



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 06:58 PM UTC

PDB ID : 2JW8 / pdb_00002jw8
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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

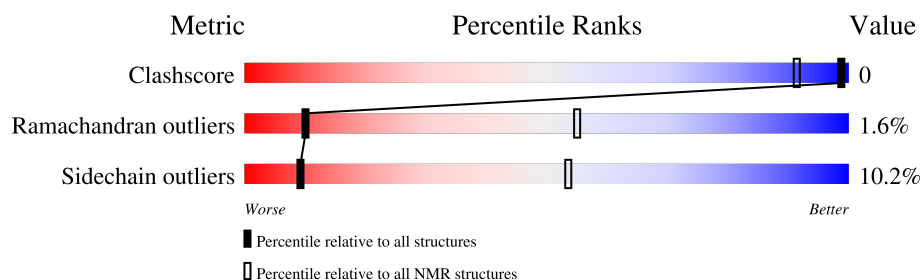
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	128	 79% • 9% 8%
1	B	128	 80% • 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)	1.05	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:

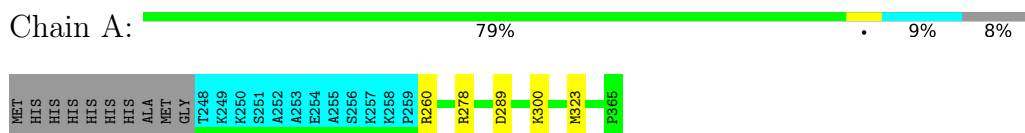
Chain	Residue	Modelled	Actual	Comment	Reference
A	238	MET	-	expression tag	UNP P59595
A	239	HIS	-	expression tag	UNP P59595
A	240	HIS	-	expression tag	UNP P59595
A	241	HIS	-	expression tag	UNP P59595
A	242	HIS	-	expression tag	UNP P59595
A	243	HIS	-	expression tag	UNP P59595
A	244	HIS	-	expression tag	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

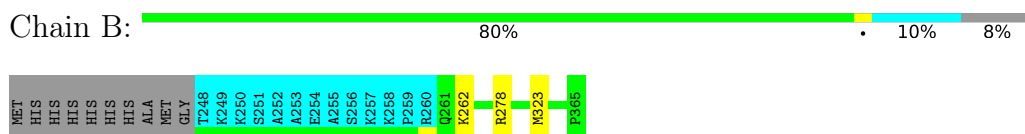
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein

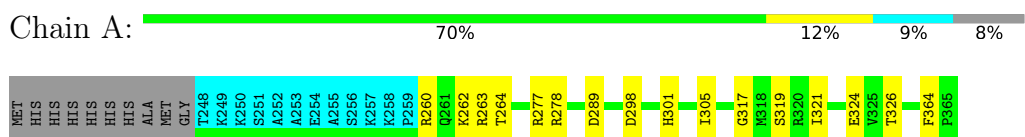


4.2 Scores per residue for each member of the ensemble

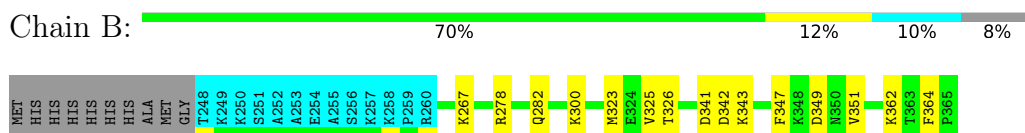
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Nucleocapsid protein

