Full wwPDB NMR Structure Validation Report (i)

Feb 20, 2022 – 01:40 AM EST

PDB ID	:	1V32
Title	:	Solution structure of the SWIB/MDM2 domain of the hypothetical protein At5g08430 from Arabidopsis thaliana
Authors	:	Yoneyama, M.; Tochio, N.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2003-10-24

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:

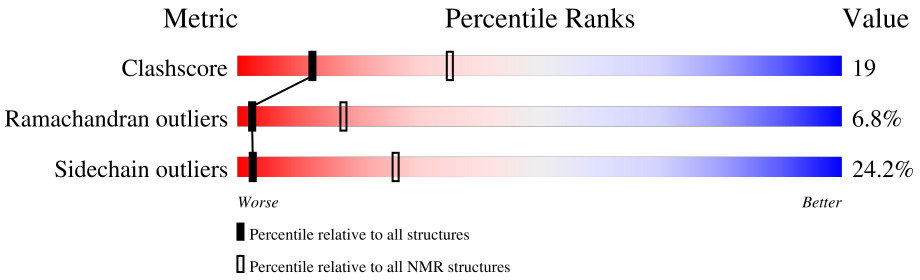
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	101	27% 47% 5% 22%

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:12-A:90 (79)	0.27	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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1608 atoms, of which 807 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical protein RAFL09-47-K03.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1608	506	807	139	153	3	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9FT92
A	2	SER	-	cloning artifact	UNP Q9FT92
A	3	SER	-	cloning artifact	UNP Q9FT92
A	4	GLY	-	cloning artifact	UNP Q9FT92
A	5	SER	-	cloning artifact	UNP Q9FT92
A	6	SER	-	cloning artifact	UNP Q9FT92
A	7	GLY	-	cloning artifact	UNP Q9FT92
A	96	SER	-	cloning artifact	UNP Q9FT92
A	97	GLY	-	cloning artifact	UNP Q9FT92
A	98	PRO	-	cloning artifact	UNP Q9FT92
A	99	SER	-	cloning artifact	UNP Q9FT92
A	100	SER	-	cloning artifact	UNP Q9FT92
A	101	GLY	-	cloning artifact	UNP Q9FT92

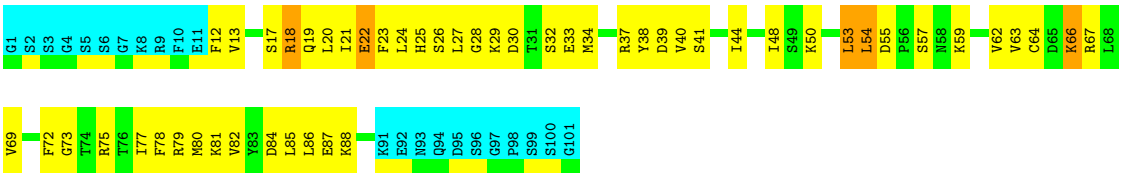
4 Residue-property plots (i)

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 RAFL09-47-K03

Chain A: 27% 47% 5% 22%



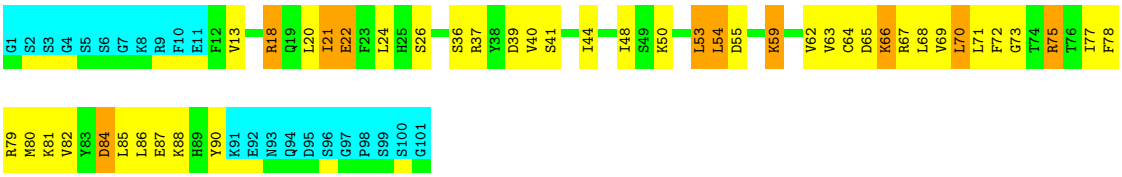
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: hypothetical protein RAFL09-47-K03

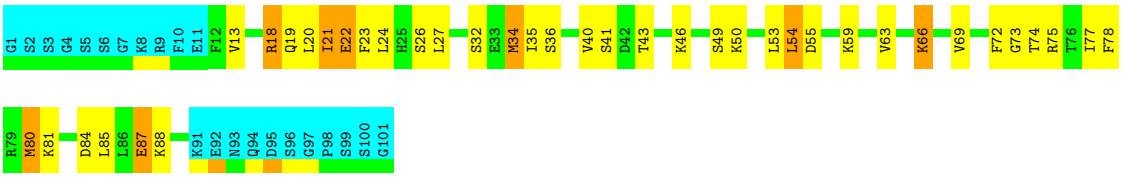
Chain A: 35% 34% 10% 22%



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: hypothetical protein RAFL09-47-K03

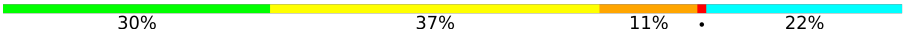
Chain A: 40% 31% 8% 22%

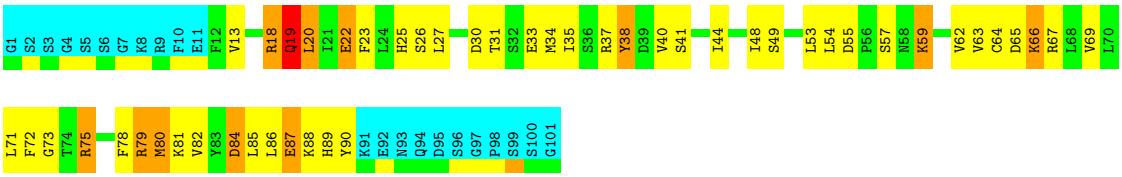


4.2.3 Score per residue for model 3

- Molecule 1: hypothetical protein RAFL09-47-K03

Chain A:

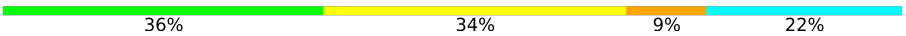


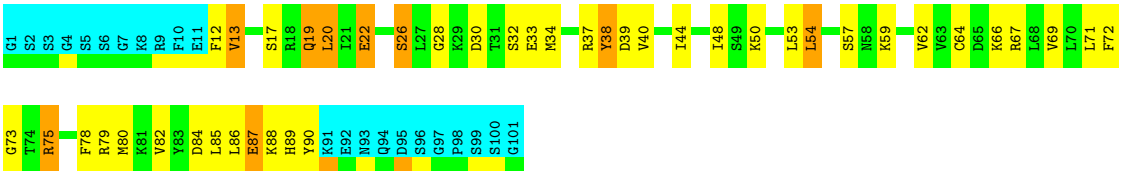


4.2.4 Score per residue for model 4

- Molecule 1: hypothetical protein RAFL09-47-K03

Chain A:

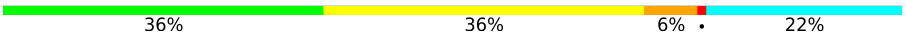




4.2.5 Score per residue for model 5

- Molecule 1: hypothetical protein RAFL09-47-K03

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: hypothetical protein RAFL09-47-K03

Chain A: 42% 28% 9% 22%

G1 S2 S3 G4 S5 S6 G7 K8 R9 F10 E11 F12 V13 S17 R18 Q19 L20 I21 E22 F23 L24 L27 E33 M34 I35 S36 R37 V40 S41 I44 Y47 I48 L53 L54 D55 K59 V62 V63 C64 D65 K66 R67 L68 V69 F72 G73 T74 R75 K81

V82 Y83 D84 L85 K88 K91 E92 N93 Q94 D95 S96 G97 P98 S99 S100 G101

4.2.7 Score per residue for model 7

- Molecule 1: hypothetical protein RAFL09-47-K03

Chain A: 43% 31% 5% 22%

G1 S2 S3 G4 S5 S6 G7 K8 R9 F10 E11 F12 L20 I21 E22 F23 L24 H25 S26 L27 G28 K29 S32 R37 Y38 D39 V40 S41 D42 T43 I44 K50 L53 L54 D55 N58 K59 V62 V63 C64 D65 K66 R67 L70 L71 F72 R75 T76 I77 V82

Y83 D84 L85 L86 E87 K88 K91 E92 N93 Q94 D95 S96 G97 P98 S99 S100 G101

4.2.8 Score per residue for model 8

- Molecule 1: hypothetical protein RAFL09-47-K03

Chain A: 29% 43% 6% • 22%

G1 S2 S3 G4 S5 S6 G7 K8 R9 F10 E11 F12 V13 G14 W15 R18 Q19 L20 I21 E22 F23 L24 H25 S26 L27 G28 K29 D30 T31 S32 E33 M34 R37 Y38 D39 V40 S41 I44 K50 L53 L54 D55 P56 S57 N58 K59 V63 C64 D65 K66 R67 L68 V69

F72 G73 T74 R75 F78 R79 M80 K81 V82 Y83 D84 L85 L86 E87 K88 H89 Y90 K91 E92 N93 Q94 D95 S96 G97 P98 S99 S100 G101

4.2.9 Score per residue for model 9

- Molecule 1: hypothetical protein RAFL09-47-K03

Chain A: 40% 31% 8% 22%

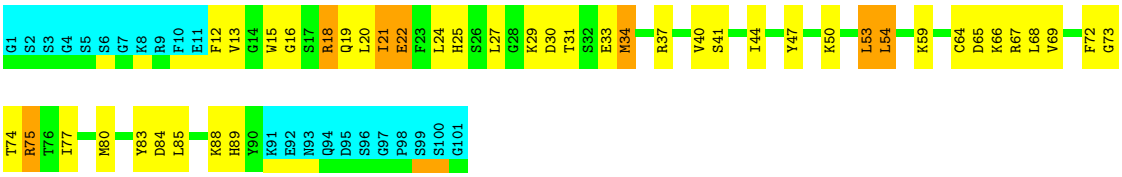
G1 S2 S3 G4 S5 S6 G7 K8 R9 F10 E11 F12 V13 G14 W15 G16 S17 R18 Q19 L20 I21 E22 F23 L24 H25 S26 L27 G28 S32 E33 M34 R37 S41 I44 K50 L53 L54 D55 K59 V63 C64 D65 K66 R67 L68 V69 L70 L71 F72 G73 T74 R75

F78 R79 M80 D84 L85 L86 K91 E92 N93 Q94 D95 S96 G97 P98 S99 S100 G101

4.2.10 Score per residue for model 10

- Molecule 1: hypothetical protein RAFL09-47-K03

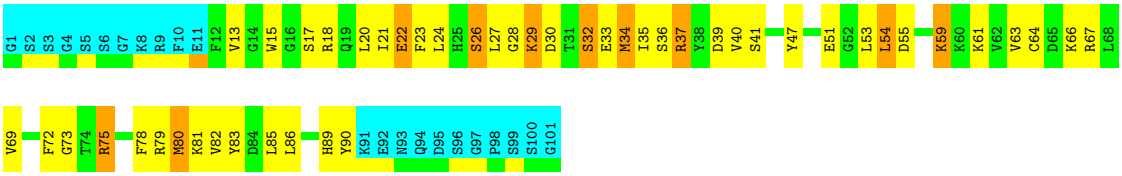
Chain A: 36% 36% 7% 22%



4.2.11 Score per residue for model 11

- Molecule 1: hypothetical protein RAFL09-47-K03

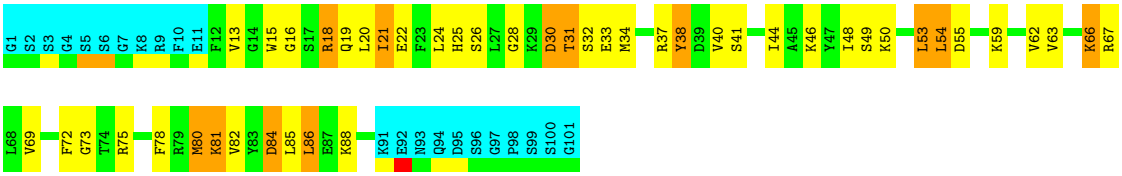
Chain A: 31% 38% 10% 22%



4.2.12 Score per residue for model 12

- Molecule 1: hypothetical protein RAFL09-47-K03

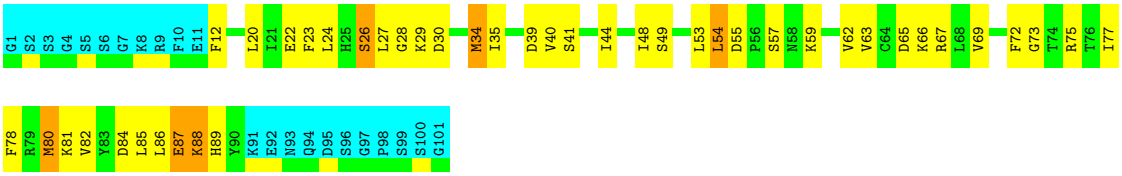
Chain A: 33% 34% 12% 22%



4.2.13 Score per residue for model 13

- Molecule 1: hypothetical protein RAFL09-47-K03

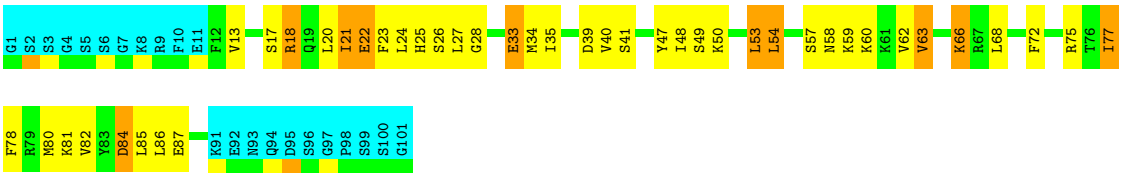
Chain A: 36% 37% 6% 22%



4.2.14 Score per residue for model 14

- Molecule 1: hypothetical protein RAFL09-47-K03

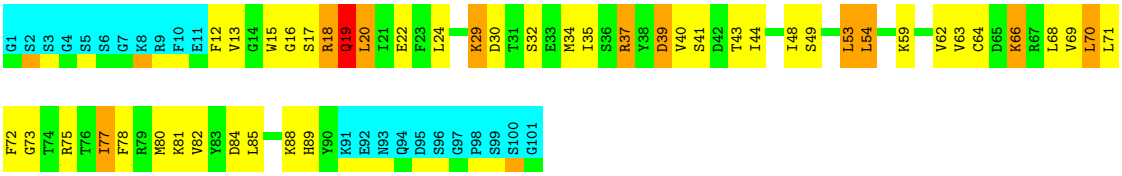
Chain A: 36% 33% 10% 22%



4.2.15 Score per residue for model 15

- Molecule 1: hypothetical protein RAFL09-47-K03

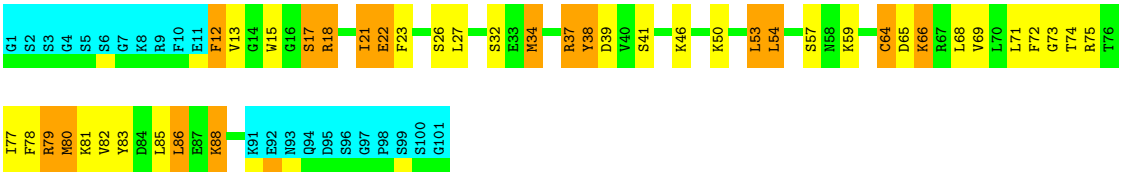
Chain A: 33% 35% 10% • 22%



4.2.16 Score per residue for model 16

- Molecule 1: hypothetical protein RAFL09-47-K03

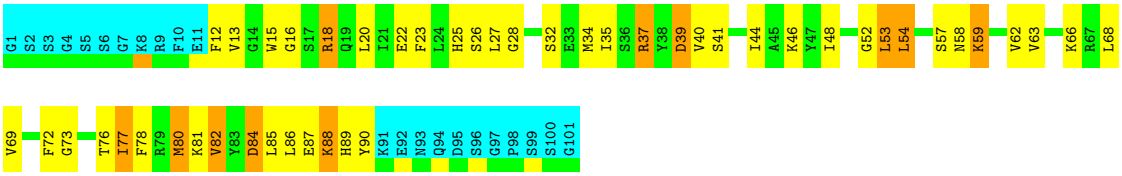
Chain A: 37% 26% 16% 22%



4.2.17 Score per residue for model 17

- Molecule 1: hypothetical protein RAFL09-47-K03

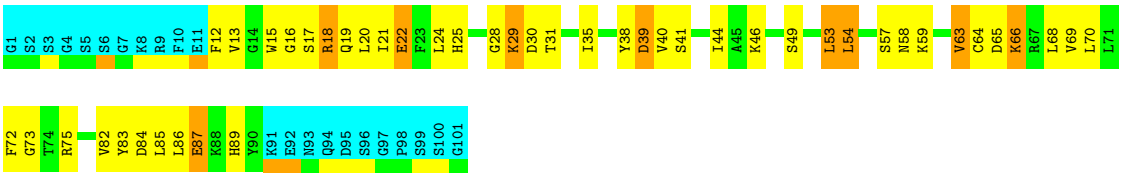
Chain A: 31% 37% 11% 22%



4.2.18 Score per residue for model 18

- Molecule 1: hypothetical protein RAFL09-47-K03

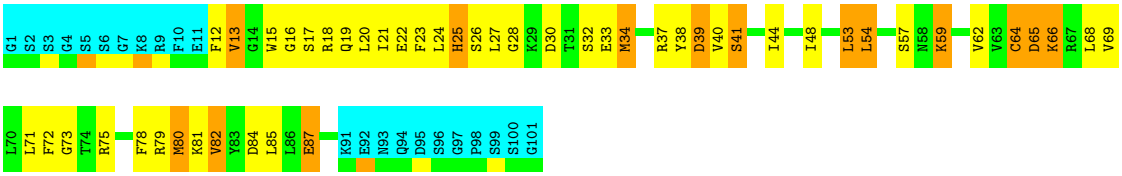
Chain A: 33% 37% 9% 22%



4.2.19 Score per residue for model 19

- Molecule 1: hypothetical protein RAFL09-47-K03

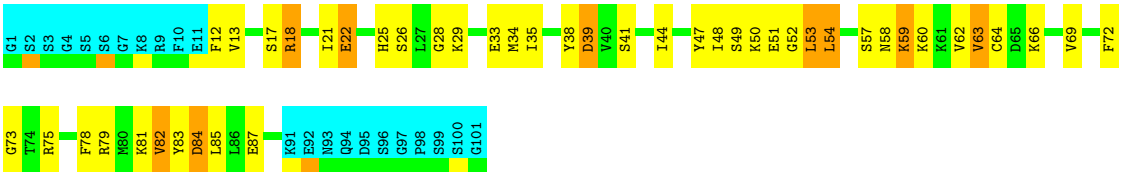
Chain A: 30% 35% 14% 22%



4.2.20 Score per residue for model 20

- Molecule 1: hypothetical protein RAFL09-47-K03

Chain A: 34% 36% 9% 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, structures with the lowest energy, target function*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.7
CYANA	refinement	1.0.7

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	649	672	672	25±6
All	All	12980	13440	13440	503

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD11	1:A:40:VAL:HG11	0.90	1.43	11	15
1:A:71:LEU:HD12	1:A:89:HIS:CE1	0.78	2.13	4	2
1:A:71:LEU:HD21	1:A:72:PHE:CE1	0.78	2.14	3	4
1:A:20:LEU:HD13	1:A:86:LEU:HD22	0.77	1.56	11	5
1:A:54:LEU:HD22	1:A:59:LYS:O	0.76	1.80	7	20
1:A:13:VAL:HG21	1:A:18:ARG:HG3	0.76	1.57	18	5
1:A:23:PHE:CZ	1:A:27:LEU:HD11	0.69	2.22	5	11
1:A:71:LEU:CD2	1:A:72:PHE:CE1	0.69	2.76	3	3
1:A:13:VAL:HG13	1:A:21:ILE:HG13	0.68	1.66	20	10
1:A:20:LEU:HG	1:A:24:LEU:HD12	0.68	1.66	6	8
1:A:29:LYS:NZ	1:A:35:ILE:HD13	0.68	2.04	18	1
1:A:53:LEU:HD23	1:A:68:LEU:CD1	0.67	2.20	14	6
1:A:55:ASP:OD1	1:A:63:VAL:HG21	0.66	1.90	3	11
1:A:13:VAL:HG11	1:A:18:ARG:HG3	0.64	1.69	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ILE:HD12	1:A:86:LEU:HD11	0.64	1.67	3	6
1:A:13:VAL:HG22	1:A:13:VAL:O	0.63	1.91	19	3
1:A:48:ILE:CD1	1:A:62:VAL:HG11	0.63	2.24	13	7
1:A:71:LEU:CD1	1:A:89:HIS:CE1	0.62	2.83	4	1
1:A:13:VAL:HG21	1:A:18:ARG:CG	0.62	2.25	8	2
1:A:44:ILE:CD1	1:A:86:LEU:HD11	0.62	2.25	4	2
1:A:20:LEU:CD1	1:A:40:VAL:HG11	0.58	2.26	3	4
1:A:44:ILE:HG21	1:A:82:VAL:HG11	0.57	1.77	20	4
1:A:25:HIS:CD2	1:A:31:THR:OG1	0.57	2.57	12	1
1:A:53:LEU:HD11	1:A:65:ASP:HB3	0.57	1.76	16	1
1:A:20:LEU:HD11	1:A:40:VAL:CG1	0.57	2.29	18	4
1:A:30:ASP:O	1:A:35:ILE:HD11	0.56	2.00	11	2
1:A:13:VAL:O	1:A:13:VAL:HG22	0.56	2.01	20	1
1:A:71:LEU:HD21	1:A:72:PHE:CZ	0.55	2.35	3	5
1:A:89:HIS:O	1:A:90:TYR:CD2	0.55	2.59	11	2
1:A:20:LEU:HD11	1:A:40:VAL:HG21	0.55	1.77	19	1
1:A:44:ILE:HG21	1:A:82:VAL:CG1	0.55	2.32	20	5
1:A:53:LEU:HD23	1:A:68:LEU:HD11	0.54	1.79	14	2
1:A:48:ILE:HD13	1:A:62:VAL:HG11	0.53	1.80	13	1
1:A:29:LYS:HZ3	1:A:35:ILE:HD13	0.53	1.63	18	1
1:A:29:LYS:O	1:A:31:THR:HG23	0.53	2.03	10	3
1:A:15:TRP:CE3	1:A:16:GLY:N	0.53	2.77	12	7
1:A:64:CYS:SG	1:A:69:VAL:CG2	0.53	2.97	20	4
1:A:66:LYS:HD3	1:A:70:LEU:HD22	0.52	1.81	1	1
1:A:44:ILE:CG2	1:A:82:VAL:HG11	0.52	2.35	20	6
1:A:35:ILE:CG2	1:A:39:ASP:CB	0.52	2.87	17	3
1:A:13:VAL:HG21	1:A:18:ARG:HB2	0.52	1.82	11	1
1:A:48:ILE:HA	1:A:53:LEU:HD22	0.51	1.82	14	3
1:A:89:HIS:O	1:A:90:TYR:CD1	0.51	2.64	8	2
1:A:13:VAL:HG21	1:A:18:ARG:CD	0.51	2.36	8	1
1:A:54:LEU:CD2	1:A:59:LYS:O	0.50	2.60	6	19
1:A:86:LEU:O	1:A:88:LYS:N	0.50	2.44	5	5
1:A:72:PHE:CZ	1:A:85:LEU:HB3	0.50	2.42	11	4
1:A:88:LYS:HG3	1:A:89:HIS:CD2	0.49	2.42	17	1
1:A:23:PHE:C	1:A:23:PHE:CD1	0.49	2.85	9	1
1:A:53:LEU:HD23	1:A:68:LEU:HD12	0.49	1.85	14	8
1:A:55:ASP:OD1	1:A:63:VAL:CG2	0.49	2.61	7	8
1:A:12:PHE:CE2	1:A:89:HIS:O	0.48	2.66	13	1
1:A:23:PHE:CZ	1:A:44:ILE:HG12	0.48	2.44	19	2
1:A:72:PHE:CE2	1:A:85:LEU:HD13	0.48	2.43	16	4
1:A:12:PHE:CZ	1:A:89:HIS:O	0.48	2.67	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD12	1:A:89:HIS:ND1	0.48	2.24	4	1
1:A:33:GLU:O	1:A:33:GLU:CG	0.48	2.62	11	1
1:A:72:PHE:CE1	1:A:85:LEU:HB3	0.48	2.44	20	20
1:A:23:PHE:CZ	1:A:27:LEU:CD1	0.48	2.96	5	1
1:A:13:VAL:O	1:A:13:VAL:CG2	0.47	2.62	19	2
1:A:77:ILE:CD1	1:A:85:LEU:HD13	0.47	2.39	1	1
1:A:84:ASP:O	1:A:87:GLU:CB	0.47	2.63	3	1
1:A:13:VAL:HG11	1:A:18:ARG:HA	0.47	1.86	1	1
1:A:65:ASP:N	1:A:65:ASP:OD1	0.46	2.47	16	1
1:A:48:ILE:CG2	1:A:62:VAL:HG13	0.46	2.40	1	1
1:A:15:TRP:CE2	1:A:34:MET:HA	0.46	2.46	10	4
1:A:13:VAL:HG21	1:A:18:ARG:HD2	0.46	1.86	8	1
1:A:69:VAL:O	1:A:73:GLY:N	0.46	2.49	12	18
1:A:33:GLU:CA	1:A:33:GLU:OE1	0.46	2.64	11	1
1:A:71:LEU:HG	1:A:72:PHE:CD1	0.46	2.45	3	1
1:A:12:PHE:CZ	1:A:17:SER:HB2	0.46	2.46	16	1
1:A:37:ARG:HA	1:A:40:VAL:HG12	0.46	1.87	19	1
1:A:74:THR:OG1	1:A:77:ILE:CG2	0.46	2.64	16	4
1:A:71:LEU:CD2	1:A:72:PHE:CZ	0.46	2.99	3	1
1:A:37:ARG:HG3	1:A:90:TYR:CE2	0.46	2.46	11	1
1:A:62:VAL:CG2	1:A:79:ARG:CG	0.45	2.94	1	1
1:A:77:ILE:HD11	1:A:82:VAL:HG22	0.45	1.88	15	1
1:A:41:SER:O	1:A:44:ILE:N	0.45	2.50	8	4
1:A:18:ARG:O	1:A:22:GLU:N	0.45	2.50	16	7
1:A:62:VAL:N	1:A:77:ILE:O	0.45	2.50	7	1
1:A:37:ARG:HB3	1:A:83:TYR:CE1	0.45	2.46	11	1
1:A:77:ILE:HD12	1:A:85:LEU:CD1	0.45	2.42	1	1
1:A:37:ARG:O	1:A:40:VAL:N	0.45	2.50	3	3
1:A:40:VAL:HG13	1:A:41:SER:N	0.45	2.26	19	1
1:A:20:LEU:HD21	1:A:90:TYR:CE1	0.45	2.47	1	1
1:A:64:CYS:N	1:A:75:ARG:O	0.45	2.50	9	11
1:A:19:GLN:O	1:A:20:LEU:C	0.45	2.55	4	3
1:A:26:SER:C	1:A:28:GLY:N	0.45	2.70	8	12
1:A:24:LEU:HD22	1:A:29:LYS:HE3	0.45	1.88	15	1
1:A:53:LEU:N	1:A:53:LEU:CD1	0.44	2.80	14	1
1:A:84:ASP:O	1:A:87:GLU:N	0.44	2.50	3	3
1:A:48:ILE:HD13	1:A:62:VAL:HG21	0.44	1.89	17	2
1:A:21:ILE:O	1:A:24:LEU:N	0.44	2.50	10	6
1:A:33:GLU:O	1:A:35:ILE:N	0.44	2.50	14	1
1:A:48:ILE:O	1:A:52:GLY:N	0.44	2.50	20	2
1:A:47:TYR:CE1	1:A:51:GLU:HG3	0.44	2.47	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:VAL:HA	1:A:85:LEU:HD12	0.44	1.90	12	1
1:A:53:LEU:HD11	1:A:65:ASP:CG	0.44	2.33	19	1
1:A:78:PHE:O	1:A:80:MET:N	0.44	2.51	11	8
1:A:78:PHE:C	1:A:80:MET:N	0.44	2.71	3	11
1:A:37:ARG:CZ	1:A:37:ARG:HB2	0.44	2.43	11	3
1:A:72:PHE:CE2	1:A:77:ILE:HD13	0.44	2.47	13	1
1:A:76:THR:O	1:A:77:ILE:CG2	0.44	2.65	17	1
1:A:39:ASP:O	1:A:40:VAL:C	0.44	2.56	19	1
1:A:77:ILE:HD13	1:A:85:LEU:HD13	0.43	1.89	16	2
1:A:22:GLU:O	1:A:25:HIS:N	0.43	2.51	14	3
1:A:25:HIS:NE2	1:A:31:THR:OG1	0.43	2.52	3	2
1:A:25:HIS:O	1:A:28:GLY:N	0.43	2.51	18	2
1:A:62:VAL:CG2	1:A:79:ARG:HG3	0.43	2.44	1	1
1:A:19:GLN:O	1:A:22:GLU:N	0.43	2.51	4	2
1:A:78:PHE:O	1:A:81:LYS:N	0.43	2.52	14	6
1:A:80:MET:C	1:A:82:VAL:N	0.43	2.71	17	1
1:A:58:ASN:OD1	1:A:58:ASN:N	0.43	2.52	7	1
1:A:24:LEU:HD21	1:A:40:VAL:HG13	0.43	1.91	11	1
1:A:84:ASP:C	1:A:86:LEU:N	0.43	2.71	14	2
1:A:23:PHE:CE1	1:A:27:LEU:HD11	0.42	2.49	16	3
1:A:24:LEU:O	1:A:29:LYS:N	0.42	2.50	13	1
1:A:48:ILE:HD13	1:A:62:VAL:CG1	0.42	2.44	13	1
1:A:77:ILE:CD1	1:A:85:LEU:CD1	0.42	2.97	1	1
1:A:81:LYS:O	1:A:82:VAL:C	0.42	2.58	17	12
1:A:27:LEU:HD21	1:A:47:TYR:CD1	0.42	2.49	6	2
1:A:29:LYS:O	1:A:31:THR:N	0.42	2.52	18	1
1:A:35:ILE:CG2	1:A:36:SER:N	0.42	2.83	2	1
1:A:13:VAL:HG13	1:A:13:VAL:O	0.42	2.14	2	1
1:A:37:ARG:O	1:A:38:TYR:C	0.42	2.58	16	4
1:A:15:TRP:CZ2	1:A:35:ILE:HG13	0.42	2.48	11	1
1:A:53:LEU:O	1:A:63:VAL:N	0.42	2.49	20	3
1:A:35:ILE:CG2	1:A:39:ASP:HB3	0.42	2.45	17	3
1:A:64:CYS:HB2	1:A:69:VAL:HG23	0.42	1.91	18	1
1:A:84:ASP:O	1:A:85:LEU:C	0.42	2.58	5	4
1:A:33:GLU:O	1:A:33:GLU:OE1	0.42	2.38	11	1
1:A:40:VAL:HG13	1:A:41:SER:H	0.42	1.75	19	1
1:A:72:PHE:CZ	1:A:85:LEU:CB	0.41	3.04	3	1
1:A:37:ARG:HB3	1:A:83:TYR:CZ	0.41	2.50	7	1
1:A:37:ARG:NH2	1:A:83:TYR:CE2	0.41	2.88	16	1
1:A:18:ARG:O	1:A:19:GLN:C	0.41	2.57	10	3
1:A:48:ILE:HG12	1:A:62:VAL:HG11	0.41	1.93	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:GLN:CG	1:A:70:LEU:O	0.41	2.68	15	1
1:A:35:ILE:HG23	1:A:39:ASP:CB	0.41	2.45	17	1
1:A:35:ILE:HG22	1:A:36:SER:N	0.41	2.30	2	1
1:A:61:LYS:HG3	1:A:78:PHE:CE1	0.41	2.50	11	1
1:A:15:TRP:CD1	1:A:33:GLU:O	0.41	2.73	11	1
1:A:18:ARG:O	1:A:19:GLN:O	0.41	2.39	15	1
1:A:20:LEU:O	1:A:21:ILE:C	0.41	2.59	10	3
1:A:26:SER:O	1:A:28:GLY:N	0.41	2.53	8	3
1:A:30:ASP:C	1:A:31:THR:OG1	0.41	2.59	12	1
1:A:86:LEU:C	1:A:88:LYS:N	0.41	2.72	13	1
1:A:37:ARG:HB2	1:A:37:ARG:CZ	0.41	2.45	17	2
1:A:19:GLN:HB2	1:A:89:HIS:CE1	0.41	2.50	10	2
1:A:47:TYR:CE2	1:A:53:LEU:HD21	0.41	2.51	14	1
1:A:40:VAL:CG1	1:A:86:LEU:HD13	0.41	2.46	17	1
1:A:44:ILE:HD13	1:A:82:VAL:HG13	0.41	1.93	20	1
1:A:17:SER:O	1:A:18:ARG:C	0.40	2.59	6	1
1:A:86:LEU:O	1:A:87:GLU:C	0.40	2.60	13	1
1:A:48:ILE:O	1:A:53:LEU:N	0.40	2.50	12	1
1:A:37:ARG:HA	1:A:40:VAL:CG1	0.40	2.46	19	1
1:A:21:ILE:O	1:A:22:GLU:C	0.40	2.59	6	1
1:A:15:TRP:CG	1:A:34:MET:HA	0.40	2.52	11	1
1:A:78:PHE:O	1:A:79:ARG:C	0.40	2.60	16	1
1:A:33:GLU:O	1:A:34:MET:C	0.40	2.60	5	1
1:A:76:THR:C	1:A:77:ILE:HG23	0.40	2.36	17	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	79/101 (78%)	55±2 (70±3%)	18±2 (23±3%)	5±2 (7±2%)	2 17
All	All	1580/2020 (78%)	1107 (70%)	366 (23%)	107 (7%)	2 17

All 18 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	54	LEU	18
1	A	66	LYS	14
1	A	12	PHE	12
1	A	34	MET	11
1	A	21	ILE	9
1	A	87	GLU	6
1	A	19	GLN	5
1	A	82	VAL	5
1	A	32	SER	5
1	A	79	ARG	4
1	A	86	LEU	4
1	A	58	ASN	4
1	A	77	ILE	3
1	A	35	ILE	2
1	A	64	CYS	2
1	A	29	LYS	1
1	A	31	THR	1
1	A	30	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	73/90 (81%)	55±3 (76±4%)	18±3 (24±4%)	2 26
All	All	1460/1800 (81%)	1107 (76%)	353 (24%)	2 26

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	22	GLU	20
1	A	53	LEU	20
1	A	41	SER	17
1	A	75	ARG	17
1	A	18	ARG	16
1	A	66	LYS	15
1	A	80	MET	15
1	A	39	ASP	14

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Mol	Chain	Res	Type	Models (Total)
1	A	84	ASP	14
1	A	50	LYS	12
1	A	88	LYS	12
1	A	67	ARG	11
1	A	57	SER	11
1	A	17	SER	11
1	A	34	MET	10
1	A	32	SER	9
1	A	49	SER	9
1	A	33	GLU	9
1	A	37	ARG	9
1	A	59	LYS	8
1	A	65	ASP	8
1	A	87	GLU	8
1	A	26	SER	7
1	A	30	ASP	7
1	A	38	TYR	7
1	A	46	LYS	6
1	A	70	LEU	5
1	A	79	ARG	5
1	A	29	LYS	5
1	A	63	VAL	5
1	A	78	PHE	4
1	A	83	TYR	4
1	A	25	HIS	4
1	A	43	THR	3
1	A	20	LEU	3
1	A	81	LYS	3
1	A	36	SER	2
1	A	19	GLN	2
1	A	13	VAL	2
1	A	60	LYS	2
1	A	58	ASN	1
1	A	77	ILE	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