Full wwPDB NMR Structure Validation Report (i)

Oct 11, 2021 – 12:41 PM EDT

PDB ID	:	2EBI
Title	:	Arabidopsis GT-1 DNA-binding domain with T133D phosphomimetic mutation
Authors	:	Nagata, T.; Noto, K.; Niyada, E.; Ikeda, Y.; Yamamoto, Y.; Uesugi, S.; Murata, J.; Hiratsuka, K.; Katahira, M.
Deposited on	:	2007-02-08

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:

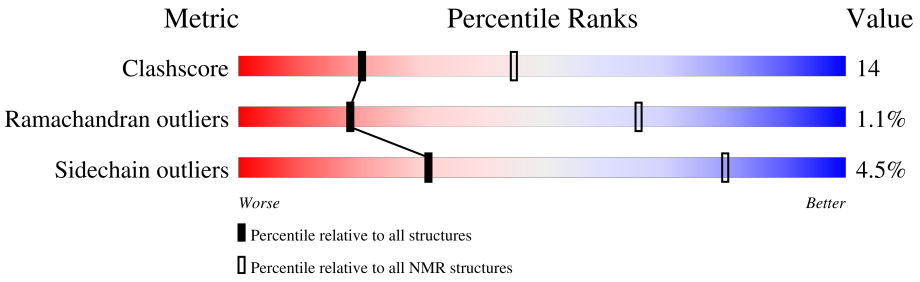
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	86	53% 16% 30%

2 Ensemble composition and analysis (i)

This entry contains 20 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: *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:87-A:146 (60)	0.33	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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 7, 8, 11, 12, 13, 17, 18, 19
2	14, 15
3	9, 20
4	2, 6
Single-model clusters	10; 16

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1443 atoms, of which 719 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA binding protein GT-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1443	450	719	138	130	6	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	ASP	THR	engineered mutation	UNP Q9FX53

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: DNA binding protein GT-1

Chain A: 53% 16% 30%

K81 K82 R83 A84 E85 T86 W87 V88 E91 S94 F98 R99 M102 D103 F106 H114 L115 M123 W139 L142 F146 K147 K148 A149 K150 H151 H152 D153 R154 G155 N156 G157 S158 A159 K160 M161 S162 Y163 Y164 K165 E166

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: DNA binding protein GT-1

Chain A: 42% 28% 30%

K81 K82 R83 A84 E85 T86 E91 T92 R93 S94 M97 F98 R99 R100 G101 M102 D103 G104 L105 F106 K113 H114 L115 W116 E117 M123 G127 F128 T136 W139 L142 L143 F146 K147 K148 A149 K150 H151 H152 D153 R154 G155 N156 G157 S158 A159 K160 M161 S162 Y163 Y164

K165 E166

4.2.2 Score per residue for model 2

• Molecule 1: DNA binding protein GT-1

Chain A: 45% 23% • 30%

K81 K82 R83 A84 E85 T86 W87 V88 Q89 D90 E91 T92 R93 S94 F98 R99 F106 L115 W116 M123 R124 E125 K126 G127 F128 D129 R130 W139 L142 K147 K148 A149 K150 H151 H152 D153 R154 G155 N156 G157 S158 A159 K160 M161 S162 Y163 Y164 K165 E166

4.2.3 Score per residue for model 3

• Molecule 1: DNA binding protein GT-1

Chain A: 55% 14% • 30%

4.2.4 Score per residue for model 4

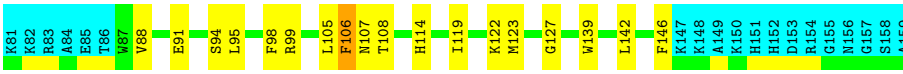
• Molecule 1: DNA binding protein GT-1

Chain A: 48% 22% 30%

4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: DNA binding protein GT-1

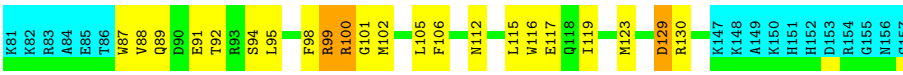
Chain A: 49% 20% • 30%



4.2.6 Score per residue for model 6

• Molecule 1: DNA binding protein GT-1

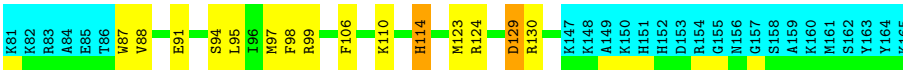
Chain A: 44% 22% • 30%



4.2.7 Score per residue for model 7

• Molecule 1: DNA binding protein GT-1

Chain A: 52% 15% • 30%



4.2.8 Score per residue for model 8

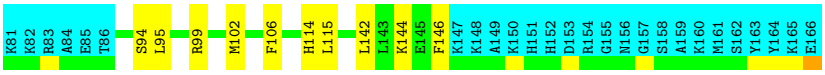
- Molecule 1: DNA binding protein GT-1

Chain A: 51% 19% 30%

4.2.9 Score per residue for model 9

- Molecule 1: DNA binding protein GT-1

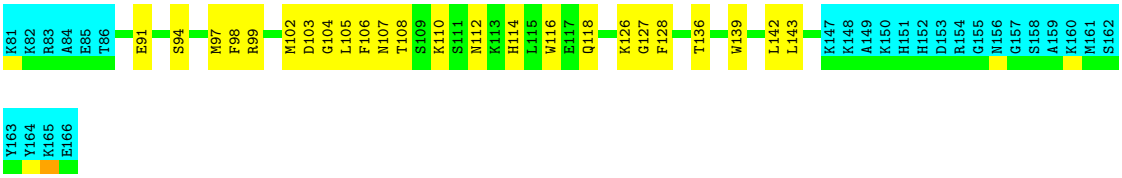
Chain A: 58% 12% 30%



4.2.10 Score per residue for model 10

- Molecule 1: DNA binding protein GT-1

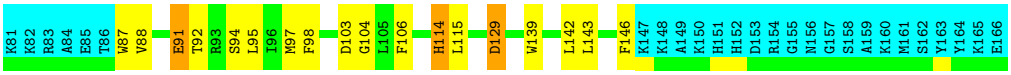
Chain A: 42% 28% 30%



4.2.11 Score per residue for model 11

- Molecule 1: DNA binding protein GT-1

Chain A: 49% 17% • 30%



4.2.12 Score per residue for model 12

- Molecule 1: DNA binding protein GT-1

Chain A: 52% 16% • 30%

4.2.13 Score per residue for model 13

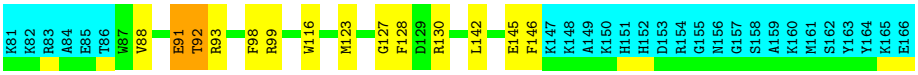
- Molecule 1: DNA binding protein GT-1

Chain A:

4.2.14 Score per residue for model 14

- Molecule 1: DNA binding protein GT-1

Chain A:



4.2.15 Score per residue for model 15

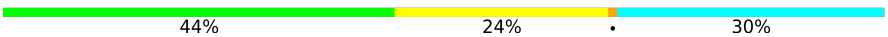
- Molecule 1: DNA binding protein GT-1

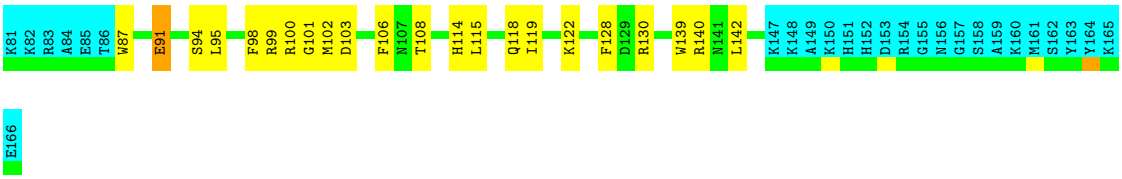
Chain A:

4.2.16 Score per residue for model 16

- Molecule 1: DNA binding protein GT-1

Chain A:





