



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1BC9 / pdb_00001bc9
Title : CYTOHESIN-1/B2-1 SEC7 DOMAIN, NMR, MINIMIZED AVERAGE STRUCTURE
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Deposited on : 1998-05-06

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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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

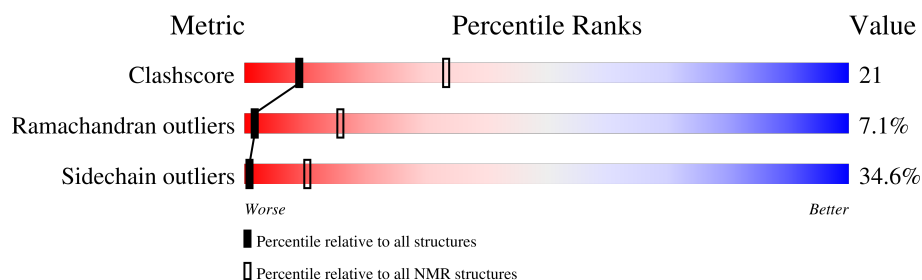
1 Overall quality at a glance

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	200	46% 39% 15%

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 3262 atoms, of which 1621 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYTOHESIN-1.

Mol	Chain	Residues	Atoms						Trace
1	A	200	Total	C	H	N	O	S	0
			3262	1038	1621	291	300	12	

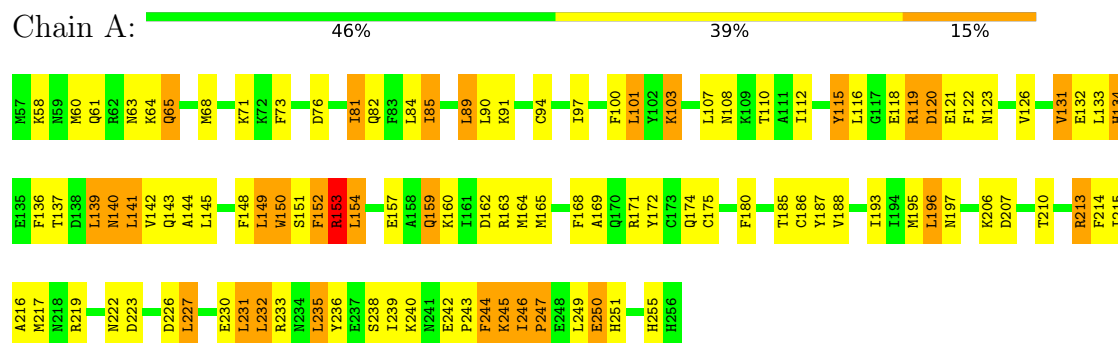
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	LEU	ASP	conflict	UNP Q15438
A	250	GLU	ASP	conflict	UNP Q15438
A	251	HIS	GLY	conflict	UNP Q15438
A	252	HIS	ASN	conflict	UNP Q15438
A	253	HIS	ASP	conflict	UNP Q15438
A	254	HIS	LEU	conflict	UNP Q15438
A	255	HIS	THR	conflict	UNP Q15438

4 Residue-property plots

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: CYTOHESIN-1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY/ SIMULATED ANNEALING*.

Of the 287 calculated structures, 1 were deposited, based on the following criterion: *MINIMIZED AVERAGE*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	3.1

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 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	1641	1621	1609	67
All	All	1641	1621	1609	67

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:142:VAL:HG22	1:A:193:ILE:HD13	1.04	1.18
1:A:101:LEU:HD13	1:A:115:TYR:CZ	0.81	2.10
1:A:142:VAL:CG2	1:A:193:ILE:HD13	0.79	2.06
1:A:222:ASN:ND2	1:A:227:LEU:HD23	0.77	1.94
1:A:139:LEU:HD22	1:A:143:GLN:HB3	0.72	1.61
1:A:100:PHE:CE1	1:A:107:LEU:HD11	0.69	2.22
1:A:231:LEU:HD12	1:A:231:LEU:O	0.67	1.89
1:A:139:LEU:HD22	1:A:143:GLN:CB	0.66	2.20
1:A:148:PHE:CE1	1:A:149:LEU:HD11	0.66	2.25
1:A:145:LEU:CD1	1:A:193:ILE:HD12	0.64	2.22
1:A:197:ASN:HB2	1:A:239:ILE:HD12	0.64	1.68
1:A:137:THR:HG23	1:A:175:CYS:HA	0.62	1.69
1:A:246:ILE:HD12	1:A:247:PRO:O	0.61	1.94
1:A:169:ALA:HB1	1:A:186:CYS:HB3	0.59	1.75
1:A:141:LEU:HD21	1:A:186:CYS:SG	0.59	2.38

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:101:LEU:HD13	1:A:115:TYR:CE2	0.58	2.32
1:A:213:ARG:O	1:A:216:ALA:HB3	0.58	1.98
1:A:142:VAL:HA	1:A:145:LEU:HD12	0.57	1.74
1:A:90:LEU:HD23	1:A:91:LYS:N	0.56	2.16
1:A:136:PHE:CE2	1:A:172:TYR:CE1	0.54	2.94
1:A:227:LEU:HD12	1:A:231:LEU:CD2	0.54	2.32
1:A:73:PHE:CD1	1:A:107:LEU:HD22	0.54	2.37
1:A:141:LEU:HD23	1:A:180:PHE:CE2	0.53	2.38
1:A:214:PHE:CD2	1:A:232:LEU:HD13	0.53	2.39
1:A:136:PHE:CZ	1:A:172:TYR:CD1	0.52	2.97
1:A:145:LEU:HD13	1:A:193:ILE:HB	0.51	1.82
1:A:142:VAL:HG13	1:A:193:ILE:HG21	0.51	1.80
1:A:245:LYS:HE3	1:A:246:ILE:HG23	0.50	1.82
1:A:227:LEU:HD12	1:A:231:LEU:HD23	0.49	1.84
1:A:231:LEU:CD1	1:A:235:LEU:HD13	0.49	2.37
1:A:85:ILE:CD1	1:A:90:LEU:HD22	0.49	2.36
1:A:136:PHE:CE2	1:A:172:TYR:CZ	0.48	3.01
1:A:172:TYR:CE1	1:A:175:CYS:HB3	0.48	2.44
1:A:154:LEU:HD23	1:A:154:LEU:O	0.48	2.09
1:A:101:LEU:HD22	1:A:115:TYR:CE2	0.47	2.44
1:A:131:VAL:HG11	1:A:168:PHE:HA	0.47	1.87
1:A:244:PHE:CD1	1:A:245:LYS:N	0.46	2.84
1:A:85:ILE:HD11	1:A:90:LEU:HD22	0.46	1.86
1:A:149:LEU:HD13	1:A:246:ILE:HG22	0.45	1.88
1:A:101:LEU:HD13	1:A:115:TYR:CE1	0.45	2.44
1:A:168:PHE:CD1	1:A:169:ALA:N	0.45	2.84
1:A:122:PHE:CE1	1:A:126:VAL:CG2	0.45	3.00
1:A:115:TYR:CE2	1:A:116:LEU:CD1	0.45	3.00
1:A:136:PHE:CD2	1:A:144:ALA:HB2	0.45	2.47
1:A:103:LYS:O	1:A:112:ILE:HD11	0.44	2.12
1:A:148:PHE:CE1	1:A:149:LEU:CD1	0.44	3.00
1:A:65:GLN:HG2	1:A:89:LEU:HD13	0.44	1.90
1:A:231:LEU:HD11	1:A:235:LEU:HD13	0.44	1.90
1:A:139:LEU:O	1:A:140:ASN:CB	0.44	2.65
1:A:84:LEU:HD22	1:A:89:LEU:HD22	0.43	1.89
1:A:187:TYR:CD2	1:A:188:VAL:N	0.43	2.86
1:A:152:PHE:CD1	1:A:153:ARG:N	0.43	2.87
1:A:142:VAL:HG23	1:A:235:LEU:HG	0.43	1.89
1:A:148:PHE:CE2	1:A:165:MET:HE1	0.42	2.49
1:A:214:PHE:CE2	1:A:232:LEU:HD13	0.42	2.49
1:A:142:VAL:CG1	1:A:239:ILE:HG12	0.42	2.43
1:A:231:LEU:HD12	1:A:231:LEU:C	0.42	2.40

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:134:HIS:HB2	1:A:136:PHE:CE1	0.42	2.50
1:A:140:ASN:CG	1:A:235:LEU:HD11	0.42	2.39
1:A:215:ILE:HG22	1:A:219:ARG:HD2	0.41	1.91
1:A:150:TRP:O	1:A:152:PHE:CD2	0.41	2.74
1:A:250:GLU:O	1:A:251:HIS:CG	0.41	2.74
1:A:136:PHE:CD2	1:A:144:ALA:CB	0.41	3.04
1:A:185:THR:HG23	1:A:222:ASN:HA	0.41	1.92
1:A:196:LEU:HD23	1:A:236:TYR:CD1	0.41	2.51
1:A:81:ILE:HG22	1:A:85:ILE:CD1	0.40	2.46
1:A:115:TYR:CD1	1:A:115:TYR:O	0.40	2.74

6.3 Torsion angles [i](#)

6.3.1 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 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	198/200 (99%)	136 (69%)	48 (24%)	14 (7%)	2	16
All	All	198/200 (99%)	136 (69%)	48 (24%)	14 (7%)	2	16

All 14 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	58	LYS
1	A	119	ARG
1	A	120	ASP
1	A	140	ASN
1	A	152	PHE
1	A	153	ARG
1	A	159	GLN
1	A	206	LYS
1	A	227	LEU
1	A	243	PRO
1	A	245	LYS
1	A	246	ILE
1	A	247	PRO

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Mol	Chain	Res	Type
1	A	255	HIS

6.3.2 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 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	179/179 (100%)	117 (65%)	62 (35%)	1	10
All	All	179/179 (100%)	117 (65%)	62 (35%)	1	10

All 62 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	60	MET
1	A	61	GLN
1	A	63	ASN
1	A	64	LYS
1	A	65	GLN
1	A	68	MET
1	A	71	LYS
1	A	76	ASP
1	A	81	ILE
1	A	82	GLN
1	A	85	ILE
1	A	89	LEU
1	A	94	CYS
1	A	97	ILE
1	A	101	LEU
1	A	103	LYS
1	A	108	ASN
1	A	110	THR
1	A	115	TYR
1	A	118	GLU
1	A	119	ARG
1	A	120	ASP
1	A	121	GLU
1	A	123	ASN

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Mol	Chain	Res	Type
1	A	131	VAL
1	A	132	GLU
1	A	133	LEU
1	A	134	HIS
1	A	139	LEU
1	A	141	LEU
1	A	149	LEU
1	A	150	TRP
1	A	151	SER
1	A	153	ARG
1	A	154	LEU
1	A	157	GLU
1	A	159	GLN
1	A	160	LYS
1	A	162	ASP
1	A	163	ARG
1	A	164	MET
1	A	171	ARG
1	A	174	GLN
1	A	195	MET
1	A	196	LEU
1	A	207	ASP
1	A	210	THR
1	A	213	ARG
1	A	217	MET
1	A	223	ASP
1	A	226	ASP
1	A	230	GLU
1	A	231	LEU
1	A	232	LEU
1	A	233	ARG
1	A	235	LEU
1	A	238	SER
1	A	240	LYS
1	A	242	GLU
1	A	244	PHE
1	A	249	LEU
1	A	250	GLU

6.3.3 RNA ⓘ

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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided