



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:23 PM BST

PDB ID : 1P4W
Title : Solution structure of the DNA-binding domain of the Erwinia amylovora RcsB protein
Authors : Pristovsek, P.; Sengupta, K.; Loehr, F.; Schaefer, B.; Wehland von Trebra, M.; Rueterjans, H.; Bernhard, F.
Deposited on : 2003-04-24

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

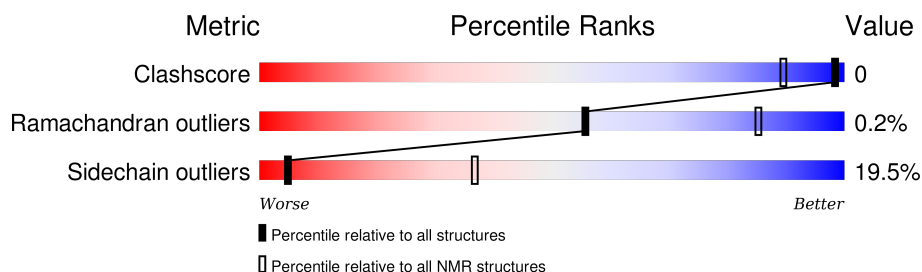
1 Overall quality at a glance

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	A	99	<div> <div>55%</div> <div>17%</div> <div>•</div> <div>13%</div> <div>12%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:132-A:143, A:152-A:213 (74)	0.34	12

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1369 atoms, of which 700 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called rcsB.

Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1369	425	700	111	130	3	

There are 12 discrepancies between the modelled and reference sequences:

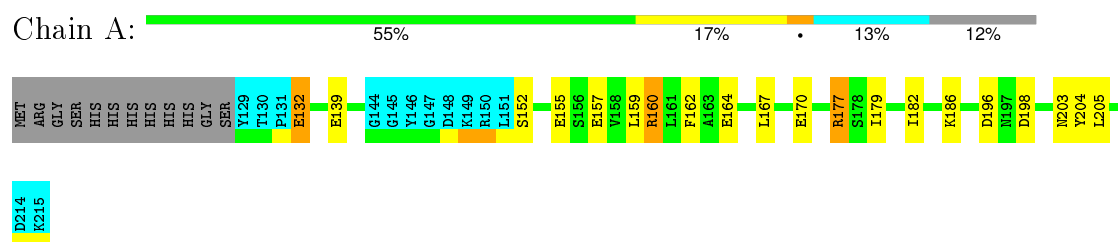
Chain	Residue	Modelled	Actual	Comment	Reference
A	117	MET	-	CLONING ARTIFACT	UNP P96320
A	118	ARG	-	CLONING ARTIFACT	UNP P96320
A	119	GLY	-	CLONING ARTIFACT	UNP P96320
A	120	SER	-	CLONING ARTIFACT	UNP P96320
A	121	HIS	-	EXPRESSION TAG	UNP P96320
A	122	HIS	-	EXPRESSION TAG	UNP P96320
A	123	HIS	-	EXPRESSION TAG	UNP P96320
A	124	HIS	-	EXPRESSION TAG	UNP P96320
A	125	HIS	-	EXPRESSION TAG	UNP P96320
A	126	HIS	-	EXPRESSION TAG	UNP P96320
A	127	GLY	-	CLONING ARTIFACT	UNP P96320
A	128	SER	-	CLONING ARTIFACT	UNP P96320

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: rcsB

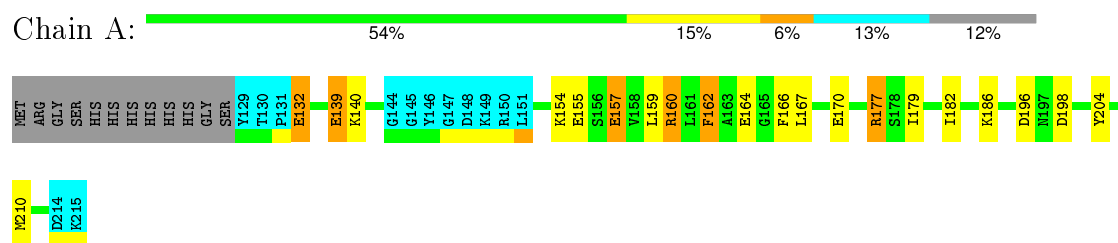


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

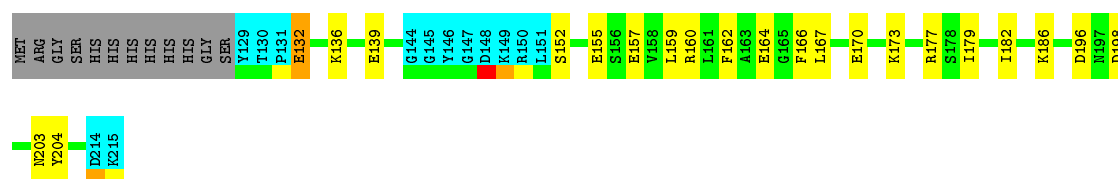
- Molecule 1: rcsB



4.2.2 Score per residue for model 2

- Molecule 1: rcsB

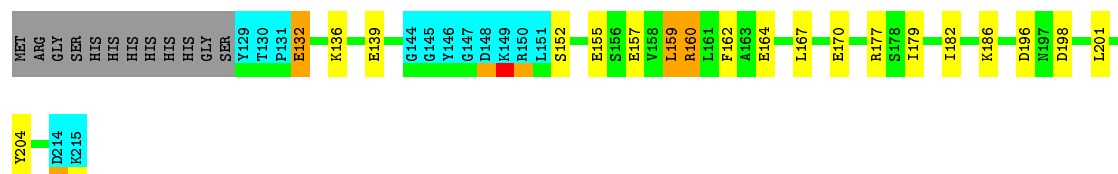




4.2.3 Score per residue for model 3

- Molecule 1: rcsB

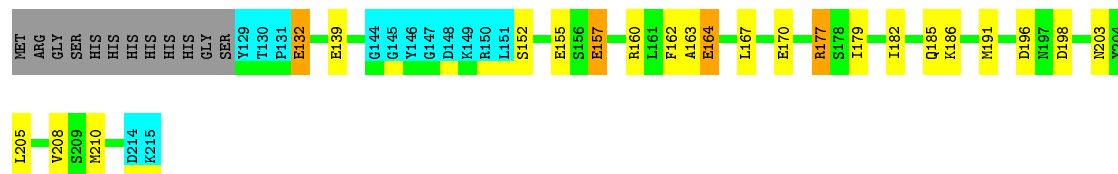
Chain A: 55% 17% 13% 12%



4.2.4 Score per residue for model 4

- Molecule 1: rcsB

Chain A: 52% 19% 13% 12%



4.2.5 Score per residue for model 5

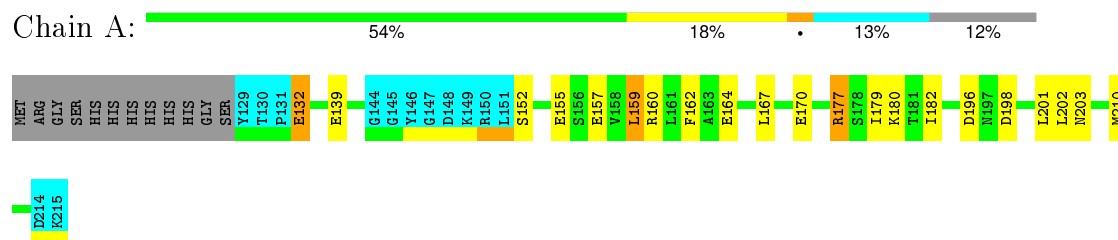
- Molecule 1: rcsB

Chain A: 51% 22% 13% 12%



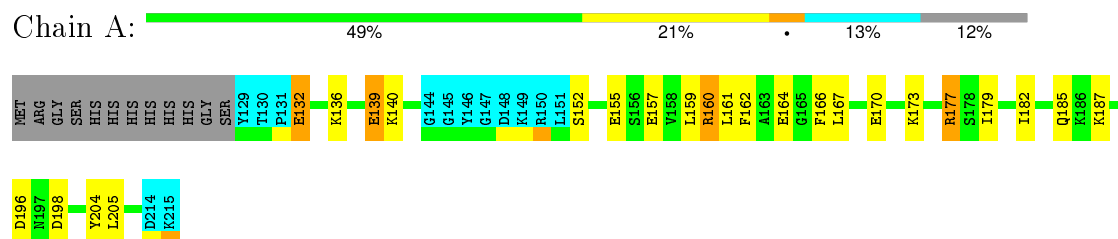
4.2.6 Score per residue for model 6

- Molecule 1: rcsB



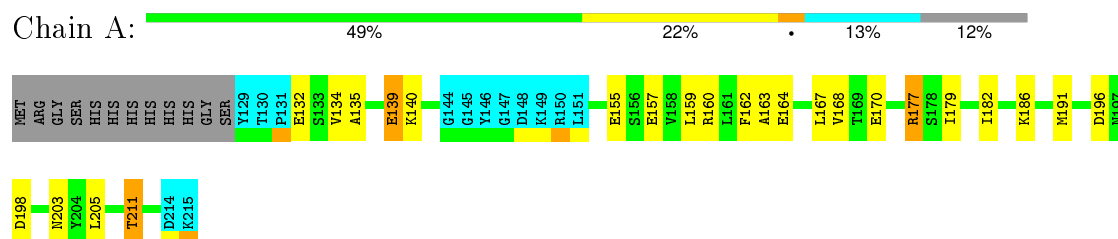
4.2.7 Score per residue for model 7

- Molecule 1: rcsB



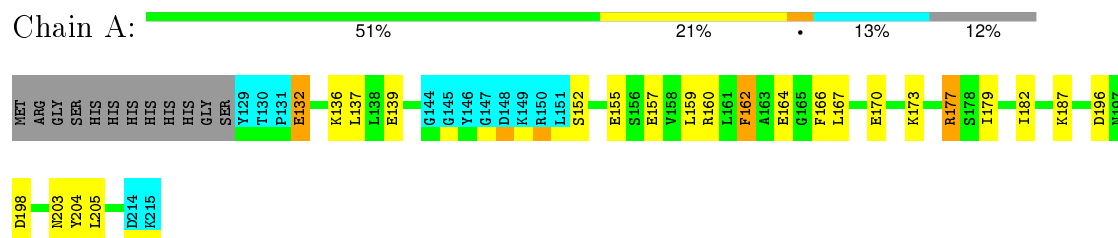
4.2.8 Score per residue for model 8

- Molecule 1: rcsB



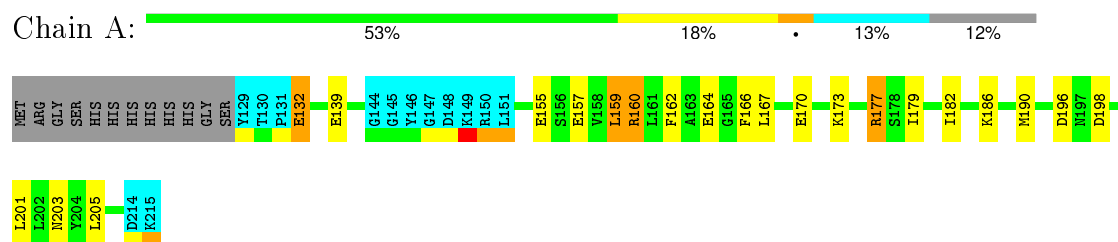
4.2.9 Score per residue for model 9

- Molecule 1: rcsB



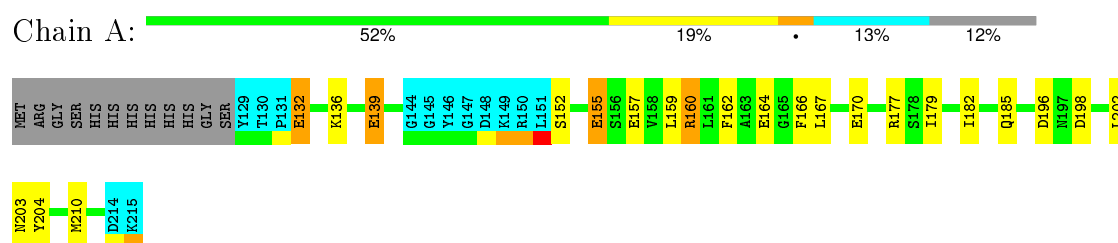
4.2.10 Score per residue for model 10

- Molecule 1: rcsB



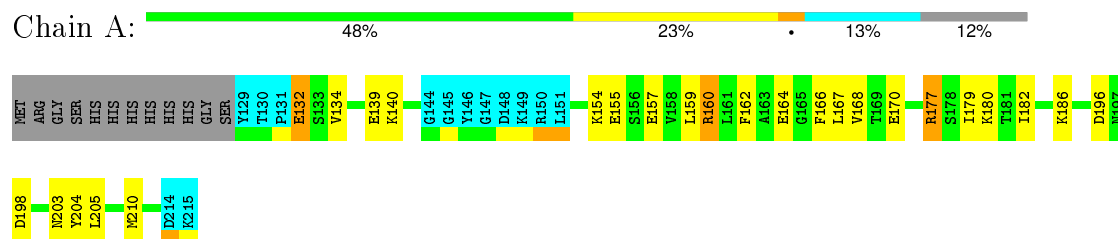
4.2.11 Score per residue for model 11

- Molecule 1: rcsB



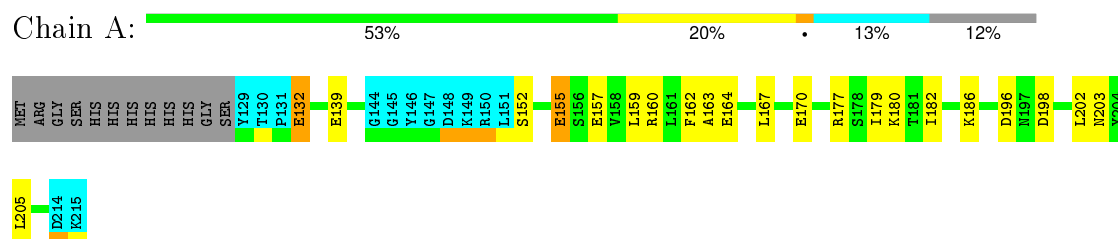
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: rcsB



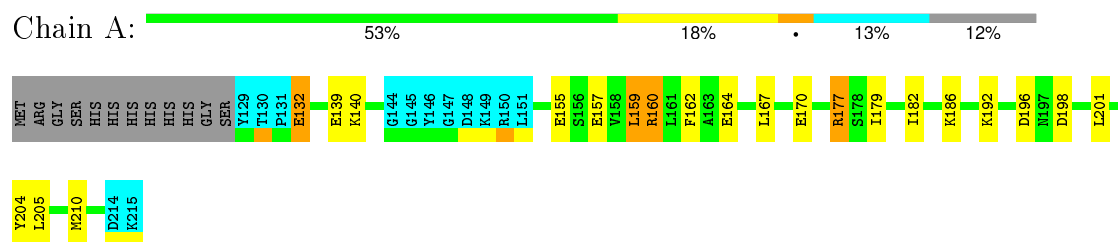
4.2.13 Score per residue for model 13

- Molecule 1: rcsB



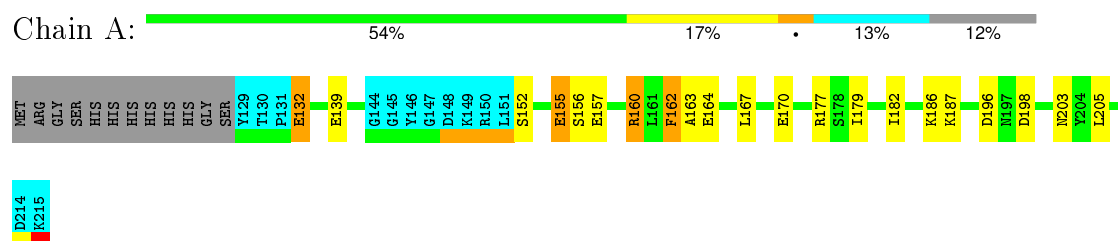
4.2.14 Score per residue for model 14

- Molecule 1: rcsB



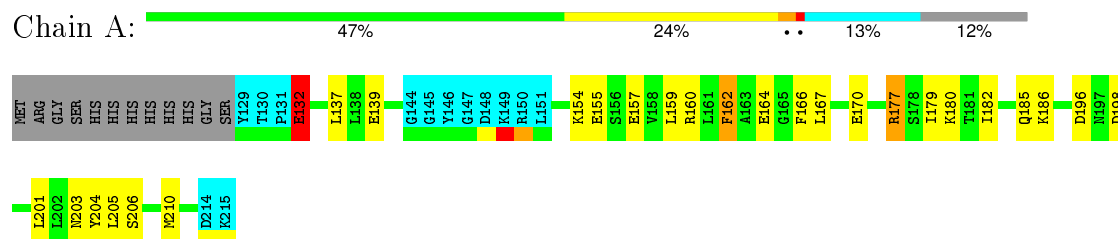
4.2.15 Score per residue for model 15

- Molecule 1: rcsB



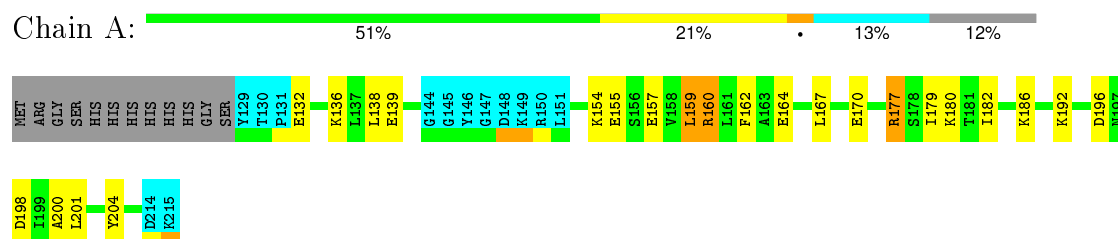
4.2.16 Score per residue for model 16

- Molecule 1: rcsB



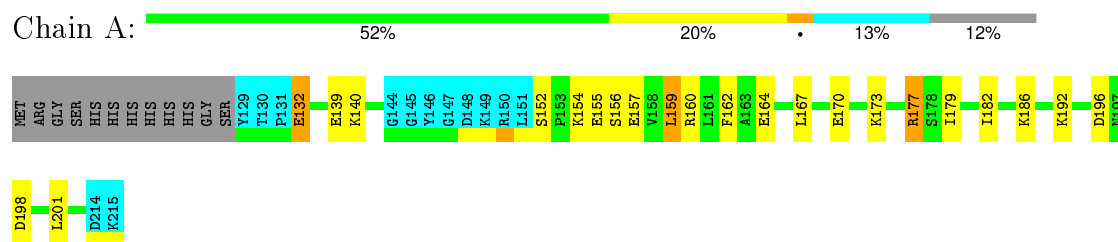
4.2.17 Score per residue for model 17

- Molecule 1: rcsB



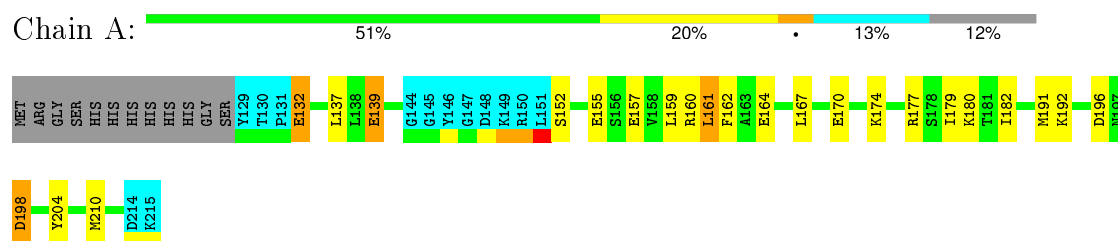
4.2.18 Score per residue for model 18

- Molecule 1: rcsB



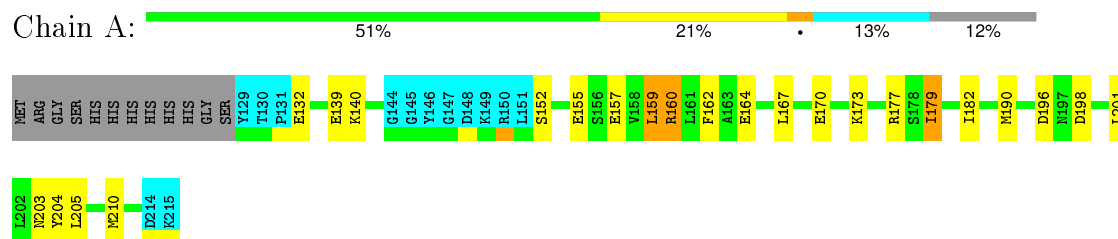
4.2.19 Score per residue for model 19

- Molecule 1: rcsB



4.2.20 Score per residue for model 20

- Molecule 1: rcsB



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *The submitted conformer models are those with the fewest number of constraint violations*.

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

Software name	Classification	Version
nmr2st	refinement	1.05
DYANA	structure solution	1.5

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.58±0.01	7±1/570 (1.2±0.1%)	1.54±0.02	8±1/765 (1.1±0.2%)
All	All	1.58	140/11400 (1.2%)	1.54	164/15300 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.8±0.9
All	All	0	35

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	164	GLU	CD-OE1	10.73	1.37	1.25	16	5
1	A	139	GLU	CD-OE2	10.71	1.37	1.25	19	15
1	A	132	GLU	CD-OE1	10.54	1.37	1.25	2	7
1	A	164	GLU	CD-OE2	10.52	1.37	1.25	19	15
1	A	132	GLU	CD-OE2	10.51	1.37	1.25	13	13
1	A	155	GLU	CD-OE2	10.45	1.37	1.25	15	10
1	A	157	GLU	CD-OE2	10.44	1.37	1.25	4	16
1	A	170	GLU	CD-OE2	10.43	1.37	1.25	8	14
1	A	139	GLU	CD-OE1	10.39	1.37	1.25	1	5
1	A	170	GLU	CD-OE1	10.34	1.37	1.25	12	6
1	A	155	GLU	CD-OE1	10.34	1.37	1.25	4	10
1	A	157	GLU	CD-OE1	10.26	1.36	1.25	2	4
1	A	196	ASP	CG-OD2	5.16	1.37	1.25	5	7
1	A	198	ASP	CG-OD1	5.13	1.37	1.25	1	4
1	A	196	ASP	CG-OD1	5.13	1.37	1.25	7	5
1	A	198	ASP	CG-OD2	5.10	1.37	1.25	3	4

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	177	ARG	NE-CZ-NH1	9.20	124.90	120.30	9	20
1	A	160	ARG	NE-CZ-NH1	8.67	124.64	120.30	20	20
1	A	196	ASP	CB-CG-OD1	7.62	125.16	118.30	12	20
1	A	196	ASP	CB-CG-OD2	-7.61	111.45	118.30	11	20
1	A	198	ASP	CB-CG-OD2	-7.43	111.61	118.30	2	20
1	A	198	ASP	CB-CG-OD1	7.34	124.90	118.30	17	20
1	A	177	ARG	NE-CZ-NH2	-6.48	117.06	120.30	14	14
1	A	132	GLU	N-CA-CB	-5.84	100.09	110.60	17	6
1	A	162	PHE	CB-CG-CD2	-5.73	116.79	120.80	15	2
1	A	166	PHE	CB-CG-CD1	-5.70	116.81	120.80	11	5
1	A	211	THR	CA-CB-CG2	5.47	120.06	112.40	8	1
1	A	163	ALA	N-CA-CB	-5.46	102.46	110.10	8	3
1	A	160	ARG	NE-CZ-NH2	-5.39	117.60	120.30	7	9
1	A	166	PHE	CB-CG-CD2	-5.36	117.05	120.80	7	2
1	A	208	VAL	CA-CB-CG2	5.29	118.84	110.90	4	1
1	A	162	PHE	CB-CG-CD1	5.12	124.39	120.80	15	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	132	GLU	Mainchain	16
1	A	204	TYR	Sidechain	12
1	A	177	ARG	Sidechain	3
1	A	162	PHE	Sidechain	2
1	A	160	ARG	Sidechain	2

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	A	565	603	612	0±1
All	All	11300	12060	12240	10

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:LEU:HD21	1:A:201:LEU:HD22	0.76	1.58	6	6
1:A:161:LEU:HD11	1:A:174:LYS:HG3	0.49	1.83	19	1
1:A:159:LEU:HD11	1:A:201:LEU:HD22	0.44	1.88	3	2
1:A:138:LEU:HD22	1:A:200:ALA:HB2	0.41	1.92	17	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	74/99 (75%)	66±2 (89±3%)	8±2 (11±3%)	0±0 (0±0%)	56	85
All	All	1480/1980 (75%)	1316 (89%)	161 (11%)	3 (0%)	56	85

All 2 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	168	VAL	2
1	A	179	ILE	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	66/86 (77%)	53±2 (81±3%)	13±2 (19±3%)	5	37
All	All	1320/1720 (77%)	1063 (81%)	257 (19%)	5	37

All 37 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	167	LEU	20
1	A	162	PHE	20
1	A	182	ILE	20
1	A	179	ILE	20
1	A	159	LEU	17
1	A	186	LYS	13
1	A	203	ASN	13
1	A	152	SER	12
1	A	205	LEU	11
1	A	210	MET	10
1	A	177	ARG	10
1	A	160	ARG	8
1	A	173	LYS	7
1	A	136	LYS	7
1	A	140	LYS	7
1	A	180	LYS	6
1	A	139	GLU	5
1	A	192	LYS	5
1	A	154	LYS	5
1	A	202	LEU	4
1	A	185	GLN	4
1	A	137	LEU	4
1	A	134	VAL	3
1	A	191	MET	3
1	A	187	LYS	3
1	A	155	GLU	3
1	A	132	GLU	3
1	A	161	LEU	2
1	A	166	PHE	2
1	A	190	MET	2
1	A	157	GLU	2
1	A	211	THR	1
1	A	184	SER	1
1	A	156	SER	1
1	A	198	ASP	1
1	A	206	SER	1
1	A	164	GLU	1

6.3.3 RNA ⓘ

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

No chemical shift data were provided