



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2KOT / pdb\_00002kot  
Title : Solution structure of S100A13 with a drug amlexanox  
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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](mailto: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 types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**  
Mogul : 2022.3.0, CSD as543be (2022)  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

## 2 Ensemble composition and analysis

This entry contains 18 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: *fewest violations*.

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:1-A:98, B:1-B:98 (196)	0.52	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 4 clusters and 2 single-model clusters were found.

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

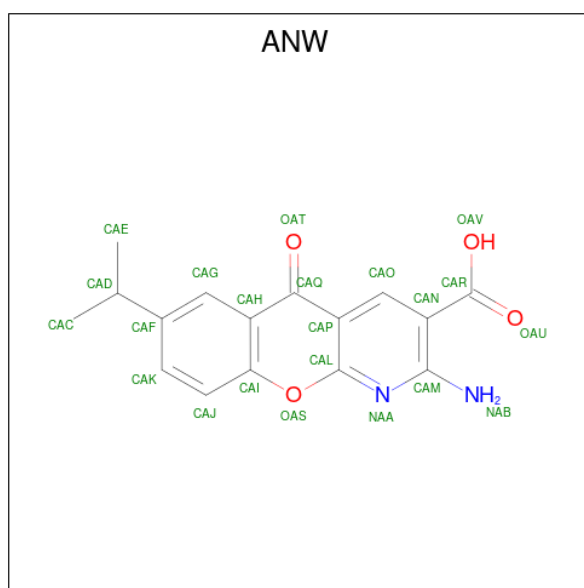
### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3349 atoms, of which 1692 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein S100-A13.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	98	1640	512	834	136	156	2	0
1	B	98	1639	512	832	136	157	2	0

- Molecule 2 is 2-amino-7-(1-methylethyl)-5-oxo-5H-chromeno[2,3-b]pyridine-3-carboxylic acid (CCD ID: ANW) (formula: C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	35	16	13	2	4
2	B	1	35	16	13	2	4

## 4 Residue-property plots

### 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: Protein S100-A13

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Protein S100-A13

Chain B:  100%

There are no outlier residues in this chain.

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

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Protein S100-A13

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Protein S100-A13

Chain B:  100%

There are no outlier residues in this chain.

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, DGSA-distance geometry simulated annealing, distance geometry, simulated annealing.*

Of the 200 calculated structures, 18 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	Classification	Version
ARIA	structure solution	2.2
ARIA	refinement	2.2

No chemical shift data was provided.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.2 Too-close contacts [i](#)

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### 6.3 Torsion angles [i](#)

#### 6.3.1 Protein backbone [i](#)

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#### 6.3.2 Protein sidechains [i](#)

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#### 6.3.3 RNA [i](#)

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### 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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### 6.5 Carbohydrates [i](#)

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### 6.6 Ligand geometry [i](#)

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### 6.7 Other polymers [i](#)

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## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided