



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:40 PM UTC

PDB ID : 2RAN / pdb_00002ran
Title : RAT ANNEXIN V CRYSTAL STRUCTURE: CA2+-INDUCED CONFORMATIONAL CHANGES
Authors : Concha, N.O.; Head, J.F.; Kaetzel, M.A.; Dedman, J.R.; Seaton, B.A.
Deposited on : 1994-09-01
Resolution : 1.89 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

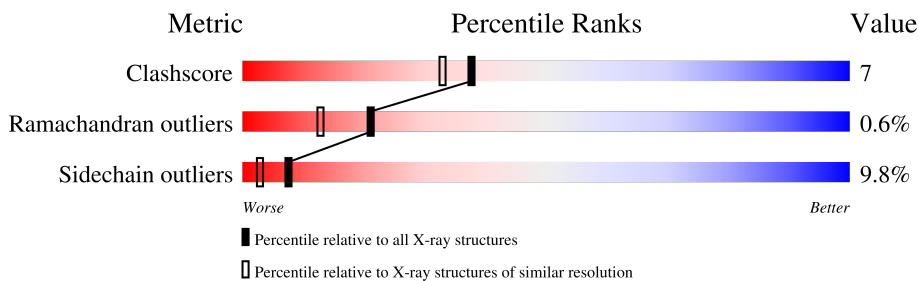
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	316	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	327	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3185 atoms, of which 573 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.

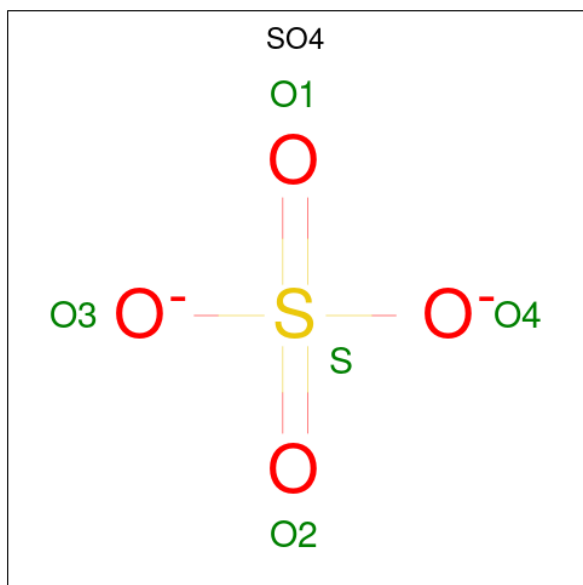
- Molecule 1 is a protein called ANNEXIN V.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	H	N	O	S	0	0	0
			3060	1564	573	423	492	8			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Ca	0	0
			7	7		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

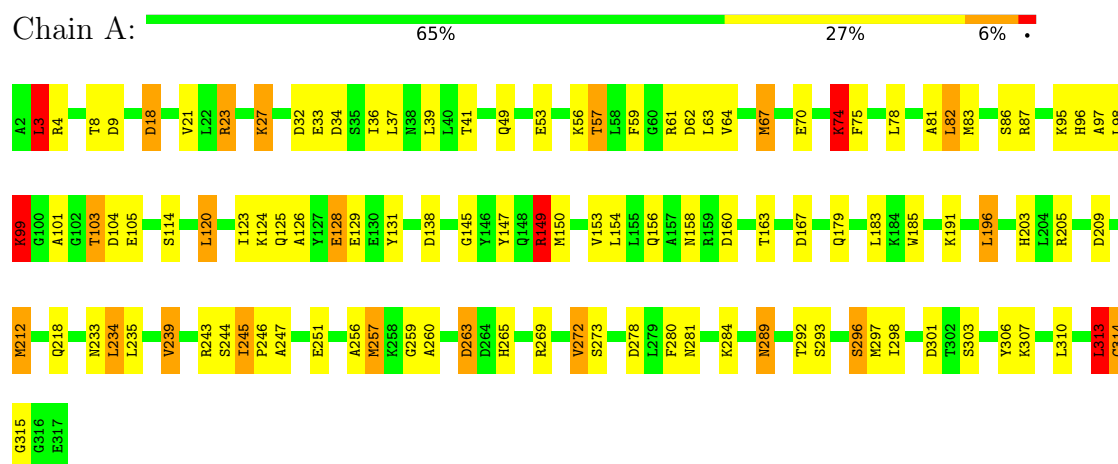
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total 108	O 108	0	0

3 Residue-property plots

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. 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



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	156.90Å 156.90Å 37.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	21.32 – 1.89	Depositor
% Data completeness (in resolution range)	83.0 (21.32-1.89)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3185	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.19	9/2519 (0.4%)	1.94	62/3391 (1.8%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	LEU	C-N	-13.45	1.16	1.33
1	A	315	GLY	C-N	-8.93	1.19	1.33
1	A	153	VAL	CA-CB	6.40	1.61	1.54
1	A	245	ILE	CA-CB	6.17	1.57	1.54
1	A	239	VAL	CA-CB	5.99	1.61	1.54
1	A	203	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	265	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	57	THR	CA-CB	5.58	1.62	1.53
1	A	96	HIS	CD2-NE2	-5.01	1.32	1.37

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	LYS	N-CA-C	9.82	125.64	110.42
1	A	104	ASP	CA-CB-CG	9.47	122.07	112.60
1	A	160	ASP	CA-CB-CG	9.32	121.92	112.60
1	A	70	GLU	N-CA-C	9.11	120.90	110.97
1	A	218	GLN	OE1-CD-NE2	-8.33	114.27	122.60
1	A	167	ASP	CA-CB-CG	-7.83	104.77	112.60
1	A	289	ASN	OD1-CG-ND2	-7.78	114.83	122.60
1	A	272	VAL	CA-C-O	-7.66	113.09	121.29
1	A	269	ARG	CA-C-O	-7.51	112.87	120.90
1	A	289	ASN	CB-CG-ND2	7.36	127.43	116.40
1	A	128	GLU	CB-CG-CD	7.09	124.65	112.60
1	A	23	ARG	CB-CG-CD	7.00	127.41	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	289	ASN	CA-CB-CG	6.81	119.41	112.60
1	A	315	GLY	O-C-N	-6.74	116.11	123.05
1	A	278	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	34	ASP	CA-C-O	-6.61	112.64	120.10
1	A	99	LYS	O-C-N	6.55	130.43	123.03
1	A	18	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	114	SER	N-CA-C	6.49	121.19	113.28
1	A	313	LEU	CA-C-O	-6.41	114.10	120.70
1	A	314	CYS	CB-CA-C	-6.38	101.13	110.96
1	A	33	GLU	CB-CA-C	-6.34	99.90	110.68
1	A	149	ARG	N-CA-C	6.33	118.18	111.28
1	A	218	GLN	CG-CD-NE2	6.06	125.50	116.40
1	A	263	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	101	ALA	N-CA-C	-5.97	104.46	110.97
1	A	105	GLU	CA-CB-CG	-5.91	102.28	114.10
1	A	273	SER	N-CA-C	5.91	118.48	111.33
1	A	3	LEU	O-C-N	5.87	129.59	122.96
1	A	75	PHE	N-CA-C	-5.76	105.08	111.36
1	A	49	GLN	CG-CD-NE2	5.70	124.95	116.40
1	A	123	ILE	CB-CA-C	-5.70	104.57	112.04
1	A	21	VAL	CB-CA-C	-5.70	104.45	112.14
1	A	212	MET	CA-C-N	5.64	128.63	120.79
1	A	212	MET	C-N-CA	5.64	128.63	120.79
1	A	81	ALA	CA-C-O	5.64	126.53	120.55
1	A	126	ALA	O-C-N	-5.60	116.18	122.12
1	A	191	LYS	N-CA-C	5.60	117.06	111.07
1	A	59	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	36	ILE	CA-C-N	5.59	129.20	120.82
1	A	36	ILE	C-N-CA	5.59	129.20	120.82
1	A	32	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	4	ARG	CA-C-N	-5.55	116.58	122.30
1	A	4	ARG	C-N-CA	-5.55	116.58	122.30
1	A	167	ASP	N-CA-C	5.54	118.08	111.71
1	A	123	ILE	CA-C-O	-5.40	115.43	121.05
1	A	37	LEU	CA-CB-CG	5.37	135.10	116.30
1	A	74	LYS	CA-CB-CG	5.37	124.83	114.10
1	A	203	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	23	ARG	CB-CA-C	-5.24	102.66	110.88
1	A	185	TRP	CG-CD2-CE3	5.23	139.13	133.90
1	A	233	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	96	HIS	CA-CB-CG	-5.20	108.60	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	GLU	CA-CB-CG	5.16	124.41	114.10
1	A	103	THR	N-CA-C	-5.14	99.59	108.69
1	A	257	MET	CG-SD-CE	-5.14	89.59	100.90
1	A	63	LEU	N-CA-C	5.12	116.86	111.28
1	A	49	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	86	SER	N-CA-C	5.08	117.21	111.11
1	A	156	GLN	OE1-CD-NE2	-5.08	117.53	122.60
1	A	205	ARG	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

There are no planarity outliers.

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	2487	573	2495	35	0
2	A	7	0	0	0	0
3	A	10	0	0	2	0
4	A	108	0	0	2	0
All	All	2612	573	2495	35	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 7.

All (35) 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:209:ASP:O	1:A:212:MET:HB3	1.95	0.66
1:A:27:LYS:NZ	3:A:327:SO4:S	2.73	0.61
1:A:18:ASP:HB3	1:A:39:LEU:HD21	1.83	0.60
1:A:196:LEU:HD23	1:A:235:LEU:HD22	1.82	0.59
1:A:99:LYS:HA	1:A:99:LYS:HE2	1.88	0.56
1:A:298:ILE:HD12	1:A:314:CYS:SG	2.45	0.56
1:A:64:VAL:HA	1:A:67:MET:HE2	1.87	0.55
1:A:98:LEU:HD13	1:A:138:ASP:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:SER:HB3	1:A:247:ALA:HB3	1.91	0.52
1:A:147:TYR:CD1	1:A:234:LEU:HD12	2.44	0.52
1:A:245:ILE:HB	1:A:246:PRO:HD3	1.92	0.51
1:A:128:GLU:HG2	4:A:507:HOH:O	2.09	0.51
1:A:239:VAL:O	1:A:243:ARG:HG3	2.11	0.51
1:A:67:MET:HE1	1:A:83:MET:HG3	1.93	0.50
1:A:257:MET:HG3	1:A:297:MET:HE2	1.93	0.49
1:A:97:ALA:O	1:A:103:THR:HA	2.12	0.49
1:A:120:LEU:O	1:A:124:LYS:HG3	2.12	0.49
1:A:74:LYS:HG2	1:A:306:TYR:CE2	2.49	0.47
1:A:56:LYS:HE3	1:A:62:ASP:HA	1.97	0.47
1:A:3:LEU:HA	1:A:281:ASN:OD1	2.14	0.47
1:A:82:LEU:HD13	1:A:272:VAL:HG22	1.97	0.46
1:A:256:ALA:HB1	1:A:263:ASP:HB3	1.99	0.45
1:A:145:GLY:O	1:A:149:ARG:HD3	2.18	0.43
1:A:78:LEU:O	1:A:82:LEU:HB2	2.19	0.43
1:A:147:TYR:HD1	1:A:234:LEU:HD12	1.83	0.42
1:A:61:ARG:NH2	4:A:403:HOH:O	2.51	0.42
1:A:280:PHE:CE2	1:A:284:LYS:HE2	2.54	0.42
1:A:150:MET:HE2	1:A:235:LEU:HD23	2.00	0.42
1:A:41:THR:HB	1:A:313:LEU:HD13	2.02	0.41
1:A:95:LYS:HG2	1:A:131:TYR:CE1	2.56	0.41
1:A:303:SER:HA	1:A:307:LYS:HD3	2.02	0.41
1:A:27:LYS:NZ	3:A:327:SO4:O1	2.52	0.41
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.90	0.41
1:A:179:GLN:HA	1:A:183:LEU:HB2	2.02	0.40
1:A:293:SER:HB3	1:A:296:SER:OG	2.21	0.40

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	314/316 (99%)	303 (96%)	9 (3%)	2 (1%)	21	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	GLY
1	A	260	ALA

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	266/266 (100%)	240 (90%)	26 (10%)	7	3

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	8	THR
1	A	23	ARG
1	A	27	LYS
1	A	53	GLU
1	A	57	THR
1	A	67	MET
1	A	74	LYS
1	A	82	LEU
1	A	87	ARG
1	A	99	LYS
1	A	120	LEU
1	A	125	GLN
1	A	129	GLU
1	A	149	ARG
1	A	154	LEU
1	A	158	ASN
1	A	163	THR
1	A	196	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	234	LEU
1	A	289	ASN
1	A	292	THR
1	A	296	SER
1	A	301	ASP
1	A	310	LEU
1	A	313	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	A	327	-	4,4,4	0.63	0	6,6,6	0.30	0
3	SO4	A	328	-	4,4,4	0.43	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	327	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	315:GLY	C	316:GLY	N	1.19
1	A	3:LEU	C	4:ARG	N	1.16

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.