Full wwPDB NMR Structure Validation Report (i)

Mar 5, 2022 – 02:36 PM EST

PDB ID	:	2K7C
Title	:	NMR Structure of Mg2+-bound CaBP1 C-domain
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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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

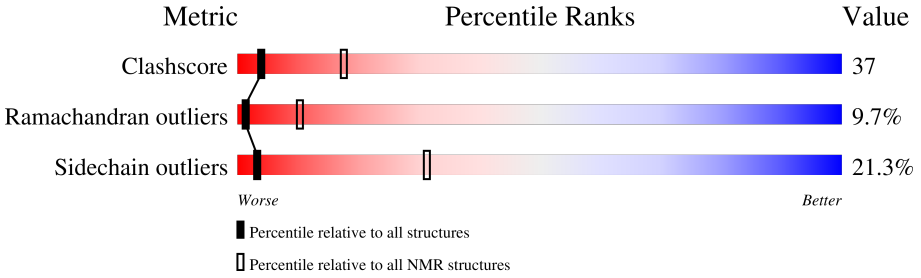
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	72	24% 53% 11% • 11%

2 Ensemble composition and analysis (i)

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
			Total	C	H	N	O	S	
1	A	72	1141	353	559	108	117	4	0

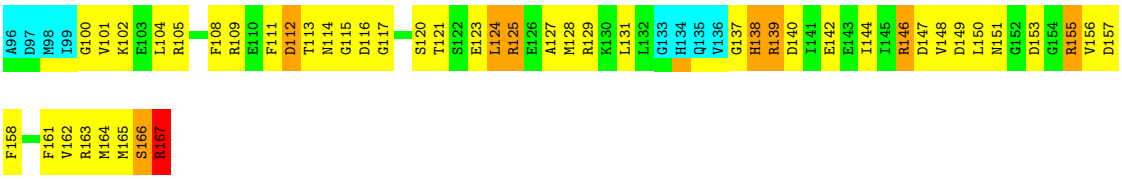
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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-binding protein 1

Chain A: 24% 53% 11% • 11%



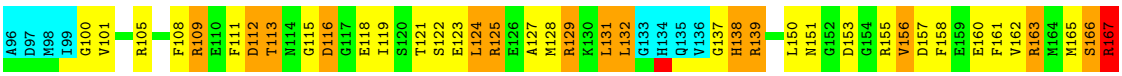
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Calcium-binding protein 1

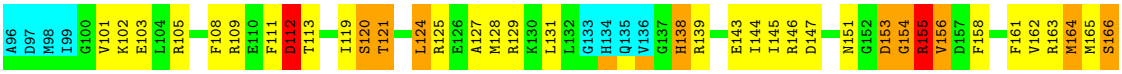
Chain A: 35% 33% 19% • 11%



4.2.2 Score per residue for model 2

• Molecule 1: Calcium-binding protein 1

Chain A: 36% 36% 12% • 11%



R167

4.2.3 Score per residue for model 3

- Molecule 1: Calcium-binding protein 1

Chain A: 29% 49% 10% • 11%

A96 D97 M98 I99 K102 R105 F108 R109 E110 F111 D112 T113 N114 G115 D116 G117 E118 I119 S120 T121 L124 R125 E126 A127 M128 R129 K130 L131 L132 G133 H134 Q135 V136 G137 H138 R139 D140 I141 E142 E143 I144 I145 R146 D147 V148 D149 L150 N151 G152 D153 V156 D157 F158 F161

V162 R163 M164 M165 S166 R167

4.2.4 Score per residue for model 4

- Molecule 1: Calcium-binding protein 1

Chain A: 28% 38% 18% 6% 11%

A96 D97 M98 I99 E103 L104 R105 D106 A107 F108 F111 D112 T113 N114 G115 D116 G117 E118 I119 S120 T121 R125 E126 A127 M128 R129 K130 L131 L132 G133 H134 Q135 V136 G137 H138 R139 D140 I141 E142 E143 I144 I145 R146 D147 V148 D149 L150 D153 G154 R155 V156 D157 F158 E159 E160 F161

V162 R163 M164 M165 S166 R167

4.2.5 Score per residue for model 5

- Molecule 1: Calcium-binding protein 1

Chain A: 36% 35% 12% 6% 11%

A96 D97 M98 I99 G100 V101 K102 E103 L104 R105 F108 R109 E110 F111 D112 T113 N114 G115 D116 G117 E118 L124 R125 E126 A127 M128 R129 K130 L131 L132 G133 H134 Q135 V136 G137 H138 R139 I145 R146 L150 N151 G152 D153 G154 R155 V156 D157 F158 F161 V162 R163 M164 M165 S166 R167

4.2.6 Score per residue for model 6

- Molecule 1: Calcium-binding protein 1

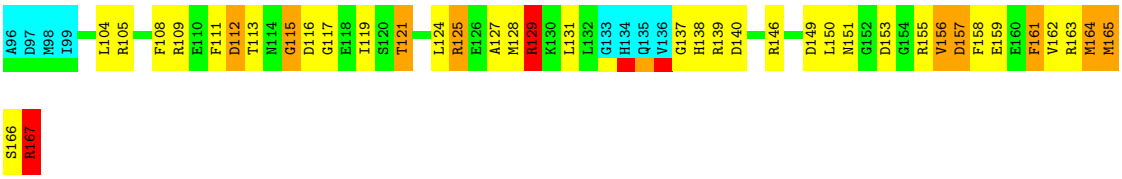
Chain A: 26% 31% 25% 7% 11%

A96 D97 M98 I99 G100 V101 K102 E103 L104 R105 F108 R109 E110 F111 D112 T113 E118 I119 S120 T121 S122 E123 L124 R125 E126 A127 M128 R129 K130 G133 H134 Q135 V136 G137 H138 R139 E142 I145 R146 D147 V148 D149 L150 N151 G152 D153 G154 R155 V156 D157 F158 E159 E160 F161 V162

4.2.7 Score per residue for model 7

• Molecule 1: Calcium-binding protein 1

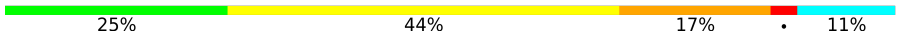
Chain A:

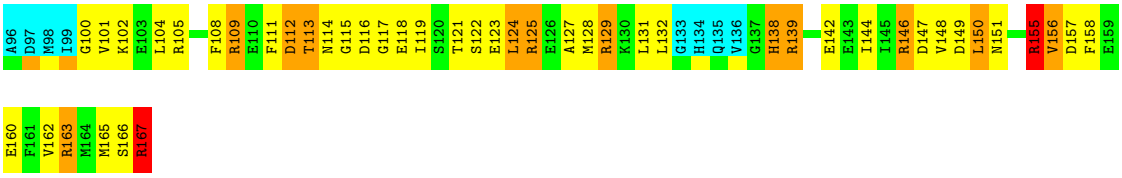


4.2.8 Score per residue for model 8

• Molecule 1: Calcium-binding protein 1

Chain A:

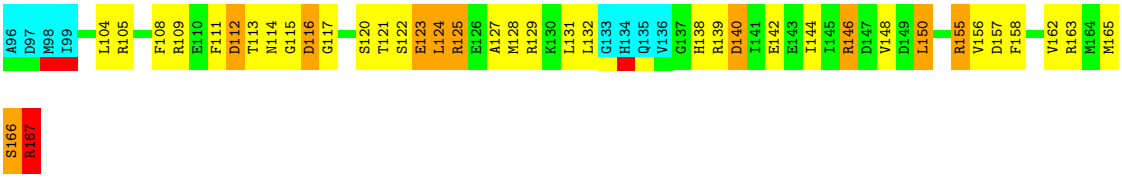




4.2.9 Score per residue for model 9

• Molecule 1: Calcium-binding protein 1

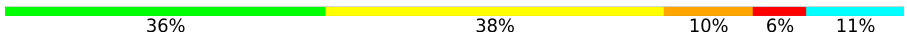
Chain A:



4.2.10 Score per residue for model 10 (medoid)

• Molecule 1: Calcium-binding protein 1

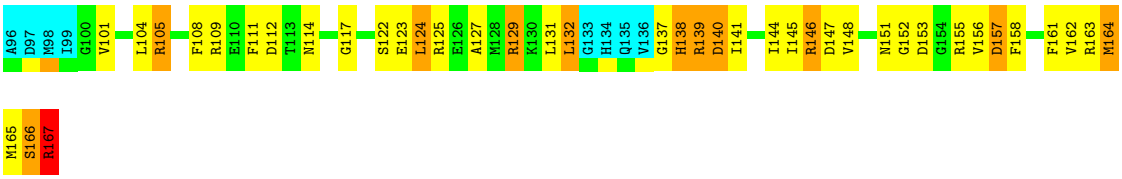
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: Calcium-binding protein 1

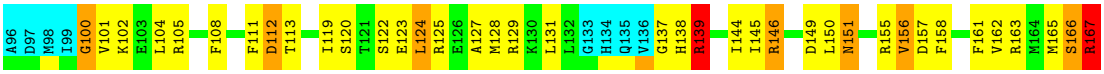
Chain A: 32% 40% 15% • 11%



4.2.12 Score per residue for model 12

- Molecule 1: Calcium-binding protein 1

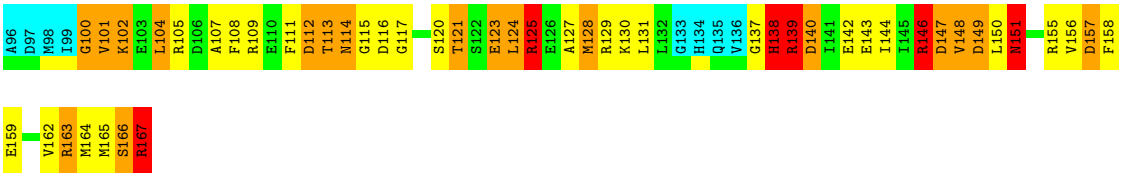
Chain A: 36% 40% 10% • 11%



4.2.13 Score per residue for model 13

- Molecule 1: Calcium-binding protein 1

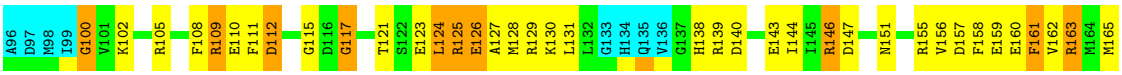
Chain A: 21% 35% 25% 8% 11%



4.2.14 Score per residue for model 14

- Molecule 1: Calcium-binding protein 1

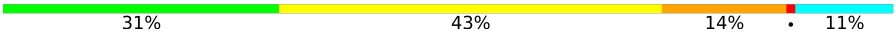
Chain A: 33% 39% 15% • 11%

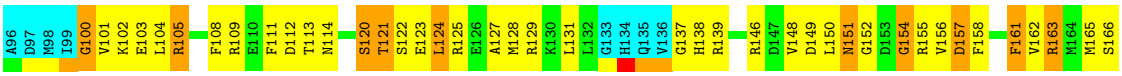


4.2.15 Score per residue for model 15

- Molecule 1: Calcium-binding protein 1

Chain A:





5 Refinement protocol and experimental data overview (i)

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.

6 Model quality (i)

6.1 Standard geometry (i)

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	129	ARG	Sidechain	15
1	A	139	ARG	Sidechain	15
1	A	163	ARG	Sidechain	15
1	A	167	ARG	Sidechain	15
1	A	125	ARG	Sidechain	14
1	A	146	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 (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	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:HD23	1:A:150:LEU:N	0.83	1.88	7	2
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	4
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:HD12	1:A:131:LEU:O	0.77	1.79	12	6
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:HG13	1:A:148:VAL:O	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:N	1:A:118:GLU:CD	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:C	1:A:164:MET:SD	0.65	2.74	7	2
1:A:150:LEU:N	1:A:150:LEU:CD2	0.65	2.59	4	4
1:A:104:LEU:N	1:A:104:LEU:CD1	0.65	2.59	15	5

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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	2
1:A:108:PHE:CD2	1:A:112:ASP:OD2	0.64	2.51	9	2
1:A:108:PHE:CZ	1:A:158:PHE:N	0.64	2.65	14	11
1:A:114:ASN:H	1:A:114:ASN:ND2	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:N	1:A:103:GLU:CD	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:N	1:A:138:HIS:ND1	0.62	2.47	4	2
1:A:150:LEU:N	1:A:150:LEU:HD22	0.62	2.08	4	2
1:A:153:ASP:N	1:A:153:ASP:OD1	0.61	2.31	6	3
1:A:122:SER:OG	1:A:123:GLU:N	0.61	2.33	8	5
1:A:157:ASP:OD1	1:A:159:GLU:N	0.61	2.33	6	2
1:A:131:LEU:CD1	1:A:131:LEU:N	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:N	1:A:126:GLU:OE1	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:157:ASP:OD1	1:A:158:PHE:N	0.58	2.36	3	3
1:A:103:GLU:OE1	1:A:103:GLU:N	0.58	2.35	15	1
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:157:ASP:OD1	1:A:160:GLU:N	0.56	2.31	1	1
1:A:149:ASP:OD2	1:A:151:ASN:ND2	0.56	2.38	12	1
1:A:131:LEU:HD12	1:A:131:LEU:C	0.56	2.21	7	5
1:A:151:ASN:HD22	1:A:152:GLY:H	0.56	1.40	6	1
1:A:157:ASP:OD1	1:A:157:ASP:N	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:128:MET:SD	1:A:165:MET:HE2	0.55	2.42	2	1
1:A:150:LEU:N	1:A:150:LEU:CD1	0.55	2.70	15	2
1:A:148:VAL:O	1:A:150:LEU:N	0.55	2.40	3	1
1:A:114:ASN:C	1:A:114:ASN:ND2	0.55	2.61	5	1
1:A:165:MET:O	1:A:167:ARG:N	0.54	2.40	6	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:GLY:O	1:A:117:GLY:N	0.54	2.40	4	2
1:A:118:GLU:N	1:A:118:GLU:OE1	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:111:PHE:O	1:A:113:THR:N	0.53	2.41	8	13
1:A:158:PHE:CZ	1:A:162:VAL:CG2	0.53	2.91	7	9
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:137:GLY:N	1:A:140:ASP:OD1	0.53	2.42	7	1
1:A:112:ASP:O	1:A:114:ASN:N	0.53	2.42	13	1
1:A:111:PHE:CD1	1:A:123:GLU:OE1	0.53	2.61	12	1
1:A:139:ARG:N	1:A:139:ARG:CD	0.53	2.72	13	1
1:A:167:ARG:CD	1:A:167:ARG:C	0.53	2.77	1	1
1:A:158:PHE:CE2	1:A:162:VAL:HG21	0.53	2.39	9	6
1:A:124:LEU:HD23	1:A:145:ILE:CD1	0.53	2.34	12	3
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:116:ASP:N	1:A:116:ASP:OD1	0.52	2.42	10	2
1:A:120:SER:O	1:A:122:SER:N	0.52	2.42	10	2
1:A:101:VAL:O	1:A:104:LEU:N	0.52	2.42	15	2
1:A:113:THR:O	1:A:115:GLY:N	0.52	2.42	13	3
1:A:128:MET:SD	1:A:165:MET:HE1	0.52	2.44	13	3
1:A:150:LEU:HD12	1:A:150:LEU:H	0.52	1.65	8	1
1:A:117:GLY:C	1:A:118:GLU:CD	0.52	2.68	5	1
1:A:104:LEU:HD21	1:A:165:MET:CB	0.52	2.35	12	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:146:ARG:C	1:A:148:VAL:N	0.52	2.63	13	3
1:A:112:ASP:OD2	1:A:117:GLY:N	0.52	2.43	14	1
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	5
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: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:114:ASN:O	1:A:114:ASN:ND2	0.51	2.42	11	2
1:A:140:ASP:CG	1:A:141:ILE:N	0.51	2.63	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:GLU:OE1	1:A:142:GLU:N	0.51	2.44	6	1
1:A:115:GLY:C	1:A:117:GLY:N	0.50	2.65	8	2
1:A:127:ALA:O	1:A:130:LYS:N	0.50	2.43	6	3
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:138:HIS:CD2	1:A:139:ARG:N	0.50	2.79	1	1
1:A:164:MET:SD	1:A:164:MET:O	0.50	2.70	4	2
1:A:108:PHE:O	1:A:112:ASP:N	0.50	2.39	15	7
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:120:SER:C	1:A:122:SER:N	0.49	2.62	10	3
1:A:113:THR:C	1:A:115:GLY:N	0.49	2.65	13	4
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:C	1:A:150:LEU:HD12	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:N	1:A:104:LEU:HD22	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:OD1	1:A:149:ASP:C	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:104:LEU:N	1:A:104:LEU:HD12	0.48	2.22	15	2
1:A:148:VAL:O	1:A:148:VAL:CG1	0.48	2.61	15	2
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:CD	1:A:125:ARG:C	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:100:GLY:C	1:A:102:LYS:H	0.47	2.12	13	3
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:142:GLU:CD	1:A:142:GLU:C	0.47	2.74	4	1
1:A:112:ASP:OD1	1:A:112:ASP:N	0.47	2.45	7	2
1:A:123:GLU:OE1	1:A:123:GLU:N	0.47	2.48	6	2
1:A:151:ASN:HD22	1:A:152:GLY:N	0.47	2.06	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:O	1:A:131:LEU:CD1	0.47	2.62	8	2
1:A:144:ILE:HG23	1:A:164:MET:SD	0.47	2.50	11	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:HE	1:A:167:ARG:C	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:157:ASP:OD1	1:A:157:ASP:C	0.45	2.54	1	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:120:SER:O	1:A:123:GLU:N	0.45	2.49	15	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:163:ARG:O	1:A:163:ARG:CG	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: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
1:A:157:ASP:OD2	1:A:160:GLU:N	0.43	2.49	14	1
1:A:138:HIS:CG	1:A:139:ARG:N	0.43	2.87	8	1
1:A:137:GLY:C	1:A:139:ARG:H	0.43	2.17	6	1
1:A:159:GLU:O	1:A:163:ARG:CB	0.43	2.67	14	1
1:A:122:SER:OG	1:A:123:GLU:OE1	0.43	2.36	1	1
1:A:150:LEU:O	1:A:150:LEU:HD23	0.43	2.14	6	1
1:A:155:ARG:O	1:A:155:ARG:CG	0.43	2.66	8	1
1:A:121:THR:O	1:A:125:ARG:N	0.42	2.45	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:LEU:N	1:A:104:LEU:HD23	0.42	2.27	8	1
1:A:113:THR:O	1:A:114:ASN:CB	0.42	2.65	8	1
1:A:108:PHE:CE2	1:A:158:PHE:HB2	0.42	2.49	11	5
1:A:108:PHE:O	1:A:112:ASP:CB	0.42	2.66	15	1
1:A:125:ARG:NH1	1:A:129:ARG:NH1	0.42	2.66	5	1
1:A:108:PHE:CE2	1:A:112:ASP:CG	0.42	2.93	6	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:145:ILE:O	1:A:145:ILE:CG2	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:111:PHE:CE2	1:A:127:ALA:CA	0.42	3.03	3	1
1:A:146:ARG:O	1:A:147:ASP:C	0.42	2.57	3	2
1:A:108:PHE:CE2	1:A:112:ASP:OD1	0.42	2.73	6	1
1:A:161:PHE:C	1:A:161:PHE:CD1	0.42	2.90	6	1
1:A:143:GLU:O	1:A:146:ARG:N	0.42	2.53	14	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:101:VAL:O	1:A:102:LYS:C	0.42	2.58	15	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:108:PHE:CE1	1:A:158:PHE:HB2	0.41	2.51	6	3
1:A:166:SER:O	1:A:167:ARG:C	0.41	2.58	10	4
1:A:120:SER:O	1:A:121:THR:C	0.41	2.59	3	6
1:A:158:PHE:O	1:A:162:VAL:N	0.41	2.41	2	3
1:A:154:GLY:C	1:A:155:ARG:CG	0.41	2.89	15	1
1:A:104:LEU:HG	1:A:165:MET:SD	0.41	2.55	12	1
1:A:104:LEU:HD11	1:A:165:MET:CG	0.41	2.44	8	1
1:A:112:ASP:C	1:A:114:ASN:N	0.41	2.74	13	1
1:A:153:ASP:CG	1:A:154:GLY:N	0.41	2.73	6	1
1:A:150:LEU:O	1:A:151:ASN:CB	0.41	2.66	13	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:150:LEU:C	1:A:150:LEU:CD1	0.41	2.89	5	1
1:A:104:LEU:HD23	1:A:162:VAL:HG13	0.41	1.91	9	1
1:A:105:ARG:O	1:A:105:ARG:NE	0.41	2.52	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:ASP:O	1:A:112:ASP:CG	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:151:ASN:O	1:A:153:ASP:N	0.40	2.54	7	1
1:A:107:ALA:CB	1:A:131:LEU:HD21	0.40	2.46	13	1

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	63/72 (88%)	48±3 (77±4%)	9±2 (14±3%)	6±2 (10±4%)	1 10
All	All	945/1080 (88%)	724 (77%)	129 (14%)	92 (10%)	1 10

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	100	GLY	5
1	A	101	VAL	5
1	A	154	GLY	4
1	A	149	ASP	4
1	A	113	THR	3
1	A	147	ASP	3
1	A	150	LEU	3
1	A	114	ASN	3
1	A	148	VAL	3
1	A	152	GLY	3
1	A	153	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	137	GLY	2
1	A	138	HIS	2
1	A	115	GLY	2
1	A	132	LEU	2
1	A	121	THR	1

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	56/62 (90%)	44±3 (79±5%)	12±3 (21±5%)	3 31
All	All	840/930 (90%)	661 (79%)	179 (21%)	3 31

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	164	MET	6
1	A	157	ASP	6
1	A	128	MET	5
1	A	129	ARG	5
1	A	138	HIS	5
1	A	123	GLU	5
1	A	109	ARG	4
1	A	116	ASP	4
1	A	151	ASN	4
1	A	140	ASP	4
1	A	118	GLU	3
1	A	120	SER	3
1	A	125	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	130	LYS	3
1	A	142	GLU	3
1	A	105	ARG	3
1	A	149	ASP	3
1	A	139	ARG	3
1	A	101	VAL	2
1	A	131	LEU	2
1	A	153	ASP	2
1	A	102	LYS	2
1	A	112	ASP	2
1	A	114	ASN	2
1	A	126	GLU	2
1	A	146	ARG	2
1	A	132	LEU	1
1	A	141	ILE	1
1	A	159	GLU	1
1	A	103	GLU	1
1	A	150	LEU	1
1	A	165	MET	1
1	A	113	THR	1
1	A	160	GLU	1
1	A	106	ASP	1
1	A	163	ARG	1
1	A	104	LEU	1
1	A	110	GLU	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 monosaccharides 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 (i)

No chemical shift data were provided