



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 6, 2017 – 04:51 PM EST

PDB ID : 5H1Q
EMDB ID: : EMD-9570
Title : C. elegans INX-6 gap junction hemichannel
Authors : Oshima, A.; Tani, K.; Fujiyoshi, Y.
Deposited on : 2016-10-11
Resolution : 3.30 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

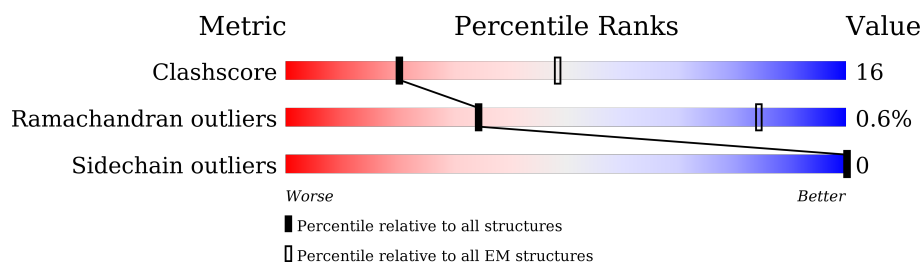
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 ≥ 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	
1	B	389	
1	C	389	
1	D	389	
1	E	389	
1	F	389	
1	G	389	
1	H	389	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23784 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.

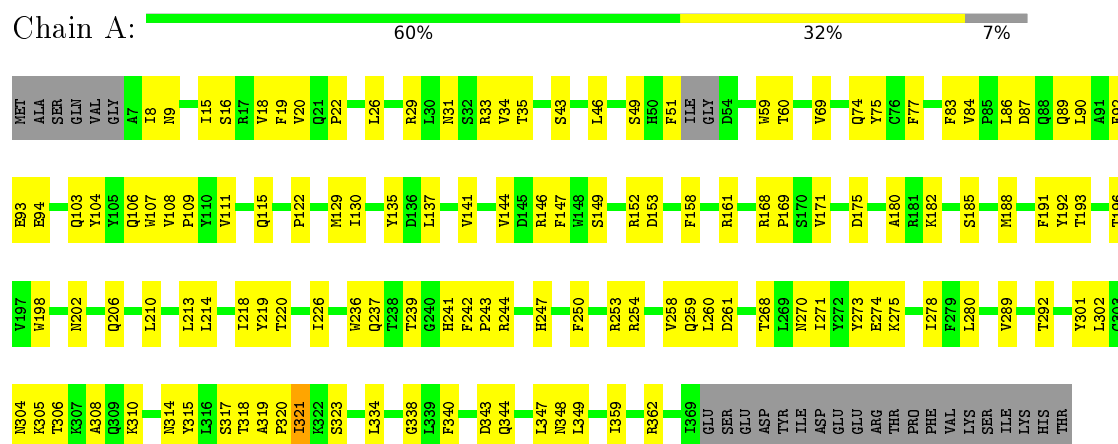
- Molecule 1 is a protein called Innexin-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total 2973	C 1956	N 488	O 517	S 12	0	0
1	B	361	Total 2973	C 1956	N 488	O 517	S 12	0	0
1	C	361	Total 2973	C 1956	N 488	O 517	S 12	0	0
1	D	361	Total 2973	C 1956	N 488	O 517	S 12	0	0
1	E	361	Total 2973	C 1956	N 488	O 517	S 12	0	0
1	F	361	Total 2973	C 1956	N 488	O 517	S 12	0	0
1	G	361	Total 2973	C 1956	N 488	O 517	S 12	0	0
1	H	361	Total 2973	C 1956	N 488	O 517	S 12	0	0

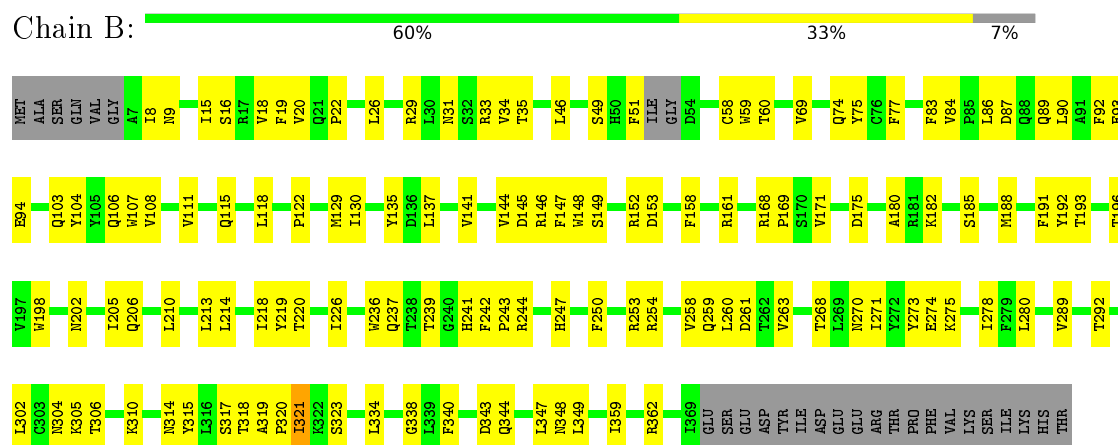
3 Residue-property plots

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.

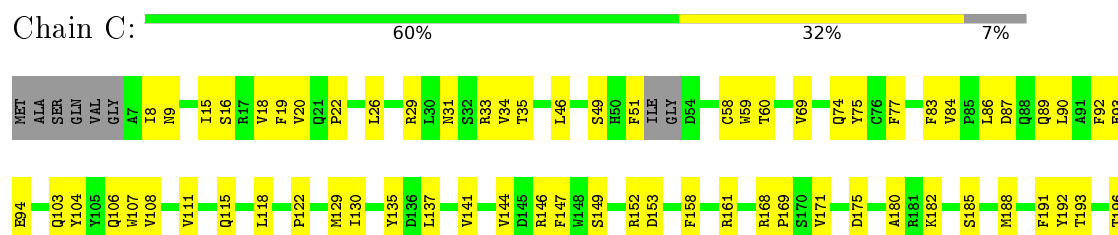
• Molecule 1: Innexin-6



• Molecule 1: Innexin-6



• Molecule 1: Innexin-6



V197	W198	N202	Q206	L210	L213	L214	L218	Y219	T220	T226	W236	Q237	T238	T239	G240	H241	F242	P243	R244	H247	F250	R253	R254	V258	Q259	L260	D261	T262	V263	T268	L269	N270	I271	V272	Y273	E274	K275	L278	F279	L280	V289	T292	L302		
C303	N304	K305	T306	K310	N314	Y315	S317	T318	A319	P320	K321	K322	S323	L334	G338	L339	F340	D343	Q344	L347	N348	L349	I359	R362	I369	GLU	Q259	SER	ASP	TYR	ILE	ASP	GLU	GLU	ARG	THR	PRO	PHE	VAL	LYS	SER	ILE	LYS	HIS	THR

- Molecule 1: Innexin-6

Chain D:  59% 33% 7%

NET	ALA	SER	GLN	VAL	GLY	A7	I8	N9	I15	S16	R17	V18	F19	V20	Q21	P22	L26	R29	L30	N31	D32	R33	V34	T35	S43	L46	S49	F50	F51	ILE	GLY	D54	W59	T60	V69	Q74	Y75	C76	F77	F83	W84	P85	L86	S87	Q88	Q89	A91	F92
E93	E94	Q103	Y104	Y105	Q106	W107	P109	Y110	V111	Q115	L118	L119	P122	M129	I130	Y135	L136	D137	V141	V144	D145	R146	F147	W148	S149	R152	D153	F158	R161	R168	P169	S170	V171	D175	A180	R181	K182	S185	M188	F191	Y192	T193						

L302	C303	N304	K305	T306	K307	A308	Q309	K310		N314	Y315	L316	S317	T318	A319	P320	L321	K322	S323		L334	G338	I341	Q344	L347	N348	L349	I359	R362		I369	GLU	SER	GLU	GLU	ASP	TYR	ILE	ASP	GLU	GLU	ARG	THR	PRO	PHE	VAL	LYS	SER	ILE	LYS	HIS	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																

- Molecule 1: Innexin-6

Chain E:  60% 32% 7%

Met	ALA	SER	GLN	VAL	GLY	A7	I8	N9	I15	S16	R17	V18	F19	V20	Q21	P22	L26	R29	L30	N31	D136	L137	V141	V144	D145	R146	F147	W148	S149	H50	F51	ILE	GLY	D54	W59	T60	V69	Q74	Y75	C76	F77	F83	W84	P85	L86	D87	Q88	Q89	A91	F191	Y192	T193	Y196	E93	E94
Q103	Y104	Y105	Q106	W107	V108	V111	Q115	L118	P122	M129	I130	Y135	D136	L137	V141	V144	D145	R146	F147	W148	S149	R152	D153	F158	R161	R168	P169	S170	V171	D175	A180	R181	K182	S185	M188	F191	Y192	T193	Y196	E93	E94														

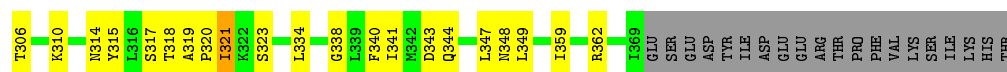
K305	T306	K307	A308	Q309	K310		N314	Y315	L316	S317	T318	A319	P320	K321	K322	S323		L334	G338	L339	F340	L341	K342	D343	Q344		L347	N348	L349		I359		R362		I369	GLU	Q259	SER	ASP	TYR	ILE	ASP	GLU	GLU	ARG	THR	PRO	PHE	VAL	LYS	SER	ILE	LYS	HIS	THR
W198	N202	Q206		L210	L213	L214		L218	L219	T220		T226		W236	Q237	T238	T239	G240	H241	F242	P243	R244		H247		F250		R253	R254		V258	Q259	L260	D261	T268	L269	N270	I271	V272	E273	E274	K275		L278	F279	L280		V289		T292		Y301	L302	N303	N304

- Molecule 1: Innexin-6

Chain F:  61% 32% 7%

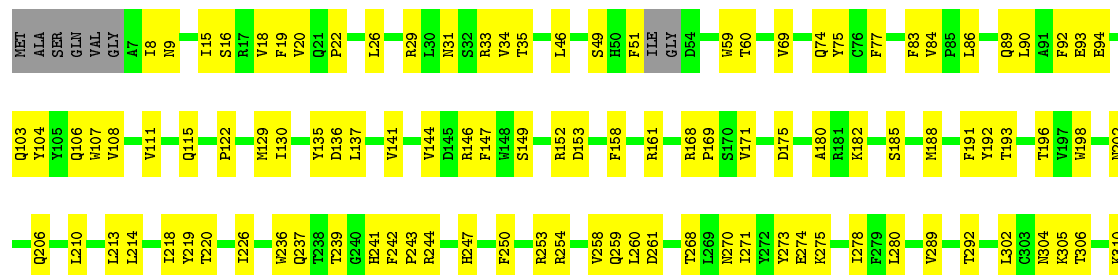
Met	ALA	SER	GLN	VAL	GLY	A7	I8	N9	I15	S16	R17	V18	F19	V20	Q21	P22	L26	R29	L30	N31	D136	L137	V141	V144	D145	R146	F147	W148	S149	R152	D153	F158	R161	R168	P169	S170	V171	D175	A180	R181	K182	S185	M188	F191	Y192	T193	T196
	Q103	Y104	Y105	Q106	W107	V108	V111	Q115	L118	P122	M129	I130	Y135	D136	L137	V141	V144	D145	R146	F147	W148	S149	R152	D153	F158	R161	R168	P169	S170	V171	D175	A180	R181	K182	S185	M188	F191	Y192	T193	T196							

W198	N202	Q206	L210	L213	L214	L218	Y219	T220	T226	W236	Q237	T238	T239	G240	H241	F242	P243	R244	H247	F250	R253	R254	V258	Q259	L260	D261	T268	L269	N270	I271	V272	Y273	E274	K275	L278	F279	L280	V289	T292	L302	G303	N304	K305
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



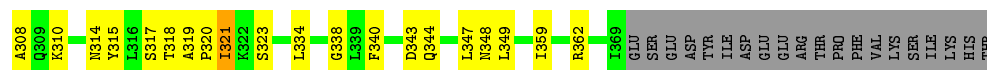
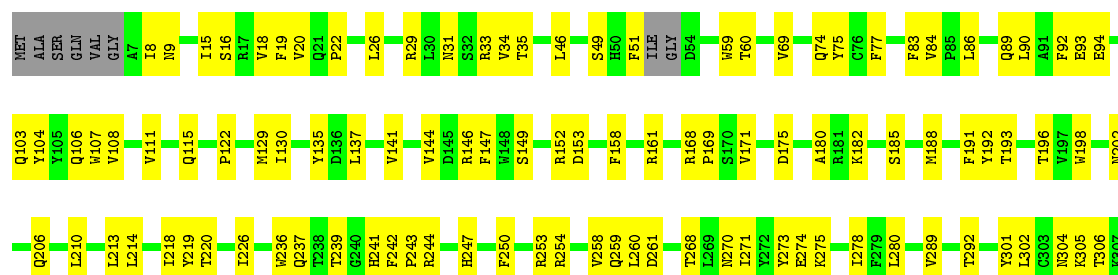
• Molecule 1: Innexin-6

Chain G: 61% 32% 7%



• Molecule 1: Innexin-6

Chain H: 61% 32% 7%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	74398	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	0.47	0/3059	0.58	0/4166
1	B	0.47	0/3059	0.58	0/4166
1	C	0.47	0/3059	0.58	0/4166
1	D	0.47	0/3059	0.58	0/4166
1	E	0.47	0/3059	0.58	0/4166
1	F	0.47	0/3059	0.58	0/4166
1	G	0.47	0/3059	0.58	0/4166
1	H	0.47	0/3059	0.58	0/4166
All	All	0.47	0/24472	0.58	0/33328

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	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	SER	Peptide
1	A	86	LEU	Peptide
1	B	185	SER	Peptide
1	B	86	LEU	Peptide
1	C	86	LEU	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	2973	0	2939	105	0
1	B	2973	0	2939	108	0
1	C	2973	0	2939	105	0
1	D	2973	0	2939	108	0
1	E	2973	0	2939	105	0
1	F	2973	0	2939	104	0
1	G	2973	0	2939	105	0
1	H	2973	0	2939	103	0
All	All	23784	0	23512	755	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 16.

The worst 5 of 755 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:C:168:ARG:HH21	1:D:153:ASP:HA	1.30	0.96
1:B:243:PRO:O	1:B:270:ASN:ND2	2.00	0.95
1:C:243:PRO:O	1:C:270:ASN:ND2	2.00	0.95
1:D:168:ARG:HH21	1:E:153:ASP:HA	1.31	0.94
1:A:243:PRO:O	1:A:270:ASN:ND2	2.00	0.94

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	357/389 (92%)	310 (87%)	45 (13%)	2 (1%)	30	68
1	B	357/389 (92%)	310 (87%)	45 (13%)	2 (1%)	30	68
1	C	357/389 (92%)	310 (87%)	45 (13%)	2 (1%)	30	68
1	D	357/389 (92%)	310 (87%)	45 (13%)	2 (1%)	30	68
1	E	357/389 (92%)	310 (87%)	45 (13%)	2 (1%)	30	68
1	F	357/389 (92%)	310 (87%)	45 (13%)	2 (1%)	30	68
1	G	357/389 (92%)	310 (87%)	45 (13%)	2 (1%)	30	68
1	H	357/389 (92%)	310 (87%)	45 (13%)	2 (1%)	30	68
All	All	2856/3112 (92%)	2480 (87%)	360 (13%)	16 (1%)	34	68

5 of 16 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	321/346 (93%)	321 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	321/346 (93%)	321 (100%)	0	100	100
1	C	321/346 (93%)	321 (100%)	0	100	100
1	D	321/346 (93%)	321 (100%)	0	100	100
1	E	321/346 (93%)	321 (100%)	0	100	100
1	F	321/346 (93%)	321 (100%)	0	100	100
1	G	321/346 (93%)	321 (100%)	0	100	100
1	H	321/346 (93%)	321 (100%)	0	100	100
All	All	2568/2768 (93%)	2568 (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 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	115	GLN
1	H	115	GLN
1	F	115	GLN
1	C	115	GLN
1	E	115	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.