4.2.17 Score per residue for model 17

• Molecule 1: DNA binding protein GT-1

Chain A: 51% 17% • 30%

4.2.18 Score per residue for model 18

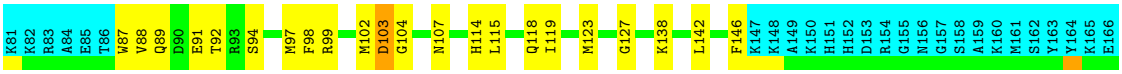
• Molecule 1: DNA binding protein GT-1

Chain A: 45% 23% • 30%

4.2.19 Score per residue for model 19

• Molecule 1: DNA binding protein GT-1

Chain A: 44% 24% • 30%



4.2.20 Score per residue for model 20

• Molecule 1: DNA binding protein GT-1

Chain A: 52% 17% 30%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *SIMULATED ANNEALING, TORSION ANGLE DYNAMICS*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	511	501	501	14±4
All	All	10220	10020	10020	276

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:TRP:CD1	1:A:143:LEU:HD11	0.78	2.12	11	2
1:A:139:TRP:HA	1:A:142:LEU:HD12	0.74	1.59	4	12
1:A:139:TRP:NE1	1:A:143:LEU:HD11	0.67	2.05	1	3
1:A:108:THR:HG23	1:A:108:THR:O	0.64	1.93	16	1
1:A:99:ARG:NH1	1:A:119:ILE:HD11	0.63	2.09	12	1
1:A:99:ARG:NH2	1:A:116:TRP:CZ3	0.62	2.67	1	1
1:A:102:MET:HE1	1:A:118:GLN:HB2	0.62	1.72	10	1
1:A:95:LEU:HD11	1:A:99:ARG:NH1	0.61	2.10	16	1
1:A:99:ARG:CZ	1:A:106:PHE:CD2	0.60	2.84	3	2
1:A:99:ARG:NH1	1:A:106:PHE:CE1	0.60	2.70	9	3
1:A:91:GLU:CD	1:A:128:PHE:CD2	0.60	2.75	12	2
1:A:91:GLU:OE1	1:A:128:PHE:CE1	0.59	2.56	14	2
1:A:91:GLU:OE2	1:A:128:PHE:CD2	0.59	2.55	16	2
1:A:99:ARG:CD	1:A:106:PHE:CE1	0.58	2.87	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:HIS:CD2	1:A:115:LEU:N	0.58	2.72	9	1
1:A:106:PHE:CD1	1:A:115:LEU:HD13	0.58	2.33	8	1
1:A:142:LEU:O	1:A:146:PHE:CD2	0.57	2.56	14	12
1:A:99:ARG:NH1	1:A:106:PHE:CZ	0.57	2.73	9	3
1:A:99:ARG:CD	1:A:106:PHE:CZ	0.56	2.89	7	1
1:A:99:ARG:HE	1:A:119:ILE:HD13	0.56	1.59	16	1
1:A:139:TRP:CE2	1:A:143:LEU:HD21	0.56	2.36	11	1
1:A:114:HIS:CD2	1:A:115:LEU:HD23	0.56	2.36	18	2
1:A:87:TRP:CZ3	1:A:95:LEU:HD22	0.55	2.36	11	4
1:A:95:LEU:HD11	1:A:99:ARG:NH2	0.55	2.16	15	2
1:A:102:MET:HE1	1:A:115:LEU:O	0.54	2.02	17	1
1:A:99:ARG:NH1	1:A:106:PHE:CG	0.54	2.75	3	2
1:A:91:GLU:OE1	1:A:128:PHE:CE2	0.54	2.61	16	2
1:A:98:PHE:CE2	1:A:123:MET:HB3	0.53	2.38	14	9
1:A:91:GLU:OE1	1:A:128:PHE:CD2	0.53	2.61	12	1
1:A:90:ASP:OD1	1:A:128:PHE:CE1	0.53	2.61	2	1
1:A:102:MET:HE1	1:A:118:GLN:CB	0.53	2.32	10	1
1:A:99:ARG:NH1	1:A:106:PHE:CD2	0.53	2.76	20	2
1:A:88:VAL:HG22	1:A:91:GLU:OE1	0.53	2.04	19	2
1:A:91:GLU:OE2	1:A:128:PHE:CD1	0.53	2.61	3	1
1:A:114:HIS:CD2	1:A:115:LEU:CD2	0.53	2.92	18	2
1:A:95:LEU:HD11	1:A:99:ARG:HH12	0.52	1.63	16	1
1:A:145:GLU:OE2	1:A:146:PHE:CG	0.52	2.63	14	1
1:A:88:VAL:HG22	1:A:91:GLU:CD	0.52	2.25	18	2
1:A:106:PHE:CZ	1:A:115:LEU:HB2	0.52	2.39	17	2
1:A:94:SER:O	1:A:98:PHE:CD2	0.51	2.63	11	1
1:A:91:GLU:HG2	1:A:128:PHE:CD1	0.51	2.40	10	1
1:A:106:PHE:CD1	1:A:115:LEU:HD12	0.51	2.41	6	3
1:A:116:TRP:CZ2	1:A:136:THR:HG23	0.51	2.41	10	1
1:A:98:PHE:CE2	1:A:123:MET:HA	0.51	2.41	2	2
1:A:114:HIS:CD2	1:A:114:HIS:N	0.51	2.77	7	2
1:A:108:THR:O	1:A:108:THR:HG23	0.51	2.06	10	2
1:A:130:ARG:CZ	1:A:135:CYS:SG	0.50	3.00	15	1
1:A:99:ARG:HD2	1:A:106:PHE:CE1	0.50	2.42	7	1
1:A:99:ARG:NH2	1:A:106:PHE:CD1	0.50	2.79	12	1
1:A:91:GLU:OE1	1:A:130:ARG:NE	0.49	2.45	6	1
1:A:88:VAL:HG23	1:A:91:GLU:H	0.49	1.67	15	3
1:A:98:PHE:CE2	1:A:123:MET:CB	0.49	2.95	7	7
1:A:95:LEU:HD11	1:A:99:ARG:CZ	0.49	2.38	16	1
1:A:139:TRP:CZ2	1:A:143:LEU:HD21	0.49	2.42	10	2
1:A:123:MET:SD	1:A:124:ARG:N	0.49	2.85	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:TRP:CH2	1:A:130:ARG:HD2	0.49	2.42	18	1
1:A:106:PHE:CZ	1:A:115:LEU:CB	0.49	2.95	17	3
1:A:106:PHE:CZ	1:A:115:LEU:HB3	0.48	2.43	16	1
1:A:108:THR:HG23	1:A:109:SER:N	0.48	2.24	15	1
1:A:98:PHE:CD2	1:A:123:MET:HB3	0.48	2.44	6	5
1:A:94:SER:OG	1:A:98:PHE:CZ	0.48	2.66	6	1
1:A:91:GLU:CG	1:A:128:PHE:CD1	0.48	2.96	10	1
1:A:122:LYS:O	1:A:125:GLU:CG	0.48	2.62	3	1
1:A:102:MET:SD	1:A:119:ILE:CG1	0.48	3.02	12	1
1:A:115:LEU:O	1:A:117:GLU:N	0.48	2.47	6	1
1:A:105:LEU:O	1:A:107:ASN:N	0.47	2.47	5	2
1:A:114:HIS:CD2	1:A:114:HIS:H	0.47	2.27	7	2
1:A:94:SER:HB3	1:A:98:PHE:CE2	0.47	2.44	4	2
1:A:102:MET:HE3	1:A:115:LEU:HD22	0.47	1.86	9	1
1:A:91:GLU:CD	1:A:128:PHE:CG	0.47	2.88	12	1
1:A:87:TRP:CZ2	1:A:130:ARG:HD2	0.47	2.44	7	2
1:A:87:TRP:CH2	1:A:130:ARG:NH1	0.47	2.83	15	1
1:A:87:TRP:CZ3	1:A:130:ARG:NH1	0.47	2.82	15	1
1:A:105:LEU:HD13	1:A:115:LEU:HD22	0.47	1.87	12	1
1:A:103:ASP:CG	1:A:104:GLY:N	0.46	2.68	19	1
1:A:99:ARG:HD3	1:A:106:PHE:CZ	0.46	2.45	7	1
1:A:99:ARG:HD3	1:A:106:PHE:CE1	0.46	2.45	1	1
1:A:99:ARG:HG2	1:A:139:TRP:CZ2	0.46	2.45	2	2
1:A:91:GLU:OE1	1:A:91:GLU:CA	0.46	2.63	11	1
1:A:103:ASP:O	1:A:105:LEU:N	0.46	2.49	10	2
1:A:94:SER:HB2	1:A:98:PHE:CE2	0.46	2.45	2	4
1:A:94:SER:OG	1:A:98:PHE:CE2	0.46	2.60	6	1
1:A:130:ARG:NE	1:A:135:CYS:SG	0.46	2.89	15	1
1:A:94:SER:O	1:A:97:MET:N	0.46	2.49	1	5
1:A:88:VAL:CG2	1:A:91:GLU:OE2	0.46	2.64	11	1
1:A:89:GLN:O	1:A:92:THR:N	0.46	2.49	2	1
1:A:99:ARG:O	1:A:102:MET:N	0.45	2.48	16	5
1:A:99:ARG:CZ	1:A:116:TRP:CZ3	0.45	3.00	14	1
1:A:99:ARG:NH2	1:A:106:PHE:CD2	0.45	2.84	5	1
1:A:99:ARG:NH1	1:A:139:TRP:CE2	0.45	2.85	8	2
1:A:99:ARG:NH2	1:A:102:MET:C	0.45	2.69	12	1
1:A:99:ARG:O	1:A:99:ARG:NH1	0.45	2.50	19	1
1:A:99:ARG:O	1:A:100:ARG:C	0.45	2.55	16	2
1:A:124:ARG:O	1:A:125:GLU:C	0.45	2.55	2	1
1:A:129:ASP:CG	1:A:129:ASP:O	0.45	2.55	12	3
1:A:99:ARG:CZ	1:A:106:PHE:CE1	0.45	2.99	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:MET:C	1:A:123:MET:SD	0.45	2.95	3	2
1:A:116:TRP:CD2	1:A:136:THR:OG1	0.45	2.66	10	1
1:A:91:GLU:O	1:A:92:THR:C	0.45	2.55	19	2
1:A:116:TRP:CH2	1:A:136:THR:HA	0.44	2.47	10	2
1:A:106:PHE:CG	1:A:115:LEU:HD12	0.44	2.47	6	1
1:A:124:ARG:O	1:A:126:LYS:N	0.44	2.51	2	1
1:A:94:SER:HB3	1:A:98:PHE:CZ	0.44	2.47	4	1
1:A:119:ILE:O	1:A:120:SER:C	0.44	2.55	4	1
1:A:129:ASP:O	1:A:129:ASP:CG	0.44	2.55	11	1
1:A:99:ARG:HG2	1:A:139:TRP:CH2	0.44	2.48	4	1
1:A:129:ASP:O	1:A:130:ARG:CZ	0.44	2.66	2	1
1:A:91:GLU:O	1:A:95:LEU:CB	0.44	2.66	6	3
1:A:114:HIS:CD2	1:A:118:GLN:NE2	0.44	2.86	15	1
1:A:105:LEU:O	1:A:106:PHE:C	0.44	2.56	6	3
1:A:91:GLU:OE2	1:A:128:PHE:CG	0.44	2.70	16	1
1:A:106:PHE:HE2	1:A:119:ILE:HD11	0.44	1.73	17	1
1:A:87:TRP:CH2	1:A:130:ARG:CD	0.44	3.01	18	1
1:A:88:VAL:O	1:A:89:GLN:C	0.43	2.56	4	4
1:A:95:LEU:CD1	1:A:99:ARG:NH1	0.43	2.81	16	1
1:A:106:PHE:CE1	1:A:112:ASN:HB2	0.43	2.48	10	1
1:A:118:GLN:O	1:A:122:LYS:CG	0.43	2.67	16	1
1:A:110:LYS:O	1:A:111:SER:C	0.43	2.55	18	2
1:A:99:ARG:NH1	1:A:139:TRP:CD2	0.43	2.86	1	1
1:A:142:LEU:HB3	1:A:146:PHE:CE2	0.43	2.49	9	1
1:A:106:PHE:CE1	1:A:115:LEU:HB3	0.43	2.49	11	2
1:A:102:MET:O	1:A:103:ASP:C	0.43	2.57	19	1
1:A:91:GLU:OE1	1:A:91:GLU:N	0.42	2.52	11	1
1:A:87:TRP:CE2	1:A:138:LYS:CG	0.42	3.02	19	1
1:A:118:GLN:CG	1:A:119:ILE:N	0.42	2.82	20	1
1:A:105:LEU:C	1:A:107:ASN:N	0.42	2.72	5	1
1:A:123:MET:SD	1:A:123:MET:C	0.42	2.98	6	1
1:A:96:ILE:O	1:A:97:MET:C	0.42	2.58	8	1
1:A:94:SER:O	1:A:95:LEU:C	0.42	2.58	4	4
1:A:103:ASP:O	1:A:104:GLY:C	0.42	2.58	4	5
1:A:95:LEU:HD11	1:A:99:ARG:HH22	0.42	1.74	16	1
1:A:100:ARG:CG	1:A:101:GLY:N	0.42	2.83	6	1
1:A:126:LYS:N	1:A:126:LYS:HE2	0.42	2.30	13	1
1:A:130:ARG:HG2	1:A:131:SER:N	0.42	2.29	18	1
1:A:99:ARG:O	1:A:101:GLY:N	0.42	2.53	16	2
1:A:99:ARG:NH1	1:A:119:ILE:CD1	0.42	2.81	12	1
1:A:99:ARG:NH2	1:A:139:TRP:NE1	0.42	2.67	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:GLN:O	1:A:90:ASP:C	0.42	2.58	12	3
1:A:115:LEU:C	1:A:117:GLU:N	0.41	2.72	6	1
1:A:115:LEU:O	1:A:116:TRP:C	0.41	2.58	8	1
1:A:114:HIS:C	1:A:118:GLN:OE1	0.41	2.59	10	1
1:A:92:THR:O	1:A:93:ARG:C	0.41	2.58	14	1
1:A:87:TRP:CH2	1:A:95:LEU:HD22	0.41	2.50	7	1
1:A:97:MET:O	1:A:98:PHE:C	0.41	2.59	10	1
1:A:102:MET:HB3	1:A:105:LEU:HD12	0.41	1.91	13	1
1:A:99:ARG:NE	1:A:106:PHE:CZ	0.41	2.88	7	1
1:A:88:VAL:HG22	1:A:91:GLU:OE2	0.41	2.16	14	1
1:A:108:THR:O	1:A:108:THR:CG2	0.41	2.64	16	1
1:A:87:TRP:CZ2	1:A:130:ARG:HG2	0.41	2.51	8	1
1:A:145:GLU:OE2	1:A:146:PHE:CD1	0.41	2.74	14	1
1:A:114:HIS:O	1:A:117:GLU:N	0.41	2.53	1	1
1:A:102:MET:HE1	1:A:119:ILE:HG13	0.41	1.93	6	1
1:A:91:GLU:CD	1:A:128:PHE:CD1	0.41	2.94	1	1
1:A:106:PHE:CE2	1:A:119:ILE:HD11	0.41	2.51	17	1
1:A:118:GLN:HG3	1:A:119:ILE:N	0.41	2.31	19	1
1:A:102:MET:CE	1:A:119:ILE:HG13	0.40	2.46	6	1
1:A:99:ARG:NH1	1:A:116:TRP:CZ2	0.40	2.89	2	1
1:A:91:GLU:O	1:A:94:SER:N	0.40	2.54	19	1
1:A:119:ILE:O	1:A:122:LYS:N	0.40	2.54	5	1
1:A:139:TRP:NE1	1:A:143:LEU:HD21	0.40	2.31	12	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	60/86 (70%)	48±3 (81±5%)	11±3 (18±5%)	1±1 (1±1%)	18	66
All	All	1200/1720 (70%)	968 (81%)	219 (18%)	13 (1%)	18	66

All 6 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	127	GLY	7
1	A	104	GLY	2
1	A	125	GLU	1
1	A	106	PHE	1
1	A	116	TRP	1
1	A	110	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	57/78 (73%)	54±1 (96±3%)	3±1 (4±3%)	31	80
All	All	1140/1560 (73%)	1089 (96%)	51 (4%)	31	80

All 20 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	103	ASP	6
1	A	129	ASP	5
1	A	91	GLU	4
1	A	114	HIS	4
1	A	92	THR	4
1	A	110	LYS	4
1	A	113	LYS	3
1	A	93	ARG	3
1	A	107	ASN	3
1	A	99	ARG	2
1	A	112	ASN	2
1	A	130	ARG	2
1	A	90	ASP	2
1	A	124	ARG	1
1	A	100	ARG	1
1	A	144	LYS	1
1	A	126	LYS	1
1	A	97	MET	1
1	A	140	ARG	1
1	A	89	GLN	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