



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2022 – 01:59 PM EST

PDB ID : 2K7D
Title : NMR Structure of Ca²⁺-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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

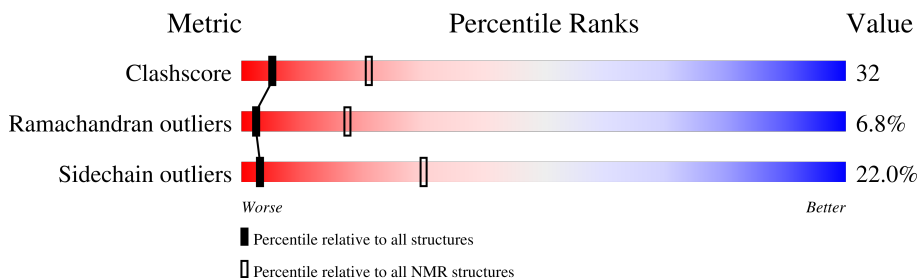
1 Overall quality at a glance i

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	72	

2 Ensemble composition and analysis

This entry contains 15 models. Model 5 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:101-A:167 (67)	0.72	5

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1143 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

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

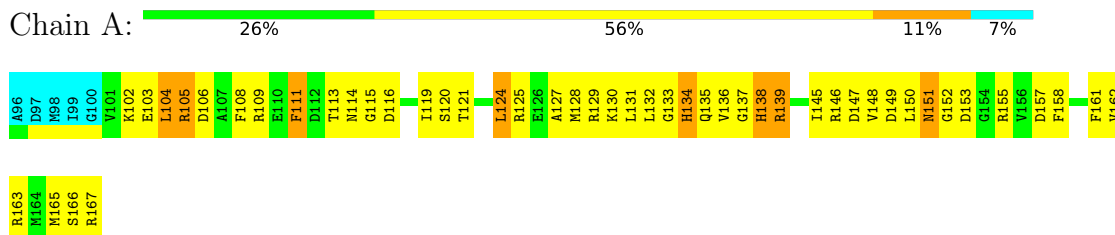
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

4 Residue-property plots

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

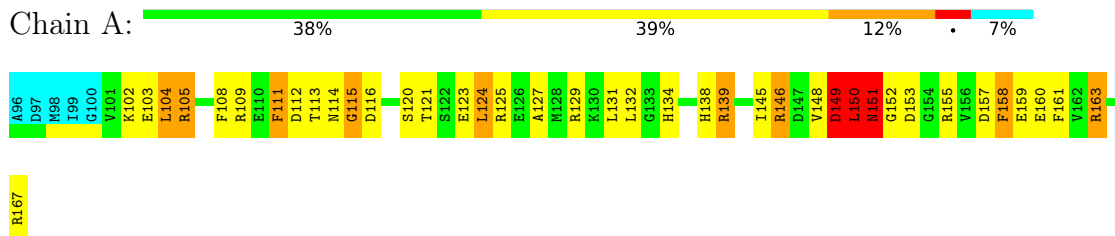


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

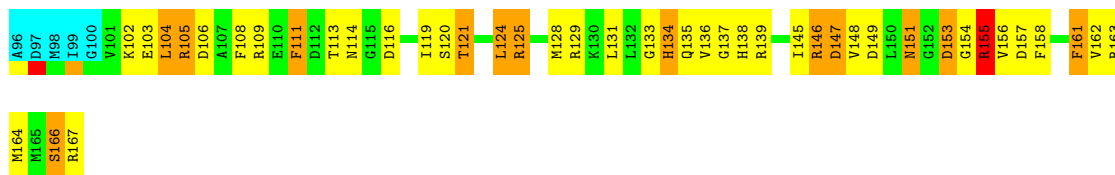
- Molecule 1: Calcium-binding protein 1



4.2.2 Score per residue for model 2

- Molecule 1: Calcium-binding protein 1





4.2.3 Score per residue for model 3

- Molecule 1: Calcium-binding protein 1

Chain A: 44% 35% 12% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Calcium-binding protein 1

