Full wwPDB NMR Structure Validation Report (i)

Feb 24, 2022 – 07:27 AM EST

PDB ID	:	1YYC
Title	:	Solution Structure of a putative late embryogenesis abundant (LEA) protein At2g46140.1
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Deposited on	:	2005-02-24

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:

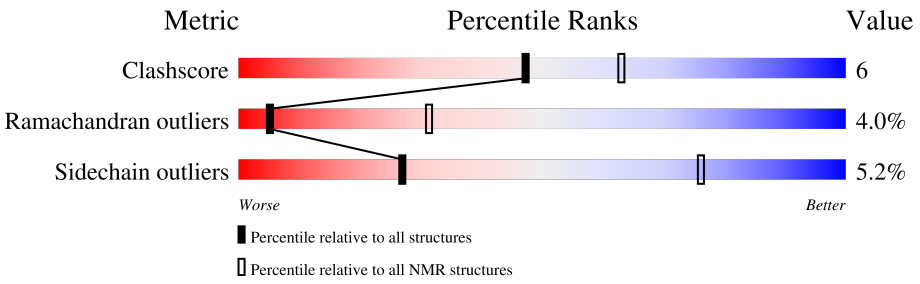
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	174	83% 9% 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 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:13-A:173 (161)	0.75	2

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 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2657 atoms, of which 1330 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called putative late embryogenesis abundant protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	174	2657	845	1330	216	262	4	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP O82355
A	2	HIS	-	cloning artifact	UNP O82355
A	3	HIS	-	cloning artifact	UNP O82355
A	4	HIS	-	cloning artifact	UNP O82355
A	5	HIS	-	cloning artifact	UNP O82355
A	6	HIS	-	cloning artifact	UNP O82355
A	7	HIS	-	cloning artifact	UNP O82355
A	8	LEU	-	cloning artifact	UNP O82355
A	9	GLU	MET	cloning artifact	UNP O82355

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: putative late embryogenesis abundant protein

Chain A: 83% 9% 7%

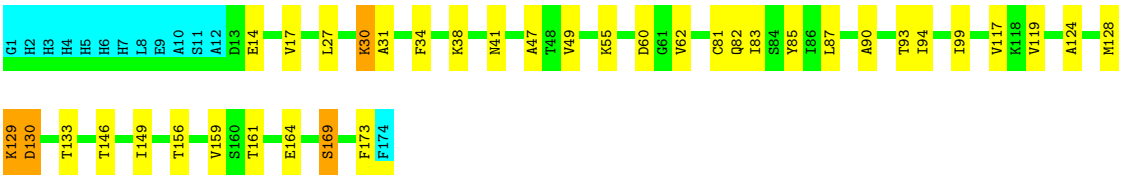
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: putative late embryogenesis abundant protein

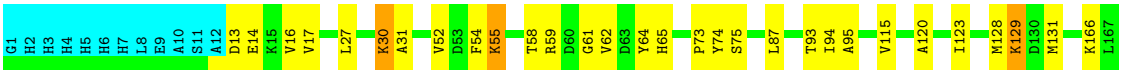
Chain A: 71% 19% • 7%



4.2.2 Score per residue for model 2 (medoid)

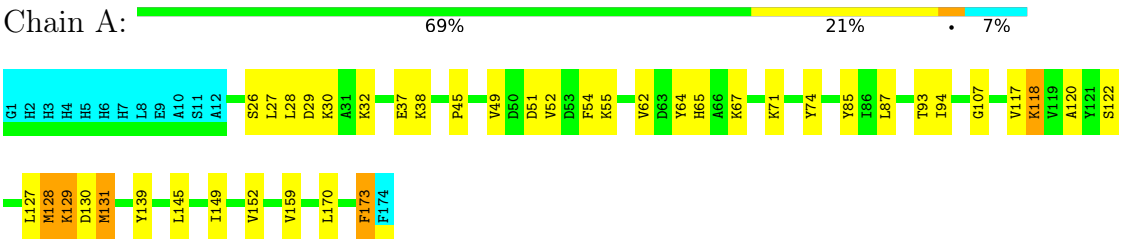
• Molecule 1: putative late embryogenesis abundant protein

