



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:08 PM UTC

PDB ID : 1DGU / pdb_00001dgu
Title : HOMOLOGY-BASED MODEL OF CALCIUM-SATURATED CIB
(CALCIUM-AND INTEGRIN-BINDING PROTEIN)
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Deposited on : 1999-11-25

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

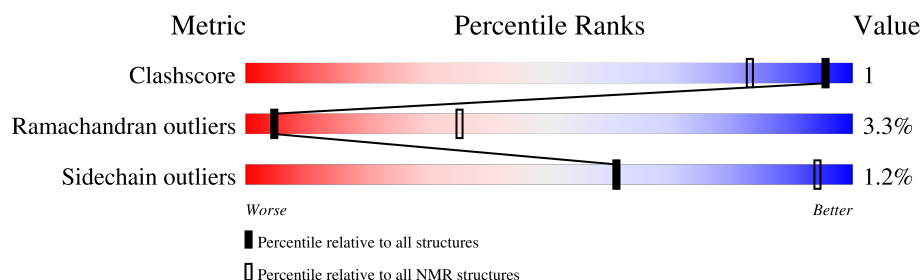
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	183	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2937 atoms, of which 1461 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CALCIUM-SATURATED CIB.

Mol	Chain	Residues	Atoms						Trace
1	A	183	Total	C	H	N	O	S	0
			2937	929	1461	246	297	4	

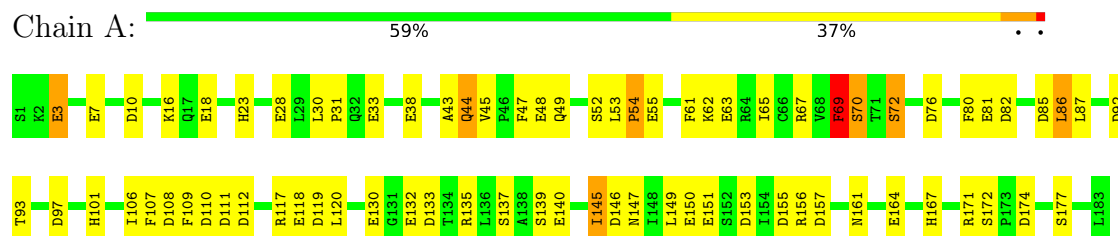
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	SER	THR	conflict	UNP Q99828

4 Residue-property plots [i](#)

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: CALCIUM-SATURATED CIB



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

6 Model quality

6.1 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 (average) 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	2.11	40/1501 (2.7%)	2.08	46/2025 (2.3%)
All	All	2.11	40/1501 (2.7%)	2.08	46/2025 (2.3%)

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	Planarity
1	A	0	5
All	All	0	5

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	VAL	CA-C	6.46	1.58	1.53
1	A	153	ASP	CG-OD2	6.10	1.36	1.25
1	A	150	GLU	CD-OE2	6.01	1.36	1.25
1	A	155	ASP	CG-OD2	6.01	1.36	1.25
1	A	85	ASP	CG-OD2	5.99	1.36	1.25
1	A	38	GLU	CD-OE2	5.97	1.36	1.25
1	A	3	GLU	CD-OE2	5.95	1.36	1.25
1	A	82	ASP	CG-OD2	5.95	1.36	1.25
1	A	63	GLU	CD-OE2	5.92	1.36	1.25
1	A	119	ASP	CG-OD2	5.90	1.36	1.25
1	A	133	ASP	CG-OD2	5.90	1.36	1.25
1	A	118	GLU	CD-OE2	5.89	1.36	1.25
1	A	81	GLU	CD-OE2	5.85	1.36	1.25
1	A	146	ASP	CG-OD2	5.85	1.36	1.25
1	A	28	GLU	CD-OE2	5.85	1.36	1.25
1	A	18	GLU	CD-OE2	5.84	1.36	1.25
1	A	132	GLU	CD-OE2	5.84	1.36	1.25
1	A	55	GLU	CD-OE2	5.83	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	GLU	CD-OE2	5.83	1.36	1.25
1	A	48	GLU	CD-OE2	5.83	1.36	1.25
1	A	112	ASP	CG-OD2	5.82	1.36	1.25
1	A	151	GLU	CD-OE2	5.81	1.36	1.25
1	A	97	ASP	CG-OD2	5.81	1.36	1.25
1	A	130	GLU	CD-OE2	5.80	1.36	1.25
1	A	140	GLU	CD-OE2	5.80	1.36	1.25
1	A	111	ASP	CG-OD2	5.78	1.36	1.25
1	A	10	ASP	CG-OD2	5.78	1.36	1.25
1	A	110	ASP	CG-OD2	5.76	1.36	1.25
1	A	174	ASP	CG-OD2	5.75	1.36	1.25
1	A	92	ASP	CG-OD2	5.74	1.36	1.25
1	A	76	ASP	CG-OD2	5.73	1.36	1.25
1	A	157	ASP	CG-OD2	5.72	1.36	1.25
1	A	33	GLU	CD-OE2	5.71	1.36	1.25
1	A	108	ASP	CG-OD2	5.53	1.35	1.25
1	A	23	HIS	ND1-CE1	5.45	1.38	1.32
1	A	172	SER	CA-C	5.44	1.58	1.52
1	A	164	GLU	CD-OE2	5.24	1.35	1.25
1	A	23	HIS	CG-CD2	5.12	1.41	1.35
1	A	53	LEU	CA-C	5.09	1.59	1.53
1	A	30	LEU	CA-C	5.04	1.58	1.52

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	SER	O-C-N	-12.20	109.83	121.79
1	A	69	PHE	CA-CB-CG	12.18	125.98	113.80
1	A	167	HIS	ND1-CE1-NE2	11.66	120.06	108.40
1	A	101	HIS	ND1-CE1-NE2	11.64	120.04	108.40
1	A	23	HIS	ND1-CE1-NE2	11.58	119.98	108.40
1	A	101	HIS	CE1-NE2-CD2	-9.31	99.69	109.00
1	A	23	HIS	CE1-NE2-CD2	-9.19	99.81	109.00
1	A	167	HIS	CE1-NE2-CD2	-9.17	99.83	109.00
1	A	65	ILE	N-CA-CB	-8.66	101.53	110.62
1	A	155	ASP	CA-CB-CG	8.64	121.24	112.60
1	A	109	PHE	CA-CB-CG	8.38	122.19	113.80
1	A	65	ILE	CB-CA-C	8.01	121.95	111.70
1	A	86	LEU	N-CA-C	7.83	119.50	110.97
1	A	61	PHE	CA-CB-CG	7.58	121.38	113.80
1	A	44	GLN	O-C-N	-7.50	114.67	123.22
1	A	101	HIS	CA-CB-CG	7.21	121.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ARG	N-CA-C	6.53	119.23	111.33
1	A	30	LEU	N-CA-C	6.45	121.53	112.75
1	A	167	HIS	CA-CB-CG	6.39	120.19	113.80
1	A	155	ASP	N-CA-C	6.14	119.88	112.38
1	A	157	ASP	CA-CB-CG	6.11	118.70	112.60
1	A	72	SER	CB-CA-C	6.10	122.19	110.17
1	A	47	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	54	PRO	N-CA-C	6.03	124.90	112.47
1	A	49	GLN	N-CA-CB	-6.03	100.94	110.28
1	A	106	ILE	CB-CA-C	6.00	120.24	112.14
1	A	119	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	112	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	23	HIS	CG-ND1-CE1	-5.82	99.41	109.30
1	A	107	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	167	HIS	CG-ND1-CE1	-5.75	99.53	109.30
1	A	101	HIS	CG-ND1-CE1	-5.73	99.56	109.30
1	A	145	ILE	N-CA-C	5.73	116.38	110.36
1	A	161	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	16	LYS	N-CA-C	5.54	118.04	111.33
1	A	52	SER	N-CA-C	5.50	117.98	111.33
1	A	80	PHE	N-CA-C	5.48	117.25	111.28
1	A	67	ARG	N-CA-C	5.40	117.17	111.28
1	A	177	SER	N-CA-C	5.36	118.03	111.82
1	A	62	LYS	N-CA-C	5.31	117.07	111.28
1	A	147	ASN	N-CA-C	5.22	116.97	111.28
1	A	120	LEU	CB-CA-C	5.21	119.44	110.79
1	A	137	SER	N-CA-C	5.17	117.65	111.71
1	A	139	SER	N-CA-C	5.15	117.56	111.33
1	A	45	VAL	N-CA-C	5.08	113.46	107.77
1	A	157	ASP	N-CA-C	5.04	121.54	110.80

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	44	GLN	Peptide
1	A	69	PHE	Sidechain
1	A	70	SER	Mainchain,Peptide
1	A	171	ARG	Peptide

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1476	1461	1448	3
All	All	1476	1461	1448	3

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 1.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:86:LEU:HD12	1:A:87:LEU:N	0.46	2.26
1:A:117:ARG:O	1:A:145:ILE:HD11	0.44	2.12
1:A:69:PHE:CG	1:A:86:LEU:HD22	0.42	2.49

6.3 Torsion angles

6.3.1 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 NMR 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	181/183 (99%)	152 (84%)	23 (13%)	6 (3%)	5	35
All	All	181/183 (99%)	152 (84%)	23 (13%)	6 (3%)	5	35

All 6 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	31	PRO
1	A	43	ALA
1	A	54	PRO
1	A	72	SER
1	A	93	THR
1	A	156	ARG

6.3.2 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 PDB entries followed by that with respect to all NMR 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	170/170 (100%)	168 (99%)	2 (1%)	61	94
All	All	170/170 (100%)	168 (99%)	2 (1%)	61	94

All 2 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	3	GLU
1	A	149	LEU

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided