



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 11, 2019 – 12:03 AM EST

PDB ID : 6N4Q  
EMDB ID: : EMD-0341  
Title : CryoEM structure of Nav1.7 VSD2 (activated state) in complex with the gating modifier toxin ProTx2  
Authors : Xu, H.; Rohou, A.; Arthur, C.P.; Estevez, A.; Ciferri, C.; Payandeh, J.; Koth, C.M.  
Deposited on : 2018-11-20  
Resolution : 3.60 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](mailto: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.

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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) : 2.4

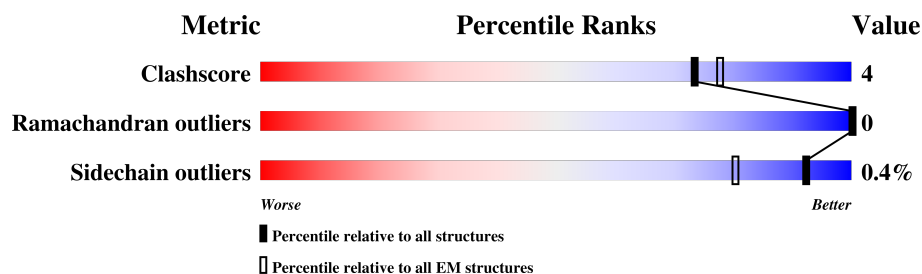
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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  $\geq 3$ , 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	288	82% 8% 9%
1	B	288	82% 9% 9%
1	C	288	81% 10% 9%
1	D	288	82% 9% 9%
2	E	30	87% 13%
2	F	30	87% 13%
2	G	30	87% 13%
2	H	30	83% 17%
3	I	215	88% 12%

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Mol	Chain	Length	Quality of chain
3	K	215	 89%10%
4	J	228	 88%12%
4	L	228	 88%12%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16358 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 Nav1.7 VSD2-NavAb chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	261	Total	C	N	O	S	0	0
			2136	1430	328	364	14		
1	B	262	Total	C	N	O	S	0	0
			2150	1439	332	365	14		
1	C	261	Total	C	N	O	S	0	0
			2136	1430	328	364	14		
1	D	262	Total	C	N	O	S	0	0
			2150	1439	332	365	14		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	MET	-	initiating methionine	UNP A8EVM5
A	705	ASP	-	expression tag	UNP A8EVM5
A	706	TYR	-	expression tag	UNP A8EVM5
A	707	LYS	-	expression tag	UNP A8EVM5
A	708	ASP	-	expression tag	UNP A8EVM5
A	709	ASP	-	expression tag	UNP A8EVM5
A	710	ASP	-	expression tag	UNP A8EVM5
A	711	ASP	-	expression tag	UNP A8EVM5
A	712	LYS	-	expression tag	UNP A8EVM5
A	713	GLY	-	expression tag	UNP A8EVM5
A	714	SER	-	expression tag	UNP A8EVM5
A	715	LEU	-	expression tag	UNP A8EVM5
A	716	VAL	-	expression tag	UNP A8EVM5
A	717	PRO	-	expression tag	UNP A8EVM5
A	718	ARG	-	expression tag	UNP A8EVM5
A	719	GLY	-	expression tag	UNP A8EVM5
A	720	SER	-	expression tag	UNP A8EVM5
A	721	HIS	-	expression tag	UNP A8EVM5
A	941	CYS	ILE	conflict	UNP A8EVM5
B	704	MET	-	initiating methionine	UNP A8EVM5
B	705	ASP	-	expression tag	UNP A8EVM5
B	706	TYR	-	expression tag	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	707	LYS	-	expression tag	UNP A8EVM5
B	708	ASP	-	expression tag	UNP A8EVM5
B	709	ASP	-	expression tag	UNP A8EVM5
B	710	ASP	-	expression tag	UNP A8EVM5
B	711	ASP	-	expression tag	UNP A8EVM5
B	712	LYS	-	expression tag	UNP A8EVM5
B	713	GLY	-	expression tag	UNP A8EVM5
B	714	SER	-	expression tag	UNP A8EVM5
B	715	LEU	-	expression tag	UNP A8EVM5
B	716	VAL	-	expression tag	UNP A8EVM5
B	717	PRO	-	expression tag	UNP A8EVM5
B	718	ARG	-	expression tag	UNP A8EVM5
B	719	GLY	-	expression tag	UNP A8EVM5
B	720	SER	-	expression tag	UNP A8EVM5
B	721	HIS	-	expression tag	UNP A8EVM5
B	941	CYS	ILE	conflict	UNP A8EVM5
C	704	MET	-	initiating methionine	UNP A8EVM5
C	705	ASP	-	expression tag	UNP A8EVM5
C	706	TYR	-	expression tag	UNP A8EVM5
C	707	LYS	-	expression tag	UNP A8EVM5
C	708	ASP	-	expression tag	UNP A8EVM5
C	709	ASP	-	expression tag	UNP A8EVM5
C	710	ASP	-	expression tag	UNP A8EVM5
C	711	ASP	-	expression tag	UNP A8EVM5
C	712	LYS	-	expression tag	UNP A8EVM5
C	713	GLY	-	expression tag	UNP A8EVM5
C	714	SER	-	expression tag	UNP A8EVM5
C	715	LEU	-	expression tag	UNP A8EVM5
C	716	VAL	-	expression tag	UNP A8EVM5
C	717	PRO	-	expression tag	UNP A8EVM5
C	718	ARG	-	expression tag	UNP A8EVM5
C	719	GLY	-	expression tag	UNP A8EVM5
C	720	SER	-	expression tag	UNP A8EVM5
C	721	HIS	-	expression tag	UNP A8EVM5
C	941	CYS	ILE	conflict	UNP A8EVM5
D	704	MET	-	initiating methionine	UNP A8EVM5
D	705	ASP	-	expression tag	UNP A8EVM5
D	706	TYR	-	expression tag	UNP A8EVM5
D	707	LYS	-	expression tag	UNP A8EVM5
D	708	ASP	-	expression tag	UNP A8EVM5
D	709	ASP	-	expression tag	UNP A8EVM5
D	710	ASP	-	expression tag	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	711	ASP	-	expression tag	UNP A8EVM5
D	712	LYS	-	expression tag	UNP A8EVM5
D	713	GLY	-	expression tag	UNP A8EVM5
D	714	SER	-	expression tag	UNP A8EVM5
D	715	LEU	-	expression tag	UNP A8EVM5
D	716	VAL	-	expression tag	UNP A8EVM5
D	717	PRO	-	expression tag	UNP A8EVM5
D	718	ARG	-	expression tag	UNP A8EVM5
D	719	GLY	-	expression tag	UNP A8EVM5
D	720	SER	-	expression tag	UNP A8EVM5
D	721	HIS	-	expression tag	UNP A8EVM5
D	941	CYS	ILE	conflict	UNP A8EVM5

- Molecule 2 is a protein called Beta/omega-theraphotoxin-Tp2a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	30	Total	C	N	O	S	0	0
			262	168	46	40	8		
2	F	30	Total	C	N	O	S	0	0
			262	168	46	40	8		
2	G	30	Total	C	N	O	S	0	0
			262	168	46	40	8		
2	H	30	Total	C	N	O	S	0	0
			262	168	46	40	8		

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	215	Total	C	N	O	S	0	0
			1649	1029	271	341	8		
3	K	215	Total	C	N	O	S	0	0
			1649	1029	271	341	8		


- Molecule 4 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	228	Total	C	N	O	S	0	0
			1720	1085	289	338	8		
4	L	228	Total	C	N	O	S	0	0
			1720	1085	289	338	8		




- Molecule 1: Nav1.7 VSD2-NavAb chimera

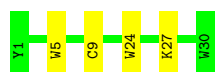


Chain E:  87% 13%



- Molecule 2: Beta/omega-theraphotoxin-Tp2a

Chain F:  87% 13%




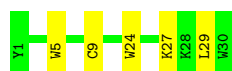
- Molecule 2: Beta/omega-theraphotoxin-Tp2a

Chain G:  87% 13%




- Molecule 2: Beta/omega-theraphotoxin-Tp2a

Chain H:  83% 17%




- Molecule 3: Fab light chain

Chain I:  88% 12%




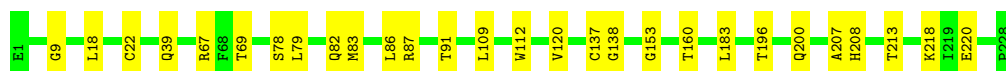
- Molecule 3: Fab light chain

Chain K:  89% 10%




- Molecule 4: Fab heavy chain

Chain J:  88% 12%



- Molecule 4: Fab heavy chain

Chain L:  88% 12%



E1	G9	L18	C22	Q39	Y57	R67	F68	T69	L79	Q82	R83	L86	R87	T91	L109	W112	V120	C137	G138	G153	T160	L183	T196	Q200	A207	H208	T213	K218	T219	E220	P228
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	187192	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	41	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.48	0/2190	0.63	0/2975
1	B	0.46	0/2204	0.60	0/2993
1	C	0.48	0/2190	0.63	0/2975
1	D	0.46	0/2204	0.60	0/2993
2	E	0.26	0/270	0.59	0/360
2	F	0.26	0/270	0.59	0/360
2	G	0.26	0/270	0.59	0/360
2	H	0.26	0/270	0.59	0/360
3	I	0.30	0/1688	0.53	0/2292
3	K	0.31	0/1688	0.53	0/2292
4	J	0.37	0/1764	0.58	0/2406
4	L	0.37	0/1764	0.57	0/2406
All	All	0.41	0/16772	0.59	0/22772

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
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	792	PHE	Peptide
1	C	792	PHE	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	2136	0	2186	15	0
1	B	2150	0	2208	17	0
1	C	2136	0	2186	19	0
1	D	2150	0	2208	16	0
2	E	262	0	254	2	0
2	F	262	0	254	2	0
2	G	262	0	254	2	0
2	H	262	0	254	3	0
3	I	1649	0	1577	14	0
3	K	1649	0	1577	12	0
4	J	1720	0	1684	15	0
4	L	1720	0	1684	15	0
All	All	16358	0	16326	119	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 119 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:B:760:GLU:OE2	1:B:763:ASN:ND2	2.29	0.65
4:J:22:CYS:HB3	4:J:79:LEU:HB3	1.78	0.65
4:L:22:CYS:HB3	4:L:79:LEU:HB3	1.78	0.65
3:K:109:ARG:NH1	3:K:171:ASP:O	2.31	0.63
3:I:109:ARG:NH1	3:I:171:ASP:O	2.31	0.63

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	259/288 (90%)	240 (93%)	19 (7%)	0	100	100
1	B	260/288 (90%)	243 (94%)	17 (6%)	0	100	100
1	C	259/288 (90%)	239 (92%)	20 (8%)	0	100	100
1	D	260/288 (90%)	246 (95%)	14 (5%)	0	100	100
2	E	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
2	F	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
2	G	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
2	H	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
3	I	213/215 (99%)	197 (92%)	16 (8%)	0	100	100
3	K	213/215 (99%)	197 (92%)	16 (8%)	0	100	100
4	J	226/228 (99%)	207 (92%)	19 (8%)	0	100	100
4	L	226/228 (99%)	206 (91%)	20 (9%)	0	100	100
All	All	2028/2158 (94%)	1867 (92%)	161 (8%)	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	239/265 (90%)	238 (100%)	1 (0%)	92	97
1	B	241/265 (91%)	240 (100%)	1 (0%)	92	97
1	C	239/265 (90%)	238 (100%)	1 (0%)	92	97
1	D	241/265 (91%)	240 (100%)	1 (0%)	92	97
2	E	29/29 (100%)	29 (100%)	0	100	100
2	F	29/29 (100%)	29 (100%)	0	100	100
2	G	29/29 (100%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	29/29 (100%)	29 (100%)	0	100	100
3	I	190/190 (100%)	188 (99%)	2 (1%)	76	90
3	K	190/190 (100%)	188 (99%)	2 (1%)	76	90
4	J	193/194 (100%)	193 (100%)	0	100	100
4	L	193/194 (100%)	193 (100%)	0	100	100
All	All	1842/1944 (95%)	1834 (100%)	8 (0%)	92	97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	746	ASN
3	K	213	ASN
3	I	213	ASN
1	C	746	ASN
3	I	109	ARG

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

Mol	Chain	Res	Type
3	I	39	GLN
3	I	167	GLN
3	K	167	GLN
1	D	969	ASN
3	K	213	ASN

### 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 [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](#)

There are no chain breaks in this entry.