



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 09:08 AM EST

PDB ID : 6W1N
EMDB ID : EMD-21513
Title : Pig Ryanodine Receptor (WT) in 5mM EGTA condition
Authors : Woll, K.W.; Haji-Ghassemi, O.; Van Petegem, F.
Deposited on : 2020-03-04
Resolution : 4.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

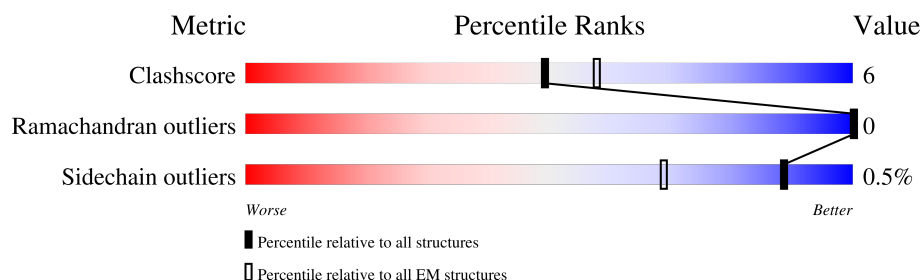
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	110	77% 17% . .
1	C	110	78% 16% . .
1	E	110	76% 18% . .
1	G	110	78% 16% . .
2	B	4624	71% 10% 20%
2	D	4624	71% 10% 20%
2	F	4624	71% 10% 20%
2	H	4624	71% 10% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 105232 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	A	106	Total	C	N	O	S	0	0
			730	465	128	133	4		
1	C	106	Total	C	N	O	S	0	0
			730	465	128	133	4		
1	E	106	Total	C	N	O	S	0	0
			730	465	128	133	4		
1	G	106	Total	C	N	O	S	0	0
			730	465	128	133	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P68106
A	-1	ASN	-	expression tag	UNP P68106
A	0	ALA	-	expression tag	UNP P68106
C	-2	SER	-	expression tag	UNP P68106
C	-1	ASN	-	expression tag	UNP P68106
C	0	ALA	-	expression tag	UNP P68106
E	-2	SER	-	expression tag	UNP P68106
E	-1	ASN	-	expression tag	UNP P68106
E	0	ALA	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	ASN	-	expression tag	UNP P68106
G	0	ALA	-	expression tag	UNP P68106

- Molecule 2 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3719	Total	C	N	O	S	1	0
			25577	16407	4433	4587	150		
2	D	3719	Total	C	N	O	S	1	0
			25577	16407	4433	4587	150		
2	F	3719	Total	C	N	O	S	1	0
			25577	16407	4433	4587	150		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	3719	Total	C	N	O	S	1	0
			25577	16407	4433	4587	150		


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

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	F	1	Total	Zn	0
			1	1	
3	H	1	Total	Zn	0
			1	1	

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

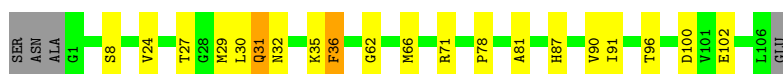
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




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

Chain C: 




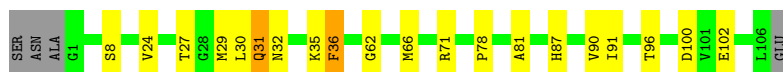
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 



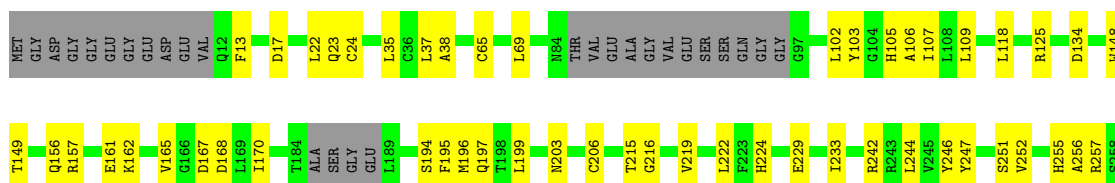
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 



- Molecule 2: Ryanodine Receptor

Chain B: 





- Molecule 2: Ryanodine Receptor

Chain D:  71% 10% 20%

T149	Q156	R157	E161	K162	V165	G166	D168	L169	I170	T184	ALA	SER	GLY	L189	S194	F195	A196	Q197	T198	L199	N203	C206	T215	G216	V219	L222	F223	H224	E229	I233	R242	T243	L244	V245	Y246	Y247	V252	H255	A256	R257	S258	P259			
Met	GLY	ASP	GLY	GLY	GLY	ASP	GLU	VAL	D12	F13	D17	L22	Q23	Q24	L35	C36	L37	A38	G65	L69	R84	THR	VAL	GLU	ALA	GLY	VAL	SER	SER	GLN	GLY	GLY	G97	L102	Y103	G104	H105	A106	I107	L108	Y109	L118	R125	D134	L149









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	52289	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/746	0.56	1/1019 (0.1%)
1	C	0.28	0/746	0.56	1/1019 (0.1%)
1	E	0.28	0/746	0.56	1/1019 (0.1%)
1	G	0.28	0/746	0.56	1/1019 (0.1%)
2	B	0.24	0/24464	0.41	1/33485 (0.0%)
2	D	0.24	0/24464	0.41	1/33485 (0.0%)
2	F	0.24	0/24464	0.41	1/33485 (0.0%)
2	H	0.24	0/24464	0.41	1/33485 (0.0%)
All	All	0.25	0/100840	0.42	8/138016 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	31	GLN	CA-CB-CG	5.80	126.15	113.40
1	A	31	GLN	CA-CB-CG	5.78	126.10	113.40
1	C	31	GLN	CA-CB-CG	5.78	126.11	113.40
1	G	31	GLN	CA-CB-CG	5.77	126.09	113.40
2	H	1554	VAL	C-N-CA	5.62	135.74	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	730	0	674	14	0
1	C	730	0	674	16	0
1	E	730	0	674	16	0
1	G	730	0	674	15	0
2	B	25577	0	21686	288	0
2	D	25577	0	21686	288	0
2	F	25577	0	21686	279	0
2	H	25577	0	21686	286	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	105232	0	89440	1180	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 6.

The worst 5 of 1180 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:F:1561:VAL:HG12	2:F:1562:ILE:HG12	1.55	0.88
2:H:1561:VAL:HG12	2:H:1562:ILE:HG12	1.55	0.88
2:D:1561:VAL:HG12	2:D:1562:ILE:HG12	1.55	0.88
2:B:1561:VAL:HG12	2:B:1562:ILE:HG12	1.55	0.86
2:H:252:VAL:HA	2:H:255:HIS:HD2	1.45	0.81

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	104/110 (94%)	99 (95%)	5 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	104/110 (94%)	99 (95%)	5 (5%)	0	100	100
1	E	104/110 (94%)	99 (95%)	5 (5%)	0	100	100
1	G	104/110 (94%)	99 (95%)	5 (5%)	0	100	100
2	B	3319/4624 (72%)	3275 (99%)	44 (1%)	0	100	100
2	D	3319/4624 (72%)	3273 (99%)	46 (1%)	0	100	100
2	F	3319/4624 (72%)	3275 (99%)	44 (1%)	0	100	100
2	H	3319/4624 (72%)	3275 (99%)	44 (1%)	0	100	100
All	All	13692/18936 (72%)	13494 (99%)	198 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	67/90 (74%)	65 (97%)	2 (3%)	41	64
1	C	67/90 (74%)	65 (97%)	2 (3%)	41	64
1	E	67/90 (74%)	65 (97%)	2 (3%)	41	64
1	G	67/90 (74%)	65 (97%)	2 (3%)	41	64
2	B	2115/3648 (58%)	2106 (100%)	9 (0%)	91	94
2	D	2115/3648 (58%)	2106 (100%)	9 (0%)	91	94
2	F	2115/3648 (58%)	2106 (100%)	9 (0%)	91	94
2	H	2115/3648 (58%)	2106 (100%)	9 (0%)	91	94
All	All	8728/14952 (58%)	8684 (100%)	44 (0%)	89	93

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	2128	GLN
2	H	165	VAL

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Mol	Chain	Res	Type
2	F	2157	LEU
2	F	4878	MET
2	H	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	495	ASN
2	H	4712	ASN
2	D	4712	ASN
2	F	255	HIS
2	F	495	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	B	25
2	D	25
2	F	25
2	H	25

The worst 5 of 100 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3606:UNK	C	3634:MET	N	44.08
1	D	3606:UNK	C	3634:MET	N	44.08
1	F	3606:UNK	C	3634:MET	N	44.08
1	H	3606:UNK	C	3634:MET	N	44.08
1	B	2939:ARG	C	2956:UNK	N	30.87