



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 10:42 PM BST

PDB ID : 2K7C
Title : NMR Structure of Mg²⁺-bound CaBP1 C-domain
Authors : Ames, J.
Deposited on : 2008-08-08

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
<http://wwpdb.org/validation/2016/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
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

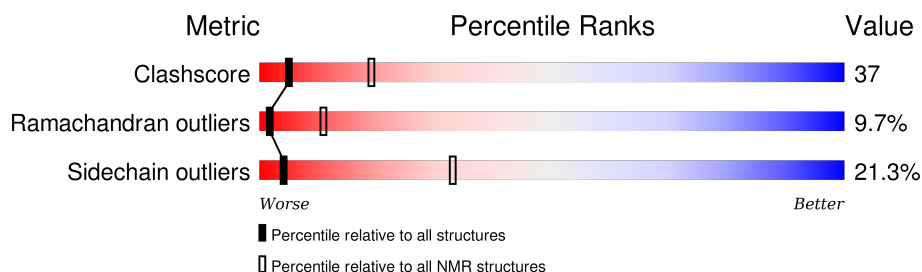
1 Overall quality at a glance

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 ≥ 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	72	

2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:100-A:132, A:137-A:167 (64)	0.76	10

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 4 clusters and 5 single-model clusters were found.

Cluster number	Models
1	3, 5, 9, 14
2	1, 8
3	12, 15
4	7, 10
Single-model clusters	2; 4; 6; 11; 13

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1141 atoms, of which 559 are hydrogens and 0 are deuteriums.

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

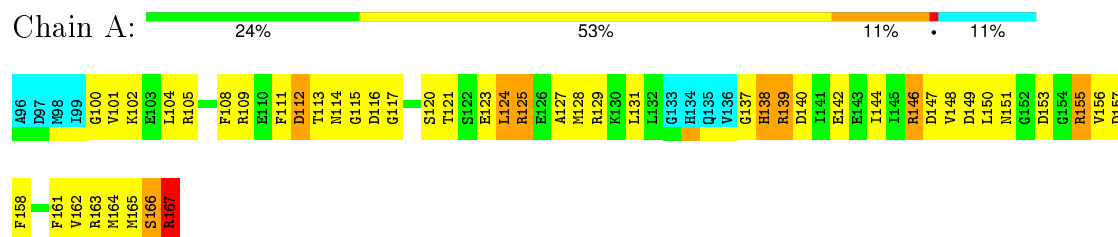
Mol	Chain	Residues	Atoms						Trace
1	A	72	Total	C	H	N	O	S	0
			1141	353	559	108	117	4	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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: Calcium-binding protein 1

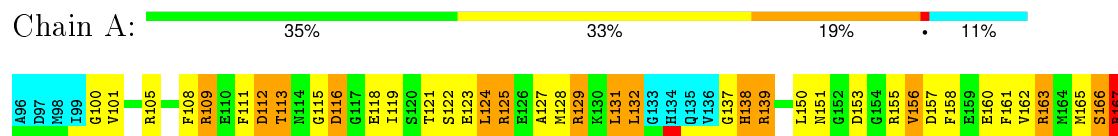


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

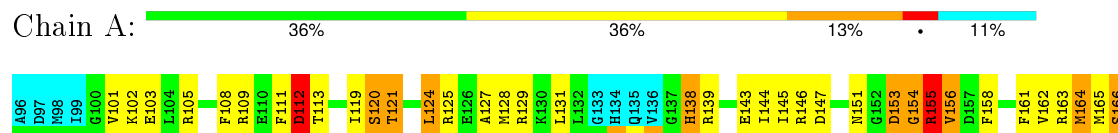
4.2.1 Score per residue for model 1

- Molecule 1: Calcium-binding protein 1



4.2.2 Score per residue for model 2

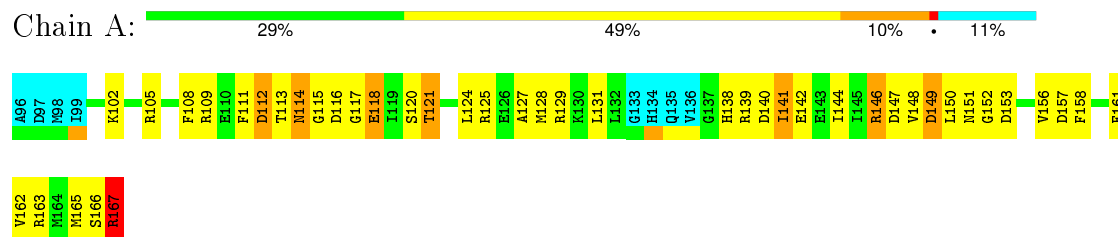
- Molecule 1: Calcium-binding protein 1



R167

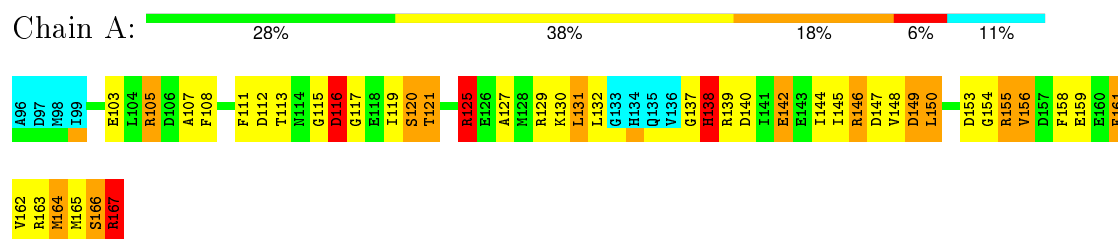
4.2.3 Score per residue for model 3

- Molecule 1: Calcium-binding protein 1



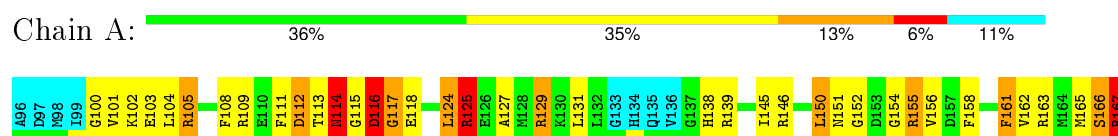
4.2.4 Score per residue for model 4

- Molecule 1: Calcium-binding protein 1



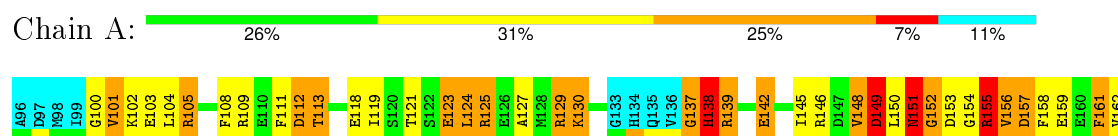
4.2.5 Score per residue for model 5

- Molecule 1: Calcium-binding protein 1



4.2.6 Score per residue for model 6

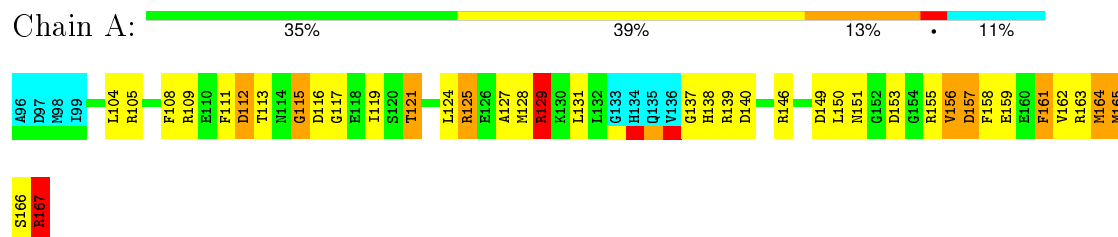
- Molecule 1: Calcium-binding protein 1



R163
M164
M165
S166
R167

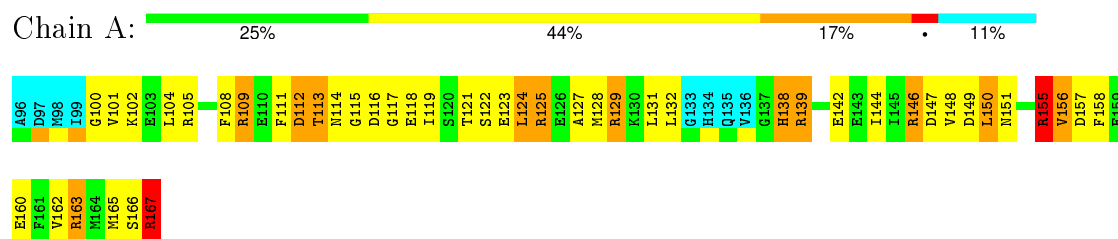
4.2.7 Score per residue for model 7

- Molecule 1: Calcium-binding protein 1



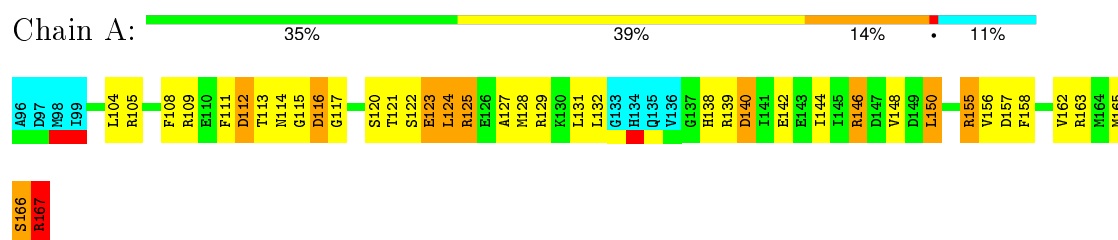
4.2.8 Score per residue for model 8

- Molecule 1: Calcium-binding protein 1



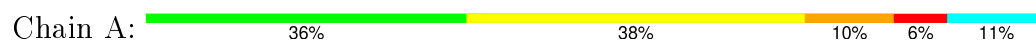
4.2.9 Score per residue for model 9

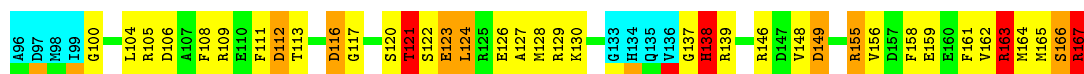
- Molecule 1: Calcium-binding protein 1



4.2.10 Score per residue for model 10 (medoid)

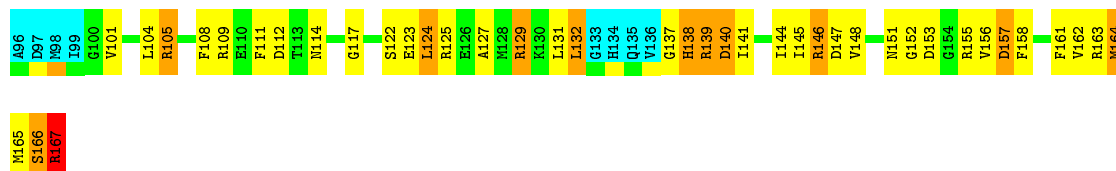
- Molecule 1: Calcium-binding protein 1





4.2.11 Score per residue for model 11

- Molecule 1: Calcium-binding protein 1



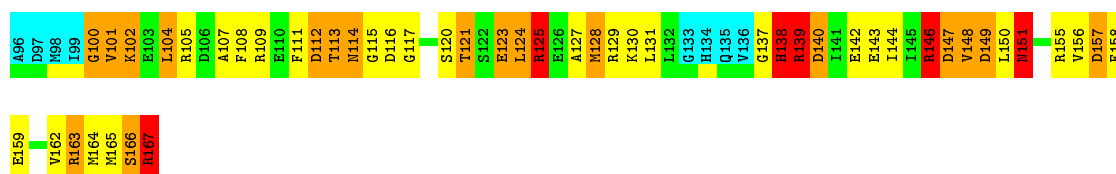
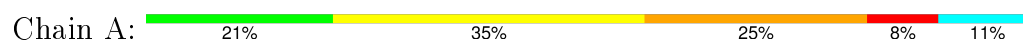
4.2.12 Score per residue for model 12

- Molecule 1: Calcium-binding protein 1



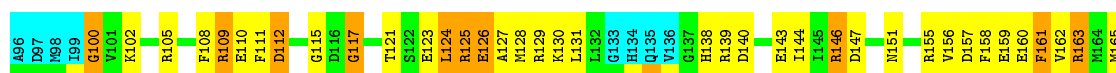
4.2.13 Score per residue for model 13

- Molecule 1: Calcium-binding protein 1



4.2.14 Score per residue for model 14

- Molecule 1: Calcium-binding protein 1

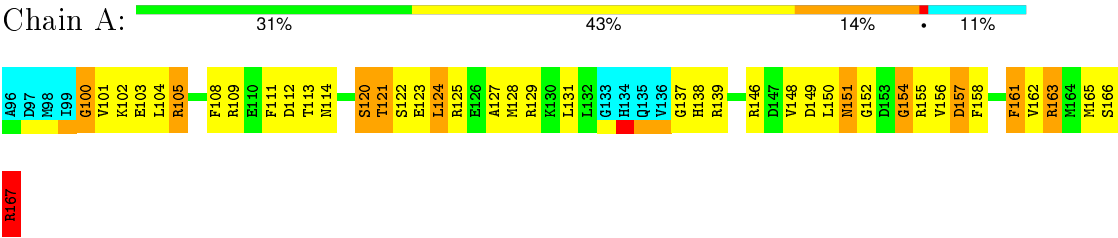


S166

R167

4.2.15 Score per residue for model 15

- Molecule 1: Calcium-binding protein 1



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	refinement	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

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	1.12±0.00	1±0/527 (0.2±0.0%)	1.26±0.00	0±0/699 (0.0±0.0%)
All	All	1.12	15/7905 (0.2%)	1.26	0/10485 (0.0%)

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	0.0±0.0	8.5±0.5
All	All	0	128

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	138	HIS	CG-ND1	-6.15	1.25	1.38	2	15

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	105	ARG	Sidechain	15
1	A	163	ARG	Sidechain	15
1	A	129	ARG	Sidechain	15
1	A	139	ARG	Sidechain	15
1	A	167	ARG	Sidechain	15
1	A	146	ARG	Sidechain	14
1	A	125	ARG	Sidechain	14
1	A	155	ARG	Sidechain	13

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	109	ARG	Sidechain	12

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	523	503	503	38±6
All	All	7845	7545	7545	577

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:LEU:HD21	1:A:165:MET:SD	0.89	2.06	12	2
1:A:150:LEU:N	1:A:150:LEU:HD23	0.83	1.88	7	1
1:A:111:PHE:CE2	1:A:127:ALA:HB2	0.81	2.11	6	14
1:A:108:PHE:CE1	1:A:158:PHE:N	0.80	2.50	14	14
1:A:131:LEU:C	1:A:131:LEU:HD12	0.79	1.97	4	5
1:A:161:PHE:CZ	1:A:165:MET:SD	0.78	2.77	4	1
1:A:161:PHE:CE1	1:A:165:MET:SD	0.78	2.76	4	2
1:A:131:LEU:O	1:A:131:LEU:HD12	0.77	1.79	12	5
1:A:158:PHE:CE1	1:A:162:VAL:CG2	0.77	2.68	7	13
1:A:158:PHE:CZ	1:A:162:VAL:HG21	0.76	2.16	14	13
1:A:158:PHE:O	1:A:162:VAL:HG23	0.74	1.82	10	10
1:A:108:PHE:CE2	1:A:158:PHE:N	0.72	2.58	10	1
1:A:104:LEU:CD2	1:A:165:MET:SD	0.72	2.78	12	1
1:A:128:MET:SD	1:A:165:MET:CE	0.71	2.78	2	6
1:A:108:PHE:CE1	1:A:158:PHE:CA	0.69	2.76	14	10
1:A:148:VAL:O	1:A:148:VAL:HG13	0.68	1.89	9	2
1:A:111:PHE:CE2	1:A:127:ALA:CB	0.68	2.76	3	13
1:A:118:GLU:CD	1:A:118:GLU:N	0.67	2.48	5	1
1:A:114:ASN:HD22	1:A:114:ASN:H	0.66	1.34	3	1
1:A:164:MET:SD	1:A:164:MET:C	0.65	2.74	7	2
1:A:150:LEU:CD2	1:A:150:LEU:N	0.65	2.59	4	2
1:A:104:LEU:N	1:A:104:LEU:CD1	0.65	2.59	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:VAL:HG12	1:A:149:ASP:N	0.65	2.05	6	2
1:A:150:LEU:HD12	1:A:150:LEU:N	0.65	2.07	15	1
1:A:108:PHE:CD2	1:A:112:ASP:OD2	0.64	2.51	9	2
1:A:150:LEU:N	1:A:150:LEU:CD2	0.64	2.61	7	2
1:A:108:PHE:CZ	1:A:158:PHE:N	0.64	2.65	14	11
1:A:114:ASN:ND2	1:A:114:ASN:H	0.64	1.91	3	1
1:A:108:PHE:CE2	1:A:112:ASP:OD2	0.64	2.50	9	2
1:A:103:GLU:CD	1:A:103:GLU:N	0.63	2.52	2	1
1:A:111:PHE:CD2	1:A:127:ALA:HB2	0.62	2.29	3	4
1:A:165:MET:C	1:A:167:ARG:N	0.62	2.50	8	15
1:A:138:HIS:ND1	1:A:138:HIS:N	0.62	2.47	4	2
1:A:150:LEU:HD22	1:A:150:LEU:N	0.62	2.08	4	2
1:A:122:SER:OG	1:A:123:GLU:N	0.61	2.33	8	5
1:A:153:ASP:OD1	1:A:153:ASP:N	0.61	2.31	6	3
1:A:157:ASP:OD1	1:A:159:GLU:N	0.61	2.33	6	2
1:A:131:LEU:N	1:A:131:LEU:CD1	0.61	2.62	13	1
1:A:119:ILE:O	1:A:156:VAL:HG13	0.61	1.96	1	7
1:A:108:PHE:CE2	1:A:158:PHE:CA	0.61	2.84	10	1
1:A:126:GLU:OE1	1:A:126:GLU:N	0.60	2.35	14	1
1:A:165:MET:C	1:A:167:ARG:H	0.60	2.00	12	15
1:A:131:LEU:HD12	1:A:132:LEU:N	0.59	2.12	4	3
1:A:158:PHE:CE1	1:A:162:VAL:HG21	0.59	2.32	14	4
1:A:104:LEU:CD2	1:A:104:LEU:N	0.58	2.66	6	1
1:A:103:GLU:N	1:A:103:GLU:OE1	0.58	2.35	15	1
1:A:157:ASP:OD1	1:A:158:PHE:N	0.58	2.36	3	3
1:A:124:LEU:CD1	1:A:161:PHE:CD1	0.57	2.88	15	3
1:A:124:LEU:HD11	1:A:164:MET:CE	0.57	2.30	2	2
1:A:149:ASP:OD2	1:A:150:LEU:N	0.57	2.37	4	1
1:A:162:VAL:O	1:A:166:SER:N	0.56	2.38	2	14
1:A:144:ILE:CG2	1:A:164:MET:SD	0.56	2.93	11	1
1:A:149:ASP:OD2	1:A:151:ASN:ND2	0.56	2.38	12	1
1:A:157:ASP:OD1	1:A:160:GLU:N	0.56	2.31	1	1
1:A:131:LEU:HD12	1:A:131:LEU:C	0.56	2.21	7	4
1:A:104:LEU:CD1	1:A:104:LEU:N	0.56	2.67	9	2
1:A:151:ASN:HD22	1:A:152:GLY:H	0.56	1.40	6	1
1:A:157:ASP:N	1:A:157:ASP:OD1	0.55	2.37	13	3
1:A:132:LEU:C	1:A:132:LEU:HD12	0.55	2.22	4	1
1:A:104:LEU:CD1	1:A:131:LEU:HD23	0.55	2.31	13	1
1:A:150:LEU:HD23	1:A:150:LEU:N	0.55	2.16	1	1
1:A:128:MET:SD	1:A:165:MET:HE2	0.55	2.42	2	1
1:A:150:LEU:CD1	1:A:150:LEU:N	0.55	2.70	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:VAL:O	1:A:150:LEU:N	0.55	2.40	3	1
1:A:114:ASN:ND2	1:A:114:ASN:C	0.55	2.61	5	1
1:A:165:MET:O	1:A:167:ARG:N	0.54	2.40	6	15
1:A:115:GLY:O	1:A:117:GLY:N	0.54	2.40	4	2
1:A:118:GLU:OE1	1:A:118:GLU:N	0.54	2.40	5	1
1:A:100:GLY:O	1:A:102:LYS:N	0.54	2.40	5	5
1:A:113:THR:C	1:A:115:GLY:H	0.54	2.06	5	3
1:A:114:ASN:ND2	1:A:114:ASN:O	0.54	2.41	5	1
1:A:104:LEU:CG	1:A:165:MET:SD	0.53	2.96	12	1
1:A:158:PHE:CZ	1:A:162:VAL:CG2	0.53	2.91	7	9
1:A:111:PHE:O	1:A:113:THR:N	0.53	2.41	8	13
1:A:114:ASN:ND2	1:A:114:ASN:N	0.53	2.55	3	1
1:A:149:ASP:O	1:A:151:ASN:N	0.53	2.42	8	2
1:A:112:ASP:O	1:A:114:ASN:N	0.53	2.42	13	1
1:A:137:GLY:N	1:A:140:ASP:OD1	0.53	2.42	7	1
1:A:111:PHE:CD1	1:A:123:GLU:OE1	0.53	2.61	12	1
1:A:139:ARG:CD	1:A:139:ARG:N	0.53	2.72	13	1
1:A:167:ARG:C	1:A:167:ARG:CD	0.53	2.77	1	1
1:A:124:LEU:HD23	1:A:145:ILE:CD1	0.53	2.34	12	3
1:A:158:PHE:CE2	1:A:162:VAL:HG21	0.53	2.39	9	6
1:A:146:ARG:O	1:A:148:VAL:N	0.52	2.42	4	3
1:A:100:GLY:C	1:A:102:LYS:N	0.52	2.63	5	5
1:A:162:VAL:O	1:A:165:MET:N	0.52	2.42	7	2
1:A:101:VAL:O	1:A:104:LEU:N	0.52	2.42	15	2
1:A:120:SER:O	1:A:122:SER:N	0.52	2.42	10	2
1:A:116:ASP:OD1	1:A:116:ASP:N	0.52	2.42	10	2
1:A:128:MET:SD	1:A:165:MET:HE1	0.52	2.44	13	3
1:A:113:THR:O	1:A:115:GLY:N	0.52	2.42	13	3
1:A:150:LEU:H	1:A:150:LEU:HD12	0.52	1.65	8	1
1:A:104:LEU:HD21	1:A:165:MET:CB	0.52	2.35	12	1
1:A:117:GLY:C	1:A:118:GLU:CD	0.52	2.68	5	1
1:A:153:ASP:CG	1:A:154:GLY:H	0.52	2.09	6	2
1:A:150:LEU:HD22	1:A:150:LEU:H	0.52	1.64	4	1
1:A:112:ASP:OD2	1:A:117:GLY:N	0.52	2.43	14	1
1:A:146:ARG:C	1:A:148:VAL:N	0.52	2.63	13	3
1:A:159:GLU:O	1:A:163:ARG:N	0.51	2.42	14	3
1:A:112:ASP:OD1	1:A:112:ASP:C	0.51	2.48	14	3
1:A:131:LEU:C	1:A:131:LEU:CD1	0.51	2.68	4	1
1:A:104:LEU:HD11	1:A:165:MET:SD	0.51	2.45	5	1
1:A:150:LEU:O	1:A:152:GLY:N	0.51	2.41	5	1
1:A:114:ASN:O	1:A:114:ASN:ND2	0.51	2.42	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:GLU:O	1:A:147:ASP:N	0.51	2.44	13	2
1:A:115:GLY:C	1:A:117:GLY:H	0.51	2.09	8	1
1:A:140:ASP:CG	1:A:141:ILE:N	0.51	2.63	11	1
1:A:142:GLU:OE1	1:A:142:GLU:N	0.51	2.44	6	1
1:A:127:ALA:O	1:A:130:LYS:N	0.50	2.43	6	3
1:A:115:GLY:C	1:A:117:GLY:N	0.50	2.65	8	2
1:A:163:ARG:C	1:A:165:MET:N	0.50	2.63	1	2
1:A:148:VAL:CG1	1:A:149:ASP:N	0.50	2.75	8	2
1:A:124:LEU:HD12	1:A:161:PHE:CD1	0.50	2.42	15	3
1:A:137:GLY:O	1:A:140:ASP:N	0.50	2.45	4	1
1:A:137:GLY:O	1:A:139:ARG:N	0.50	2.45	6	4
1:A:164:MET:SD	1:A:164:MET:O	0.50	2.70	4	2
1:A:138:HIS:CD2	1:A:139:ARG:N	0.50	2.79	1	1
1:A:108:PHE:O	1:A:112:ASP:N	0.50	2.39	15	7
1:A:120:SER:C	1:A:122:SER:N	0.49	2.62	10	3
1:A:115:GLY:C	1:A:116:ASP:CG	0.49	2.71	1	1
1:A:148:VAL:O	1:A:149:ASP:CB	0.49	2.60	6	1
1:A:113:THR:C	1:A:115:GLY:N	0.49	2.65	13	4
1:A:131:LEU:HD12	1:A:131:LEU:O	0.49	2.06	2	1
1:A:140:ASP:N	1:A:140:ASP:OD1	0.49	2.44	13	2
1:A:131:LEU:O	1:A:132:LEU:CB	0.49	2.59	1	1
1:A:124:LEU:HD23	1:A:125:ARG:N	0.49	2.23	9	6
1:A:150:LEU:HD12	1:A:150:LEU:C	0.49	2.27	5	1
1:A:115:GLY:C	1:A:116:ASP:OD1	0.49	2.52	5	1
1:A:158:PHE:CD1	1:A:162:VAL:CG2	0.48	2.96	7	3
1:A:104:LEU:HD22	1:A:104:LEU:N	0.48	2.23	6	1
1:A:161:PHE:CD1	1:A:161:PHE:C	0.48	2.87	14	4
1:A:149:ASP:C	1:A:149:ASP:OD1	0.48	2.51	10	1
1:A:147:ASP:O	1:A:149:ASP:N	0.48	2.46	13	1
1:A:112:ASP:C	1:A:114:ASN:H	0.48	2.10	13	1
1:A:148:VAL:O	1:A:148:VAL:CG1	0.48	2.61	15	2
1:A:104:LEU:HD12	1:A:104:LEU:N	0.48	2.22	15	2
1:A:150:LEU:N	1:A:150:LEU:HD12	0.48	2.23	9	1
1:A:115:GLY:O	1:A:116:ASP:CB	0.48	2.62	7	2
1:A:147:ASP:OD1	1:A:147:ASP:C	0.47	2.53	8	1
1:A:125:ARG:C	1:A:125:ARG:CD	0.47	2.83	4	1
1:A:128:MET:SD	1:A:144:ILE:HG21	0.47	2.49	8	1
1:A:138:HIS:ND1	1:A:139:ARG:N	0.47	2.63	6	1
1:A:140:ASP:OD1	1:A:141:ILE:N	0.47	2.47	11	1
1:A:112:ASP:C	1:A:112:ASP:OD1	0.47	2.53	2	2
1:A:100:GLY:C	1:A:102:LYS:H	0.47	2.12	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:ASP:CG	1:A:158:PHE:N	0.47	2.68	9	3
1:A:150:LEU:HD23	1:A:150:LEU:H	0.47	1.67	7	1
1:A:131:LEU:O	1:A:131:LEU:CD1	0.47	2.62	8	2
1:A:142:GLU:C	1:A:142:GLU:CD	0.47	2.74	4	1
1:A:144:ILE:HG23	1:A:164:MET:SD	0.47	2.50	11	1
1:A:112:ASP:OD1	1:A:112:ASP:N	0.47	2.45	7	1
1:A:123:GLU:N	1:A:123:GLU:OE1	0.47	2.48	6	1
1:A:151:ASN:HD22	1:A:152:GLY:N	0.47	2.06	6	1
1:A:146:ARG:C	1:A:148:VAL:H	0.47	2.12	13	2
1:A:131:LEU:HD12	1:A:132:LEU:HB2	0.47	1.87	11	1
1:A:149:ASP:CG	1:A:150:LEU:N	0.47	2.67	4	1
1:A:142:GLU:O	1:A:146:ARG:N	0.47	2.45	8	2
1:A:104:LEU:CD1	1:A:161:PHE:CZ	0.46	2.98	6	1
1:A:137:GLY:C	1:A:139:ARG:N	0.46	2.67	6	4
1:A:150:LEU:C	1:A:151:ASN:CG	0.46	2.74	1	1
1:A:167:ARG:C	1:A:167:ARG:HE	0.46	2.14	9	1
1:A:158:PHE:CD1	1:A:162:VAL:HG23	0.45	2.47	7	1
1:A:149:ASP:N	1:A:149:ASP:OD1	0.45	2.47	15	1
1:A:120:SER:O	1:A:123:GLU:N	0.45	2.49	15	1
1:A:141:ILE:HG22	1:A:142:GLU:N	0.45	2.25	3	1
1:A:131:LEU:N	1:A:131:LEU:HD12	0.45	2.27	13	1
1:A:157:ASP:C	1:A:157:ASP:OD1	0.45	2.54	1	1
1:A:104:LEU:HD22	1:A:104:LEU:H	0.45	1.72	13	1
1:A:149:ASP:O	1:A:150:LEU:CB	0.45	2.64	6	1
1:A:111:PHE:CE1	1:A:123:GLU:O	0.45	2.70	6	1
1:A:147:ASP:O	1:A:148:VAL:C	0.44	2.54	13	1
1:A:138:HIS:CD2	1:A:139:ARG:HG3	0.44	2.48	1	1
1:A:112:ASP:N	1:A:112:ASP:OD1	0.44	2.51	5	1
1:A:163:ARG:CG	1:A:163:ARG:O	0.44	2.66	8	1
1:A:151:ASN:CG	1:A:152:GLY:N	0.44	2.70	3	1
1:A:108:PHE:CE1	1:A:158:PHE:HA	0.44	2.45	14	2
1:A:100:GLY:O	1:A:103:GLU:N	0.44	2.51	6	1
1:A:148:VAL:HG23	1:A:149:ASP:N	0.43	2.27	3	1
1:A:129:ARG:CD	1:A:129:ARG:O	0.43	2.66	7	1
1:A:153:ASP:O	1:A:155:ARG:N	0.43	2.51	2	1
1:A:104:LEU:HD11	1:A:165:MET:CE	0.43	2.43	6	1
1:A:111:PHE:CE2	1:A:127:ALA:HA	0.43	2.49	3	1
1:A:157:ASP:OD2	1:A:160:GLU:N	0.43	2.49	14	1
1:A:108:PHE:CD2	1:A:158:PHE:HA	0.43	2.48	10	1
1:A:101:VAL:HA	1:A:104:LEU:HD23	0.43	1.90	13	1
1:A:104:LEU:N	1:A:104:LEU:HD13	0.43	2.29	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:HIS:CG	1:A:139:ARG:N	0.43	2.87	8	1
1:A:159:GLU:O	1:A:163:ARG:CB	0.43	2.67	14	1
1:A:123:GLU:OE1	1:A:123:GLU:N	0.43	2.51	13	1
1:A:161:PHE:C	1:A:161:PHE:CD1	0.43	2.91	7	1
1:A:137:GLY:C	1:A:139:ARG:H	0.43	2.17	6	1
1:A:155:ARG:O	1:A:155:ARG:CG	0.43	2.66	8	1
1:A:122:SER:OG	1:A:123:GLU:OE1	0.43	2.36	1	1
1:A:150:LEU:HD23	1:A:150:LEU:O	0.43	2.14	6	1
1:A:121:THR:O	1:A:125:ARG:N	0.42	2.45	7	2
1:A:113:THR:O	1:A:114:ASN:CB	0.42	2.65	8	1
1:A:104:LEU:HD23	1:A:104:LEU:N	0.42	2.27	8	1
1:A:108:PHE:O	1:A:112:ASP:CB	0.42	2.66	15	1
1:A:108:PHE:CE2	1:A:158:PHE:HB2	0.42	2.49	11	5
1:A:125:ARG:NH1	1:A:129:ARG:NH1	0.42	2.66	5	1
1:A:167:ARG:C	1:A:167:ARG:NE	0.42	2.73	9	1
1:A:131:LEU:HD12	1:A:132:LEU:CB	0.42	2.44	11	1
1:A:108:PHE:CE2	1:A:112:ASP:CG	0.42	2.93	6	1
1:A:145:ILE:CG2	1:A:145:ILE:O	0.42	2.67	4	1
1:A:151:ASN:C	1:A:153:ASP:N	0.42	2.73	7	1
1:A:108:PHE:CZ	1:A:158:PHE:HB2	0.42	2.49	14	5
1:A:143:GLU:O	1:A:146:ARG:N	0.42	2.53	14	1
1:A:146:ARG:O	1:A:147:ASP:C	0.42	2.58	14	2
1:A:111:PHE:CE2	1:A:127:ALA:CA	0.42	3.03	3	1
1:A:108:PHE:CE2	1:A:112:ASP:OD1	0.42	2.73	6	1
1:A:101:VAL:O	1:A:102:LYS:C	0.42	2.58	15	1
1:A:102:LYS:HD2	1:A:102:LYS:N	0.42	2.30	3	1
1:A:104:LEU:HD11	1:A:165:MET:HG2	0.42	1.92	8	1
1:A:105:ARG:HA	1:A:158:PHE:CZ	0.42	2.50	4	2
1:A:111:PHE:CZ	1:A:127:ALA:HA	0.42	2.49	3	2
1:A:100:GLY:O	1:A:101:VAL:C	0.42	2.57	6	1
1:A:118:GLU:CD	1:A:118:GLU:C	0.41	2.79	3	1
1:A:140:ASP:OD1	1:A:140:ASP:C	0.41	2.58	11	2
1:A:107:ALA:HB2	1:A:131:LEU:HD21	0.41	1.92	13	1
1:A:166:SER:O	1:A:167:ARG:C	0.41	2.58	10	4
1:A:108:PHE:CE1	1:A:158:PHE:HB2	0.41	2.51	6	3
1:A:120:SER:O	1:A:121:THR:C	0.41	2.57	4	6
1:A:154:GLY:C	1:A:155:ARG:CG	0.41	2.89	15	1
1:A:158:PHE:O	1:A:162:VAL:N	0.41	2.41	2	3
1:A:104:LEU:HG	1:A:165:MET:SD	0.41	2.55	12	1
1:A:112:ASP:C	1:A:114:ASN:N	0.41	2.74	13	1
1:A:104:LEU:HD11	1:A:165:MET:CG	0.41	2.44	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:LEU:O	1:A:151:ASN:CB	0.41	2.66	13	1
1:A:153:ASP:CG	1:A:154:GLY:N	0.41	2.73	6	1
1:A:124:LEU:CD2	1:A:145:ILE:CD1	0.41	2.98	2	2
1:A:151:ASN:ND2	1:A:152:GLY:H	0.41	2.11	6	1
1:A:115:GLY:O	1:A:116:ASP:C	0.41	2.59	4	1
1:A:104:LEU:HD23	1:A:162:VAL:HG13	0.41	1.91	9	1
1:A:150:LEU:CD1	1:A:150:LEU:C	0.41	2.89	5	1
1:A:105:ARG:NE	1:A:105:ARG:O	0.41	2.52	6	1
1:A:112:ASP:CG	1:A:112:ASP:O	0.40	2.60	1	1
1:A:103:GLU:O	1:A:107:ALA:HB2	0.40	2.15	4	1
1:A:118:GLU:OE1	1:A:155:ARG:NH1	0.40	2.54	6	1
1:A:162:VAL:HG12	1:A:166:SER:OG	0.40	2.15	2	1
1:A:107:ALA:CB	1:A:131:LEU:HD21	0.40	2.46	13	1
1:A:151:ASN:O	1:A:153:ASP:N	0.40	2.54	7	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	63/72 (88%)	48±3 (77±4%)	9±2 (14±3%)	6±2 (10±4%)	2	11
All	All	945/1080 (88%)	724 (77%)	129 (14%)	92 (10%)	2	11

All 21 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	112	ASP	13
1	A	166	SER	12
1	A	117	GLY	8
1	A	151	ASN	6
1	A	116	ASP	6
1	A	101	VAL	5
1	A	100	GLY	5
1	A	149	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	154	GLY	4
1	A	114	ASN	3
1	A	152	GLY	3
1	A	148	VAL	3
1	A	147	ASP	3
1	A	150	LEU	3
1	A	113	THR	3
1	A	138	HIS	2
1	A	137	GLY	2
1	A	115	GLY	2
1	A	153	ASP	2
1	A	132	LEU	2
1	A	121	THR	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	56/62 (90%)	44±3 (79±5%)	12±3 (21±5%)	4	33
All	All	840/930 (90%)	661 (79%)	179 (21%)	4	33

All 45 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	156	VAL	15
1	A	167	ARG	15
1	A	124	LEU	14
1	A	121	THR	12
1	A	161	PHE	9
1	A	144	ILE	7
1	A	155	ARG	7
1	A	157	ASP	6
1	A	164	MET	6
1	A	129	ARG	5
1	A	123	GLU	5
1	A	138	HIS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	128	MET	5
1	A	116	ASP	4
1	A	151	ASN	4
1	A	109	ARG	4
1	A	140	ASP	4
1	A	118	GLU	3
1	A	142	GLU	3
1	A	130	LYS	3
1	A	105	ARG	3
1	A	120	SER	3
1	A	125	ARG	3
1	A	139	ARG	3
1	A	149	ASP	3
1	A	114	ASN	2
1	A	146	ARG	2
1	A	112	ASP	2
1	A	102	LYS	2
1	A	153	ASP	2
1	A	101	VAL	2
1	A	131	LEU	2
1	A	126	GLU	2
1	A	106	ASP	1
1	A	160	GLU	1
1	A	132	LEU	1
1	A	165	MET	1
1	A	159	GLU	1
1	A	141	ILE	1
1	A	110	GLU	1
1	A	104	LEU	1
1	A	163	ARG	1
1	A	150	LEU	1
1	A	113	THR	1
1	A	103	GLU	1

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