



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:35 pm BST

PDB ID : 2KBM
Title : Ca-S100A1 interacting with TRTK12
Authors : Wright, N.T.; Varney, K.M.; Cannon, B.R.; Morgan, M.; Weber, D.J.
Deposited on : 2008-12-02

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

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	X:5-X:12, Y:5-Y:12, A:1-A:90, B:2-B:90 (195)	0.45	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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3322 atoms, of which 1644 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called F-actin-capping protein subunit alpha-2.

Mol	Chain	Residues	Atoms					Trace
1	X	12	Total	C	H	N	O	0
			217	66	113	19	19	
1	Y	12	Total	C	H	N	O	0
			217	66	113	19	19	

- Molecule 2 is a protein called Protein S100-A1.

Mol	Chain	Residues	Atoms					Trace	
2	A	93	Total	C	H	N	O	S	0
			1442	462	709	115	153	3	
2	B	93	Total	C	H	N	O	S	0
			1442	462	709	115	153	3	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

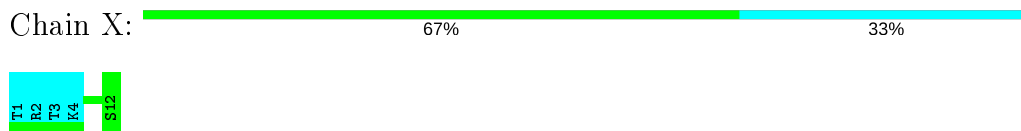
Mol	Chain	Residues	Atoms	
3	B	2	Total	Ca
			2	2
3	A	2	Total	Ca
			2	2

4 Residue-property plots

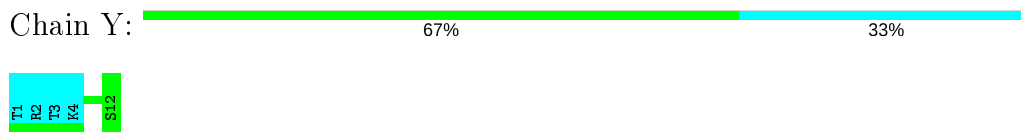
4.1 Average score per residue in the NMR ensemble

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.

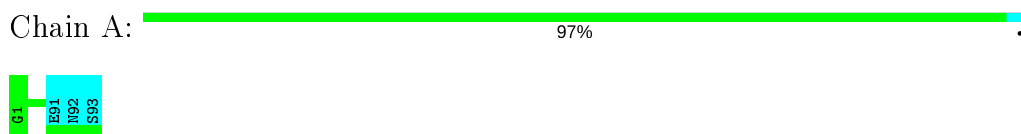
- Molecule 1: F-actin-capping protein subunit alpha-2



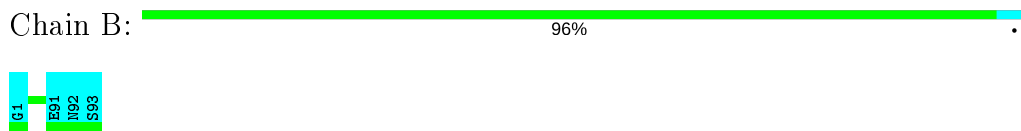
- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 2: Protein S100-A1



- Molecule 2: Protein S100-A1



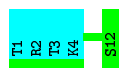
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

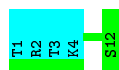
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X:  67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y:  67% 33%



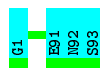
- Molecule 2: Protein S100-A1

Chain A:  97%



- Molecule 2: Protein S100-A1

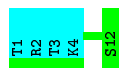
Chain B:  96%



4.2.2 Score per residue for model 2

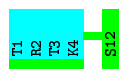
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X:  67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y:  67% 33%

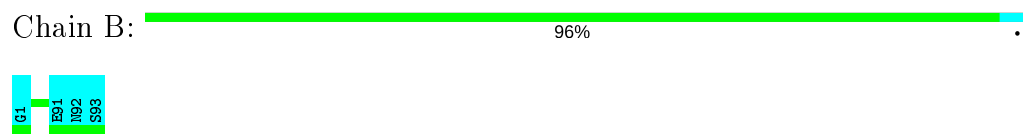


- Molecule 2: Protein S100-A1

Chain A:  97%

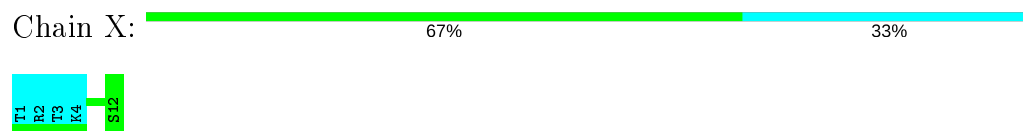


- Molecule 2: Protein S100-A1

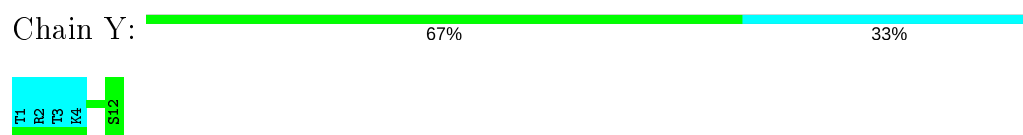


4.2.3 Score per residue for model 3

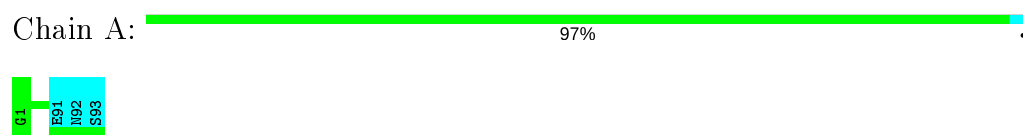
- Molecule 1: F-actin-capping protein subunit alpha-2



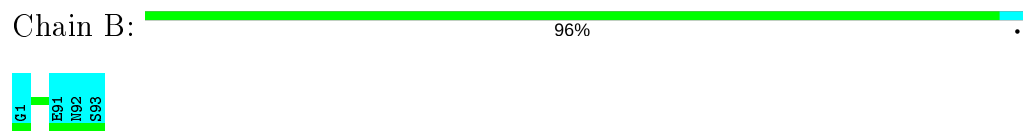
- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 2: Protein S100-A1

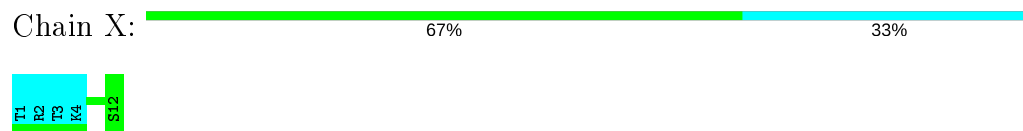


- Molecule 2: Protein S100-A1



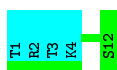
4.2.4 Score per residue for model 4

- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 1: F-actin-capping protein subunit alpha-2





- Molecule 2: Protein S100-A1

Chain A: 97%



- Molecule 2: Protein S100-A1

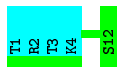
Chain B: 96%



4.2.5 Score per residue for model 5

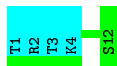
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X: 67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y: 67% 33%



- Molecule 2: Protein S100-A1

Chain A: 97%



- Molecule 2: Protein S100-A1

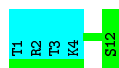
Chain B: 96%



4.2.6 Score per residue for model 6

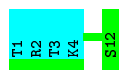
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X:  67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y:  67% 33%



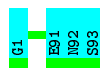
- Molecule 2: Protein S100-A1

Chain A:  97%



- Molecule 2: Protein S100-A1

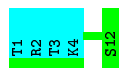
Chain B:  96%




4.2.7 Score per residue for model 7

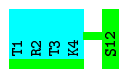
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X:  67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y:  67% 33%

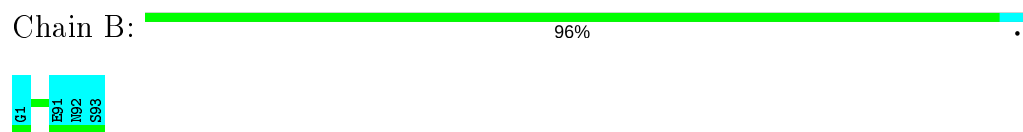


- Molecule 2: Protein S100-A1

Chain A:  97%

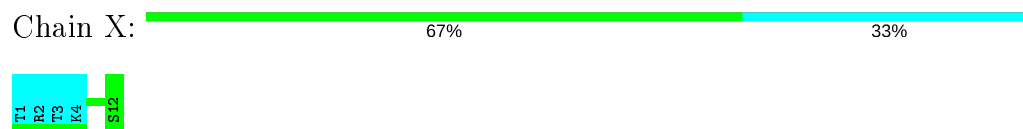


- Molecule 2: Protein S100-A1

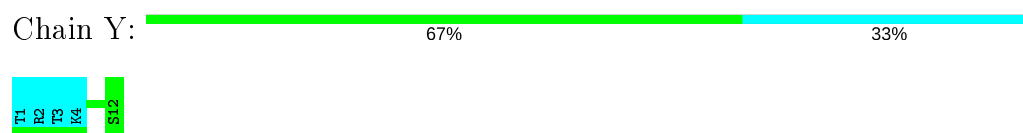


4.2.8 Score per residue for model 8

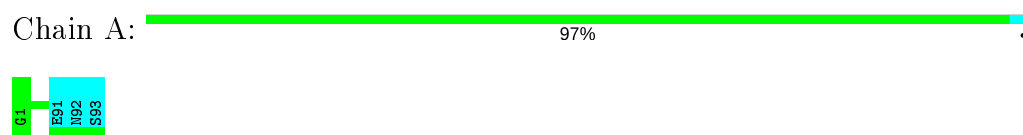
- Molecule 1: F-actin-capping protein subunit alpha-2



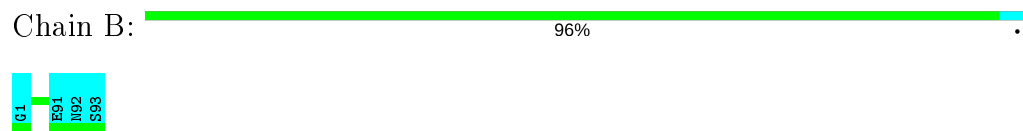
- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 2: Protein S100-A1

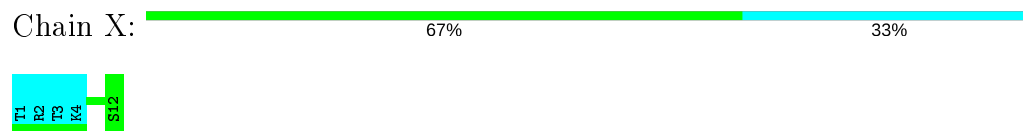


- Molecule 2: Protein S100-A1



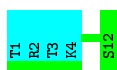
4.2.9 Score per residue for model 9

- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 1: F-actin-capping protein subunit alpha-2





- Molecule 2: Protein S100-A1

Chain A: 97%



- Molecule 2: Protein S100-A1

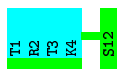
Chain B: 96%



4.2.10 Score per residue for model 10

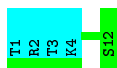
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X: 67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y: 67% 33%



- Molecule 2: Protein S100-A1

Chain A: 97%



- Molecule 2: Protein S100-A1

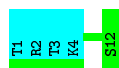
Chain B: 96%



4.2.11 Score per residue for model 11

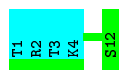
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X:  67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y:  67% 33%



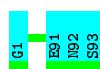
- Molecule 2: Protein S100-A1

Chain A:  97%



- Molecule 2: Protein S100-A1

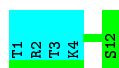
Chain B:  96%



4.2.12 Score per residue for model 12

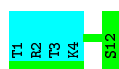
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X:  67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y:  67% 33%

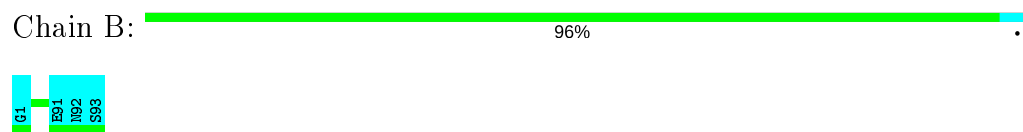


- Molecule 2: Protein S100-A1

Chain A:  97%

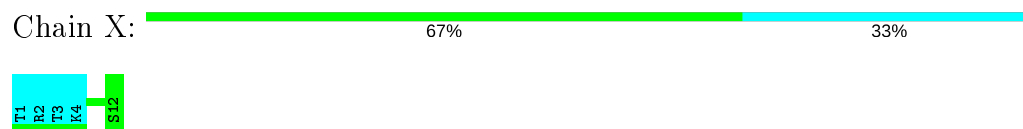


- Molecule 2: Protein S100-A1

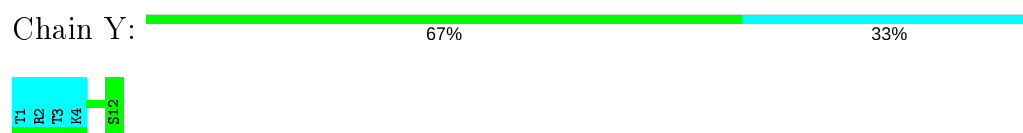


4.2.13 Score per residue for model 13

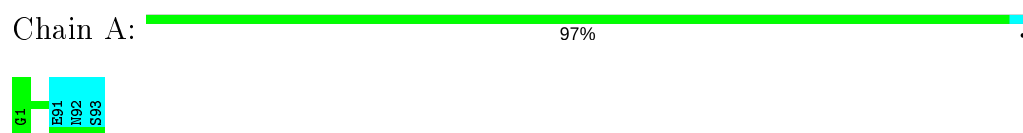
- Molecule 1: F-actin-capping protein subunit alpha-2



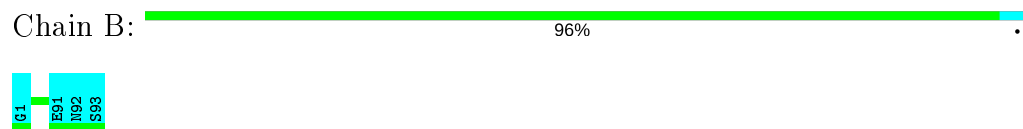
- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 2: Protein S100-A1

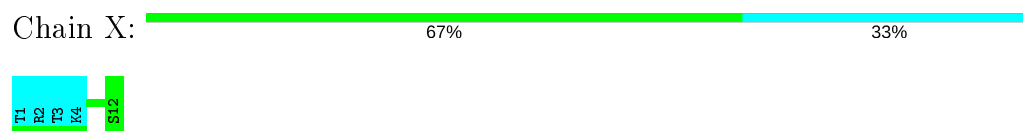


- Molecule 2: Protein S100-A1



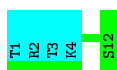
4.2.14 Score per residue for model 14

- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 1: F-actin-capping protein subunit alpha-2





- Molecule 2: Protein S100-A1

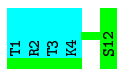


- Molecule 2: Protein S100-A1

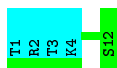


4.2.15 Score per residue for model 15

- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 2: Protein S100-A1



- Molecule 2: Protein S100-A1



4.2.16 Score per residue for model 16

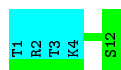
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X:  67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y:  67% 33%



- Molecule 2: Protein S100-A1

Chain A:  97%



- Molecule 2: Protein S100-A1

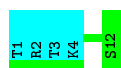
Chain B:  96%



4.2.17 Score per residue for model 17

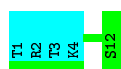
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X:  67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y:  67% 33%

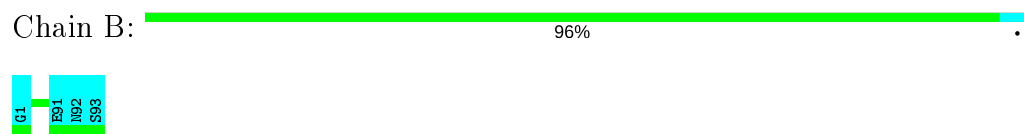


- Molecule 2: Protein S100-A1

Chain A:  97%

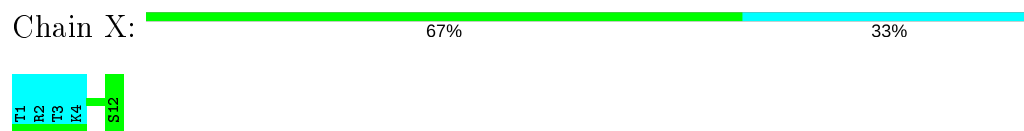


- Molecule 2: Protein S100-A1

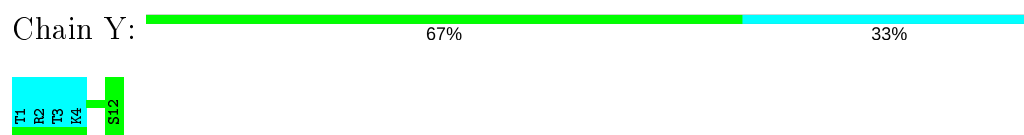


4.2.18 Score per residue for model 18

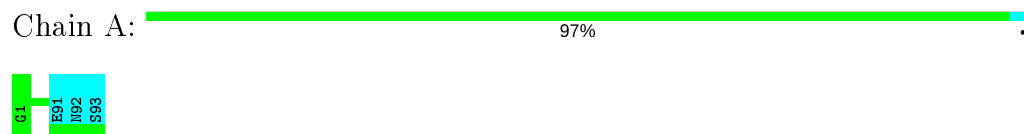
- Molecule 1: F-actin-capping protein subunit alpha-2



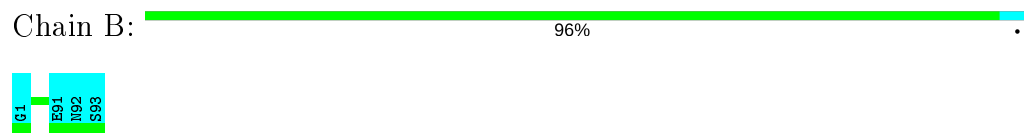
- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 2: Protein S100-A1

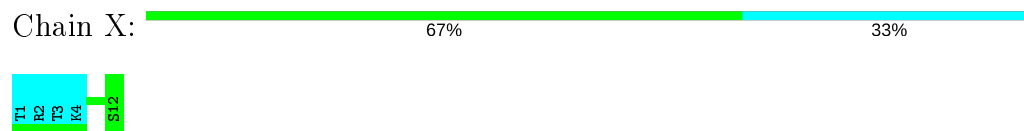


- Molecule 2: Protein S100-A1



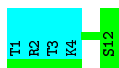
4.2.19 Score per residue for model 19

- Molecule 1: F-actin-capping protein subunit alpha-2



- Molecule 1: F-actin-capping protein subunit alpha-2





- Molecule 2: Protein S100-A1

Chain A: 97%



- Molecule 2: Protein S100-A1

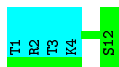
Chain B: 96%



4.2.20 Score per residue for model 20

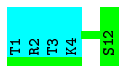
- Molecule 1: F-actin-capping protein subunit alpha-2

Chain X: 67% 33%



- Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y: 67% 33%



- Molecule 2: Protein S100-A1

Chain A: 97%



- Molecule 2: Protein S100-A1

Chain B: 96%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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](#)

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

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
All	All	31160	30460	0	-

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 -.

There are no clashes.

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	X	0	-	-	-	-
1	Y	0	-	-	-	-
2	A	0	-	-	-	-
2	B	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	0	-	-	-	-

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	X	0	-	-	-
1	Y	0	-	-	-
2	A	0	-	-	-
2	B	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

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 4 ligands modelled in this entry, 4 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

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided