



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1BC9  
Title : CYTOHESIN-1/B2-1 SEC7 DOMAIN, NMR, MINIMIZED AVERAGE STRUCTURE  
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This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

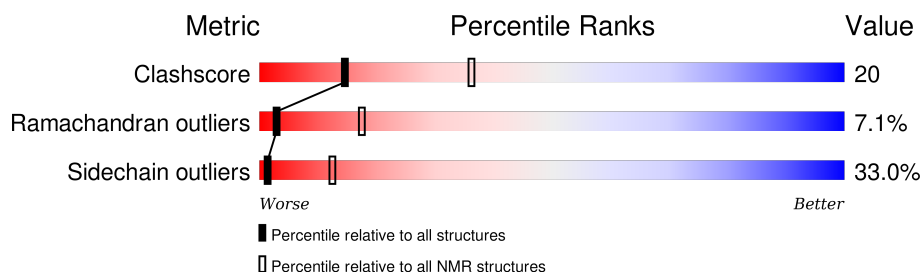
# 1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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  $\geq 3$ , 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	

## 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	

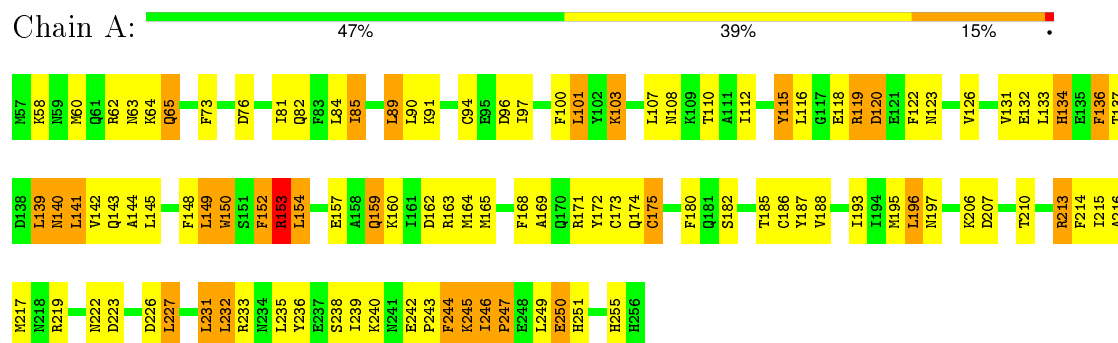
There are 7 discrepancies between the modelled and reference sequences:

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 [i](#)

These plots are provided for all protein, RNA and DNA 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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 ⓘ

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	65
All	All	1641	1621	1609	65

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 20.

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:O	1:A:231:LEU:HD12	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:227:LEU:HD12	1:A:231:LEU:CD2	0.54	2.32
1:A:136:PHE:CE2	1:A:172:TYR:CE1	0.54	2.94
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:148:PHE:CE1	1:A:149:LEU:CD1	0.44	3.00
1:A:103:LYS:O	1:A:112:ILE:HD11	0.44	2.12
1:A:139:LEU:O	1:A:140:ASN:CB	0.44	2.65
1:A:231:LEU:HD11	1:A:235:LEU:HD13	0.44	1.90
1:A:65:GLN:HG2	1:A:89:LEU:HD13	0.44	1.90
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: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:134:HIS:HB2	1:A:136:PHE:CE1	0.42	2.50
1:A:215:ILE:HG22	1:A:219:ARG:HD2	0.41	1.91

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:148:PHE:CZ	1:A:165:MET:HE1	0.41	2.50
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

### 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	198/200 (99%)	136 (69%)	48 (24%)	14 (7%)	3	17
All	All	198/200 (99%)	136 (69%)	48 (24%)	14 (7%)	3	17

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

Mol	Chain	Res	Type
1	A	153	ARG
1	A	140	ASN
1	A	255	HIS
1	A	227	LEU
1	A	120	ASP
1	A	246	ILE
1	A	247	PRO
1	A	152	PHE
1	A	159	GLN
1	A	243	PRO
1	A	119	ARG
1	A	245	LYS
1	A	58	LYS
1	A	206	LYS

### 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%)	120 (67%)	59 (33%)	1	12
All	All	179/179 (100%)	120 (67%)	59 (33%)	1	12

All 59 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	171	ARG
1	A	223	ASP
1	A	85	ILE
1	A	136	PHE
1	A	244	PHE
1	A	240	LYS
1	A	134	HIS
1	A	207	ASP
1	A	119	ARG
1	A	163	ARG
1	A	103	LYS
1	A	159	GLN
1	A	231	LEU
1	A	76	ASP
1	A	157	GLU
1	A	132	GLU
1	A	226	ASP
1	A	96	ASP
1	A	213	ARG
1	A	64	LYS
1	A	196	LEU
1	A	232	LEU
1	A	115	TYR
1	A	65	GLN
1	A	89	LEU
1	A	210	THR
1	A	242	GLU
1	A	97	ILE
1	A	63	ASN

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Mol	Chain	Res	Type
1	A	153	ARG
1	A	160	LYS
1	A	149	LEU
1	A	139	LEU
1	A	118	GLU
1	A	110	THR
1	A	133	LEU
1	A	173	CYS
1	A	94	CYS
1	A	233	ARG
1	A	150	TRP
1	A	162	ASP
1	A	249	LEU
1	A	238	SER
1	A	141	LEU
1	A	250	GLU
1	A	182	SER
1	A	164	MET
1	A	101	LEU
1	A	175	CYS
1	A	60	MET
1	A	174	GLN
1	A	217	MET
1	A	62	ARG
1	A	195	MET
1	A	108	ASN
1	A	154	LEU
1	A	123	ASN
1	A	120	ASP
1	A	82	GLN

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates 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