Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 08:14 AM EST

PDB ID	:	1WK1
Title	:	Solution structure of Lectin C-type domain derived from a hypothetical protein from C. elegans
Authors	:	Kobayashi, N.; Koshiba, S.; Inoue, M.; Tochio, N.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-05-29

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:

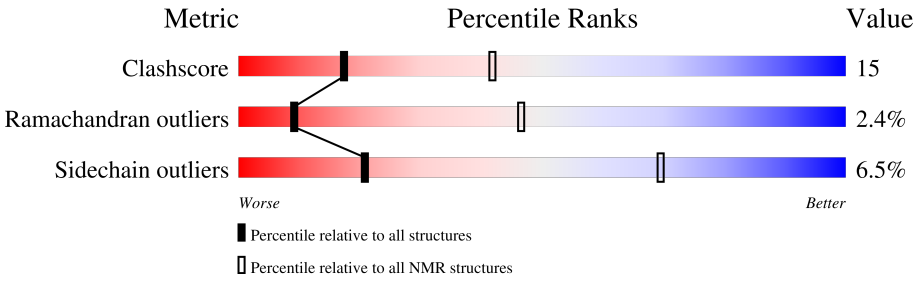
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	150	58% 17% • 22%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:8-A:105, A:110-A:128 (117)	0.20	1

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, 4, 5, 7, 8, 10, 11, 13, 14, 15, 16, 17, 18, 19, 20
2	6, 9
Single-model clusters	12

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2213 atoms, of which 1057 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein yk1067a12.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	150	2213	717	1057	201	233	5	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q19853
A	2	SER	-	cloning artifact	UNP Q19853
A	3	SER	-	cloning artifact	UNP Q19853
A	4	GLY	-	cloning artifact	UNP Q19853
A	5	SER	-	cloning artifact	UNP Q19853
A	6	SER	-	cloning artifact	UNP Q19853
A	7	GLY	-	cloning artifact	UNP Q19853
A	145	SER	-	cloning artifact	UNP Q19853
A	146	GLY	-	cloning artifact	UNP Q19853
A	147	PRO	-	cloning artifact	UNP Q19853
A	148	SER	-	cloning artifact	UNP Q19853
A	149	SER	-	cloning artifact	UNP Q19853
A	150	GLY	-	cloning artifact	UNP Q19853

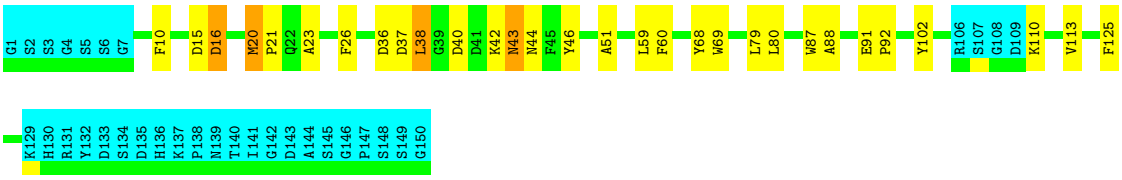
4 Residue-property plots (i)

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: Hypothetical protein yk1067a12

Chain A: 58% 17% • 22%



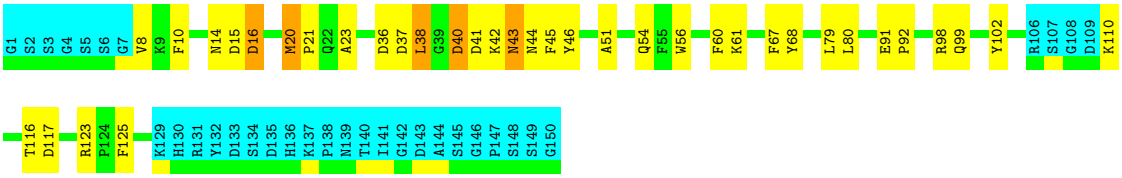
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Hypothetical protein yk1067a12

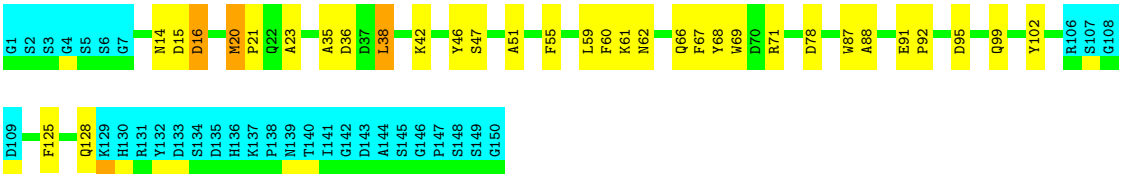
Chain A: 53% 21% • 22%



4.2.2 Score per residue for model 2

• Molecule 1: Hypothetical protein yk1067a12

Chain A: 56% 20% • 22%



4.2.3 Score per residue for model 3

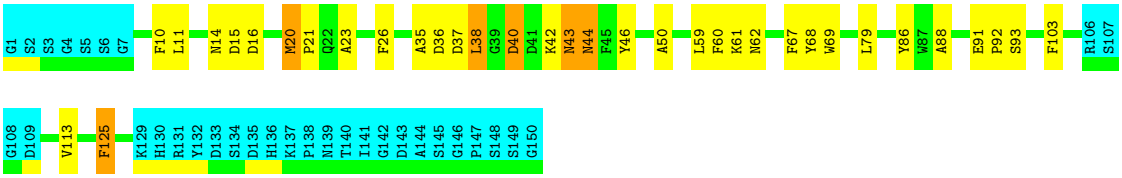
- Molecule 1: Hypothetical protein yk1067a12

Chain A:

4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical protein yk1067a12

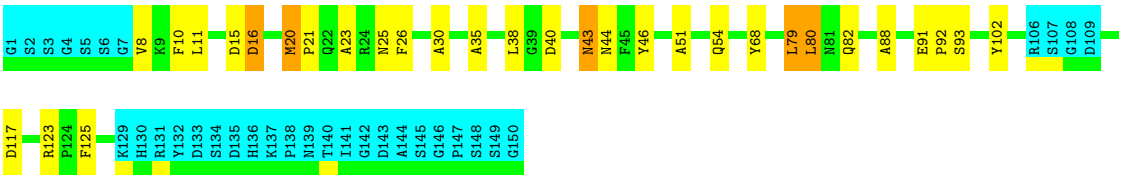
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Hypothetical protein yk1067a12

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical protein yk1067a12

Chain A: 60% 14% • 22%

G1 S2 S3 G4 S5 S6 G7 D15 D16 M20 P21 Q22 A23 D36 D37 L38 G39 D40 N43 N44 A51 F55 W56 F60 L79 L80 Y86 W87 E91 P92 Y102 F103 D104 G105 R106 S107 G108 D109 V113 W114 T115 T116 F125 K129 H130 R131

Y132 D133 S134 D135 H136 K137 P138 N139 T140 I141 G142 D143 A144 S145 G146 P147 S148 S149 G150

4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical protein yk1067a12

Chain A: 49% 24% 5% 22%

G1 S2 S3 G4 S5 S6 G7 V8 K9 F10 L11 T12 V13 N14 D15 D16 M20 P21 F26 S29 D36 D37 L38 G39 D40 D41 K42 N43 N44 F45 Y46 S47 A50 A51 N52 T53 Q54 F55 W56 L59 N62 Y68 W69 L79 L80 Y86 W87 A88 N89 G90

E91 P92 S93 Y102 F103 R106 S107 G108 D109 T116 R123 P124 F125 K129 H130 R131 Y132 D133 S134 D135 H136 K137 P138 N139 T140 I141 G142 D143 A144 S145 G146 P147 S148 S149 G150

4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical protein yk1067a12

Chain A: 55% 20% • 22%

G1 S2 S3 G4 S5 S6 G7 N14 D15 D16 M20 P21 N25 L38 D41 K42 N43 N44 F45 A51 N52 L59 F60 K61 N62 Y68 W69 L79 Q82 Y86 W87 E91 P92 D95 Q99 G100 V101 Y102 F103 R106 S107 G108 D109 K110

V113 T116 D117 T118 T121 K129 H130 R131 Y132 D133 S134 D135 H136 K137 P138 N139 T140 I141 G142 D143 A144 S145 G146 P147 S148 S149 G150

4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical protein yk1067a12

Chain A: 55% 19% • • 22%

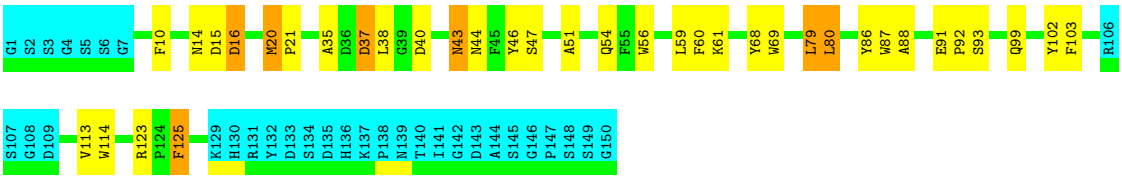
G1 S2 S3 G4 S5 S6 G7 F10 L11 T12 D15 D16 M20 P21 Q22 A23 R24 N25 F26 C27 G32 Y33 L34 A35 L38 G39 D40 D41 K42 N43 Y46 S47 S48 W56 F60 Y68 L79 L80 E91 P92 V101 Y102 R106 S107 G108 D109 K110

V113 T116 D117 F125 K129 H130 R131 Y132 D133 S134 D135 H136 K137 P138 N139 T140 I141 G142 D143 A144 S145 G146 P147 S148 S149 G150

4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical protein yk1067a12

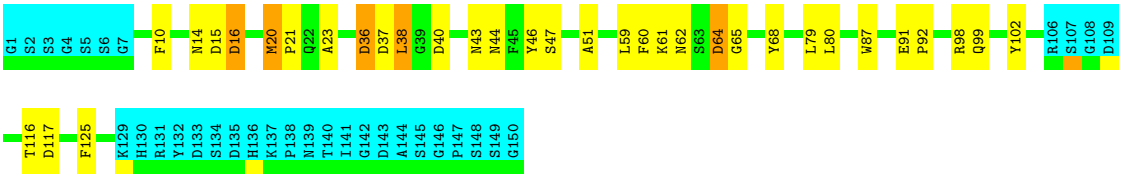
Chain A: 53% 20% 5% 22%



4.2.11 Score per residue for model 11

- Molecule 1: Hypothetical protein yk1067a12

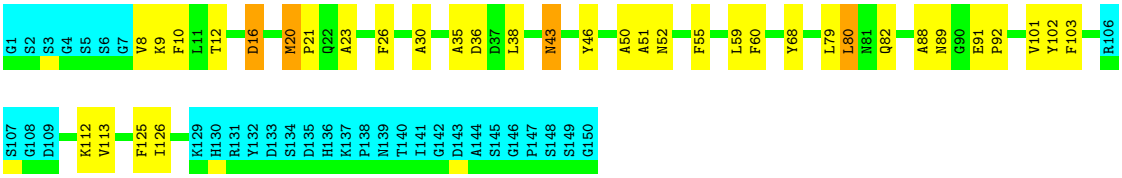
Chain A: 55% 19% • 22%



4.2.12 Score per residue for model 12

- Molecule 1: Hypothetical protein yk1067a12

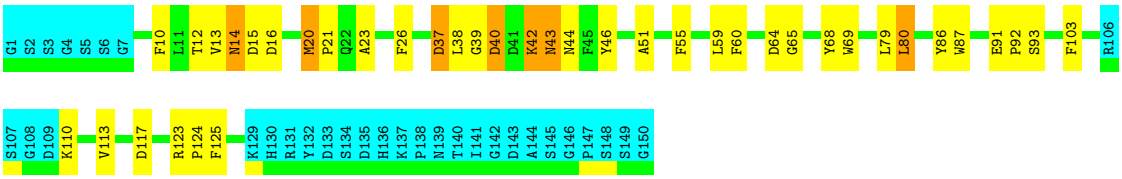
Chain A: 54% 21% • 22%



4.2.13 Score per residue for model 13

- Molecule 1: Hypothetical protein yk1067a12

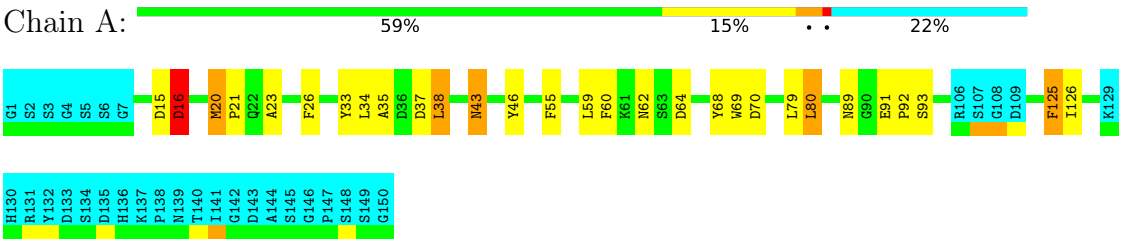
Chain A: 51% 22% 5% 22%



4.2.14 Score per residue for model 14

- Molecule 1: Hypothetical protein yk1067a12

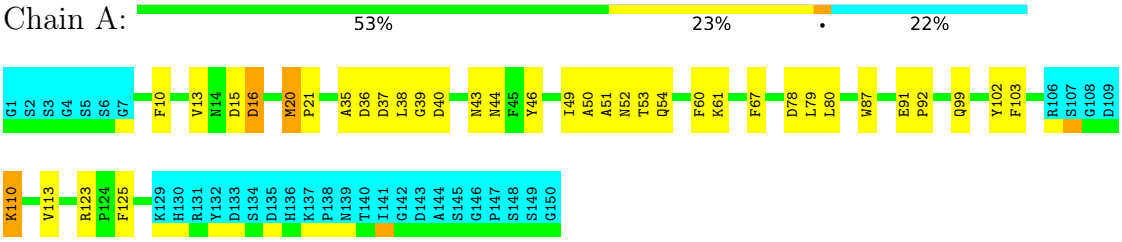
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Hypothetical protein yk1067a12

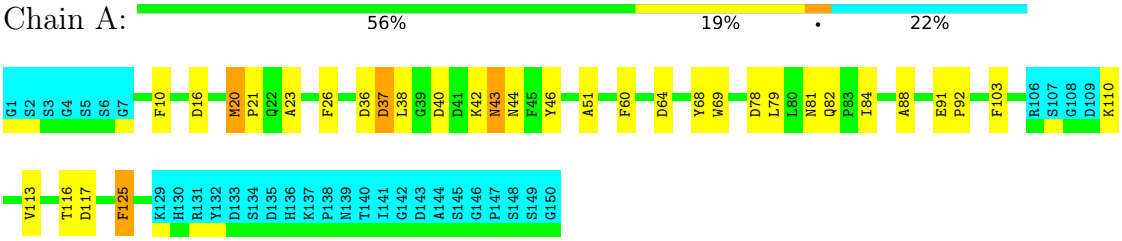
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Hypothetical protein yk1067a12

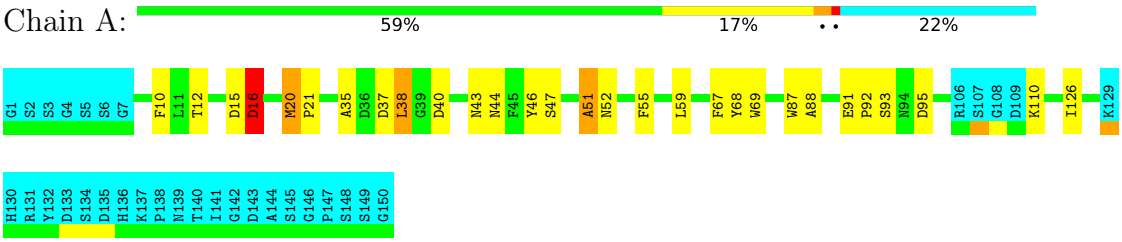
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Hypothetical protein yk1067a12

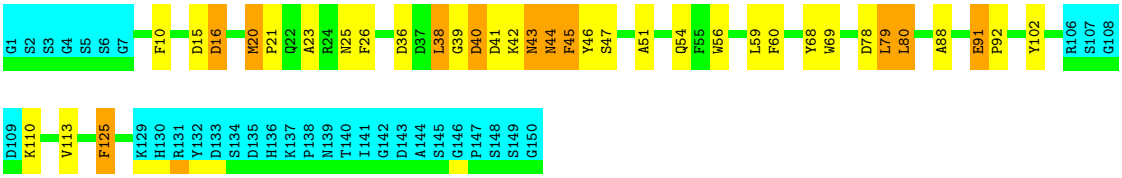
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Hypothetical protein yk1067a12

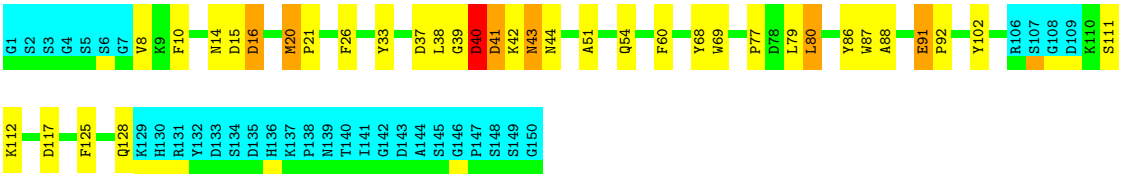
Chain A: 54% 17% 7% 22%



4.2.19 Score per residue for model 19

- Molecule 1: Hypothetical protein yk1067a12

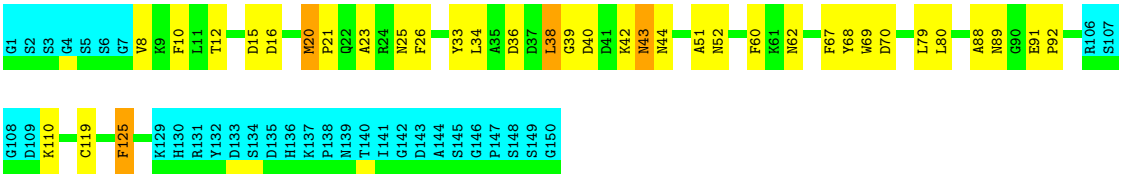
Chain A: 54% 19% • • 22%



4.2.20 Score per residue for model 20

- Molecule 1: Hypothetical protein yk1067a12

Chain A: 54% 21% • 22%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, 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	928	855	855	27±5
All	All	18560	17100	17100	542

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:HD12	1:A:38:LEU:O	0.80	1.76	9	4
1:A:35:ALA:HB1	1:A:46:TYR:OH	0.72	1.83	4	9
1:A:103:PHE:CE2	1:A:113:VAL:HG21	0.68	2.23	8	3
1:A:91:GLU:OE1	1:A:116:THR:HG23	0.66	1.89	16	4
1:A:101:VAL:HG22	1:A:116:THR:HG22	0.66	1.68	9	2
1:A:38:LEU:HD21	1:A:69:TRP:CE2	0.65	2.26	8	1
1:A:102:TYR:CE2	1:A:123:ARG:NH1	0.64	2.65	10	1
1:A:23:ALA:HB1	1:A:125:PHE:CD2	0.64	2.28	12	9
1:A:88:ALA:HB3	1:A:91:GLU:OE2	0.64	1.92	19	1
1:A:88:ALA:HB3	1:A:91:GLU:HG3	0.64	1.70	16	3
1:A:103:PHE:CE1	1:A:113:VAL:HG21	0.64	2.28	4	4
1:A:68:TYR:CZ	1:A:79:LEU:HD23	0.63	2.29	9	9
1:A:23:ALA:HB1	1:A:125:PHE:CG	0.62	2.29	14	12
1:A:79:LEU:HD13	1:A:80:LEU:N	0.61	2.10	5	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:MET:N	1:A:21:PRO:HD2	0.61	2.11	3	20
1:A:38:LEU:HD23	1:A:69:TRP:CE2	0.60	2.31	19	1
1:A:60:PHE:CD1	1:A:60:PHE:O	0.59	2.56	13	13
1:A:42:LYS:O	1:A:46:TYR:CD2	0.59	2.56	7	4
1:A:36:ASP:CG	1:A:38:LEU:HD21	0.59	2.17	4	2
1:A:37:ASP:OD1	1:A:46:TYR:CE2	0.57	2.56	1	5
1:A:125:PHE:CD1	1:A:125:PHE:N	0.56	2.73	20	17
1:A:59:LEU:HD13	1:A:69:TRP:CZ2	0.55	2.37	18	6
1:A:38:LEU:H	1:A:38:LEU:HD23	0.55	1.61	17	1
1:A:13:VAL:HG11	1:A:53:THR:HG21	0.55	1.79	15	3
1:A:68:TYR:CZ	1:A:79:LEU:CD2	0.55	2.89	9	5
1:A:59:LEU:HD21	1:A:87:TRP:CH2	0.55	2.37	8	4
1:A:38:LEU:HD23	1:A:38:LEU:N	0.54	2.17	17	5
1:A:110:LYS:O	1:A:113:VAL:HG13	0.54	2.02	18	2
1:A:43:ASN:CB	1:A:86:TYR:CZ	0.53	2.91	6	4
1:A:59:LEU:HD23	1:A:101:VAL:HG21	0.53	1.81	12	1
1:A:14:ASN:OD1	1:A:125:PHE:CD1	0.53	2.61	13	1
1:A:43:ASN:HD22	1:A:44:ASN:N	0.53	2.01	7	5
1:A:79:LEU:HD13	1:A:79:LEU:C	0.53	2.24	12	7
1:A:67:PHE:CE2	1:A:87:TRP:CH2	0.53	2.97	3	2
1:A:55:PHE:CE2	1:A:126:ILE:HD12	0.52	2.39	17	3
1:A:68:TYR:CE2	1:A:79:LEU:HD23	0.52	2.40	9	7
1:A:60:PHE:C	1:A:60:PHE:CD1	0.52	2.83	10	4
1:A:56:TRP:CZ2	1:A:123:ARG:NH1	0.51	2.78	1	1
1:A:60:PHE:CD1	1:A:60:PHE:C	0.51	2.84	18	11
1:A:43:ASN:ND2	1:A:43:ASN:C	0.51	2.64	13	12
1:A:79:LEU:HD23	1:A:80:LEU:N	0.51	2.20	20	1
1:A:10:PHE:O	1:A:12:THR:HG23	0.51	2.05	20	3
1:A:104:ASP:O	1:A:113:VAL:HG12	0.51	2.06	6	1
1:A:20:MET:N	1:A:21:PRO:CD	0.50	2.74	20	20
1:A:69:TRP:O	1:A:77:PRO:CB	0.50	2.60	19	1
1:A:36:ASP:CB	1:A:38:LEU:HD21	0.50	2.36	11	1
1:A:37:ASP:OD2	1:A:103:PHE:CE1	0.50	2.65	16	1
1:A:39:GLY:O	1:A:42:LYS:N	0.50	2.45	18	7
1:A:38:LEU:HD11	1:A:69:TRP:CD1	0.50	2.42	16	1
1:A:36:ASP:CB	1:A:38:LEU:CD2	0.50	2.89	11	3
1:A:43:ASN:HB2	1:A:86:TYR:CE2	0.50	2.42	13	3
1:A:64:ASP:OD1	1:A:65:GLY:N	0.50	2.45	11	2
1:A:88:ALA:HB3	1:A:91:GLU:CG	0.49	2.37	12	1
1:A:91:GLU:OE1	1:A:93:SER:N	0.49	2.45	17	5
1:A:79:LEU:C	1:A:79:LEU:CD1	0.49	2.79	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ALA:O	1:A:26:PHE:N	0.49	2.46	12	7
1:A:46:TYR:O	1:A:48:SER:N	0.49	2.46	9	1
1:A:102:TYR:CD1	1:A:102:TYR:C	0.49	2.86	15	8
1:A:40:ASP:OD1	1:A:44:ASN:ND2	0.49	2.45	6	1
1:A:102:TYR:CD1	1:A:102:TYR:O	0.49	2.66	15	3
1:A:56:TRP:CE3	1:A:102:TYR:HB3	0.49	2.43	9	6
1:A:61:LYS:CB	1:A:99:GLN:O	0.49	2.61	2	6
1:A:34:LEU:HD12	1:A:70:ASP:OD2	0.49	2.07	20	1
1:A:64:ASP:CG	1:A:65:GLY:N	0.48	2.66	11	1
1:A:8:VAL:HG11	1:A:30:ALA:HB1	0.48	1.84	5	1
1:A:36:ASP:HB2	1:A:38:LEU:HD21	0.48	1.86	11	1
1:A:69:TRP:HE1	1:A:80:LEU:HD12	0.48	1.69	18	1
1:A:38:LEU:O	1:A:38:LEU:CD1	0.48	2.59	3	3
1:A:40:ASP:O	1:A:44:ASN:ND2	0.48	2.46	10	5
1:A:45:PHE:C	1:A:45:PHE:CD1	0.48	2.86	18	1
1:A:36:ASP:CG	1:A:38:LEU:CD2	0.48	2.82	4	1
1:A:43:ASN:HB2	1:A:86:TYR:CZ	0.48	2.44	4	3
1:A:38:LEU:HD11	1:A:69:TRP:NE1	0.48	2.24	16	1
1:A:21:PRO:CD	1:A:119:CYS:O	0.48	2.62	20	1
1:A:56:TRP:CH2	1:A:123:ARG:NH1	0.48	2.82	1	1
1:A:38:LEU:HD23	1:A:69:TRP:CD2	0.48	2.44	19	1
1:A:67:PHE:CD2	1:A:87:TRP:CZ2	0.47	3.02	15	2
1:A:50:ALA:O	1:A:52:ASN:N	0.47	2.46	12	3
1:A:82:GLN:NE2	1:A:84:ILE:O	0.47	2.46	16	1
1:A:40:ASP:O	1:A:42:LYS:N	0.47	2.46	1	1
1:A:42:LYS:HG3	1:A:46:TYR:CE2	0.47	2.43	7	3
1:A:44:ASN:OD1	1:A:44:ASN:C	0.47	2.52	18	4
1:A:38:LEU:CD2	1:A:82:GLN:OE1	0.47	2.61	12	3
1:A:61:LYS:HE3	1:A:67:PHE:CZ	0.47	2.44	4	3
1:A:55:PHE:CD1	1:A:55:PHE:N	0.47	2.83	2	3
1:A:26:PHE:C	1:A:26:PHE:CD1	0.47	2.88	13	2
1:A:9:LYS:HD2	1:A:12:THR:HG21	0.47	1.87	12	1
1:A:98:ARG:NE	1:A:116:THR:O	0.46	2.49	1	1
1:A:67:PHE:O	1:A:79:LEU:HD12	0.46	2.10	3	1
1:A:44:ASN:OD1	1:A:45:PHE:N	0.46	2.48	1	1
1:A:91:GLU:HA	1:A:92:PRO:C	0.46	2.31	4	20
1:A:62:ASN:HB2	1:A:68:TYR:CD1	0.46	2.45	11	6
1:A:15:ASP:O	1:A:16:ASP:C	0.46	2.53	7	16
1:A:110:LYS:HA	1:A:113:VAL:HG13	0.46	1.88	9	5
1:A:38:LEU:HD21	1:A:69:TRP:NE1	0.46	2.26	8	1
1:A:43:ASN:C	1:A:43:ASN:ND2	0.46	2.69	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LYS:HD2	1:A:46:TYR:CE2	0.46	2.46	13	1
1:A:8:VAL:HG13	1:A:8:VAL:O	0.46	2.10	20	3
1:A:60:PHE:CE2	1:A:70:ASP:OD1	0.46	2.69	14	1
1:A:62:ASN:HB2	1:A:68:TYR:CE1	0.46	2.46	11	3
1:A:37:ASP:OD2	1:A:46:TYR:CD2	0.46	2.69	13	2
1:A:55:PHE:O	1:A:103:PHE:N	0.46	2.49	6	1
1:A:38:LEU:CD2	1:A:69:TRP:CE2	0.46	2.98	8	1
1:A:37:ASP:OD2	1:A:103:PHE:CD1	0.45	2.69	16	1
1:A:23:ALA:CB	1:A:125:PHE:CD2	0.45	3.00	13	1
1:A:54:GLN:HB3	1:A:102:TYR:CE1	0.45	2.47	5	4
1:A:46:TYR:O	1:A:47:SER:C	0.45	2.55	2	8
1:A:85:THR:HB	1:A:87:TRP:CD1	0.45	2.47	3	1
1:A:59:LEU:HB2	1:A:69:TRP:CZ3	0.45	2.47	17	2
1:A:55:PHE:CE1	1:A:103:PHE:HB3	0.45	2.46	7	1
1:A:39:GLY:O	1:A:41:ASP:N	0.45	2.50	19	1
1:A:51:ALA:O	1:A:52:ASN:CG	0.44	2.56	17	4
1:A:88:ALA:C	1:A:91:GLU:OE1	0.44	2.55	10	1
1:A:10:PHE:O	1:A:126:ILE:HG23	0.44	2.12	12	1
1:A:14:ASN:O	1:A:15:ASP:C	0.44	2.55	13	8
1:A:36:ASP:HB3	1:A:38:LEU:CD2	0.44	2.43	2	2
1:A:38:LEU:HD23	1:A:82:GLN:OE1	0.44	2.12	8	1
1:A:27:CYS:O	1:A:32:GLY:N	0.44	2.51	9	1
1:A:98:ARG:NH2	1:A:117:ASP:OD2	0.44	2.50	11	1
1:A:11:LEU:HD22	1:A:11:LEU:N	0.44	2.27	4	1
1:A:54:GLN:CB	1:A:123:ARG:NH1	0.44	2.80	5	1
1:A:39:GLY:O	1:A:40:ASP:C	0.44	2.56	19	4
1:A:67:PHE:C	1:A:68:TYR:CD1	0.44	2.91	20	1
1:A:56:TRP:CZ3	1:A:102:TYR:HB3	0.44	2.47	10	3
1:A:33:TYR:O	1:A:34:LEU:C	0.44	2.56	14	3
1:A:66:GLN:HB2	1:A:68:TYR:CE1	0.44	2.48	2	1
1:A:86:TYR:O	1:A:87:TRP:C	0.44	2.56	10	3
1:A:43:ASN:ND2	1:A:44:ASN:N	0.44	2.66	18	1
1:A:102:TYR:CE1	1:A:123:ARG:NH1	0.44	2.86	7	2
1:A:36:ASP:C	1:A:37:ASP:OD1	0.44	2.56	7	1
1:A:68:TYR:CE2	1:A:79:LEU:CD2	0.44	3.01	7	2
1:A:38:LEU:HD21	1:A:69:TRP:CZ2	0.44	2.48	16	1
1:A:40:ASP:O	1:A:44:ASN:CG	0.43	2.56	3	5
1:A:38:LEU:HD11	1:A:69:TRP:CE2	0.43	2.47	16	1
1:A:9:LYS:CB	1:A:12:THR:OG1	0.43	2.67	12	2
1:A:59:LEU:HD13	1:A:69:TRP:CH2	0.43	2.49	13	3
1:A:80:LEU:CD1	1:A:82:GLN:OE1	0.43	2.66	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:TYR:CD1	1:A:68:TYR:N	0.43	2.86	17	1
1:A:38:LEU:HD21	1:A:82:GLN:OE1	0.43	2.13	5	1
1:A:88:ALA:CB	1:A:91:GLU:OE2	0.43	2.63	19	1
1:A:40:ASP:C	1:A:42:LYS:N	0.43	2.72	1	1
1:A:87:TRP:CZ3	1:A:92:PRO:HB3	0.43	2.48	17	1
1:A:40:ASP:O	1:A:43:ASN:N	0.43	2.52	1	1
1:A:43:ASN:OD1	1:A:86:TYR:CD1	0.43	2.72	7	1
1:A:46:TYR:HD1	1:A:49:ILE:HD11	0.43	1.72	15	1
1:A:8:VAL:HG21	1:A:26:PHE:CE1	0.43	2.49	19	1
1:A:33:TYR:OH	1:A:128:GLN:NE2	0.42	2.52	19	1
1:A:69:TRP:N	1:A:78:ASP:O	0.42	2.51	16	1
1:A:89:ASN:O	1:A:89:ASN:CG	0.42	2.58	7	2
1:A:43:ASN:CG	1:A:86:TYR:CE1	0.42	2.93	7	1
1:A:41:ASP:O	1:A:45:PHE:CB	0.42	2.68	18	2
1:A:87:TRP:CG	1:A:92:PRO:HD3	0.42	2.50	19	1
1:A:36:ASP:OD1	1:A:71:ARG:NH2	0.42	2.53	2	1
1:A:89:ASN:N	1:A:112:LYS:HE3	0.42	2.30	12	1
1:A:81:ASN:C	1:A:81:ASN:OD1	0.42	2.57	16	1
1:A:88:ALA:HB3	1:A:91:GLU:HG2	0.42	1.91	18	2
1:A:46:TYR:O	1:A:50:ALA:N	0.42	2.53	4	1
1:A:8:VAL:HG11	1:A:30:ALA:CB	0.42	2.44	12	1
1:A:35:ALA:CB	1:A:46:TYR:OH	0.41	2.68	15	1
1:A:79:LEU:HG	1:A:80:LEU:N	0.41	2.30	15	2
1:A:54:GLN:OE1	1:A:123:ARG:CZ	0.41	2.68	15	1
1:A:38:LEU:HD22	1:A:69:TRP:CE2	0.41	2.50	20	2
1:A:61:LYS:HE3	1:A:67:PHE:CE1	0.41	2.50	4	1
1:A:93:SER:CB	1:A:116:THR:OG1	0.41	2.68	7	1
1:A:13:VAL:HG13	1:A:124:PRO:HB2	0.41	1.91	13	1
1:A:26:PHE:CD1	1:A:26:PHE:C	0.41	2.93	14	1
1:A:67:PHE:CZ	1:A:87:TRP:CH2	0.41	3.08	15	1
1:A:86:TYR:C	1:A:111:SER:O	0.41	2.59	19	1
1:A:91:GLU:N	1:A:91:GLU:CD	0.41	2.73	8	1
1:A:80:LEU:HD12	1:A:82:GLN:OE1	0.41	2.15	5	1
1:A:26:PHE:O	1:A:29:SER:N	0.41	2.54	7	1
1:A:46:TYR:C	1:A:48:SER:N	0.41	2.74	9	1
1:A:103:PHE:CZ	1:A:113:VAL:HG21	0.41	2.51	13	2
1:A:79:LEU:HD23	1:A:80:LEU:C	0.41	2.37	20	1
1:A:89:ASN:OD1	1:A:89:ASN:C	0.41	2.58	20	1
1:A:36:ASP:HB2	1:A:38:LEU:CD2	0.40	2.47	1	1
1:A:118:THR:CG2	1:A:121:THR:OG1	0.40	2.69	8	1
1:A:67:PHE:CD2	1:A:87:TRP:CH2	0.40	3.09	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ASP:HA	1:A:44:ASN:ND2	0.40	2.32	18	1
1:A:8:VAL:CG1	1:A:30:ALA:HB1	0.40	2.47	5	1
1:A:117:ASP:OD2	1:A:123:ARG:NH1	0.40	2.54	13	1
1:A:116:THR:O	1:A:117:ASP:OD1	0.40	2.40	16	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	117/150 (78%)	99±3 (85±3%)	15±3 (13±3%)	3±1 (2±1%)	9	46
All	All	2340/3000 (78%)	1988 (85%)	297 (13%)	55 (2%)	9	46

All 11 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	16	ASP	19
1	A	51	ALA	15
1	A	80	LEU	9
1	A	88	ALA	4
1	A	114	TRP	2
1	A	41	ASP	1
1	A	79	LEU	1
1	A	103	PHE	1
1	A	93	SER	1
1	A	47	SER	1
1	A	40	ASP	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	100/125 (80%)	94±2 (94±2%)	6±2 (6±2%)	21 69
All	All	2000/2500 (80%)	1871 (94%)	129 (6%)	21 69

All 27 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	20	MET	20
1	A	43	ASN	18
1	A	38	LEU	13
1	A	40	ASP	8
1	A	125	PHE	8
1	A	25	ASN	6
1	A	37	ASP	6
1	A	36	ASP	6
1	A	79	LEU	5
1	A	110	LYS	4
1	A	117	ASP	4
1	A	64	ASP	4
1	A	44	ASN	4
1	A	16	ASP	4
1	A	78	ASP	3
1	A	95	ASP	3
1	A	93	SER	2
1	A	91	GLU	2
1	A	33	TYR	1
1	A	70	ASP	1
1	A	111	SER	1
1	A	54	GLN	1
1	A	14	ASN	1
1	A	42	LYS	1
1	A	12	THR	1
1	A	45	PHE	1
1	A	41	ASP	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