Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 03:11 PM EST

PDB ID	:	1V5U
Title	:	Solution Structure of the C-terminal Pleckstrin Homology Domain of Sbf1 from Mouse
Authors	:	Li, H.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2003-11-25

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:

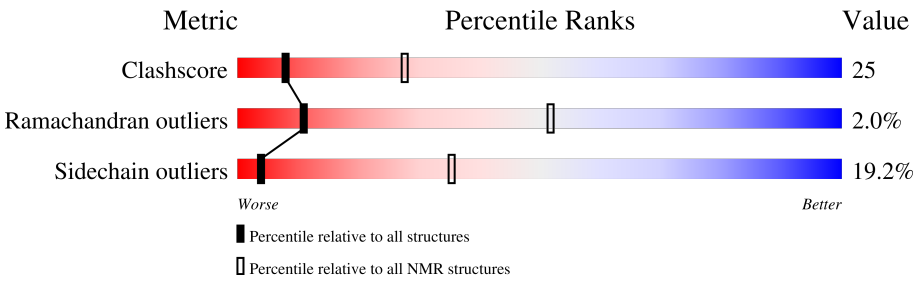
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	117	36% 32% • 28%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 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:10-A:17, A:24-A:41, A:52-A:109 (84)	0.27	4

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 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1814 atoms, of which 897 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SET binding factor 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	117	1814	579	897	161	172	5	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	GB 26344980
A	2	SER	-	cloning artifact	GB 26344980
A	3	SER	-	cloning artifact	GB 26344980
A	4	GLY	-	cloning artifact	GB 26344980
A	5	SER	-	cloning artifact	GB 26344980
A	6	SER	-	cloning artifact	GB 26344980
A	7	GLY	-	cloning artifact	GB 26344980
A	112	SER	-	cloning artifact	GB 26344980
A	113	GLY	-	cloning artifact	GB 26344980
A	114	PRO	-	cloning artifact	GB 26344980
A	115	SER	-	cloning artifact	GB 26344980
A	116	SER	-	cloning artifact	GB 26344980
A	117	GLY	-	cloning artifact	GB 26344980

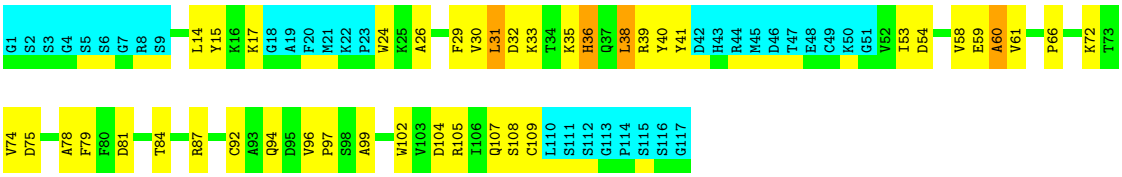
4 Residue-property plots (i)

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: SET binding factor 1

Chain A: 36% 32% • 28%



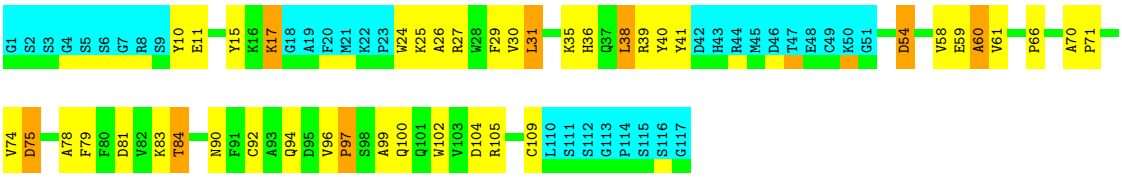
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: SET binding factor 1

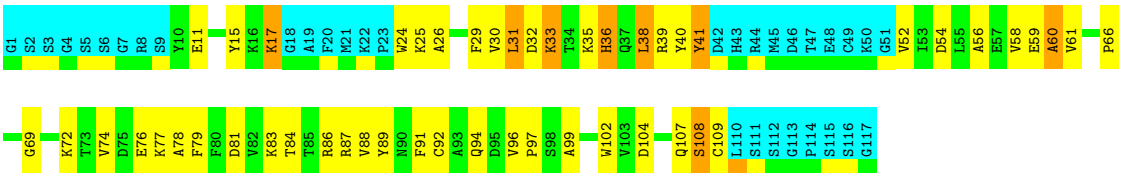
Chain A: 35% 30% 7% 28%



4.2.2 Score per residue for model 2

• Molecule 1: SET binding factor 1

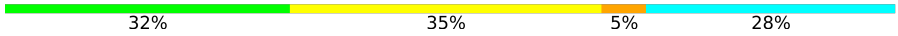
Chain A: 29% 36% 7% 28%

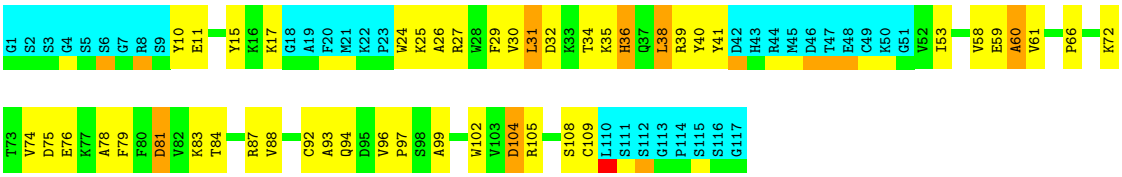


4.2.3 Score per residue for model 3

- Molecule 1: SET binding factor 1

Chain A:

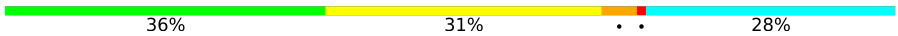


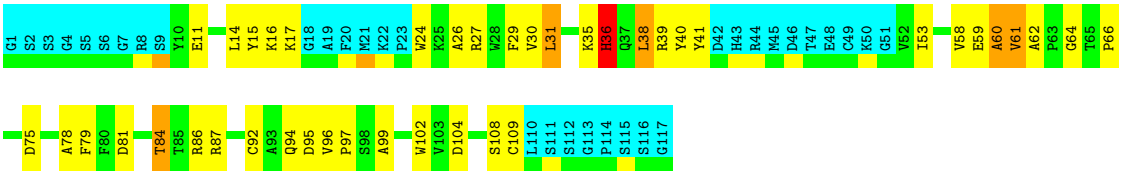


4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: SET binding factor 1

Chain A:

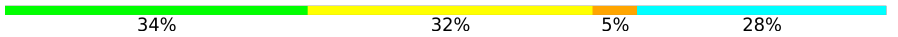


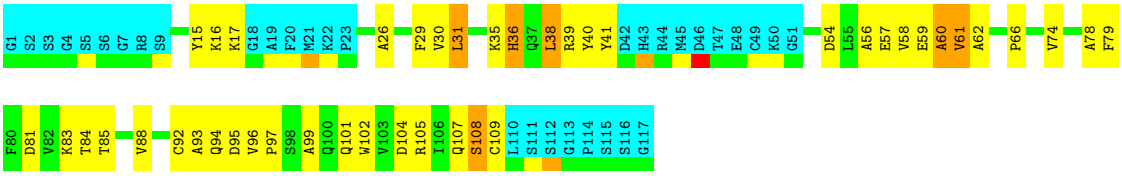


4.2.5 Score per residue for model 5

- Molecule 1: SET binding factor 1

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: SET binding factor 1

Chain A: 35% 31% 6% 28%

G1 S2 S3 G4 S5 S6 G7 R8 S9 L14 Y15 K16 K17 G18 A19 F20 M21 K22 P23 W24 K25 A26 F29 V30 L31 D32 K33 T34 K35 H36 Q37 L38 R39 Y40 Y41 D42 H43 R44 M45 D46 T47 E48 C49 K50 G51 D54 V58 E59 A60 V61 V74 D75 E76 K77 A78

D81 T84 T85 R86 Y89 N90 F91 C92 A93 Q94 D95 V96 P97 S98 A99 W102 V103 D104 R105 I106 Q107 S108 C109 L110 S111 S112 G113 P114 S115 S116 G117

4.2.7 Score per residue for model 7

- Molecule 1: SET binding factor 1

Chain A: 31% 36% 5% 28%

G1 S2 S3 G4 S5 S6 G7 R8 S9 Y10 L14 Y15 K16 K17 G18 A19 F20 M21 K22 P23 W24 K25 A26 R27 W28 F29 V30 L31 D32 K33 T34 K35 H36 Q37 L38 R39 Y40 Y41 D42 H43 R44 M45 D46 T47 E48 C49 K50 G51 V52 I53 D54 L55 A56 E57 V58 E59 A60 V61

P66 A70 P71 K72 D75 A78 F79 F80 D81 V82 K83 T84 T85 R86 R87 F91 C92 A93 Q94 D95 V96 P97 S98 A99 W102 V103 D104 R105 S108 C109 L110 S111 S112 G113 P114 S115 S116 G117

4.2.8 Score per residue for model 8

- Molecule 1: SET binding factor 1

Chain A: 25% 38% 9% 28%

G1 S2 S3 G4 S5 S6 G7 R8 S9 G12 I13 L14 Y15 K16 K17 G18 A19 F20 M21 K22 P23 W24 K25 A26 R27 W28 F29 V30 L31 D32 K33 H36 Q37 L38 R39 Y40 Y41 D42 H43 R44 M45 D46 T47 E48 C49 K50 G51 V52 I53 E57 V58 E59 A60 V61 A62 P66

G69 A70 P71 K72 T73 V74 D75 E76 K77 A78 F79 F80 D81 T84 T85 R86 R87 N90 F91 C92 A93 Q94 D95 V96 P97 S98 A99 W102 V103 D104 R105 I106 Q107 S108 C109 L110 S111 S112 G113 P114 S115 S116 G117

4.2.9 Score per residue for model 9

- Molecule 1: SET binding factor 1

Chain A: 43% 24% 5% 28%

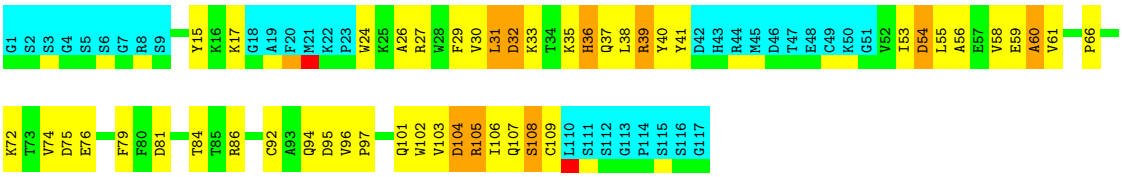
G1 S2 S3 G4 S5 S6 G7 R8 S9 L14 K17 G18 A19 F20 M21 K22 P23 W24 F29 V30 L31 H36 Q37 L38 R39 Y40 Y41 D42 H43 R44 M45 D46 T47 E48 C49 K50 G51 V52 I53 V58 E59 A60 V61 A62 P66 D75 A78 F79 F80 D81 T84

T85 R86 R87 C92 A93 Q94 D95 V96 P97 S98 A99 W102 R105 I106 C109 L110 S111 S112 G113 P114 S115 S116 G117

4.2.10 Score per residue for model 10

- Molecule 1: SET binding factor 1

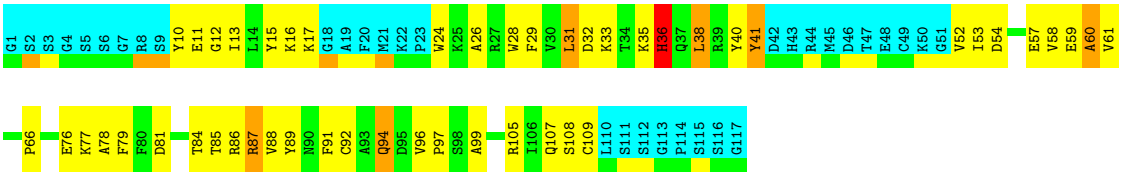
Chain A: 31% 33% 8% 28%



4.2.11 Score per residue for model 11

- Molecule 1: SET binding factor 1

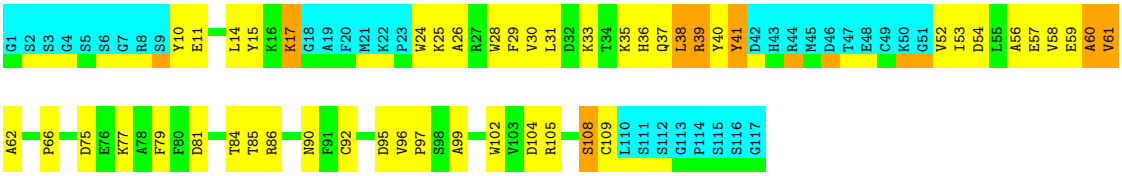
Chain A: 30% 36% 5% • 28%



4.2.12 Score per residue for model 12

- Molecule 1: SET binding factor 1

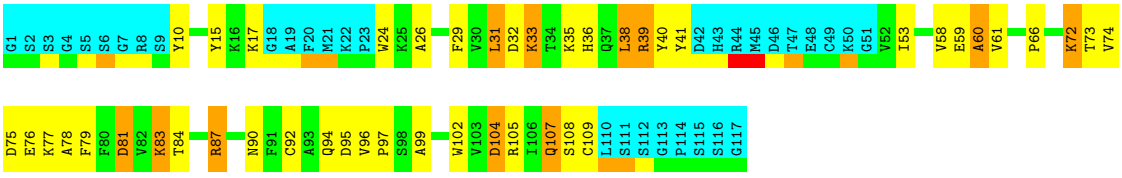
Chain A: 30% 36% 6% 28%



4.2.13 Score per residue for model 13

- Molecule 1: SET binding factor 1

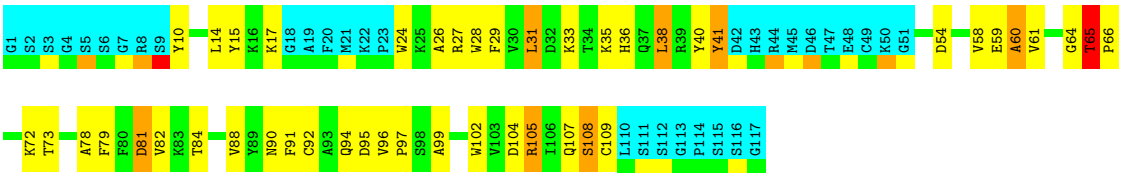
Chain A: 32% 30% 9% 28%



4.2.14 Score per residue for model 14

- Molecule 1: SET binding factor 1

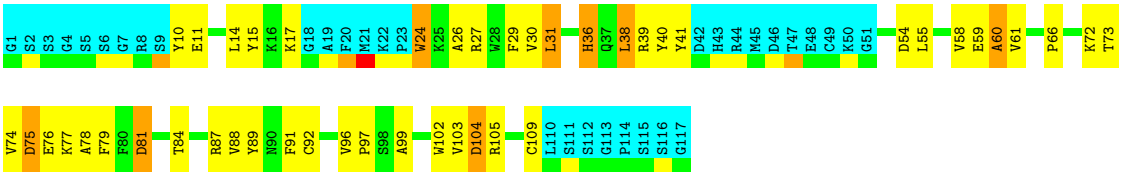
Chain A: 32% 32% 6% • 28%



4.2.15 Score per residue for model 15

- Molecule 1: SET binding factor 1

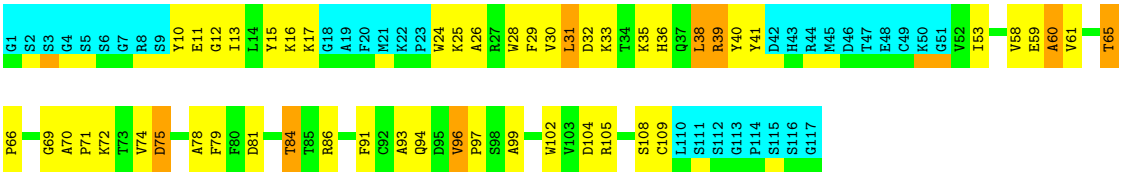
Chain A: 32% 32% 7% 28%



4.2.16 Score per residue for model 16

- Molecule 1: SET binding factor 1

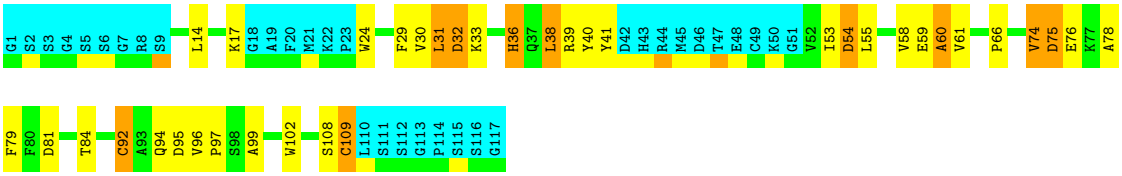
Chain A: 28% 37% 7% 28%



4.2.17 Score per residue for model 17

- Molecule 1: SET binding factor 1

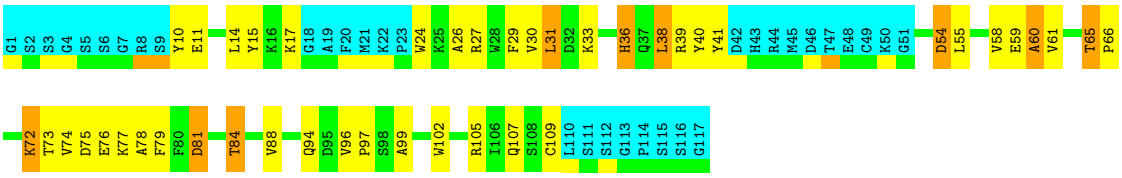
Chain A: 40% 23% 9% 28%



4.2.18 Score per residue for model 18

- Molecule 1: SET binding factor 1

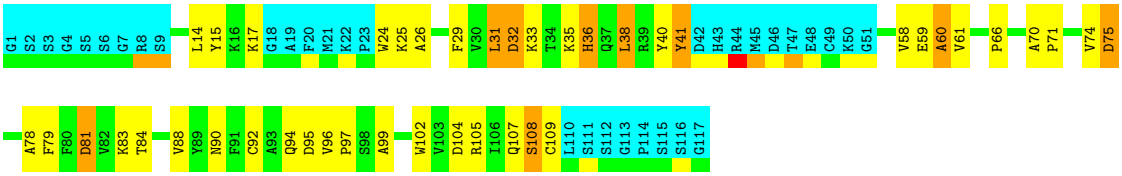
Chain A: 34% 30% 8% 28%



4.2.19 Score per residue for model 19

- Molecule 1: SET binding factor 1

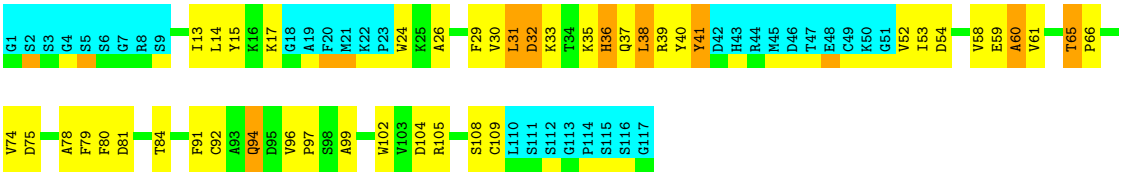
Chain A: 35% 29% 8% 28%



4.2.20 Score per residue for model 20

- Molecule 1: SET binding factor 1

Chain A: 33% 32% 7% 28%



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	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	693	689	689	35±6
All	All	13860	13780	13780	691

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:TYR:CE2	1:A:26:ALA:HB2	0.94	1.96	7	18
1:A:29:PHE:CD2	1:A:38:LEU:HD21	0.90	2.02	15	20
1:A:70:ALA:HB1	1:A:71:PRO:HD2	0.81	1.50	8	4
1:A:15:TYR:CZ	1:A:26:ALA:HB2	0.80	2.11	20	6
1:A:65:THR:HG22	1:A:66:PRO:HD2	0.78	1.56	14	1
1:A:70:ALA:HB1	1:A:71:PRO:CD	0.77	2.09	8	1
1:A:54:ASP:OD2	1:A:56:ALA:HB3	0.74	1.82	12	1
1:A:58:VAL:HG22	1:A:84:THR:CG2	0.73	2.13	12	20
1:A:58:VAL:HG22	1:A:84:THR:HG22	0.73	1.60	2	17
1:A:14:LEU:HD23	1:A:92:CYS:O	0.70	1.85	20	8
1:A:10:TYR:CD1	1:A:105:ARG:CZ	0.70	2.75	11	5
1:A:10:TYR:CD2	1:A:105:ARG:CD	0.68	2.76	1	5
1:A:74:VAL:CG2	1:A:78:ALA:HB3	0.68	2.19	15	1
1:A:55:LEU:HD13	1:A:109:CYS:SG	0.68	2.27	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:PHE:CD2	1:A:38:LEU:CD2	0.67	2.77	9	14
1:A:57:GLU:O	1:A:85:THR:HG23	0.67	1.89	5	3
1:A:14:LEU:HD11	1:A:102:TRP:CD2	0.66	2.26	6	7
1:A:57:GLU:OE1	1:A:85:THR:HG21	0.66	1.90	11	1
1:A:10:TYR:CD2	1:A:105:ARG:NE	0.65	2.65	1	3
1:A:59:GLU:O	1:A:60:ALA:HB2	0.64	1.93	16	20
1:A:17:LYS:CD	1:A:24:TRP:CZ2	0.64	2.81	14	9
1:A:96:VAL:N	1:A:97:PRO:CD	0.64	2.61	15	20
1:A:78:ALA:O	1:A:99:ALA:HB1	0.64	1.93	2	6
1:A:74:VAL:CG1	1:A:78:ALA:HB3	0.63	2.23	13	2
1:A:10:TYR:CD1	1:A:105:ARG:NH2	0.63	2.66	16	3
1:A:41:TYR:CD1	1:A:41:TYR:N	0.63	2.66	2	20
1:A:29:PHE:HD2	1:A:38:LEU:HD21	0.61	1.55	12	16
1:A:10:TYR:CG	1:A:105:ARG:NE	0.60	2.70	3	6
1:A:35:LYS:O	1:A:36:HIS:CD2	0.60	2.54	7	14
1:A:36:HIS:CE1	1:A:109:CYS:SG	0.60	2.95	8	2
1:A:24:TRP:CD1	1:A:69:GLY:O	0.60	2.54	8	3
1:A:15:TYR:CE2	1:A:26:ALA:CB	0.59	2.83	15	1
1:A:89:TYR:CB	1:A:91:PHE:CE2	0.58	2.86	15	2
1:A:29:PHE:CD1	1:A:40:TYR:CB	0.58	2.87	12	2
1:A:83:LYS:HG2	1:A:88:VAL:HG22	0.58	1.75	2	3
1:A:54:ASP:OD1	1:A:56:ALA:HB3	0.57	1.99	5	4
1:A:39:ARG:NH2	1:A:52:VAL:HG11	0.56	2.14	12	1
1:A:77:LYS:HB2	1:A:96:VAL:HG22	0.56	1.77	13	2
1:A:79:PHE:CG	1:A:92:CYS:SG	0.56	2.99	17	1
1:A:74:VAL:HG21	1:A:93:ALA:O	0.56	2.01	5	1
1:A:74:VAL:CG2	1:A:78:ALA:CB	0.55	2.84	15	1
1:A:35:LYS:O	1:A:36:HIS:CG	0.54	2.59	12	6
1:A:58:VAL:HA	1:A:84:THR:HG22	0.54	1.78	18	9
1:A:74:VAL:HG12	1:A:79:PHE:CE2	0.54	2.38	19	5
1:A:58:VAL:CG2	1:A:84:THR:HG22	0.54	2.31	2	7
1:A:93:ALA:HB3	1:A:99:ALA:HB2	0.54	1.80	8	4
1:A:38:LEU:HD22	1:A:53:ILE:HD12	0.54	1.80	10	12
1:A:89:TYR:HB3	1:A:91:PHE:CE2	0.53	2.38	15	3
1:A:74:VAL:HG22	1:A:93:ALA:O	0.53	2.03	16	1
1:A:17:LYS:HD3	1:A:24:TRP:CZ2	0.53	2.39	4	5
1:A:29:PHE:CD1	1:A:40:TYR:HB3	0.53	2.39	12	1
1:A:78:ALA:HA	1:A:99:ALA:HB3	0.53	1.80	17	8
1:A:78:ALA:HB2	1:A:96:VAL:HA	0.52	1.79	11	3
1:A:37:GLN:NE2	1:A:52:VAL:HG21	0.52	2.19	12	2
1:A:39:ARG:CZ	1:A:52:VAL:HG11	0.52	2.35	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LYS:HD2	1:A:24:TRP:CZ2	0.52	2.40	1	15
1:A:79:PHE:CD2	1:A:92:CYS:HB3	0.52	2.40	2	4
1:A:96:VAL:N	1:A:97:PRO:HD2	0.51	2.20	15	20
1:A:40:TYR:CD1	1:A:40:TYR:O	0.51	2.64	2	2
1:A:77:LYS:O	1:A:96:VAL:HG22	0.51	2.06	18	3
1:A:31:LEU:HB2	1:A:102:TRP:CZ3	0.51	2.40	8	18
1:A:79:PHE:CD1	1:A:92:CYS:HB3	0.51	2.41	11	2
1:A:75:ASP:CB	1:A:96:VAL:HG23	0.51	2.36	8	3
1:A:10:TYR:CG	1:A:105:ARG:CZ	0.51	2.93	13	4
1:A:59:GLU:O	1:A:60:ALA:CB	0.51	2.59	16	20
1:A:10:TYR:CD2	1:A:105:ARG:HD3	0.51	2.40	7	2
1:A:74:VAL:HG11	1:A:92:CYS:HB2	0.51	1.83	10	1
1:A:15:TYR:CD2	1:A:26:ALA:HB2	0.50	2.40	15	4
1:A:87:ARG:CG	1:A:88:VAL:N	0.50	2.71	11	1
1:A:74:VAL:HG22	1:A:78:ALA:HB3	0.50	1.81	15	1
1:A:78:ALA:O	1:A:92:CYS:CB	0.50	2.60	13	1
1:A:81:ASP:OD2	1:A:88:VAL:CG1	0.49	2.60	15	4
1:A:74:VAL:CG2	1:A:93:ALA:O	0.49	2.60	5	1
1:A:74:VAL:HG12	1:A:78:ALA:HB3	0.49	1.83	17	2
1:A:78:ALA:HB1	1:A:99:ALA:HB2	0.49	1.83	15	1
1:A:72:LYS:C	1:A:73:THR:CG2	0.49	2.80	8	1
1:A:57:GLU:OE1	1:A:85:THR:CG2	0.49	2.60	11	1
1:A:75:ASP:O	1:A:79:PHE:CE2	0.49	2.66	20	2
1:A:24:TRP:N	1:A:24:TRP:CD1	0.48	2.79	20	2
1:A:10:TYR:CD2	1:A:105:ARG:HD2	0.48	2.43	11	1
1:A:75:ASP:O	1:A:79:PHE:CD2	0.48	2.66	20	3
1:A:40:TYR:CD1	1:A:40:TYR:C	0.48	2.86	2	1
1:A:12:GLY:HA2	1:A:28:TRP:CH2	0.48	2.44	11	2
1:A:78:ALA:O	1:A:79:PHE:C	0.48	2.52	15	2
1:A:37:GLN:N	1:A:55:LEU:HD12	0.48	2.23	10	1
1:A:78:ALA:HA	1:A:99:ALA:CB	0.47	2.39	15	15
1:A:13:ILE:O	1:A:94:GLN:NE2	0.47	2.47	11	1
1:A:66:PRO:HB3	1:A:79:PHE:CZ	0.47	2.44	14	4
1:A:66:PRO:HB3	1:A:79:PHE:CE1	0.47	2.45	9	12
1:A:14:LEU:CD2	1:A:92:CYS:O	0.47	2.63	9	2
1:A:13:ILE:HG21	1:A:94:GLN:HG3	0.47	1.87	8	2
1:A:30:VAL:N	1:A:39:ARG:O	0.46	2.48	7	15
1:A:24:TRP:CD1	1:A:70:ALA:HA	0.46	2.45	7	1
1:A:74:VAL:HG13	1:A:79:PHE:CE1	0.46	2.46	2	1
1:A:14:LEU:HD11	1:A:102:TRP:CE2	0.46	2.45	8	3
1:A:66:PRO:HB3	1:A:79:PHE:CE2	0.46	2.46	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:TRP:CE3	1:A:92:CYS:SG	0.46	3.09	12	1
1:A:99:ALA:O	1:A:102:TRP:N	0.46	2.49	13	6
1:A:104:ASP:O	1:A:108:SER:N	0.46	2.49	2	10
1:A:75:ASP:CB	1:A:96:VAL:CG2	0.45	2.94	17	2
1:A:29:PHE:CD1	1:A:40:TYR:HB2	0.45	2.46	12	3
1:A:101:GLN:O	1:A:105:ARG:NE	0.45	2.49	10	1
1:A:17:LYS:HG3	1:A:24:TRP:CE2	0.45	2.46	17	5
1:A:16:LYS:HG3	1:A:91:PHE:CE1	0.45	2.45	11	3
1:A:32:ASP:OD2	1:A:36:HIS:N	0.45	2.49	17	5
1:A:75:ASP:HB2	1:A:96:VAL:HG23	0.45	1.87	15	2
1:A:14:LEU:HD11	1:A:102:TRP:CE3	0.45	2.46	18	1
1:A:75:ASP:O	1:A:78:ALA:N	0.45	2.49	8	1
1:A:39:ARG:NH1	1:A:41:TYR:OH	0.45	2.50	13	1
1:A:79:PHE:CD2	1:A:92:CYS:CB	0.45	2.99	2	2
1:A:105:ARG:O	1:A:108:SER:N	0.45	2.49	12	6
1:A:97:PRO:O	1:A:100:GLN:N	0.45	2.50	1	1
1:A:101:GLN:O	1:A:105:ARG:CD	0.45	2.65	5	1
1:A:79:PHE:CD1	1:A:92:CYS:CB	0.45	3.00	11	1
1:A:36:HIS:C	1:A:55:LEU:HD12	0.45	2.32	18	1
1:A:24:TRP:NE1	1:A:69:GLY:O	0.45	2.49	16	1
1:A:11:GLU:N	1:A:11:GLU:OE2	0.44	2.50	16	1
1:A:97:PRO:O	1:A:99:ALA:N	0.44	2.51	1	1
1:A:32:ASP:OD1	1:A:34:THR:N	0.44	2.50	3	2
1:A:16:LYS:HG3	1:A:91:PHE:CD1	0.44	2.47	11	1
1:A:54:ASP:N	1:A:54:ASP:OD1	0.44	2.50	1	1
1:A:74:VAL:HG22	1:A:75:ASP:N	0.44	2.26	1	1
1:A:106:ILE:O	1:A:109:CYS:N	0.44	2.47	10	1
1:A:35:LYS:C	1:A:36:HIS:CG	0.44	2.91	10	3
1:A:70:ALA:CB	1:A:71:PRO:CD	0.43	2.81	8	1
1:A:86:ARG:CG	1:A:87:ARG:N	0.43	2.81	11	1
1:A:82:VAL:HG12	1:A:84:THR:HG23	0.43	1.89	14	1
1:A:32:ASP:OD1	1:A:33:LYS:N	0.43	2.52	10	4
1:A:78:ALA:O	1:A:99:ALA:CB	0.43	2.64	2	1
1:A:14:LEU:HB2	1:A:29:PHE:CG	0.43	2.48	8	5
1:A:10:TYR:CE1	1:A:105:ARG:CZ	0.43	3.02	11	1
1:A:55:LEU:O	1:A:58:VAL:N	0.43	2.50	18	1
1:A:40:TYR:C	1:A:41:TYR:CD1	0.43	2.92	16	1
1:A:97:PRO:C	1:A:99:ALA:N	0.43	2.70	1	1
1:A:81:ASP:OD2	1:A:90:ASN:ND2	0.43	2.52	13	1
1:A:32:ASP:OD2	1:A:39:ARG:CD	0.43	2.66	16	1
1:A:66:PRO:HD3	1:A:76:GLU:CB	0.43	2.44	13	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:TRP:CD1	1:A:70:ALA:N	0.43	2.86	7	1
1:A:73:THR:O	1:A:73:THR:OG1	0.43	2.34	8	1
1:A:65:THR:OG1	1:A:66:PRO:HD2	0.43	2.13	18	3
1:A:80:PHE:CZ	1:A:91:PHE:CB	0.42	3.02	20	2
1:A:83:LYS:HG3	1:A:88:VAL:HG22	0.42	1.91	19	1
1:A:11:GLU:N	1:A:11:GLU:OE1	0.42	2.52	2	1
1:A:81:ASP:OD1	1:A:90:ASN:ND2	0.42	2.52	19	2
1:A:59:GLU:N	1:A:83:LYS:O	0.42	2.50	13	1
1:A:86:ARG:NE	1:A:89:TYR:OH	0.42	2.52	11	1
1:A:90:ASN:O	1:A:91:PHE:CD1	0.42	2.73	14	1
1:A:75:ASP:O	1:A:76:GLU:C	0.42	2.57	8	1
1:A:106:ILE:O	1:A:109:CYS:SG	0.42	2.77	9	1
1:A:29:PHE:CE1	1:A:40:TYR:CB	0.42	3.03	12	1
1:A:74:VAL:HG12	1:A:75:ASP:N	0.42	2.30	6	1
1:A:74:VAL:HG23	1:A:78:ALA:CB	0.42	2.44	15	1
1:A:54:ASP:OD1	1:A:54:ASP:N	0.42	2.53	17	1
1:A:36:HIS:CD2	1:A:109:CYS:HB3	0.42	2.49	3	1
1:A:72:LYS:C	1:A:74:VAL:N	0.42	2.73	15	1
1:A:72:LYS:O	1:A:74:VAL:O	0.42	2.38	15	2
1:A:75:ASP:HB2	1:A:96:VAL:CG2	0.42	2.45	17	1
1:A:35:LYS:C	1:A:36:HIS:CD2	0.41	2.93	4	2
1:A:35:LYS:O	1:A:36:HIS:C	0.41	2.58	20	2
1:A:72:LYS:O	1:A:73:THR:C	0.41	2.58	13	3
1:A:64:GLY:O	1:A:65:THR:C	0.41	2.58	14	1
1:A:36:HIS:O	1:A:55:LEU:N	0.41	2.52	15	1
1:A:17:LYS:CD	1:A:24:TRP:CE2	0.41	3.04	4	2
1:A:64:GLY:N	1:A:79:PHE:O	0.41	2.53	4	1
1:A:75:ASP:O	1:A:77:LYS:N	0.41	2.53	8	1
1:A:84:THR:OG1	1:A:87:ARG:O	0.41	2.39	2	8
1:A:75:ASP:HB3	1:A:96:VAL:CG2	0.41	2.46	18	1
1:A:61:VAL:CG2	1:A:62:ALA:N	0.41	2.84	9	5
1:A:17:LYS:HA	1:A:24:TRP:CD2	0.41	2.50	10	1
1:A:65:THR:HG22	1:A:66:PRO:CD	0.41	2.38	14	1
1:A:74:VAL:CG1	1:A:79:PHE:CE2	0.41	3.04	3	1
1:A:75:ASP:C	1:A:77:LYS:N	0.41	2.74	8	1
1:A:87:ARG:HB3	1:A:87:ARG:CZ	0.41	2.46	15	1
1:A:31:LEU:HD22	1:A:31:LEU:HA	0.40	1.80	2	1
1:A:24:TRP:CZ3	1:A:79:PHE:CE2	0.40	3.09	4	1
1:A:16:LYS:O	1:A:17:LYS:C	0.40	2.60	5	1
1:A:24:TRP:CD1	1:A:24:TRP:N	0.40	2.89	7	1
1:A:72:LYS:O	1:A:73:THR:HG22	0.40	2.17	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD23	1:A:102:TRP:HZ3	0.40	1.76	7	1
1:A:102:TRP:O	1:A:103:VAL:C	0.40	2.60	10	1
1:A:10:TYR:CG	1:A:11:GLU:N	0.40	2.89	12	1
1:A:75:ASP:HB3	1:A:96:VAL:HG23	0.40	1.93	12	1
1:A:12:GLY:O	1:A:13:ILE:C	0.40	2.59	16	1
1:A:95:ASP:N	1:A:95:ASP:OD1	0.40	2.54	6	1
1:A:103:VAL:O	1:A:104:ASP:C	0.40	2.59	6	2
1:A:77:LYS:O	1:A:78:ALA:C	0.40	2.59	8	1
1:A:80:PHE:CE2	1:A:91:PHE:HB2	0.40	2.51	8	1
1:A:29:PHE:CE2	1:A:91:PHE:CE1	0.40	3.09	7	1
1:A:38:LEU:N	1:A:53:ILE:O	0.40	2.54	9	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	84/117 (72%)	70±3 (83±3%)	13±3 (15±3%)	2±1 (2±1%)	11	52
All	All	1680/2340 (72%)	1390 (83%)	257 (15%)	33 (2%)	11	52

All 7 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	60	ALA	20
1	A	36	HIS	7
1	A	54	ASP	2
1	A	97	PRO	1
1	A	65	THR	1
1	A	24	TRP	1
1	A	74	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	73/98 (74%)	59±2 (81±3%)	14±2 (19±3%)	4 35
All	All	1460/1960 (74%)	1180 (81%)	280 (19%)	4 35

All 38 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	31	LEU	20
1	A	61	VAL	20
1	A	81	ASP	20
1	A	38	LEU	18
1	A	94	GLN	18
1	A	75	ASP	13
1	A	109	CYS	13
1	A	33	LYS	13
1	A	108	SER	11
1	A	104	ASP	9
1	A	95	ASP	9
1	A	27	ARG	8
1	A	54	ASP	8
1	A	86	ARG	8
1	A	36	HIS	8
1	A	41	TYR	7
1	A	72	LYS	7
1	A	107	GLN	7
1	A	105	ARG	7
1	A	11	GLU	6
1	A	25	LYS	6
1	A	84	THR	5
1	A	39	ARG	5
1	A	32	ASP	5
1	A	76	GLU	4
1	A	65	THR	4
1	A	17	LYS	3
1	A	83	LYS	3
1	A	90	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	96	VAL	2
1	A	92	CYS	2
1	A	87	ARG	2
1	A	35	LYS	1
1	A	16	LYS	1
1	A	53	ILE	1
1	A	52	VAL	1
1	A	73	THR	1
1	A	77	LYS	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