALA	PRO	VAL	HIS	K2927	R2807	THR	I2562	GLU	GLU
R3904	ALA	ALA	ALA	ALA	PRO	THR	ILE	ILE	GLY	GLN	F2929	R2807	THR	I2562	GLU	GLU
T3905	C3839	GLU	LEU	VAL	VAL	SER	ILE	PRO	ASN	ILE	L2930	R2807	THR	I2562	GLU	GLU
T3905	S3840	GLU	LEU	VAL	VAL	THR	ILE	VAL	THR	LYS	L2930	R2807	THR	I2562	GLU	GLU
I3915	L3842	GLU	GLU	ILE	ILE	ILE	V3346	VAL	THR	LYS	N2933	R2807	THR	I2562	GLU	GLU
I3916	D3843	VAL	VAL	ALA	ALA	ALA	V3346	VAL	THR	LYS	N2933	R2807	THR	I2562	GLU	GLU
T3919	R3849	GLY	GLY	THR	THR	P3519	ARG	ALA	P3138	PHE	T2938	R2807	THR	I2562	GLU	GLU
V3920	F3852	GLY	GLY	GLU	GLU	P3527	ARG	ASP	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
Y3922	ALA	ALA	ALA	HIS	HIS	THR	ARG	ASP	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
L3923	GLY	GLY	GLY	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
L3924	GLY	GLY	GLY	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
L3925	GLY	GLY	GLY	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
Q3927	GLY	GLY	GLY	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
E3928	VAL	VAL	VAL	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
S3929	ASN	ASN	ASN	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
Y3936	GLY	GLY	GLY	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
Y3937	GLY	GLY	GLY	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
S3938	THR	THR	THR	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU
	VAL	VAL	VAL	PRO	PRO	THR	ARG	GLY	F3152	GLY	T2938	R2807	THR	I2562	GLU	GLU

Chain E: 46% 26% . 27%










- Molecule 1: Ryanodine receptor 1

T149	T150	E159	K162	V163	R164	V165	G166	D167	D168	L169	I170	L171	V172	S176	E177	R178	Y179	L182	S183	T184	ALA	SER	GLY	GLU	L189	Q190	V191	F195	M196	Q197	T198	L199	Q200	N201	N202	N203	P204	I205	C206	S207	C208	C209	E210	Y213	V214	T215	G216	G217	R221	L222	F223	F224	E70	Q71	R76	T84	THR	VAL	GLU	ASP	GLY	VAL	Q12	R15	T16	D17	D18	E19	V20	L22	Q23	C24	S25	A26	T27	V28	L29	L30	E31	Q32	L33	K34	L35	C36	L37	F42	R45	L46	C47	F48	L49	S53	N54	A55	Q56	N57	P59	P60	D61	L62	A63	I64	C65	L60
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PRO	GLY	ASP	PRO	ARG	A1227	Q1144	GLN	ASP	V840	L682	M617	N543	Q465	G382	V300	R295
GLN	THR	GLN	THR	CYS	M1230	D1147	SER	ASN	G841	R683	Q618	L544	S466	G382	V301	HIS
PRO	GLN	PRO	THR	THR	Q1231	V1148	ARG	LEU	P842	V764	Q619	N546	S467	D386	V302	MET
VAL	GLY	VAL	GLY	GLY	R1232	V1149	LVS	LVS	G845	L688	L620	N547	L468	D387	D303	ASP
ALA	ALA	ALA	THR	THR	T1235	M1152	LVS	THR	SER	V767	L621	N548	R472	F388	A304	C230
PRO	PRO	PRO	PRO	PRO	T1236	T1153	LEU	LEU	THR	F768	T622	K550	R474	L390	H308	L231
LEU	LEU	LEU	LEU	LEU	T1237	T1154	PRO	PRO	THR	P694	L626	K551	Q475	A400	A311	L232
ALA	ALA	ALA	ALA	ALA	F1238	T1155	LVS	LVS	THR	V695	P627	N552	S476	A401	T312	S234
ARG	ARG	ARG	ARG	ARG	T1156	T1156	THR	THR	F851	L776	N638	N553	L477	R402	A235	A235
ALA	ALA	ALA	ALA	ALA	E1157	N1158	LVS	LVS	N652	G697	G628	N554	F478	N403	S313	A236
GLY	GLY	GLY	GLY	GLY	Q1243	N1158	THR	THR	P853	F777	G629	N555	F481	L404	F314	D237
LEU	LEU	LEU	LEU	LEU	F1245	T1159	THR	THR	P879	F779	E630	N556	E481	H405	C315	S238
GLN	GLN	GLN	GLN	GLN	P1249	I1160	Y1081	Y1081	D857	F780	L631	N560	L484	L410	F316	R242
PRO	PRO	PRO	PRO	PRO	T1250	F1162	T1082	L984	T858	V781	Q634	N561	S485	Y411	R317	R242
ALA	ALA	ALA	ALA	ALA	E1251	T1163	V1083	L988	V859	S782	T635	N564	L486	Y411	K320	L244
THR	THR	THR	THR	THR	H1252	L1164	L988	A989	L863	G704	N636	N564	F414	F414	E321	V245
ASP	ASP	ASP	ASP	ASP	P1253	L1164	A989	E990	P864	G706	L637	N565	I491	I415	K322	V246
GLU	GLU	GLU	GLU	GLU	T1254	V1168	THR	THR	P865	G706	N638	N566	D492	I416	L323	T247
ALA	ALA	ALA	ALA	ALA	Y1255	L1169	LVS	LVS	R789	L711	N639	N567	R493	R417	ASP	E248
ASN	ASN	ASN	ASN	ASN	E1256	MET	F1090	H993	R790	L712	Y640	N568	L494	L418	THR	G249
ALA	ALA	ALA	ALA	ALA	V1257	SER	F1091	Q1003	R871	L712	N641	N569	N495	L418	ALA	
LVS	LVS	LVS	LVS	LVS	A1258	ASP	F1092	GLY	A875	G715	T642	N570	T499	F421	PRO	V252
ARG	ARG	ARG	ARG	ARG	R1259	SER	F1092	TRP	I887	F716	S643	N571	ALA	K328	C253	C253
GLY	GLY	GLY	GLY	GLY	M1260	GLY	E1093	SER	T887	L719	L644	N572	ALA	R426	L254	L254
PRO	PRO	PRO	PRO	PRO	D1261	SER	T1096	THR	T887	L719	R645	N573	ALA	GLY	Y341	H255
GLY	GLY	GLY	GLY	GLY	E1262	GLY	T1096	THR	T887	L719	R646	N574	HIS	SER	G342	A256
THR	THR	THR	THR	THR	GLY	GLY	T1096	THR	T887	L719	P646	N575	PHE	GLY	R257	R257
VAL	VAL	VAL	VAL	VAL	THR	THR	E1099	ALA	N891	L721	N647	N576	ALA	PRO	C346	
ASP	ASP	ASP	ASP	ASP	THR	THR	M1100	VAL	N896	L722	N648	N576	ALA	PRO	C347	
GLU	GLU	GLU	GLU	GLU	F1179	F1179	R1101	GLN	N897	L723	N649	N577	GLU	PRO	F348	V260
LEU	LEU	LEU	LEU	LEU	R1180	R1180	R1101	ASP	N898	G724	N650	N577	ALA	ALA	V349	R261
LVS	LVS	LVS	LVS	LVS	Q1187	Q1187	V1102	ILE	N899	H725	G651	N580	GLY	PRO	H350	G271
ALA	ALA	ALA	ALA	ALA	A1105	A1105	A1105	ALA	N900	R728	N652	N581	ALA	ALA	V351	S272
ALA	ALA	ALA	ALA	ALA	L1109	L1109	L1109	ALA	L907	P806	GLY	N582	K516	L436	A352	R273
GLY	GLY	GLY	GLY	GLY	R1110	R1110	R1110	ALA	V908	S732	GLY	N583	V519	F437	L355	Q278
GLY	GLY	GLY	GLY	GLY	P1111	P1111	P1111	SER	V815	H736	THR	N589	N520	I439	K356	
GLY	GLY	GLY	GLY	GLY	D1112	D1112	D1112	THR	L816	L737	GLN	N590	L521	V441	A361	P279
THR	THR	THR	THR	THR	V1113	V1113	V1113	THR	R818	L737	THR	N591	L522	I442	PRO	L280
PRO	PRO	PRO	PRO	PRO	E1114	E1114	E1114	GLN	P914	L738	GLN	N592	L523	L443	R281	
ALA	ALA	ALA	ALA	ALA	L1115	L1115	L1115	GLN	E915	A739	GLY	N593	L524	S444	ASP	T282
ALA	ALA	ALA	ALA	ALA	G1116	G1116	G1116	THR	P916	P740	G660	N594	L525	L445	PRO	R283
GLY	GLY	GLY	GLY	GLY	L1120	L1120	L1120	THR	E741	E741	F664	N595	L526	Q446	LVS	A283
GLY	GLY	GLY	GLY	GLY	A1121	A1121	A1121	THR	E824	D742	R665	N596	L527	Q446	ALA	V285
LVS	LVS	LVS	LVS	LVS	G1205	G1205	G1205	THR	P825	V743	V666	N597	L528	D447	LEU	T286
GLY	GLY	GLY	GLY	GLY	Q1206	Q1206	Q1206	THR	I826	V744	M667	N598	L529	I448	ARG	T287
ALA	ALA	ALA	ALA	ALA	L1126	L1126	L1126	THR	K827	S745	V668	N599	L530	I449	LEU	G288
PRO	PRO	PRO	PRO	PRO	N1126	N1126	N1126	THR	E828	S745	D669	N600	L531	G450	GLY	R289
ALA	ALA	ALA	ALA	ALA	T931	T931	T931	THR	R829	L748	P673	N602	G532	Y451	GLY	Y290
GLY	GLY	GLY	GLY	GLY	Q936	Q936	Q936	GLN	R830	D749	F674	N606	N533	F452	V371	
GLY	GLY	GLY	GLY	GLY	L935	L935	L935	GLN	R831	L750	L675	N607	N536	P455	K375	L291
VAL	VAL	VAL	VAL	VAL	G937	G937	G937	GLY	E832	S751	L676	N608	C537	S456	A376	A292
VAL	VAL	VAL	VAL	VAL	H938	H938	H938	THR	G833	P752	T676	N609	C538	S456	I377	L293
PRO	PRO	PRO	PRO	PRO	Q1220	Q1220	Q1220	GLN	P834	P753	A677	N610	A538	L459	L378	T294
GLY	GLY	GLY	GLY	GLY	F1223	F1223	F1223	VAL	R835	S754	Q678	N610	L539	L459	L378	E295
HIS	HIS	HIS	HIS	HIS	F1223	F1223	F1223	VAL	R838	I755	A679	N613	F540	L459	R379	D296
GLY	GLY	GLY	GLY	GLY	F1226	F1226	F1226	ASN	L839	R758	T680	A613	S541	E462	Q380	L299


WORLDWIDE PDB
 PROTEIN DATA BANK

EMDataBank
 Unified Data Resource for 3DEM

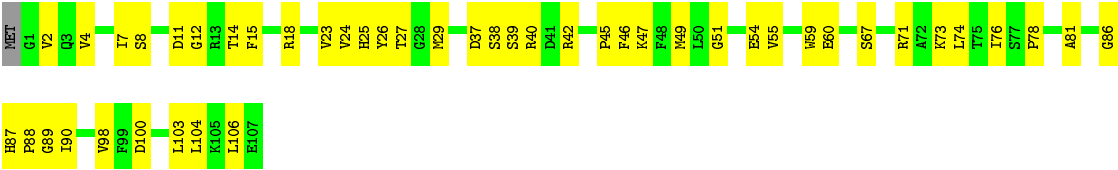



● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:

56%

43%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	119000	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: 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.85	25/27395 (0.1%)	0.86	68/37119 (0.2%)
1	C	0.85	27/27395 (0.1%)	0.86	64/37119 (0.2%)
1	E	0.85	24/27395 (0.1%)	0.86	63/37119 (0.2%)
1	G	0.84	26/27395 (0.1%)	0.85	59/37119 (0.2%)
2	B	0.64	0/851	0.68	0/1146
2	D	0.64	0/851	0.68	0/1146
2	F	0.64	0/851	0.68	0/1146
2	H	0.66	0/851	0.69	0/1146
All	All	0.84	102/112984 (0.1%)	0.85	254/153060 (0.2%)

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	17
1	C	0	17
1	E	0	17
1	G	0	16
All	All	0	67

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2853	GLU	CD-OE1	17.93	1.45	1.25
1	E	2853	GLU	CD-OE1	17.88	1.45	1.25
1	G	2853	GLU	CD-OE1	17.49	1.44	1.25
1	C	2853	GLU	CD-OE1	17.32	1.44	1.25
1	G	4988	TYR	CG-CD1	-9.48	1.26	1.39

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	4032	GLU	OE1-CD-OE2	-7.83	113.91	123.30
1	G	4985	LEU	CB-CG-CD1	-7.61	98.06	111.00
1	G	2118	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	3773	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	G	4563	ARG	NE-CZ-NH2	7.46	124.03	120.30

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1187	GLY	Mainchain
1	A	31	GLU	Mainchain,Peptide
1	A	322	LYS	Peptide
1	A	841	GLY	Mainchain,Peptide
1	A	857	ASP	Mainchain,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	26926	0	24467	1003	0
1	C	26926	0	24467	1022	0
1	E	26926	0	24467	1004	0
1	G	26926	0	24467	952	0
2	B	832	0	831	41	0
2	D	832	0	831	41	0
2	F	832	0	831	41	0
2	H	832	0	831	40	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	111036	0	101192	3945	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 19.

The worst 5 of 3945 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:G:1808:ARG:NH1	1:G:1858:ASP:OD2	1.79	1.16
1:E:1808:ARG:NH1	1:E:1858:ASP:OD2	1.79	1.16
1:C:1808:ARG:NH1	1:C:1858:ASP:OD2	1.79	1.15
1:A:1808:ARG:NH1	1:A:1858:ASP:OD2	1.79	1.14
1:A:1243:PRO:HD2	1:A:1458:HIS:HB3	1.20	1.10

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	3499/5037 (70%)	3211 (92%)	199 (6%)	89 (2%)	7	49
1	C	3499/5037 (70%)	3211 (92%)	201 (6%)	87 (2%)	7	49
1	E	3499/5037 (70%)	3211 (92%)	199 (6%)	89 (2%)	7	49
1	G	3499/5037 (70%)	3211 (92%)	199 (6%)	89 (2%)	7	49
2	B	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	D	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	H	105/108 (97%)	97 (92%)	7 (7%)	1 (1%)	19	66
All	All	14416/20580 (70%)	13232 (92%)	829 (6%)	355 (2%)	11	49

5 of 355 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	A	737	LEU
1	A	858	THR

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Mol	Chain	Res	Type
1	A	896	VAL
1	A	916	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2503/4276 (58%)	2489 (99%)	14 (1%)	90	96
1	C	2504/4276 (59%)	2490 (99%)	14 (1%)	90	96
1	E	2504/4276 (59%)	2490 (99%)	14 (1%)	90	96
1	G	2502/4276 (58%)	2489 (100%)	13 (0%)	92	97
2	B	89/90 (99%)	89 (100%)	0	100	100
2	D	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10369/17464 (59%)	10314 (100%)	55 (0%)	92	97

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1096	THR
1	E	510	GLU
1	G	1055	PRO
1	C	2066	LEU
1	C	4972	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4153	HIS
1	E	593	HIS
1	G	3851	ASN

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Mol	Chain	Res	Type
1	C	4650	HIS
1	E	111	HIS

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.