



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 04:47 pm BST

PDB ID : 1ANX
Title : THE CRYSTAL STRUCTURE OF A NEW HIGH-CALCIUM FORM OF ANNEXIN V
Authors : Sopkova, J.; Renouard, M.; Lewit-Bentley, A.
Deposited on : 1993-10-26
Resolution : 1.90 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

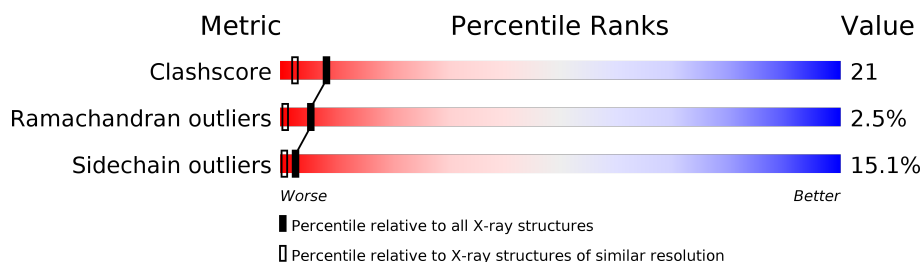
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	319	<div> <div>49%</div> <div>34%</div> <div>13%</div> <div>• •</div> </div>
1	B	319	<div> <div>53%</div> <div>31%</div> <div>11%</div> <div>• •</div> </div>
1	C	319	<div> <div>55%</div> <div>26%</div> <div>13%</div> <div>6%</div> <div>•</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7990 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
1	A	316	Total	C	N	O	S	0	5	0
			2519	1587	428	496	8			
1	B	316	Total	C	N	O	S	0	4	0
			2513	1584	425	496	8			
1	C	316	Total	C	N	O	S	0	4	0
			2513	1584	425	496	8			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Ca	0	0
			4	4		
2	A	4	Total	Ca	0	0
			4	4		
2	C	4	Total	Ca	0	0
			4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

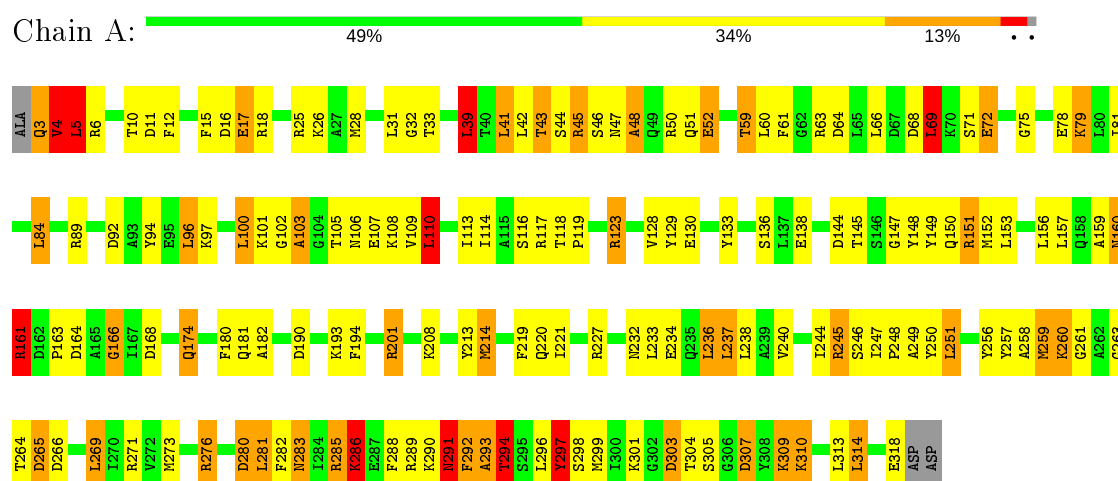
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	133	Total	O	0	0
			133	133		
4	C	134	Total	O	0	0
			134	134		

3 Residue-property plots

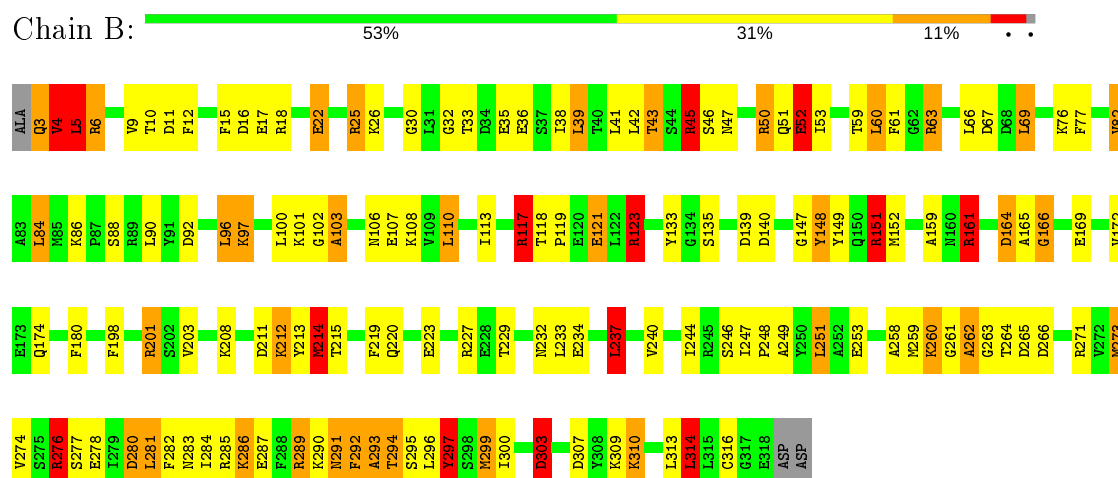
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: ANNEXIN V

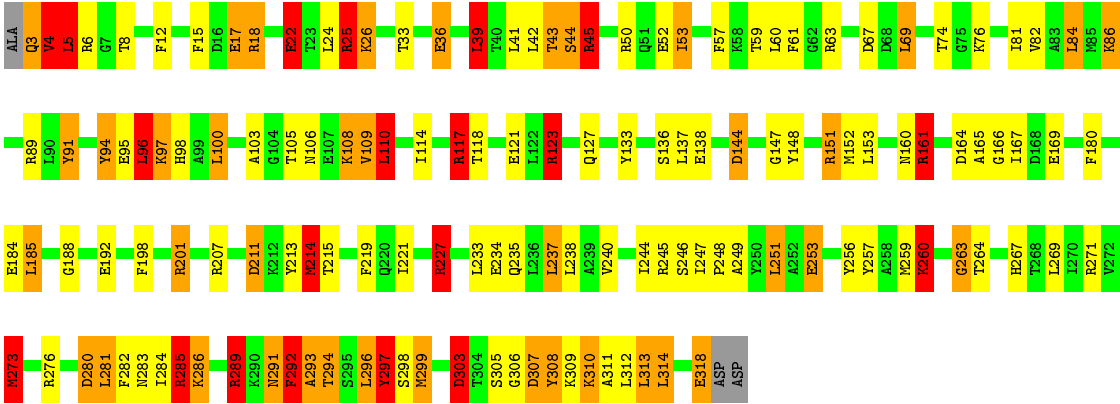


• Molecule 1: ANNEXIN V



• Molecule 1: ANNEXIN V





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.20 Å 91.30 Å 36.20 Å 82.40° 82.40° 118.20°	Depositor
Resolution (Å)	12.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7990	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4

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	0.92	1/2579 (0.0%)	2.19	98/3468 (2.8%)
1	B	0.92	1/2568 (0.0%)	2.07	89/3454 (2.6%)
1	C	0.94	1/2568 (0.0%)	2.10	112/3454 (3.2%)
All	All	0.93	3/7715 (0.0%)	2.12	299/10376 (2.9%)

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	3
1	B	0	7
1	C	0	9
All	All	0	19

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	SER	C-N	-6.32	1.19	1.34
1	A	234	GLU	CD-OE1	-5.39	1.19	1.25
1	C	263	GLY	C-N	-5.09	1.22	1.34

The worst 5 of 299 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151[A]	ARG	CD-NE-CZ	27.49	162.09	123.60
1	A	151[B]	ARG	CD-NE-CZ	27.49	162.09	123.60
1	B	45	ARG	NE-CZ-NH2	20.95	130.77	120.30
1	B	25	ARG	NE-CZ-NH2	19.00	129.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH2	16.55	128.57	120.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	A	45	ARG	Sidechain
1	A	63	ARG	Sidechain
1	B	25	ARG	Sidechain
1	B	45	ARG	Sidechain

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	2519	0	2540	112	0
1	B	2513	0	2530	105	0
1	C	2513	0	2530	104	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	151	0	0	7	0
4	B	133	0	0	6	0
4	C	134	0	0	9	0
All	All	7990	0	7600	321	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 21.

The worst 5 of 321 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:3:GLN:HG2	1:A:247:ILE:HD13	1.28	1.07
1:B:3:GLN:HG2	1:B:247:ILE:HD13	1.33	1.07
1:B:123:ARG:NH2	1:B:159:ALA:O	1.94	0.99
1:B:3:GLN:N	4:B:378:HOH:O	1.99	0.96
1:A:41:LEU:HD13	1:A:45:ARG:HH11	1.32	0.94

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	319/319 (100%)	293 (92%)	18 (6%)	8 (2%)	5	1
1	B	318/319 (100%)	296 (93%)	13 (4%)	9 (3%)	5	1
1	C	318/319 (100%)	294 (92%)	17 (5%)	7 (2%)	6	1
All	All	955/957 (100%)	883 (92%)	48 (5%)	24 (2%)	5	1

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	103	ALA
1	A	292	PHE
1	A	294	THR
1	B	5	LEU

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	274/271 (101%)	233 (85%)	41 (15%)	3	1
1	B	273/271 (101%)	236 (86%)	37 (14%)	3	1
1	C	273/271 (101%)	226 (83%)	47 (17%)	2	0
All	All	820/813 (101%)	695 (85%)	125 (15%)	3	1

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	LYS
1	B	286	LYS
1	C	286	LYS
1	B	151[A]	ARG
1	B	212	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	150	GLN
1	B	220	GLN
1	C	232	ASN
1	B	98	HIS
1	C	150	GLN

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

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	322	2	4,4,4	1.50	1 (25%)	6,6,6	0.56	0
3	SO4	A	322	2	4,4,4	1.48	1 (25%)	6,6,6	0.94	0
3	SO4	C	322	2	4,4,4	1.63	1 (25%)	6,6,6	0.99	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	322	SO4	O1-S	2.82	1.61	1.46
3	B	322	SO4	O1-S	2.64	1.60	1.46
3	A	322	SO4	O1-S	2.44	1.59	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	88:SER	C	89:ARG	N	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.