Full wwPDB NMR Structure Validation Report (i)

Feb 24, 2022 – 07:41 AM EST

PDB ID	:	1Z9B
Title	:	Solution structure of the C1-subdomain of Bacillus stearothermophilus translation initiation factor IF2
Authors	:	Wienk, H.; Tomaselli, S.; Bernard, C.; Spurio, R.; Picone, D.; Gualerzi, C.O.; Boelens, R.
Deposited on	:	2005-04-01

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:

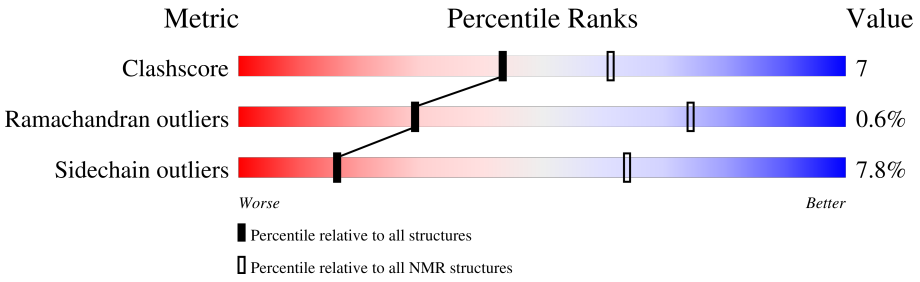
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	135	43% 10% 47%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 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:43-A:63, A:71-A:120 (71)	0.35	8

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 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2088 atoms, of which 1051 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	135	2088	645	1051	186	204	2	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASN	-	cloning artifact	UNP P04766
A	2	GLU	-	cloning artifact	UNP P04766
A	3	PHE	-	cloning artifact	UNP P04766
A	4	GLU	-	cloning artifact	UNP P04766
A	5	LEU	-	cloning artifact	UNP P04766
A	6	GLY	-	cloning artifact	UNP P04766
A	7	THR	-	cloning artifact	UNP P04766
A	8	ARG	-	cloning artifact	UNP P04766
A	9	GLY	-	cloning artifact	UNP P04766
A	10	SER	-	cloning artifact	UNP P04766
A	11	SER	-	cloning artifact	UNP P04766
A	12	ARG	-	cloning artifact	UNP P04766
A	13	VAL	-	cloning artifact	UNP P04766
A	14	ASP	-	cloning artifact	UNP P04766

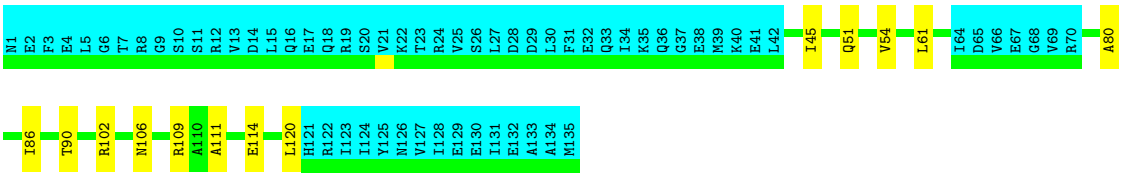
4 Residue-property plots (i)

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: Translation initiation factor IF-2

Chain A: 43% 10% 47%



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: Translation initiation factor IF-2

Chain A: 40% 12% • 47%

4.2.2 Score per residue for model 2

• Molecule 1: Translation initiation factor IF-2

Chain A: 36% 16% • 47%

4.2.3 Score per residue for model 3

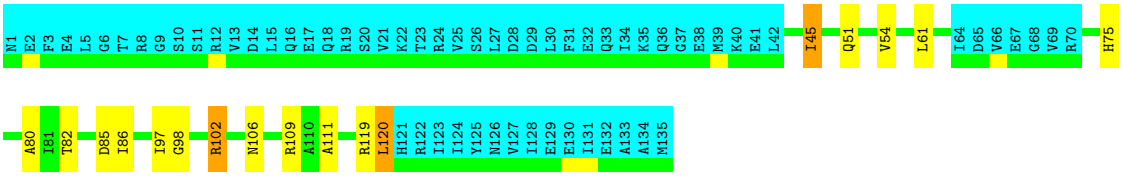
- Molecule 1: Translation initiation factor IF-2

Chain A: 38% 13% • 47%

4.2.4 Score per residue for model 4

- Molecule 1: Translation initiation factor IF-2

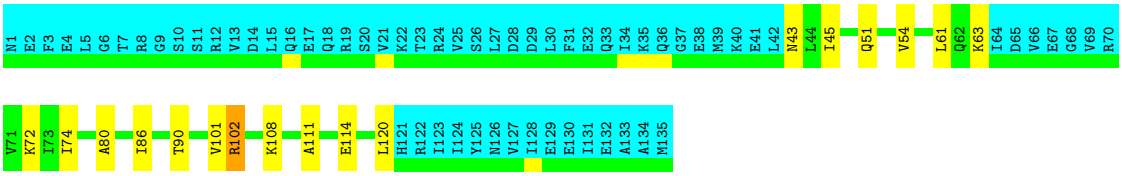
Chain A: 40% 10% • 47%



4.2.5 Score per residue for model 5

- Molecule 1: Translation initiation factor IF-2

Chain A: 40% 12% • 47%



4.2.6 Score per residue for model 6

- Molecule 1: Translation initiation factor IF-2

Chain A: 44% 8% • 47%

N1 E2 F3 E4 L5 G6 T7 R8 G9 S10 S11 R12 V13 D14 L15 Q16 E17 Q18 R19 S20 V21 K22 T23 R24 V25 S26 L27 D28 D29 L30 F31 E32 Q33 I34 K35 Q36 G37 E38 M39 K40 E41 L42 I45 Q51 V54 L61 I64 D65 V66 E67 G68 V69 R70 T90

N93 V96 R102 N106 R109 E114 L120 H121 R122 I123 I124 Y125 N126 V127 I128 E129 E130 I131 E132 A133 A134 M135

4.2.7 Score per residue for model 7

- Molecule 1: Translation initiation factor IF-2

Chain A: 39% 13% • 47%

N1 E2 F3 E4 L5 G6 T7 R8 G9 S10 S11 R12 V13 D14 L15 Q16 E17 Q18 R19 S20 V21 K22 T23 R24 V25 S26 L27 D28 D29 L30 F31 E32 Q33 I34 K35 Q36 G37 E38 M39 K40 E41 L42 N43 L44 I45 Q51 V54 L61 I64 D65 V66 E67 G68 V69 R70 V71

A80 I86 T90 A94 I97 R102 N106 R109 A110 A111 E114 R119 L120 H121 R122 I123 I124 Y125 N126 V127 I128 E129 E130 I131 E132 A133 A134 M135

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Translation initiation factor IF-2

Chain A: 41% 12% 47%

N1 E2 F3 E4 L5 G6 T7 R8 G9 S10 S11 R12 V13 D14 L15 Q16 E17 Q18 R19 S20 V21 K22 T23 R24 V25 S26 L27 D28 D29 L30 F31 E32 Q33 I34 K35 Q36 G37 E38 M39 K40 E41 L42 I45 V46 Q51 V54 L61 I64 D65 V66 E67 G68 V69 R70

A76 A80 E83 I86 T90 V96 V101 R102 A111 E114 K115 H121 R122 I123 I124 Y125 N126 V127 I128 E129 E130 I131 E132 A133 A134 M135

4.2.9 Score per residue for model 9

- Molecule 1: Translation initiation factor IF-2

Chain A: 41% 10% • 47%

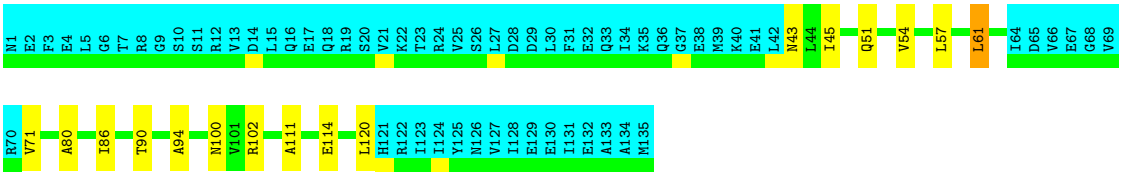
N1 E2 F3 E4 L5 G6 T7 R8 G9 S10 S11 R12 V13 D14 L15 Q16 E17 Q18 R19 S20 V21 K22 T23 R24 V25 S26 L27 D28 D29 L30 F31 E32 Q33 I34 K35 Q36 G37 E38 M39 K40 E41 L42 I45 Q51 V54 A60 L61 Q62 K63 I64 D65 V66 E67 G68 V69 R70

V71 A80 T90 G98 R102 N106 R109 E114 L120 H121 R122 I123 I124 Y125 N126 V127 I128 E129 E130 I131 E132 A133 A134 M135

4.2.10 Score per residue for model 10

- Molecule 1: Translation initiation factor IF-2

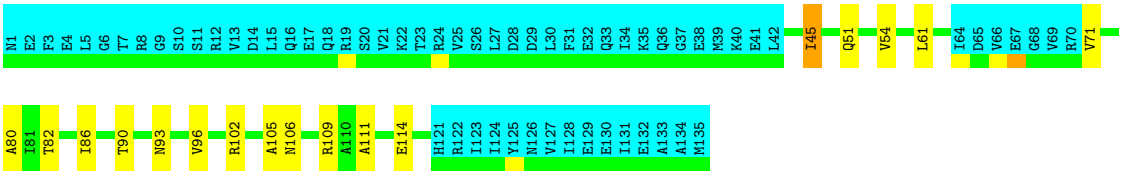
Chain A: 41% 11% • 47%



4.2.11 Score per residue for model 11

- Molecule 1: Translation initiation factor IF-2

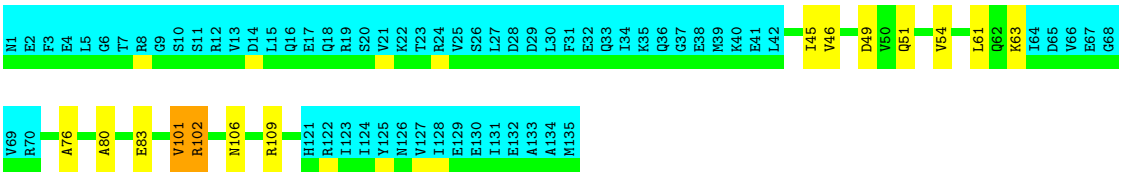
Chain A: 40% 12% • 47%



4.2.12 Score per residue for model 12

- Molecule 1: Translation initiation factor IF-2

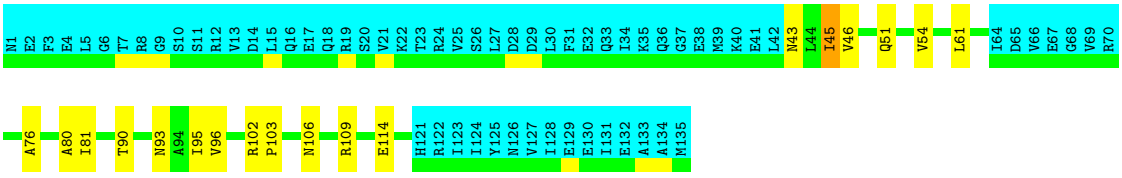
Chain A: 42% 9% • 47%



4.2.13 Score per residue for model 13

- Molecule 1: Translation initiation factor IF-2

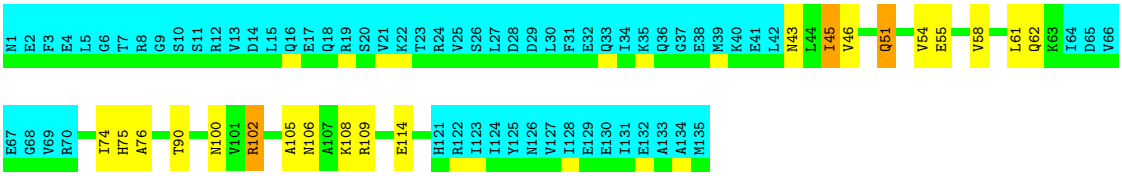
Chain A: 39% 13% • 47%



4.2.14 Score per residue for model 14

- Molecule 1: Translation initiation factor IF-2

Chain A: 38% 13% • 47%



4.2.15 Score per residue for model 15

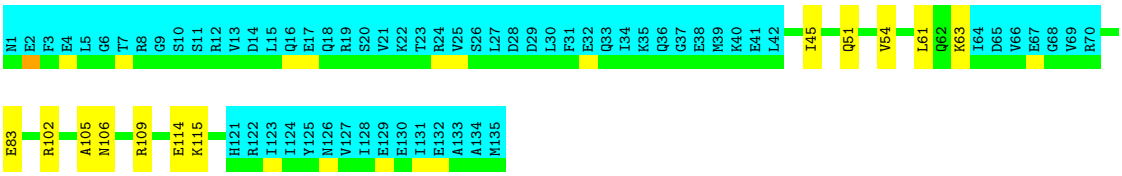
- Molecule 1: Translation initiation factor IF-2

Chain A: 35% 16% • 47%

4.2.16 Score per residue for model 16

- Molecule 1: Translation initiation factor IF-2

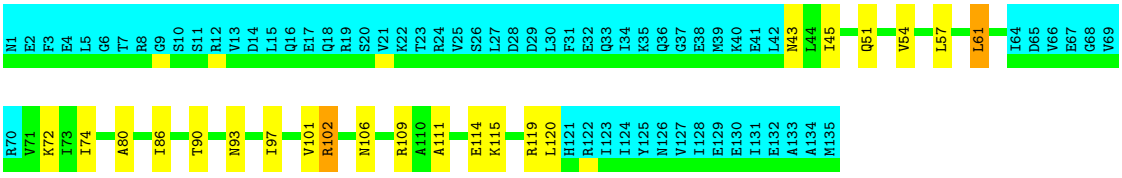
Chain A: 44% 9% 47%



4.2.17 Score per residue for model 17

- Molecule 1: Translation initiation factor IF-2

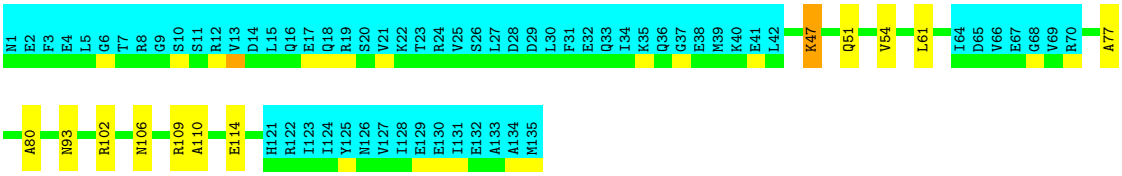
Chain A: 36% 15% • 47%



4.2.18 Score per residue for model 18

- Molecule 1: Translation initiation factor IF-2

Chain A: 44% 8% • 47%



4.2.19 Score per residue for model 19

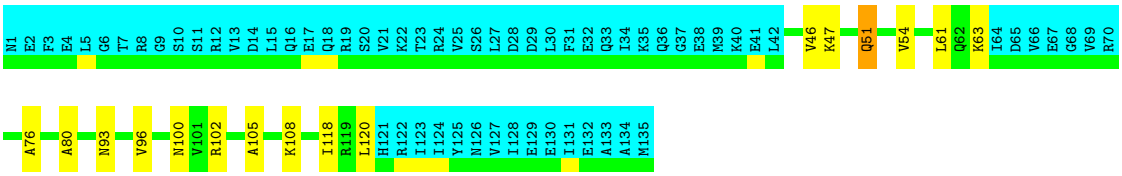
- Molecule 1: Translation initiation factor IF-2

Chain A: 37% 13% • 47%

4.2.20 Score per residue for model 20

- Molecule 1: Translation initiation factor IF-2

Chain A: 41% 11% • 47%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *intial fold determination with CNS in ARIA followed by iterative automatic assignment and simulated annealing in CYANA2.0, followed by a round of annealing in ARIA and final water refinement using CNS procedure re_h2o.inp.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	refinement	1.1
CYANA	structure solution	2.0

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	517	541	549	7±3
All	All	10340	10820	10980	149

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:GLN:O	1:A:54:VAL:HG22	0.68	1.89	19	20
1:A:96:VAL:HB	1:A:118:ILE:HG22	0.58	1.74	20	3
1:A:43:ASN:HB3	1:A:74:ILE:HD11	0.58	1.73	5	2
1:A:86:ILE:HD13	1:A:111:ALA:HB2	0.56	1.75	17	4
1:A:80:ALA:HB1	1:A:102:ARG:O	0.54	2.02	1	16
1:A:43:ASN:O	1:A:94:ALA:HA	0.54	2.03	15	4
1:A:46:VAL:O	1:A:76:ALA:HA	0.54	2.03	20	9
1:A:106:ASN:O	1:A:109:ARG:HB2	0.54	2.03	19	15
1:A:97:ILE:HA	1:A:119:ARG:O	0.53	2.03	15	5
1:A:45:ILE:HD13	1:A:75:HIS:CD2	0.52	2.39	4	3
1:A:90:THR:HB	1:A:114:GLU:O	0.52	2.05	8	14
1:A:89:ALA:HA	1:A:94:ALA:O	0.51	2.04	1	1
1:A:100:ASN:O	1:A:102:ARG:HD3	0.51	2.06	14	1
1:A:51:GLN:O	1:A:55:GLU:HG2	0.51	2.06	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:HG23	1:A:96:VAL:HA	0.50	1.84	11	5
1:A:80:ALA:HA	1:A:101:VAL:HB	0.49	1.82	15	4
1:A:57:LEU:O	1:A:61:LEU:HB2	0.48	2.08	17	3
1:A:86:ILE:HG21	1:A:111:ALA:HA	0.48	1.85	8	7
1:A:105:ALA:O	1:A:108:LYS:HG2	0.47	2.10	20	4
1:A:98:GLY:O	1:A:120:LEU:HA	0.46	2.10	4	2
1:A:105:ALA:O	1:A:109:ARG:HG3	0.46	2.11	11	4
1:A:47:LYS:HE3	1:A:85:ASP:CG	0.45	2.31	3	1
1:A:114:GLU:O	1:A:115:LYS:HB2	0.45	2.11	1	5
1:A:43:ASN:HA	1:A:72:LYS:O	0.45	2.11	5	2
1:A:60:ALA:O	1:A:63:LYS:HG2	0.43	2.13	2	1
1:A:45:ILE:HD12	1:A:75:HIS:CD2	0.43	2.48	19	3
1:A:86:ILE:CG2	1:A:111:ALA:HA	0.43	2.44	10	2
1:A:110:ALA:HB1	1:A:114:GLU:OE1	0.42	2.15	18	1
1:A:47:LYS:HA	1:A:77:ALA:O	0.41	2.14	18	1
1:A:82:THR:HG22	1:A:85:ASP:OD2	0.41	2.15	4	1
1:A:83:GLU:H	1:A:83:GLU:CD	0.41	2.18	2	1
1:A:43:ASN:OD1	1:A:74:ILE:HD11	0.41	2.16	14	1
1:A:58:VAL:O	1:A:62:GLN:HG2	0.40	2.16	14	1
1:A:45:ILE:HD12	1:A:75:HIS:O	0.40	2.17	3	1
1:A:81:ILE:O	1:A:103:PRO:HA	0.40	2.17	13	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	71/135 (53%)	67±1 (94±2%)	4±1 (5±2%)	0±0 (1±1%)	29	74
All	All	1420/2700 (53%)	1338 (94%)	74 (5%)	8 (1%)	29	74

All 3 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	102	ARG	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	101	VAL	1
1	A	100	ASN	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	54/112 (48%)	50±1 (92±2%)	4±1 (8±2%)	16 64
All	All	1080/2240 (48%)	996 (92%)	84 (8%)	16 64

All 16 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	61	LEU	20
1	A	45	ILE	17
1	A	120	LEU	12
1	A	93	ASN	7
1	A	63	LYS	5
1	A	51	GLN	4
1	A	83	GLU	4
1	A	102	ARG	4
1	A	108	LYS	2
1	A	97	ILE	2
1	A	47	LYS	2
1	A	82	THR	1
1	A	49	ASP	1
1	A	101	VAL	1
1	A	43	ASN	1
1	A	95	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