



wwPDB EM Map/Model Validation Report

Sep 14, 2016 – 11:13 AM EDT

PDB ID : 5GL1
EMDB ID: : EMD-9521
Title : Structure of RyR1 in an open state
Authors : Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-07
Resolution : 5.70 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

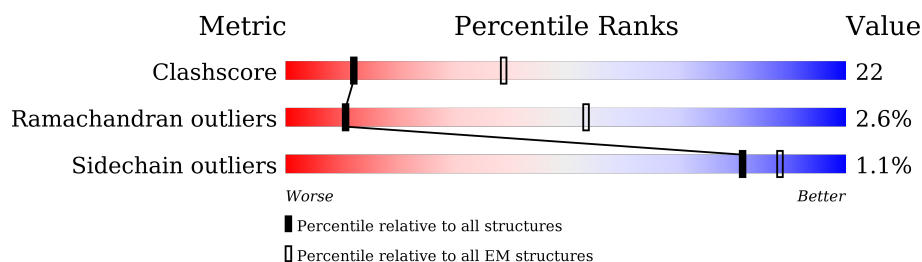
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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 110704 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	3645	Total	C	N	O	S	0	0
			26843	17063	4667	4956	157		
1	C	3645	Total	C	N	O	S	0	0
			26843	17063	4667	4956	157		
1	E	3645	Total	C	N	O	S	0	0
			26843	17063	4667	4956	157		
1	G	3645	Total	C	N	O	S	0	0
			26843	17063	4667	4956	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		

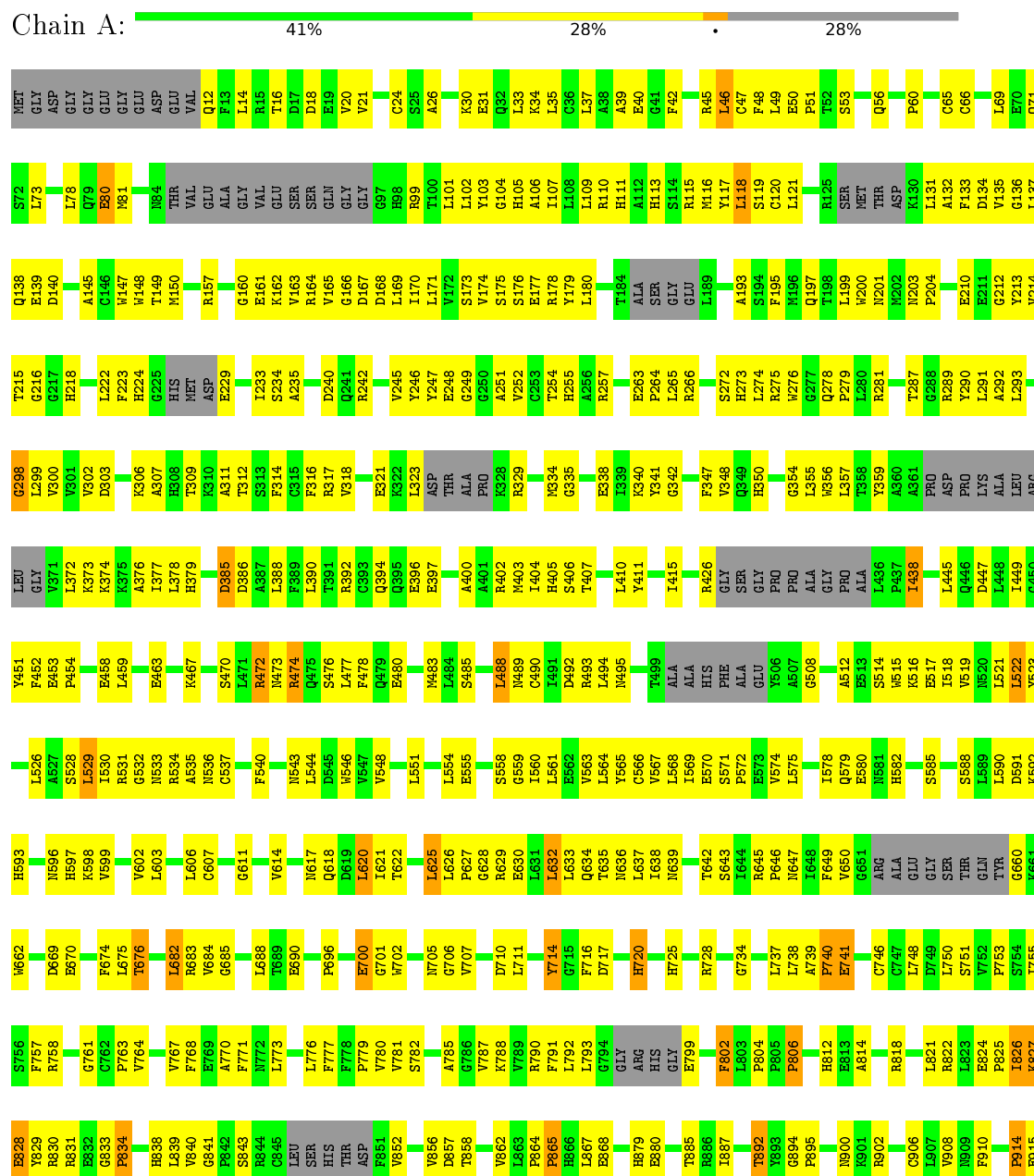
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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









WORLDWIDE
PDB
PROTEIN DATA BANK

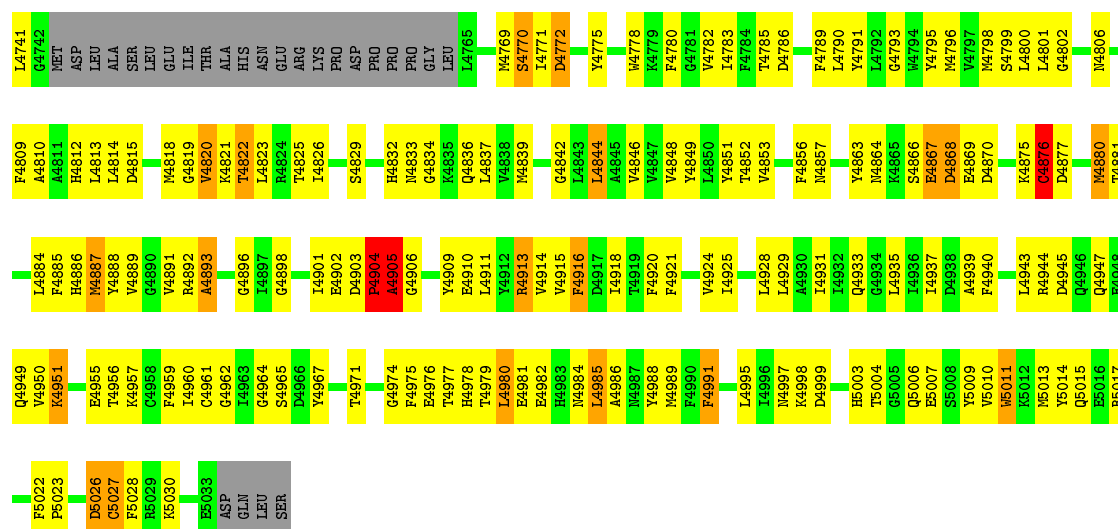
 **EMDataBank**
Unified Data Resource for 3DEM



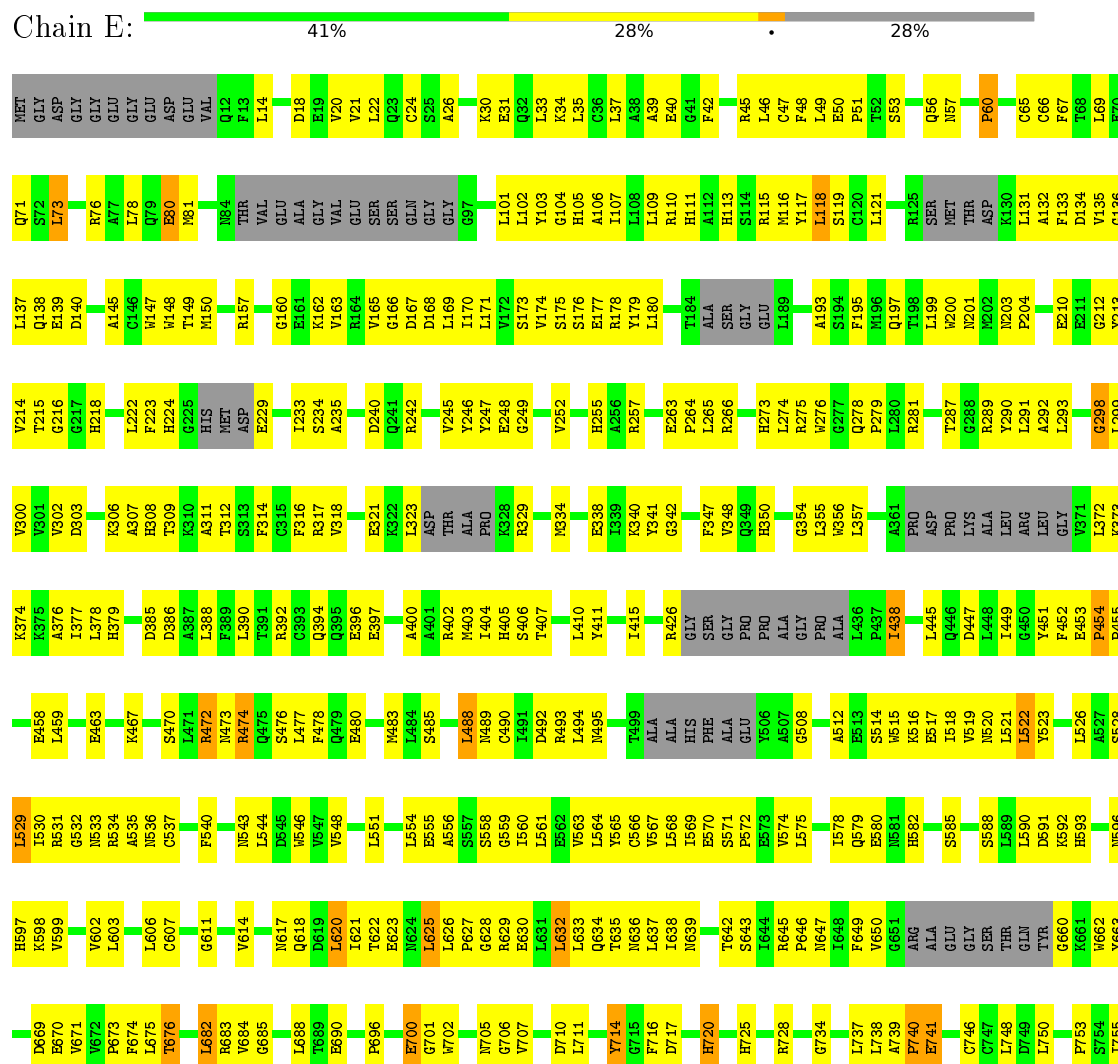






• Molecule 1: Ryanodine receptor 1









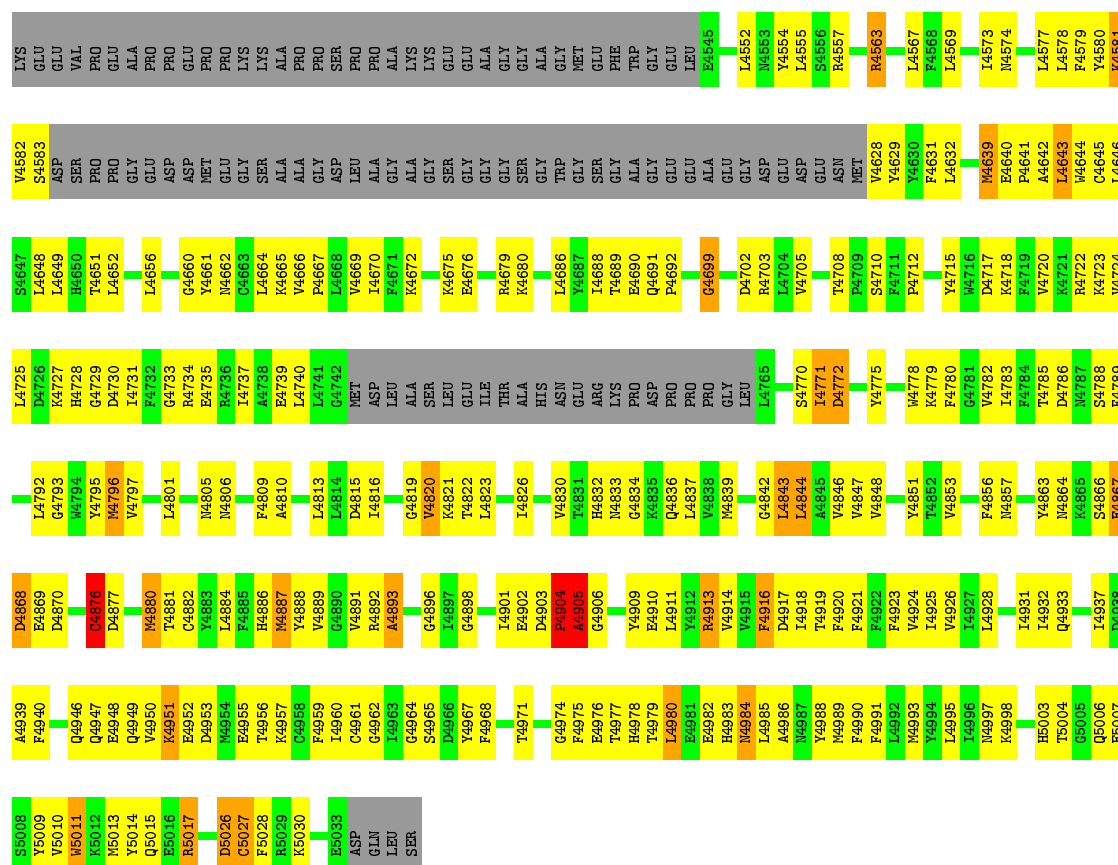






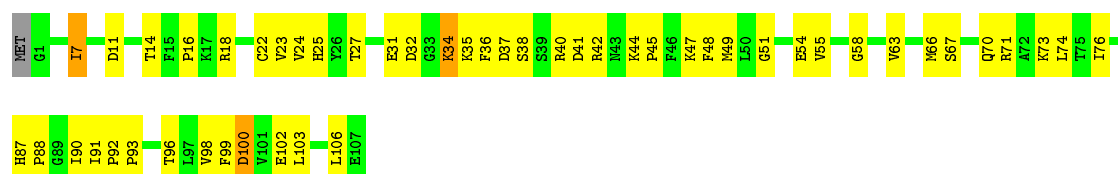
VAL	A2913	K2814	P2711	ALA	MET	HIS	V2352	T2206	H2125	T2057	GLU	GLU	PRO
VAL	K2914	A2818	P2712	P2567	SER	LEU	V2353	V2207	R2126	S2058	PHE	ALA	ALA
SER	R2819	A2819	ASP	I2577	ALA	H2420	R2354	M2208	Q2127	L2059	SER	ARG	ARG
GLY	E2820	E2820	VAL	V2586	F2494	M2423	L2356	V2210	L2129	R2062	PRO	L1798	L1798
VAL	K2825	E2821	ASP	T2586	P2495	S2424	L2357	M2211	G2130	L2063	PRO	P1868	P1868
GLU	K2825	K2825	SER	T2586	P2496	S2424	L2358	V2212	G2130	L2063	GLN	L1801	L1801
LYS	E2830	E2830	TYR	T2586	D2497	A2427	L2359	M2213	L2134	S2065	GLU	L1802	L1802
SER	L2926	L2926	TYR	ARG	H2498	A2428	L2360	L2214	L2135	L2066	ILE	E1805	E1805
SER	L2927	L2927	SER	LEU	K2499	A2428	P2361	L2215	L2136	G2130	ASP	A1806	A1806
HIS	K2928	K2928	LYS	R2591	A2500	L2429	E2362	L2216	A2137	S1934	MET	L1807	L1807
GLU	F2929	F2929	ALA	L2595	S2501	I2430	CYS	GLY	L2138	S1934	LEU	R1808	R1808
GLN	L2930	L2930	GLU	L2595	M2502	D2431	PHE	GLU	P2139	L1937	LEU	D1809	D1809
ILE	Y2935	Y2935	LYS	M2608	V2503	A2437	GLY	THR	R2140	M1941	HIS	K1810	K1810
LYS	A2936	A2936	LYS	A2609	R2508	PRO	ALA	THR	R2141	L1942	PHE	GLU	GLU
PHE	V2937	V2937	ALA	LEU	V2509	GLU	LEU	LYS	Y2142	L1943	GLU	R1813	R1813
PHE	T2938	T2938	THR	CYS	Y2510	MET	ARG	ILE	L2156	L1944	ASP	M1814	M1814
ALA	R2939	R2939	VAL	ARG	GLY	HIS	GLY	ARG	P2146	Y1945	GLU	L1815	L1815
LYS	G2940	G2940	ASP	TYR	ILE	LEU	GLU	PHE	D2151	F1946	ALA	V1819	V1819
ILE	L2941	L2941	GLY	ILE	GLU	ILE	GLY	P2226	L2155	C1947	ASP	GLU	GLU
LEU	L2942	L2942	GLY	GLY	GLY	GLN	GLY	GLY	L2156	D1948	GLU	H1825	H1825
LEU	L2943	L2943	GLY	GLY	GLY	GLY	GLY	GLY	E2157	Q1949	GLU	A1826	A1826
LEU	L2944	L2944	GLY	GLY	GLY	GLY	GLY	GLY	C2158	E1950	GLU	R1827	R1827
PRO	M2945	M2945	GLY	GLY	GLY	GLY	GLY	GLY	L2159	L1951	PRO	D1828	D1828
LEU	L2946	L2946	GLY	GLY	GLY	GLY	GLY	GLY	L2159	V1955	GLU	P1830	P1830
ILE	Y2947	Y2947	GLY	GLY	GLY	GLY	GLY	GLY	L2162	A1959	GLU	V1830	V1830
GLY	L2948	L2948	GLY	GLY	GLY	GLY	GLY	GLY	R2163	A1960	GLU	S1833	S1833
GLY	L2949	L2949	GLY	GLY	GLY	GLY	GLY	GLY	L2167	F1961	GLU	V1834	V1834
GLY	L2950	L2950	GLY	GLY	GLY	GLY	GLY	GLY	V2168	F1962	LYS	E1835	E1835
GLY	L2951	L2951	GLY	GLY	GLY	GLY	GLY	GLY	GLN	Y1965	GLU	F1836	F1836
GLY	L2952	L2952	GLY	GLY	GLY	GLY	GLY	GLY	GLY	V1966	ASP	F1837	F1837
GLY	L2953	L2953	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Q1973	GLU	V1839	V1839
GLY	L2954	L2954	GLY	GLY	GLY	GLY	GLY	GLY	PRO	R1974	GLU	P1840	P1840
GLY	L2955	L2955	GLY	GLY	GLY	GLY	GLY	GLY	GLY	S1975	GLU	V1841	V1841
GLY	L2956	L2956	GLY	GLY	GLY	GLY	GLY	GLY	E2174	R1976	GLU	L1842	L1842
GLY	L2957	L2957	GLY	GLY	GLY	GLY	GLY	GLY	M2178	TYR	LYS	L1844	L1844
GLY	L2958	L2958	GLY	GLY	GLY	GLY	GLY	GLY	L2182	ASP	LEU	V1845	V1845
GLY	L2959	L2959	GLY	GLY	GLY	GLY	GLY	GLY	G2183	V2102	LEU	S1846	S1846
GLY	L2960	L2960	GLY	GLY	GLY	GLY	GLY	GLY	M2184	V2103	ALA	T1847	T1847
GLY	L2961	L2961	GLY	GLY	GLY	GLY	GLY	GLY	L2184	R2104	HIS	L1848	L1848
GLY	L2962	L2962	GLY	GLY	GLY	GLY	GLY	GLY	N2188	CYS	LYS	L1849	L1849
GLY	L2963	L2963	GLY	GLY	GLY	GLY	GLY	GLY	F2191	ALA	ALA	V1850	V1850
GLY	L2964	L2964	GLY	GLY	GLY	GLY	GLY	GLY	L2196	ILE	PHE	M1851	M1851
GLY	L2965	L2965	GLY	GLY	GLY	GLY	GLY	GLY	L2197	THR	GLU	G1852	G1852
GLY	L2966	L2966	GLY	GLY	GLY	GLY	GLY	GLY	M2198	GLU	GLU	F1853	F1853
GLY	L2967	L2967	GLY	GLY	GLY	GLY	GLY	GLY	R2199	ALA	ALA	G1854	G1854
GLY	L2968	L2968	GLY	GLY	GLY	GLY	GLY	GLY	A2200	GLU	GLU	D1855	D1855
GLY	L2969	L2969	GLY	GLY	GLY	GLY	GLY	GLY	M2201	LYS	LYS	V1856	V1856
GLY	L2970	L2970	GLY	GLY	GLY	GLY	GLY	GLY	G2202	ALA	ALA	K1860	K1860
GLY	L2971	L2971	GLY	GLY	GLY	GLY	GLY	GLY	M2203	ARG	ARG	Q1861	Q1861
GLY	L2972	L2972	GLY	GLY	GLY	GLY	GLY	GLY	H2204	THR	THR	L1862	L1862
GLY	L2973	L2973	GLY	GLY	GLY	GLY	GLY	GLY	E2205	GLU	GLU	L1863	L1863



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

Chain B: 53% 44%



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

Chain D: 56% 40%



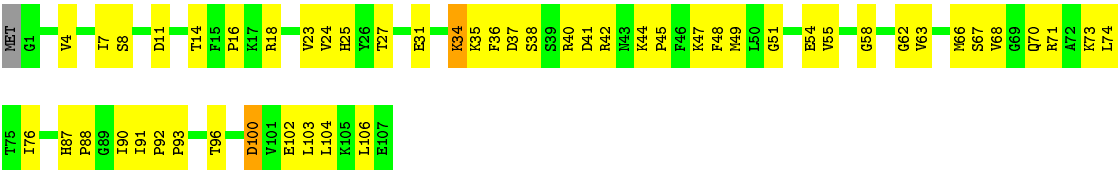
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 56% 40%





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



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	30000	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	1.21	41/27312 (0.2%)	1.12	151/37004 (0.4%)
1	C	1.20	39/27312 (0.1%)	1.12	154/37004 (0.4%)
1	E	1.21	35/27312 (0.1%)	1.12	158/37004 (0.4%)
1	G	1.21	38/27312 (0.1%)	1.11	145/37004 (0.4%)
2	B	0.91	1/851 (0.1%)	0.93	2/1146 (0.2%)
2	D	0.91	1/851 (0.1%)	0.92	2/1146 (0.2%)
2	F	0.91	1/851 (0.1%)	0.92	2/1146 (0.2%)
2	H	0.93	1/851 (0.1%)	0.90	0/1146
All	All	1.20	157/112652 (0.1%)	1.11	614/152600 (0.4%)

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	36
1	C	0	35
1	E	0	36
1	G	0	34
All	All	0	141

The worst 5 of 157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	80	GLU	CG-CD	11.12	1.68	1.51
1	G	3661	TRP	CB-CG	10.06	1.68	1.50
1	A	3661	TRP	CB-CG	9.81	1.68	1.50
1	G	1976	ARG	NE-CZ	9.78	1.45	1.33
1	A	741	GLU	CG-CD	9.74	1.66	1.51

The worst 5 of 614 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	80	GLU	OE1-CD-OE2	-10.92	110.20	123.30
1	A	1212	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	G	4796	MET	CG-SD-CE	10.33	116.73	100.20
1	G	1976	ARG	CD-NE-CZ	10.23	137.93	123.60
1	C	1212	ARG	NE-CZ-NH1	10.17	125.39	120.30

There are no chirality outliers.

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	GLU	Mainchain,Peptide
1	A	329	ARG	Mainchain,Peptide
1	A	734	GLY	Peptide
1	A	841	GLY	Mainchain,Peptide
1	A	894	GLY	Mainchain

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	26843	0	24428	1190	0
1	C	26843	0	24428	1200	0
1	E	26843	0	24428	1194	0
1	G	26843	0	24427	1209	0
2	B	832	0	831	58	0
2	D	832	0	831	54	0
2	F	832	0	831	58	0
2	H	832	0	831	58	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	110704	0	101035	4733	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 22.

The worst 5 of 4733 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:A:4880:MET:HA	1:G:4578:LEU:HD11	1.26	1.17
1:A:4578:LEU:HD11	1:C:4880:MET:HA	1.18	1.17
1:E:4578:LEU:HD11	1:G:4880:MET:HA	1.25	1.16
1:C:4578:LEU:HD11	1:E:4880:MET:HA	1.17	1.10
1:A:4822:THR:HG22	1:C:4839:MET:SD	1.93	1.08

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	3483/5037 (69%)	3132 (90%)	258 (7%)	93 (3%)	6	44
1	C	3483/5037 (69%)	3133 (90%)	254 (7%)	96 (3%)	6	44
1	E	3483/5037 (69%)	3134 (90%)	255 (7%)	94 (3%)	6	44
1	G	3483/5037 (69%)	3137 (90%)	252 (7%)	94 (3%)	6	44
2	B	105/108 (97%)	95 (90%)	9 (9%)	1 (1%)	19	65
2	D	105/108 (97%)	95 (90%)	9 (9%)	1 (1%)	19	65
2	F	105/108 (97%)	96 (91%)	8 (8%)	1 (1%)	19	65
2	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
All	All	14352/20580 (70%)	12919 (90%)	1053 (7%)	380 (3%)	11	45

5 of 380 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	806	PRO
1	A	900	ASN
1	A	914	PRO

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Mol	Chain	Res	Type
1	A	916	PRO
1	A	971	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	2502/4276 (58%)	2472 (99%)	30 (1%)	78	90
1	C	2504/4276 (59%)	2476 (99%)	28 (1%)	80	91
1	E	2501/4276 (58%)	2472 (99%)	29 (1%)	78	90
1	G	2501/4276 (58%)	2474 (99%)	27 (1%)	80	91
2	B	89/90 (99%)	88 (99%)	1 (1%)	80	91
2	D	89/90 (99%)	88 (99%)	1 (1%)	80	91
2	F	89/90 (99%)	88 (99%)	1 (1%)	80	91
2	H	89/90 (99%)	88 (99%)	1 (1%)	80	91
All	All	10364/17464 (59%)	10246 (99%)	118 (1%)	81	91

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3987	ASP
1	E	928	THR
1	G	2518	LEU
1	C	4039	MET
2	D	34	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3896	ASN
1	E	543	ASN
1	G	3809	ASN

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Mol	Chain	Res	Type
1	C	3906	GLN
1	E	113	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.