Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 09:40 PM BST

PDB ID	:	2JW8
Title	:	Solution structure of stereo-array isotope labelled (SAIL) C-terminal dimerization domain of SARS coronavirus nucleocapsid protein
Authors	:	Takeda, M.; Chang, C.; Ikeya, T.; Guntert, P.; Chang, Y.; Hsu, Y.; Huang, T.; Kainosho, M.
Deposited on	:	2007-10-06

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 (i) symbol.

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

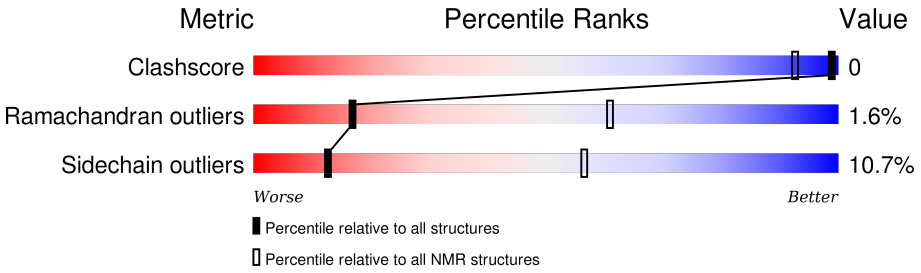
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 is 64%.

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	128	78% 5% 9% 8%
1	B	128	79% • 10% 8%

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:260-A:365, B:261-B:365 (211)	0.61	16

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3732 atoms, of which 1850 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleocapsid protein.

Mol	Chain	Residues	Atoms						Trace
1	A	118	Total	C	H	N	O	S	0
			1866	595	925	170	174	2	
1	B	118	Total	C	H	N	O	S	0
			1866	595	925	170	174	2	

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	MET	-	EXPRESSION TAG	UNP P59595
A	239	HIS	-	EXPRESSION TAG	UNP P59595
A	240	HIS	-	EXPRESSION TAG	UNP P59595
A	241	HIS	-	EXPRESSION TAG	UNP P59595
A	242	HIS	-	EXPRESSION TAG	UNP P59595
A	243	HIS	-	EXPRESSION TAG	UNP P59595
A	244	HIS	-	EXPRESSION TAG	UNP P59595
A	245	ALA	-	EXPRESSION TAG	UNP P59595
A	246	MET	-	EXPRESSION TAG	UNP P59595
A	247	GLY	-	EXPRESSION TAG	UNP P59595
B	238	MET	-	EXPRESSION TAG	UNP P59595
B	239	HIS	-	EXPRESSION TAG	UNP P59595
B	240	HIS	-	EXPRESSION TAG	UNP P59595
B	241	HIS	-	EXPRESSION TAG	UNP P59595
B	242	HIS	-	EXPRESSION TAG	UNP P59595
B	243	HIS	-	EXPRESSION TAG	UNP P59595
B	244	HIS	-	EXPRESSION TAG	UNP P59595
B	245	ALA	-	EXPRESSION TAG	UNP P59595
B	246	MET	-	EXPRESSION TAG	UNP P59595
B	247	GLY	-	EXPRESSION TAG	UNP P59595

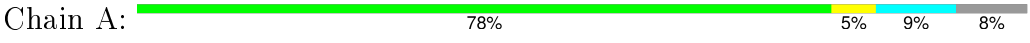
4 Residue-property plots

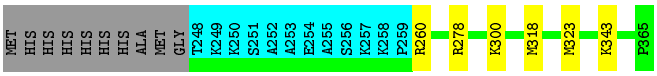
4.1 Average score per residue in the NMR ensemble

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: Nucleocapsid protein

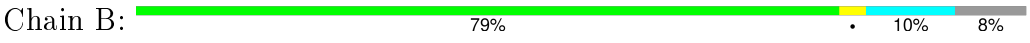
Chain A:

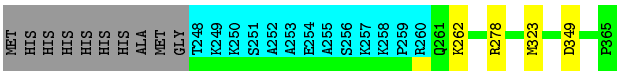




- Molecule 1: Nucleocapsid protein

Chain B:





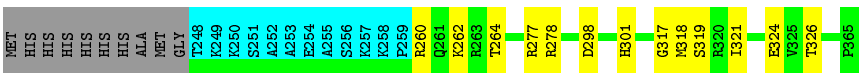
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Nucleocapsid protein

Chain A:



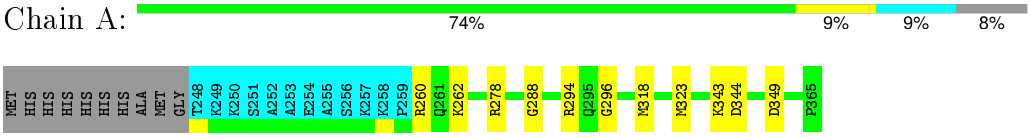
- Molecule 1: Nucleocapsid protein

Chain B:

4.2.2 Score per residue for model 2

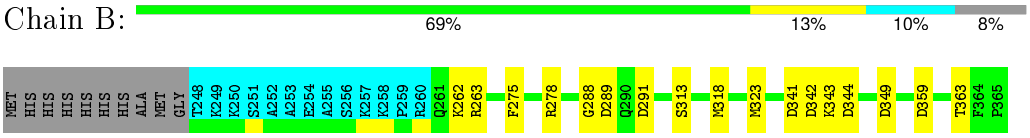
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

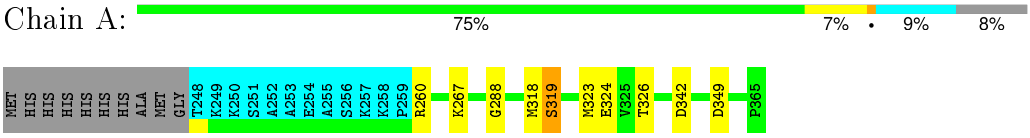
Chain B:



4.2.3 Score per residue for model 3

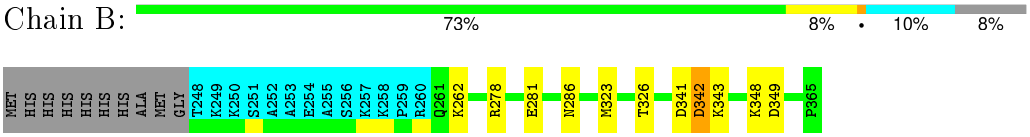
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

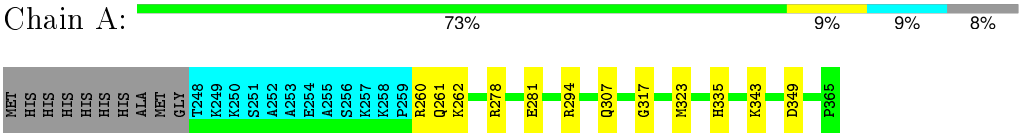
Chain B:



4.2.4 Score per residue for model 4

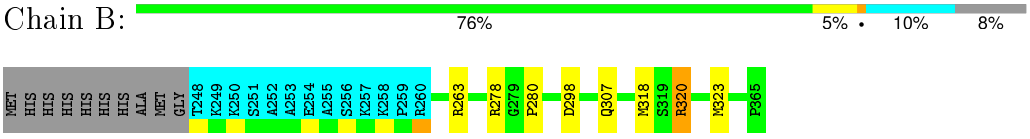
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

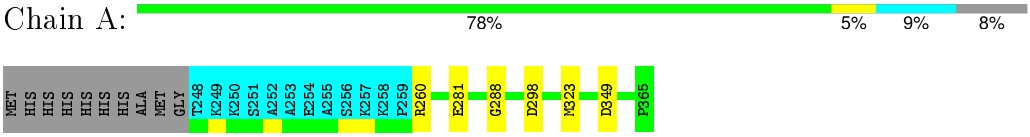
Chain B:



4.2.5 Score per residue for model 5

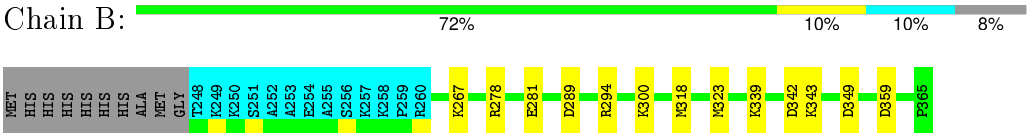
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

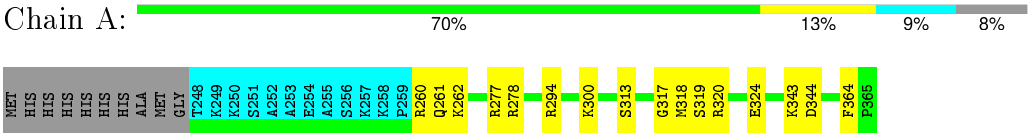
Chain B:



4.2.6 Score per residue for model 6

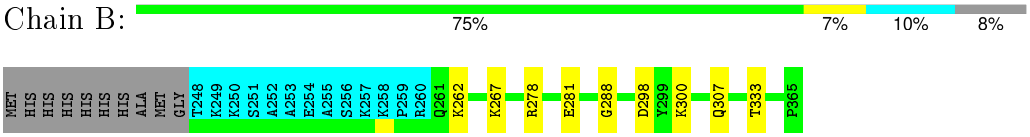
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

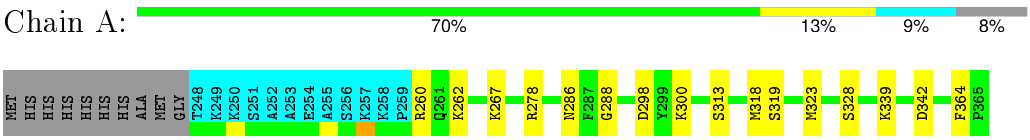
Chain B:



4.2.7 Score per residue for model 7

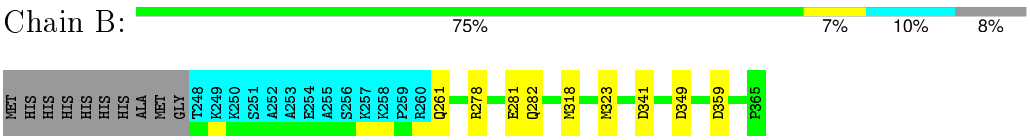
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

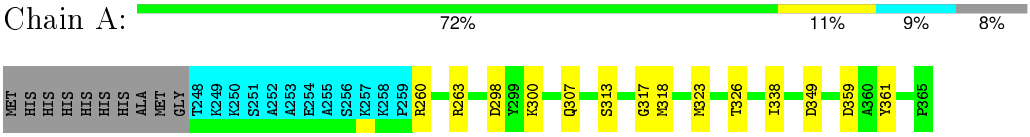
Chain B:



4.2.8 Score per residue for model 8

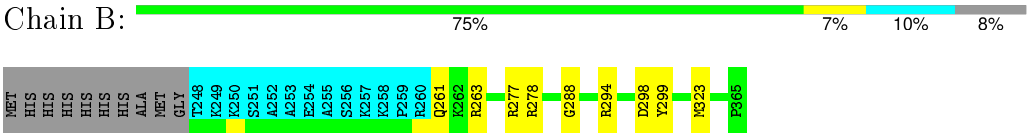
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

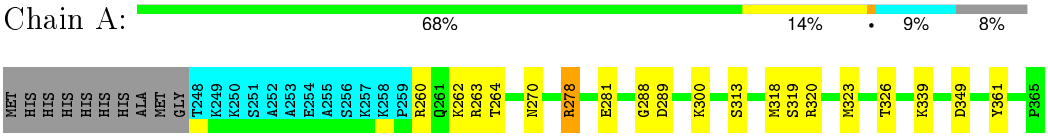
Chain B:



4.2.9 Score per residue for model 9

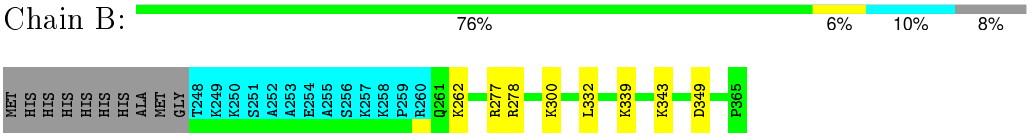
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

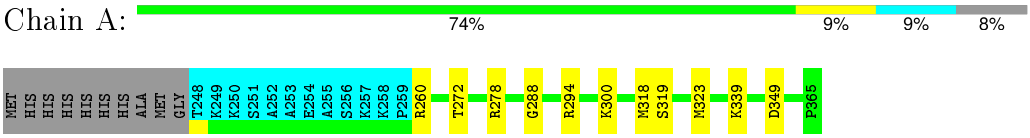
Chain B:



4.2.10 Score per residue for model 10

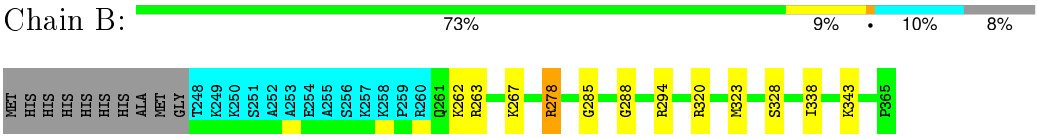
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

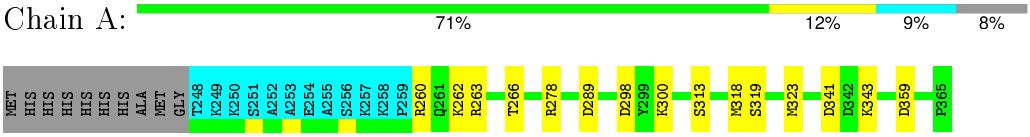
Chain B:



4.2.11 Score per residue for model 11

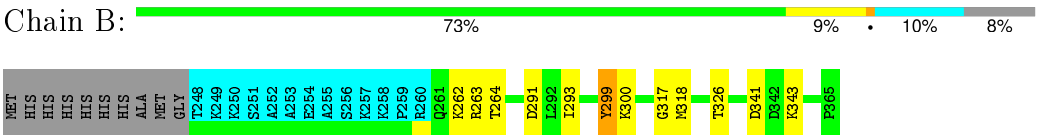
- Molecule 1: Nucleocapsid protein

Chain A:



- Molecule 1: Nucleocapsid protein

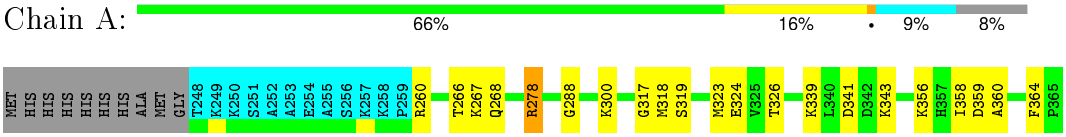
Chain B:



4.2.12 Score per residue for model 12

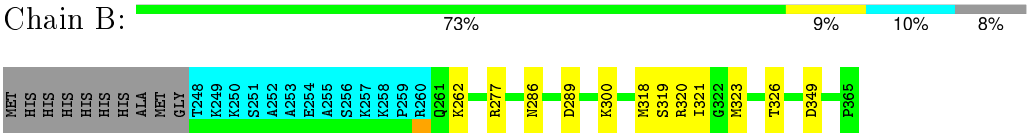
- Molecule 1: Nucleocapsid protein

Chain A:



- Molecule 1: Nucleocapsid protein

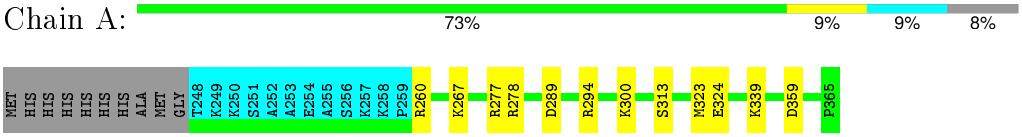
Chain B:



4.2.13 Score per residue for model 13

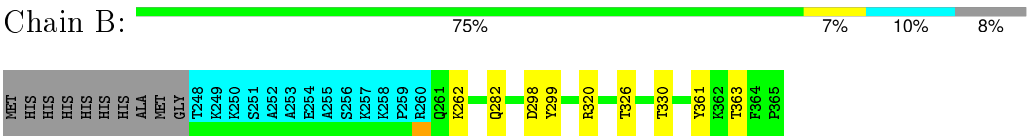
- Molecule 1: Nucleocapsid protein

Chain A:



- Molecule 1: Nucleocapsid protein

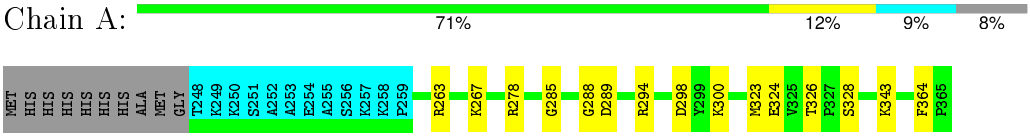
Chain B:



4.2.14 Score per residue for model 14

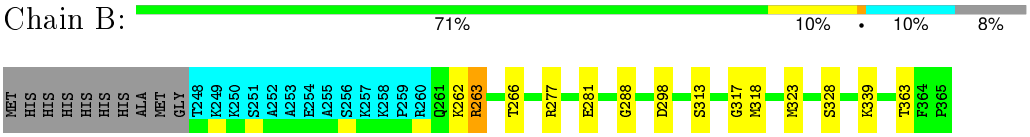
- Molecule 1: Nucleocapsid protein

Chain A:



- Molecule 1: Nucleocapsid protein

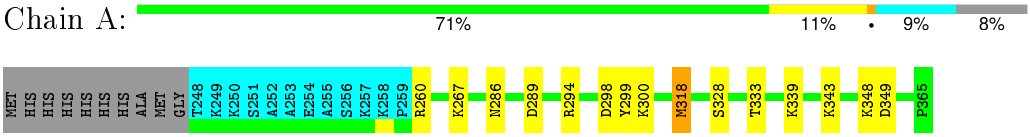
Chain B:



4.2.15 Score per residue for model 15

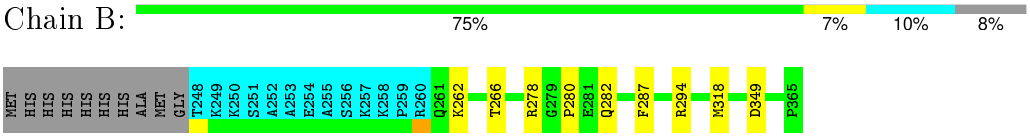
- Molecule 1: Nucleocapsid protein

Chain A:



- Molecule 1: Nucleocapsid protein

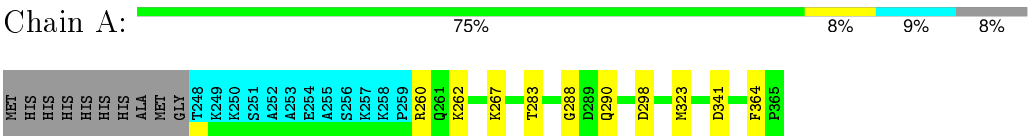
Chain B:



4.2.16 Score per residue for model 16 (medoid)

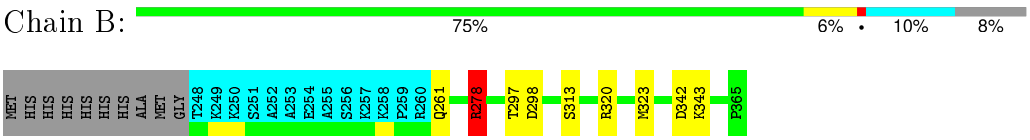
- Molecule 1: Nucleocapsid protein

Chain A:



- Molecule 1: Nucleocapsid protein

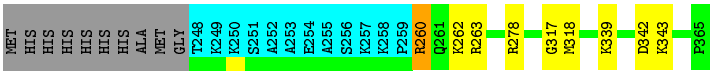
Chain B:



4.2.17 Score per residue for model 17

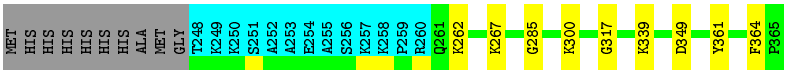
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

Chain B:



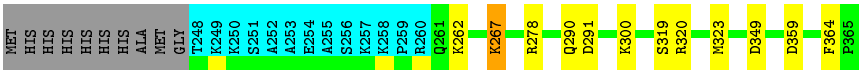
4.2.18 Score per residue for model 18

• Molecule 1: Nucleocapsid protein

Chain A:

• Molecule 1: Nucleocapsid protein

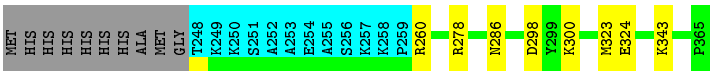
Chain B:



4.2.19 Score per residue for model 19

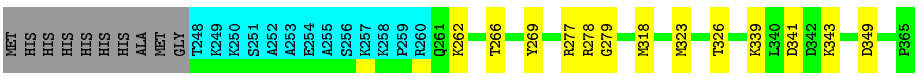
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

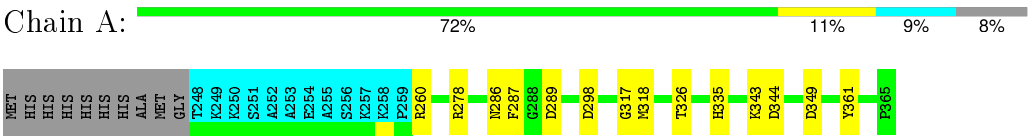
Chain B:



4.2.20 Score per residue for model 20

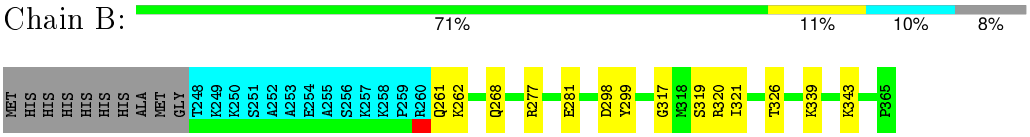
• Molecule 1: Nucleocapsid protein

Chain A:



• Molecule 1: Nucleocapsid protein

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, TORSION ANGLE DYNAMICS.*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	structure solution	2.2
CYANA	refinement	2.2

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 15511
Number of chemical shift lists	1
Total number of shifts	2090
Number of shifts mapped to atoms	2090
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

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	0.63±0.00	0±0/878 (0.0±0.0%)	0.99±0.03	0±0/1186 (0.0±0.0%)
1	B	0.63±0.01	0±0/867 (0.0±0.0%)	1.00±0.02	0±1/1172 (0.0±0.0%)
All	All	0.63	0/34900 (0.0%)	1.00	9/47160 (0.0%)

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	0.8±0.9
1	B	0.0±0.0	0.9±0.8
All	All	0	33

There are no bond-length outliers.

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	278	ARG	NE-CZ-NH2	-6.33	117.14	120.30	19	1
1	B	278	ARG	NE-CZ-NH2	-6.10	117.25	120.30	16	2
1	B	364	PHE	CB-CG-CD2	-5.66	116.84	120.80	18	1
1	A	294	ARG	NE-CZ-NH2	-5.37	117.61	120.30	14	1
1	B	320	ARG	NE-CZ-NH1	5.17	122.88	120.30	10	1
1	B	263	ARG	NE-CZ-NH1	5.14	122.87	120.30	4	1
1	B	341	ASP	C-N-CA	5.08	134.41	121.70	3	1
1	B	277	ARG	NE-CZ-NH2	-5.02	117.79	120.30	8	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	294	ARG	Sidechain	6
1	B	299	TYR	Sidechain	4
1	B	294	ARG	Sidechain	4
1	B	278	ARG	Sidechain	4
1	A	263	ARG	Sidechain	2
1	B	263	ARG	Sidechain	2
1	B	320	ARG	Sidechain	2
1	B	361	TYR	Sidechain	2
1	A	278	ARG	Sidechain	2
1	A	260	ARG	Sidechain	2
1	A	277	ARG	Sidechain	1
1	A	299	TYR	Sidechain	1
1	A	361	TYR	Sidechain	1

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	844	815	815	0±0
1	A	855	828	828	0±1
All	All	33980	32860	32860	6

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:360:ALA:HB1	1:A:364:PHE:CZ	0.56	2.35	12	1
1:A:360:ALA:HB1	1:A:364:PHE:CE2	0.54	2.37	12	1
1:A:356:LYS:O	1:A:360:ALA:HB2	0.48	2.08	12	1
1:B:291:ASP:HB3	1:B:299:TYR:CE1	0.42	2.49	11	1
1:A:358:ILE:HD11	1:B:321:ILE:HG22	0.41	1.93	12	1
1:B:347:PHE:O	1:B:351:VAL:HG23	0.41	2.15	1	1

6.3 Torsion angles

6.3.1 Protein backbone

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	105/128 (82%)	94±3 (89±3%)	9±2 (9±2%)	2±1 (2±1%)	16	59
1	B	104/128 (81%)	94±3 (90±3%)	9±2 (9±2%)	2±1 (2±1%)	18	63
All	All	4180/5120 (82%)	3748 (90%)	365 (9%)	67 (2%)	17	61

All 25 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	288	GLY	10
1	A	319	SER	8
1	A	317	GLY	7
1	B	342	ASP	5
1	B	288	GLY	5
1	B	317	GLY	4
1	A	342	ASP	3
1	B	319	SER	3
1	B	320	ARG	2
1	A	267	LYS	2
1	B	285	GLY	2
1	B	280	PRO	2
1	B	318	MET	2
1	A	285	GLY	1
1	A	301	HIS	1
1	B	290	GLN	1
1	A	296	GLY	1
1	A	318	MET	1
1	B	261	GLN	1
1	B	278	ARG	1
1	B	279	GLY	1
1	B	267	LYS	1
1	B	286	ASN	1
1	A	278	ARG	1
1	B	263	ARG	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	89/106 (84%)	79±3 (88±3%)	11±3 (12±3%)	11	53
1	B	88/106 (83%)	80±2 (90±2%)	8±2 (10±2%)	15	60
All	All	3540/4240 (83%)	3162 (89%)	378 (11%)	13	56

All 85 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	260	ARG	18
1	A	323	MET	15
1	A	318	MET	14
1	B	262	LYS	14
1	B	323	MET	13
1	A	278	ARG	13
1	A	300	LYS	12
1	A	343	LYS	11
1	B	349	ASP	11
1	B	343	LYS	10
1	B	278	ARG	10
1	A	298	ASP	10
1	A	349	ASP	10
1	A	262	LYS	9
1	A	339	LYS	8
1	B	300	LYS	8
1	A	326	THR	8
1	B	318	MET	8
1	A	289	ASP	7
1	A	324	GLU	7
1	A	313	SER	7
1	B	326	THR	7
1	B	298	ASP	7
1	B	281	GLU	6
1	B	267	LYS	6
1	A	267	LYS	6
1	B	339	LYS	6
1	A	359	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	B	277	ARG	5
1	B	359	ASP	4
1	B	282	GLN	4
1	A	286	ASN	4
1	A	364	PHE	4
1	B	263	ARG	4
1	B	341	ASP	4
1	B	261	GLN	3
1	A	341	ASP	3
1	B	266	THR	3
1	A	263	ARG	3
1	B	313	SER	3
1	A	328	SER	3
1	B	363	THR	3
1	A	281	GLU	3
1	B	320	ARG	3
1	B	289	ASP	3
1	A	344	ASP	3
1	A	277	ARG	2
1	A	320	ARG	2
1	A	307	GLN	2
1	B	291	ASP	2
1	B	328	SER	2
1	A	335	HIS	2
1	A	266	THR	2
1	A	261	GLN	2
1	B	307	GLN	2
1	A	361	TYR	2
1	A	264	THR	2
1	B	332	LEU	1
1	A	270	ASN	1
1	B	297	THR	1
1	B	333	THR	1
1	B	364	PHE	1
1	A	321	ILE	1
1	B	330	THR	1
1	B	269	TYR	1
1	B	275	PHE	1
1	A	348	LYS	1
1	B	264	THR	1
1	B	338	ILE	1
1	A	268	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	B	287	PHE	1
1	A	290	GLN	1
1	B	286	ASN	1
1	B	342	ASP	1
1	B	344	ASP	1
1	A	272	THR	1
1	A	333	THR	1
1	B	348	LYS	1
1	B	268	GLN	1
1	A	319	SER	1
1	B	321	ILE	1
1	A	287	PHE	1
1	A	283	THR	1
1	B	293	ILE	1
1	A	338	ILE	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

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

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 64% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 15511

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2090
Number of shifts mapped to atoms	2090
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	232	-0.46 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	208	0.42 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	220	0.46 ± 0.32	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 64%, i.e. 1696 atoms were assigned a chemical shift out of a possible 2663. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	790/1031 (77%)	386/410 (94%)	207/422 (49%)	197/199 (99%)
Sidechain	772/1352 (57%)	403/801 (50%)	347/474 (73%)	22/77 (29%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	134/280 (48%)	68/150 (45%)	62/120 (52%)	4/10 (40%)
Overall	1696/2663 (64%)	857/1361 (63%)	616/1016 (61%)	223/286 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 64%, i.e. 1886 atoms were assigned a chemical shift out of a possible 2970. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	886/1152 (77%)	434/458 (95%)	232/472 (49%)	220/222 (99%)
Sidechain	866/1538 (56%)	450/914 (49%)	394/536 (74%)	22/88 (25%)
Aromatic	134/280 (48%)	68/150 (45%)	62/120 (52%)	4/10 (40%)
Overall	1886/2970 (64%)	952/1522 (63%)	688/1128 (61%)	246/320 (77%)

7.1.4 Statistically unusual chemical shifts (i)

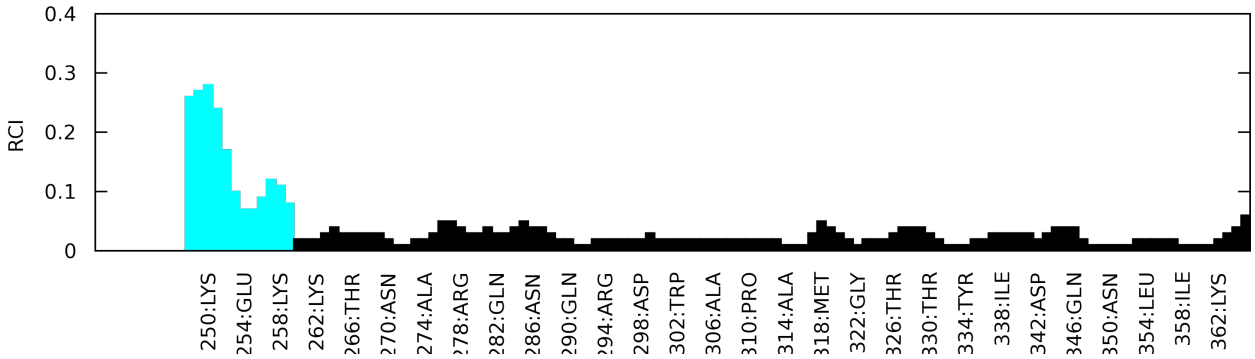
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	274	ALA	HB2	-0.24	2.61 – 0.11	-6.4
1	A	274	ALA	HB1	-0.24	2.61 – 0.11	-6.4
1	B	274	ALA	HB1	-0.24	2.61 – 0.11	-6.4
1	B	274	ALA	HB2	-0.24	2.61 – 0.11	-6.4
1	A	274	ALA	HB3	-0.24	2.61 – 0.11	-6.4
1	B	274	ALA	HB3	-0.24	2.61 – 0.11	-6.4
1	A	339	LYS	HG3	-0.18	2.76 – -0.04	-5.5
1	B	339	LYS	HG3	-0.18	2.76 – -0.04	-5.5
1	B	310	PRO	HD3	1.58	5.52 – 1.72	-5.4
1	A	310	PRO	HD3	1.58	5.52 – 1.72	-5.4
1	A	361	TYR	HA	1.63	7.42 – 1.82	-5.3
1	B	361	TYR	HA	1.63	7.42 – 1.82	-5.3

7.1.5 Random Coil Index (RCI) plots (i)

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B: