Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:55 PM GMT

PDB ID	:	1HVG
Title	:	STRUCTURAL AND ELECTROPHYSIOLOGICAL ANALYSIS OF ANNEXIN V MUTANTS. MUTAGENESIS OF HUMAN ANNEXIN V, AN IN VITRO VOLTAGE-GATED CALCIUM CHANNEL, PROVIDES INFORMATION ABOUT THE STRUCTURAL FEATURES OF THE ION PATHWAY, THE VOLTAGE SENSOR AND THE ION SELECTIVITY FILTER
Authors	:	Burger, A.; Huber, R.
Deposited on	:	1994-06-29
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

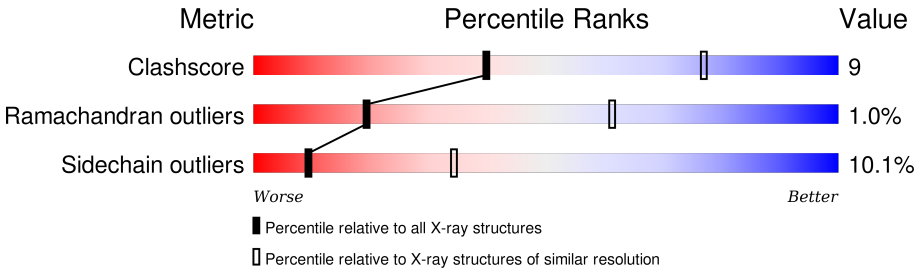
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 on the lower 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	319	68% 25% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2474 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 ANNEXIN V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2474	1562	417	487	8	82	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLN	GLU	CONFLICT	UNP P08758

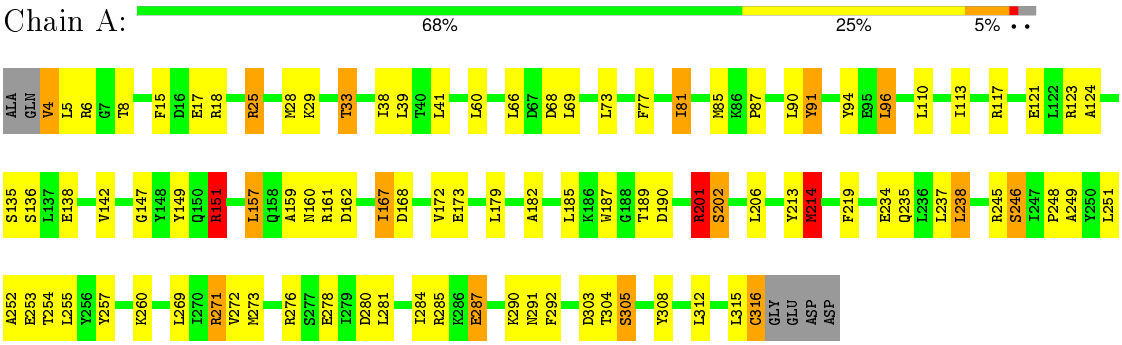
3 Residue-property plots (i)

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 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.

Note EDS was not executed.

- Molecule 1: ANNEXIN V

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	156.90Å 156.90Å 36.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2474	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

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	0.77	0/2508	1.49	28/3376 (0.8%)

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

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	GLU	CA-CB-CG	9.13	133.49	113.40
1	A	187	TRP	CD1-CG-CD2	8.03	112.73	106.30
1	A	201	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	A	245	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	316	CYS	CA-CB-SG	7.28	127.10	114.00
1	A	161	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	187	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	201	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	235	GLN	CA-CB-CG	6.86	128.49	113.40
1	A	39	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	214	MET	CA-CB-CG	6.60	124.52	113.30
1	A	91	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	A	151	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	161	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	271	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	25	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	308	TYR	CB-CG-CD2	-5.92	117.44	121.00
1	A	123	ARG	NE-CZ-NH1	5.84	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	149	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	A	202	SER	CA-CB-OG	5.49	126.01	111.20
1	A	213	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	A	117	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	18	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	257	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	85	MET	CG-SD-CE	-5.13	91.99	100.20
1	A	168	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	41	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	A	276	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	TYR	Sidechain

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	2474	0	2491	42	0
All	All	2474	0	2491	42	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 9.

All (42) 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:A:66:LEU:HA	1:A:69:LEU:HD12	1.71	0.73
1:A:96:LEU:HD21	1:A:113:ILE:HG21	1.77	0.66
1:A:285:ARG:HD2	1:A:316:CYS:HB2	1.78	0.65
1:A:4:VAL:HA	1:A:280:ASP:HB3	1.78	0.65
1:A:138:GLU:O	1:A:142:VAL:HG23	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HD11	1:A:172:VAL:HG21	1.81	0.61
1:A:255:LEU:HD13	1:A:272:VAL:HB	1.83	0.61
1:A:147:GLY:O	1:A:151:ARG:HD3	2.04	0.58
1:A:201:ARG:HB3	1:A:206:LEU:HG	1.86	0.57
1:A:73:LEU:HD22	1:A:81:ILE:HG21	1.88	0.56
1:A:246:SER:HB3	1:A:249:ALA:HB3	1.88	0.55
1:A:8:THR:HG21	1:A:316:CYS:HA	1.89	0.53
1:A:87:PRO:HG2	1:A:90:LEU:HD12	1.91	0.53
1:A:304:THR:HG22	1:A:305:SER:H	1.78	0.49
1:A:304:THR:HG21	1:A:312:LEU:HD12	1.95	0.48
1:A:4:VAL:CA	1:A:280:ASP:HB3	2.44	0.48
1:A:121:GLU:O	1:A:124:ALA:HB3	2.13	0.48
1:A:162:ASP:O	1:A:202:SER:HB3	2.13	0.48
1:A:96:LEU:HD12	1:A:110:LEU:HD12	1.96	0.47
1:A:312:LEU:O	1:A:315:LEU:HB2	2.14	0.47
1:A:6:ARG:O	1:A:280:ASP:HA	2.14	0.47
1:A:214:MET:HA	1:A:219:PHE:O	2.15	0.47
1:A:28:MET:SD	1:A:68:ASP:HB3	2.56	0.46
1:A:269:LEU:O	1:A:273:MET:HG2	2.15	0.46
1:A:290:LYS:HE2	1:A:291:ASN:OD1	2.16	0.46
1:A:69:LEU:O	1:A:73:LEU:HB2	2.16	0.46
1:A:25:ARG:O	1:A:29:LYS:HB2	2.15	0.46
1:A:28:MET:HA	1:A:33:THR:HG23	1.97	0.45
1:A:91:TYR:OH	1:A:271:ARG:HA	2.16	0.45
1:A:312:LEU:HA	1:A:315:LEU:HD12	1.98	0.45
1:A:17:GLU:H	1:A:17:GLU:CD	2.20	0.45
1:A:252:ALA:HB2	1:A:284:ILE:HG23	1.99	0.43
1:A:248:PRO:HA	1:A:284:ILE:HG12	2.00	0.43
1:A:77:PHE:O	1:A:81:ILE:HB	2.20	0.42
1:A:25:ARG:HA	1:A:25:ARG:HD2	1.83	0.42
1:A:234:GLU:O	1:A:238:LEU:HB2	2.19	0.42
1:A:253:GLU:HG3	1:A:292:PHE:CZ	2.54	0.41
1:A:157:LEU:HA	1:A:157:LEU:HD12	1.90	0.41
1:A:96:LEU:CD2	1:A:113:ILE:HG21	2.48	0.41
1:A:249:ALA:HA	1:A:287:GLU:HG2	2.03	0.40
1:A:33:THR:HG22	1:A:38:ILE:HD11	2.03	0.40
1:A:182:ALA:HB1	1:A:190:ASP:HB3	2.02	0.40

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 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	311/319 (98%)	289 (93%)	19 (6%)	3 (1%)	19 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	159	ALA
1	A	260	LYS

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 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	267/271 (98%)	240 (90%)	27 (10%)	9 34

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	15	PHE
1	A	33	THR
1	A	60	LEU
1	A	81	ILE
1	A	96	LEU
1	A	135	SER
1	A	136	SER

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Mol	Chain	Res	Type
1	A	151	ARG
1	A	157	LEU
1	A	160	ASN
1	A	167	ILE
1	A	179	LEU
1	A	185	LEU
1	A	189	THR
1	A	201	ARG
1	A	214	MET
1	A	237	LEU
1	A	238	LEU
1	A	246	SER
1	A	251	LEU
1	A	254	THR
1	A	278	GLU
1	A	281	LEU
1	A	287	GLU
1	A	303	ASP
1	A	305	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	232	ASN
1	A	235	GLN
1	A	283	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

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.