wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2E5O
Title	:	'Solution structure of the TRIP_4C domain of target of activating signal cointegrator 1
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This is a wwPDB NMR Structure Validation Summary 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:

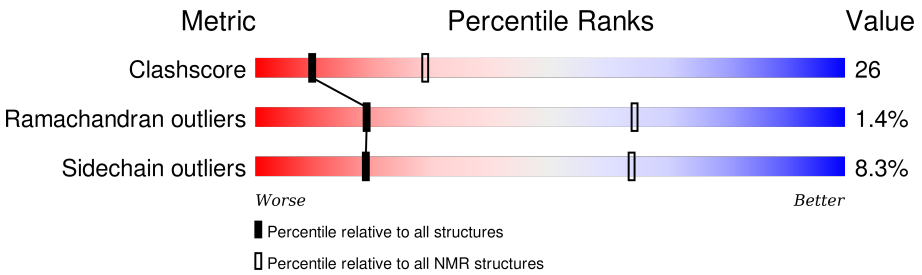
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	154	48% 43% • 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:7-A:147 (141)	0.13	1

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 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2452 atoms, of which 1233 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Activating signal cointegrator 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	154	2452	779	1233	216	217	7	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q15650
A	2	SER	-	EXPRESSION TAG	UNP Q15650
A	3	SER	-	EXPRESSION TAG	UNP Q15650
A	4	GLY	-	EXPRESSION TAG	UNP Q15650
A	5	SER	-	EXPRESSION TAG	UNP Q15650
A	6	SER	-	EXPRESSION TAG	UNP Q15650
A	7	GLY	-	EXPRESSION TAG	UNP Q15650

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: Activating signal cointegrator 1

Chain A: 48% 43% • 8%

G1 S2 S3 G4 S5 S6 G7 W8 V12 H13 Q14 P15 W16 A17 L20 R26 V27 E28 G29 R30 S31 W32 Y33 T34 W41 A44 T45 K48 Q52 E53 V54 L57 Q58 R62 G66 K67 D68 V69 E70 F71 P72 Y75 P76 L80 L81 G82 C83

I87 L90 S91 Q92 K93 Q94 F95 K96 E97 I102 S103 Q104 E105 S106 D107 S108 V111 F112 I113 N116 P117 M120 F124 K127 K131 I132 W133 D136 S137 K138 I139 H140 Q141 G142 A143 K144 K145 M148 K149 Q150 N151 K152 A153 V154

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Activating signal cointegrator 1

Chain A: 46% 44% • 8%

G1 S2 S3 G4 S5 S6 G7 W8 V12 H13 Q14 P15 W16 A17 S18 L19 L20 V21 R22 R25 E28 G29 R30 S31 W32 Y33 T34 P35 H36 W41 A44 T45 K48 P49 Q52 E53 V54 L57 Q58 R62 G66 K67 D68 V69 E70 F71 P72 Y75 P76

L80 L81 G82 C83 L86 I87 D88 C89 L90 S91 Q92 K93 Q94 F95 K96 E97 I102 S103 Q104 E105 S106 D107 S108 V111 F112 I113 N116 P117 V121 F124 K127 K131 I132 W133 D136 S137 K138 I139 H140 Q141 G142 A143 K144 M148 K149 Q150 N151 K152 A153

V154

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function.*

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided. 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	1132	1144	1144	59±6
All	All	22640	22880	22880	1177

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 26.

5 of 213 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:GLY:O	1:A:69:VAL:HG13	0.95	1.62	2	20
1:A:95:PHE:CD2	1:A:111:VAL:HG21	0.78	2.14	15	14
1:A:54:VAL:HG12	1:A:58:GLN:NE2	0.77	1.95	6	14
1:A:41:TRP:CZ3	1:A:143:ALA:HB1	0.75	2.16	5	13
1:A:102:ILE:HG22	1:A:105:GLU:CD	0.75	2.03	6	15

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	141/154 (92%)	119±2 (84±1%)	20±3 (14±2%)	2±1 (1±1%)	19 64
All	All	2820/3080 (92%)	2374 (84%)	407 (14%)	39 (1%)	19 64

5 of 7 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	THR	10
1	A	92	GLN	8
1	A	67	LYS	7
1	A	16	TRP	6
1	A	146	GLY	6

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	125/135 (93%)	115±2 (92±2%)	10±2 (8±2%)	19 64
All	All	2500/2700 (93%)	2292 (92%)	208 (8%)	19 64

5 of 33 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	87	ILE	20
1	A	113	ILE	20
1	A	116	ASN	20
1	A	80	LEU	20
1	A	67	LYS	14

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)

No chemical shift data were provided