wwPDB X-ray Structure Validation Summary Report (i)

Jun 1, 2022 – 01:12 am BST

PDB ID	:	7PG8
Title	:	NaV_Ae1/Sp1CTD_pore-ANT05 complex
Authors	:	Lolicato, M.; Arrigoni, C.
Deposited on	:	2021-08-13
Resolution	:	4.50 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

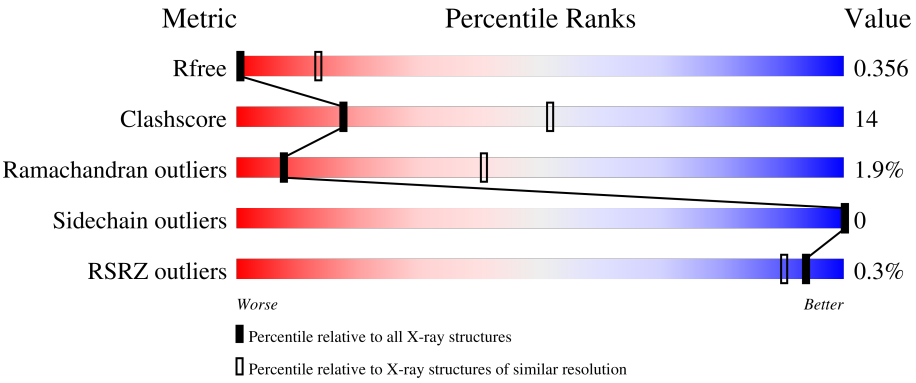
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	217	86% 13%
1	D	217	86% 13%
1	G	217	85% 14%
1	J	217	85% 14%
1	M	217	86% 13%

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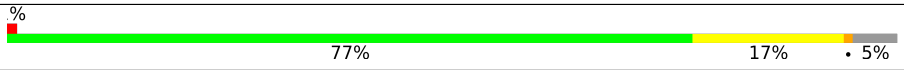
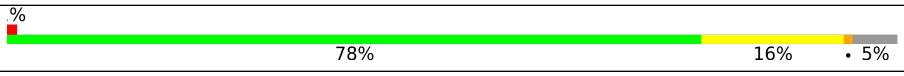
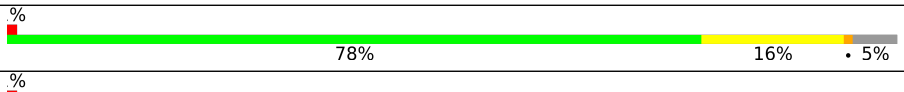
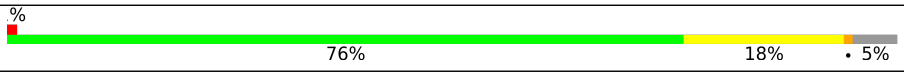
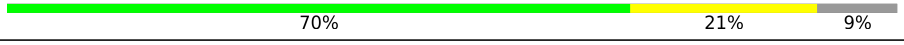
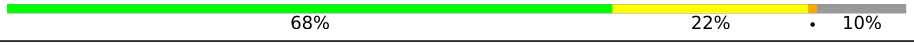
Mol	Chain	Length	Quality of chain
1	P	217	
1	S	217	
1	V	217	
2	B	233	
2	F	233	
2	I	233	
2	L	233	
2	N	233	
2	R	233	
2	U	233	
2	X	233	
3	C	143	
3	E	143	
3	H	143	
3	K	143	
3	O	143	
3	Q	143	
3	T	143	
3	W	143	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22623 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ANT05 H12 fab fragment, light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	P	215	Total 1086	C 656	N 215	O 215	0	0	0
1	M	215	Total 1086	C 656	N 215	O 215	0	0	0
1	V	215	Total 1086	C 656	N 215	O 215	0	0	0
1	S	215	Total 1086	C 656	N 215	O 215	0	0	0
1	G	215	Total 1086	C 656	N 215	O 215	0	0	0
1	D	215	Total 1086	C 656	N 215	O 215	0	0	0
1	J	215	Total 1086	C 656	N 215	O 215	0	0	0
1	A	215	Total 1086	C 656	N 215	O 215	0	0	0

- Molecule 2 is a protein called ANT05 H12 fab fragment, heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	221	Total 1106	C 664	N 221	O 221	0	0	0
2	F	221	Total 1106	C 664	N 221	O 221	0	0	0
2	I	221	Total 1106	C 664	N 221	O 221	0	0	0
2	L	221	Total 1106	C 664	N 221	O 221	0	0	0
2	N	221	Total 1106	C 664	N 221	O 221	0	0	0
2	R	221	Total 1106	C 664	N 221	O 221	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	221	Total 1106	C 664	N 221	O 221	0	0	0
2	X	221	Total 1106	C 664	N 221	O 221	0	0	0

- Molecule 3 is a protein called Ion transport protein,Voltage-gated sodium channel.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	127	Total 628	C 374	N 127	O 127	0	0	0
3	E	128	Total 633	C 377	N 128	O 128	0	0	0
3	H	130	Total 643	C 383	N 130	O 130	0	0	0
3	K	129	Total 638	C 380	N 129	O 129	0	0	0
3	O	130	Total 643	C 383	N 130	O 130	0	0	0
3	Q	126	Total 623	C 371	N 126	O 126	0	0	0
3	T	130	Total 641	C 381	N 130	O 130	0	0	0
3	W	129	Total 638	C 380	N 129	O 129	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	137	GLY	-	expression tag	UNP Q0ABW0
C	138	PRO	-	expression tag	UNP Q0ABW0
C	139	SER	-	expression tag	UNP Q0ABW0
C	140	SER	-	expression tag	UNP Q0ABW0
C	141	PRO	-	expression tag	UNP Q0ABW0
C	142	SER	-	expression tag	UNP Q0ABW0
E	137	GLY	-	expression tag	UNP Q0ABW0
E	138	PRO	-	expression tag	UNP Q0ABW0
E	139	SER	-	expression tag	UNP Q0ABW0
E	140	SER	-	expression tag	UNP Q0ABW0
E	141	PRO	-	expression tag	UNP Q0ABW0
E	142	SER	-	expression tag	UNP Q0ABW0
H	137	GLY	-	expression tag	UNP Q0ABW0
H	138	PRO	-	expression tag	UNP Q0ABW0

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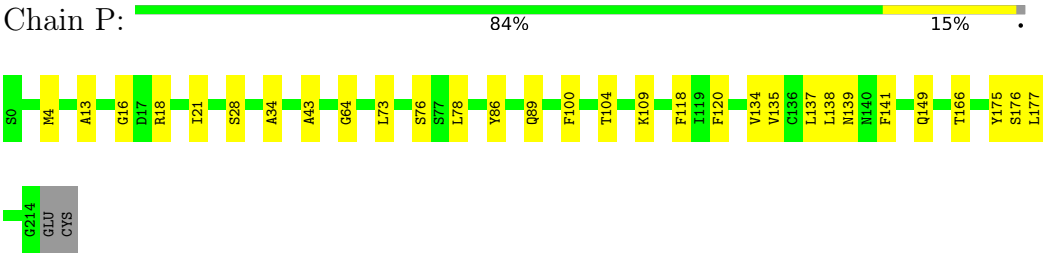
Chain	Residue	Modelled	Actual	Comment	Reference
H	139	SER	-	expression tag	UNP Q0ABW0
H	140	SER	-	expression tag	UNP Q0ABW0
H	141	PRO	-	expression tag	UNP Q0ABW0
H	142	SER	-	expression tag	UNP Q0ABW0
K	137	GLY	-	expression tag	UNP Q0ABW0
K	138	PRO	-	expression tag	UNP Q0ABW0
K	139	SER	-	expression tag	UNP Q0ABW0
K	140	SER	-	expression tag	UNP Q0ABW0
K	141	PRO	-	expression tag	UNP Q0ABW0
K	142	SER	-	expression tag	UNP Q0ABW0
O	137	GLY	-	expression tag	UNP Q0ABW0
O	138	PRO	-	expression tag	UNP Q0ABW0
O	139	SER	-	expression tag	UNP Q0ABW0
O	140	SER	-	expression tag	UNP Q0ABW0
O	141	PRO	-	expression tag	UNP Q0ABW0
O	142	SER	-	expression tag	UNP Q0ABW0
Q	137	GLY	-	expression tag	UNP Q0ABW0
Q	138	PRO	-	expression tag	UNP Q0ABW0
Q	139	SER	-	expression tag	UNP Q0ABW0
Q	140	SER	-	expression tag	UNP Q0ABW0
Q	141	PRO	-	expression tag	UNP Q0ABW0
Q	142	SER	-	expression tag	UNP Q0ABW0
T	137	GLY	-	expression tag	UNP Q0ABW0
T	138	PRO	-	expression tag	UNP Q0ABW0
T	139	SER	-	expression tag	UNP Q0ABW0
T	140	SER	-	expression tag	UNP Q0ABW0
T	141	PRO	-	expression tag	UNP Q0ABW0
T	142	SER	-	expression tag	UNP Q0ABW0
W	137	GLY	-	expression tag	UNP Q0ABW0
W	138	PRO	-	expression tag	UNP Q0ABW0
W	139	SER	-	expression tag	UNP Q0ABW0
W	140	SER	-	expression tag	UNP Q0ABW0
W	141	PRO	-	expression tag	UNP Q0ABW0
W	142	SER	-	expression tag	UNP Q0ABW0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

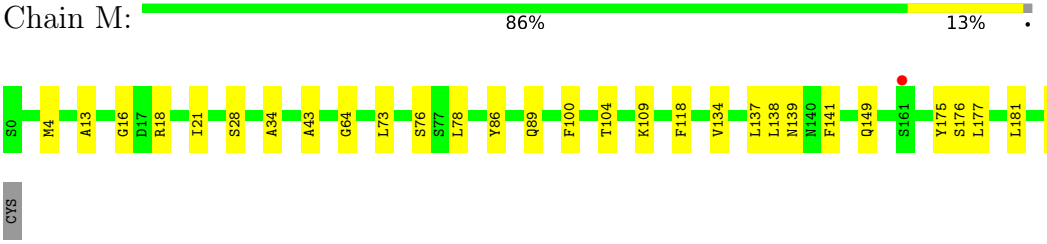
• Molecule 1: ANT05 H12 fab fragment, light chain

Chain P:



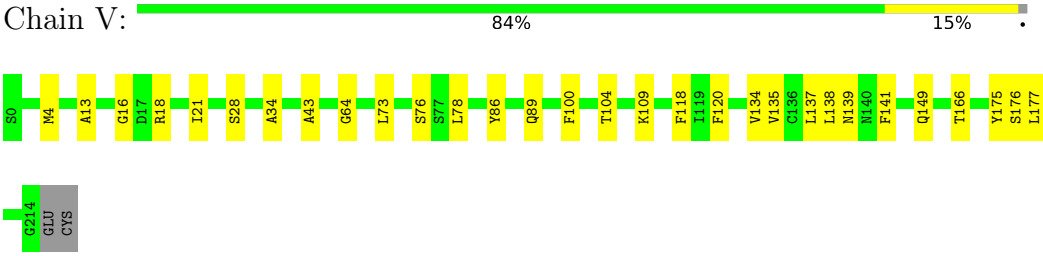
• Molecule 1: ANT05 H12 fab fragment, light chain

Chain M:



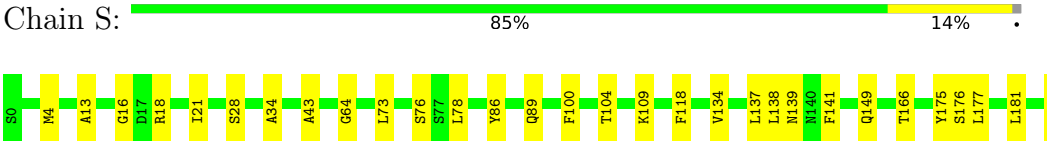
• Molecule 1: ANT05 H12 fab fragment, light chain

Chain V:



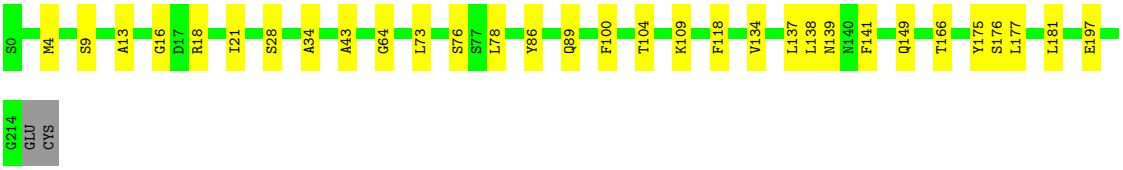
• Molecule 1: ANT05 H12 fab fragment, light chain

Chain S:



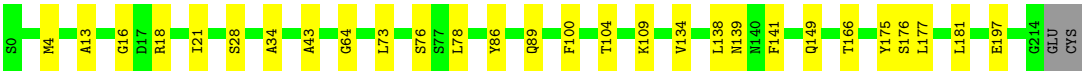
• Molecule 1: ANT05 H12 fab fragment, light chain

Chain G:



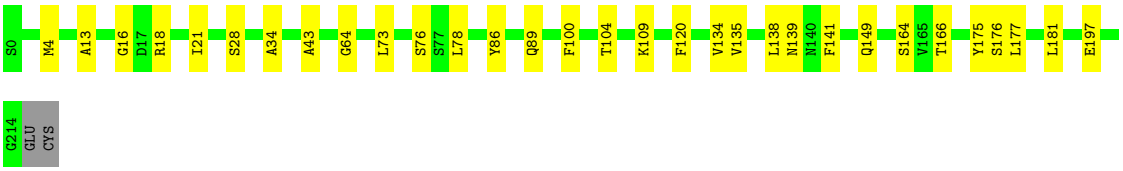
• Molecule 1: ANT05 H12 fab fragment, light chain

Chain D:



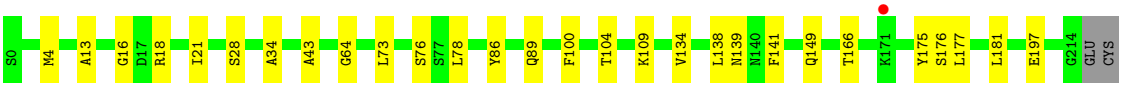
• Molecule 1: ANT05 H12 fab fragment, light chain

Chain J:



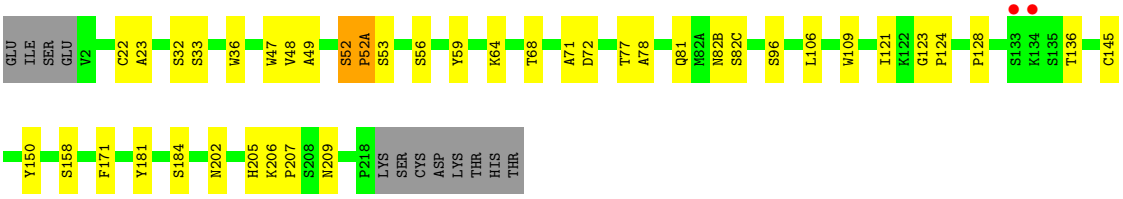
• Molecule 1: ANT05 H12 fab fragment, light chain

Chain A:



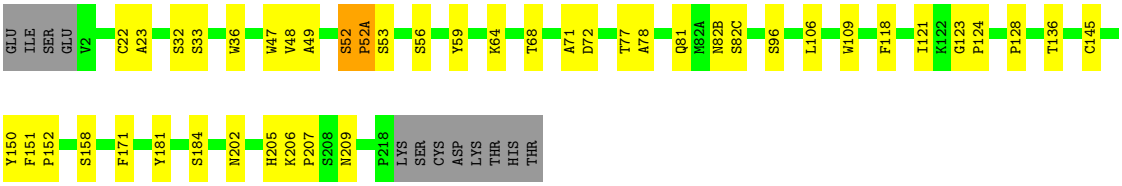
• Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain B:



• Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain F:

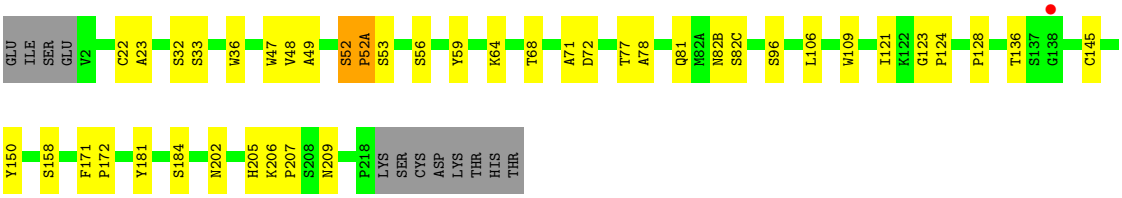


• Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain I:

• Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain L:

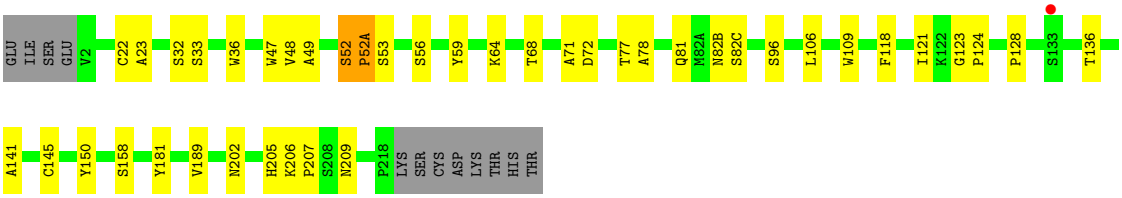


• Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain N:

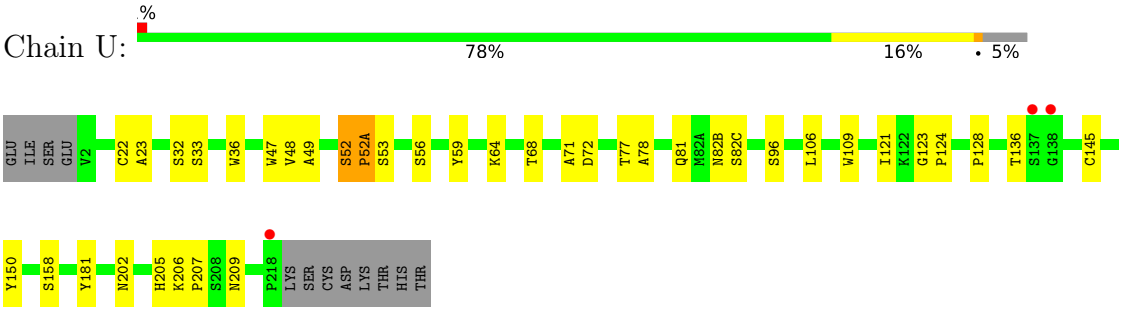
• Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain R:



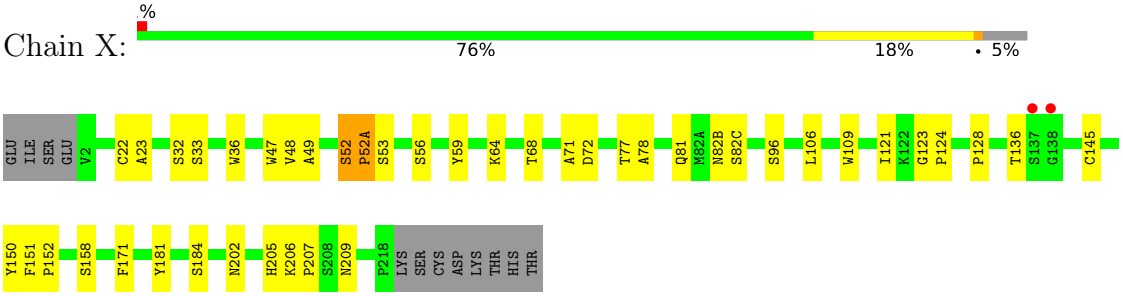
• Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain U:



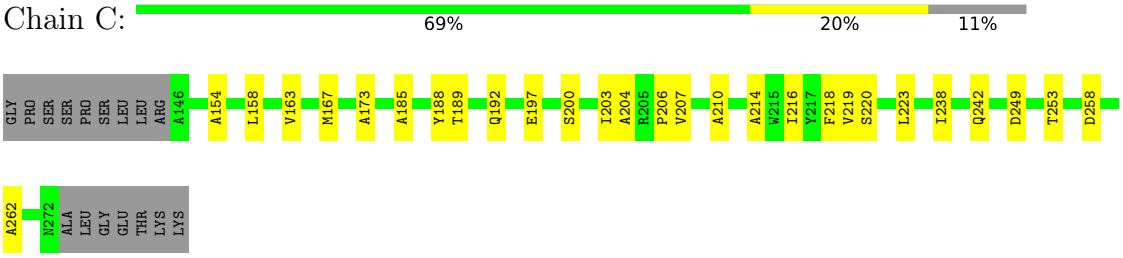
• Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain X:



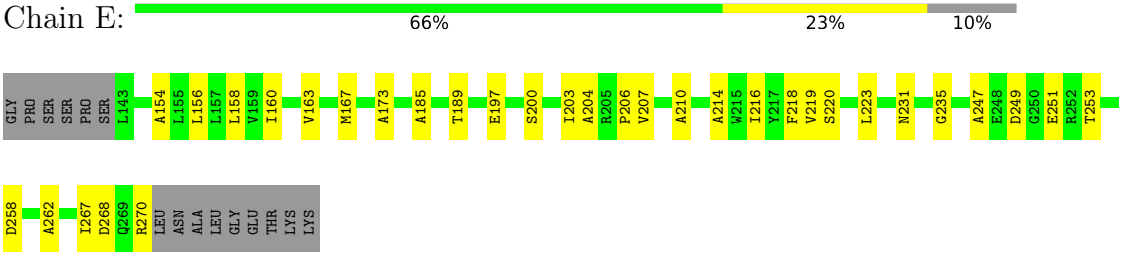
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain C:



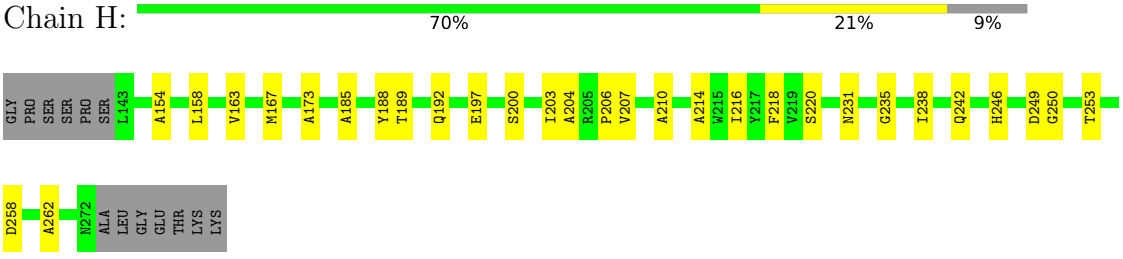
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain E:



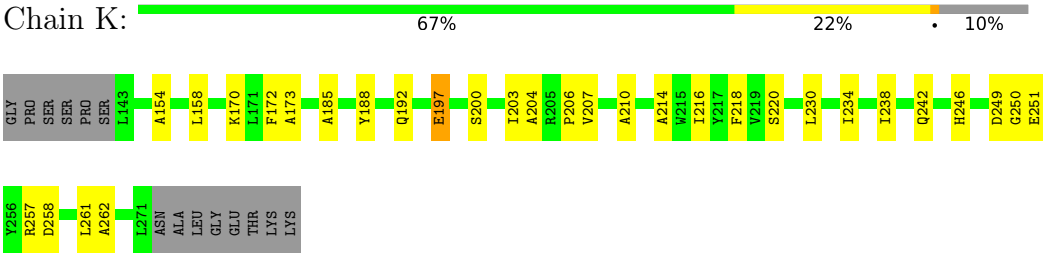
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain H:



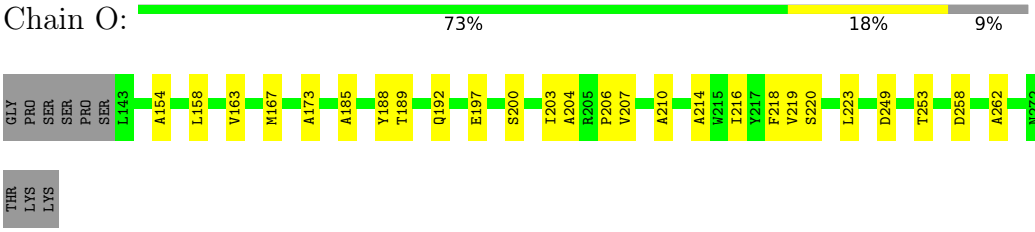
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain K:



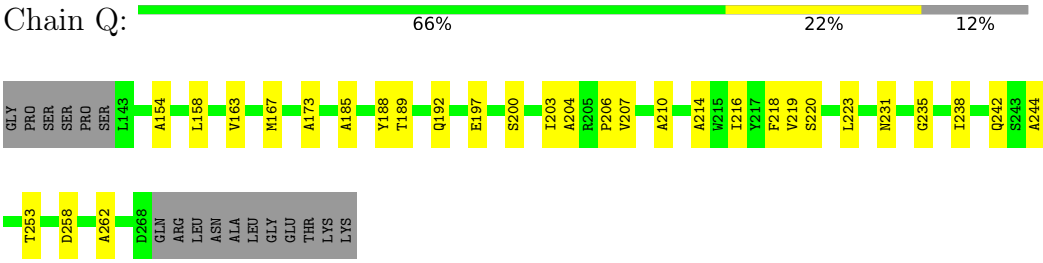
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain O:



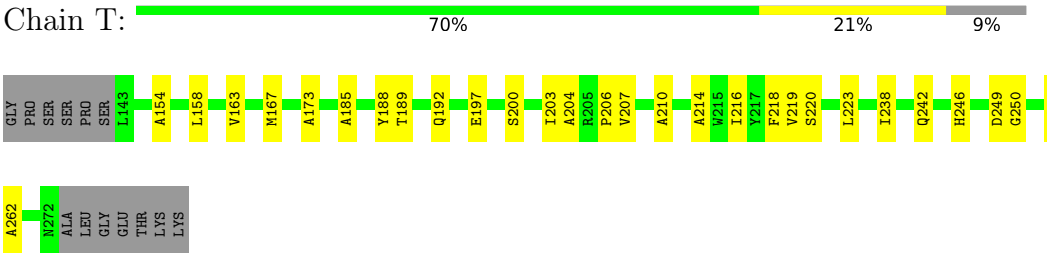
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain Q:



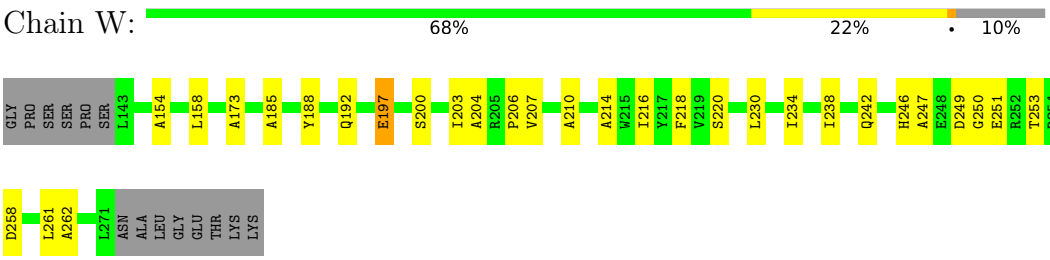
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain T:



• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	127.17Å 127.17Å 445.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 4.50 19.96 – 4.46	Depositor EDS
% Data completeness (in resolution range)	96.4 (15.00-4.50) 98.3 (19.96-4.46)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 4.54Å)	Xtriage
Refinement program	REFMAC 5.8.0	Depositor
R, R_{free}	0.303 , 0.352 0.317 , 0.356	Depositor DCC
R_{free} test set	2117 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	254.6	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.349 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22623	wwPDB-VP
Average B, all atoms (Å^2)	251.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.82	0/1096	0.84	0/1535
1	D	0.82	0/1096	0.84	0/1535
1	G	0.82	0/1096	0.84	0/1535
1	J	0.82	0/1096	0.84	0/1535
1	M	0.82	0/1096	0.84	0/1535
1	P	0.82	0/1096	0.84	0/1535
1	S	0.82	0/1096	0.84	0/1535
1	V	0.82	0/1096	0.84	0/1535
2	B	0.84	0/1111	0.86	0/1540
2	F	0.84	0/1111	0.86	0/1540
2	I	0.83	0/1111	0.86	0/1540
2	L	0.83	0/1111	0.86	0/1540
2	N	0.83	0/1111	0.85	0/1540
2	R	0.84	0/1111	0.86	0/1540
2	U	0.83	0/1111	0.86	0/1540
2	X	0.83	0/1111	0.86	0/1540
3	C	0.86	0/627	0.96	0/872
3	E	0.85	0/632	0.95	0/879
3	H	0.85	0/642	0.98	0/893
3	K	0.87	0/637	1.06	0/886
3	O	0.86	0/642	0.96	0/893
3	Q	0.85	0/621	0.96	0/862
3	T	0.86	0/640	0.97	0/889
3	W	0.87	0/637	1.06	0/886
All	All	0.84	0/22734	0.88	0/31660

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
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	I	0	1
2	L	0	1
2	N	0	1
2	R	0	1
2	U	0	1
2	X	0	1
3	C	0	1
3	E	0	2
3	H	0	1
3	K	0	1
3	O	0	1
3	Q	0	1
3	T	0	1
3	W	0	1
All	All	0	17

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	52	SER	Peptide
2	F	52	SER	Peptide
2	I	52	SER	Peptide
2	L	52	SER	Peptide
2	N	52	SER	Peptide

5.2 Too-close contacts (i)

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	1086	0	540	16	0
1	D	1086	0	540	16	0
1	G	1086	0	540	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1086	0	540	18	0
1	M	1086	0	540	16	0
1	P	1086	0	540	18	0
1	S	1086	0	540	17	0
1	V	1086	0	540	18	0
2	B	1106	0	563	26	0
2	F	1106	0	563	25	0
2	I	1106	0	563	25	0
2	L	1106	0	563	26	0
2	N	1106	0	563	25	0
2	R	1106	0	563	25	0
2	U	1106	0	563	24	0
2	X	1106	0	563	27	0
3	C	628	0	295	15	0
3	E	633	0	297	17	0
3	H	643	0	301	16	0
3	K	638	0	299	19	0
3	O	643	0	301	14	0
3	Q	623	0	292	17	0
3	T	641	0	296	16	0
3	W	638	0	299	19	0
All	All	22623	0	11204	463	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 14.

The worst 5 of 463 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:52(A):PRO:HG3	2:F:56:SER:CB	2.16	0.76
2:I:52(A):PRO:HG3	2:I:56:SER:CB	2.17	0.75
2:X:52(A):PRO:HG3	2:X:56:SER:CB	2.17	0.75
2:R:52(A):PRO:HG3	2:R:56:SER:CB	2.16	0.74
2:U:52(A):PRO:HG3	2:U:56:SER:CB	2.17	0.74

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 X-ray entries followed by that with respect to entries of similar resolution.

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	213/217 (98%)	188 (88%)	23 (11%)	2 (1%)	17	56
1	D	213/217 (98%)	188 (88%)	23 (11%)	2 (1%)	17	56
1	G	213/217 (98%)	186 (87%)	24 (11%)	3 (1%)	11	47
1	J	213/217 (98%)	187 (88%)	24 (11%)	2 (1%)	17	56
1	M	213/217 (98%)	188 (88%)	23 (11%)	2 (1%)	17	56
1	P	213/217 (98%)	188 (88%)	23 (11%)	2 (1%)	17	56
1	S	213/217 (98%)	186 (87%)	25 (12%)	2 (1%)	17	56
1	V	213/217 (98%)	187 (88%)	24 (11%)	2 (1%)	17	56
2	B	211/233 (91%)	179 (85%)	25 (12%)	7 (3%)	4	30
2	F	211/233 (91%)	179 (85%)	24 (11%)	8 (4%)	3	27
2	I	211/233 (91%)	180 (85%)	24 (11%)	7 (3%)	4	30
2	L	211/233 (91%)	180 (85%)	24 (11%)	7 (3%)	4	30
2	N	211/233 (91%)	179 (85%)	25 (12%)	7 (3%)	4	30
2	R	211/233 (91%)	180 (85%)	23 (11%)	8 (4%)	3	27
2	U	211/233 (91%)	180 (85%)	24 (11%)	7 (3%)	4	30
2	X	211/233 (91%)	180 (85%)	24 (11%)	7 (3%)	4	30
3	C	125/143 (87%)	117 (94%)	7 (6%)	1 (1%)	19	60
3	E	126/143 (88%)	116 (92%)	9 (7%)	1 (1%)	19	60
3	H	128/143 (90%)	117 (91%)	10 (8%)	1 (1%)	19	60
3	K	127/143 (89%)	116 (91%)	10 (8%)	1 (1%)	19	60
3	O	128/143 (90%)	120 (94%)	7 (6%)	1 (1%)	19	60
3	Q	122/143 (85%)	113 (93%)	8 (7%)	1 (1%)	19	60
3	T	128/143 (90%)	118 (92%)	9 (7%)	1 (1%)	19	60
3	W	127/143 (89%)	116 (91%)	10 (8%)	1 (1%)	19	60
All	All	4403/4744 (93%)	3868 (88%)	452 (10%)	83 (2%)	8	41

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	121	ILE
2	F	121	ILE
2	I	121	ILE
2	L	121	ILE
2	N	121	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	11/192 (6%)	11 (100%)	0	100	100
1	D	11/192 (6%)	11 (100%)	0	100	100
1	G	11/192 (6%)	11 (100%)	0	100	100
1	J	11/192 (6%)	11 (100%)	0	100	100
1	M	11/192 (6%)	11 (100%)	0	100	100
1	P	11/192 (6%)	11 (100%)	0	100	100
1	S	11/192 (6%)	11 (100%)	0	100	100
1	V	11/192 (6%)	11 (100%)	0	100	100
2	B	12/195 (6%)	12 (100%)	0	100	100
2	F	12/195 (6%)	12 (100%)	0	100	100
2	I	12/195 (6%)	12 (100%)	0	100	100
2	L	12/195 (6%)	12 (100%)	0	100	100
2	N	12/195 (6%)	12 (100%)	0	100	100
2	R	12/195 (6%)	12 (100%)	0	100	100
2	U	12/195 (6%)	12 (100%)	0	100	100
2	X	12/195 (6%)	12 (100%)	0	100	100
All	All	184/3096 (6%)	184 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L	6
2	B	6
2	F	6
2	I	6
2	N	6
2	R	6
2	U	6
2	X	6
3	Q	1

The worst 5 of 49 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	51:ILE	C	52:SER	N	4.00
1	B	51:ILE	C	52:SER	N	3.99
1	F	51:ILE	C	52:SER	N	3.99
1	I	51:ILE	C	52:SER	N	3.99
1	N	51:ILE	C	52:SER	N	3.99

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	215/217 (99%)	-0.90	1 (0%) 91 85	147, 298, 423, 525	0
1	D	215/217 (99%)	-0.97	0 100 100	148, 269, 366, 492	0
1	G	215/217 (99%)	-0.98	0 100 100	117, 234, 324, 439	0
1	J	215/217 (99%)	-1.02	0 100 100	129, 232, 297, 349	0
1	M	215/217 (99%)	-0.90	1 (0%) 91 85	139, 303, 434, 496	0
1	P	215/217 (99%)	-0.96	0 100 100	145, 264, 363, 524	0
1	S	215/217 (99%)	-0.99	0 100 100	128, 229, 331, 409	0
1	V	215/217 (99%)	-1.02	0 100 100	143, 244, 309, 329	0
2	B	221/233 (94%)	-0.93	2 (0%) 84 77	127, 258, 436, 544	0
2	F	221/233 (94%)	-0.96	0 100 100	113, 230, 360, 430	0
2	I	221/233 (94%)	-0.93	1 (0%) 91 85	103, 216, 320, 638	0
2	L	221/233 (94%)	-0.94	1 (0%) 91 85	109, 223, 347, 541	0
2	N	221/233 (94%)	-0.92	2 (0%) 84 77	138, 255, 448, 599	0
2	R	221/233 (94%)	-0.94	1 (0%) 91 85	109, 225, 386, 472	0
2	U	221/233 (94%)	-0.92	3 (1%) 75 66	116, 218, 347, 613	0
2	X	221/233 (94%)	-0.95	2 (0%) 84 77	111, 223, 343, 534	0
3	C	127/143 (88%)	-1.11	0 100 100	168, 262, 456, 528	0
3	E	128/143 (89%)	-1.06	0 100 100	177, 263, 374, 428	0
3	H	130/143 (90%)	-1.10	0 100 100	139, 223, 322, 342	0
3	K	129/143 (90%)	-1.15	0 100 100	113, 218, 310, 382	0
3	O	130/143 (90%)	-1.14	0 100 100	149, 260, 364, 455	0
3	Q	126/143 (88%)	-1.07	0 100 100	177, 252, 339, 423	0
3	T	130/143 (90%)	-1.12	0 100 100	147, 229, 326, 362	0
3	W	129/143 (90%)	-1.13	0 100 100	120, 228, 319, 365	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	4517/4744 (95%)	-0.99	14 (0%)	94	90	103, 243, 373, 638	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	137	SER	8.4
2	I	137	SER	7.0
2	L	138	GLY	3.6
2	U	138	GLY	3.1
2	X	138	GLY	2.8

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.