



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 11, 2019 – 12:31 AM EST

PDB ID : 6N4R
EMDB ID: : EMD-0342
Title : CryoEM structure of Nav1.7 VSD2 (deactivated 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 : 4.20 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) : 2.4

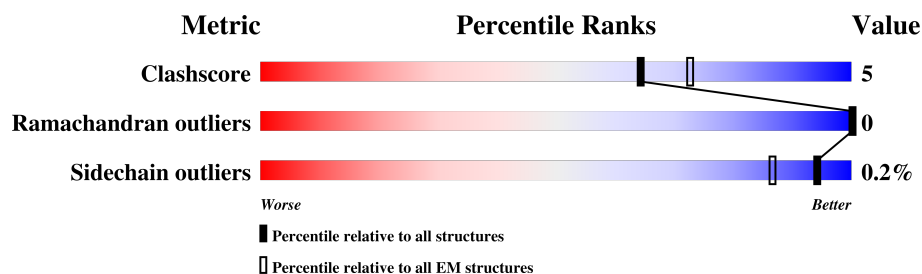
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	288	73% 12% 16%
1	B	288	67% 11% 22%
1	C	288	73% 12% 16%
1	D	288	66% 13% 22%
2	E	30	87% 13%
2	F	30	87% 13%
2	G	30	87% 13%
2	H	30	83% 17%
3	I	215	90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	K	215	 90%10%
4	J	228	 86%14%
4	L	228	 88%12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15444 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	B	225	Total	C	N	O	S	0	0
			1841	1249	279	300	13		
1	C	243	Total	C	N	O	S	0	0
			1984	1336	303	331	14		
1	D	225	Total	C	N	O	S	0	0
			1841	1249	279	300	13		
1	A	243	Total	C	N	O	S	0	0
			1984	1336	303	331	14		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	704	MET	-	initiating methionine	UNP A8EVM5
B	705	ASP	-	expression tag	UNP A8EVM5
B	706	TYR	-	expression tag	UNP A8EVM5
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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		

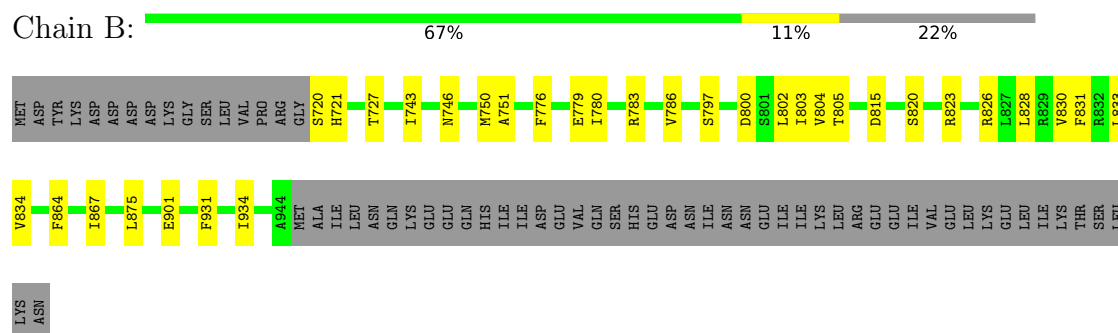
- Molecule 4 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	228	Total	C	N	O	S	0	0
			1724	1087	289	340	8		
4	L	228	Total	C	N	O	S	0	0
			1724	1087	289	340	8		

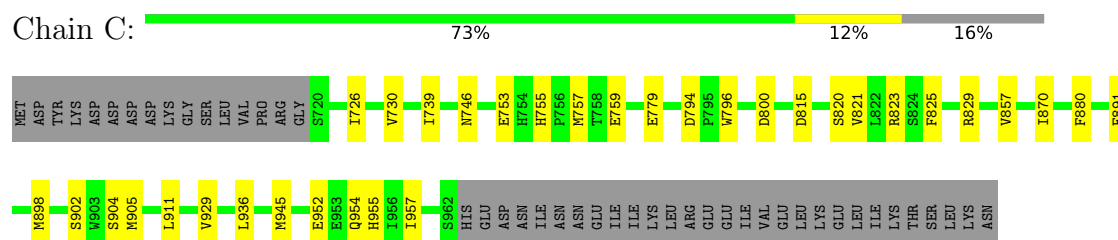
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

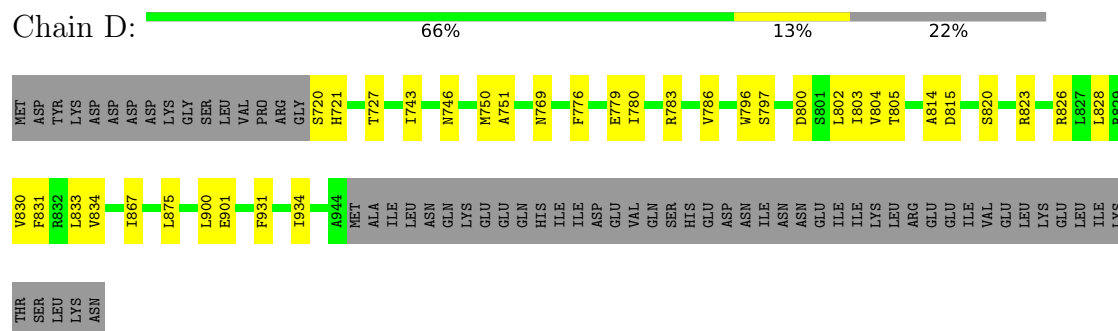
- Molecule 1: Nav1.7 VSD2-NavAb chimera



- Molecule 1: Nav1.7 VSD2-NavAb chimera

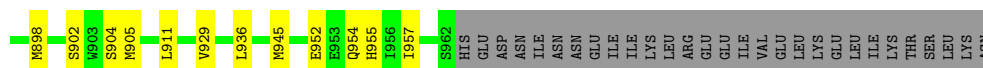
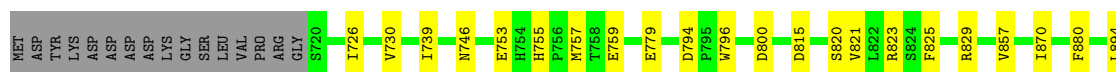


- Molecule 1: Nav1.7 VSD2-NavAb chimera



- Molecule 1: Nav1.7 VSD2-NavAb chimera

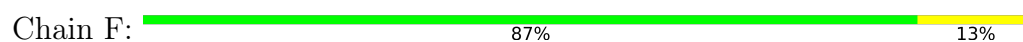




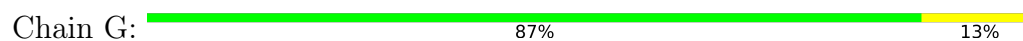
- Molecule 2: Beta/omega-theraphotoxin-Tp2a



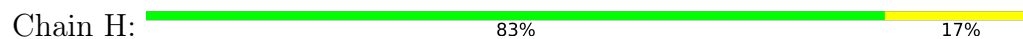
- Molecule 2: Beta/omega-theraphotoxin-Tp2a



- Molecule 2: Beta/omega-theraphotoxin-Tp2a



- Molecule 2: Beta/omega-theraphotoxin-Tp2a



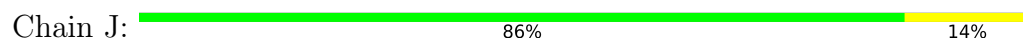
- Molecule 3: Fab light chain



- Molecule 3: Fab light chain

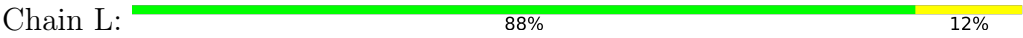


- Molecule 4: Fab heavy chain





● Molecule 4: Fab heavy chain



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	53206	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	0.49	0/2037	0.63	0/2769
1	B	0.47	0/1893	0.66	0/2574
1	C	0.49	0/2037	0.63	0/2769
1	D	0.47	0/1893	0.66	0/2574
2	E	0.29	0/270	0.64	0/360
2	F	0.29	0/270	0.64	0/360
2	G	0.28	0/270	0.64	0/360
2	H	0.28	0/270	0.64	0/360
3	I	0.37	0/1688	0.57	0/2292
3	K	0.37	0/1688	0.56	0/2292
4	J	0.42	0/1768	0.60	0/2411
4	L	0.42	0/1768	0.60	0/2411
All	All	0.43	0/15852	0.62	0/21532

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	B	0	1
1	D	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	B	931	PHE	Peptide
1	D	931	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	1984	0	2036	22	0
1	B	1841	0	1904	22	0
1	C	1984	0	2036	22	0
1	D	1841	0	1904	25	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	12	0
3	K	1649	0	1577	11	0
4	J	1724	0	1688	17	0
4	L	1724	0	1688	15	0
All	All	15444	0	15426	141	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 5.

The worst 5 of 141 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)
3:I:18:LYS:HA	3:I:76:ILE:O	1.80	0.81
3:K:18:LYS:HA	3:K:76:ILE:O	1.80	0.80
4:J:218:LYS:NZ	4:J:220:GLU:OE2	2.22	0.72
4:L:218:LYS:NZ	4:L:220:GLU:OE2	2.22	0.71
1:B:779:GLU:OE2	1:B:783:ARG:NH2	2.27	0.67

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	241/288 (84%)	228 (95%)	13 (5%)	0	100	100
1	B	223/288 (77%)	212 (95%)	11 (5%)	0	100	100
1	C	241/288 (84%)	228 (95%)	13 (5%)	0	100	100
1	D	223/288 (77%)	212 (95%)	11 (5%)	0	100	100
2	E	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	F	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	G	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	H	28/30 (93%)	25 (89%)	3 (11%)	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%)	207 (92%)	19 (8%)	0	100	100
All	All	1918/2158 (89%)	1788 (93%)	130 (7%)	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	221/265 (83%)	220 (100%)	1 (0%)	90	94
1	B	205/265 (77%)	204 (100%)	1 (0%)	90	94
1	C	221/265 (83%)	220 (100%)	1 (0%)	90	94
1	D	205/265 (77%)	204 (100%)	1 (0%)	90	94
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	29/29 (100%)	29 (100%)	0	100	100
3	I	190/190 (100%)	190 (100%)	0	100	100
3	K	190/190 (100%)	190 (100%)	0	100	100
4	J	194/194 (100%)	194 (100%)	0	100	100
4	L	194/194 (100%)	194 (100%)	0	100	100
All	All	1736/1944 (89%)	1732 (100%)	4 (0%)	94	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	746	ASN
1	C	746	ASN
1	D	746	ASN
1	A	746	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	39	GLN
4	J	99	HIS
1	A	746	ASN
3	I	91	GLN
4	L	99	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 [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.