



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:07 pm BST

PDB ID : 2LM5
Title : Solution structure of Ca²⁺-CIB1 in complex with the cytoplasmic domain of the integrin α Ib subunit
Authors : Huang, H.; Vogel, H.J.
Deposited on : 2011-11-22

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 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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

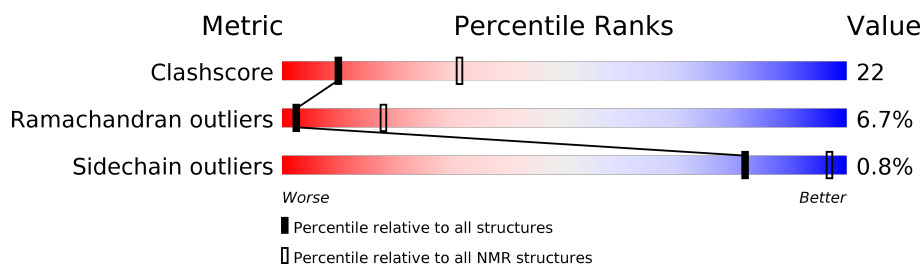
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 42%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	214	

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:190 (183)	0.33	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 9, 10
2	7, 8
3	2, 6

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2943 atoms, of which 1457 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium and integrin-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	184	Total	C	H	N	O	S	0
			2941	935	1457	247	298	4	

There are 23 discrepancies between the modelled and reference sequences:

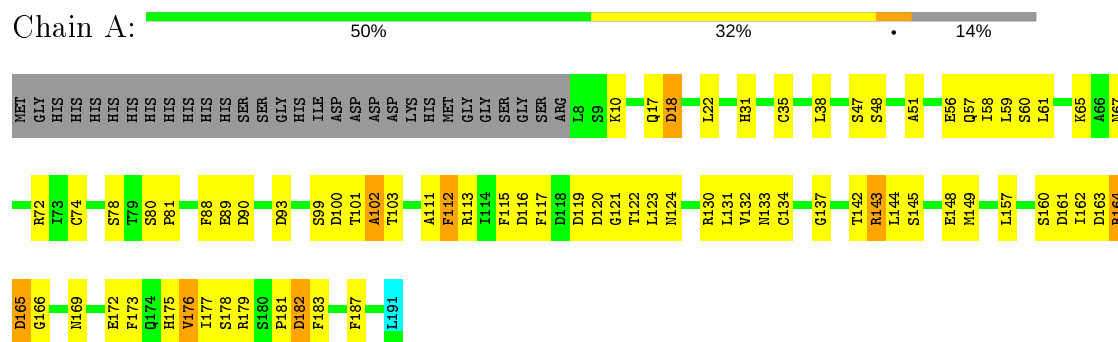
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q99828
A	-21	GLY	-	EXPRESSION TAG	UNP Q99828
A	-20	HIS	-	EXPRESSION TAG	UNP Q99828
A	-19	HIS	-	EXPRESSION TAG	UNP Q99828
A	-18	HIS	-	EXPRESSION TAG	UNP Q99828
A	-17	HIS	-	EXPRESSION TAG	UNP Q99828
A	-16	HIS	-	EXPRESSION TAG	UNP Q99828
A	-15	HIS	-	EXPRESSION TAG	UNP Q99828
A	-14	HIS	-	EXPRESSION TAG	UNP Q99828
A	-13	HIS	-	EXPRESSION TAG	UNP Q99828
A	-12	HIS	-	EXPRESSION TAG	UNP Q99828
A	-11	HIS	-	EXPRESSION TAG	UNP Q99828
A	-10	SER	-	EXPRESSION TAG	UNP Q99828
A	-9	SER	-	EXPRESSION TAG	UNP Q99828
A	-8	GLY	-	EXPRESSION TAG	UNP Q99828
A	-7	HIS	-	EXPRESSION TAG	UNP Q99828
A	-6	ILE	-	EXPRESSION TAG	UNP Q99828
A	-5	ASP	-	EXPRESSION TAG	UNP Q99828
A	-4	ASP	-	EXPRESSION TAG	UNP Q99828
A	-3	ASP	-	EXPRESSION TAG	UNP Q99828
A	-2	ASP	-	EXPRESSION TAG	UNP Q99828
A	-1	LYS	-	EXPRESSION TAG	UNP Q99828
A	0	HIS	-	EXPRESSION TAG	UNP Q99828

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

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

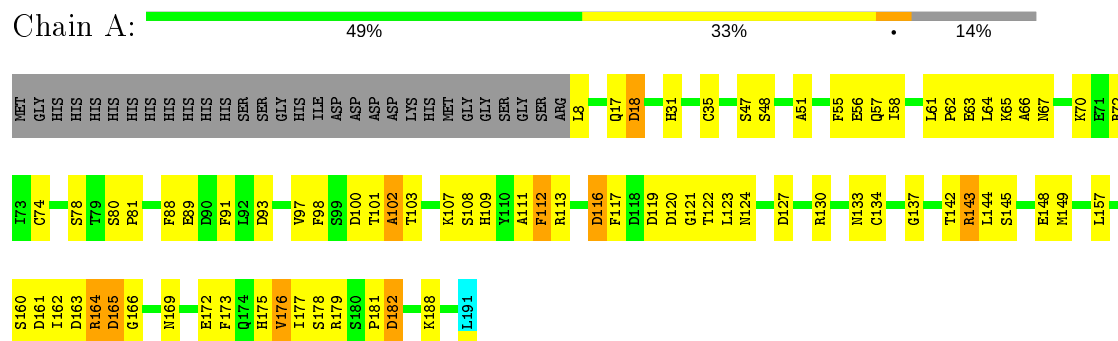
4.2.5 Score per residue for model 5

- Molecule 1: Calcium and integrin-binding protein 1



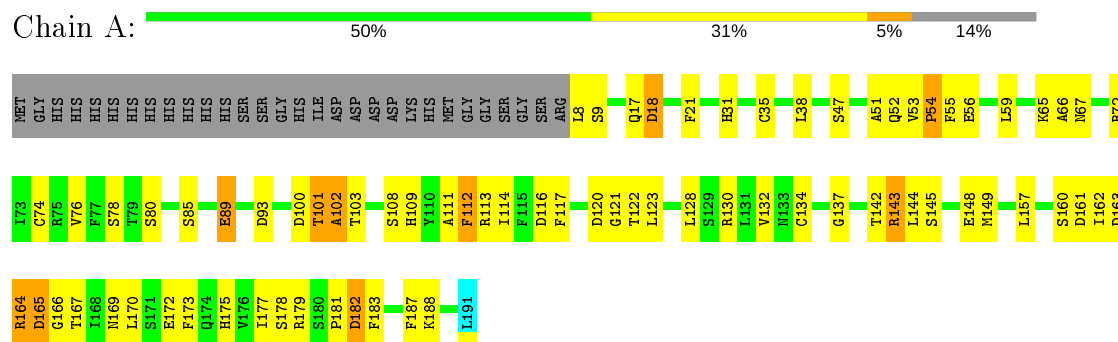
4.2.6 Score per residue for model 6

- Molecule 1: Calcium and integrin-binding protein 1



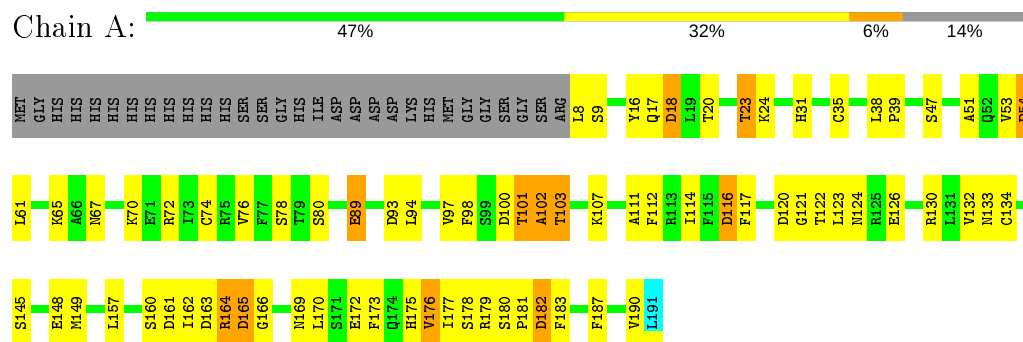
4.2.7 Score per residue for model 7

- Molecule 1: Calcium and integrin-binding protein 1



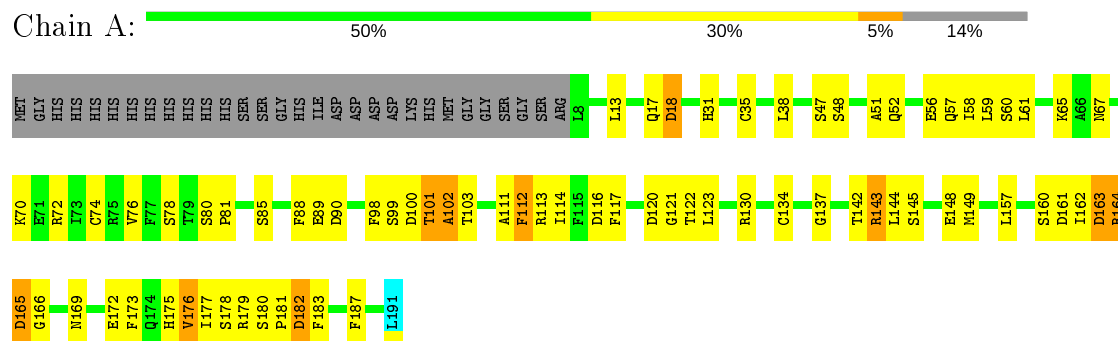
4.2.8 Score per residue for model 8

- Molecule 1: Calcium and integrin-binding protein 1



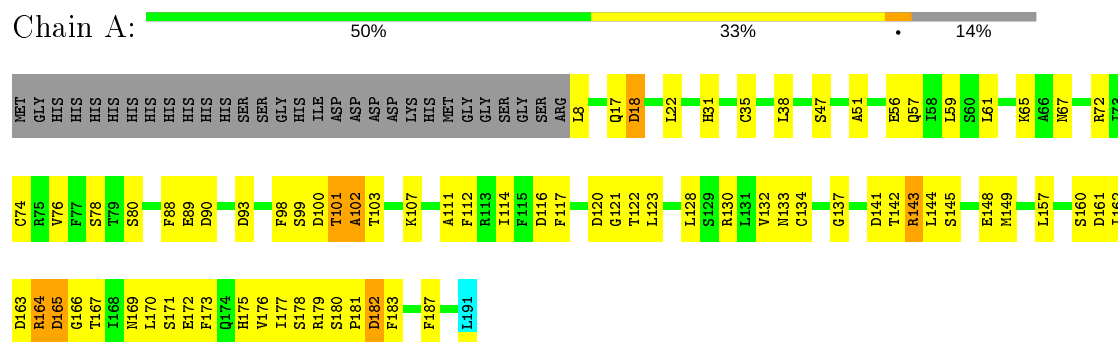
4.2.9 Score per residue for model 9

- Molecule 1: Calcium and integrin-binding protein 1



4.2.10 Score per residue for model 10

- Molecule 1: Calcium and integrin-binding protein 1



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest RDC energy*.

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

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

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1119
Number of shifts mapped to atoms	1119
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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	1475	1446	1445	64±5
All	All	14770	14460	14450	638

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ARG:NE	1:A:117:PHE:CE1	0.62	2.68	10	7
1:A:72:ARG:NH2	1:A:117:PHE:CZ	0.62	2.68	5	5
1:A:72:ARG:NE	1:A:117:PHE:CZ	0.62	2.68	10	4
1:A:72:ARG:NE	1:A:117:PHE:CE2	0.62	2.68	2	1
1:A:72:ARG:NH2	1:A:117:PHE:CE2	0.60	2.69	4	2
1:A:31:HIS:CE1	1:A:35:CYS:SG	0.59	2.96	1	1
1:A:122:THR:HG22	1:A:123:LEU:N	0.57	2.15	6	10
1:A:97:VAL:O	1:A:102:ALA:HB2	0.56	2.00	2	2
1:A:94:LEU:HD23	1:A:94:LEU:C	0.56	2.20	8	1
1:A:115:PHE:CE2	1:A:131:LEU:CD2	0.56	2.89	1	2
1:A:72:ARG:CZ	1:A:117:PHE:CZ	0.56	2.88	2	1
1:A:101:THR:O	1:A:103:THR:N	0.55	2.40	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ALA:O	1:A:114:ILE:N	0.55	2.40	10	7
1:A:31:HIS:CD2	1:A:48:SER:HG	0.55	2.20	3	7
1:A:116:ASP:OD2	1:A:120:ASP:N	0.54	2.40	10	8
1:A:175:HIS:O	1:A:179:ARG:N	0.54	2.40	2	10
1:A:112:PHE:CZ	1:A:121:GLY:O	0.54	2.61	2	4
1:A:180:SER:O	1:A:182:ASP:N	0.54	2.41	2	7
1:A:116:ASP:OD2	1:A:121:GLY:N	0.54	2.41	7	10
1:A:187:PHE:CG	1:A:187:PHE:O	0.54	2.61	7	4
1:A:142:THR:O	1:A:143:ARG:C	0.54	2.46	10	10
1:A:74:CYS:O	1:A:78:SER:N	0.53	2.41	5	7
1:A:160:SER:O	1:A:179:ARG:NH1	0.53	2.42	4	9
1:A:112:PHE:CE2	1:A:121:GLY:O	0.53	2.61	6	3
1:A:133:ASN:ND2	1:A:144:LEU:CD1	0.53	2.71	5	2
1:A:103:THR:O	1:A:107:LYS:N	0.53	2.42	2	5
1:A:187:PHE:O	1:A:187:PHE:CG	0.53	2.62	8	4
1:A:183:PHE:O	1:A:187:PHE:N	0.53	2.42	7	7
1:A:175:HIS:O	1:A:178:SER:N	0.53	2.41	2	10
1:A:31:HIS:NE2	1:A:48:SER:OG	0.53	2.42	5	5
1:A:169:ASN:OD1	1:A:171:SER:N	0.52	2.42	2	2
1:A:88:PHE:CE2	1:A:89:GLU:OE2	0.52	2.62	1	8
1:A:17:GLN:NE2	1:A:90:ASP:OD2	0.52	2.42	1	4
1:A:124:ASN:ND2	1:A:127:ASP:OD2	0.52	2.42	2	1
1:A:187:PHE:CD2	1:A:187:PHE:O	0.51	2.63	5	3
1:A:157:LEU:O	1:A:161:ASP:N	0.51	2.43	9	2
1:A:88:PHE:CZ	1:A:89:GLU:OE2	0.51	2.63	6	2
1:A:130:ARG:O	1:A:134:CYS:SG	0.51	2.69	4	10
1:A:124:ASN:N	1:A:124:ASN:OD1	0.51	2.43	8	1
1:A:163:ASP:O	1:A:165:ASP:N	0.51	2.44	10	10
1:A:116:ASP:OD1	1:A:119:ASP:N	0.51	2.44	3	2
1:A:111:ALA:O	1:A:113:ARG:N	0.50	2.44	6	8
1:A:31:HIS:O	1:A:35:CYS:SG	0.49	2.70	7	10
1:A:97:VAL:O	1:A:102:ALA:N	0.49	2.44	8	1
1:A:108:SER:OG	1:A:109:HIS:N	0.49	2.45	6	2
1:A:108:SER:O	1:A:111:ALA:N	0.49	2.46	6	1
1:A:164:ARG:O	1:A:166:GLY:N	0.49	2.46	7	10
1:A:22:LEU:HD21	1:A:93:ASP:OD1	0.49	2.06	10	1
1:A:132:VAL:HG23	1:A:133:ASN:N	0.49	2.22	1	5
1:A:100:ASP:C	1:A:102:ALA:N	0.48	2.67	9	8
1:A:115:PHE:CE2	1:A:131:LEU:CD1	0.48	2.96	5	1
1:A:67:ASN:ND2	1:A:67:ASN:N	0.48	2.60	8	1
1:A:65:LYS:O	1:A:67:ASN:N	0.48	2.47	6	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:ASP:O	1:A:102:ALA:N	0.48	2.46	9	7
1:A:124:ASN:OD1	1:A:124:ASN:N	0.48	2.46	5	1
1:A:169:ASN:ND2	1:A:172:GLU:CD	0.48	2.67	4	8
1:A:70:LYS:O	1:A:74:CYS:SG	0.48	2.70	6	5
1:A:22:LEU:CD2	1:A:93:ASP:OD1	0.48	2.62	10	1
1:A:65:LYS:C	1:A:67:ASN:N	0.47	2.66	8	10
1:A:173:PHE:O	1:A:177:ILE:CG1	0.47	2.62	10	9
1:A:144:LEU:HG	1:A:145:SER:N	0.47	2.24	10	10
1:A:160:SER:O	1:A:179:ARG:CZ	0.47	2.62	5	5
1:A:17:GLN:NE2	1:A:90:ASP:CG	0.47	2.68	5	3
1:A:164:ARG:C	1:A:166:GLY:N	0.47	2.67	6	10
1:A:58:ILE:CG2	1:A:91:PHE:CG	0.47	2.97	6	1
1:A:169:ASN:HD21	1:A:172:GLU:CD	0.47	2.13	6	2
1:A:165:ASP:OD1	1:A:166:GLY:N	0.47	2.48	5	10
1:A:162:ILE:C	1:A:164:ARG:N	0.47	2.68	8	10
1:A:59:LEU:CD1	1:A:70:LYS:NZ	0.47	2.78	8	1
1:A:98:PHE:CE2	1:A:190:VAL:O	0.46	2.68	8	1
1:A:93:ASP:O	1:A:97:VAL:HG23	0.46	2.10	1	2
1:A:157:LEU:O	1:A:161:ASP:O	0.46	2.34	8	10
1:A:186:SER:C	1:A:188:LYS:N	0.46	2.68	2	1
1:A:17:GLN:HE21	1:A:90:ASP:CG	0.46	2.14	5	5
1:A:56:GLU:O	1:A:59:LEU:N	0.46	2.49	8	2
1:A:98:PHE:CZ	1:A:190:VAL:O	0.46	2.68	8	1
1:A:13:LEU:HD23	1:A:113:ARG:NH1	0.46	2.26	2	1
1:A:111:ALA:O	1:A:112:PHE:C	0.46	2.54	10	10
1:A:74:CYS:O	1:A:78:SER:CB	0.46	2.64	1	10
1:A:53:VAL:O	1:A:54:PRO:O	0.46	2.34	8	2
1:A:98:PHE:CD2	1:A:98:PHE:O	0.46	2.69	1	1
1:A:170:LEU:HD23	1:A:170:LEU:O	0.46	2.10	3	4
1:A:94:LEU:HD23	1:A:94:LEU:O	0.45	2.10	8	1
1:A:122:THR:CG2	1:A:123:LEU:N	0.45	2.79	6	5
1:A:171:SER:O	1:A:175:HIS:ND1	0.45	2.42	10	1
1:A:187:PHE:O	1:A:187:PHE:CD2	0.45	2.69	9	3
1:A:124:ASN:C	1:A:126:GLU:N	0.45	2.69	8	1
1:A:98:PHE:O	1:A:98:PHE:CG	0.45	2.70	9	2
1:A:17:GLN:O	1:A:18:ASP:O	0.45	2.34	10	10
1:A:47:SER:O	1:A:51:ALA:HB3	0.45	2.12	7	10
1:A:103:THR:OG1	1:A:106:ILE:CG1	0.45	2.65	2	1
1:A:98:PHE:O	1:A:98:PHE:CD2	0.45	2.70	6	2
1:A:65:LYS:C	1:A:67:ASN:H	0.45	2.16	4	8
1:A:56:GLU:CG	1:A:57:GLN:N	0.45	2.79	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:THR:O	1:A:144:LEU:N	0.44	2.49	10	8
1:A:173:PHE:CE1	1:A:177:ILE:HD11	0.44	2.47	5	2
1:A:124:ASN:HD21	1:A:126:GLU:CD	0.44	2.15	8	1
1:A:148:GLU:CG	1:A:149:MET:N	0.44	2.81	1	9
1:A:124:ASN:ND2	1:A:127:ASP:CG	0.44	2.70	2	1
1:A:163:ASP:C	1:A:165:ASP:N	0.44	2.70	10	7
1:A:170:LEU:O	1:A:170:LEU:HD23	0.44	2.12	10	2
1:A:10:LYS:HZ2	1:A:113:ARG:HD3	0.44	1.72	5	1
1:A:124:ASN:O	1:A:126:GLU:N	0.44	2.51	8	1
1:A:116:ASP:OD2	1:A:122:THR:O	0.44	2.36	6	2
1:A:116:ASP:OD1	1:A:120:ASP:OD1	0.44	2.36	8	3
1:A:120:ASP:N	1:A:120:ASP:OD1	0.44	2.48	8	1
1:A:8:LEU:HD23	1:A:9:SER:N	0.43	2.29	8	2
1:A:165:ASP:OD2	1:A:167:THR:O	0.43	2.37	7	2
1:A:162:ILE:O	1:A:164:ARG:N	0.43	2.52	8	3
1:A:55:PHE:CD1	1:A:55:PHE:C	0.43	2.92	7	2
1:A:61:LEU:O	1:A:63:GLU:N	0.43	2.51	6	2
1:A:175:HIS:O	1:A:176:VAL:C	0.43	2.56	2	9
1:A:52:GLN:NE2	1:A:85:SER:OG	0.43	2.51	9	2
1:A:8:LEU:C	1:A:8:LEU:HD23	0.43	2.34	10	3
1:A:116:ASP:OD1	1:A:122:THR:O	0.43	2.37	4	4
1:A:31:HIS:NE2	1:A:35:CYS:SG	0.43	2.91	7	2
1:A:165:ASP:OD1	1:A:167:THR:O	0.43	2.37	1	2
1:A:180:SER:C	1:A:182:ASP:N	0.43	2.72	1	4
1:A:35:CYS:O	1:A:38:LEU:O	0.43	2.36	8	6
1:A:89:GLU:O	1:A:93:ASP:OD2	0.43	2.36	8	2
1:A:58:ILE:C	1:A:60:SER:N	0.43	2.71	1	6
1:A:181:PRO:O	1:A:182:ASP:O	0.42	2.37	10	9
1:A:99:SER:O	1:A:100:ASP:OD1	0.42	2.37	9	6
1:A:116:ASP:OD2	1:A:120:ASP:OD1	0.42	2.37	9	6
1:A:59:LEU:C	1:A:61:LEU:H	0.42	2.18	4	7
1:A:64:LEU:HD12	1:A:91:PHE:CE2	0.42	2.49	6	1
1:A:58:ILE:CG2	1:A:91:PHE:CE2	0.42	3.03	3	1
1:A:31:HIS:NE2	1:A:48:SER:CB	0.42	2.83	5	2
1:A:100:ASP:C	1:A:102:ALA:H	0.42	2.17	8	1
1:A:124:ASN:ND2	1:A:126:GLU:CD	0.42	2.73	8	1
1:A:186:SER:O	1:A:188:LYS:N	0.42	2.52	2	1
1:A:8:LEU:HD23	1:A:8:LEU:C	0.42	2.35	1	4
1:A:72:ARG:O	1:A:76:VAL:HG23	0.42	2.14	3	5
1:A:52:GLN:OE1	1:A:85:SER:OG	0.42	2.36	7	1
1:A:120:ASP:CG	1:A:121:GLY:N	0.42	2.72	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ALA:O	1:A:115:PHE:N	0.42	2.44	2	1
1:A:124:ASN:OD1	1:A:127:ASP:N	0.42	2.50	2	2
1:A:162:ILE:C	1:A:164:ARG:H	0.42	2.18	8	2
1:A:23:THR:OG1	1:A:24:LYS:N	0.42	2.52	8	1
1:A:132:VAL:CG2	1:A:133:ASN:N	0.42	2.82	1	1
1:A:116:ASP:O	1:A:119:ASP:OD1	0.42	2.37	5	1
1:A:64:LEU:O	1:A:67:ASN:OD1	0.42	2.37	4	1
1:A:21:PHE:O	1:A:93:ASP:OD1	0.42	2.37	7	1
1:A:132:VAL:HG21	1:A:149:MET:CE	0.42	2.45	8	1
1:A:13:LEU:CD2	1:A:113:ARG:HH12	0.41	2.28	3	3
1:A:47:SER:O	1:A:51:ALA:CB	0.41	2.68	6	2
1:A:47:SER:O	1:A:51:ALA:N	0.41	2.53	6	1
1:A:141:ASP:OD1	1:A:141:ASP:O	0.41	2.37	10	2
1:A:22:LEU:HD21	1:A:93:ASP:OD2	0.41	2.15	5	1
1:A:101:THR:O	1:A:101:THR:HG22	0.41	2.16	3	1
1:A:169:ASN:O	1:A:173:PHE:N	0.41	2.54	8	1
1:A:53:VAL:O	1:A:53:VAL:HG13	0.41	2.15	8	2
1:A:128:LEU:O	1:A:132:VAL:HG22	0.41	2.16	10	3
1:A:61:LEU:C	1:A:63:GLU:N	0.41	2.75	1	2
1:A:17:GLN:HE22	1:A:79:THR:HG23	0.41	1.75	3	1
1:A:61:LEU:C	1:A:63:GLU:H	0.41	2.19	6	1
1:A:94:LEU:CD2	1:A:94:LEU:C	0.41	2.90	8	1
1:A:120:ASP:OD1	1:A:120:ASP:N	0.41	2.52	7	1
1:A:13:LEU:HD23	1:A:113:ARG:HH12	0.40	1.75	1	1
1:A:16:TYR:O	1:A:20:THR:OG1	0.40	2.36	8	1
1:A:101:THR:HG22	1:A:101:THR:O	0.40	2.16	9	1
1:A:132:VAL:O	1:A:136:THR:OG1	0.40	2.33	1	1
1:A:187:PHE:O	1:A:188:LYS:O	0.40	2.38	2	1

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	182/214 (85%)	143±2 (79±1%)	26±3 (15±2%)	12±2 (7±1%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1820/2140 (85%)	1434 (79%)	264 (15%)	122 (7%)	2 18

All 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	143	ARG	10
1	A	164	ARG	10
1	A	137	GLY	10
1	A	18	ASP	10
1	A	165	ASP	10
1	A	102	ALA	10
1	A	182	ASP	10
1	A	176	VAL	8
1	A	112	PHE	8
1	A	101	THR	6
1	A	81	PRO	5
1	A	188	LYS	5
1	A	181	PRO	4
1	A	66	ALA	4
1	A	89	GLU	2
1	A	54	PRO	2
1	A	116	ASP	2
1	A	142	THR	2
1	A	23	THR	1
1	A	111	ALA	1
1	A	62	PRO	1
1	A	39	PRO	1

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	170/196 (87%)	169±0 (99±0%)	1±0 (1±0%)	82 97
All	All	1700/1960 (87%)	1687 (99%)	13 (1%)	82 97

All 3 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	80	SER	10
1	A	103	THR	2
1	A	163	ASP	1

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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 42% for the well-defined parts and 42% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1119
Number of shifts mapped to atoms	1119
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	176	-0.13 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	172	0.95 ± 0.15	Should be applied
$^{13}\text{C}'$	174	-0.40 ± 0.09	None needed (< 0.5 ppm)
^{15}N	159	0.77 ± 0.15	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 42%, i.e. 974 atoms were assigned a chemical shift out of a possible 2306. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	662/901 (73%)	158/359 (44%)	346/366 (95%)	158/176 (90%)
Sidechain	312/1242 (25%)	70/727 (10%)	242/458 (53%)	0/57 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/163 (0%)	0/90 (0%)	0/70 (0%)	0/3 (0%)
Overall	974/2306 (42%)	228/1176 (19%)	588/894 (66%)	158/236 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 42%, i.e. 979 atoms were assigned a chemical shift out of a possible 2320. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	666/906 (74%)	159/361 (44%)	348/368 (95%)	159/177 (90%)
Sidechain	313/1251 (25%)	70/732 (10%)	243/462 (53%)	0/57 (0%)
Aromatic	0/163 (0%)	0/90 (0%)	0/70 (0%)	0/3 (0%)
Overall	979/2320 (42%)	229/1183 (19%)	591/900 (66%)	159/237 (67%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

