



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:43 AM BST

PDB ID : 2ODD
Title : Solution structure of the MYND domain from AML1-ETO complexed with SMRT, a corepressor
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Deposited on : 2006-12-22

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 ⓘ 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
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

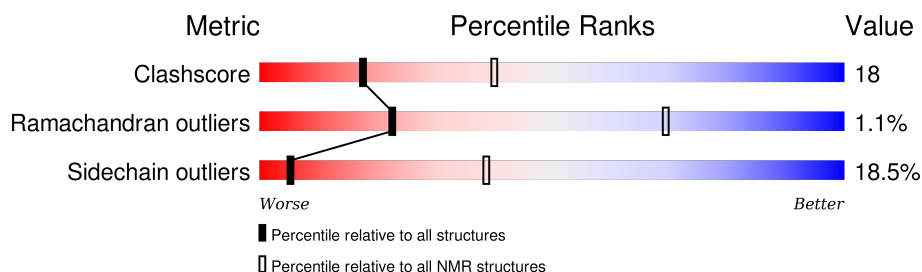
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	B	17	<div> <div>35%</div> <div>12%</div> <div>29%</div> <div>24%</div> </div>
2	A	64	<div> <div>31%</div> <div>25%</div> <div>•</div> <div>19%</div> <div>22%</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 25 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: *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	B:1104-B:1111, A:662-A:699 (46)	0.07	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 5 single-model clusters were found.

Cluster number	Models
1	2, 5, 13, 16, 19
2	7, 15, 18, 21, 24
3	6, 8, 9, 11, 23
4	4, 12, 20
5	10, 25
Single-model clusters	1; 3; 14; 17; 22

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 925 atoms, of which 440 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SMRT.

Mol	Chain	Residues	Atoms					Trace
1	B	13	Total	C	H	N	O	0
			192	59	100	15	18	

- Molecule 2 is a protein called Protein CBFA2T1.

Mol	Chain	Residues	Atoms						Trace
2	A	50	Total	C	H	N	O	S	0
			731	230	340	76	78	7	

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	644	GLU	-	CLONING ARTIFACT	UNP Q06455
A	645	ASN	-	CLONING ARTIFACT	UNP Q06455
A	646	LEU	-	CLONING ARTIFACT	UNP Q06455
A	647	TYR	-	CLONING ARTIFACT	UNP Q06455
A	648	PHE	-	CLONING ARTIFACT	UNP Q06455
A	649	GLN	-	CLONING ARTIFACT	UNP Q06455
A	650	GLY	-	CLONING ARTIFACT	UNP Q06455
A	651	GLU	-	CLONING ARTIFACT	UNP Q06455
A	652	ASN	-	CLONING ARTIFACT	UNP Q06455
A	653	LEU	-	CLONING ARTIFACT	UNP Q06455
A	654	TYR	-	CLONING ARTIFACT	UNP Q06455
A	655	PHE	-	CLONING ARTIFACT	UNP Q06455
A	656	GLN	-	CLONING ARTIFACT	UNP Q06455
A	657	GLY	-	CLONING ARTIFACT	UNP Q06455

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

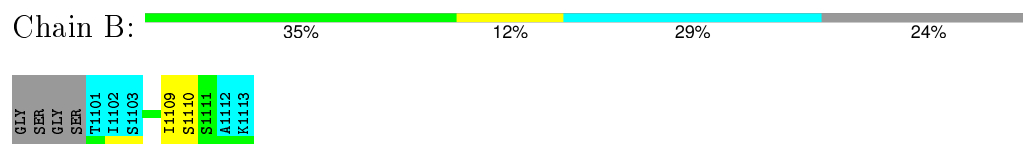
Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

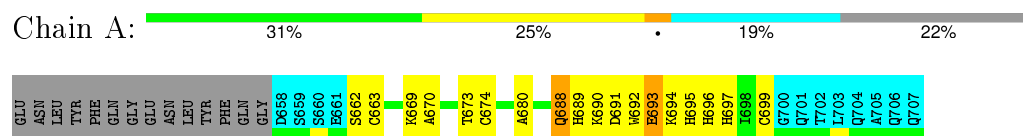
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA 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: SMRT



- Molecule 2: Protein CBFA2T1

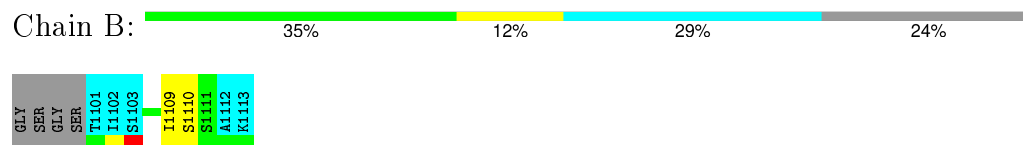


4.2 Scores per residue for each member of the ensemble

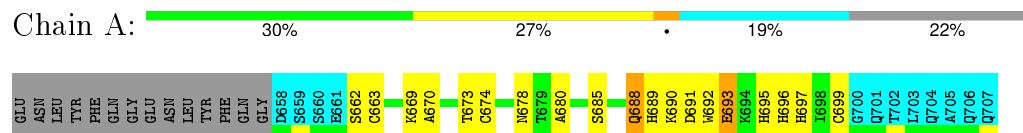
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: SMRT

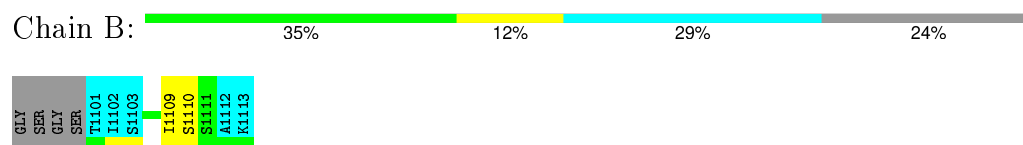


- Molecule 2: Protein CBFA2T1

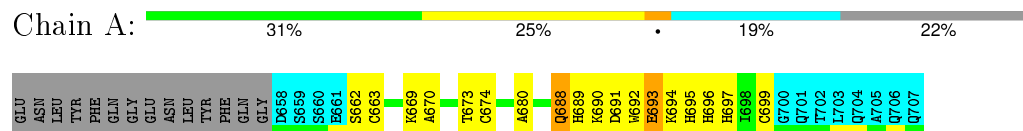


4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: SMRT

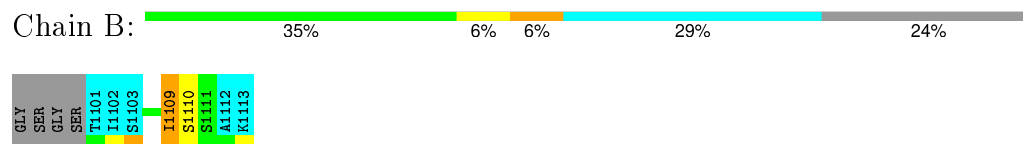


- Molecule 2: Protein CBFA2T1

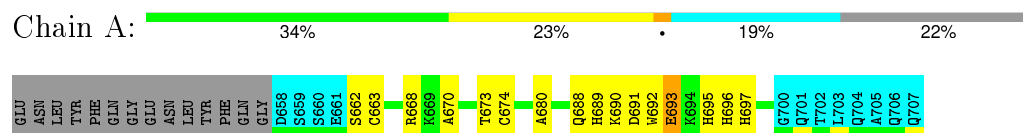


4.2.3 Score per residue for model 3

- Molecule 1: SMRT

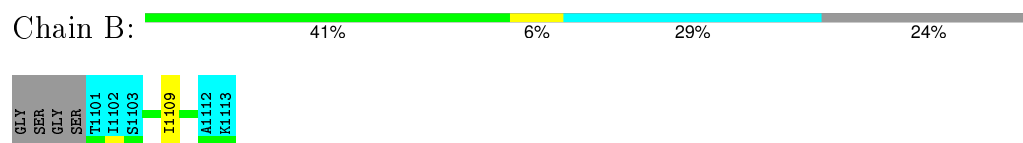


- Molecule 2: Protein CBFA2T1

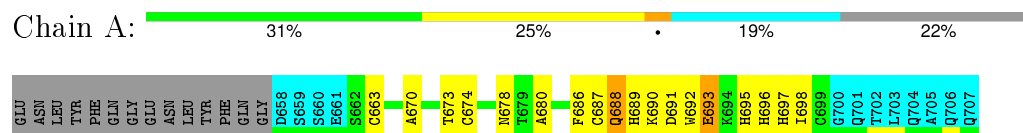


4.2.4 Score per residue for model 4

- Molecule 1: SMRT

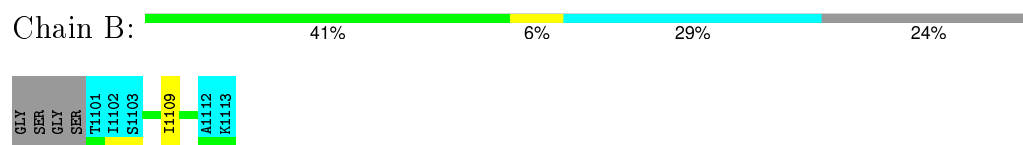


- Molecule 2: Protein CBFA2T1

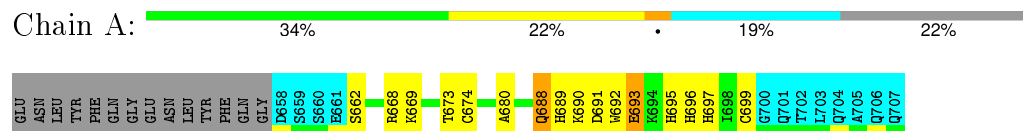


4.2.5 Score per residue for model 5

- Molecule 1: SMRT

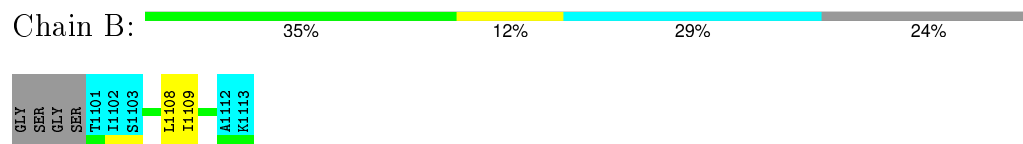


- Molecule 2: Protein CBFA2T1

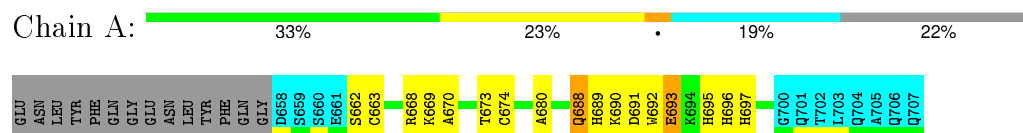


4.2.6 Score per residue for model 6

- Molecule 1: SMRT

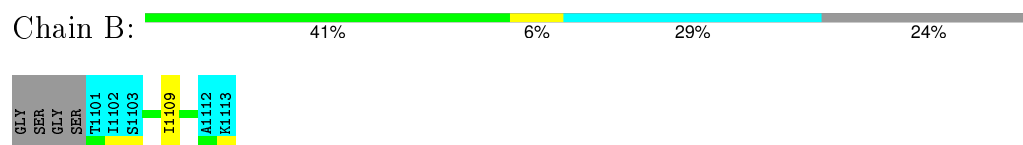


- Molecule 2: Protein CBFA2T1

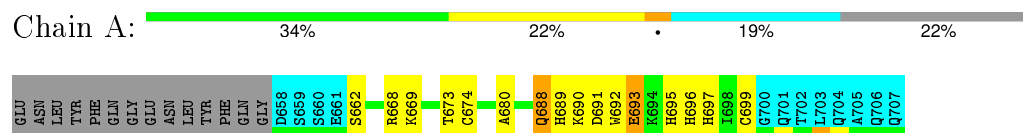


4.2.7 Score per residue for model 7

- Molecule 1: SMRT

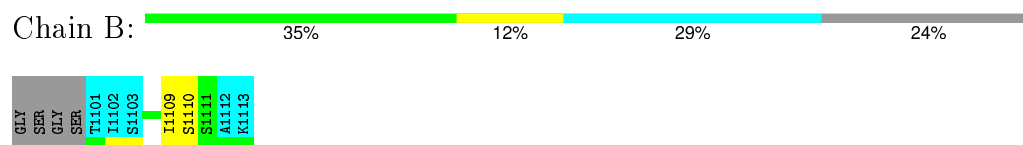


- Molecule 2: Protein CBFA2T1

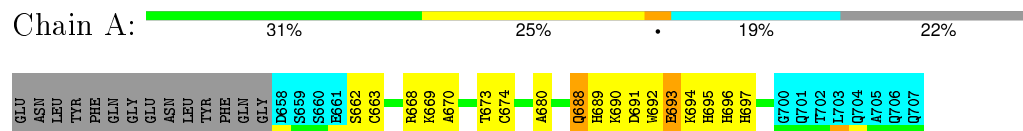


4.2.8 Score per residue for model 8

- Molecule 1: SMRT

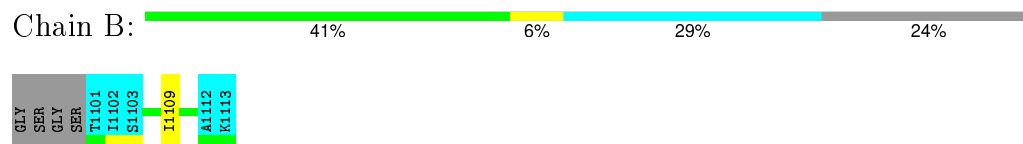


- Molecule 2: Protein CBFA2T1

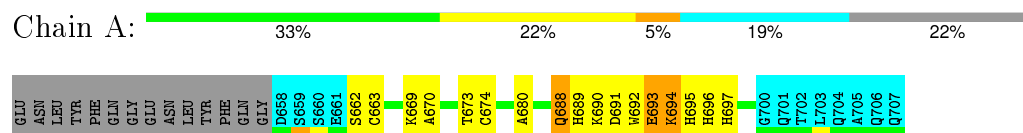


4.2.9 Score per residue for model 9

- Molecule 1: SMRT

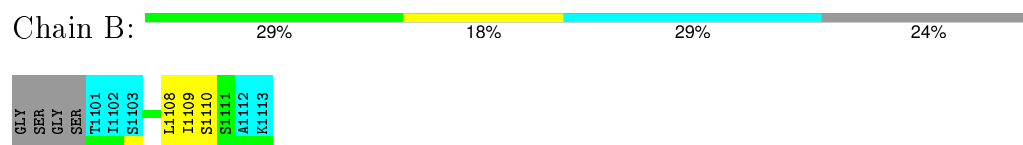


- Molecule 2: Protein CBFA2T1

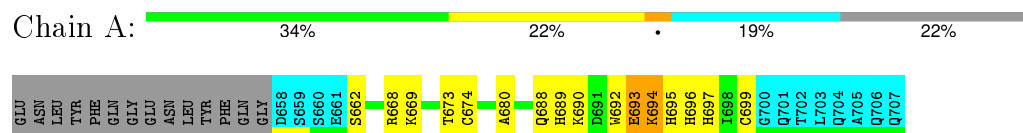


4.2.10 Score per residue for model 10

- Molecule 1: SMRT

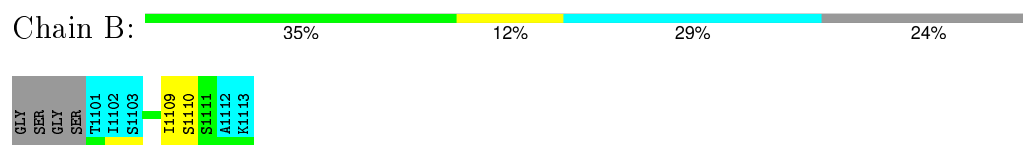


- Molecule 2: Protein CBFA2T1

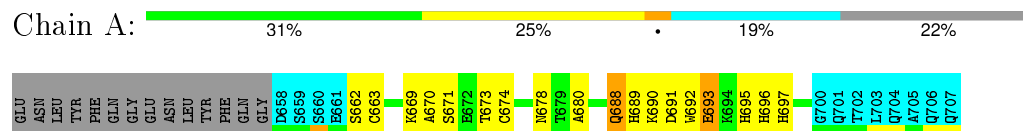


4.2.11 Score per residue for model 11

- Molecule 1: SMRT

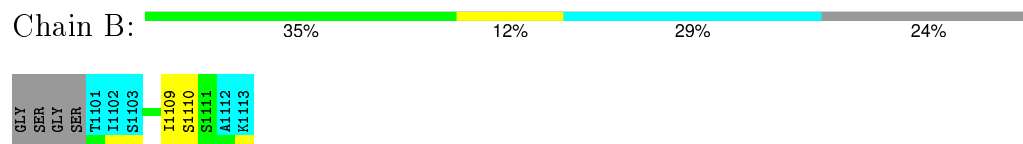


- Molecule 2: Protein CBFA2T1

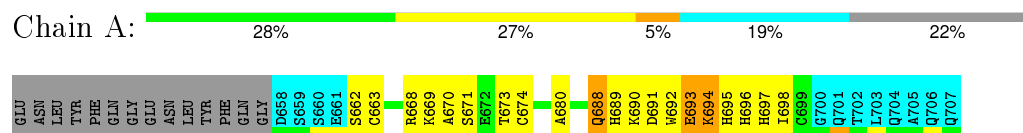


4.2.12 Score per residue for model 12

- Molecule 1: SMRT

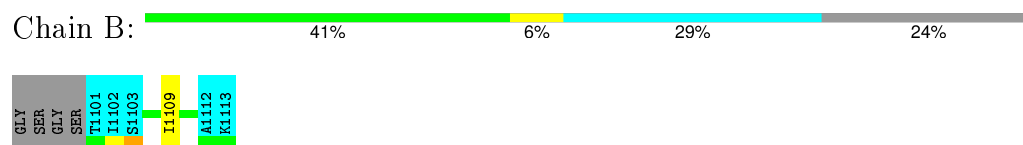


- Molecule 2: Protein CBFA2T1

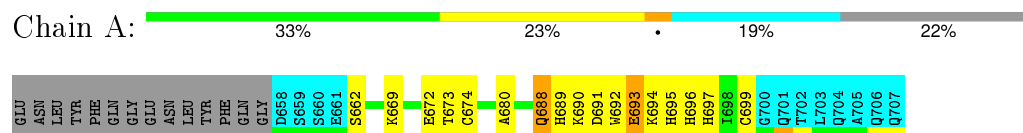


4.2.13 Score per residue for model 13

- Molecule 1: SMRT

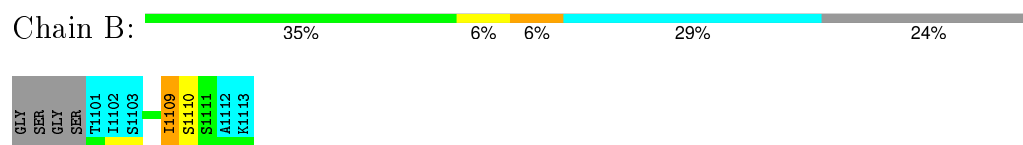


- Molecule 2: Protein CBFA2T1

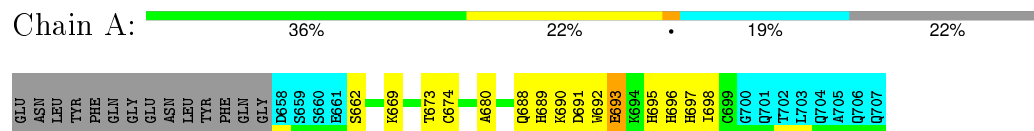


4.2.14 Score per residue for model 14

- Molecule 1: SMRT

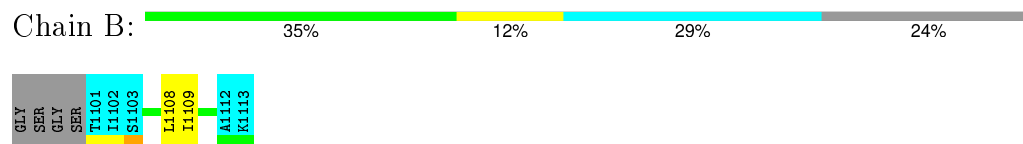


- Molecule 2: Protein CBFA2T1

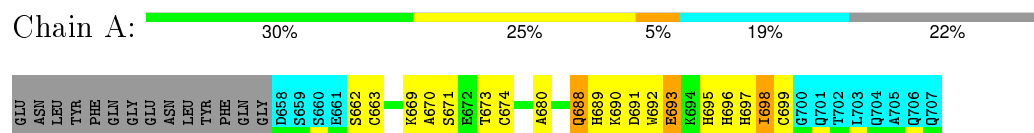


4.2.15 Score per residue for model 15

- Molecule 1: SMRT

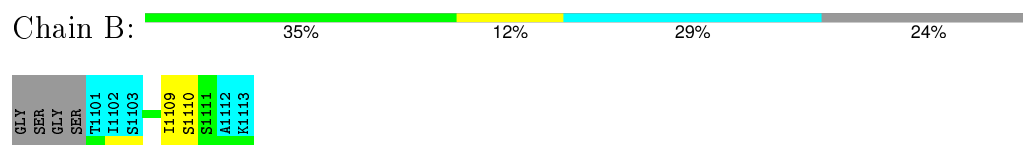


- Molecule 2: Protein CBFA2T1

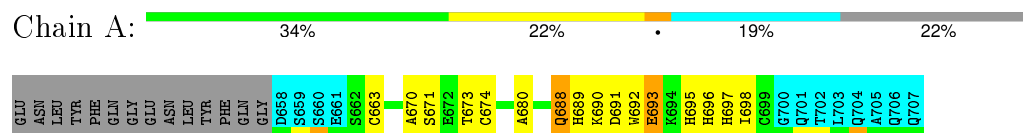


4.2.16 Score per residue for model 16

- Molecule 1: SMRT

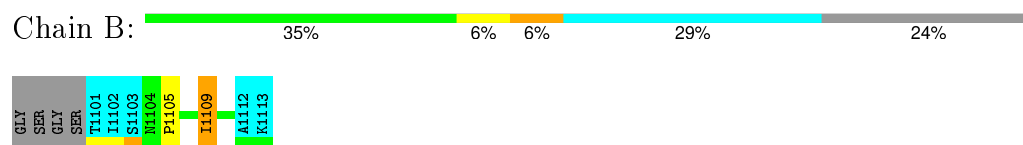


- Molecule 2: Protein CBFA2T1

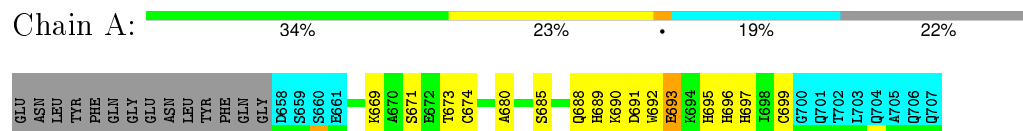


4.2.17 Score per residue for model 17

- Molecule 1: SMRT

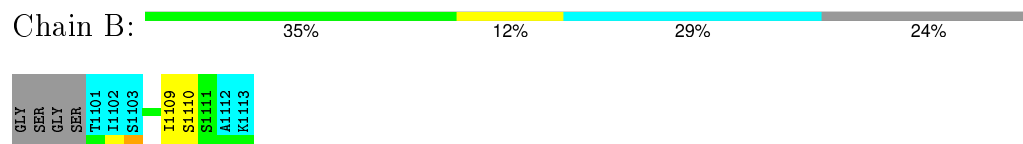


- Molecule 2: Protein CBFA2T1

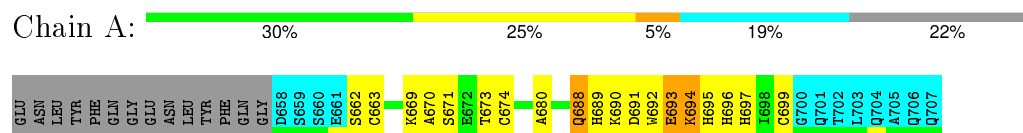


4.2.18 Score per residue for model 18

- Molecule 1: SMRT

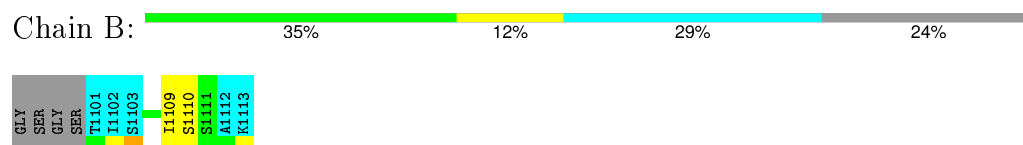


- Molecule 2: Protein CBFA2T1

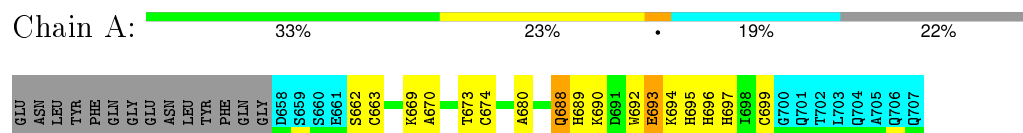


4.2.19 Score per residue for model 19

- Molecule 1: SMRT

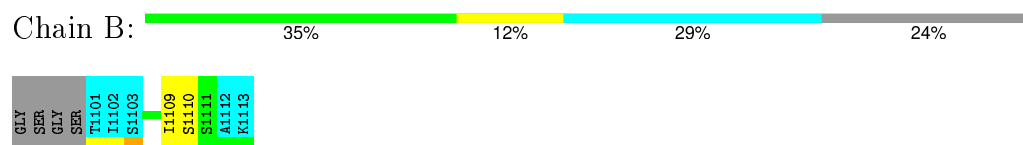


- Molecule 2: Protein CBFA2T1

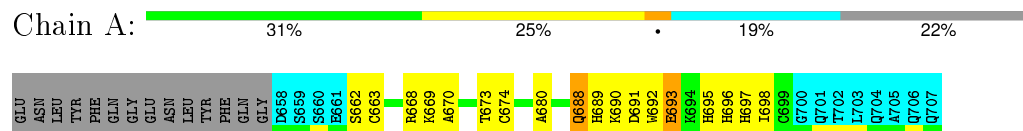


4.2.20 Score per residue for model 20

- Molecule 1: SMRT

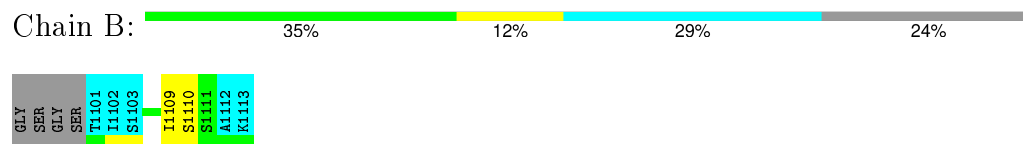


- Molecule 2: Protein CBFA2T1

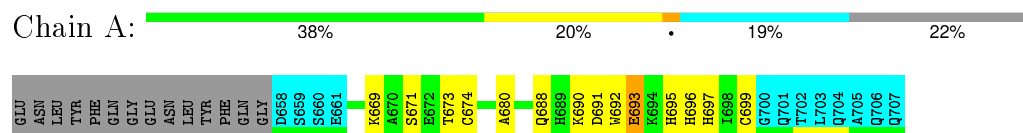


4.2.21 Score per residue for model 21

- Molecule 1: SMRT

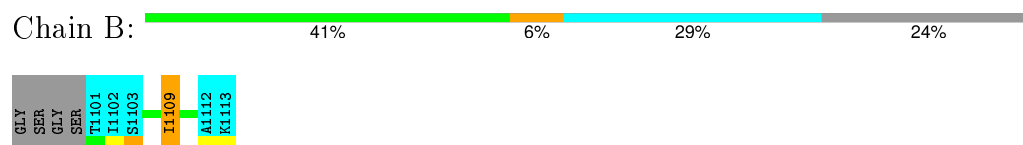


- Molecule 2: Protein CBFA2T1

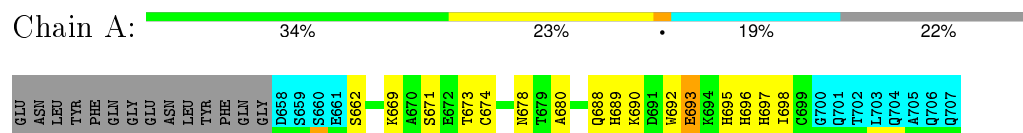


4.2.22 Score per residue for model 22

- Molecule 1: SMRT

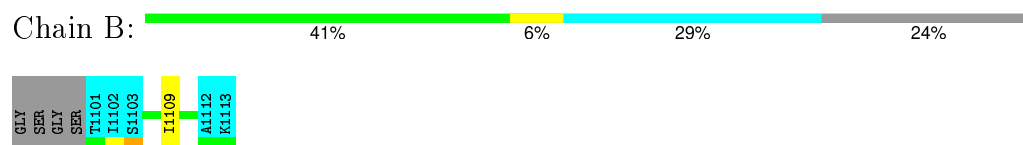


- Molecule 2: Protein CBFA2T1

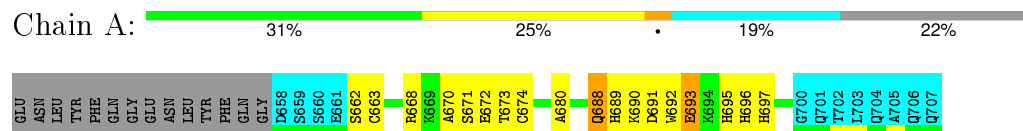


4.2.23 Score per residue for model 23

- Molecule 1: SMRT

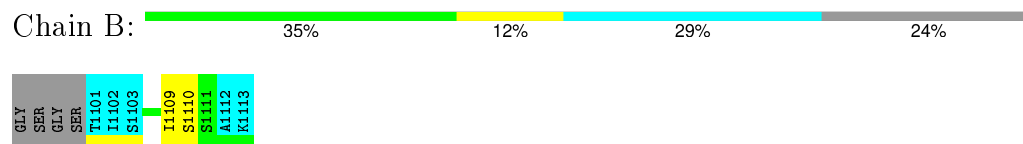


- Molecule 2: Protein CBFA2T1

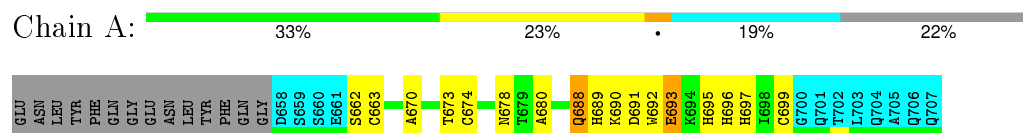


4.2.24 Score per residue for model 24

- Molecule 1: SMRT

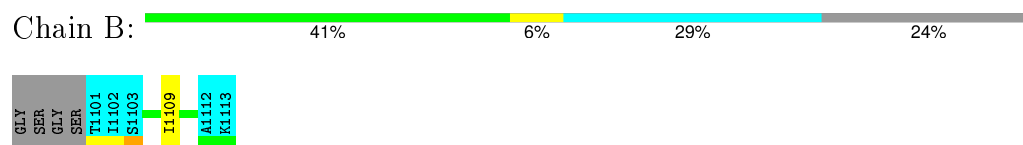


- Molecule 2: Protein CBFA2T1

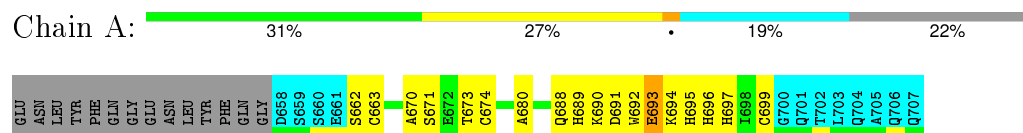


4.2.25 Score per residue for model 25

- Molecule 1: SMRT



- Molecule 2: Protein CBFA2T1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics*.

Of the 100 calculated structures, 25 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
CNS	structure solution	
CNS	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 ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	B	57	59	59	2±1
2	A	301	262	259	12±2
All	All	9000	8025	7950	299

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:680:ALA:HB2	2:A:695:HIS:CE1	0.88	2.04	5	25
2:A:674:CYS:CB	2:A:680:ALA:HB3	0.60	2.27	21	25
2:A:696:HIS:CE1	2:A:697:HIS:CE1	0.57	2.93	12	25
1:B:1108:LEU:HD11	2:A:688:GLN:HG2	0.56	1.78	15	2
2:A:680:ALA:HB2	2:A:695:HIS:NE2	0.54	2.17	15	25
2:A:674:CYS:HB2	2:A:680:ALA:HB3	0.54	1.79	3	17
2:A:693:GLU:HA	2:A:696:HIS:CD2	0.49	2.42	2	25
2:A:694:LYS:HA	2:A:697:HIS:CD2	0.49	2.42	18	7
1:B:1109:ILE:HG13	2:A:673:THR:O	0.48	2.09	14	25
2:A:688:GLN:HG3	2:A:689:HIS:N	0.48	2.24	17	11
2:A:663:CYS:CA	2:A:670:ALA:HB2	0.46	2.41	16	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:688:GLN:OE1	2:A:689:HIS:CD2	0.46	2.69	11	16
2:A:663:CYS:HA	2:A:670:ALA:HB2	0.46	1.86	16	17
2:A:692:TRP:O	2:A:696:HIS:CD2	0.43	2.71	23	25
2:A:674:CYS:HB3	2:A:680:ALA:HB3	0.43	1.90	24	3
1:B:1109:ILE:HG13	2:A:673:THR:HB	0.42	1.91	14	8
1:B:1109:ILE:CG1	2:A:673:THR:O	0.42	2.67	20	19
1:B:1105:PRO:HB3	2:A:692:TRP:CD2	0.42	2.50	17	1
1:B:1108:LEU:HD11	2:A:688:GLN:HB3	0.42	1.91	10	1
2:A:695:HIS:HA	2:A:698:ILE:HD12	0.41	1.91	15	1
2:A:686:PHE:CE2	2:A:687:CYS:SG	0.41	3.14	4	1
2:A:693:GLU:CG	2:A:694:LYS:N	0.40	2.84	9	4
2:A:693:GLU:O	2:A:696:HIS:NE2	0.40	2.54	9	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	B	8/17 (47%)	7±0 (94±6%)	1±0 (6±6%)	0±0 (0±0%)	100	100
2	A	38/64 (59%)	34±0 (90±1%)	3±1 (9±2%)	1±0 (1±1%)	19	64
All	All	1150/2025 (57%)	1038 (90%)	99 (9%)	13 (1%)	23	69

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	A	699	CYS	13

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	B	8/14 (57%)	7±1 (91±8%)	1±1 (9±8%)	16	61
2	A	33/55 (60%)	26±1 (79±3%)	7±1 (21±3%)	4	34
All	All	1025/1725 (59%)	835 (81%)	190 (19%)	5	39

All 15 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)
2	A	690	LYS	25
2	A	693	GLU	25
2	A	691	ASP	22
2	A	662	SER	21
2	A	669	LYS	19
2	A	688	GLN	19
1	B	1110	SER	14
2	A	671	SER	10
2	A	668	ARG	9
2	A	698	ILE	7
2	A	694	LYS	6
2	A	678	ASN	5
1	B	1109	ILE	4
2	A	672	GLU	2
2	A	685	SER	2

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 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

No chemical shift data were provided