Chain A: 36% 36% 19% 7%



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Calcium-binding protein 1

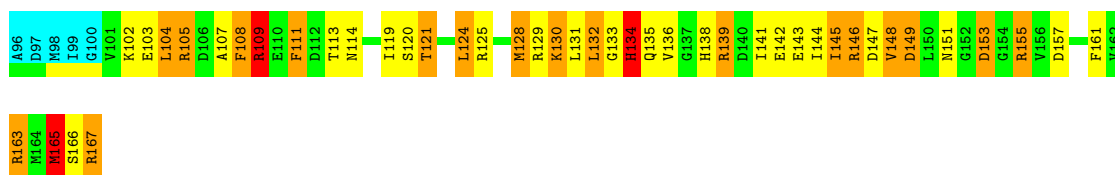
Chain A: 31% 42% 21% 7%



4.2.6 Score per residue for model 6

- Molecule 1: Calcium-binding protein 1

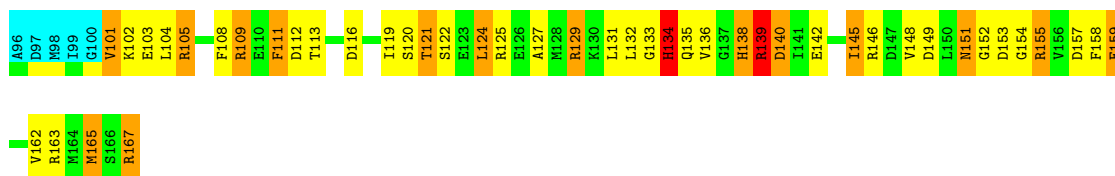
Chain A: 32% 32% 25% 7%



4.2.7 Score per residue for model 7

- Molecule 1: Calcium-binding protein 1

Chain A: 31% 39% 21% 7%



4.2.8 Score per residue for model 8

- Molecule 1: Calcium-binding protein 1

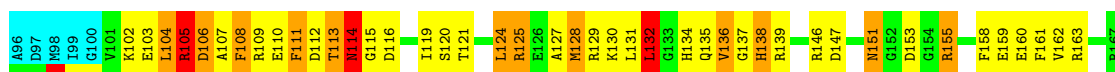
Chain A: 39% 39% 14% 7%



4.2.9 Score per residue for model 9

- Molecule 1: Calcium-binding protein 1

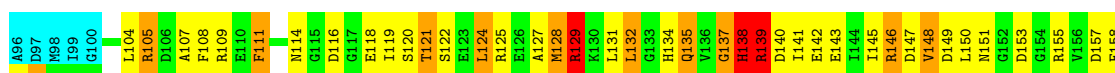
Chain A: 33% 39% 17% 7%



4.2.10 Score per residue for model 10

- Molecule 1: Calcium-binding protein 1

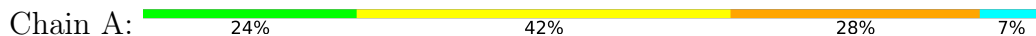
Chain A: 31% 43% 15% 7%





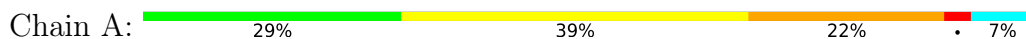
4.2.11 Score per residue for model 11

- Molecule 1: Calcium-binding protein 1



4.2.12 Score per residue for model 12

- Molecule 1: Calcium-binding protein 1



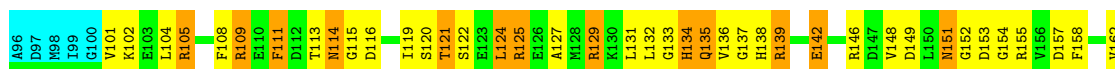
4.2.13 Score per residue for model 13

- Molecule 1: Calcium-binding protein 1



4.2.14 Score per residue for model 14

- Molecule 1: Calcium-binding protein 1





4.2.15 Score per residue for model 15

- Molecule 1: Calcium-binding protein 1

Chain A: 36% 40% 15% 7%



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.

6 Model quality i

6.1 Standard geometry i

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

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	1.14±0.01	2±0/554 (0.4± 0.0%)	1.25±0.00	0±0/736 (0.0± 0.0%)
All	All	1.14	30/8310 (0.4%)	1.25	0/11040 (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	8.7±0.5
All	All	0	130

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	134	HIS	CG-ND1	-6.21	1.25	1.38	5	15
1	A	138	HIS	CG-ND1	-6.17	1.25	1.38	7	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	146	ARG	Sidechain	15

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	163	ARG	Sidechain	15
1	A	109	ARG	Sidechain	14
1	A	125	ARG	Sidechain	14
1	A	155	ARG	Sidechain	14
1	A	167	ARG	Sidechain	13

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	549	527	527	35±7
2	A	2	0	0	0±0
All	All	8265	7905	7905	524

