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Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:27 am BST

PDB ID	:	2N9P
Title	:	Solution structure of RNF126 N-terminal zinc finger domain in complex with BAG6 Ubiquitin-like domain
Authors	:	Martinez-Lumbreras, S.; Krysztofinska, E.M.; Thapaliya, A.; Isaacson, R.L.
Deposited on	:	2015-12-01

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 ⓘ symbol.

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

|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
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	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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		27
Ramachandran outliers		4.7%
Sidechain outliers		15.1%

Worse ... *Better*

■ Percentile relative to all structures
▯ Percentile relative to all NMR structures
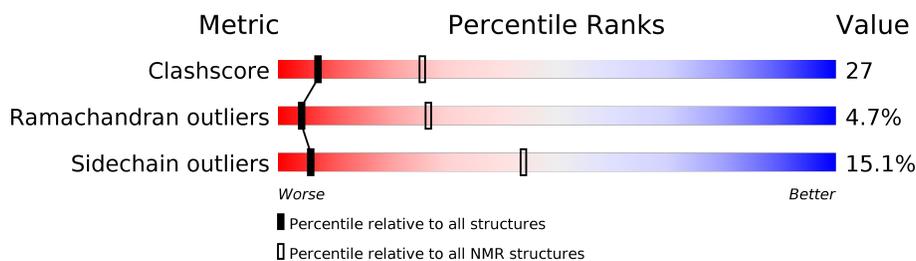
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	42	31% · 36% · 7% · 26%
2	C	100	30% · 31% · · · 34%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 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:40, C:16-C:23, C:28-C:85 (97)	0.35	10

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 5 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2220 atoms, of which 1101 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase RNF126.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	42	630	204	304	55	61	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q9BV68
A	0	SER	-	EXPRESSION TAG	UNP Q9BV68

- Molecule 2 is a protein called Large proline-rich protein BAG6.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	C	100	1589	493	797	147	149	3	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	MET	-	EXPRESSION TAG	UNP P46379
C	3	ALA	-	EXPRESSION TAG	UNP P46379
C	4	HIS	-	EXPRESSION TAG	UNP P46379
C	5	HIS	-	EXPRESSION TAG	UNP P46379
C	6	HIS	-	EXPRESSION TAG	UNP P46379
C	7	HIS	-	EXPRESSION TAG	UNP P46379
C	8	HIS	-	EXPRESSION TAG	UNP P46379
C	9	HIS	-	EXPRESSION TAG	UNP P46379
C	10	VAL	-	EXPRESSION TAG	UNP P46379
C	11	ASP	-	EXPRESSION TAG	UNP P46379
C	12	ASP	-	EXPRESSION TAG	UNP P46379
C	13	ASP	-	EXPRESSION TAG	UNP P46379
C	14	ASP	-	EXPRESSION TAG	UNP P46379
C	15	LYS	-	EXPRESSION TAG	UNP P46379
C	16	MET	-	EXPRESSION TAG	UNP P46379

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	1	1	1

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: E3 ubiquitin-protein ligase RNF126
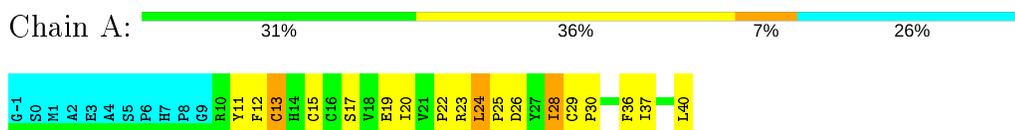
- Molecule 2: Large proline-rich protein BAG6
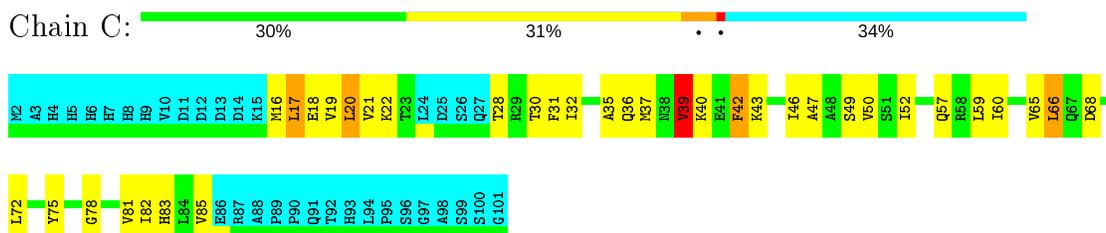
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: E3 ubiquitin-protein ligase RNF126
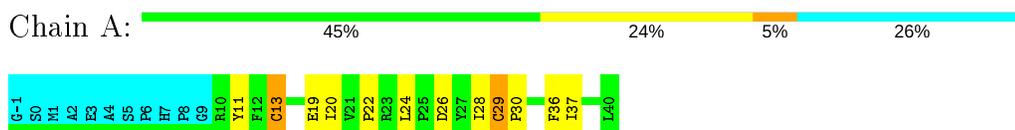
- Molecule 2: Large proline-rich protein BAG6
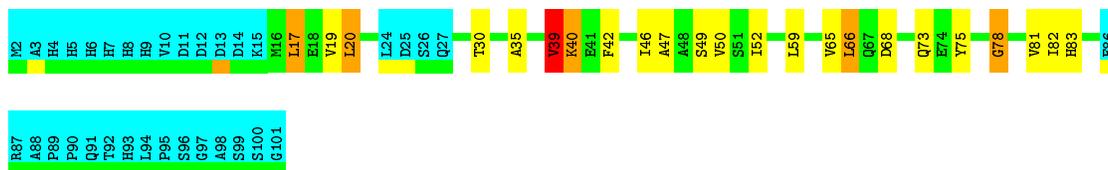
4.2.2 Score per residue for model 2

• Molecule 1: E3 ubiquitin-protein ligase RNF126
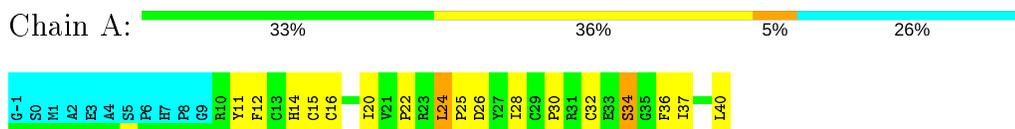

• Molecule 2: Large proline-rich protein BAG6
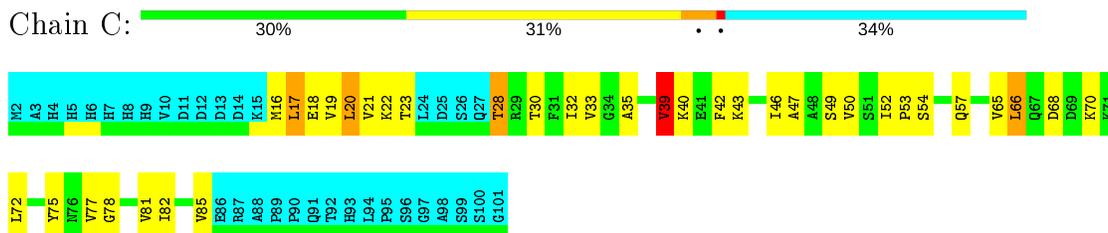
4.2.3 Score per residue for model 3

• Molecule 1: E3 ubiquitin-protein ligase RNF126
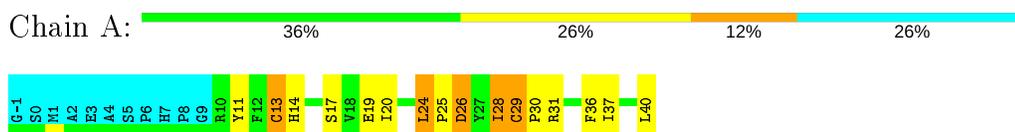
• Molecule 2: Large proline-rich protein BAG6
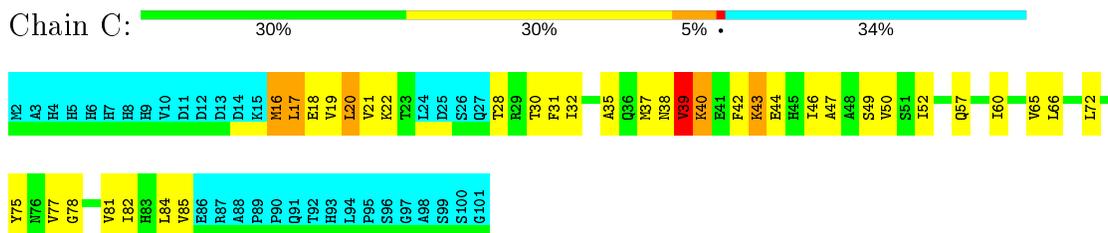
4.2.4 Score per residue for model 4

• Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A: 38%   29%   7%   26%

- Molecule 2: Large proline-rich protein BAG6

Chain C: 34%   24%   7%   34%
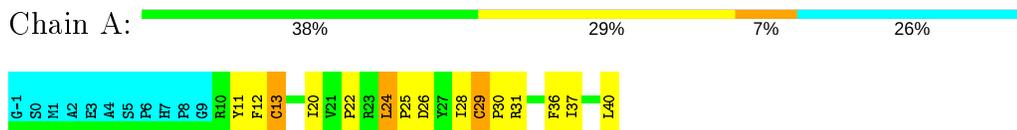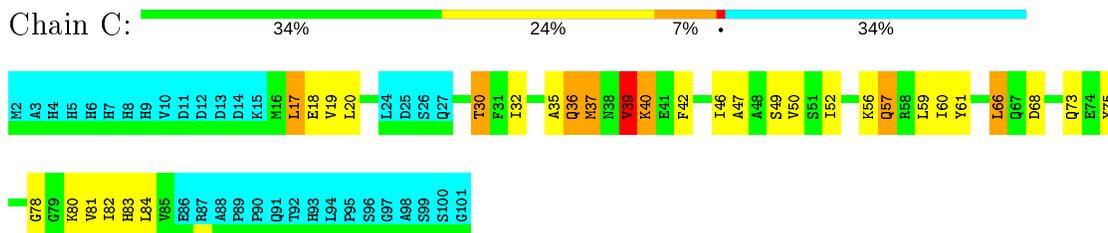
4.2.5 Score per residue for model 5

- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A: 33%   24%   17%   26%

- Molecule 2: Large proline-rich protein BAG6

Chain C: 28%   33%   34%
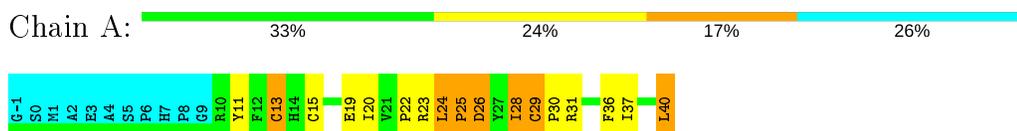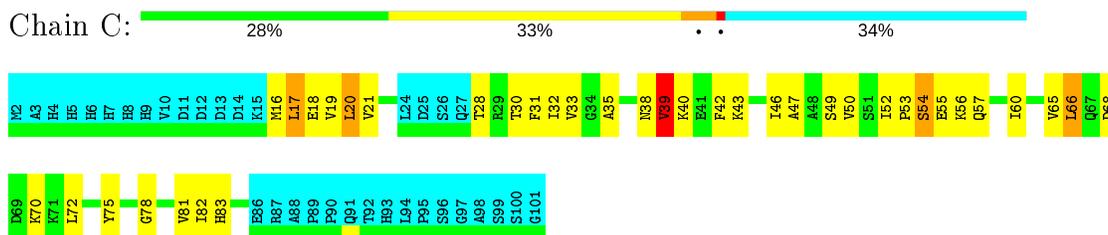
4.2.6 Score per residue for model 6

- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A: 36%   29%   10%   26%

- Molecule 2: Large proline-rich protein BAG6

Chain C: 32%   29%   34%
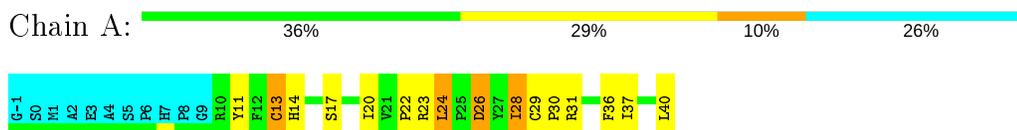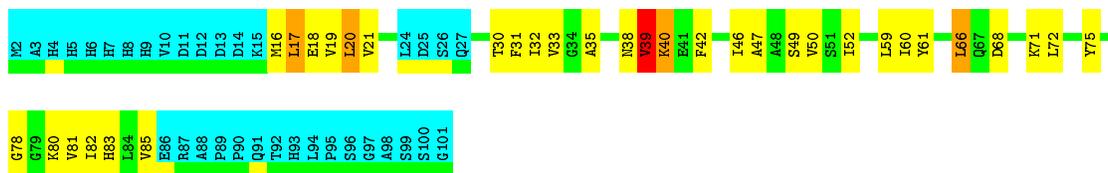
4.2.7 Score per residue for model 7

• Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

• Molecule 2: Large proline-rich protein BAG6

Chain C:
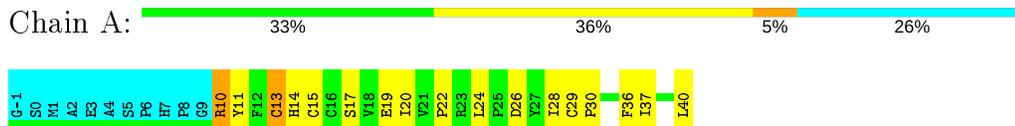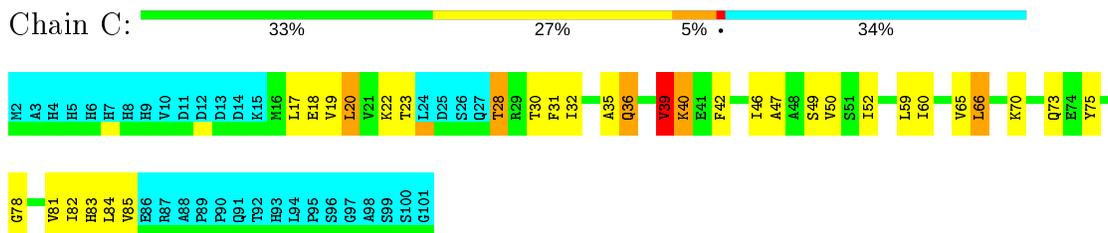
4.2.8 Score per residue for model 8

• Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

• Molecule 2: Large proline-rich protein BAG6

Chain C:
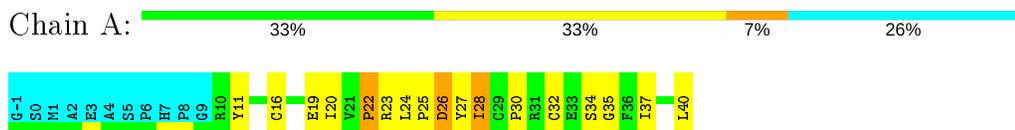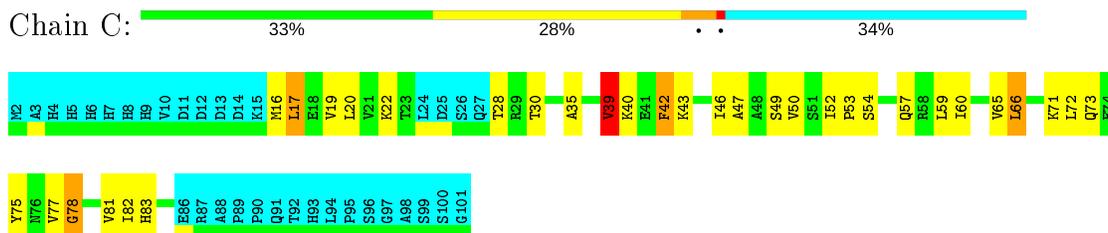
4.2.9 Score per residue for model 9

• Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

- Molecule 2: Large proline-rich protein BAG6

Chain C:
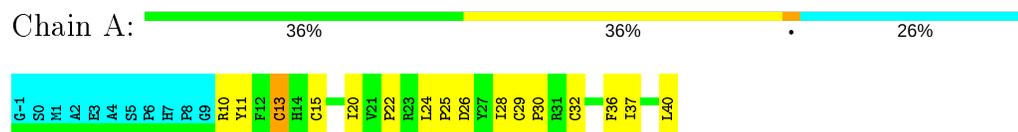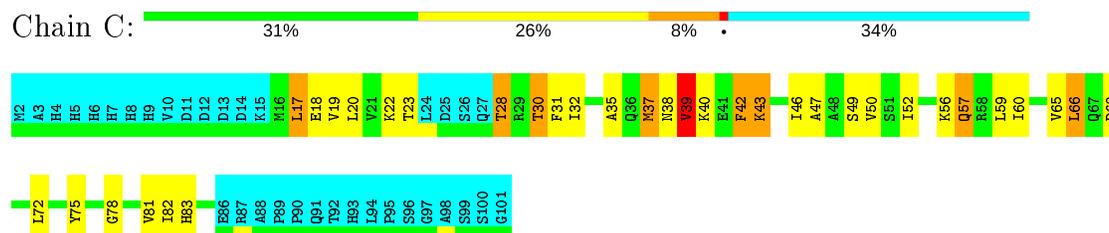
4.2.10　Score per residue for model 10 (medoid)

- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

- Molecule 2: Large proline-rich protein BAG6

Chain C:
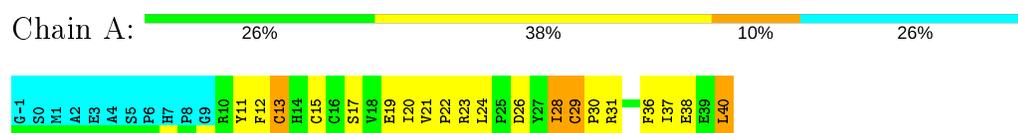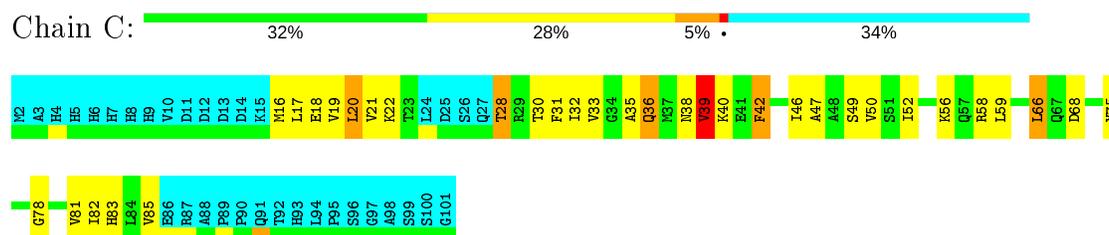
4.2.11　Score per residue for model 11

- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

- Molecule 2: Large proline-rich protein BAG6

Chain C:
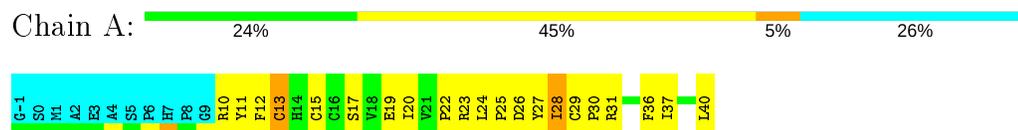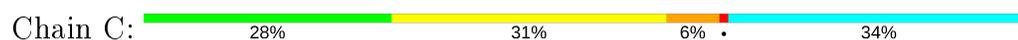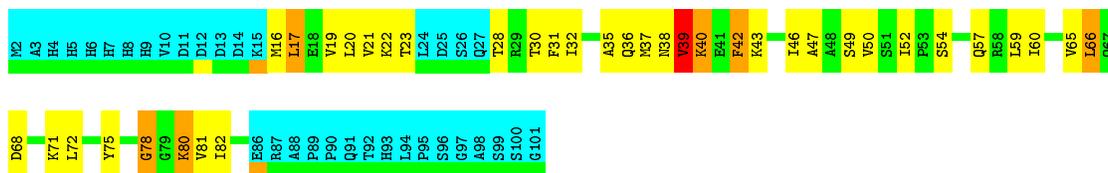
4.2.12 Score per residue for model 12

• Molecule 1: E3 ubiquitin-protein ligase RNF126

• Molecule 2: Large proline-rich protein BAG6
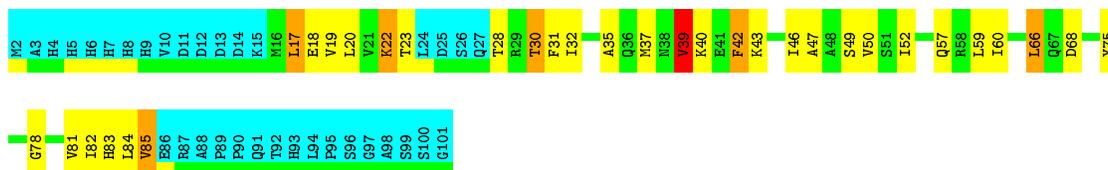
4.2.13 Score per residue for model 13

• Molecule 1: E3 ubiquitin-protein ligase RNF126
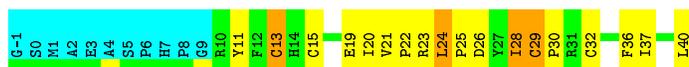
• Molecule 2: Large proline-rich protein BAG6
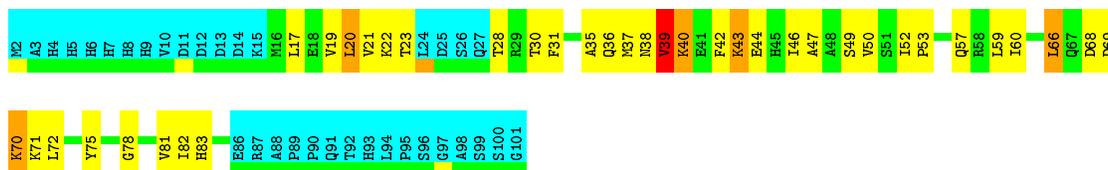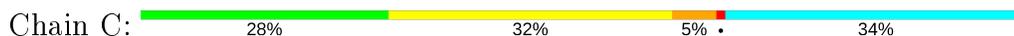
4.2.14 Score per residue for model 14

• Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

- Molecule 2: Large proline-rich protein BAG6

Chain C:
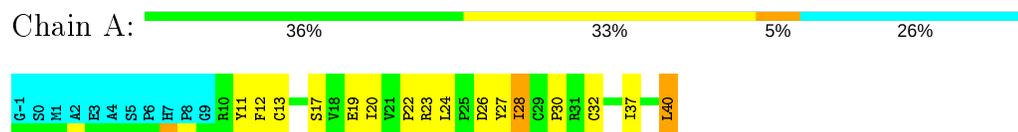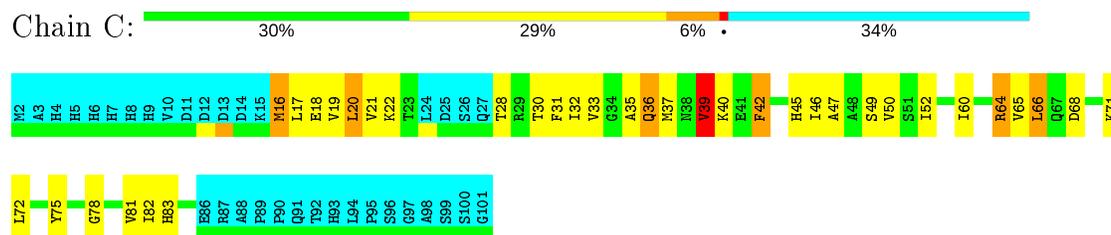
4.2.15   Score per residue for model 15

- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

- Molecule 2: Large proline-rich protein BAG6

Chain C:
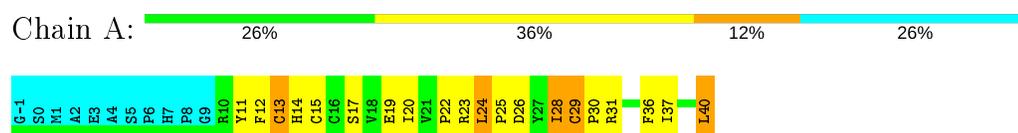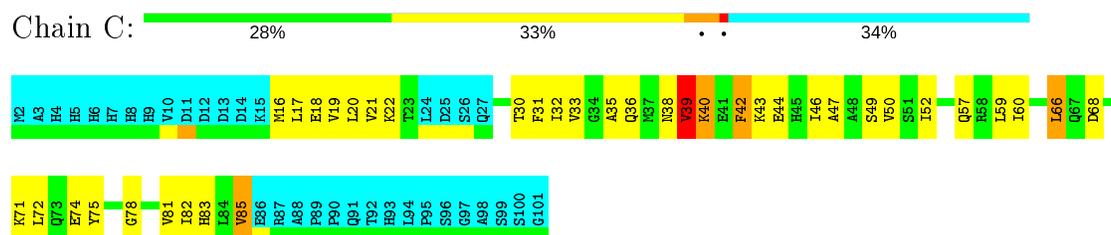
4.2.16   Score per residue for model 16

- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

- Molecule 2: Large proline-rich protein BAG6

Chain C:

M2 A3 H4 H5 H6 H7 H8 H9 V10 D11 D12 D13 K15 M16 L17 E18 V19 L20 V21 K22 T23 L24 D25 S26 Q27 T28 R29 T30 F31 I32 V33 G34 A35 V39 K40 E41 F42 I46 A47 A48 S49 V50 S51 I52 L59 I60 L66 Q67 D68 L72 Y75 G78

V81 V85 E86 R87 A88 P89 P90 Q91 T92 H93 L94 P95 S96 G97 A98 S99 S100 G101
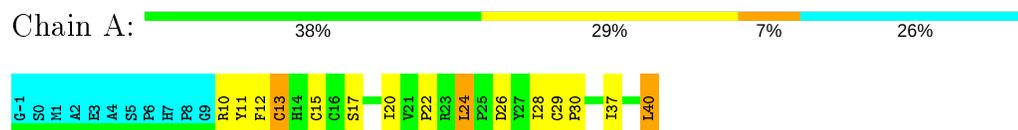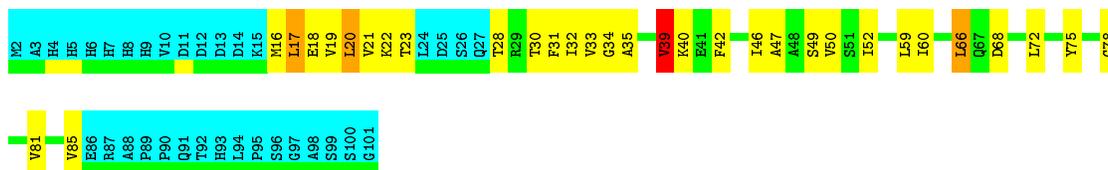
4.2.17   Score per residue for model 17

• Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A: 45%   21%   7%   26%

G-1 S0 M1 A2 E3 A4 S5 P6 H7 P8 G9 F12 C13 S17 I20 R23 L24 P25 D26 Y27 I28 C29 P30 I37 I40

• Molecule 2: Large proline-rich protein BAG6

Chain C: 31%   29%   6%   34%

M2 A3 H4 H5 H6 H7 H8 H9 V10 D11 D12 D13 D14 K15 M16 L17 E18 V19 L20 V21 K22 T23 L24 D25 S26 Q27 T28 R29 T30 F31 I32 V33 G34 Q36 M37 N38 V39 K40 E41 F42 I46 A47 A48 S49 V50 S51 I52 Q57 R58 L59 I60 Y61 V65 L66 K70

K71 L72 V77 G78 V81 I82 E86 R87 A88 P89 P90 Q91 T92 H93 L94 P95 S96 G97 A98 S99 S100 G101
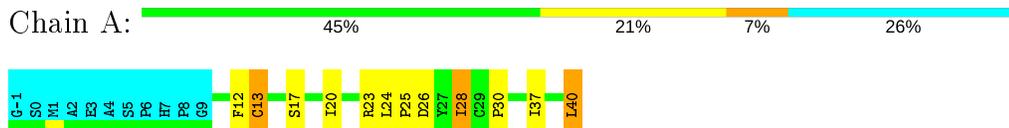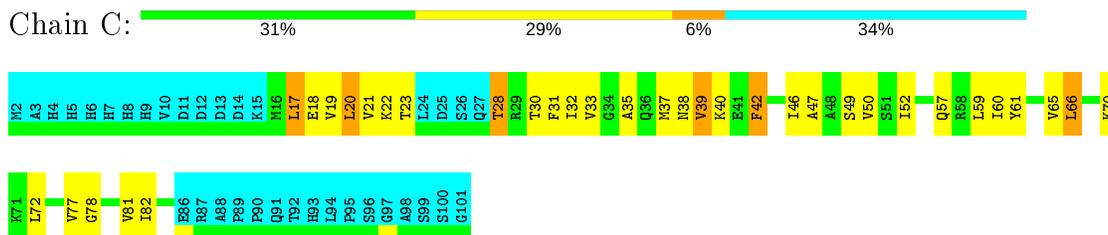
4.2.18   Score per residue for model 18

• Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A: 29%   36%   10%   26%

G-1 S0 M1 A2 E3 A4 S5 P6 H7 P8 G9 R10 Y11 F12 C13 H14 C15 C16 S17 I20 V21 P22 R23 L24 P25 D26 Y27 I28 C29 P30 R31 C32 F36 I37 L40

• Molecule 2: Large proline-rich protein BAG6

Chain C: 32%   31%   ••   34%

M2 A3 H4 H5 H6 H7 H8 H9 V10 D11 D12 D13 D14 K15 M16 L17 E18 V19 L20 V21 K22 T23 L24 D25 S26 Q27 T28 F31 I32 V33 G34 A35 Q36 V39 K40 E41 F42 K43 I46 A47 A48 S49 V50 S51 I52 L59 I60 L66 Q67 D68 L72 Y75 N76

V77 G78 V81 I82 H83 L84 V85 E86 R87 A88 P89 P90 Q91 T92 H93 L94 P95 S96 G97 A98 S99 S100 G101
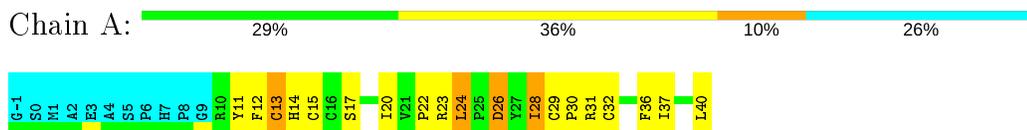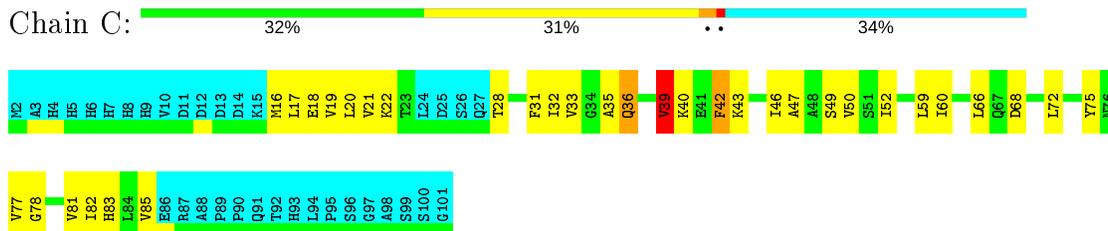
4.2.19   Score per residue for model 19

• Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

40%　　26%　　7%　　26%

G-1 S0 M1 A2 E3 A4 S5 P6 H7 P8 G9 R10 Y11 F12 C13 H14 C15 I20 V21 P22 R23 L24 P25 D26 Y27 I28 C29 P30 R31 C32 F36 I37 L40

• Molecule 2: Large proline-rich protein BAG6

Chain C:

39%　　21%　　5% •　　34%

M2 A3 H4 H5 H6 H7 H8 H9 V10 D11 D12 D13 D14 K15 M16 L17 E18 V19 L20 L24 D25 S26 Q27 T30 F31 I32 A35 Q36 M37 N38 V39 K40 E41 F42 K43 I46 A47 V50 S51 I52 Q57 R58 L59 V65 L66 Q67 D68 L72 Y75 N76 V77

G78 V81 E86 R87 A88 P89 P90 Q91 T92 H93 L94 P95 S96 G97 A98 S99 S100 G101
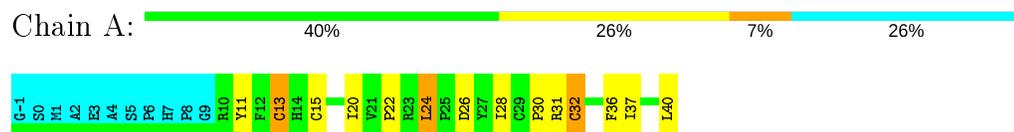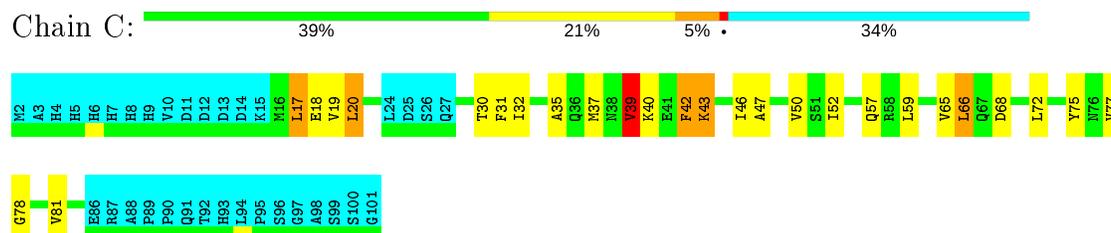
4.2.20　Score per residue for model 20

• Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:

36%　　29%　　10%　　26%

G-1 S0 M1 A2 E3 A4 S5 P6 H7 P8 G9 R10 Y11 F12 C13 S17 I20 V21 P22 R23 L24 P25 D26 Y27 I28 C29 P30 R31 F36 I37 L40

• Molecule 2: Large proline-rich protein BAG6

Chain C:

30%　　31%　　5%　　34%

M2 A3 H4 H5 H6 H7 H8 H9 V10 D11 D12 D13 D14 K15 M16 L17 E18 V19 L20 V21 K22 T23 L24 D25 S26 Q27 T28 R29 T30 F31 I32 V33 G34 A35 Q36 V39 K40 E41 F42 I46 A47 A48 S49 V50 S51 I52 Q57 R58 L59 G63 R64 V65 L66 Q67 D68 D69

K70 K71 L72 Y75 G78 V81 I82 H83 L84 V85 E86 R87 A88 P89 P90 Q91 T92 H93 L94 P95 S96 G97 A98 S99 S100 G101
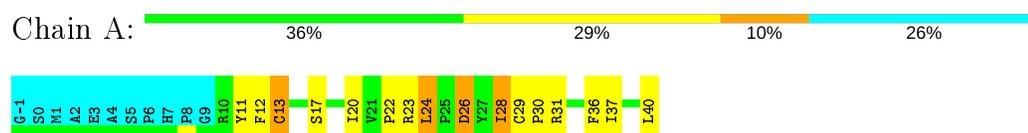
5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

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
ARIA	structure solution	2.1
ARIA	refinement	2.1
CcpNMR Analysis	structure solution	2.3

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)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	1547
Number of shifts mapped to atoms	1547
Number of unparsed shifts	0
Number of shifts with mapping errors	0
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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	255	239	238	14±2
2	C	528	562	560	30±5
All	All	15680	16020	15960	844

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
2:C:20:LEU:HB3	2:C:81:VAL:HG12	0.83	1.50	11	6
1:A:20:ILE:HD11	1:A:37:ILE:HG21	0.79	1.51	8	18
2:C:21:VAL:O	2:C:28:THR:HA	0.79	1.78	17	6
2:C:17:LEU:HD11	2:C:35:ALA:HA	0.76	1.56	3	13
2:C:17:LEU:HD22	2:C:35:ALA:HA	0.74	1.57	8	5
2:C:35:ALA:O	2:C:36:GLN:HB2	0.73	1.82	4	5
1:A:20:ILE:CD1	1:A:37:ILE:HG21	0.72	2.13	8	20
2:C:17:LEU:CD2	2:C:35:ALA:HA	0.69	2.18	6	7
2:C:20:LEU:HB3	2:C:81:VAL:CG1	0.67	2.20	11	3
1:A:20:ILE:HD12	1:A:30:PRO:HD3	0.66	1.67	17	20
1:A:15:CYS:SG	1:A:36:PHE:HB2	0.65	2.32	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:C:17:LEU:HD21	2:C:35:ALA:HA	0.64	1.68	11	2
2:C:59:LEU:O	2:C:66:LEU:HG	0.64	1.92	16	11
2:C:42:PHE:O	2:C:46:ILE:HG23	0.64	1.93	10	7
2:C:36:GLN:H	2:C:72:LEU:HD12	0.64	1.52	14	1
1:A:11:TYR:CG	1:A:22:PRO:HG3	0.63	2.29	6	18
1:A:13:CYS:SG	1:A:15:CYS:SG	0.62	2.96	15	4
1:A:14:HIS:CG	2:C:85:VAL:HG13	0.62	2.30	6	1
2:C:22:LYS:HG2	2:C:28:THR:OG1	0.62	1.94	8	5
2:C:35:ALA:O	2:C:72:LEU:HB2	0.61	1.95	8	7
2:C:39:VAL:O	2:C:43:LYS:HD2	0.60	1.96	3	3
2:C:46:ILE:HD11	2:C:57:GLN:OE1	0.60	1.96	19	6
1:A:22:PRO:HB3	1:A:37:ILE:CD1	0.59	2.27	8	8
1:A:20:ILE:HB	1:A:30:PRO:CD	0.59	2.28	16	20
2:C:17:LEU:HB3	2:C:78:GLY:HA2	0.59	1.74	20	15
2:C:17:LEU:HD21	2:C:35:ALA:HB2	0.58	1.74	20	1
2:C:35:ALA:O	2:C:36:GLN:HB3	0.58	1.97	18	1
2:C:39:VAL:CA	2:C:42:PHE:HB3	0.58	2.28	18	20
1:A:11:TYR:O	1:A:19:GLU:HG3	0.58	1.97	11	11
2:C:66:LEU:HD22	2:C:75:TYR:CD1	0.58	2.34	3	17
2:C:20:LEU:CB	2:C:81:VAL:HG12	0.58	2.29	14	15
2:C:46:ILE:O	2:C:50:VAL:HG22	0.58	1.97	9	19
2:C:43:LYS:HG3	2:C:57:GLN:OE1	0.57	1.99	19	3
2:C:47:ALA:HA	2:C:52:ILE:O	0.57	1.98	3	20
1:A:23:ARG:HB2	1:A:28:ILE:HG13	0.57	1.75	10	9
2:C:16:MET:HA	2:C:33:VAL:O	0.56	2.00	2	8
2:C:33:VAL:HG21	2:C:72:LEU:HD13	0.56	1.74	2	4
2:C:19:VAL:O	2:C:30:THR:HA	0.56	2.00	6	19
2:C:19:VAL:HB	2:C:31:PHE:O	0.56	2.01	16	10
2:C:20:LEU:HB2	2:C:81:VAL:HG12	0.56	1.76	14	6
2:C:20:LEU:O	2:C:81:VAL:HA	0.56	2.01	3	13
1:A:13:CYS:SG	1:A:15:CYS:HB3	0.56	2.41	7	4
2:C:43:LYS:HB2	2:C:57:GLN:OE1	0.55	2.01	13	2
1:A:29:CYS:SG	1:A:31:ARG:HB2	0.55	2.41	15	9
1:A:13:CYS:HB2	1:A:37:ILE:HG22	0.55	1.76	9	7
2:C:61:TYR:CD2	2:C:77:VAL:HG12	0.55	2.36	17	1
1:A:13:CYS:HB2	1:A:37:ILE:CG2	0.55	2.32	19	12
2:C:20:LEU:HB2	2:C:81:VAL:CG1	0.55	2.32	17	4
2:C:33:VAL:HG11	2:C:42:PHE:CD1	0.55	2.37	20	1
2:C:39:VAL:HG23	2:C:72:LEU:HD21	0.54	1.77	13	4
2:C:40:LYS:O	2:C:43:LYS:HG2	0.54	2.03	11	3
2:C:39:VAL:HA	2:C:42:PHE:CD2	0.54	2.38	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:12:PHE:CB	1:A:40:LEU:HD11	0.54	2.31	15	6
2:C:17:LEU:HB3	2:C:78:GLY:CA	0.54	2.33	2	14
2:C:38:ASN:O	2:C:39:VAL:HG12	0.53	2.04	11	6
1:A:20:ILE:HD13	1:A:37:ILE:HG21	0.53	1.81	19	7
2:C:43:LYS:HB3	2:C:57:GLN:OE1	0.53	2.04	5	1
2:C:21:VAL:HG21	2:C:31:PHE:CE2	0.53	2.39	18	3
1:A:12:PHE:HB2	1:A:40:LEU:HD21	0.53	1.81	2	1
2:C:20:LEU:C	2:C:81:VAL:HA	0.53	2.24	7	13
1:A:22:PRO:HG2	1:A:24:LEU:CD2	0.53	2.34	6	1
1:A:14:HIS:CE1	2:C:85:VAL:HB	0.53	2.39	15	1
1:A:11:TYR:CD2	1:A:22:PRO:HG3	0.52	2.39	1	9
2:C:21:VAL:HG22	2:C:82:ILE:HB	0.52	1.82	14	7
2:C:19:VAL:CG1	2:C:31:PHE:HB2	0.52	2.34	14	12
1:A:37:ILE:O	2:C:60:ILE:HG21	0.52	2.04	9	15
2:C:33:VAL:HG11	2:C:42:PHE:CD2	0.52	2.40	14	4
2:C:54:SER:HA	2:C:57:GLN:OE1	0.52	2.04	5	1
1:A:12:PHE:CB	1:A:40:LEU:HD21	0.51	2.34	2	5
2:C:43:LYS:HG2	2:C:57:GLN:OE1	0.51	2.04	12	3
2:C:39:VAL:HG13	2:C:68:ASP:HA	0.51	1.82	9	13
2:C:35:ALA:O	2:C:36:GLN:CB	0.51	2.57	4	2
2:C:50:VAL:HG21	2:C:57:GLN:OE1	0.51	2.04	20	1
1:A:10:ARG:O	1:A:10:ARG:HG3	0.51	2.04	11	1
2:C:19:VAL:O	2:C:19:VAL:HG12	0.51	2.06	9	2
2:C:59:LEU:O	2:C:66:LEU:HB2	0.50	2.06	18	1
2:C:20:LEU:HB2	2:C:81:VAL:HA	0.50	1.83	14	12
2:C:35:ALA:C	2:C:72:LEU:HB2	0.50	2.27	20	1
1:A:22:PRO:HB3	1:A:37:ILE:HD12	0.50	1.84	2	2
1:A:23:ARG:HB2	1:A:28:ILE:CD1	0.50	2.36	20	3
2:C:39:VAL:H	2:C:42:PHE:HB3	0.49	1.67	15	5
2:C:40:LYS:HE2	2:C:70:LYS:O	0.49	2.07	7	1
2:C:40:LYS:HA	2:C:68:ASP:CB	0.49	2.37	6	3
2:C:39:VAL:N	2:C:42:PHE:HB3	0.49	2.23	18	11
2:C:38:ASN:O	2:C:40:LYS:HD2	0.49	2.08	6	1
2:C:66:LEU:HG	2:C:75:TYR:CD1	0.49	2.42	18	1
2:C:82:ILE:HG22	2:C:83:HIS:N	0.49	2.23	18	14
2:C:22:LYS:HG3	2:C:81:VAL:CG2	0.48	2.38	11	10
2:C:66:LEU:HB3	2:C:75:TYR:CD2	0.48	2.42	10	1
2:C:22:LYS:HG3	2:C:81:VAL:CB	0.48	2.37	11	3
2:C:38:ASN:O	2:C:39:VAL:HB	0.48	2.08	17	1
1:A:13:CYS:HA	1:A:36:PHE:O	0.48	2.07	13	10
1:A:10:ARG:HG2	1:A:40:LEU:HD12	0.48	1.86	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:C:22:LYS:HG3	2:C:81:VAL:HB	0.48	1.86	12	6
2:C:61:TYR:OH	2:C:80:LYS:HD3	0.47	2.09	4	1
2:C:17:LEU:HG	2:C:78:GLY:CA	0.47	2.38	6	2
2:C:21:VAL:HG21	2:C:31:PHE:HE2	0.47	1.68	20	4
2:C:39:VAL:HA	2:C:42:PHE:HB3	0.47	1.86	3	15
2:C:42:PHE:C	2:C:42:PHE:CD1	0.47	2.87	14	5
2:C:20:LEU:CD2	2:C:30:THR:HG22	0.47	2.40	5	11
1:A:12:PHE:HB2	1:A:40:LEU:HD11	0.47	1.86	15	5
2:C:64:ARG:HD3	2:C:65:VAL:N	0.47	2.24	14	1
2:C:17:LEU:O	2:C:32:ILE:HG23	0.47	2.10	11	1
2:C:52:ILE:HG22	2:C:57:GLN:HB2	0.47	1.86	17	1
2:C:18:GLU:HA	2:C:32:ILE:HG13	0.47	1.86	14	15
2:C:66:LEU:HD12	2:C:82:ILE:HD13	0.47	1.85	3	2
2:C:36:GLN:HG3	2:C:73:GLN:CB	0.47	2.40	4	1
2:C:36:GLN:N	2:C:72:LEU:HD12	0.47	2.24	14	1
1:A:15:CYS:SG	1:A:34:SER:HB2	0.47	2.49	2	1
1:A:14:HIS:CD2	2:C:85:VAL:HG12	0.47	2.44	7	1
1:A:26:ASP:HB3	1:A:28:ILE:HG12	0.46	1.87	12	6
1:A:15:CYS:SG	1:A:32:CYS:SG	0.46	3.13	13	3
2:C:52:ILE:CG2	2:C:57:GLN:HB3	0.46	2.41	11	2
1:A:10:ARG:O	1:A:10:ARG:HG2	0.46	2.10	7	1
2:C:18:GLU:HG2	2:C:32:ILE:HG12	0.46	1.86	12	1
2:C:22:LYS:HE3	2:C:81:VAL:HG21	0.46	1.88	15	3
2:C:53:PRO:O	2:C:57:GLN:HG3	0.46	2.11	5	1
1:A:11:TYR:CD1	1:A:22:PRO:HG3	0.46	2.46	6	3
2:C:35:ALA:O	2:C:73:GLN:HB2	0.46	2.11	7	1
2:C:20:LEU:HB2	2:C:80:LYS:C	0.46	2.31	11	1
1:A:31:ARG:O	1:A:32:CYS:HB3	0.46	2.10	19	1
1:A:29:CYS:SG	1:A:30:PRO:HD2	0.46	2.51	20	7
2:C:17:LEU:CD1	2:C:35:ALA:HA	0.46	2.40	18	2
2:C:19:VAL:O	2:C:31:PHE:N	0.46	2.48	18	8
2:C:52:ILE:HG22	2:C:57:GLN:HG3	0.46	1.88	5	1
2:C:43:LYS:HA	2:C:57:GLN:OE1	0.45	2.11	3	1
2:C:16:MET:H	2:C:34:GLY:HA2	0.45	1.71	16	1
2:C:46:ILE:HG13	2:C:57:GLN:NE2	0.45	2.26	5	1
2:C:18:GLU:HA	2:C:32:ILE:CG1	0.45	2.42	10	4
2:C:66:LEU:HD21	2:C:77:VAL:HG11	0.45	1.89	18	1
2:C:22:LYS:HE3	2:C:28:THR:OG1	0.45	2.11	3	1
1:A:23:ARG:C	1:A:25:PRO:HD2	0.45	2.32	5	1
1:A:14:HIS:HD2	1:A:38:GLU:OE1	0.45	1.94	12	1
2:C:59:LEU:HB3	2:C:82:ILE:HG21	0.44	1.88	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:39:VAL:HG11	2:C:70:LYS:HA	0.44	1.89	17	1
2:C:37:MET:HG3	2:C:38:ASN:OD1	0.44	2.11	3	2
2:C:19:VAL:HG11	2:C:42:PHE:CZ	0.44	2.47	4	1
2:C:59:LEU:O	2:C:66:LEU:N	0.44	2.51	11	5
2:C:52:ILE:HG22	2:C:57:GLN:CG	0.44	2.43	5	1
1:A:10:ARG:H	1:A:10:ARG:HD3	0.43	1.72	7	1
1:A:11:TYR:HB2	1:A:22:PRO:HD3	0.43	1.90	8	4
2:C:72:LEU:HA	2:C:75:TYR:CD2	0.43	2.48	5	2
1:A:37:ILE:O	2:C:63:GLY:HA2	0.43	2.13	20	1
2:C:35:ALA:O	2:C:73:GLN:N	0.43	2.51	1	2
2:C:42:PHE:CD1	2:C:42:PHE:C	0.43	2.92	19	3
2:C:19:VAL:HG22	2:C:77:VAL:HG23	0.43	1.90	2	1
2:C:59:LEU:HD23	2:C:84:LEU:HD21	0.43	1.90	7	1
1:A:14:HIS:CD2	2:C:85:VAL:HG21	0.43	2.48	18	2
2:C:20:LEU:HB2	2:C:81:VAL:CA	0.43	2.44	5	4
1:A:14:HIS:CE1	2:C:85:VAL:HG13	0.43	2.48	2	1
2:C:53:PRO:O	2:C:57:GLN:HB2	0.43	2.14	8	3
2:C:55:GLU:HG3	2:C:56:LYS:HG3	0.42	1.91	5	1
1:A:27:TYR:C	1:A:37:ILE:HD11	0.42	2.35	14	2
1:A:12:PHE:CZ	1:A:17:SER:HA	0.42	2.48	20	1
2:C:54:SER:HA	2:C:57:GLN:HG2	0.42	1.90	11	1
2:C:69:ASP:O	2:C:70:LYS:HB2	0.42	2.14	13	1
1:A:27:TYR:O	1:A:35:GLY:HA2	0.42	2.14	8	1
2:C:71:LYS:HB3	2:C:74:GLU:CG	0.42	2.45	15	1
2:C:22:LYS:HE2	2:C:28:THR:OG1	0.42	2.14	18	1
2:C:39:VAL:O	2:C:43:LYS:HG3	0.42	2.14	18	1
2:C:36:GLN:HG3	2:C:73:GLN:HB3	0.42	1.92	4	1
2:C:66:LEU:HA	2:C:75:TYR:CZ	0.42	2.50	6	1
2:C:23:THR:HG22	2:C:84:LEU:O	0.42	2.15	12	1
2:C:40:LYS:O	2:C:43:LYS:HB2	0.41	2.15	3	1
2:C:50:VAL:HG11	2:C:84:LEU:CD1	0.41	2.46	12	1
2:C:39:VAL:CG1	2:C:70:LYS:HA	0.41	2.44	2	1
2:C:22:LYS:HA	2:C:28:THR:HA	0.41	1.90	3	1
2:C:39:VAL:H	2:C:42:PHE:CB	0.41	2.28	8	3
2:C:61:TYR:CZ	2:C:80:LYS:HB3	0.41	2.50	6	1
2:C:33:VAL:CG2	2:C:72:LEU:HD13	0.41	2.46	18	1
2:C:22:LYS:HG3	2:C:81:VAL:HG21	0.41	1.92	11	1
1:A:26:ASP:CB	1:A:28:ILE:HG12	0.41	2.46	20	1
2:C:22:LYS:N	2:C:82:ILE:O	0.41	2.48	11	2
2:C:59:LEU:HB2	2:C:66:LEU:HB2	0.41	1.92	18	1
1:A:26:ASP:HB3	1:A:28:ILE:CG1	0.40	2.46	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:43:LYS:HE3	2:C:54:SER:OG	0.40	2.16	2	2
1:A:24:LEU:O	1:A:26:ASP:N	0.40	2.49	12	1
2:C:22:LYS:CD	2:C:81:VAL:HG21	0.40	2.46	15	1
2:C:66:LEU:HG	2:C:75:TYR:CG	0.40	2.51	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	30/42 (71%)	23±1 (76±3%)	5±1 (18±2%)	2±1 (6±2%)	3	20
2	C	66/100 (66%)	51±2 (77±3%)	13±2 (19±3%)	3±1 (4±2%)	5	30
All	All	1920/2840 (68%)	1472 (77%)	357 (19%)	91 (5%)	4	27

All 14 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	24	LEU	20
2	C	39	VAL	20
1	A	25	PRO	11
2	C	28	THR	8
2	C	36	GLN	7
2	C	16	MET	4
2	C	37	MET	4
2	C	85	VAL	3
2	C	70	LYS	3
1	A	32	CYS	3
2	C	78	GLY	3
2	C	71	LYS	3
1	A	26	ASP	1
1	A	22	PRO	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	30/37 (81%)	25±1 (82±3%)	5±1 (18±3%)	4	37
2	C	59/88 (67%)	51±2 (86±3%)	8±2 (14±3%)	7	47
All	All	1780/2500 (71%)	1511 (85%)	269 (15%)	6	44

All 37 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)
2	C	40	LYS	20
1	A	28	ILE	20
1	A	26	ASP	19
2	C	49	SER	19
2	C	66	LEU	18
2	C	39	VAL	18
1	A	13	CYS	18
2	C	17	LEU	14
1	A	40	LEU	13
2	C	20	LEU	12
1	A	17	SER	11
1	A	24	LEU	11
2	C	65	VAL	11
2	C	42	PHE	10
1	A	29	CYS	8
2	C	37	MET	5
2	C	23	THR	4
2	C	43	LYS	4
2	C	30	THR	3
2	C	44	GLU	3
2	C	77	VAL	3
1	A	34	SER	2
1	A	32	CYS	2
1	A	16	CYS	2
1	A	10	ARG	2
2	C	84	LEU	2
2	C	71	LYS	2
2	C	85	VAL	2

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Mol	Chain	Res	Type	Models (Total)
2	C	36	GLN	2
2	C	57	GLN	2
2	C	16	MET	1
2	C	54	SER	1
2	C	22	LYS	1
2	C	80	LYS	1
2	C	45	HIS	1
2	C	64	ARG	1
1	A	38	GLU	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 81% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

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	486
Number of shifts mapped to atoms	486
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	42	-0.11 ± 0.19	None needed (< 0.5 ppm)
$^{13}C_\beta$	39	0.02 ± 0.45	None needed (< 0.5 ppm)
$^{13}C'$	40	0.08 ± 0.29	None needed (< 0.5 ppm)
^{15}N	35	0.06 ± 0.66	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 29%, i.e. 363 atoms were assigned a chemical shift out of a possible 1250. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	148/477 (31%)	59/190 (31%)	61/194 (31%)	28/93 (30%)
Sidechain	179/681 (26%)	112/400 (28%)	64/249 (26%)	3/32 (9%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	36/92 (39%)	19/48 (40%)	17/38 (45%)	0/6 (0%)
Overall	363/1250 (29%)	190/638 (30%)	142/481 (30%)	31/131 (24%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 26%, i.e. 455 atoms were assigned a chemical shift out of a possible 1755. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	194/692 (28%)	77/275 (28%)	82/284 (29%)	35/133 (26%)
Sidechain	224/907 (25%)	141/537 (26%)	80/332 (24%)	3/38 (8%)
Aromatic	37/156 (24%)	20/80 (25%)	17/54 (31%)	0/22 (0%)
Overall	455/1755 (26%)	238/892 (27%)	179/670 (27%)	38/193 (20%)

### 7.1.4   Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5   Random Coil Index (RCI) plots (i)

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:
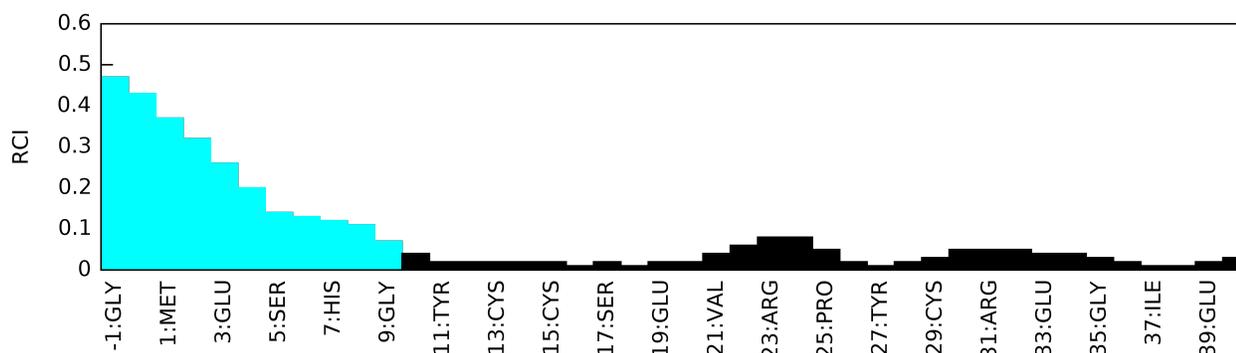
7.2   Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	1061
Number of shifts mapped to atoms	1061
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	89	-0.30 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_\beta$	81	0.15 ± 0.26	None needed (< 0.5 ppm)
$^{13}C'$	77	-0.11 ± 0.10	None needed (< 0.5 ppm)
^{15}N	87	-0.43 ± 0.66	None needed (< 0.5 ppm)

7.2.3 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 58%, i.e. 726 atoms were assigned a chemical shift out of a possible 1250. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	318/477 (67%)	129/190 (68%)	124/194 (64%)	65/93 (70%)
Sidechain	376/681 (55%)	230/400 (58%)	137/249 (55%)	9/32 (28%)
Aromatic	32/92 (35%)	16/48 (33%)	16/38 (42%)	0/6 (0%)
Overall	726/1250 (58%)	375/638 (59%)	277/481 (58%)	74/131 (56%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 966 atoms were assigned a chemical shift out of a possible 1755. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	429/692 (62%)	176/275 (64%)	166/284 (58%)	87/133 (65%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	505/907 (56%)	312/537 (58%)	182/332 (55%)	11/38 (29%)
Aromatic	32/156 (21%)	16/80 (20%)	16/54 (30%)	0/22 (0%)
Overall	966/1755 (55%)	504/892 (57%)	364/670 (54%)	98/193 (51%)

7.2.4 Statistically unusual chemical shifts (i)

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
3	C	46	ILE	HG23	-0.87	$2.13 - -0.57$	-6.1
3	C	46	ILE	HG22	-0.87	$2.13 - -0.57$	-6.1
3	C	46	ILE	HG21	-0.87	$2.13 - -0.57$	-6.1

7.2.5 Random Coil Index (RCI) plots (i)

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 C: