W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 09:01 PM BST

PDB ID	:	2GS0
Title	:	NMR structure of the complex between the PH domain of the Tfb1 subunit from TFIIH and the activation domain of p53
Authors	:	Di Lello, P.; Jones, T.N.; Nguyen, B.D.; Legault, P.; Omichinski, J.G.
Deposited on	:	2006-04-25

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
http://wwpdb.org/validation/2016/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:

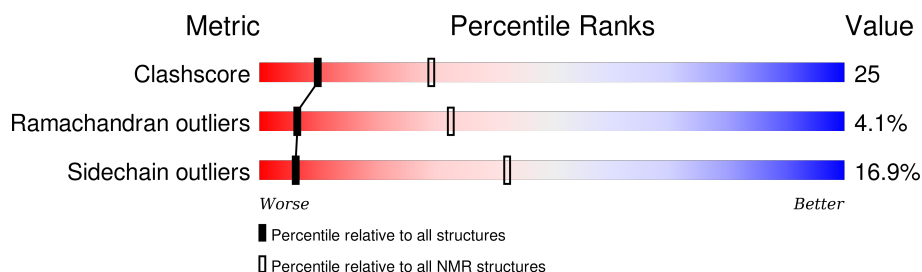|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 is 87%.

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	Percentile Ranks	Value
Clashscore		25
Ramachandran outliers		4.1%
Sidechain outliers		16.9%

Worse   *Better*

■ Percentile relative to all structures

▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	115	57% 34% 6% •
2	B	54	26% 74%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 19 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:2-A:65, A:85-A:112 (92)	0.25	19
2	A:66-A:84 (19)	0.29	9

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2039 atoms, of which 1018 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA polymerase II transcription factor B subunit 1.

Mol	Chain	Residues	Atoms						Trace
1	A	115	Total	C	H	N	O	S	0
			1821	559	919	161	177	5	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	MET	ENGINEERED	UNP P32776

- Molecule 2 is a protein called Cellular tumor antigen p53.

| Mol	Chain	Residues	Atoms					Trace
2	B	14	Total	C	H	N	O	0
			218	76	99	16	27	

4   Residue-property plots ⓘ

4.1   Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: RNA polymerase II transcription factor B subunit 1
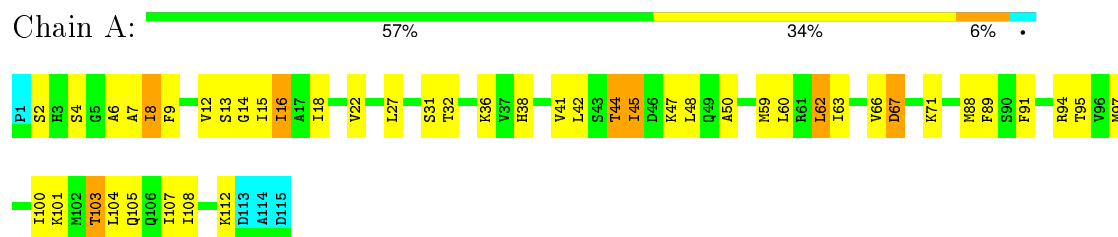
- Molecule 2: Cellular tumor antigen p53
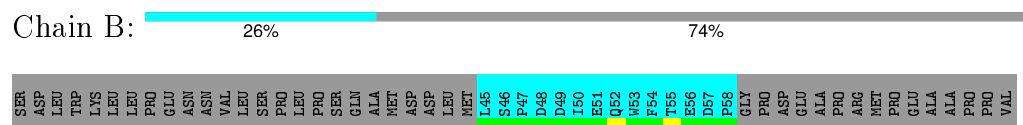
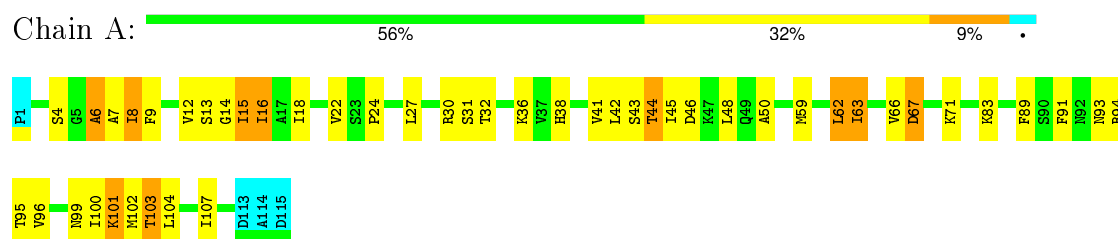## 4.2   Scores per residue for each member of the ensemble

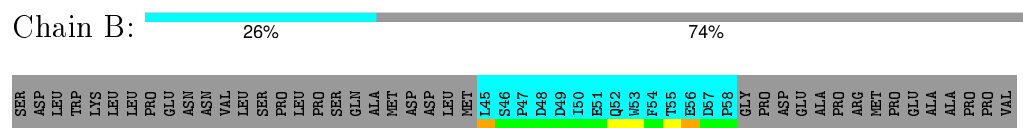Colouring as in section 4.1 above.

4.2.1   Score per residue for model 1

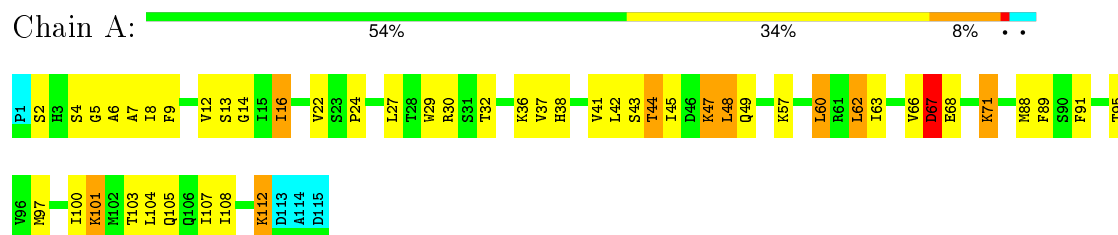- Molecule 1: RNA polymerase II transcription factor B subunit 1
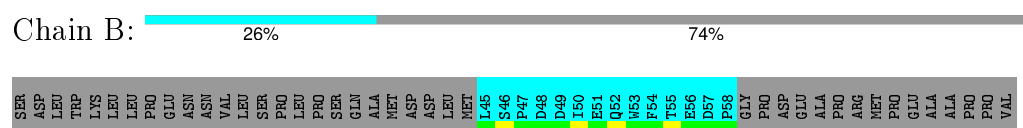

- Molecule 2: Cellular tumor antigen p53

Chain B:

26%

74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL

4.2.2 Score per residue for model 2

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A:

54%

34%

8%

P1 S2 H3 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 V22 S23 P24 L27 T28 W29 R30 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 K57 L60 R61 L62 I63 V66 D67 E68 K71 M88 F89 S90 F91 T95

V96 M97 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B:

26%

74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL

4.2.3 Score per residue for model 3

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A:

57%

30%

10%

P1 S2 H3 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 L27 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 M59 L62 I63 V66 D67 K71 F89 S90 F91 T95 V96 M97 I100 K101

M102 T103 L104 Q105 Q106 I107 I108 Y111 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B:

26%

74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL
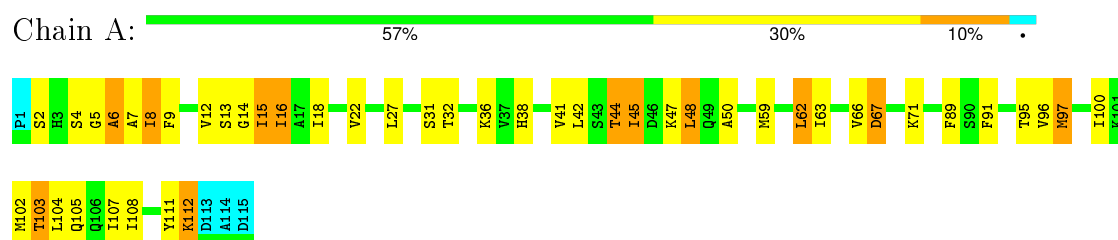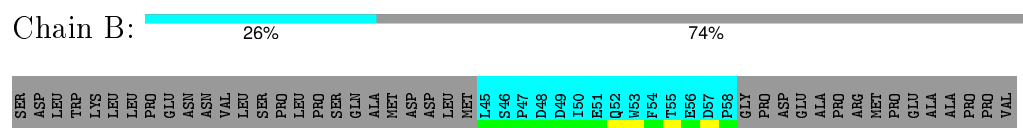
4.2.4 Score per residue for model 4

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 　　56%　　　　　　31%　　　　10%　·

P1 S2 H3 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 V22 S23 P24 L27 T28 W29 R30 S31 T32 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 M59 L60 R61 L62 I63 V66 D67 K71 P84 F89 S90 F91 T95 I100

T103 L104 Q105 Q106 I107 I108 Y111 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 　26%　　　　　　　74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO VAL
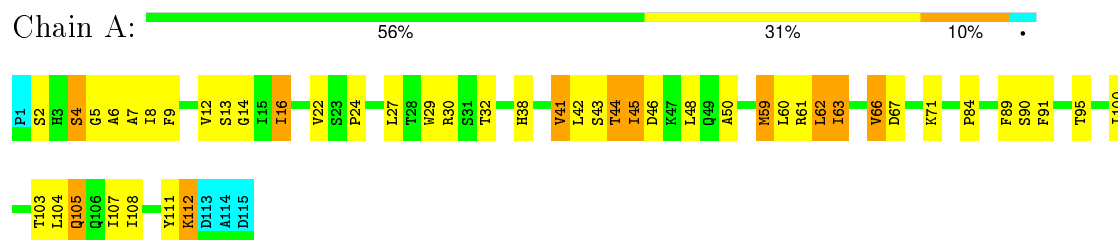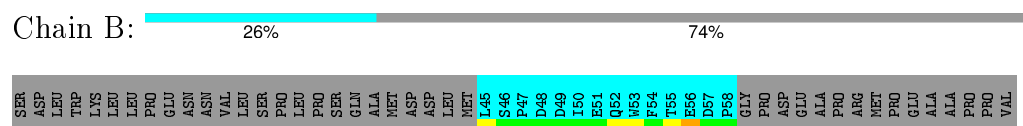
4.2.5　Score per residue for model 5

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 　　56%　　　　　　33%　　　8%　·

P1 S2 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 L27 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 M58 M59 L60 R61 L62 I63 G64 K65 V66 D67 E68 K71 V81 R86 F89 S90 F91 N92 N93 R94

T95 V96 M97 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 　26%　　　　　　　74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO VAL

4.2.6　Score per residue for model 6

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 　　52%　　　　　　36%　　　9%　·

P1 S2 H3 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 S23 L27 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 L48 Q49 A50 L60 R61 L62 V66 D67 E68 K71 R72 V81 M88 F89 S90 F91 N92 N93 R94

T95 V96 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 Y111 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26% 74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL
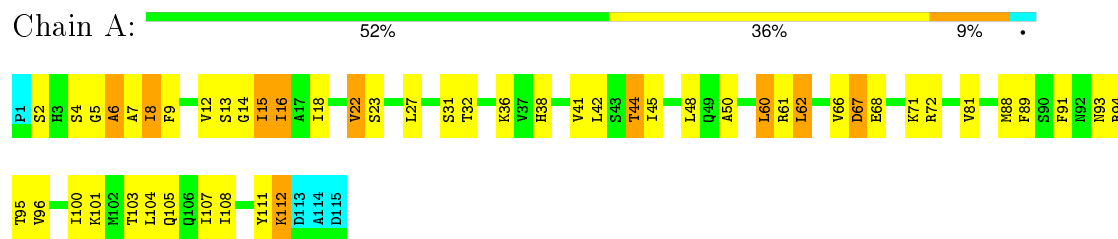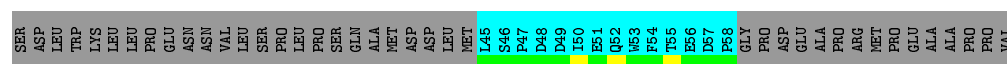
4.2.7 Score per residue for model 7

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 54% 35% 8% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 S23 L27 T28 W29 R30 S31 T32 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 M59 L62 I63 V66 D67 K70 K71 N78 Q85 R86 F89 S90

F91 T95 V96 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26% 74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL
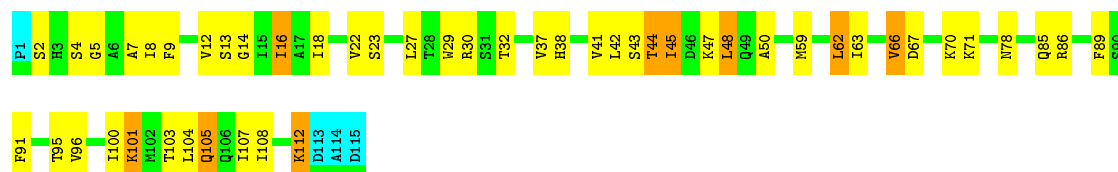
4.2.8 Score per residue for model 8
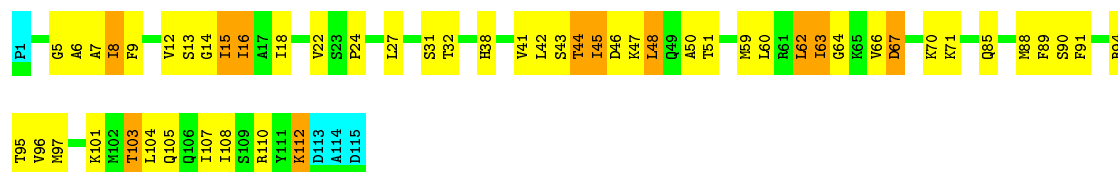
• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 50% 37% 10% •

P1 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 S23 P24 L27 S31 T32 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 M59 L60 R61 L62 I63 G64 K65 V66 D67 K70 K71 Q85 M88 F89 S90 F91 R94

T95 V96 M97 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26% 74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL
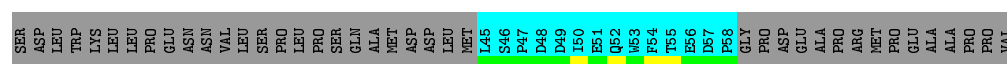
4.2.9 Score per residue for model 9

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 56% 33% 8% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 A25 E26 L27 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 M59 L60 R61 L62 I63 V66 D67 K71 F89 S90 F91 T95 I100

K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26% 74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO VAL

4.2.10 Score per residue for model 10

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 50% 37% 10% •

P1 S2 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 L27 R30 S31 T32 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 K57 M58 M59 L60 R61 L62 I63 G64 K65 V66 D67 K71 P82 K83

R86 F89 S90 F91 R94 T95 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26% 74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO VAL

4.2.11 Score per residue for model 11

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 53% 37% 6% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 L27 T28 W29 R30 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 M59 L60 R61 L62 I63 V66 D67 E68 K71 V81 Q85 M88

F89 S90 F91 T95 V96 M97 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26% 74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL

4.2.12 Score per residue for model 12

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 57% 32% 8% •

P1 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 S23 P24 L27 T28 W29 R30 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 M59 L60 R61 L62 I63 V66 D67 K71 K83 P84 M88 F89 S90 F91 T95

M102 T103 L104 Q105 Q106 I107 I108 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26% 74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL
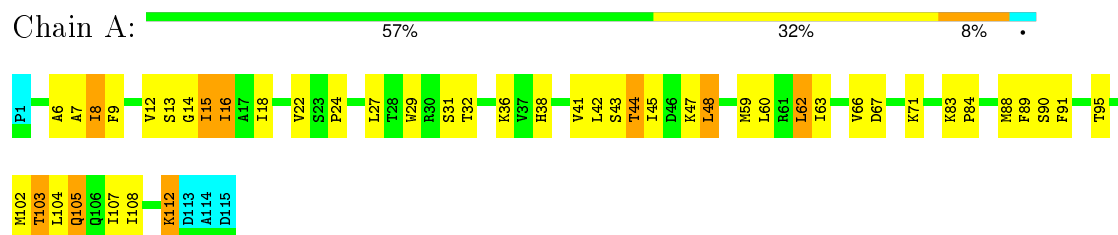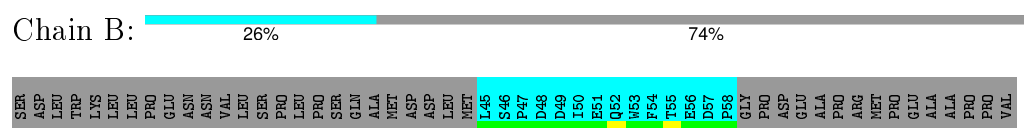
4.2.13 Score per residue for model 13

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 52% 31% 13% •

P1 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 A25 E26 L27 T28 W29 R30 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 T51 M58 M59 L60 R61 L62 I63 V66 D67 K70 K71 P82 K83 M88

F89 S90 F91 N92 N93 R94 T95 V96 M97 I100 K101 M102 T103 L104 I107 I108 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26% 74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL

4.2.14 Score per residue for model 14

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 58%   30%   9%   •

P1 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 N19 V22 L27 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 M59 L60 R61 L62 I63 V66 D67 E68 K71 R72 V81 P82 F89 S90 F91 T95

K101 M102 T103 L104 Q105 Q106 I107 I108 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26%   74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL

4.2.15   Score per residue for model 15

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 51%   32%   13%   •

P1 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 L27 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 K57 L60 R61 L62 I63 V66 D67 E68 K71 N78 V81 R86 F89 S90

F91 N92 N93 R94 T95 V96 M97 D98 N99 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26%   74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL

4.2.16   Score per residue for model 16

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 57%   34%   6%   •

P1 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 L27 T28 W29 R30 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 L60 R61 L62 I63 V66 D67 E68 R72 V81 F89 S90 F91 R94 T95

V96 M97 I100 T103 L104 Q105 Q106 I107 I108 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26%   74%

4.2.17 Score per residue for model 17

• Molecule 1: RNA polymerase II transcription factor B subunit 1
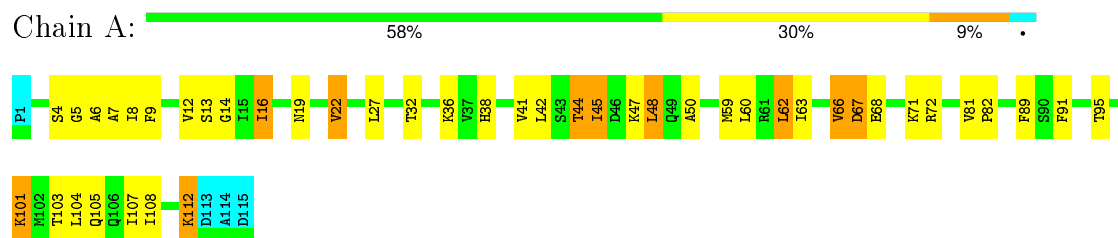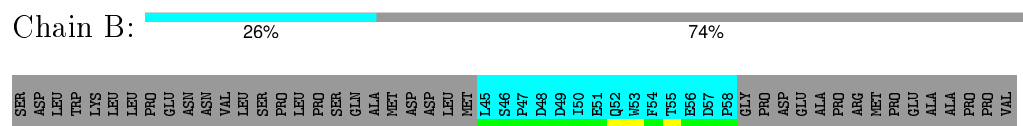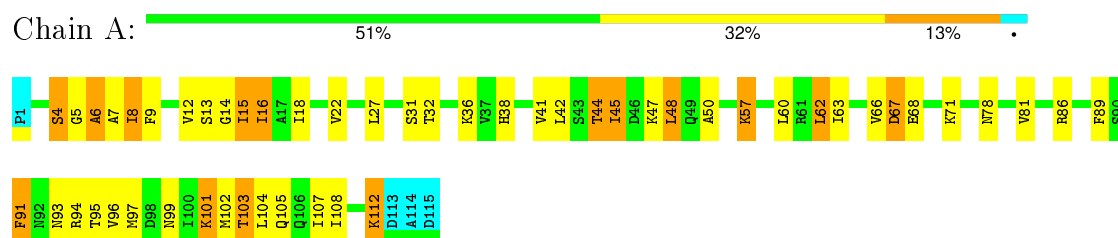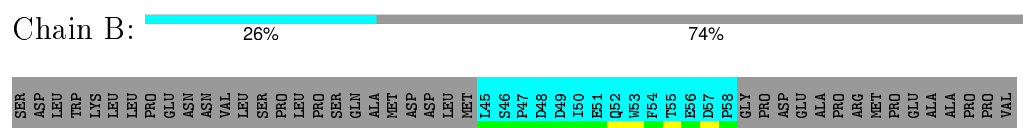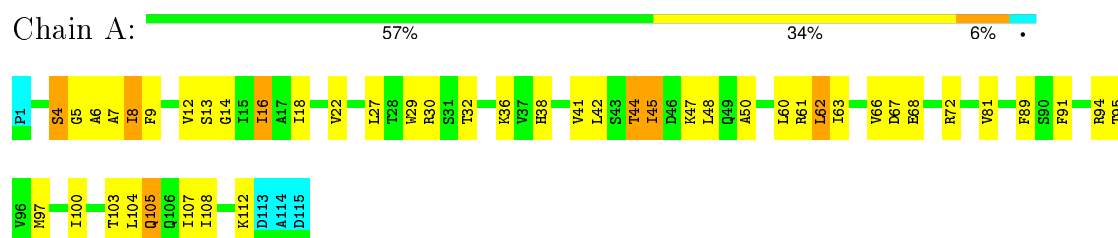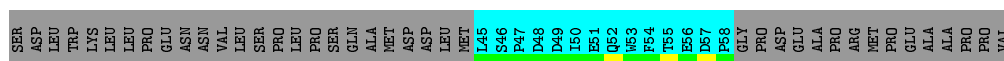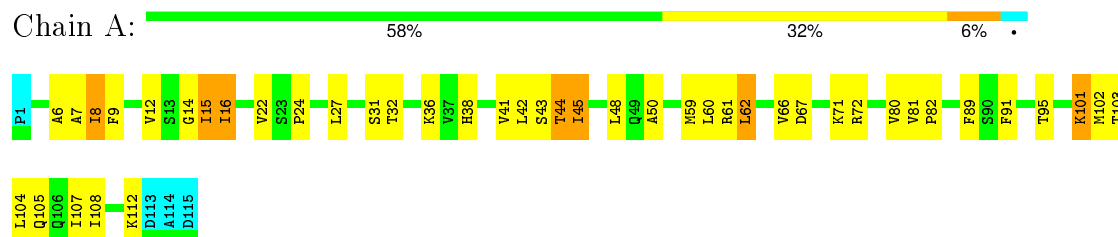
Chain A:

• Molecule 2: Cellular tumor antigen p53

Chain B:

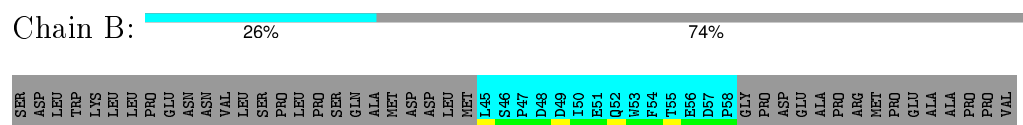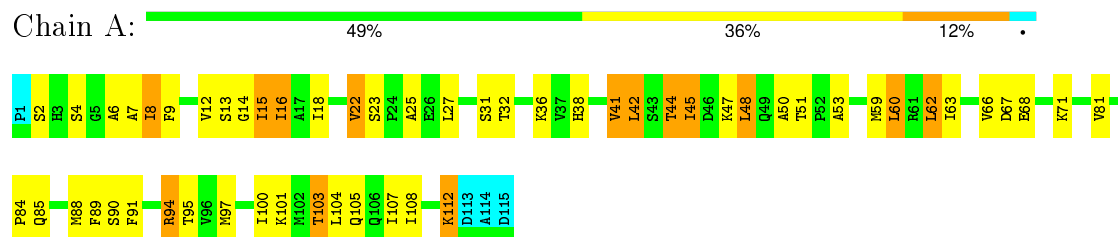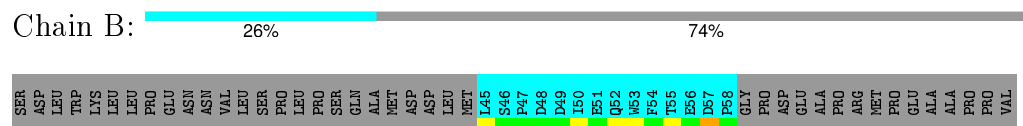## 4.2.18 Score per residue for model 18

• Molecule 1: RNA polymerase II transcription factor B subunit 1
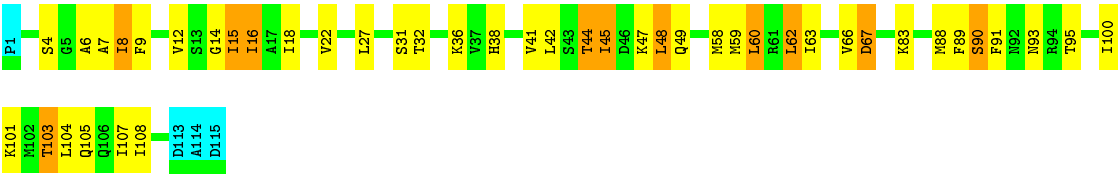
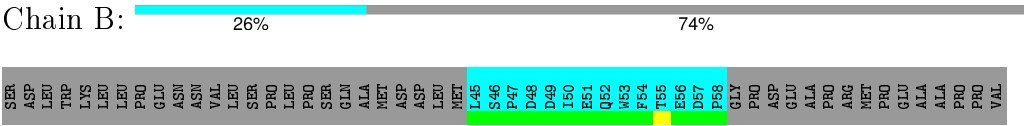Chain A:

• Molecule 2: Cellular tumor antigen p53

Chain B:

4.2.19 Score per residue for model 19 (medoid)

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A:

P1 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 V22 L27 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 D46 K47 L48 Q49 M58 M59 L60 R61 L62 I63 V66 D67 K83 M88 F89 S90 F91 N92 N93 R94 T95 I100

K101 M102 T103 L104 Q105 Q106 I107 I108 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26%   74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL

4.2.20   Score per residue for model 20

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 53%   31%   12%   •

P1 S2 H3 A6 A7 I8 F9 V12 S13 G14 I15 I16 V22 L27 T28 W29 R30 S31 T32 K36 V37 H38 V41 L42 S43 T44 I45 L48 Q49 A50 T51 K57 M58 M59 L60 R61 L62 I63 V66 D67 K71 N75 V80 V81 F89 S90 F91

T95 V96 M97 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 K112 D113 A114 D115

• Molecule 2: Cellular tumor antigen p53

Chain B: 26%   74%

SER ASP LEU TRP LYS LEU LEU PRO GLU ASN ASN VAL LEU SER PRO LEU PRO SER GLN ALA MET ASP ASP LEU MET L45 S46 P47 D48 D49 I50 E51 Q52 W53 F54 T55 E56 D57 P58 GLY PRO ASP GLU ALA PRO ARG MET PRO GLU ALA ALA PRO PRO VAL

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Simulated annealing, with a combination of torsion angle and Cartesian dynamics.*.

Of the 67 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	structure solution	1.0
CNS	refinement	1.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 6225
Number of chemical shift lists	1
Total number of shifts	1428
Number of shifts mapped to atoms	1395
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

No validations of the models with respect to experimental NMR restraints is performed at this time.

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	873	897	894	45±4
2	B	0	0	0	0±0
All	All	17460	17940	17880	899

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	Models Total
1:A:42:LEU:HD13	1:A:107:ILE:HD13	1.07	1.22	14	16
1:A:42:LEU:HD22	1:A:104:LEU:HD21	0.99	1.30	16	8
1:A:50:ALA:HB2	1:A:60:LEU:HD12	0.92	1.41	8	4
1:A:108:ILE:HG22	1:A:112:LYS:CD	0.83	2.04	8	10
1:A:42:LEU:HD22	1:A:104:LEU:CD2	0.81	2.03	20	14
1:A:42:LEU:CD1	1:A:107:ILE:HD13	0.79	2.08	2	15
1:A:42:LEU:HD13	1:A:107:ILE:CD1	0.79	2.03	12	13
1:A:27:LEU:CB	1:A:42:LEU:HD11	0.78	2.08	13	3
1:A:45:ILE:HD12	1:A:62:LEU:HB3	0.76	1.57	16	13
1:A:7:ALA:HB2	1:A:91:PHE:CE2	0.75	2.16	13	19
1:A:108:ILE:HG22	1:A:112:LYS:HD3	0.74	1.59	15	10
1:A:27:LEU:HB2	1:A:42:LEU:HD11	0.73	1.60	13	3
1:A:53:ALA:HB2	1:A:94:ARG:NH1	0.70	2.00	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD12	1:A:105:GLN:HG3	0.70	1.62	10	2
1:A:45:ILE:HG23	1:A:62:LEU:HB2	0.70	1.62	10	1
1:A:41:VAL:HG13	1:A:44:THR:CG2	0.69	2.17	17	16
1:A:18:ILE:HG23	1:A:42:LEU:HD11	0.69	1.65	6	9
1:A:7:ALA:HB2	1:A:91:PHE:CZ	0.69	2.22	1	5
1:A:49:GLN:O	1:A:60:LEU:HD23	0.69	1.87	11	4
1:A:16:ILE:HG12	1:A:27:LEU:HD21	0.68	1.65	6	19
1:A:108:ILE:HG22	1:A:112:LYS:HD2	0.68	1.65	14	5
1:A:60:LEU:HD11	1:A:101:LYS:HB3	0.68	1.64	20	1
1:A:47:LYS:HB2	1:A:63:ILE:CG1	0.67	2.19	12	12
1:A:16:ILE:HD11	1:A:89:PHE:CD2	0.67	2.25	11	8
1:A:48:LEU:HD11	1:A:104:LEU:HB3	0.66	1.67	9	6
1:A:30:ARG:HD2	1:A:37:VAL:HG22	0.66	1.65	2	1
1:A:50:ALA:HB2	1:A:60:LEU:CD1	0.65	2.21	4	5
1:A:18:ILE:HD12	1:A:103:THR:CG2	0.64	2.21	8	8
1:A:27:LEU:HB2	1:A:42:LEU:HD21	0.64	1.70	16	5
1:A:48:LEU:HD21	1:A:104:LEU:HB3	0.64	1.68	16	2
1:A:63:ILE:N	1:A:63:ILE:HD13	0.64	2.08	10	2
1:A:16:ILE:HD11	1:A:89:PHE:CD1	0.62	2.29	16	7
1:A:42:LEU:N	1:A:42:LEU:HD13	0.62	2.10	9	2
1:A:25:ALA:O	1:A:42:LEU:HD22	0.61	1.93	13	3
1:A:66:VAL:HG13	1:A:67:ASP:N	0.61	2.11	20	18
1:A:105:GLN:HA	1:A:108:ILE:HD12	0.61	1.71	2	18
1:A:50:ALA:HB3	1:A:101:LYS:NZ	0.60	2.11	7	3
1:A:16:ILE:HD11	1:A:89:PHE:CE2	0.60	2.31	9	7
1:A:104:LEU:HA	1:A:107:ILE:HD12	0.60	1.72	4	15
1:A:66:VAL:HG22	1:A:67:ASP:H	0.60	1.56	18	18
1:A:45:ILE:HG23	1:A:62:LEU:CB	0.60	2.27	10	1
1:A:50:ALA:HB1	1:A:97:MET:HE3	0.60	1.72	8	1
1:A:18:ILE:HG23	1:A:42:LEU:CD1	0.60	2.27	1	2
1:A:48:LEU:CD1	1:A:60:LEU:HD21	0.59	2.27	19	1
1:A:8:ILE:HG23	1:A:12:VAL:O	0.59	1.98	1	14
1:A:51:THR:HG23	1:A:59:MET:O	0.59	1.98	11	3
1:A:16:ILE:HD11	1:A:89:PHE:CE1	0.58	2.32	19	6
1:A:50:ALA:CB	1:A:60:LEU:HD12	0.58	2.27	16	4
1:A:42:LEU:HD13	1:A:42:LEU:N	0.58	2.14	13	1
1:A:40:VAL:CG1	1:A:45:ILE:HD11	0.58	2.29	10	1
1:A:60:LEU:HD11	1:A:101:LYS:HB2	0.58	1.75	6	2
1:A:41:VAL:HB	1:A:44:THR:HG23	0.57	1.77	10	2
1:A:4:SER:HA	1:A:16:ILE:O	0.57	2.00	7	14
1:A:41:VAL:HG13	1:A:44:THR:HG23	0.56	1.75	6	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LEU:H	1:A:42:LEU:HD22	0.56	1.59	13	2
1:A:48:LEU:HD23	1:A:105:GLN:HG2	0.56	1.78	14	4
1:A:42:LEU:HD23	1:A:107:ILE:HD13	0.56	1.78	9	2
1:A:42:LEU:HD22	1:A:42:LEU:H	0.56	1.61	18	1
1:A:48:LEU:HD13	1:A:101:LYS:O	0.56	2.01	10	1
1:A:48:LEU:HD11	1:A:104:LEU:CB	0.55	2.32	17	6
1:A:48:LEU:HD12	1:A:105:GLN:CG	0.55	2.31	10	1
1:A:68:GLU:HB3	1:A:81:VAL:HG23	0.54	1.78	6	1
1:A:7:ALA:CB	1:A:16:ILE:HD12	0.54	2.32	5	8
1:A:27:LEU:HD23	1:A:27:LEU:C	0.54	2.23	10	13
1:A:42:LEU:CD2	1:A:104:LEU:HD21	0.54	2.20	16	2
1:A:66:VAL:HG11	1:A:68:GLU:OE2	0.53	2.02	2	1
1:A:62:LEU:C	1:A:63:ILE:HD13	0.53	2.23	10	3
1:A:48:LEU:HD21	1:A:104:LEU:HD13	0.53	1.81	13	2
1:A:60:LEU:HD23	1:A:62:LEU:HD11	0.53	1.80	9	1
1:A:68:GLU:OE2	1:A:81:VAL:HG12	0.53	2.04	14	1
1:A:50:ALA:HB3	1:A:101:LYS:HE2	0.52	1.81	1	2
1:A:41:VAL:CG1	1:A:44:THR:CG2	0.52	2.87	6	18
1:A:40:VAL:HG11	1:A:45:ILE:HD11	0.52	1.80	10	1
1:A:27:LEU:C	1:A:27:LEU:HD23	0.52	2.25	7	7
1:A:9:PHE:CE2	1:A:38:HIS:CG	0.52	2.98	19	19
1:A:91:PHE:N	1:A:91:PHE:CD1	0.51	2.78	13	8
1:A:91:PHE:CD1	1:A:91:PHE:N	0.51	2.78	15	5
1:A:47:LYS:CE	1:A:63:ILE:HD13	0.51	2.35	5	1
1:A:48:LEU:HD11	1:A:101:LYS:CG	0.51	2.36	7	2
1:A:9:PHE:CD1	1:A:89:PHE:CE2	0.51	2.99	11	10
1:A:16:ILE:CG2	1:A:100:ILE:HD12	0.51	2.35	10	14
1:A:41:VAL:HG22	1:A:44:THR:HG23	0.50	1.82	20	14
1:A:50:ALA:HB3	1:A:101:LYS:HD3	0.50	1.81	8	1
1:A:27:LEU:HB3	1:A:42:LEU:HD11	0.50	1.79	13	1
1:A:15:ILE:N	1:A:15:ILE:CD1	0.50	2.74	6	9
1:A:22:VAL:CG2	1:A:23:SER:N	0.50	2.75	6	2
1:A:9:PHE:CD1	1:A:89:PHE:CE1	0.50	3.00	3	10
1:A:18:ILE:HD12	1:A:103:THR:HG22	0.50	1.82	8	1
1:A:100:ILE:HG22	1:A:104:LEU:HD12	0.50	1.82	4	3
1:A:9:PHE:CZ	1:A:38:HIS:CD2	0.50	3.00	12	19
1:A:62:LEU:CD1	1:A:62:LEU:N	0.49	2.75	16	11
1:A:68:GLU:OE1	1:A:81:VAL:HG12	0.49	2.07	5	1
1:A:18:ILE:CG1	1:A:27:LEU:HD12	0.49	2.38	16	10
1:A:93:ASN:ND2	1:A:96:VAL:HG23	0.49	2.22	15	1
1:A:15:ILE:N	1:A:15:ILE:HD13	0.49	2.23	6	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:15:ILE:CD1	1:A:15:ILE:N	0.49	2.75	3	5
1:A:66:VAL:CG2	1:A:67:ASP:N	0.49	2.75	13	2
1:A:47:LYS:HB2	1:A:63:ILE:HG13	0.49	1.85	8	9
1:A:41:VAL:HG13	1:A:44:THR:HG21	0.49	1.83	6	3
1:A:50:ALA:HB1	1:A:97:MET:HE1	0.48	1.85	20	1
1:A:50:ALA:HB1	1:A:97:MET:CE	0.48	2.38	3	2
1:A:15:ILE:HD13	1:A:15:ILE:N	0.48	2.23	3	7
1:A:48:LEU:HD11	1:A:105:GLN:CA	0.48	2.38	16	1
1:A:48:LEU:HD11	1:A:105:GLN:N	0.48	2.22	16	1
1:A:68:GLU:CB	1:A:81:VAL:HG23	0.48	2.38	6	1
1:A:9:PHE:N	1:A:12:VAL:O	0.48	2.47	14	8
1:A:81:VAL:O	1:A:81:VAL:HG13	0.48	2.08	20	2
1:A:48:LEU:HD12	1:A:60:LEU:HD21	0.48	1.86	19	1
1:A:42:LEU:HD12	1:A:104:LEU:HD21	0.48	1.84	18	2
1:A:108:ILE:HG22	1:A:112:LYS:CE	0.48	2.39	12	4
1:A:7:ALA:O	1:A:14:GLY:O	0.48	2.32	1	20
1:A:45:ILE:CG2	1:A:62:LEU:CB	0.47	2.92	10	1
1:A:48:LEU:HD22	1:A:105:GLN:N	0.47	2.25	12	1
1:A:63:ILE:HD12	1:A:86:ARG:HG2	0.47	1.85	10	1
1:A:62:LEU:N	1:A:62:LEU:CD1	0.47	2.78	18	8
1:A:12:VAL:HG21	1:A:36:LYS:NZ	0.47	2.25	11	3
1:A:107:ILE:CG2	1:A:111:TYR:CE2	0.46	2.98	3	3
1:A:80:VAL:HG12	1:A:81:VAL:N	0.46	2.25	17	1
1:A:68:GLU:HB3	1:A:81:VAL:HG13	0.46	1.88	16	1
1:A:30:ARG:HG3	1:A:37:VAL:HG22	0.46	1.87	7	1
1:A:9:PHE:CB	1:A:29:TRP:CD2	0.46	2.98	7	6
1:A:107:ILE:HG22	1:A:111:TYR:CE2	0.46	2.45	3	2
1:A:7:ALA:N	1:A:14:GLY:O	0.46	2.48	7	6
1:A:63:ILE:CG1	1:A:86:ARG:HG2	0.46	2.41	5	1
1:A:5:GLY:CA	1:A:96:VAL:HG13	0.46	2.39	3	1
1:A:7:ALA:CB	1:A:91:PHE:CZ	0.46	2.98	1	1
1:A:42:LEU:HD22	1:A:104:LEU:HD22	0.46	1.87	10	1
1:A:58:MET:HE2	1:A:92:ASN:CA	0.46	2.41	5	1
1:A:42:LEU:HA	1:A:45:ILE:HG12	0.46	1.88	13	2
1:A:2:SER:HG	1:A:3:HIS:CE1	0.46	2.27	20	1
1:A:46:ASP:N	1:A:63:ILE:O	0.46	2.49	4	4
1:A:68:GLU:CG	1:A:81:VAL:HG13	0.46	2.41	18	1
1:A:41:VAL:CG1	1:A:44:THR:HG23	0.46	2.41	12	2
1:A:7:ALA:CB	1:A:91:PHE:CE2	0.46	2.95	13	7
1:A:48:LEU:CD1	1:A:105:GLN:CB	0.45	2.95	16	1
1:A:42:LEU:HB2	1:A:107:ILE:HG21	0.45	1.88	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD23	1:A:105:GLN:HG3	0.45	1.88	2	2
1:A:48:LEU:CD2	1:A:105:GLN:CB	0.45	2.95	12	1
1:A:66:VAL:CG1	1:A:67:ASP:N	0.45	2.80	16	8
1:A:50:ALA:HB3	1:A:101:LYS:CE	0.44	2.42	14	2
1:A:48:LEU:HD21	1:A:104:LEU:CB	0.44	2.41	16	1
1:A:48:LEU:CD2	1:A:104:LEU:HD13	0.44	2.42	1	1
1:A:66:VAL:HG22	1:A:67:ASP:N	0.44	2.27	17	2
1:A:42:LEU:N	1:A:42:LEU:CD1	0.44	2.79	9	2
1:A:48:LEU:HD21	1:A:105:GLN:HG3	0.44	1.90	8	1
1:A:66:VAL:HG21	1:A:84:PRO:HD3	0.44	1.90	12	1
1:A:58:MET:HE2	1:A:92:ASN:HA	0.44	1.89	5	1
1:A:18:ILE:CG2	1:A:42:LEU:HD11	0.44	2.41	6	1
1:A:45:ILE:O	1:A:108:ILE:HG23	0.43	2.13	17	1
1:A:6:ALA:HA	1:A:15:ILE:HA	0.43	1.90	1	13
1:A:44:THR:O	1:A:65:LYS:N	0.43	2.50	10	1
1:A:47:LYS:CB	1:A:63:ILE:CG1	0.43	2.96	7	3
1:A:18:ILE:HD12	1:A:103:THR:HG21	0.43	1.89	8	2
1:A:12:VAL:CG1	1:A:13:SER:N	0.43	2.81	1	11
1:A:16:ILE:O	1:A:16:ILE:HG22	0.43	2.14	1	9
1:A:24:PRO:HB2	1:A:43:SER:CB	0.43	2.44	2	3
1:A:8:ILE:HG13	1:A:13:SER:HA	0.43	1.90	14	5
1:A:6:ALA:HA	1:A:15:ILE:HD12	0.43	1.90	1	4
1:A:80:VAL:CG2	1:A:81:VAL:N	0.43	2.82	20	1
1:A:5:GLY:O	1:A:6:ALA:C	0.42	2.57	4	4
1:A:48:LEU:HD11	1:A:101:LYS:HB2	0.42	1.90	18	2
1:A:16:ILE:CD1	1:A:89:PHE:CD1	0.42	3.01	13	1
1:A:53:ALA:HB2	1:A:94:ARG:HE	0.42	1.74	18	1
1:A:16:ILE:HG22	1:A:16:ILE:O	0.42	2.14	13	6
1:A:72:ARG:O	1:A:80:VAL:N	0.42	2.49	17	1
1:A:93:ASN:HB2	1:A:96:VAL:HG23	0.42	1.91	6	2
1:A:19:ASN:ND2	1:A:22:VAL:HG21	0.42	2.30	14	1
1:A:51:THR:HG22	1:A:57:LYS:CE	0.42	2.45	20	1
1:A:49:GLN:N	1:A:61:ARG:O	0.42	2.52	10	1
1:A:58:MET:HE1	1:A:92:ASN:O	0.42	2.14	13	1
1:A:47:LYS:HB2	1:A:63:ILE:HG12	0.42	1.91	10	1
1:A:63:ILE:CD1	1:A:63:ILE:N	0.41	2.78	10	1
1:A:18:ILE:CD1	1:A:103:THR:CG2	0.41	2.98	9	6
1:A:16:ILE:CD1	1:A:89:PHE:CD2	0.41	3.03	6	1
1:A:48:LEU:HD11	1:A:101:LYS:CB	0.41	2.45	18	1
1:A:66:VAL:HG23	1:A:84:PRO:HA	0.41	1.91	4	1
1:A:5:GLY:CA	1:A:96:VAL:CG1	0.41	2.98	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:PHE:CD1	1:A:97:MET:HG3	0.41	2.50	15	1
1:A:50:ALA:CB	1:A:60:LEU:CD1	0.41	2.99	18	1
1:A:41:VAL:HG13	1:A:41:VAL:O	0.41	2.15	12	1
1:A:63:ILE:HD13	1:A:63:ILE:N	0.41	2.31	2	1
1:A:48:LEU:CD2	1:A:105:GLN:CA	0.41	2.98	12	1
1:A:48:LEU:HD11	1:A:101:LYS:HG2	0.41	1.91	7	1
1:A:60:LEU:HB2	1:A:91:PHE:CE1	0.41	2.51	10	2
1:A:9:PHE:HB3	1:A:29:TRP:CH2	0.41	2.50	13	1
1:A:19:ASN:ND2	1:A:22:VAL:CG2	0.41	2.84	14	1
1:A:62:LEU:HD22	1:A:89:PHE:CE2	0.41	2.51	15	1
1:A:27:LEU:CB	1:A:42:LEU:HD21	0.41	2.41	16	1
1:A:24:PRO:CB	1:A:43:SER:CB	0.41	2.99	1	3
1:A:68:GLU:OE2	1:A:81:VAL:HG11	0.41	2.15	11	1
1:A:44:THR:O	1:A:46:ASP:N	0.41	2.54	8	1
1:A:9:PHE:HB3	1:A:29:TRP:CZ3	0.40	2.51	13	2
1:A:58:MET:CE	1:A:93:ASN:N	0.40	2.83	19	1
1:A:48:LEU:HD21	1:A:101:LYS:O	0.40	2.17	2	2
1:A:68:GLU:OE2	1:A:81:VAL:HG21	0.40	2.16	15	1
1:A:14:GLY:C	1:A:15:ILE:HD13	0.40	2.36	5	1
1:A:8:ILE:N	1:A:90:SER:O	0.40	2.52	19	1
1:A:43:SER:CB	1:A:111:TYR:CE2	0.40	3.04	9	1
1:A:51:THR:CG2	1:A:57:LYS:CE	0.40	2.99	20	1
1:A:41:VAL:CG2	1:A:44:THR:HG23	0.40	2.47	12	1
1:A:50:ALA:CB	1:A:101:LYS:CE	0.40	2.99	1	1
1:A:61:ARG:NH2	1:A:86:ARG:NE	0.40	2.70	5	1
1:A:108:ILE:O	1:A:112:LYS:N	0.40	2.54	7	1
1:A:42:LEU:CB	1:A:107:ILE:HG21	0.40	2.46	20	1
1:A:49:GLN:O	1:A:61:ARG:N	0.40	2.52	5	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	111/115 (97%)	99±1 (90±1%)	7±1 (6±1%)	5±1 (4±1%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	0	-	-	-	-	
All	All	2220/3380 (66%)	1989 (90%)	140 (6%)	91 (4%)	6	33

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	45	ILE	20
1	A	71	LYS	18
1	A	31	SER	15
1	A	67	ASP	11
1	A	2	SER	11
1	A	6	ALA	6
1	A	82	PRO	4
1	A	4	SER	2
1	A	66	VAL	2
1	A	64	GLY	1
1	A	78	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	100/103 (97%)	83±2 (83±2%)	17±2 (17±2%)	6	42
2	B	0	-	-	-	
All	All	2000/3040 (66%)	1663 (83%)	337 (17%)	6	42

All 49 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	44	THR	20
1	A	22	VAL	20
1	A	103	THR	20
1	A	32	THR	20
1	A	62	LEU	20
1	A	95	THR	20

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Mol	Chain	Res	Type	Models (Total)
1	A	16	ILE	20
1	A	8	ILE	15
1	A	36	LYS	14
1	A	15	ILE	14
1	A	112	LYS	12
1	A	60	LEU	11
1	A	101	LYS	11
1	A	48	LEU	10
1	A	97	MET	8
1	A	94	ARG	8
1	A	59	MET	8
1	A	90	SER	7
1	A	102	MET	6
1	A	83	LYS	5
1	A	61	ARG	5
1	A	105	GLN	5
1	A	85	GLN	4
1	A	63	ILE	4
1	A	30	ARG	4
1	A	57	LYS	4
1	A	110	ARG	4
1	A	88	MET	4
1	A	70	LYS	3
1	A	41	VAL	3
1	A	72	ARG	3
1	A	42	LEU	3
1	A	67	ASP	2
1	A	47	LYS	2
1	A	86	ARG	2
1	A	71	LYS	2
1	A	91	PHE	2
1	A	13	SER	1
1	A	84	PRO	1
1	A	65	LYS	1
1	A	4	SER	1
1	A	75	ASN	1
1	A	31	SER	1
1	A	80	VAL	1
1	A	78	ASN	1
1	A	2	SER	1
1	A	23	SER	1
1	A	66	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	43	SER	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 carbohydrates 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)

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 78% for the entire structure.

7.1   Chemical shift list 1

File name: BMRB entry 6225

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1   Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1428
Number of shifts mapped to atoms	1395
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 33 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	118	SER	HA	4.52	0.02	1
A	116	GLY	HA3	3.95	0.02	1
A	117	ASN	CG	177.2	0.35	1
A	118	SER	HB3	3.87	0.02	1
A	117	ASN	CA	53.59	0.35	1
A	117	ASN	H	8.32	0.02	1
A	119	SER	HB3	3.82	0.02	1
A	118	SER	H	8.32	0.02	1
A	119	SER	H	8.01	0.02	1
A	118	SER	C	173.73	0.35	1
A	117	ASN	ND2	113.51	0.1	1
A	116	GLY	C	174.3	0.35	1
A	119	SER	N	123.3	0.1	1
A	116	GLY	HA2	3.95	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	117	ASN	HD22	6.93	0.02	2
A	118	SER	HB2	3.9	0.02	1
A	117	ASN	HD21	7.64	0.02	2
A	119	SER	HA	4.27	0.02	1
A	116	GLY	N	108.95	0.1	1
A	117	ASN	HA	4.8	0.02	1
A	116	GLY	CA	45.6	0.35	1
A	117	ASN	CB	39.31	0.35	1
A	117	ASN	HB3	2.77	0.02	2
A	119	SER	CA	60.1	0.35	1
A	117	ASN	C	175.29	0.35	1
A	118	SER	CB	64.06	0.35	1
A	117	ASN	N	118.82	0.1	1
A	119	SER	CB	64.84	0.35	1
A	119	SER	HB2	3.82	0.02	1
A	116	GLY	H	8.24	0.02	1
A	118	SER	N	116.65	0.1	1
A	117	ASN	HB2	2.84	0.02	2
A	118	SER	CA	58.5	0.35	1

7.1.2　Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, *ppm*	Suggested action
$^{13}C_\alpha$	115	-0.30 $\pm$ 0.07	None needed ($<$ 0.5 ppm)
$^{13}C_\beta$	109	-0.21 $\pm$ 0.11	None needed ($<$ 0.5 ppm)
$^{13}C'$	108	0.19 $\pm$ 0.11	None needed ($<$ 0.5 ppm)
^{15}N	109	-0.25 $\pm$ 0.28	None needed ($<$ 0.5 ppm)

7.1.3　Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1215 atoms were assigned a chemical shift out of a possible 1390. 5 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	519/547 (95%)	208/218 (95%)	209/222 (94%)	102/107 (95%)
Sidechain	646/772 (84%)	395/453 (87%)	238/280 (85%)	13/39 (33%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	50/71 (70%)	31/37 (84%)	18/27 (67%)	1/7 (14%)
Overall	1215/1390 (87%)	634/708 (90%)	465/529 (88%)	116/153 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1249 atoms were assigned a chemical shift out of a possible 1599. 5 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	536/631 (85%)	215/251 (86%)	216/258 (84%)	105/122 (86%)
Sidechain	663/876 (76%)	406/514 (79%)	244/322 (76%)	13/40 (32%)
Aromatic	50/92 (54%)	31/48 (65%)	18/36 (50%)	1/8 (12%)
Overall	1249/1599 (78%)	652/813 (80%)	478/616 (78%)	119/170 (70%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	110	ARG	NE	111.09	92.63 − 76.73	16.6
1	A	30	ARG	NE	111.05	92.63 − 76.73	16.6
1	A	94	ARG	NE	110.01	92.63 − 76.73	15.9
1	A	10	GLU	HG3	0.75	3.31 − 1.21	-7.2
1	A	9	PHE	HB3	0.30	4.85 − 1.05	-7.0
1	A	10	GLU	HG2	0.84	3.33 − 1.23	-6.9
1	A	9	PHE	HB2	1.08	4.85 − 1.15	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: