Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 02:20 PM EST

PDB ID	:	2FH0
Title	:	NMR Ensemble of The Yeast Saccharomyces cerevisiae protein Ymr074cp core region
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Deposited on	:	2005-12-23

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

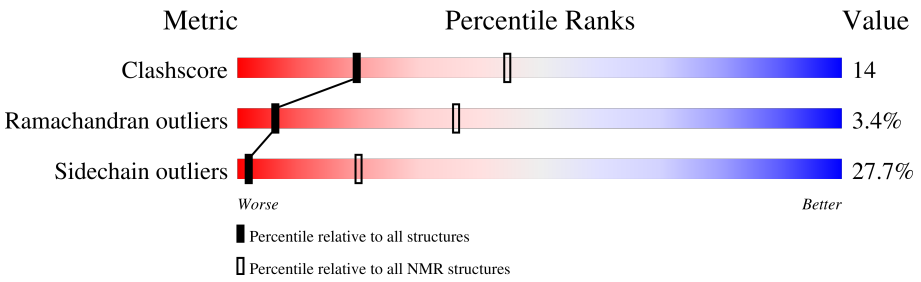
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	81	43% 28% • 27%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 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:46-A:104 (59)	0.34	16

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 3 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1277 atoms, of which 651 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	81	1277	389	651	116	121	0

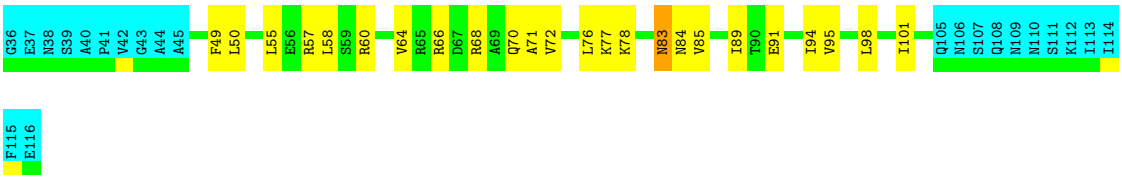
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 43% 28% • 27%



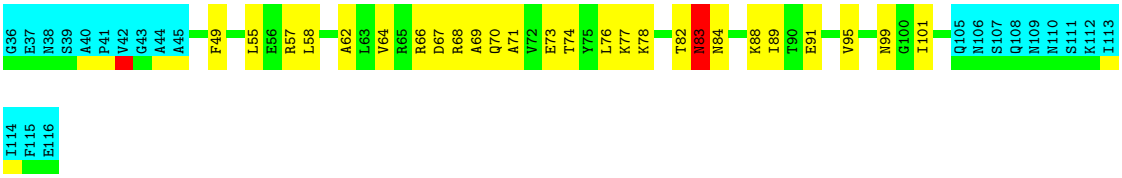
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

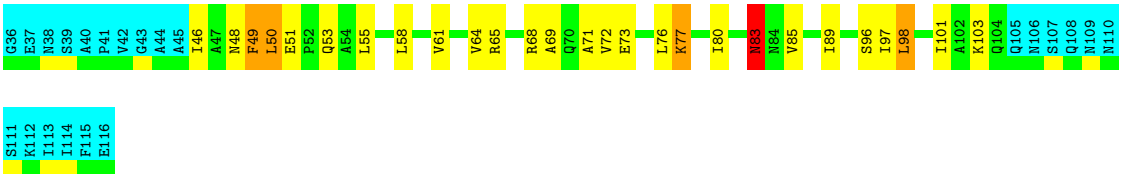
Chain A: 41% 31% • 27%



4.2.2 Score per residue for model 2

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

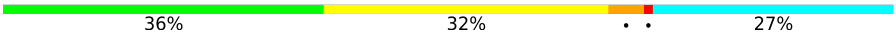
Chain A: 40% 27% 5% • 27%

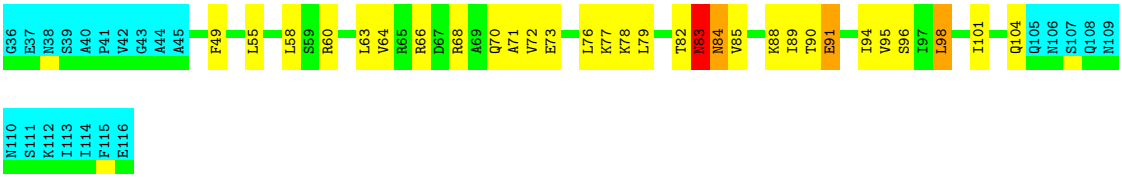


4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A:

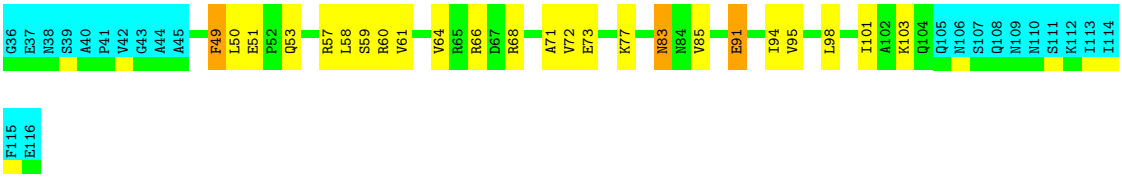




4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

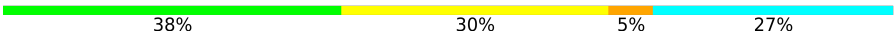
Chain A:

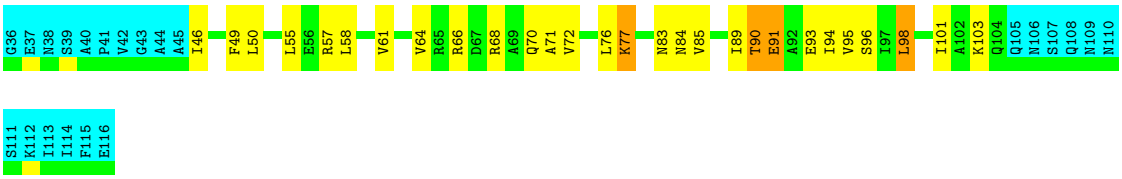


4.2.5 Score per residue for model 5

- Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 41% 30% • 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 F49 L50 Q53 E56 R57 L58 S59 R60 V61 V64 D67 R68 A69 Q70 A71 L76 K77 K78 N83 N84 K88 I89 T90 E91 I94 V95 L98 I101 A102 K103 Q104 Q105 N106 S107 Q108 N109 N110 S111 K112

I113 I114 F115 E116

4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 40% 30% • 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 N48 F49 L50 L55 E56 R57 L58 S59 R60 V61 A62 L63 V64 R68 A69 Q70 A71 V72 E73 T74 K77 K78 N83 N84 E91 I94 V95 L98 N99 G100 I101 Q105 N106 S107 Q108 N109 N110 S111 K112 I113 I114

F115 E116

4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 36% 31% 6% 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 I46 F49 Q53 R57 L58 S59 R60 L63 V64 R65 R66 D67 R68 A69 Q70 A71 V72 L76 K77 K78 L79 N83 N84 V85 K88 I89 T90 E91 A92 E93 I94 V95 S96 I101 A102 Q105 N106 S107 Q108 N109 N110

S111 K112 I113 I114 F115 E116

4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 43% 27% •• 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 F49 L50 L55 E56 R57 R60 V61 V64 R65 R66 Q70 A71 T74 Y75 L76 K77 K78 N83 N84 V85 E91 A92 E93 I94 V95 L98 I101 A102 K103 Q104 Q105 N106 S107 Q108 N109 N110 S111 K112 I113 I114

F115 E116

4.2.10 Score per residue for model 10

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 40% 30% • 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 F49 A54 L55 E56 R57 L58 S59 R60 V61 A62 L63 V64 R65 R66 D67 R68 A69 Q70 A71 V72 E73 L76 K77 I80 N83 N84 V85 I89 T90 E91 I94 V95 S96 I97 L98 I101 Q105 N106 S107 Q108 N109

N110 S111 K112 I113 I114 F115 E116

4.2.11 Score per residue for model 11

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 37% 28% 7% 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 I46 F49 L50 E51 L55 E56 R57 L58 S59 R60 L63 V64 R68 A69 Q70 A71 V72 E73 L76 K77 N83 I89 T90 E91 A92 E93 I94 V95 S96 I97 L98 I101 Q105 N106 S107 Q108 N109 N110 S111 K112 I113

I114 F115 E116

4.2.12 Score per residue for model 12

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 41% 26% 6% 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 I46 A47 N48 F49 S59 R60 L63 V64 R65 R66 D67 R68 A71 V72 E73 T74 Y75 L76 K77 K78 L79 T82 N83 N84 V85 K88 E91 V95 S96 I97 I101 Q105 N106 S107 Q108 N109 N110 S111 K112 I113 I114

F115 E116

4.2.13 Score per residue for model 13

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 36% 32% 5% 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 I46 F49 L50 Q53 A54 L55 E56 R57 L58 S59 R60 V61 V64 R68 A69 Q70 A71 V72 L76 K77 K78 N83 N84 I89 T90 E91 A92 E93 I94 V95 S96 I97 L98 I101 A102 K103 Q104 Q105 N106 S107 Q108 N109

N110 S111 K112 I113 I114 F115 E116

4.2.14 Score per residue for model 14

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 37% 32% • 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 F49 L50 E51 P52 Q53 A54 L55 E56 V61 V64 R65 R66 D67 R68 A69 Q70 A71 V72 L76 K77 K78 T82 N83 N84 V85 I89 I94 V95 S96 I97 L98 I101 A102 K103 Q104 Q105 N106 S107 Q108 N109 N110 S111 K112 I113 I114 F115 E116

4.2.15 Score per residue for model 15

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 41% 26% 5% • 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 F49 L50 E51 A54 R57 L58 S59 R60 V64 R65 R66 D67 R68 A69 Q70 A71 L76 K77 K78 T82 N83 K88 I89 T90 E91 I94 V95 S96 I101 A102 K103 Q104 Q105 N106 S107 Q108 N109 N110 S111 K112 I113 I114 F115 E116

4.2.16 Score per residue for model 16 (medoid)

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 32% 37% • • 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 I46 F49 L50 E51 R57 L58 S59 R60 L63 V64 R65 R66 D67 R68 A69 Q70 A71 V72 E73 T74 Y75 L76 K77 T82 N83 N84 K88 I89 T90 E91 A92 E93 I94 V95 L98 I101 A102 K103 Q104 Q105 N106 S107 Q108 N109 N110 S111 K112 I113 I114 F115 E116

4.2.17 Score per residue for model 17

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 33% 37% • 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 I46 F49 L50 E51 L55 E56 R57 L58 S59 R60 V61 V64 R65 R66 D67 R68 A69 Q70 A71 V72 L76 K77 K78 L79 I80 N83 N84 V85 T86 H87 K88 I89 T90 E91 V95 L98 N99 G100 I101 A102 Q105 N106 S107 Q108 N109 N110 S111 K112 I113 I114 F115 E116

4.2.18 Score per residue for model 18

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 37% 30% 6% 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 I46 F49 L55 E56 R57 L58 S59 R60 V64 R65 R66 D67 R68 A69 Q70 A71 V72 E73 T74 Y75 L76 K77 K78 L79 N83 N84 V85 I89 T90 E91 A92 E93 I94 V95 N99 G100 I101 A102 Q105 N106 S107 Q108 N109

N110 S111 K112 I113 I114 F115 E116

4.2.19 Score per residue for model 19

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 35% 33% • • 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 F49 L50 E51 A54 L55 E56 R57 L58 S59 R60 V64 R68 A71 V72 E73 T74 Y75 L76 K77 K78 L79 I80 A81 T82 N83 N84 V85 I89 T90 E91 A92 E93 I94 V96 L98 I101 Q105 N106 S107 Q108 N109

N110 S111 K112 I113 I114 F115 E116

4.2.20 Score per residue for model 20

• Molecule 1: Hypothetical 16.0 kDa protein in ABF2-CHL12 intergenic region

Chain A: 38% 30% • • 27%

G36 E37 N38 S39 A40 P41 V42 G43 A44 A45 F49 L55 E56 R57 L58 V64 R65 R66 D67 R68 A71 V72 L76 K77 K78 T82 N83 N84 V85 T86 H87 K88 I89 T90 E91 A92 E93 I94 V95 S96 I97 I101 A102 K103 Q104 Q105 N106 S107 Q108 N109 N110 S111 K112

I113 I114 F115 E116

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *with refinement program.*

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowset energy.*

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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	466	501	500	13±4
All	All	9320	10020	10000	269

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:58:LEU:HD13	1:A:94:ILE:HD11	0.87	1.44	20	12
1:A:54:ALA:HB1	1:A:94:ILE:HD11	0.83	1.48	10	1
1:A:71:ALA:HB3	1:A:101:ILE:HD13	0.78	1.55	13	20
1:A:50:LEU:O	1:A:54:ALA:HB3	0.74	1.83	15	2
1:A:91:GLU:O	1:A:95:VAL:HG23	0.69	1.88	12	15
1:A:61:VAL:HG11	1:A:98:LEU:HD11	0.69	1.63	6	1
1:A:68:ARG:O	1:A:72:VAL:HG23	0.67	1.89	14	14
1:A:97:ILE:HG22	1:A:101:ILE:CD1	0.67	2.19	14	4
1:A:76:LEU:HB2	1:A:89:ILE:HD11	0.67	1.66	2	8
1:A:61:VAL:HG21	1:A:98:LEU:HD21	0.66	1.67	14	3
1:A:49:PHE:HB3	1:A:76:LEU:HD21	0.65	1.68	2	5
1:A:91:GLU:HA	1:A:94:ILE:HD12	0.64	1.70	10	1
1:A:72:VAL:HG13	1:A:101:ILE:CD1	0.63	2.23	17	1
1:A:80:ILE:HG23	1:A:85:VAL:HG13	0.62	1.72	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ILE:HG22	1:A:101:ILE:HD12	0.62	1.69	10	2
1:A:72:VAL:HG21	1:A:98:LEU:CD2	0.60	2.27	13	1
1:A:94:ILE:O	1:A:98:LEU:HD12	0.60	1.96	16	2
1:A:80:ILE:HA	1:A:85:VAL:HG22	0.60	1.71	17	2
1:A:61:VAL:HG13	1:A:69:ALA:HB2	0.59	1.72	13	2
1:A:71:ALA:HB3	1:A:101:ILE:CD1	0.59	2.27	14	16
1:A:61:VAL:HG21	1:A:98:LEU:HD11	0.59	1.73	9	4
1:A:76:LEU:HD22	1:A:89:ILE:HD11	0.59	1.73	3	3
1:A:76:LEU:HD13	1:A:89:ILE:CD1	0.58	2.29	17	4
1:A:91:GLU:O	1:A:95:VAL:HG22	0.58	1.99	6	1
1:A:72:VAL:HG11	1:A:94:ILE:HG13	0.57	1.74	13	3
1:A:46:ILE:HD13	1:A:77:LYS:HB3	0.57	1.77	11	1
1:A:58:LEU:HD11	1:A:69:ALA:HA	0.57	1.75	17	7
1:A:76:LEU:HD13	1:A:89:ILE:HD11	0.57	1.76	6	2
1:A:82:THR:HG22	1:A:83:ASN:OD1	0.57	1.99	1	5
1:A:50:LEU:HD11	1:A:89:ILE:HD12	0.56	1.77	6	1
1:A:60:ARG:HA	1:A:63:LEU:HD12	0.56	1.76	8	4
1:A:75:TYR:CZ	1:A:79:LEU:HD11	0.55	2.36	19	3
1:A:76:LEU:HD13	1:A:89:ILE:CG1	0.55	2.33	2	4
1:A:72:VAL:HG13	1:A:101:ILE:HD12	0.55	1.77	17	1
1:A:50:LEU:CD2	1:A:94:ILE:HD11	0.54	2.31	14	1
1:A:61:VAL:HG21	1:A:98:LEU:CD2	0.54	2.32	14	2
1:A:68:ARG:HD2	1:A:102:ALA:HB2	0.54	1.79	8	1
1:A:50:LEU:HD21	1:A:94:ILE:HD11	0.54	1.80	14	1
1:A:94:ILE:HA	1:A:97:ILE:HD12	0.53	1.80	13	2
1:A:74:THR:HG23	1:A:77:LYS:CE	0.53	2.33	1	1
1:A:76:LEU:HD13	1:A:89:ILE:HG13	0.53	1.80	2	4
1:A:46:ILE:CG2	1:A:76:LEU:HD23	0.53	2.33	8	1
1:A:97:ILE:HG22	1:A:101:ILE:HD11	0.53	1.80	14	1
1:A:49:PHE:HZ	1:A:85:VAL:HG13	0.53	1.62	18	1
1:A:74:THR:HG22	1:A:78:LYS:HE3	0.52	1.79	7	1
1:A:72:VAL:HG11	1:A:94:ILE:HD12	0.52	1.81	8	3
1:A:50:LEU:HD12	1:A:76:LEU:CD2	0.52	2.34	17	1
1:A:68:ARG:HB3	1:A:98:LEU:HD23	0.52	1.81	11	2
1:A:50:LEU:HG	1:A:76:LEU:HD22	0.52	1.81	15	2
1:A:46:ILE:HG21	1:A:77:LYS:HB3	0.51	1.80	5	2
1:A:61:VAL:HG21	1:A:98:LEU:HD22	0.51	1.83	10	1
1:A:72:VAL:HG21	1:A:98:LEU:HD22	0.51	1.80	13	1
1:A:68:ARG:HE	1:A:102:ALA:HB2	0.51	1.65	18	1
1:A:94:ILE:HG22	1:A:98:LEU:CD1	0.51	2.36	14	1
1:A:68:ARG:O	1:A:72:VAL:HG22	0.51	2.06	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:ARG:HA	1:A:101:ILE:HG21	0.51	1.83	19	10
1:A:76:LEU:HD22	1:A:89:ILE:CD1	0.50	2.36	3	2
1:A:54:ALA:CB	1:A:94:ILE:HD11	0.50	2.31	10	1
1:A:74:THR:HG23	1:A:77:LYS:HE3	0.49	1.82	7	1
1:A:46:ILE:HG22	1:A:76:LEU:HD23	0.49	1.85	17	2
1:A:59:SER:O	1:A:63:LEU:HD13	0.49	2.07	10	2
1:A:68:ARG:HB2	1:A:98:LEU:HD23	0.48	1.83	16	1
1:A:58:LEU:HD21	1:A:73:GLU:HG2	0.48	1.86	2	2
1:A:58:LEU:HD22	1:A:94:ILE:HD11	0.47	1.86	7	1
1:A:46:ILE:O	1:A:50:LEU:HD12	0.47	2.10	2	3
1:A:83:ASN:O	1:A:85:VAL:HG23	0.47	2.09	9	3
1:A:50:LEU:HD12	1:A:76:LEU:HD22	0.47	1.86	14	1
1:A:62:ALA:HB2	1:A:69:ALA:CB	0.47	2.40	1	1
1:A:85:VAL:O	1:A:85:VAL:HG12	0.47	2.09	14	7
1:A:46:ILE:N	1:A:46:ILE:HD13	0.47	2.25	12	1
1:A:59:SER:O	1:A:63:LEU:HD12	0.47	2.10	12	1
1:A:74:THR:HG22	1:A:77:LYS:HE2	0.47	1.86	12	1
1:A:50:LEU:CD1	1:A:76:LEU:HD22	0.46	2.40	14	1
1:A:89:ILE:HG22	1:A:94:ILE:HG13	0.46	1.88	10	1
1:A:49:PHE:CD2	1:A:80:ILE:HD11	0.46	2.46	2	1
1:A:74:THR:HG22	1:A:78:LYS:CE	0.45	2.42	1	1
1:A:46:ILE:O	1:A:46:ILE:HG22	0.45	2.12	18	1
1:A:49:PHE:HD2	1:A:76:LEU:HD11	0.45	1.70	2	1
1:A:76:LEU:HD22	1:A:89:ILE:HD12	0.45	1.89	18	1
1:A:78:LYS:O	1:A:82:THR:HG23	0.45	2.11	14	2
1:A:72:VAL:HG13	1:A:97:ILE:HD13	0.44	1.88	2	1
1:A:72:VAL:HG11	1:A:94:ILE:CD1	0.44	2.41	8	1
1:A:68:ARG:HB3	1:A:98:LEU:HD12	0.44	1.88	13	1
1:A:68:ARG:CD	1:A:102:ALA:HB2	0.44	2.41	8	1
1:A:50:LEU:CD1	1:A:89:ILE:HD12	0.43	2.42	6	1
1:A:85:VAL:C	1:A:86:THR:HG23	0.43	2.34	20	1
1:A:89:ILE:HG22	1:A:94:ILE:HB	0.43	1.89	16	1
1:A:76:LEU:HA	1:A:79:LEU:HD12	0.43	1.88	19	1
1:A:85:VAL:HG12	1:A:86:THR:H	0.43	1.73	20	1
1:A:89:ILE:O	1:A:93:GLU:CB	0.43	2.67	19	1
1:A:76:LEU:HD13	1:A:89:ILE:HD12	0.43	1.89	17	1
1:A:74:THR:HA	1:A:77:LYS:HG2	0.42	1.91	18	3
1:A:76:LEU:HB2	1:A:89:ILE:CD1	0.42	2.44	17	1
1:A:82:THR:HG22	1:A:83:ASN:ND2	0.42	2.30	20	1
1:A:94:ILE:HG12	1:A:98:LEU:HD12	0.42	1.91	5	2
1:A:54:ALA:HB1	1:A:94:ILE:HG13	0.42	1.90	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:ARG:NE	1:A:102:ALA:HB2	0.42	2.29	17	1
1:A:68:ARG:CB	1:A:98:LEU:HD23	0.42	2.43	16	1
1:A:68:ARG:CZ	1:A:102:ALA:HB2	0.42	2.45	14	1
1:A:72:VAL:HG21	1:A:98:LEU:HG	0.41	1.91	19	1
1:A:57:ARG:HH11	1:A:98:LEU:HD13	0.41	1.75	11	1
1:A:49:PHE:CZ	1:A:85:VAL:CG1	0.41	3.03	17	1
1:A:57:ARG:NH1	1:A:98:LEU:HD13	0.41	2.30	11	1
1:A:49:PHE:O	1:A:76:LEU:HD21	0.41	2.16	17	1
1:A:75:TYR:CE1	1:A:79:LEU:HD11	0.41	2.51	19	1
1:A:89:ILE:CG2	1:A:94:ILE:HD13	0.41	2.46	14	1
1:A:49:PHE:CZ	1:A:85:VAL:HG13	0.41	2.51	4	1
1:A:67:ASP:O	1:A:70:GLN:HG3	0.41	2.16	15	1
1:A:79:LEU:HD23	1:A:84:ASN:HB3	0.40	1.93	3	1
1:A:65:ARG:CB	1:A:68:ARG:HG3	0.40	2.46	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	59/81 (73%)	54±1 (92±2%)	3±1 (5±2%)	2±1 (3±1%)	6 36
All	All	1180/1620 (73%)	1080 (92%)	60 (5%)	40 (3%)	6 36

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	83	ASN	20
1	A	84	ASN	11
1	A	90	THR	4
1	A	88	LYS	2
1	A	51	GLU	2
1	A	85	VAL	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	50/67 (75%)	36±2 (72±4%)	14±2 (28±4%)	2 20
All	All	1000/1340 (75%)	723 (72%)	277 (28%)	2 20

All 36 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	64	VAL	20
1	A	49	PHE	19
1	A	57	ARG	16
1	A	77	LYS	16
1	A	55	LEU	14
1	A	83	ASN	14
1	A	60	ARG	14
1	A	66	ARG	12
1	A	50	LEU	11
1	A	78	LYS	11
1	A	70	GLN	10
1	A	103	LYS	10
1	A	91	GLU	9
1	A	93	GLU	9
1	A	88	LYS	8
1	A	65	ARG	7
1	A	96	SER	7
1	A	98	LEU	7
1	A	67	ASP	6
1	A	68	ARG	6
1	A	51	GLU	6
1	A	53	GLN	6
1	A	73	GLU	5
1	A	56	GLU	5
1	A	99	ASN	4
1	A	59	SER	4
1	A	94	ILE	4
1	A	48	ASN	3
1	A	104	GLN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	74	THR	3
1	A	95	VAL	2
1	A	86	THR	2
1	A	90	THR	1
1	A	79	LEU	1
1	A	46	ILE	1
1	A	84	ASN	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