Chain A: 74% 16% • 7%



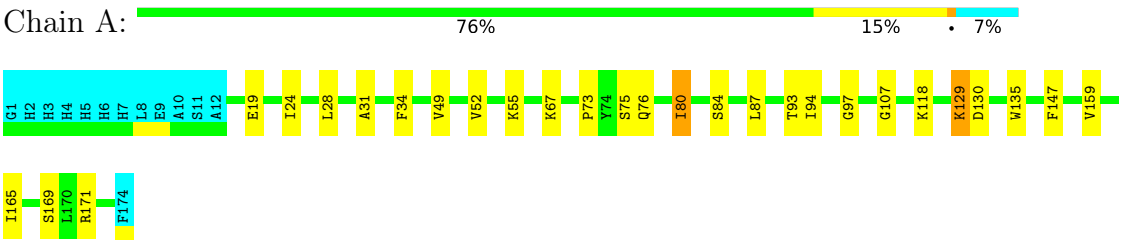
4.2.3 Score per residue for model 3

• Molecule 1: putative late embryogenesis abundant protein



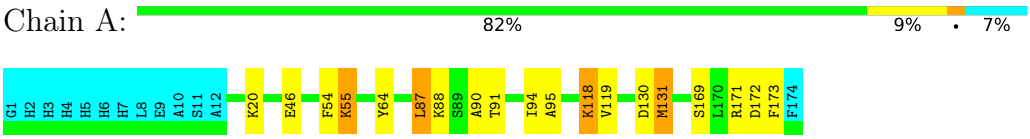
4.2.4 Score per residue for model 4

• Molecule 1: putative late embryogenesis abundant protein



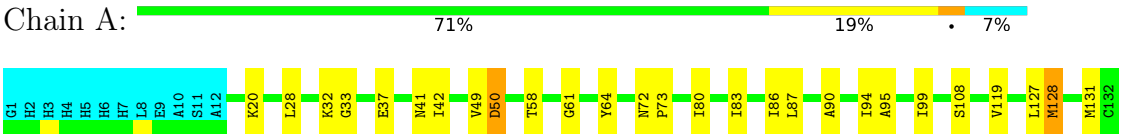
4.2.5 Score per residue for model 5

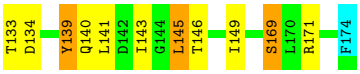
• Molecule 1: putative late embryogenesis abundant protein



4.2.6 Score per residue for model 6

• Molecule 1: putative late embryogenesis abundant protein

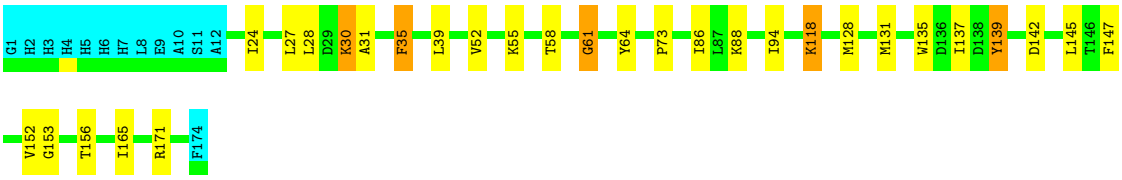




4.2.7 Score per residue for model 7

- Molecule 1: putative late embryogenesis abundant protein

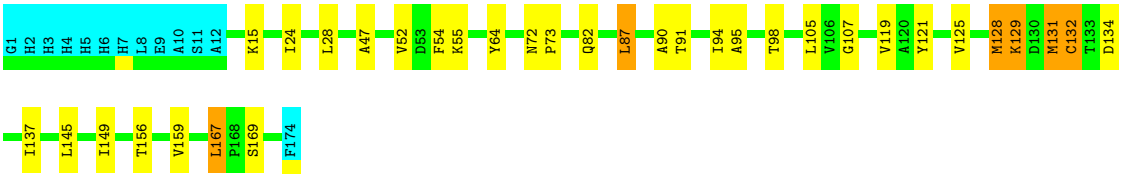
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: putative late embryogenesis abundant protein

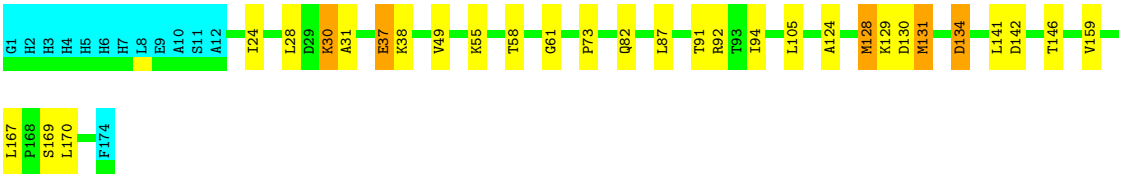
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: putative late embryogenesis abundant protein

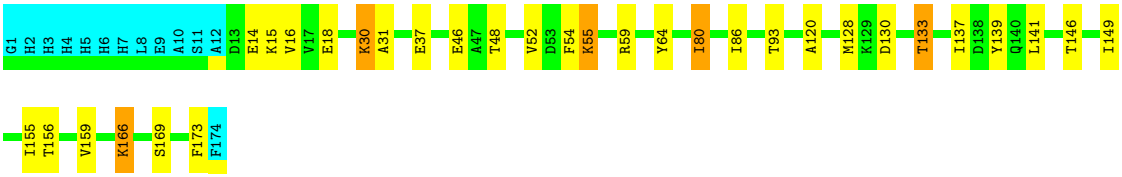
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: putative late embryogenesis abundant protein

Chain A:



4.2.11 Score per residue for model 11

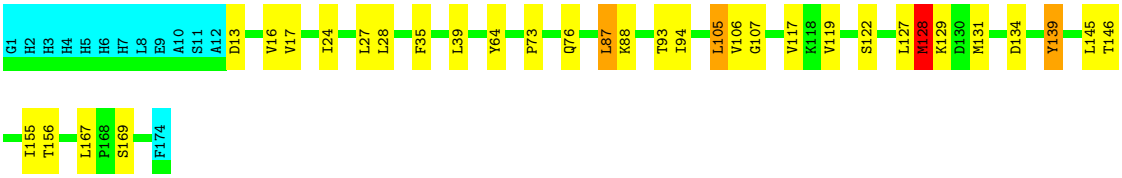
- Molecule 1: putative late embryogenesis abundant protein

Chain A:

4.2.12 Score per residue for model 12

- Molecule 1: putative late embryogenesis abundant protein

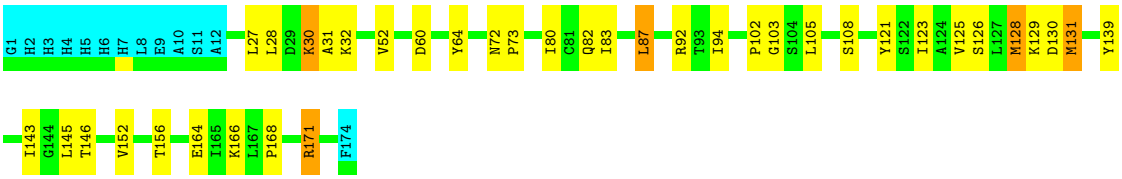
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: putative late embryogenesis abundant protein

Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: putative late embryogenesis abundant protein

Chain A: 71% 19% • 7%

G1 H2 H3 H4 H5 H6 H7 L8 E9 A10 S11 A12 D13 E14 K15 V16 V17 E18 K30 A31 K32 G33 E37 V52 D53 F54 K55 T58 G61 Y64 H65 N72 P73 Y74 L87 R92 T93 I94 A95 S108 L127 M128 K129 D130 M131 Y139 Q140

L145 T146 F147 V152 G153 D154 I155 T156 I157 S169 D172 F173 F174

4.2.15 Score per residue for model 15

- Molecule 1: putative late embryogenesis abundant protein

Chain A: 72% 18% •• 7%

G1 H2 H3 H4 H5 H6 H7 L8 E9 A10 S11 A12 K15 V16 K20 K30 F35 A36 E37 K38 L39 V49 D50 D51 F54 K55 Y64 K67 N72 P73 Y74 S75 I78 I86 S108 V119 A120 Y121 V125 D130 M131 D134 Y139

Q140 L141 T161 Q162 L170 R171 D172 F173 F174

4.2.16 Score per residue for model 16

- Molecule 1: putative late embryogenesis abundant protein

Chain A: 76% 14% • 7%

G1 H2 H3 H4 H5 H6 H7 L8 E9 A10 S11 A12 D13 V16 V17 V52 K55 G56 V57 T58 G61 Y64 H65 P73 Y74 K88 S89 A90 I94 S108 V117 K118 V119 A120 D130 M131 C132 T133 D134 W135 Y139 Q140 L145 V152 I155

S169 F174

4.2.17 Score per residue for model 17

- Molecule 1: putative late embryogenesis abundant protein

Chain A: 66% 24% •• 7%

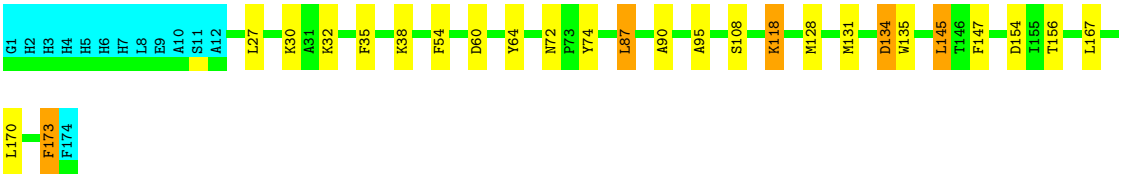
G1 H2 H3 H4 H5 H6 H7 L8 E9 A10 S11 A12 K15 V16 V17 E18 I24 L27 L28 D29 K30 G33 E37 P43 T48 V52 K55 Y64 N72 P73 Y74 S75 Q76 S77 I78 I86 T91 R92 T93 I94 A95 L105 V106 V119 A120

Y121 V125 M128 K129 D130 M131 I137 D138 Y139 Q140 I143 G144 L145 T146 F147 D148 I149 P158 V159 L167 P168 S169 D172 F173 F174

4.2.18 Score per residue for model 18

- Molecule 1: putative late embryogenesis abundant protein

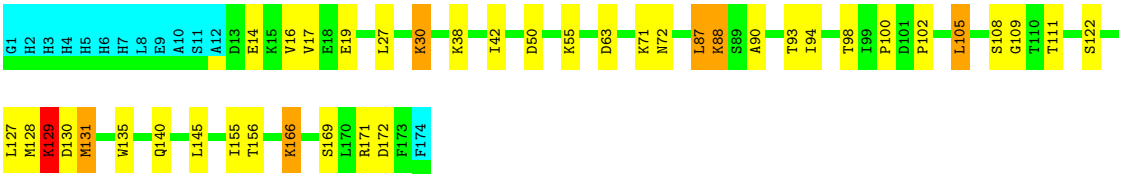
Chain A: 78% 12% • 7%



4.2.19 Score per residue for model 19

- Molecule 1: putative late embryogenesis abundant protein

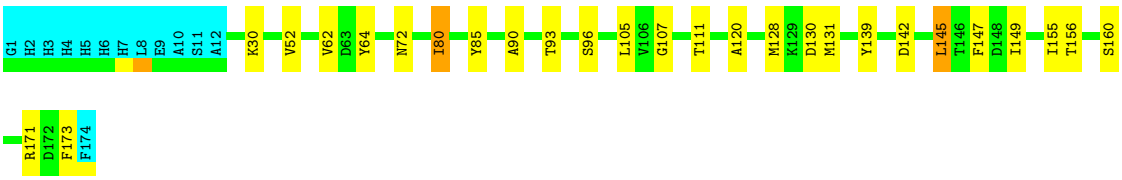
Chain A: 70% 19% • • 7%



4.2.20 Score per residue for model 20

- Molecule 1: putative late embryogenesis abundant protein

Chain A: 77% 14% • 7%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, molecular 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	1.0.6
XPLOR-NIH	refinement	2.9.3

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	0.85±0.03	0±0/1241 (0.0± 0.0%)	0.74±0.02	0±0/1693 (0.0± 0.0%)
All	All	0.86	1/24820 (0.0%)	0.74	0/33860 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	133	THR	N-CA	-6.02	1.34	1.46	10	1

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	1218	1236	1235	16±3
All	All	24360	24720	24700	312

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ASN:O	1:A:108:SER:HA	0.73	1.83	18	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:THR:HB	1:A:169:SER:OG	0.71	1.85	10	1
1:A:129:LYS:HE2	1:A:131:MET:SD	0.67	2.29	11	1
1:A:64:TYR:CD1	1:A:119:VAL:HB	0.67	2.24	5	6
1:A:123:ILE:HG23	1:A:128:MET:HA	0.66	1.66	13	1
1:A:58:THR:HB	1:A:61:GLY:O	0.64	1.92	9	6
1:A:31:ALA:HA	1:A:34:PHE:CE2	0.61	2.31	4	1
1:A:87:LEU:O	1:A:94:ILE:HB	0.60	1.95	5	11
1:A:64:TYR:CD1	1:A:119:VAL:HG13	0.59	2.32	16	1
1:A:54:PHE:HB3	1:A:64:TYR:CZ	0.58	2.33	14	5
1:A:81:CYS:O	1:A:146:THR:HB	0.58	1.98	1	1
1:A:14:GLU:O	1:A:17:VAL:HG12	0.57	1.99	19	1
1:A:170:LEU:HB3	1:A:173:PHE:CD1	0.57	2.35	15	1
1:A:118:LYS:HE3	1:A:118:LYS:HA	0.57	1.76	7	4
1:A:52:VAL:HG12	1:A:64:TYR:CD2	0.56	2.35	3	1
1:A:134:ASP:HA	1:A:167:LEU:O	0.56	2.00	8	3
1:A:55:LYS:HD2	1:A:55:LYS:N	0.56	2.14	15	1
1:A:80:ILE:HG22	1:A:147:PHE:CE1	0.56	2.36	4	1
1:A:27:LEU:O	1:A:30:LYS:HB3	0.55	2.02	3	1
1:A:38:LYS:O	1:A:42:ILE:HG12	0.54	2.03	19	1
1:A:33:GLY:O	1:A:37:GLU:HG2	0.53	2.02	14	3
1:A:147:PHE:O	1:A:154:ASP:HA	0.53	2.02	14	2
1:A:13:ASP:O	1:A:17:VAL:HG23	0.53	2.04	12	2
1:A:52:VAL:HG13	1:A:64:TYR:CD2	0.53	2.38	17	3
1:A:72:ASN:HB3	1:A:107:GLY:O	0.53	2.04	11	2
1:A:27:LEU:O	1:A:30:LYS:HG3	0.53	2.03	1	7
1:A:145:LEU:H	1:A:145:LEU:HD13	0.53	1.63	6	1
1:A:133:THR:HB	1:A:169:SER:CB	0.53	2.33	10	1
1:A:64:TYR:CZ	1:A:117:VAL:HB	0.53	2.39	16	1
1:A:88:LYS:HB2	1:A:140:GLN:HB2	0.53	1.81	19	2
1:A:131:MET:SD	1:A:171:ARG:HA	0.52	2.44	19	3
1:A:35:PHE:CD1	1:A:39:LEU:HD12	0.52	2.39	15	1
1:A:133:THR:HG22	1:A:169:SER:CB	0.52	2.34	11	1
1:A:64:TYR:CE1	1:A:119:VAL:HB	0.52	2.40	17	1
1:A:52:VAL:HG22	1:A:64:TYR:HB3	0.52	1.80	14	5
1:A:64:TYR:CE1	1:A:117:VAL:HB	0.52	2.40	16	1
1:A:129:LYS:HE3	1:A:135:TRP:CD1	0.52	2.40	4	1
1:A:129:LYS:C	1:A:131:MET:H	0.52	2.09	8	1
1:A:87:LEU:HD13	1:A:95:ALA:HB3	0.51	1.81	5	3
1:A:87:LEU:O	1:A:94:ILE:HD12	0.51	2.04	12	1
1:A:131:MET:HE1	1:A:167:LEU:HD13	0.51	1.82	12	1
1:A:20:LYS:HA	1:A:20:LYS:HE3	0.51	1.80	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:THR:HA	1:A:169:SER:HA	0.51	1.81	1	3
1:A:133:THR:HA	1:A:169:SER:OG	0.51	2.06	6	1
1:A:168:PRO:O	1:A:170:LEU:HG	0.51	2.06	11	1
1:A:55:LYS:HD3	1:A:55:LYS:C	0.51	2.25	9	2
1:A:142:ASP:OD1	1:A:160:SER:HB3	0.51	2.06	20	2
1:A:129:LYS:HD3	1:A:129:LYS:H	0.50	1.66	2	1
1:A:76:GLN:O	1:A:107:GLY:HA2	0.50	2.06	4	2
1:A:83:ILE:CG2	1:A:99:ILE:HB	0.50	2.36	1	2
1:A:131:MET:HA	1:A:131:MET:CE	0.50	2.37	16	2
1:A:54:PHE:C	1:A:55:LYS:HD2	0.50	2.27	11	1
1:A:133:THR:HA	1:A:169:SER:CB	0.50	2.37	6	1
1:A:145:LEU:HD13	1:A:145:LEU:H	0.50	1.66	18	2
1:A:34:PHE:CZ	1:A:38:LYS:HD2	0.50	2.42	1	1
1:A:86:ILE:O	1:A:141:LEU:HA	0.50	2.07	6	3
1:A:51:ASP:HB3	1:A:67:LYS:HB3	0.49	1.83	3	1
1:A:93:THR:O	1:A:122:SER:HB3	0.49	2.07	3	1
1:A:145:LEU:O	1:A:156:THR:HA	0.49	2.08	7	6
1:A:128:MET:SD	1:A:129:LYS:N	0.49	2.85	9	1
1:A:62:VAL:HG22	1:A:119:VAL:O	0.48	2.07	1	1
1:A:146:THR:OG1	1:A:156:THR:HG22	0.48	2.08	10	4
1:A:170:LEU:HB3	1:A:173:PHE:HB2	0.48	1.83	3	1
1:A:55:LYS:HD3	1:A:65:HIS:HB2	0.48	1.83	3	1
1:A:64:TYR:CE1	1:A:119:VAL:HG13	0.48	2.42	16	1
1:A:129:LYS:HG3	1:A:135:TRP:NE1	0.48	2.23	19	1
1:A:132:CYS:SG	1:A:135:TRP:HB2	0.48	2.48	11	1
1:A:105:LEU:H	1:A:105:LEU:HD23	0.48	1.68	12	1
1:A:131:MET:HA	1:A:131:MET:HE3	0.48	1.85	16	1
1:A:55:LYS:HB2	1:A:63:ASP:O	0.48	2.09	19	1
1:A:127:LEU:HD12	1:A:128:MET:N	0.47	2.25	6	4
1:A:24:ILE:O	1:A:28:LEU:HG	0.47	2.09	4	6
1:A:14:GLU:O	1:A:18:GLU:HG3	0.47	2.09	10	2
1:A:45:PRO:HA	1:A:71:LYS:O	0.47	2.09	3	1
1:A:80:ILE:HG13	1:A:102:PRO:HD2	0.47	1.87	13	1
1:A:145:LEU:HB3	1:A:147:PHE:CE2	0.47	2.45	7	3
1:A:72:ASN:ND2	1:A:105:LEU:HD21	0.47	2.25	8	1
1:A:72:ASN:ND2	1:A:105:LEU:HD23	0.47	2.25	19	1
1:A:28:LEU:O	1:A:32:LYS:HG3	0.47	2.09	6	3
1:A:20:LYS:HA	1:A:20:LYS:HE2	0.47	1.85	5	1
1:A:55:LYS:HA	1:A:55:LYS:HE3	0.47	1.86	2	1
1:A:140:GLN:HG3	1:A:161:THR:O	0.47	2.09	15	1
1:A:64:TYR:CD1	1:A:119:VAL:HG11	0.46	2.45	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:ALA:HA	1:A:123:ILE:HD13	0.46	1.86	2	1
1:A:54:PHE:HB3	1:A:64:TYR:CE2	0.46	2.45	5	1
1:A:88:LYS:HD2	1:A:93:THR:O	0.46	2.10	12	1
1:A:74:TYR:O	1:A:108:SER:HB2	0.46	2.08	14	2
1:A:80:ILE:H	1:A:80:ILE:HD13	0.46	1.71	10	2
1:A:35:PHE:HA	1:A:39:LEU:HD13	0.46	1.87	12	1
1:A:131:MET:O	1:A:132:CYS:HB2	0.46	2.10	8	1
1:A:27:LEU:O	1:A:30:LYS:HG2	0.46	2.11	18	1
1:A:131:MET:SD	1:A:170:LEU:HB2	0.46	2.50	15	1
1:A:71:LYS:HA	1:A:109:GLY:O	0.46	2.10	19	1
1:A:49:VAL:HG11	1:A:143:ILE:CG1	0.46	2.41	6	1
1:A:54:PHE:HA	1:A:64:TYR:CE1	0.46	2.45	10	1
1:A:62:VAL:O	1:A:118:LYS:HA	0.46	2.11	11	1
1:A:52:VAL:HG11	1:A:139:TYR:OH	0.46	2.11	7	1
1:A:62:VAL:CG2	1:A:119:VAL:HB	0.46	2.41	1	1
1:A:124:ALA:HA	1:A:128:MET:HA	0.46	1.88	11	1
1:A:30:LYS:HD2	1:A:31:ALA:N	0.45	2.26	1	7
1:A:155:ILE:HD12	1:A:155:ILE:O	0.45	2.11	11	1
1:A:155:ILE:HD13	1:A:155:ILE:H	0.45	1.71	16	1
1:A:124:ALA:HA	1:A:128:MET:CA	0.45	2.41	9	1
1:A:121:TYR:O	1:A:125:VAL:HG23	0.45	2.12	13	3
1:A:91:THR:C	1:A:92:ARG:HD2	0.45	2.32	9	1
1:A:48:THR:HA	1:A:159:VAL:HG21	0.45	1.88	10	3
1:A:82:GLN:HG3	1:A:98:THR:CG2	0.45	2.42	8	1
1:A:32:LYS:HA	1:A:35:PHE:CE2	0.45	2.47	18	1
1:A:127:LEU:H	1:A:127:LEU:HD23	0.45	1.72	19	1
1:A:129:LYS:HG3	1:A:130:ASP:H	0.45	1.71	1	1
1:A:49:VAL:O	1:A:50:ASP:HB2	0.45	2.12	6	1
1:A:128:MET:SD	1:A:131:MET:HG2	0.45	2.52	9	1
1:A:13:ASP:HA	1:A:16:VAL:HG22	0.45	1.89	12	1
1:A:52:VAL:HG22	1:A:64:TYR:CB	0.45	2.42	20	1
1:A:13:ASP:O	1:A:17:VAL:HG22	0.45	2.11	2	1
1:A:62:VAL:HG21	1:A:173:PHE:CE2	0.45	2.47	2	1
1:A:55:LYS:HG3	1:A:65:HIS:CD2	0.44	2.47	14	1
1:A:62:VAL:HG21	1:A:173:PHE:CZ	0.44	2.48	20	1
1:A:149:ILE:HD13	1:A:149:ILE:H	0.44	1.72	17	1
1:A:72:ASN:HD22	1:A:105:LEU:HD12	0.44	1.73	17	1
1:A:131:MET:CG	1:A:171:ARG:HA	0.44	2.43	19	1
1:A:85:TYR:O	1:A:96:SER:HA	0.44	2.12	20	1
1:A:37:GLU:HG2	1:A:38:LYS:HD3	0.44	1.89	9	1
1:A:35:PHE:HA	1:A:39:LEU:HB2	0.44	1.89	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LYS:C	1:A:15:LYS:HD3	0.44	2.33	15	2
1:A:88:LYS:O	1:A:139:TYR:HB2	0.44	2.13	7	1
1:A:91:THR:O	1:A:92:ARG:HD2	0.44	2.12	9	1
1:A:27:LEU:HD22	1:A:156:THR:OG1	0.44	2.13	12	1
1:A:131:MET:HE1	1:A:167:LEU:CD1	0.44	2.43	12	1
1:A:128:MET:O	1:A:128:MET:HG2	0.44	2.13	17	1
1:A:49:VAL:H	1:A:159:VAL:HG11	0.44	1.72	3	1
1:A:170:LEU:HD12	1:A:170:LEU:O	0.44	2.12	11	1
1:A:85:TYR:OH	1:A:117:VAL:HA	0.43	2.12	1	1
1:A:87:LEU:HD23	1:A:88:LYS:N	0.43	2.27	5	1
1:A:166:LYS:O	1:A:168:PRO:HD3	0.43	2.12	13	2
1:A:52:VAL:HB	1:A:64:TYR:CE2	0.43	2.48	10	1
1:A:105:LEU:HA	1:A:111:THR:HG21	0.43	1.90	19	2
1:A:86:ILE:HA	1:A:95:ALA:O	0.43	2.12	17	1
1:A:55:LYS:N	1:A:55:LYS:HE2	0.43	2.28	5	1
1:A:128:MET:C	1:A:129:LYS:HD3	0.43	2.33	19	1
1:A:166:LYS:HD3	1:A:166:LYS:H	0.43	1.73	19	1
1:A:41:ASN:OD1	1:A:42:ILE:HG13	0.43	2.14	6	1
1:A:52:VAL:HB	1:A:64:TYR:CD2	0.43	2.49	10	1
1:A:89:SER:OG	1:A:122:SER:HB2	0.43	2.14	11	1
1:A:170:LEU:HD21	1:A:173:PHE:CD1	0.43	2.48	18	1
1:A:17:VAL:HG11	1:A:94:ILE:O	0.43	2.14	1	2
1:A:52:VAL:HG21	1:A:165:ILE:CD1	0.43	2.44	4	1
1:A:134:ASP:H	1:A:169:SER:H	0.43	1.57	12	1
1:A:80:ILE:HG12	1:A:103:GLY:O	0.43	2.14	13	1
1:A:49:VAL:HG11	1:A:143:ILE:HG13	0.43	1.91	6	1
1:A:37:GLU:HG3	1:A:38:LYS:N	0.42	2.29	3	1
1:A:15:LYS:HD2	1:A:15:LYS:C	0.42	2.35	10	1
1:A:47:ALA:O	1:A:159:VAL:HG11	0.42	2.14	8	2
1:A:87:LEU:HB3	1:A:95:ALA:HB3	0.42	1.90	2	1
1:A:82:GLN:C	1:A:83:ILE:HD12	0.42	2.34	13	1
1:A:54:PHE:C	1:A:55:LYS:HE2	0.42	2.35	5	1
1:A:98:THR:O	1:A:100:PRO:HD3	0.42	2.14	19	1
1:A:133:THR:HG22	1:A:169:SER:HB2	0.42	1.90	11	1
1:A:76:GLN:HG3	1:A:78:ILE:HG12	0.42	1.90	17	1
1:A:65:HIS:HA	1:A:115:VAL:O	0.42	2.14	2	1
1:A:146:THR:HA	1:A:155:ILE:O	0.42	2.14	10	1
1:A:83:ILE:HG23	1:A:143:ILE:HG23	0.42	1.91	13	1
1:A:62:VAL:HG12	1:A:173:PHE:O	0.42	2.14	1	1
1:A:166:LYS:HD2	1:A:166:LYS:H	0.42	1.73	10	1
1:A:94:ILE:HD13	1:A:95:ALA:N	0.42	2.29	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:PHE:CZ	1:A:62:VAL:HG11	0.42	2.49	11	1
1:A:121:TYR:O	1:A:125:VAL:HG12	0.42	2.15	15	1
1:A:54:PHE:O	1:A:55:LYS:HE3	0.41	2.14	2	1
1:A:55:LYS:HG2	1:A:64:TYR:HA	0.41	1.92	16	1
1:A:80:ILE:HG22	1:A:147:PHE:CZ	0.41	2.50	4	1
1:A:84:SER:HA	1:A:97:GLY:O	0.41	2.15	4	1
1:A:52:VAL:CG2	1:A:64:TYR:HB3	0.41	2.43	8	1
1:A:51:ASP:HB2	1:A:67:LYS:HB3	0.41	1.92	15	1
1:A:76:GLN:HG3	1:A:78:ILE:CG1	0.41	2.45	17	1
1:A:105:LEU:HG	1:A:147:PHE:CE1	0.41	2.50	17	1
1:A:129:LYS:HG3	1:A:130:ASP:N	0.41	2.30	1	1
1:A:85:TYR:CE2	1:A:117:VAL:HG12	0.41	2.49	3	1
1:A:82:GLN:O	1:A:146:THR:HB	0.41	2.15	9	1
1:A:105:LEU:HD23	1:A:105:LEU:H	0.41	1.75	11	1
1:A:93:THR:OG1	1:A:122:SER:HB2	0.41	2.15	12	1
1:A:38:LYS:N	1:A:38:LYS:HD3	0.41	2.31	18	1
1:A:26:SER:HA	1:A:29:ASP:OD2	0.41	2.15	3	1
1:A:139:TYR:CE1	1:A:165:ILE:HD11	0.41	2.50	7	1
1:A:143:ILE:O	1:A:158:PRO:HA	0.41	2.15	17	1
1:A:62:VAL:HG11	1:A:173:PHE:CZ	0.41	2.51	3	1
1:A:20:LYS:HE3	1:A:20:LYS:HA	0.41	1.93	6	1
1:A:94:ILE:C	1:A:94:ILE:HD12	0.41	2.36	6	2
1:A:86:ILE:HB	1:A:142:ASP:HB2	0.41	1.91	7	1
1:A:131:MET:HG2	1:A:135:TRP:CD1	0.41	2.51	7	1
1:A:147:PHE:CD2	1:A:157:ILE:HD13	0.41	2.50	14	1
1:A:87:LEU:HD11	1:A:95:ALA:HB3	0.41	1.92	18	1
1:A:94:ILE:HD12	1:A:94:ILE:C	0.41	2.35	2	1
1:A:49:VAL:HG23	1:A:159:VAL:HG22	0.41	1.93	4	1
1:A:117:VAL:HG11	1:A:139:TYR:OH	0.41	2.16	12	1
1:A:80:ILE:HA	1:A:146:THR:O	0.40	2.16	6	1
1:A:105:LEU:HD23	1:A:107:GLY:H	0.40	1.76	20	2
1:A:49:VAL:HG23	1:A:161:THR:CG2	0.40	2.46	15	1
1:A:93:THR:HB	1:A:122:SER:OG	0.40	2.15	19	1
1:A:80:ILE:HG23	1:A:147:PHE:CE1	0.40	2.52	20	1
1:A:49:VAL:HG22	1:A:159:VAL:HG22	0.40	1.93	9	1
1:A:49:VAL:HB	1:A:161:THR:OG1	0.40	2.17	1	1
1:A:81:CYS:O	1:A:82:GLN:HB3	0.40	2.16	1	1
1:A:87:LEU:HG	1:A:139:TYR:CE2	0.40	2.51	12	2
1:A:35:PHE:HA	1:A:39:LEU:HD12	0.40	1.92	7	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	161/174 (93%)	137±2 (85±2%)	18±3 (11±2%)	6±2 (4±1%)	5 31
All	All	3220/3480 (93%)	2732 (85%)	358 (11%)	130 (4%)	5 31

All 30 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	130	ASP	14
1	A	73	PRO	12
1	A	169	SER	11
1	A	128	MET	9
1	A	90	ALA	8
1	A	131	MET	8
1	A	173	PHE	6
1	A	93	THR	5
1	A	74	TYR	5
1	A	129	LYS	5
1	A	152	VAL	5
1	A	171	ARG	5
1	A	172	ASP	5
1	A	134	ASP	5
1	A	60	ASP	3
1	A	75	SER	3
1	A	91	THR	3
1	A	50	ASP	3
1	A	106	VAL	3
1	A	43	PRO	2
1	A	107	GLY	1
1	A	61	GLY	1
1	A	153	GLY	1
1	A	132	CYS	1
1	A	170	LEU	1
1	A	108	SER	1
1	A	126	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	56	GLY	1
1	A	92	ARG	1
1	A	102	PRO	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	141/151 (93%)	134±2 (95±1%)	7±2 (5±1%)	27 76
All	All	2820/3020 (93%)	2673 (95%)	147 (5%)	27 76

All 42 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	30	LYS	12
1	A	139	TYR	11
1	A	55	LYS	9
1	A	131	MET	9
1	A	149	ILE	8
1	A	87	LEU	8
1	A	129	LYS	7
1	A	145	LEU	7
1	A	128	MET	6
1	A	105	LEU	6
1	A	118	LYS	5
1	A	155	ILE	5
1	A	137	ILE	4
1	A	15	LYS	4
1	A	80	ILE	3
1	A	140	GLN	3
1	A	94	ILE	3
1	A	37	GLU	3
1	A	166	LYS	3
1	A	14	GLU	2
1	A	164	GLU	2
1	A	59	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	19	GLU	2
1	A	46	GLU	2
1	A	92	ARG	2
1	A	88	LYS	2
1	A	135	TRP	2
1	A	41	ASN	1
1	A	67	LYS	1
1	A	171	ARG	1
1	A	35	PHE	1
1	A	167	LEU	1
1	A	141	LEU	1
1	A	142	ASP	1
1	A	38	LYS	1
1	A	102	PRO	1
1	A	20	LYS	1
1	A	78	ILE	1
1	A	162	GLN	1
1	A	65	HIS	1
1	A	18	GLU	1
1	A	158	PRO	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