Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1XY5
Title	:	NMR strcutre of sst1-selective somatostatin (SRIF) analog 1
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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:

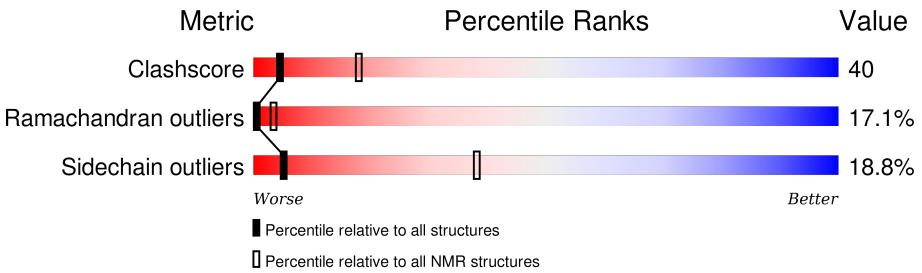
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 36%.

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	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	12	58% 8% 33%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:5, A:8-A:9, A:11-A:12 (8)	0.47	8

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 5, 7, 8, 9
2	2, 4, 6
Single-model clusters	10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 224 atoms, of which 106 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SST1-selective somatosatin analog.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	12	224	82	106	17	17	2	0

4 Residue-property plots (i)

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: SST1-selective somatosatin analog

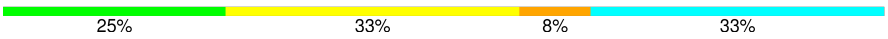
Chain A:

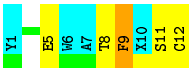
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: SST1-selective somatosatin analog

Chain A: 



4.2.2 Score per residue for model 2

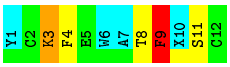
- Molecule 1: SST1-selective somatosatin analog

Chain A:

4.2.3 Score per residue for model 3

- Molecule 1: SST1-selective somatosatin analog

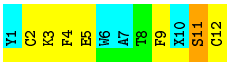
Chain A: 25% 25% 8% 8% 33%



4.2.4 Score per residue for model 4

- Molecule 1: SST1-selective somatosatin analog

Chain A: 8% 50% 8% 33%



4.2.5 Score per residue for model 5

- Molecule 1: SST1-selective somatosatin analog

Chain A: 8% 42% 17% 33%

4.2.6 Score per residue for model 6

- Molecule 1: SST1-selective somatosatin analog

Chain A: 17% 42% 8% 33%

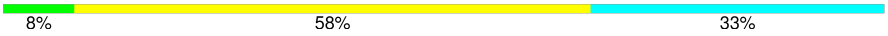
4.2.7 Score per residue for model 7

- Molecule 1: SST1-selective somatosatin analog

Chain A: 8% 33% 25% 33%

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: SST1-selective somatosatin analog

Chain A: 

4.2.9 Score per residue for model 9

- Molecule 1: SST1-selective somatosatin analog

Chain A:

4.2.10 Score per residue for model 10

- Molecule 1: SST1-selective somatosatin analog

Chain A:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Torsion angle dynamics.*

Of the 20 calculated structures, 10 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
DYANA	structure solution	1.0.6
DYANA	refinement	1.0.6

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 6423
Number of chemical shift lists	1
Total number of shifts	82
Number of shifts mapped to atoms	69
Number of unparsed shifts	0
Number of shifts with mapping errors	13
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	36%

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: IAM, DTR, 193

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	64	56	57	5±1
All	All	640	560	570	48

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:CYS:SG	1:A:12:CYS:O	0.95	2.24	2	1
1:A:11:SER:O	1:A:12:CYS:O	0.94	1.86	10	6
1:A:9:PHE:HZ	1:A:12:CYS:O	0.85	1.52	7	1
1:A:3:LYS:N	1:A:12:CYS:O	0.82	2.12	4	2
1:A:9:PHE:CZ	1:A:12:CYS:O	0.80	2.34	7	1
1:A:2:CYS:HA	1:A:12:CYS:O	0.64	1.92	6	2
1:A:9:PHE:CZ	1:A:11:SER:O	0.60	2.54	5	5
1:A:9:PHE:CE2	1:A:11:SER:O	0.59	2.55	3	1
1:A:2:CYS:CA	1:A:12:CYS:O	0.54	2.56	6	2
1:A:9:PHE:CD1	1:A:9:PHE:C	0.51	2.84	3	4
1:A:9:PHE:CE1	1:A:11:SER:O	0.46	2.68	1	3
1:A:3:LYS:O	1:A:4:PHE:O	0.46	2.34	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:CYS:CB	1:A:12:CYS:O	0.46	2.64	2	1
1:A:8:THR:O	1:A:8:THR:HG22	0.45	2.12	9	2
1:A:8:THR:O	1:A:9:PHE:C	0.45	2.55	5	7
1:A:3:LYS:O	1:A:9:PHE:CE1	0.45	2.69	4	1
1:A:8:THR:HG22	1:A:8:THR:O	0.44	2.13	1	2
1:A:11:SER:C	1:A:12:CYS:O	0.44	2.55	8	1
1:A:3:LYS:C	1:A:4:PHE:CD2	0.41	2.94	10	1
1:A:2:CYS:SG	1:A:12:CYS:C	0.41	2.99	4	3
1:A:11:SER:O	1:A:12:CYS:C	0.41	2.59	6	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	7/12 (58%)	4±1 (59±15%)	2±1 (24±11%)	1±1 (17±12%)	0 3
All	All	70/120 (58%)	41 (59%)	17 (24%)	12 (17%)	0 3

All 5 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	11	SER	6
1	A	2	CYS	2
1	A	9	PHE	2
1	A	4	PHE	1
1	A	5	GLU	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	8/9 (89%)	7±1 (81±17%)	2±1 (19±17%)	5 38
All	All	80/90 (89%)	65 (81%)	15 (19%)	5 38

All 5 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	5	GLU	5
1	A	4	PHE	3
1	A	9	PHE	3
1	A	3	LYS	3
1	A	11	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	193	A	10	1	9,11,12	2.40±0.01	1±0 (11±0%)
1	DTR	A	6	1	11,15,16	1.02±0.01	0±0 (0±0%)
1	IAM	A	7	1	14,16,17	1.13±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	193	A	10	1	8,12,14	2.73±0.00	1±0 (12±0%)
1	DTR	A	6	1	10,20,22	1.98±0.01	0±0 (0±0%)
1	IAM	A	7	1	18,20,22	1.17±0.00	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	193	A	10	1	-	0±0,9,11,13	0±0,0,0,0
1	DTR	A	6	1	-	0±0,3,6,8	0±0,2,2,2
1	IAM	A	7	1	-	0±0,9,11,13	0±0,1,1,1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	10	193	CE-ND	6.23	1.48	1.33	3	10

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	10	193	CG-ND-CE	6.73	109.45	122.79	8	10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 36% for the well-defined parts and 35% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6423

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	82
Number of shifts mapped to atoms	69
Number of unparsed shifts	0
Number of shifts with mapping errors	13
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atoms in chemical component dictionary. All 7 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	10	193	HG3	2.164	0.0	1
A	7	IAM	HK	1.112	0.004	1
A	7	IAM	HB2	3.089	0.002	1
A	10	193	HT3	3.026	0.001	1
A	7	IAM	HT	4.019	0.004	1
A	7	IAM	HB3	2.664	0.0	1
A	10	193	HZ3	1.527	0.006	1

- Residue not found in structure. All 6 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	5	DHN	HG3	1.842	0.0	1
A	5	DHN	HA	4.234	0.001	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	5	DHN	HB3	1.588	0.0	1
A	5	DHN	H	8.21	0.0	1
A	5	DHN	HG2	1.92	0.001	1
A	5	DHN	HB2	1.765	0.003	1

7.1.2 Chemical shift referencing (i)

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

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 36%, i.e. 35 atoms were assigned a chemical shift out of a possible 97. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	14/40 (35%)	14/16 (88%)	0/16 (0%)	0/8 (0%)
Sidechain	15/39 (38%)	15/24 (62%)	0/14 (0%)	0/1 (0%)
Aromatic	6/18 (33%)	6/10 (60%)	0/8 (0%)	0/0 (—%)
Overall	35/97 (36%)	35/50 (70%)	0/38 (0%)	0/9 (0%)

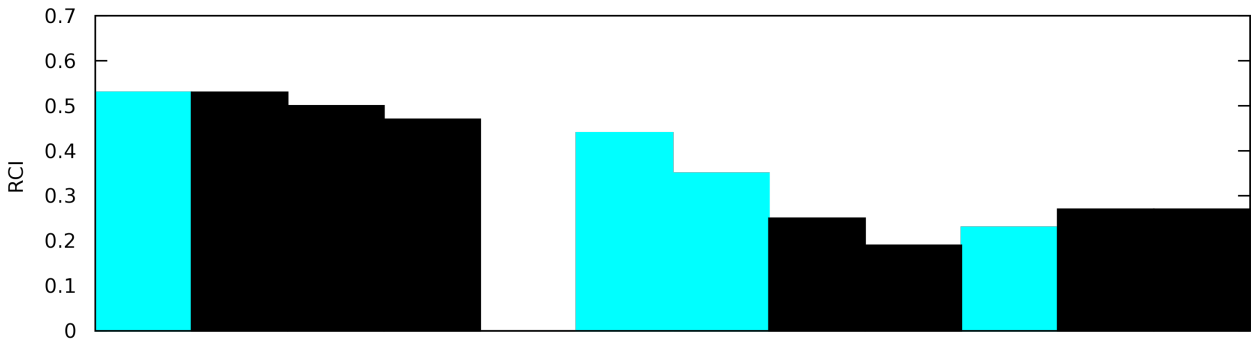
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 40 atoms were assigned a chemical shift out of a possible 113. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	15/45 (33%)	15/18 (83%)	0/18 (0%)	0/9 (0%)
Sidechain	17/42 (40%)	17/26 (65%)	0/15 (0%)	0/1 (0%)
Aromatic	8/26 (31%)	8/14 (57%)	0/12 (0%)	0/0 (—%)
Overall	40/113 (35%)	40/58 (69%)	0/45 (0%)	0/10 (0%)

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: