Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2M3H
BMRB ID	:	18963
Title	:	Structure of Dido PHD domain
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Deposited on	:	2013-01-19

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

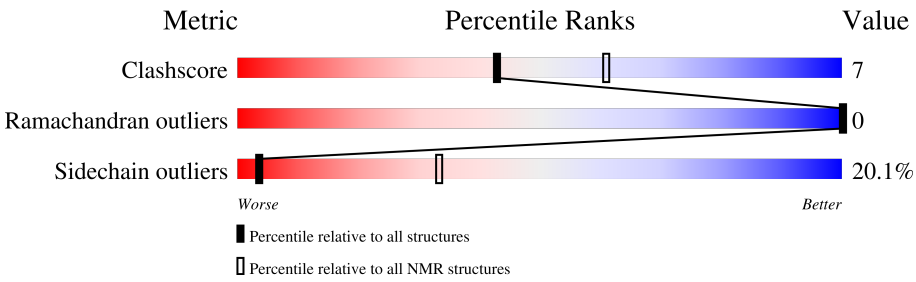
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 89%.

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	61	69% 28% .

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:3-A:61 (59)	0.27	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 931 atoms, of which 444 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Death-inducer obliterator 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	61	929	295	444	90	90	10	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9BTC0
A	2	SER	-	expression tag	UNP Q9BTC0
A	3	MET	-	expression tag	UNP Q9BTC0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

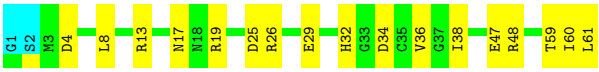
4 Residue-property plots (i)

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: Death-inducer obliterator 1

Chain A:



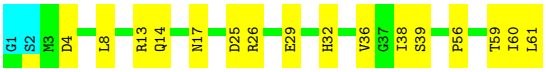
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Death-inducer obliterator 1

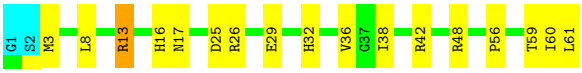
Chain A:



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Death-inducer obliterator 1

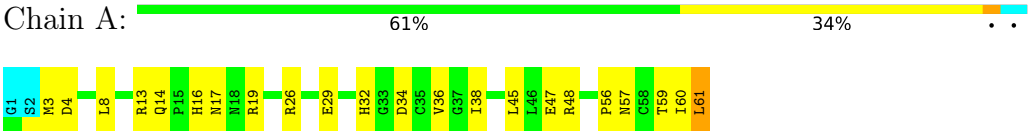
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Death-inducer obliterator 1

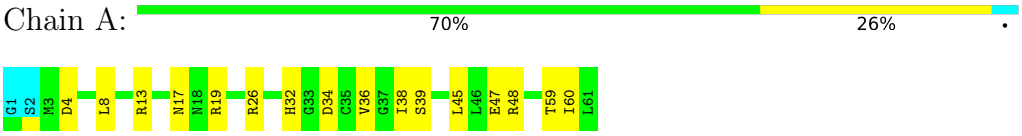
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Death-inducer obliterator 1

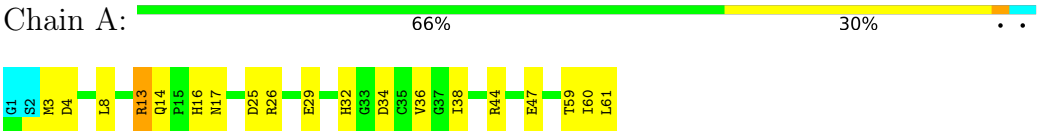
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Death-inducer obliterator 1

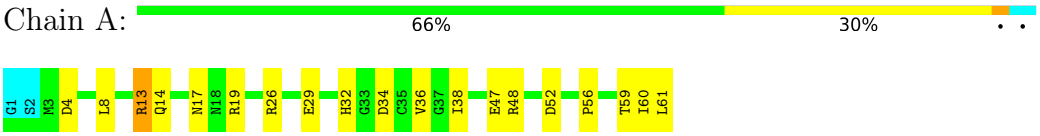
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Death-inducer obliterator 1

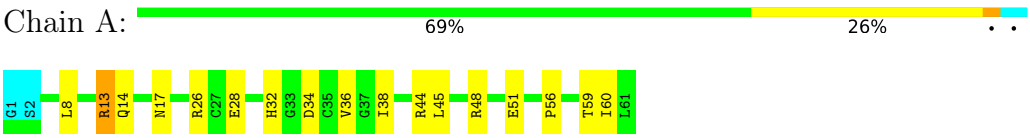
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Death-inducer obliterator 1

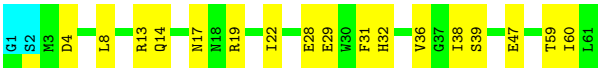
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Death-inducer obliterator 1

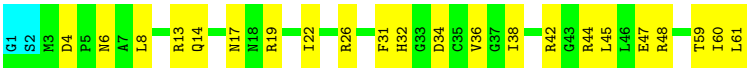
Chain A: 69% 28% •



4.2.9 Score per residue for model 9

• Molecule 1: Death-inducer obliterator 1

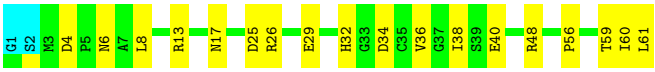
Chain A: 61% 36% •



4.2.10 Score per residue for model 10

• Molecule 1: Death-inducer obliterator 1

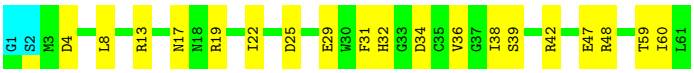
Chain A: 67% 30% •



4.2.11 Score per residue for model 11

• Molecule 1: Death-inducer obliterator 1

Chain A: 66% 31% •



4.2.12 Score per residue for model 12

• Molecule 1: Death-inducer obliterator 1

Chain A: 67% 28% • •

4.2.13 Score per residue for model 13

• Molecule 1: Death-inducer obliterator 1

Chain A: 57% 39%

G1 S2 M3 D4 L8 R13 H16 N17 N18 R19 D25 R26 E29 H32 V36 G37 I38 S39 R44 L45 L46 E47 R48 E51 P56 T59 I60 L61

4.2.14 Score per residue for model 14

• Molecule 1: Death-inducer obliterator 1

Chain A: 67% 30%

G1 S2 M3 D4 A7 L8 R13 Q14 N17 N18 R19 D25 R26 E29 H32 G33 D34 C35 V36 G37 I38 R44 P56 T59 I60 L61

4.2.15 Score per residue for model 15

• Molecule 1: Death-inducer obliterator 1

Chain A: 59% 36%

G1 S2 M3 D4 L8 R13 H16 N17 N18 R19 R26 E29 H32 G33 D34 C35 V36 G37 I38 S39 R42 G43 R44 L45 R48 E51 D52 T59 I60 L61

4.2.16 Score per residue for model 16

• Molecule 1: Death-inducer obliterator 1

Chain A: 69% 26%

G1 S2 M3 D4 L8 R13 N17 I22 D25 E29 W30 F31 H32 G33 D34 C35 V36 G37 I38 R42 T59 I60 L61

4.2.17 Score per residue for model 17

• Molecule 1: Death-inducer obliterator 1

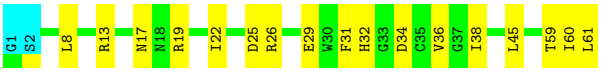
Chain A: 67% 30%

G1 S2 M3 D4 L8 R13 N17 I22 R26 E29 W30 F31 H32 V36 G37 I38 S39 R44 L45 L46 E47 T59 I60 L61

4.2.18 Score per residue for model 18

- Molecule 1: Death-inducer obliterator 1

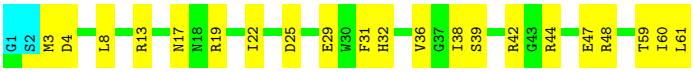
Chain A: 69% 28% •



4.2.19 Score per residue for model 19

- Molecule 1: Death-inducer obliterator 1

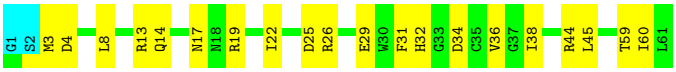
Chain A: 62% 34% •



4.2.20 Score per residue for model 20

- Molecule 1: Death-inducer obliterator 1

Chain A: 64% 33% •



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: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

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)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	1115
Number of shifts mapped to atoms	1115
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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	475	436	436	6±1
All	All	9540	8720	8720	129

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:59:THR:HG23	1:A:60:ILE:HG23	0.68	1.64	10	20
1:A:46:LEU:HD12	1:A:51:GLU:O	0.63	1.94	13	1
1:A:8:LEU:HD22	1:A:13:ARG:C	0.62	2.15	4	20
1:A:32:HIS:O	1:A:36:VAL:HG22	0.62	1.94	14	20
1:A:8:LEU:HD13	1:A:13:ARG:HB3	0.61	1.73	5	20
1:A:22:ILE:HG22	1:A:31:PHE:O	0.56	1.99	9	9
1:A:36:VAL:HG12	1:A:56:PRO:HD2	0.50	1.83	14	8
1:A:57:ASN:O	1:A:61:LEU:HD23	0.50	2.06	3	1
1:A:36:VAL:HG23	1:A:38:ILE:H	0.48	1.69	12	20
1:A:60:ILE:HD12	1:A:61:LEU:HB2	0.46	1.88	17	1
1:A:60:ILE:O	1:A:60:ILE:HD12	0.44	2.12	3	5
1:A:7:ALA:O	1:A:8:LEU:HD23	0.42	2.14	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:C	1:A:45:LEU:HD13	0.42	2.35	13	1
1:A:8:LEU:HD13	1:A:13:ARG:CB	0.42	2.44	12	1
1:A:60:ILE:HD12	1:A:60:ILE:O	0.40	2.16	10	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	58/61 (95%)	48±1 (83±1%)	10±1 (17±1%)	0±0 (0±0%)	100	100
All	All	1160/1220 (95%)	966 (83%)	194 (17%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	53/54 (98%)	42±2 (80±4%)	11±2 (20±4%)	3	33
All	All	1060/1080 (98%)	847 (80%)	213 (20%)	3	33

All 23 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	17	ASN	20
1	A	29	GLU	17
1	A	4	ASP	16
1	A	26	ARG	16
1	A	34	ASP	14

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Mol	Chain	Res	Type	Models (Total)
1	A	19	ARG	13
1	A	61	LEU	12
1	A	48	ARG	12
1	A	25	ASP	11
1	A	47	GLU	11
1	A	44	ARG	10
1	A	14	GLN	9
1	A	39	SER	9
1	A	3	MET	8
1	A	45	LEU	8
1	A	13	ARG	7
1	A	42	ARG	6
1	A	16	HIS	5
1	A	52	ASP	2
1	A	28	GLU	2
1	A	51	GLU	2
1	A	6	ASN	2
1	A	40	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are 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 89% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

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	715
Number of shifts mapped to atoms	715
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	61	-0.31 ± 0.23	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	56	-0.02 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	56	-0.03 ± 0.12	None needed (< 0.5 ppm)
^{15}N	56	-0.55 ± 0.56	None needed (imprecise)

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 88%, i.e. 705 atoms were assigned a chemical shift out of a possible 797. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	289/293 (99%)	119/119 (100%)	114/118 (97%)	56/56 (100%)
Sidechain	391/440 (89%)	257/282 (91%)	123/134 (92%)	11/24 (46%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	25/64 (39%)	24/32 (75%)	0/29 (0%)	1/3 (33%)
Overall	705/797 (88%)	400/433 (92%)	237/281 (84%)	68/83 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 714 atoms were assigned a chemical shift out of a possible 811. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	295/304 (97%)	122/124 (98%)	117/122 (96%)	56/58 (97%)
Sidechain	394/443 (89%)	259/284 (91%)	124/135 (92%)	11/24 (46%)
Aromatic	25/64 (39%)	24/32 (75%)	0/29 (0%)	1/3 (33%)
Overall	714/811 (88%)	405/440 (92%)	241/286 (84%)	68/85 (80%)

7.1.4 Statistically unusual chemical shifts (i)

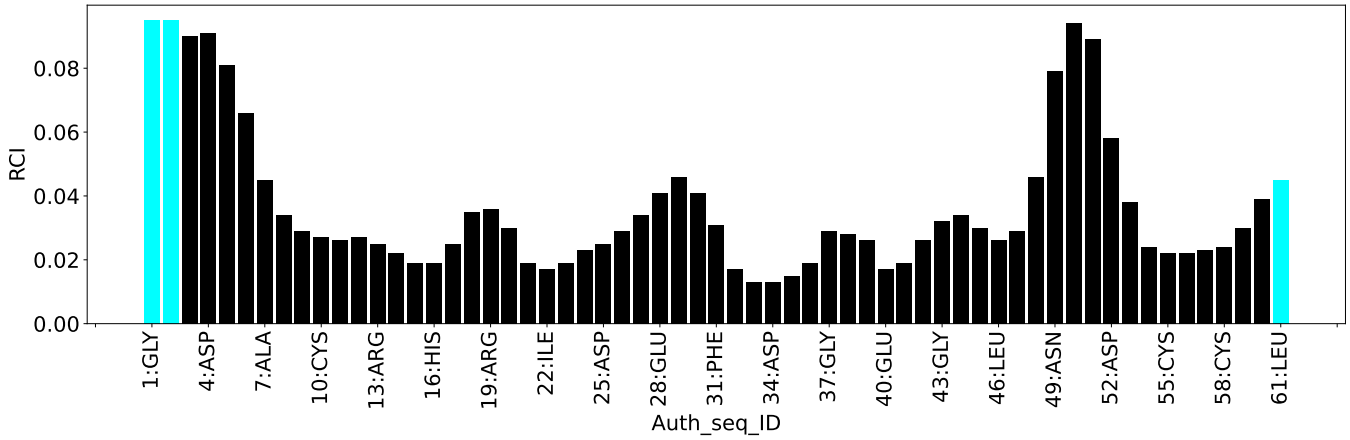
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	23	CYS	HB2	-0.03	0.81 – 5.11	-6.9

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	400
Number of shifts mapped to atoms	400
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.2.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 50%, i.e. 396 atoms were assigned a chemical shift out of a possible 797. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	118/293 (40%)	118/119 (99%)	0/118 (0%)	0/56 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	251/440 (57%)	251/282 (89%)	0/134 (0%)	0/24 (0%)
Aromatic	27/64 (42%)	27/32 (84%)	0/29 (0%)	0/3 (0%)
Overall	396/797 (50%)	396/433 (91%)	0/281 (0%)	0/83 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 399 atoms were assigned a chemical shift out of a possible 811. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	119/304 (39%)	119/124 (96%)	0/122 (0%)	0/58 (0%)
Sidechain	253/443 (57%)	253/284 (89%)	0/135 (0%)	0/24 (0%)
Aromatic	27/64 (42%)	27/32 (84%)	0/29 (0%)	0/3 (0%)
Overall	399/811 (49%)	399/440 (91%)	0/286 (0%)	0/85 (0%)

7.2.4 Statistically unusual chemical shifts (i)

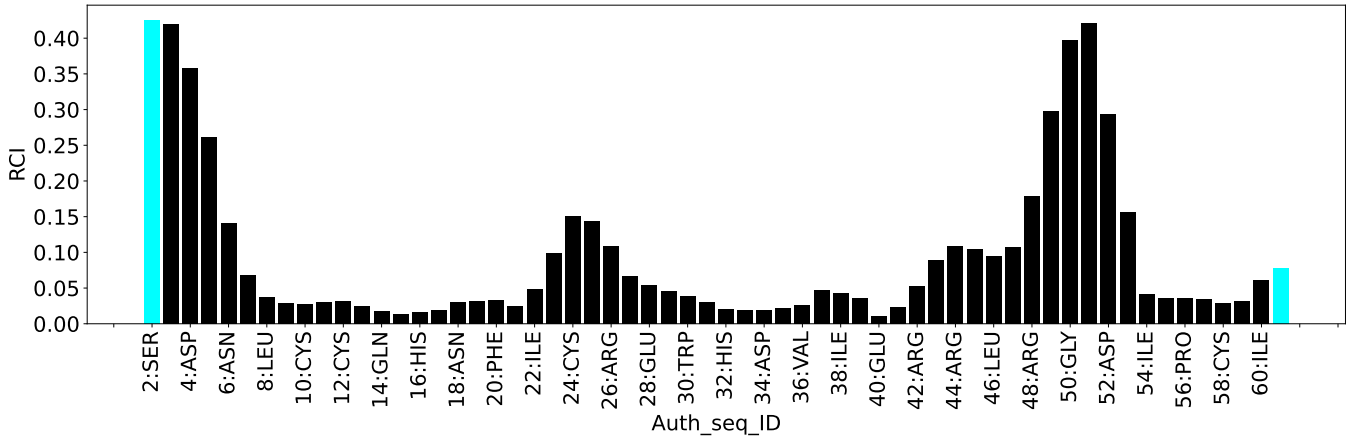
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	A	23	CYS	HB2	-0.01	0.81 – 5.11	-6.9

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
2:SER
4:ASP
6:ASN
8:LEU
10:CYS
12:CYS
14:GLN
16:HIS
18:ASN
20:PHE
22:ILE
24:CYS
26:ARG
28:GLU
30:TRP
32:HIS
34:ASP
36:VAL
38:ILE
40:GLU
42:ARG
44:ARG
46:LEU
48:ARG
50:GLY
52:ASP
54:ILE
56:PRO
58:CYS
60:ILE
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1062
Intra-residue (|i-j|=0)	266
Sequential (|i-j|=1)	264
Medium range (|i-j|>1 and |i-j|<5)	161
Long range (|i-j|≥5)	371
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	17.4
Number of long range restraints per residue[1]	6.1

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.1	0.12
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

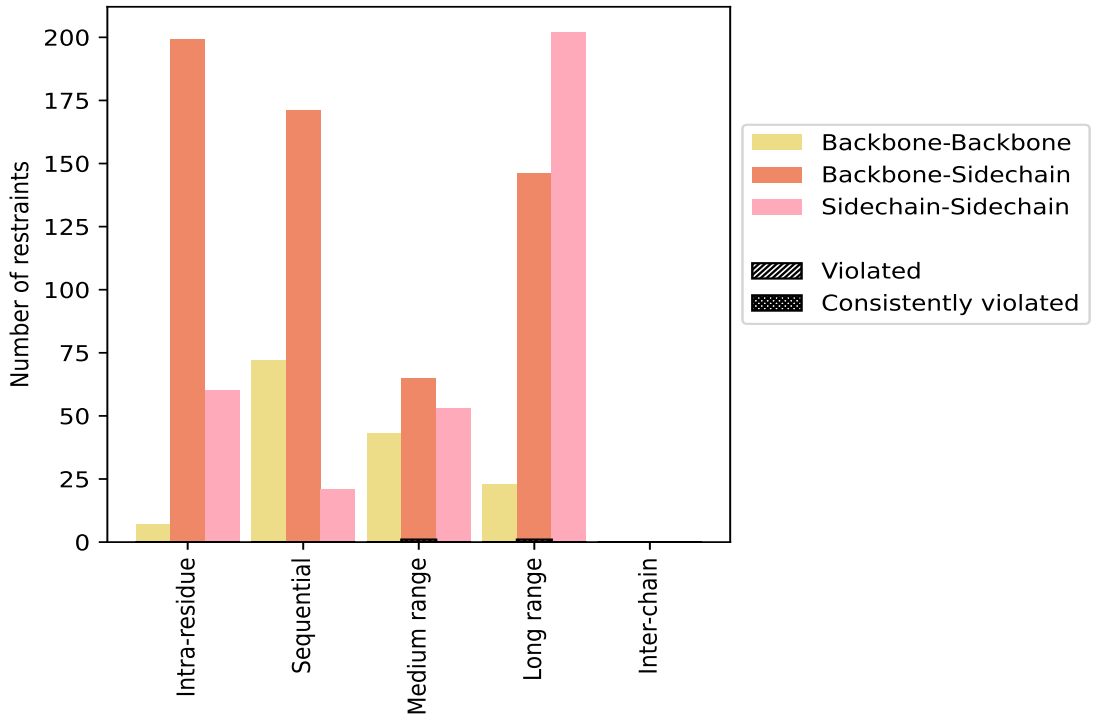
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	266	25.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	7	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	199	18.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	60	5.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	264	24.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	72	6.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	171	16.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	21	2.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	161	15.2	1	0.6	0.1	0	0.0	0.0
Backbone-Backbone	43	4.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	65	6.1	1	1.5	0.1	0	0.0	0.0
Sidechain-Sidechain	53	5.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	371	34.9	1	0.3	0.1	0	0.0	0.0
Backbone-Backbone	23	2.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	146	13.7	1	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	202	19.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1062	100.0	2	0.2	0.2	0	0.0	0.0
Backbone-Backbone	145	13.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	581	54.7	2	0.3	0.2	0	0.0	0.0
Sidechain-Sidechain	336	31.6	0	0.0	0.0	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	1	0	0	1	0.12	0.12	0.0	0.12
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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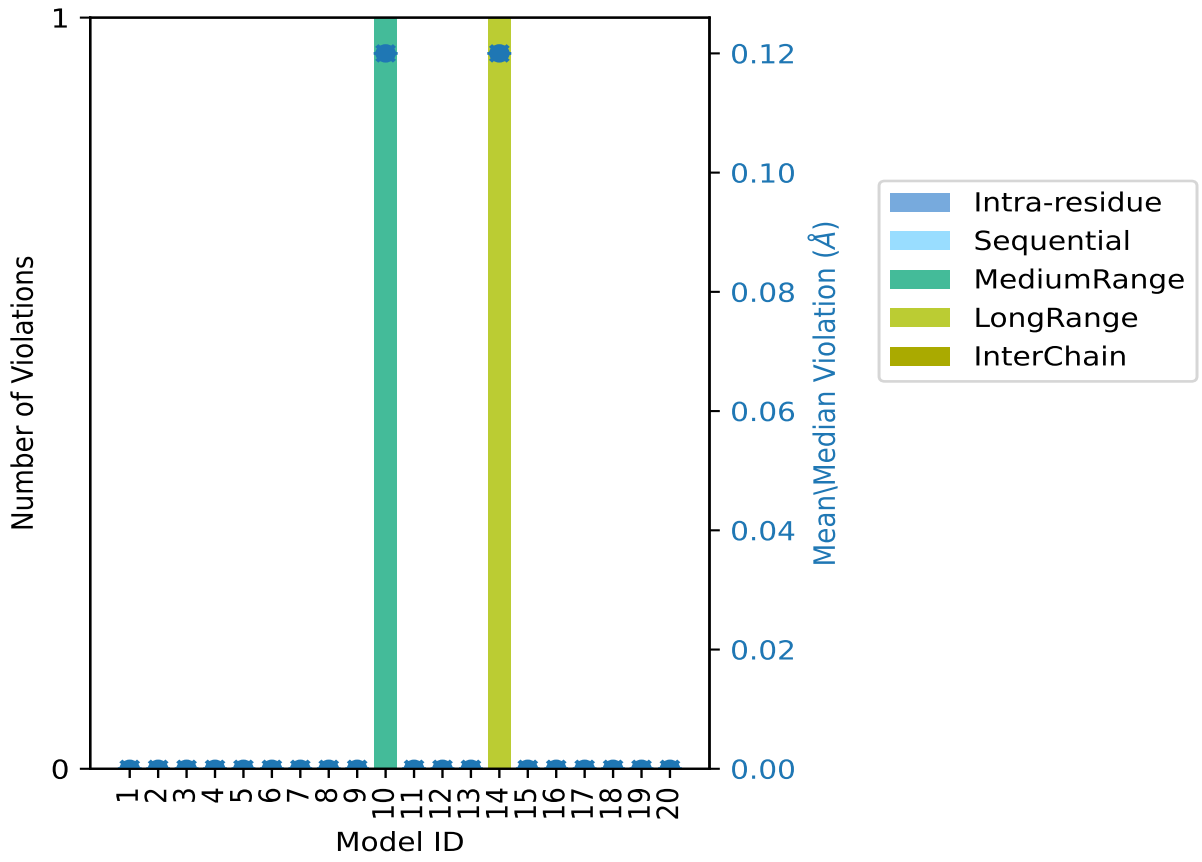
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	1	0	1	0.12	0.12	0.0	0.12
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model (i)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

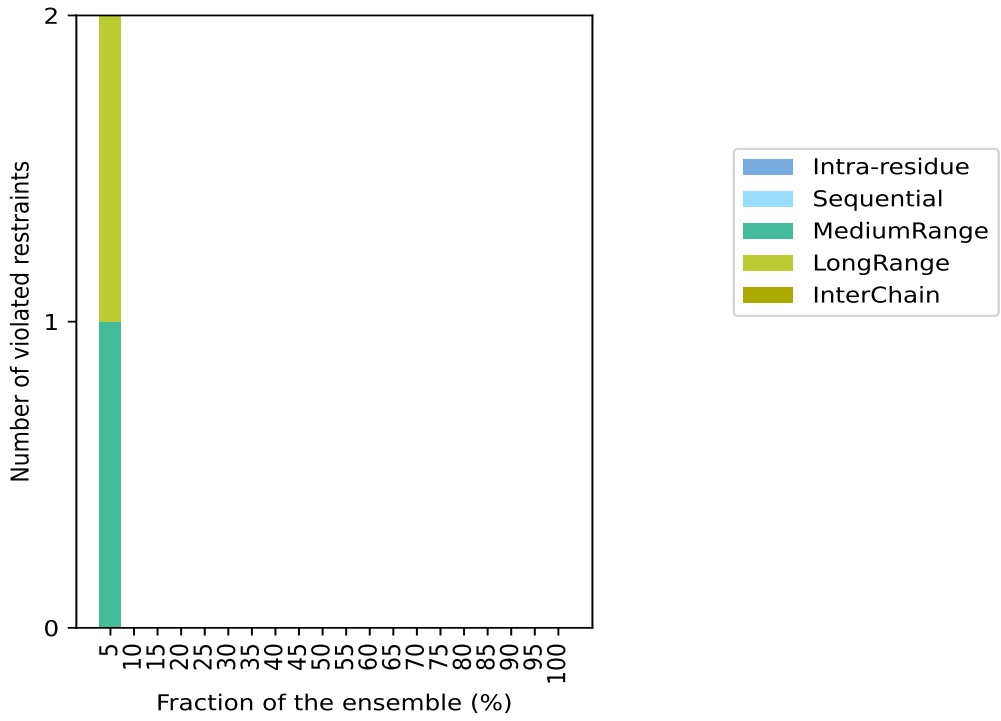
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1060(IR:266, SQ:264, MR:160, LR:370, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	1	1	0	2	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

No violations found

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
Data insufficient to plot histogram

9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:A:3:MET:HE1	1:A:17:ASN:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:A:3:MET:HE2	1:A:17:ASN:H	14	0.12
(1,455)	1:A:3:MET:HE3	1:A:17:ASN:H	14	0.12
(1,1034)	1:A:46:LEU:HA	1:A:49:ASN:HB2	10	0.12
(1,1034)	1:A:46:LEU:HA	1:A:49:ASN:HB3	10	0.12

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value