



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

Jan 23, 2017 – 08:34 PM EST

PDB ID : 5H1R  
EMDB ID: : EMD-9571  
Title : C. elegans INX-6 gap junction channel  
Authors : Oshima, A.; Tani, K.; Fujiyoshi, Y.  
Deposited on : 2016-10-11  
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  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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-20028442

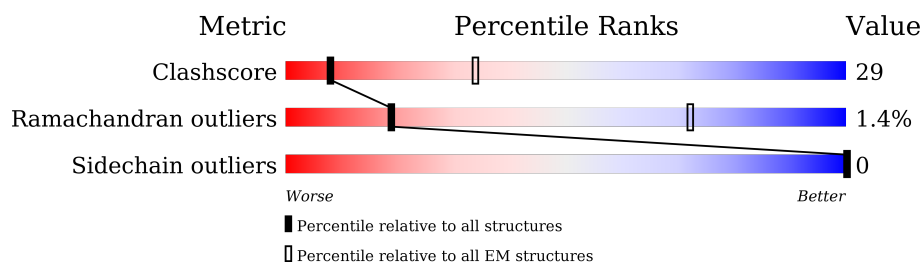
# 1 Overall quality at a glance

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.




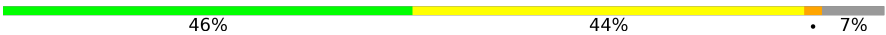



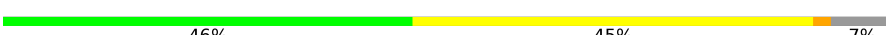
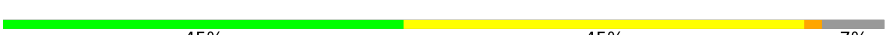
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	389	46% 44% • 7%
1	B	389	45% 45% • 7%
1	C	389	46% 44% • 7%
1	D	389	45% 45% • 7%
1	E	389	46% 44% • 7%
1	F	389	45% 45% • 7%
1	G	389	46% 45% • 7%
1	H	389	46% 45% • 7%
1	I	389	45% 45% • 7%

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Mol	Chain	Length	Quality of chain
1	J	389	 46% 44% • 7%
1	K	389	 46% 44% • 7%
1	L	389	 45% 45% • 7%
1	M	389	 46% 44% • 7%
1	N	389	 45% 45% • 7%
1	O	389	 46% 45% • 7%
1	P	389	 45% 45% • 7%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 47440 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.

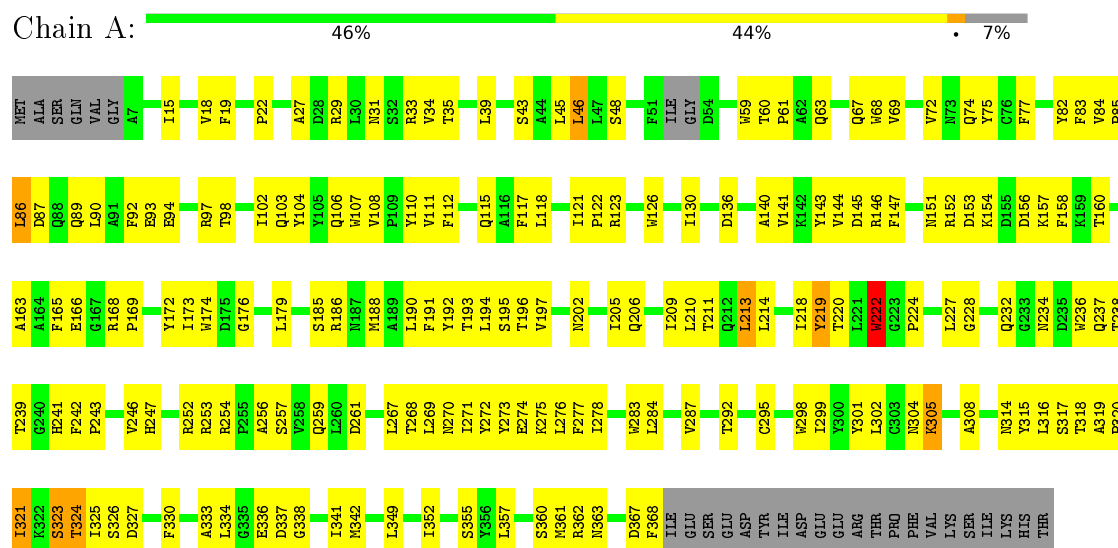
- Molecule 1 is a protein called Innexin-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	B	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	C	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	D	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	E	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	F	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	G	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	H	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	I	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	J	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	K	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	L	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	M	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	N	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	O	360	Total 2965	C 1950	N 487	O 516	S 12	0	0
1	P	360	Total 2965	C 1950	N 487	O 516	S 12	0	0

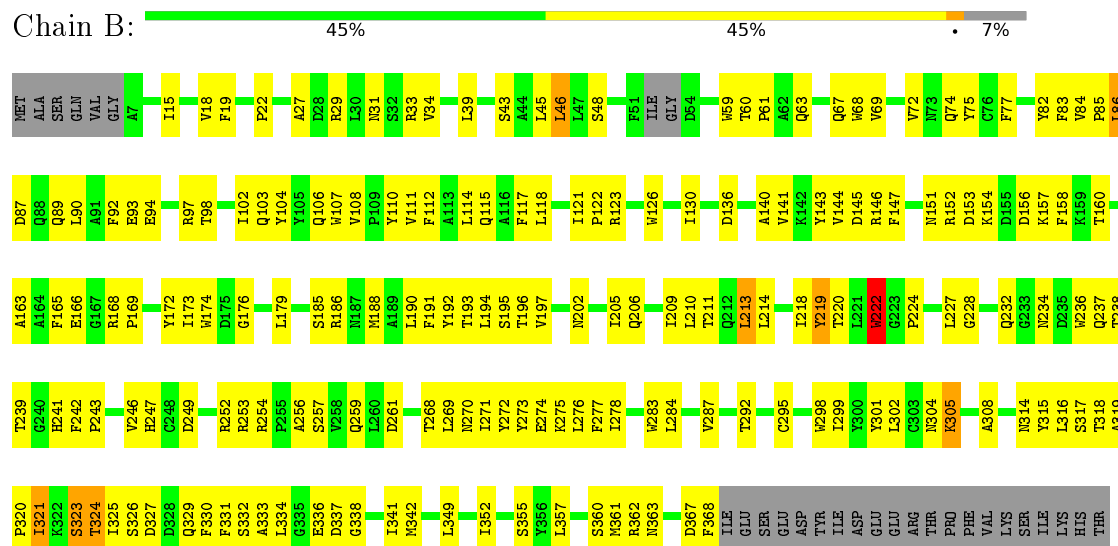
### 3 Residue-property plots

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: Innexin-6

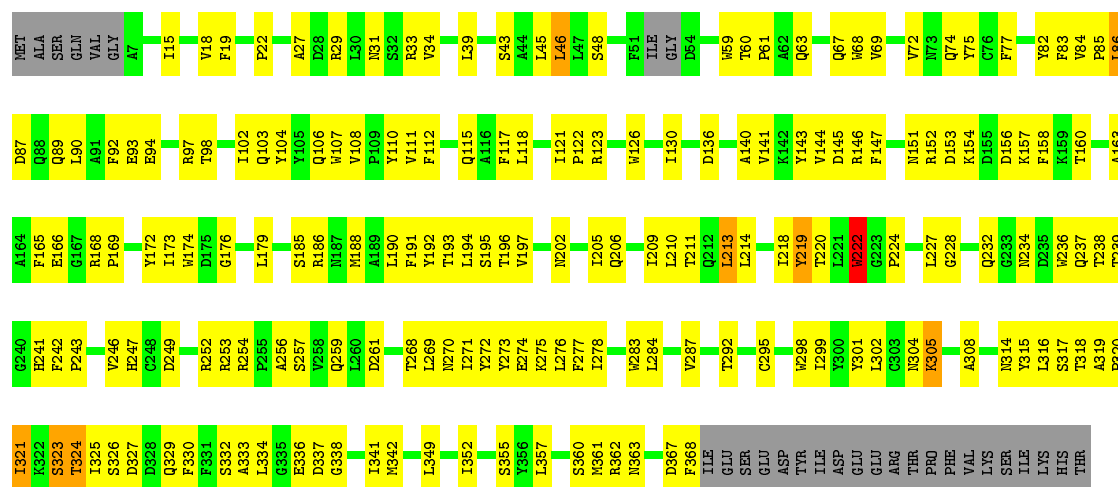


#### • Molecule 1: Innexin-6



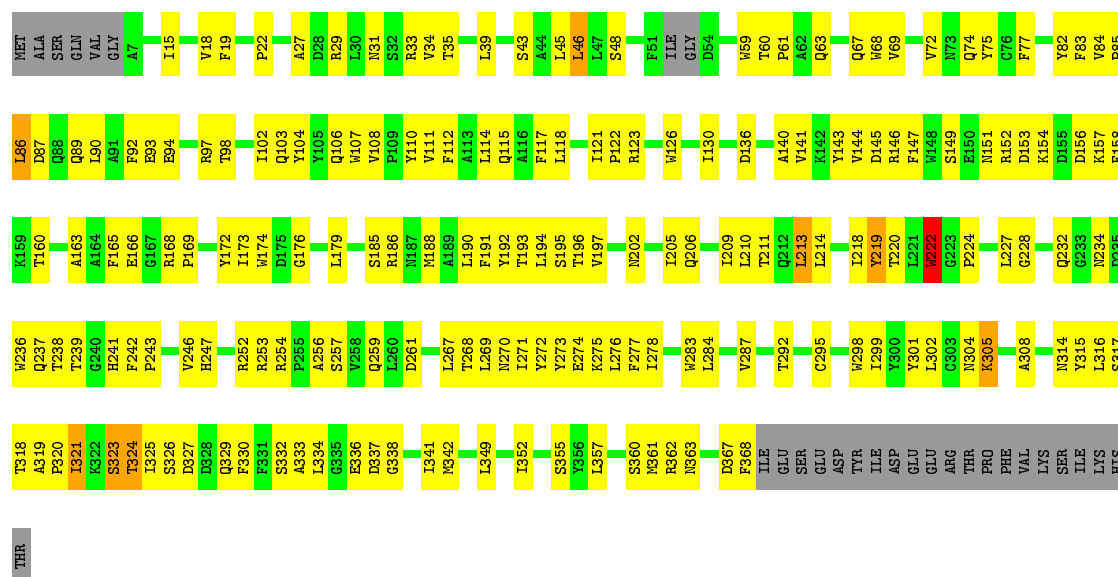
#### • Molecule 1: Innexin-6





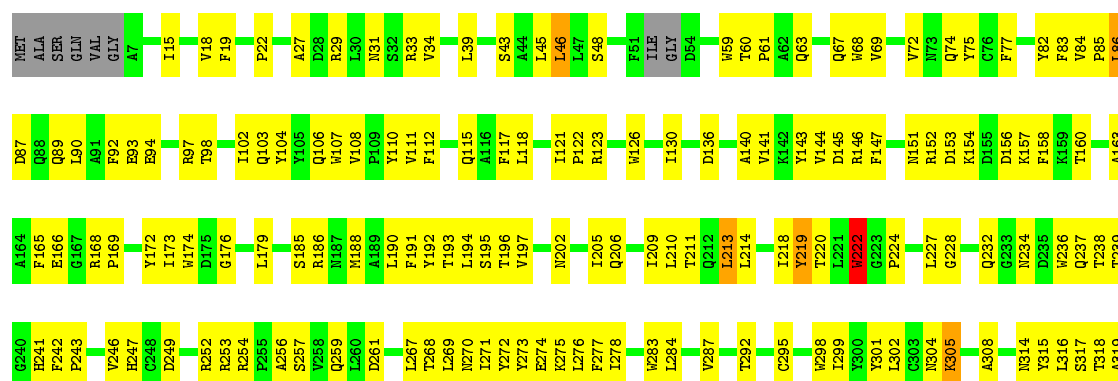
### • Molecule 1: Innexin-6

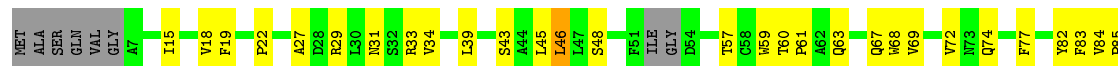
Chain D: 45% 45% 7%

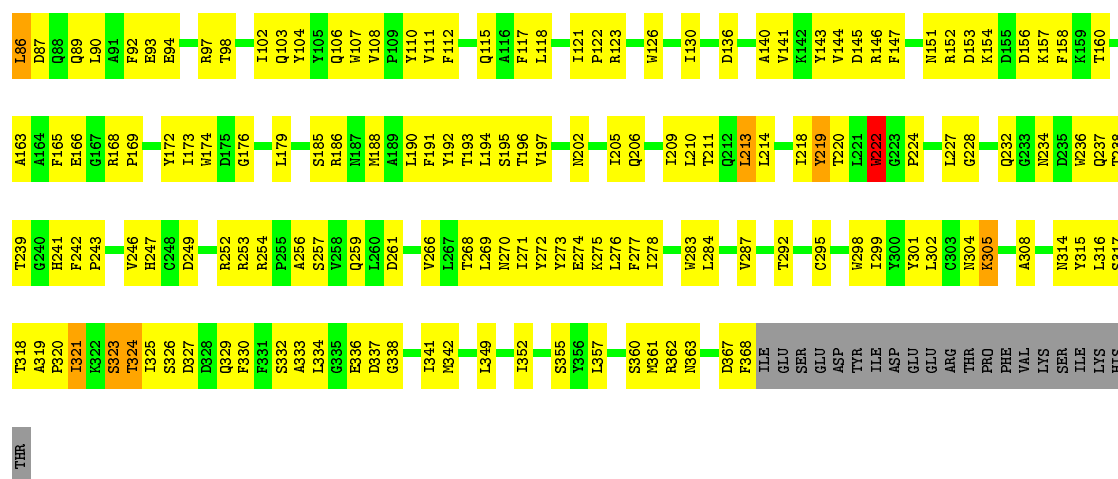


### • Molecule 1: Innexin-6

Chain E: 46% 44% 7%





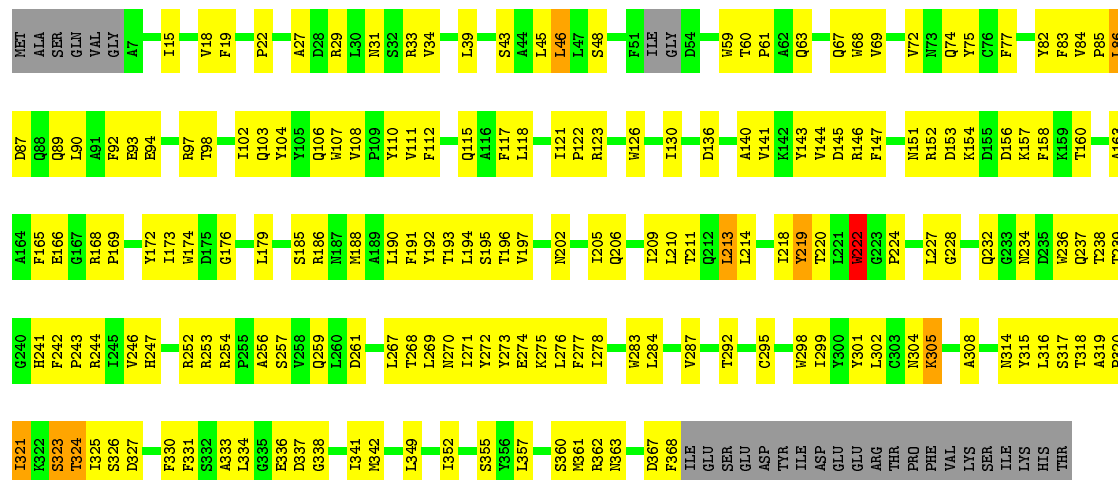






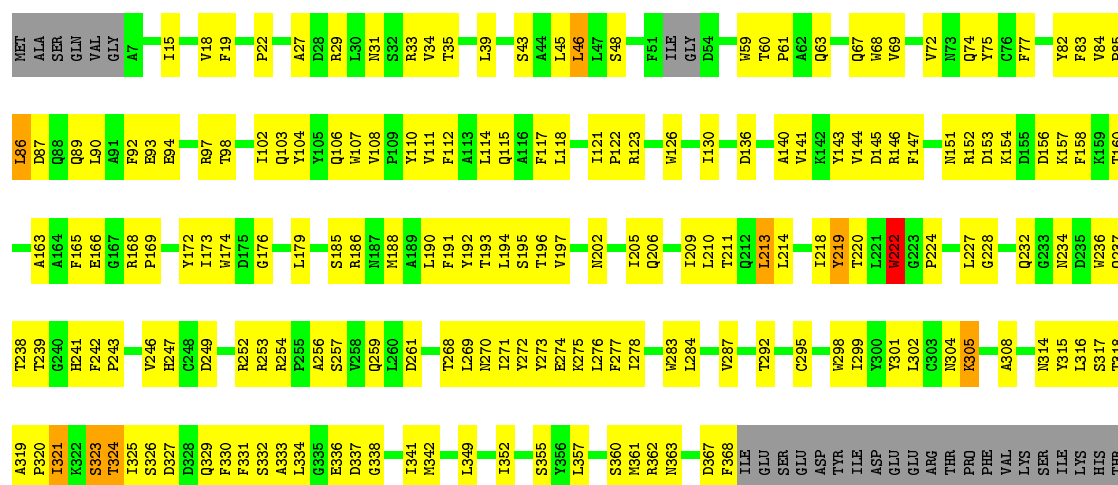
• Molecule 1: Innexin-6

Chain K: 46% 44% 7%



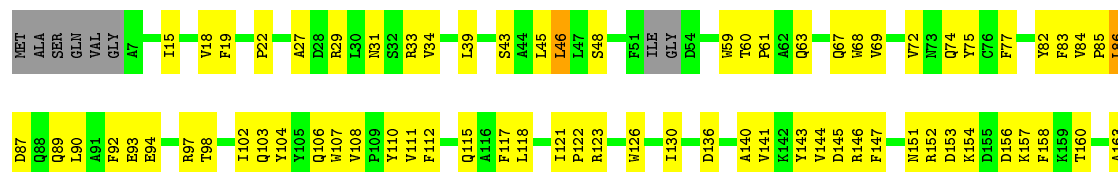
• Molecule 1: Innexin-6

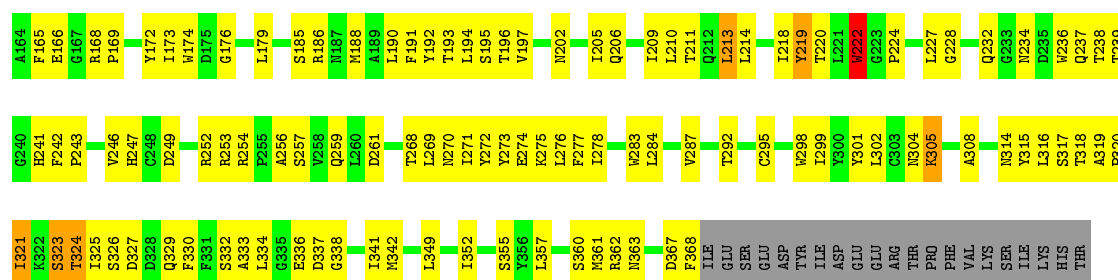
Chain L: 45% 45% 7%



• Molecule 1: Innexin-6

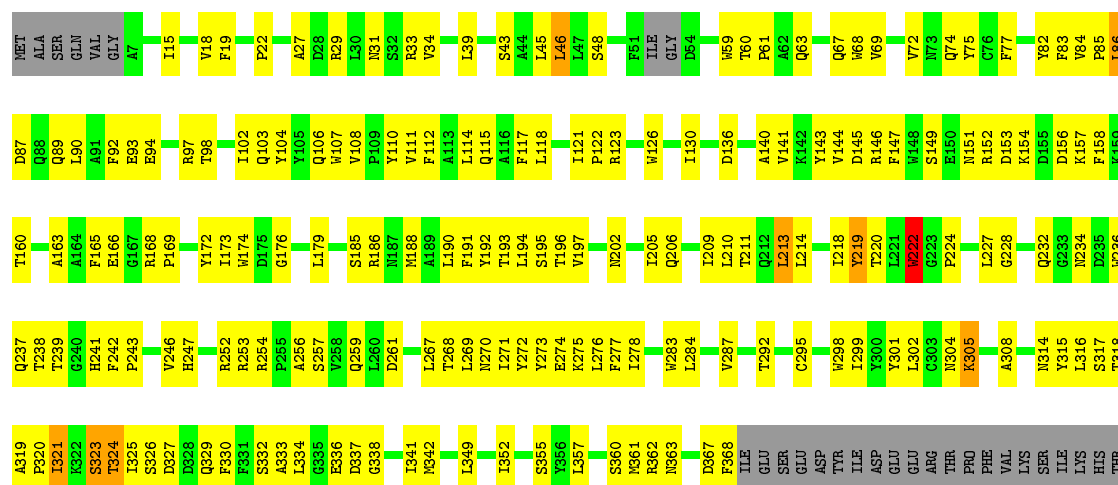
Chain M: 46% 44% 7%





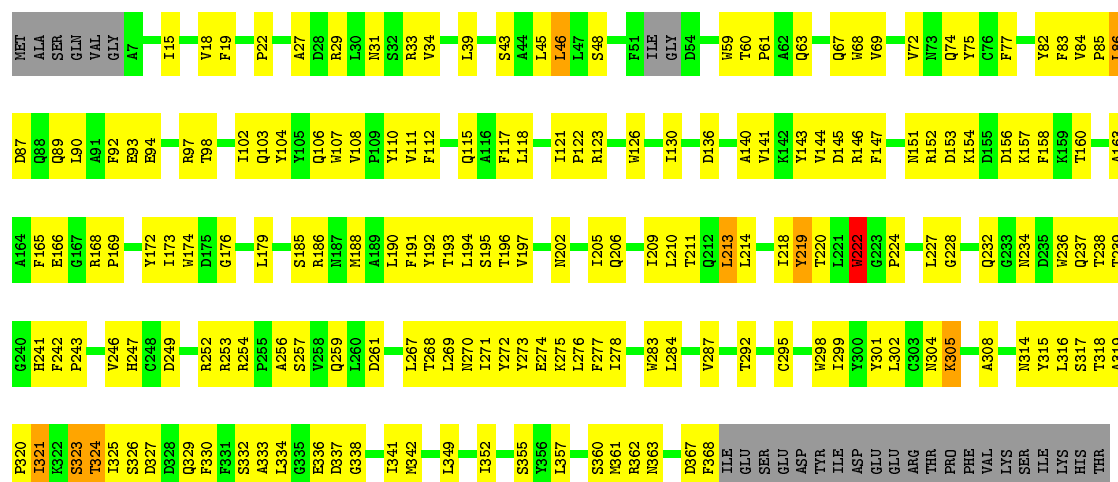
• Molecule 1: Innexin-6

Chain N: 45% 45% 7%



• Molecule 1: Innexin-6

Chain O: 46% 45% 7%



• Molecule 1: Innexin-6

Chain P: 45% 45% 7%

HIS	THR	S317	T238	A163	P85	MT
		T318	T239	A163	L86	SER
		A319	G240	A164	D87	GLN
		P320	H241	F165	Q88	VAL
		F242	F242	E166	L90	GLY
		K322	F243	G167	A91	A7
		S323		R168	F92	
		T324	V246	P169	E93	I15
		S326	G247		E94	
		S326	H248	Y172		V18
		D327	D249	I173	A97	F19
		D328		W174	T98	
		Q329	R252	G176		P22
		F330	R253		I102	A27
		F331	R254	L179	Q103	D28
		S332	T255		Y104	R29
		A333	A256	S185	T85	L30
		L334	S257	R186	Q107	N31
		G335	T258	M187	W108	S32
		G336	Q259	M188	P109	R33
		D337	L260	A189		V34
		G338	D261	L190	Y110	
				F191	V111	
		I341	V266	Y192	F112	L39
		M342	L267	T193		
		L349	T268	L194	Q115	S43
			L269	L195	A116	A44
		L352	N270	S195	F117	L45
			T271	T196	L118	L46
			T272	V197		L47
		S355	T273	N202	I121	S48
		Y356	E274	I205	P122	F51
		L357	R275	Q206	R123	I1E
			L276			GLY
		S360	F277		W126	D54
		M361	T278	I209		
		R362	W283	L210	I130	
		N363	L284	T211		T57
				Q212	D136	C58
		D367	V287	L213		M59
		F368		L214	A140	T60
					V141	P61
		GLU	T292	I218	R142	A62
		SER		Y219	V143	
		GLU	C295	T220	V144	Q63
		ASP		L221	D145	
		TYR	W298	K222	R146	Q67
		ASP	T299	G223	F147	M68
		I1E	T300	P224		V69
		GLU	Y301		N151	
		GLU	L302	G227	R152	V72
		ARG	G303	G228	D153	N73
		THR	N304		L154	Q74
		PRO	K305	Q232	D156	Y75
		PHE		G233	R157	C76
		VAL		N234	F158	F77
		LYS		D235	L159	
		SER	N314	W236		Y82
		I1E	V315	C237	T160	F83
			T316			V84

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	35608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 3000SFF	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 ⓘ

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	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	B	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	C	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	D	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	E	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	F	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	G	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	H	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	I	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	J	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	K	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	L	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	M	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	N	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	O	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
1	P	0.74	1/3051 (0.0%)	0.71	1/4155 (0.0%)
All	All	0.74	16/48816 (0.0%)	0.71	16/66480 (0.0%)

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	8
1	B	0	8
1	C	0	8
1	D	0	8
1	E	0	8
1	F	0	8
1	G	0	8
1	H	0	8
1	I	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	8
1	K	0	8
1	L	0	8
1	M	0	8
1	N	0	8
1	O	0	8
1	P	0	8
All	All	0	128

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	TRP	CB-CG	-5.08	1.41	1.50
1	D	222	TRP	CB-CG	-5.08	1.41	1.50
1	K	222	TRP	CB-CG	-5.06	1.41	1.50
1	F	222	TRP	CB-CG	-5.05	1.41	1.50
1	H	222	TRP	CB-CG	-5.05	1.41	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	46	LEU	CA-CB-CG	-6.89	99.45	115.30
1	N	46	LEU	CA-CB-CG	-6.89	99.45	115.30
1	G	46	LEU	CA-CB-CG	-6.89	99.46	115.30
1	A	46	LEU	CA-CB-CG	-6.88	99.47	115.30
1	O	46	LEU	CA-CB-CG	-6.88	99.47	115.30

There are no chirality outliers.

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	SER	Peptide
1	A	213	LEU	Peptide
1	A	222	TRP	Peptide
1	A	61	PRO	Peptide
1	A	86	LEU	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	2965	0	2928	188	0
1	B	2965	0	2928	186	0
1	C	2965	0	2928	190	0
1	D	2965	0	2928	193	0
1	E	2965	0	2928	191	0
1	F	2965	0	2928	193	0
1	G	2965	0	2928	191	0
1	H	2965	0	2928	185	0
1	I	2965	0	2928	192	0
1	J	2965	0	2928	185	0
1	K	2965	0	2928	189	0
1	L	2965	0	2928	189	0
1	M	2965	0	2928	191	0
1	N	2965	0	2928	190	0
1	O	2965	0	2928	190	0
1	P	2965	0	2928	193	0
All	All	47440	0	46848	2728	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 29.

The worst 5 of 2728 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:243:PRO:O	1:B:270:ASN:ND2	1.97	0.98
1:G:243:PRO:O	1:G:270:ASN:ND2	1.97	0.98
1:J:243:PRO:O	1:J:270:ASN:ND2	1.97	0.98
1:L:243:PRO:O	1:L:270:ASN:ND2	1.97	0.98
1:I:243:PRO:O	1:I:270:ASN:ND2	1.97	0.98

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	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	B	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	C	356/389 (92%)	304 (85%)	47 (13%)	5 (1%)	14	59
1	D	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	E	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	F	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	G	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	H	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	I	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	J	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	K	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	L	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	M	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	N	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	O	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
1	P	356/389 (92%)	305 (86%)	46 (13%)	5 (1%)	14	59
All	All	5696/6224 (92%)	4879 (86%)	737 (13%)	80 (1%)	19	59

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	ILE
1	B	321	ILE
1	C	321	ILE
1	D	321	ILE
1	E	321	ILE

### 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	320/346 (92%)	320 (100%)	0	100	100
1	B	320/346 (92%)	320 (100%)	0	100	100
1	C	320/346 (92%)	320 (100%)	0	100	100
1	D	320/346 (92%)	320 (100%)	0	100	100
1	E	320/346 (92%)	320 (100%)	0	100	100
1	F	320/346 (92%)	320 (100%)	0	100	100
1	G	320/346 (92%)	320 (100%)	0	100	100
1	H	320/346 (92%)	320 (100%)	0	100	100
1	I	320/346 (92%)	320 (100%)	0	100	100
1	J	320/346 (92%)	320 (100%)	0	100	100
1	K	320/346 (92%)	320 (100%)	0	100	100
1	L	320/346 (92%)	320 (100%)	0	100	100
1	M	320/346 (92%)	320 (100%)	0	100	100
1	N	320/346 (92%)	320 (100%)	0	100	100
1	O	320/346 (92%)	320 (100%)	0	100	100
1	P	320/346 (92%)	320 (100%)	0	100	100
All	All	5120/5536 (92%)	5120 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	241	HIS
1	I	241	HIS
1	O	241	HIS
1	G	241	HIS
1	H	241	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 [i](#)

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.