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:VAL:HG13	1:A:149:ASP:N	0.89	1.83	4	7
1:A:148:VAL:HG13	1:A:149:ASP:H	0.82	1.35	12	5
1:A:114:ASN:HD22	1:A:114:ASN:H	0.82	1.16	9	1
1:A:114:ASN:ND2	1:A:116:ASP:N	0.76	2.31	14	1
1:A:104:LEU:CD1	1:A:161:PHE:CE2	0.76	2.69	12	10
1:A:132:LEU:HD12	1:A:133:GLY:N	0.75	1.96	14	1
1:A:114:ASN:H	1:A:114:ASN:ND2	0.75	1.78	13	2
1:A:130:LYS:C	1:A:131:LEU:HD12	0.74	2.02	6	3
1:A:114:ASN:ND2	1:A:115:GLY:N	0.74	2.35	14	1
1:A:111:PHE:CD1	1:A:119:ILE:HD13	0.74	2.18	6	10
1:A:124:LEU:HD21	1:A:128:MET:SD	0.74	2.22	13	1
1:A:128:MET:SD	1:A:132:LEU:HD11	0.73	2.23	11	1
1:A:124:LEU:HD11	1:A:128:MET:SD	0.71	2.25	3	3
1:A:112:ASP:OD1	2:A:501:CA:CA	0.71	1.67	1	1
1:A:104:LEU:HD12	1:A:161:PHE:CE2	0.69	2.22	2	10
1:A:114:ASN:HD22	1:A:115:GLY:N	0.68	1.86	14	1
1:A:124:LEU:HD23	1:A:124:LEU:O	0.68	1.88	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ASN:ND2	1:A:114:ASN:N	0.68	2.42	13	3
1:A:104:LEU:HD12	1:A:162:VAL:HG22	0.67	1.66	10	4
1:A:148:VAL:CG1	1:A:149:ASP:N	0.67	2.55	4	6
1:A:104:LEU:CD1	1:A:161:PHE:CZ	0.67	2.78	2	2
1:A:118:GLU:N	1:A:118:GLU:CD	0.66	2.49	3	1
1:A:148:VAL:CG1	1:A:149:ASP:H	0.66	2.03	4	2
1:A:105:ARG:NH1	1:A:158:PHE:CG	0.66	2.64	8	1
1:A:131:LEU:CD1	1:A:131:LEU:N	0.65	2.59	4	11
1:A:108:PHE:CZ	1:A:158:PHE:N	0.65	2.65	1	8
1:A:111:PHE:CE1	1:A:119:ILE:HD13	0.65	2.27	7	8
1:A:114:ASN:ND2	1:A:116:ASP:H	0.64	1.90	14	1
1:A:114:ASN:N	1:A:114:ASN:HD22	0.64	1.89	13	1
1:A:103:GLU:CG	1:A:104:LEU:N	0.64	2.60	3	2
1:A:132:LEU:CD1	1:A:133:GLY:N	0.64	2.61	14	1
1:A:151:ASN:HD22	1:A:152:GLY:H	0.63	1.35	11	1
1:A:112:ASP:OD2	1:A:115:GLY:N	0.62	2.33	1	1
1:A:101:VAL:CG1	1:A:102:LYS:N	0.62	2.62	11	1
1:A:114:ASN:ND2	1:A:116:ASP:CG	0.62	2.53	14	1
1:A:116:ASP:OD1	1:A:117:GLY:N	0.62	2.33	12	2
1:A:149:ASP:OD2	1:A:154:GLY:N	0.61	2.33	2	1
1:A:106:ASP:N	1:A:106:ASP:OD1	0.61	2.31	5	1
1:A:151:ASN:ND2	1:A:151:ASN:H	0.61	1.92	11	1
1:A:151:ASN:HD22	1:A:152:GLY:N	0.61	1.93	11	1
1:A:166:SER:OG	1:A:167:ARG:N	0.60	2.34	2	3
1:A:153:ASP:OD2	1:A:155:ARG:N	0.60	2.33	12	2
1:A:135:GLN:H	1:A:135:GLN:CD	0.60	1.99	7	2
1:A:151:ASN:ND2	1:A:152:GLY:H	0.60	1.95	11	1
1:A:124:LEU:HD23	1:A:145:ILE:CD1	0.60	2.27	2	1
1:A:116:ASP:CG	1:A:117:GLY:N	0.60	2.54	11	1
1:A:132:LEU:HD12	1:A:132:LEU:N	0.60	2.11	1	2
1:A:138:HIS:H	1:A:138:HIS:CD2	0.60	2.10	4	1
1:A:111:PHE:CD1	1:A:119:ILE:CD1	0.60	2.85	6	8
1:A:128:MET:SD	1:A:132:LEU:CD1	0.60	2.90	11	1
1:A:151:ASN:CG	1:A:152:GLY:N	0.59	2.55	7	3
1:A:148:VAL:HG22	1:A:149:ASP:N	0.59	2.11	12	3
1:A:138:HIS:N	1:A:138:HIS:ND1	0.59	2.51	3	1
1:A:147:ASP:OD1	1:A:148:VAL:N	0.59	2.36	13	1
1:A:153:ASP:CG	1:A:154:GLY:N	0.59	2.55	8	3
1:A:110:GLU:OE2	1:A:130:LYS:NZ	0.59	2.34	12	1
1:A:151:ASN:ND2	1:A:160:GLU:OE2	0.59	2.34	4	1
1:A:136:VAL:O	1:A:136:VAL:HG23	0.59	1.98	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:LEU:HD23	1:A:150:LEU:N	0.59	2.13	1	1
1:A:114:ASN:HD22	1:A:114:ASN:C	0.59	2.01	14	1
1:A:158:PHE:O	1:A:162:VAL:HG23	0.58	1.97	14	5
1:A:122:SER:OG	1:A:123:GLU:N	0.58	2.36	8	3
1:A:111:PHE:CE1	1:A:127:ALA:CB	0.58	2.87	10	3
1:A:114:ASN:H	1:A:114:ASN:HD22	0.58	1.36	13	1
1:A:131:LEU:N	1:A:131:LEU:HD12	0.57	2.14	4	10
1:A:149:ASP:OD1	1:A:150:LEU:N	0.57	2.38	1	2
1:A:116:ASP:CG	1:A:117:GLY:H	0.56	2.04	11	1
1:A:138:HIS:CG	1:A:139:ARG:N	0.56	2.72	7	1
1:A:146:ARG:O	1:A:150:LEU:HD21	0.56	2.00	1	1
1:A:138:HIS:CD2	1:A:138:HIS:N	0.56	2.73	4	1
1:A:151:ASN:ND2	1:A:153:ASP:OD2	0.56	2.38	5	1
1:A:148:VAL:HG22	1:A:149:ASP:H	0.56	1.60	6	3
1:A:101:VAL:HG13	1:A:102:LYS:N	0.56	2.15	11	1
1:A:148:VAL:HG11	1:A:156:VAL:CG2	0.56	2.30	13	1
1:A:114:ASN:HD21	1:A:116:ASP:H	0.56	1.42	14	1
1:A:157:ASP:OD1	1:A:158:PHE:N	0.55	2.40	10	2
1:A:148:VAL:HG11	1:A:156:VAL:HG22	0.55	1.79	5	5
1:A:112:ASP:OD1	1:A:114:ASN:ND2	0.55	2.39	9	1
1:A:138:HIS:N	1:A:138:HIS:CD2	0.55	2.71	13	1
1:A:106:ASP:OD1	1:A:106:ASP:N	0.55	2.38	9	1
1:A:142:GLU:O	1:A:146:ARG:N	0.55	2.40	10	2
1:A:165:MET:O	1:A:167:ARG:N	0.55	2.40	11	2
1:A:153:ASP:OD1	1:A:154:GLY:N	0.55	2.40	14	2
1:A:109:ARG:C	1:A:111:PHE:N	0.55	2.60	12	4
1:A:147:ASP:C	1:A:149:ASP:H	0.55	2.06	10	1
1:A:149:ASP:OD1	1:A:151:ASN:ND2	0.55	2.39	11	1
1:A:104:LEU:HG	1:A:162:VAL:HG22	0.54	1.79	12	3
1:A:124:LEU:HB2	1:A:145:ILE:HD11	0.54	1.78	11	1
1:A:128:MET:O	1:A:132:LEU:N	0.54	2.37	9	3
1:A:149:ASP:OD1	1:A:160:GLU:CG	0.54	2.55	1	1
1:A:108:PHE:CD1	1:A:161:PHE:CD2	0.54	2.96	11	9
1:A:150:LEU:O	1:A:152:GLY:N	0.54	2.41	1	1
1:A:147:ASP:OD1	1:A:147:ASP:C	0.54	2.46	13	1
1:A:125:ARG:O	1:A:129:ARG:N	0.54	2.41	14	3
1:A:112:ASP:C	1:A:114:ASN:H	0.54	2.05	15	1
1:A:157:ASP:O	1:A:159:GLU:N	0.54	2.40	1	2
1:A:149:ASP:H	1:A:150:LEU:HD23	0.54	1.61	1	1
1:A:153:ASP:N	1:A:153:ASP:OD1	0.54	2.41	13	1
1:A:106:ASP:CG	1:A:107:ALA:N	0.54	2.60	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:SER:O	1:A:124:LEU:N	0.54	2.41	14	8
1:A:102:LYS:O	1:A:105:ARG:N	0.53	2.41	9	11
1:A:151:ASN:OD1	1:A:151:ASN:N	0.53	2.41	15	3
1:A:146:ARG:O	1:A:148:VAL:N	0.53	2.42	2	1
1:A:131:LEU:HD12	1:A:131:LEU:N	0.53	2.16	6	1
1:A:149:ASP:CG	1:A:150:LEU:H	0.53	2.05	12	2
1:A:151:ASN:OD1	1:A:153:ASP:N	0.53	2.41	7	1
1:A:132:LEU:N	1:A:132:LEU:CD1	0.53	2.72	12	2
1:A:157:ASP:O	1:A:161:PHE:N	0.53	2.41	12	4
1:A:134:HIS:CD2	1:A:134:HIS:N	0.53	2.76	8	1
1:A:121:THR:OG1	1:A:122:SER:N	0.52	2.40	13	1
1:A:124:LEU:HD23	1:A:124:LEU:C	0.52	2.24	13	1
1:A:124:LEU:CD1	1:A:124:LEU:C	0.52	2.77	9	8
1:A:161:PHE:CD1	1:A:161:PHE:C	0.52	2.82	11	2
1:A:150:LEU:C	1:A:152:GLY:N	0.52	2.62	1	1
1:A:106:ASP:OD1	1:A:107:ALA:N	0.52	2.43	15	1
1:A:136:VAL:HG12	1:A:137:GLY:N	0.52	2.19	5	1
1:A:138:HIS:O	1:A:140:ASP:N	0.52	2.42	7	1
1:A:114:ASN:ND2	1:A:114:ASN:C	0.52	2.60	14	1
1:A:124:LEU:O	1:A:127:ALA:N	0.52	2.43	13	10
1:A:129:ARG:O	1:A:131:LEU:N	0.52	2.43	11	1
1:A:147:ASP:O	1:A:149:ASP:N	0.51	2.43	10	1
1:A:133:GLY:O	1:A:135:GLN:N	0.51	2.43	11	2
1:A:114:ASN:HD22	1:A:116:ASP:N	0.51	2.02	14	1
1:A:151:ASN:ND2	1:A:151:ASN:N	0.51	2.56	11	3
1:A:149:ASP:CG	1:A:150:LEU:N	0.51	2.64	5	3
1:A:150:LEU:C	1:A:152:GLY:H	0.51	2.07	1	1
1:A:164:MET:SD	1:A:164:MET:O	0.51	2.69	2	1
1:A:117:GLY:C	1:A:118:GLU:CD	0.51	2.70	11	1
1:A:130:LYS:O	1:A:131:LEU:HD12	0.51	2.04	11	1
1:A:116:ASP:OD1	1:A:116:ASP:N	0.51	2.41	12	2
1:A:135:GLN:CD	1:A:135:GLN:N	0.51	2.64	4	1
1:A:106:ASP:OD1	1:A:106:ASP:C	0.51	2.49	15	1
1:A:151:ASN:CG	1:A:152:GLY:H	0.51	2.09	5	1
1:A:104:LEU:HD13	1:A:161:PHE:CE2	0.50	2.41	1	1
1:A:153:ASP:OD1	1:A:155:ARG:N	0.50	2.37	7	1
1:A:159:GLU:CG	1:A:160:GLU:N	0.50	2.74	9	1
1:A:109:ARG:C	1:A:111:PHE:H	0.50	2.09	12	1
1:A:136:VAL:CG1	1:A:137:GLY:N	0.50	2.75	5	1
1:A:112:ASP:O	1:A:114:ASN:N	0.50	2.44	4	2
1:A:157:ASP:OD1	1:A:157:ASP:N	0.50	2.44	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:MET:SD	1:A:165:MET:N	0.50	2.85	7	1
1:A:112:ASP:OD1	1:A:114:ASN:CG	0.50	2.50	9	1
1:A:147:ASP:C	1:A:149:ASP:N	0.50	2.63	10	1
1:A:134:HIS:O	1:A:136:VAL:N	0.50	2.45	2	1
1:A:149:ASP:OD2	1:A:153:ASP:N	0.50	2.44	7	1
1:A:101:VAL:O	1:A:104:LEU:N	0.50	2.45	7	1
1:A:132:LEU:HD12	1:A:132:LEU:C	0.49	2.26	14	1
1:A:109:ARG:O	1:A:111:PHE:N	0.49	2.45	12	1
1:A:134:HIS:CD2	1:A:134:HIS:H	0.49	2.26	12	1
1:A:163:ARG:HH11	1:A:163:ARG:CG	0.49	2.20	13	1
1:A:134:HIS:O	1:A:135:GLN:CB	0.49	2.61	6	1
1:A:142:GLU:O	1:A:145:ILE:N	0.49	2.46	12	3
1:A:124:LEU:CB	1:A:145:ILE:HD11	0.49	2.37	11	2
1:A:112:ASP:C	1:A:114:ASN:N	0.49	2.66	4	2
1:A:135:GLN:C	1:A:136:VAL:HG23	0.49	2.28	8	1
1:A:153:ASP:CG	1:A:154:GLY:H	0.49	2.10	8	1
1:A:153:ASP:CG	1:A:155:ARG:H	0.49	2.08	12	1
1:A:120:SER:CB	1:A:155:ARG:NE	0.48	2.76	5	1
1:A:131:LEU:O	1:A:132:LEU:C	0.48	2.51	9	1
1:A:129:ARG:C	1:A:131:LEU:N	0.48	2.66	11	1
1:A:157:ASP:CG	1:A:160:GLU:OE1	0.48	2.52	1	1
1:A:102:LYS:O	1:A:105:ARG:CB	0.48	2.62	15	6
1:A:140:ASP:O	1:A:143:GLU:N	0.48	2.47	10	1
1:A:124:LEU:HD23	1:A:145:ILE:HD11	0.48	1.85	2	2
1:A:112:ASP:OD1	1:A:116:ASP:CG	0.48	2.51	1	1
1:A:149:ASP:OD1	1:A:149:ASP:C	0.48	2.52	1	1
1:A:133:GLY:O	1:A:134:HIS:CG	0.48	2.67	15	2
1:A:138:HIS:C	1:A:140:ASP:N	0.47	2.68	7	2
1:A:149:ASP:O	1:A:150:LEU:C	0.47	2.52	1	1
1:A:111:PHE:CD2	1:A:119:ILE:CD1	0.47	2.97	2	1
1:A:103:GLU:HG3	1:A:104:LEU:N	0.47	2.24	3	2
1:A:140:ASP:C	1:A:142:GLU:N	0.47	2.66	7	1
1:A:116:ASP:N	1:A:116:ASP:OD1	0.47	2.46	5	2
1:A:130:LYS:CB	1:A:130:LYS:HZ2	0.47	2.23	12	1
1:A:161:PHE:CD1	1:A:161:PHE:O	0.47	2.67	11	2
1:A:138:HIS:ND1	1:A:139:ARG:N	0.47	2.63	10	1
1:A:145:ILE:HG22	1:A:145:ILE:O	0.47	2.09	1	1
1:A:103:GLU:O	1:A:106:ASP:N	0.47	2.48	12	3
1:A:158:PHE:CE1	1:A:162:VAL:CG2	0.47	2.98	9	1
1:A:149:ASP:OD1	1:A:153:ASP:OD2	0.47	2.32	6	1
1:A:129:ARG:NE	1:A:135:GLN:OE1	0.47	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:PHE:CD2	1:A:119:ILE:HD11	0.46	2.45	2	1
1:A:136:VAL:HG12	1:A:136:VAL:O	0.46	2.10	6	1
1:A:136:VAL:CG2	1:A:137:GLY:N	0.46	2.78	9	1
1:A:157:ASP:C	1:A:159:GLU:N	0.46	2.67	1	2
1:A:159:GLU:OE1	1:A:159:GLU:C	0.46	2.53	5	1
1:A:145:ILE:O	1:A:145:ILE:HG22	0.46	2.11	4	1
1:A:151:ASN:HD21	1:A:153:ASP:CG	0.46	2.13	5	1
1:A:157:ASP:OD2	1:A:160:GLU:OE1	0.46	2.34	1	1
1:A:105:ARG:NH1	1:A:158:PHE:CD2	0.46	2.84	8	1
1:A:146:ARG:C	1:A:148:VAL:N	0.46	2.68	2	1
1:A:104:LEU:CD1	1:A:162:VAL:HG22	0.46	2.41	7	2
1:A:140:ASP:O	1:A:142:GLU:N	0.45	2.48	7	1
1:A:121:THR:O	1:A:124:LEU:N	0.45	2.47	12	1
1:A:135:GLN:CG	1:A:136:VAL:N	0.45	2.79	14	1
1:A:103:GLU:OE1	1:A:103:GLU:C	0.45	2.55	1	1
1:A:149:ASP:OD1	1:A:160:GLU:OE2	0.45	2.34	1	1
1:A:111:PHE:CE1	1:A:124:LEU:HD13	0.45	2.46	3	1
1:A:112:ASP:OD1	1:A:112:ASP:C	0.45	2.54	9	1
1:A:148:VAL:HG21	1:A:164:MET:SD	0.45	2.51	10	1
1:A:135:GLN:CG	1:A:136:VAL:H	0.45	2.24	14	1
1:A:159:GLU:HG3	1:A:160:GLU:N	0.45	2.26	9	1
1:A:104:LEU:HD22	1:A:165:MET:SD	0.45	2.51	11	1
1:A:165:MET:C	1:A:167:ARG:N	0.45	2.70	6	1
1:A:144:ILE:HD12	1:A:144:ILE:N	0.45	2.27	6	1
1:A:118:GLU:OE1	1:A:157:ASP:OD2	0.45	2.35	10	1
1:A:157:ASP:O	1:A:158:PHE:C	0.44	2.55	14	8
1:A:114:ASN:OD1	1:A:114:ASN:N	0.44	2.49	5	1
1:A:114:ASN:CG	1:A:116:ASP:OD2	0.44	2.56	14	1
1:A:120:SER:O	1:A:123:GLU:N	0.44	2.50	1	1
1:A:116:ASP:OD1	1:A:116:ASP:C	0.44	2.54	10	1
1:A:129:ARG:C	1:A:131:LEU:H	0.44	2.16	11	1
1:A:144:ILE:N	1:A:144:ILE:CD1	0.44	2.80	6	1
1:A:120:SER:O	1:A:121:THR:C	0.44	2.56	11	11
1:A:156:VAL:C	1:A:157:ASP:OD1	0.44	2.55	5	1
1:A:104:LEU:HD12	1:A:161:PHE:CD2	0.44	2.47	1	2
1:A:104:LEU:O	1:A:107:ALA:N	0.44	2.51	10	1
1:A:137:GLY:O	1:A:139:ARG:N	0.44	2.51	10	1
1:A:112:ASP:OD2	1:A:115:GLY:CA	0.44	2.65	1	1
1:A:138:HIS:CD2	1:A:138:HIS:H	0.44	2.30	13	1
1:A:112:ASP:OD1	1:A:116:ASP:OD1	0.44	2.36	1	1
1:A:126:GLU:N	1:A:126:GLU:OE1	0.43	2.51	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:N	1:A:131:LEU:CD1	0.43	2.81	6	2
1:A:143:GLU:CD	1:A:147:ASP:OD2	0.43	2.57	6	1
1:A:149:ASP:OD1	1:A:160:GLU:CD	0.43	2.56	1	1
1:A:124:LEU:O	1:A:125:ARG:C	0.43	2.56	13	5
1:A:150:LEU:CD1	1:A:151:ASN:ND2	0.43	2.82	3	1
1:A:165:MET:O	1:A:166:SER:C	0.43	2.57	4	1
1:A:130:LYS:NZ	1:A:130:LYS:CB	0.43	2.79	12	1
1:A:112:ASP:OD1	1:A:123:GLU:OE1	0.43	2.37	8	1
1:A:125:ARG:O	1:A:129:ARG:CB	0.43	2.67	14	1
1:A:128:MET:HG3	1:A:141:ILE:HG22	0.43	1.91	12	1
1:A:138:HIS:O	1:A:139:ARG:C	0.43	2.57	11	1
1:A:148:VAL:CG2	1:A:149:ASP:H	0.43	2.26	12	1
1:A:142:GLU:OE1	1:A:142:GLU:N	0.43	2.51	14	1
1:A:114:ASN:HD21	1:A:123:GLU:CD	0.42	2.16	8	1
1:A:114:ASN:HD21	1:A:116:ASP:N	0.42	2.03	14	1
1:A:114:ASN:ND2	1:A:115:GLY:H	0.42	2.12	5	1
1:A:145:ILE:O	1:A:145:ILE:CG2	0.42	2.66	4	2
1:A:124:LEU:C	1:A:124:LEU:CD1	0.42	2.87	6	1
1:A:102:LYS:O	1:A:103:GLU:C	0.42	2.57	13	7
1:A:140:ASP:N	1:A:140:ASP:OD1	0.42	2.53	7	1
1:A:107:ALA:O	1:A:108:PHE:C	0.42	2.58	6	2
1:A:141:ILE:CG1	1:A:142:GLU:N	0.42	2.82	6	2
1:A:114:ASN:ND2	1:A:123:GLU:OE2	0.42	2.42	8	1
1:A:136:VAL:HG23	1:A:137:GLY:N	0.42	2.29	11	1
1:A:149:ASP:OD1	1:A:155:ARG:N	0.42	2.53	6	1
1:A:152:GLY:O	1:A:153:ASP:C	0.42	2.57	8	1
1:A:118:GLU:OE2	1:A:157:ASP:OD2	0.42	2.37	5	1
1:A:141:ILE:HG13	1:A:142:GLU:N	0.42	2.30	10	3
1:A:111:PHE:CG	1:A:119:ILE:CD1	0.41	3.02	2	3
1:A:135:GLN:C	1:A:136:VAL:HG12	0.41	2.34	9	1
1:A:104:LEU:O	1:A:105:ARG:C	0.41	2.58	10	1
1:A:153:ASP:OD1	1:A:153:ASP:C	0.41	2.59	7	1
1:A:150:LEU:N	1:A:150:LEU:CD2	0.41	2.82	1	1
1:A:114:ASN:CG	1:A:115:GLY:H	0.41	2.17	5	1
1:A:159:GLU:OE1	1:A:160:GLU:N	0.41	2.53	5	1
1:A:128:MET:SD	1:A:132:LEU:HB2	0.41	2.56	6	1
1:A:101:VAL:O	1:A:102:LYS:C	0.41	2.58	14	2
1:A:124:LEU:CD1	1:A:128:MET:SD	0.41	3.09	10	1
1:A:138:HIS:O	1:A:141:ILE:N	0.41	2.54	11	1
1:A:121:THR:HG22	1:A:138:HIS:NE2	0.41	2.30	15	1
1:A:147:ASP:O	1:A:148:VAL:C	0.41	2.60	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:VAL:O	1:A:136:VAL:CG2	0.41	2.67	7	1
1:A:149:ASP:C	1:A:151:ASN:H	0.41	2.19	13	1
1:A:113:THR:HG21	1:A:126:GLU:OE2	0.41	2.16	5	1
1:A:143:GLU:OE2	1:A:147:ASP:OD1	0.41	2.38	11	1
1:A:146:ARG:C	1:A:148:VAL:H	0.40	2.19	2	1
1:A:148:VAL:CG2	1:A:149:ASP:N	0.40	2.76	12	1
1:A:145:ILE:CG2	1:A:154:GLY:O	0.40	2.69	5	1
1:A:113:THR:O	1:A:114:ASN:C	0.40	2.59	9	1
1:A:138:HIS:ND1	1:A:138:HIS:N	0.40	2.70	11	1
1:A:157:ASP:CG	1:A:158:PHE:N	0.40	2.74	12	1
1:A:136:VAL:O	1:A:136:VAL:CG1	0.40	2.70	6	1
1:A:143:GLU:OE1	1:A:147:ASP:OD2	0.40	2.39	6	1
1:A:137:GLY:C	1:A:139:ARG:N	0.40	2.75	15	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	66/72 (92%)	48±3 (73±4%)	13±3 (20±4%)	4±1 (7±2%)	2	17
All	All	990/1080 (92%)	725 (73%)	198 (20%)	67 (7%)	2	17

All 24 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	115	GLY	6
1	A	152	GLY	6
1	A	149	ASP	5
1	A	135	GLN	5
1	A	134	HIS	5
1	A	133	GLY	4
1	A	137	GLY	4
1	A	166	SER	4
1	A	148	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	150	LEU	3
1	A	136	VAL	3
1	A	151	ASN	2
1	A	101	VAL	2
1	A	113	THR	2
1	A	153	ASP	2
1	A	132	LEU	2
1	A	158	PHE	1
1	A	147	ASP	1
1	A	117	GLY	1
1	A	165	MET	1
1	A	139	ARG	1
1	A	114	ASN	1
1	A	138	HIS	1
1	A	130	LYS	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	59/62 (95%)	46±2 (78±4%)	13±2 (22±4%)	3 30
All	All	885/930 (95%)	690 (78%)	195 (22%)	3 30

All 46 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	111	PHE	15
1	A	113	THR	13
1	A	124	LEU	13
1	A	151	ASN	12
1	A	104	LEU	11
1	A	114	ASN	10
1	A	128	MET	9
1	A	108	PHE	9
1	A	121	THR	8
1	A	153	ASP	8

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Mol	Chain	Res	Type	Models (Total)
1	A	139	ARG	6
1	A	132	LEU	5
1	A	157	ASP	5
1	A	163	ARG	4
1	A	138	HIS	4
1	A	122	SER	4
1	A	165	MET	4
1	A	102	LYS	3
1	A	130	LYS	3
1	A	106	ASP	3
1	A	109	ARG	3
1	A	148	VAL	3
1	A	167	ARG	3
1	A	110	GLU	3
1	A	136	VAL	3
1	A	149	ASP	2
1	A	150	LEU	2
1	A	147	ASP	2
1	A	155	ARG	2
1	A	161	PHE	2
1	A	116	ASP	2
1	A	145	ILE	2
1	A	105	ARG	2
1	A	129	ARG	2
1	A	140	ASP	2
1	A	118	GLU	1
1	A	166	SER	1
1	A	112	ASP	1
1	A	134	HIS	1
1	A	159	GLU	1
1	A	144	ILE	1
1	A	126	GLU	1
1	A	146	ARG	1
1	A	101	VAL	1
1	A	142	GLU	1
1	A	164	MET	1

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 monosaccharides 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

No chemical shift data were provided