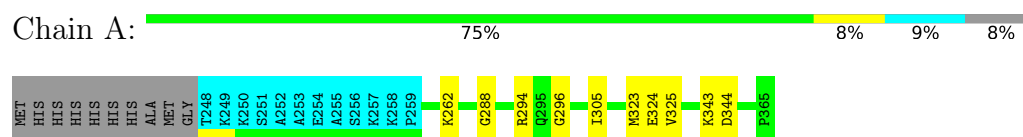


- Molecule 1: Nucleocapsid protein

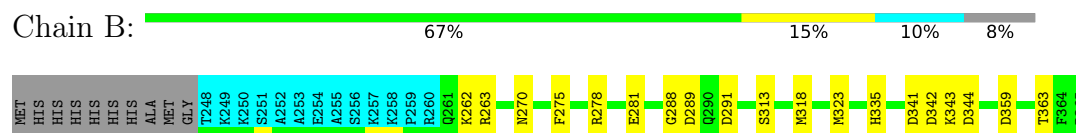


4.2.2 Score per residue for model 2

- Molecule 1: Nucleocapsid protein

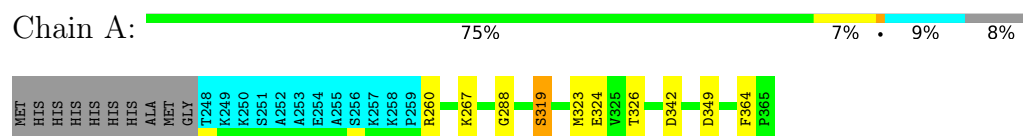


- Molecule 1: Nucleocapsid protein

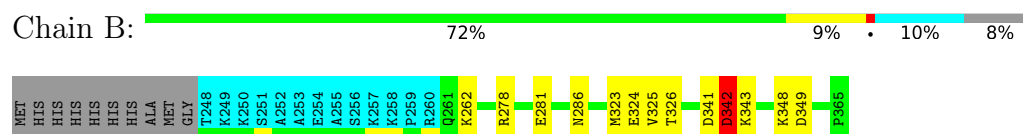


4.2.3 Score per residue for model 3

- Molecule 1: Nucleocapsid protein

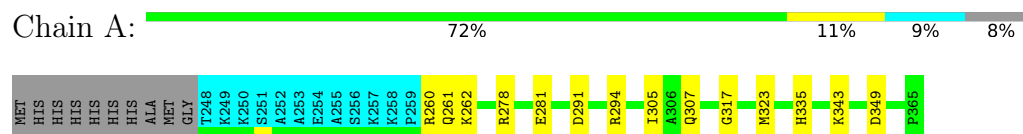


- Molecule 1: Nucleocapsid protein

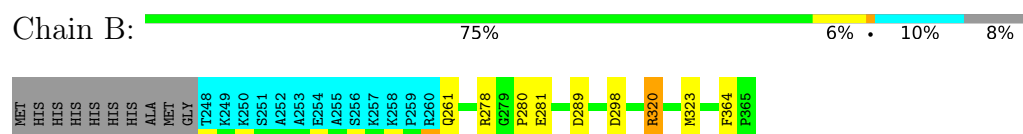


4.2.4 Score per residue for model 4

- Molecule 1: Nucleocapsid protein

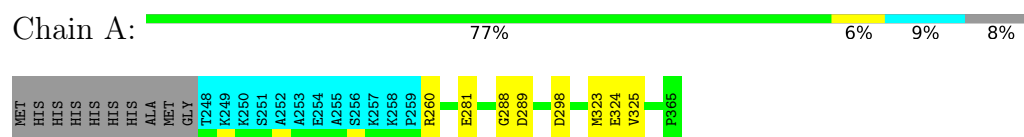


- Molecule 1: Nucleocapsid protein

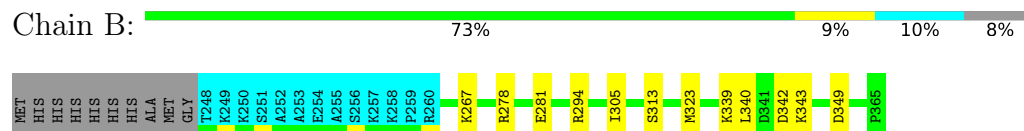


4.2.5 Score per residue for model 5

- Molecule 1: Nucleocapsid protein

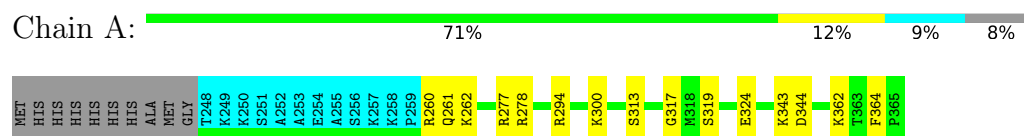


- Molecule 1: Nucleocapsid protein

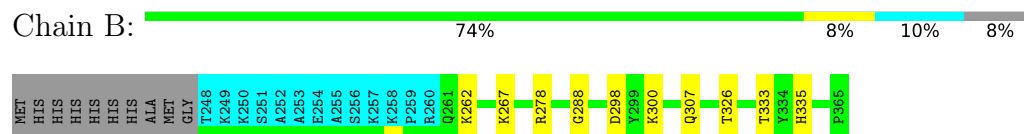


4.2.6 Score per residue for model 6

- Molecule 1: Nucleocapsid protein

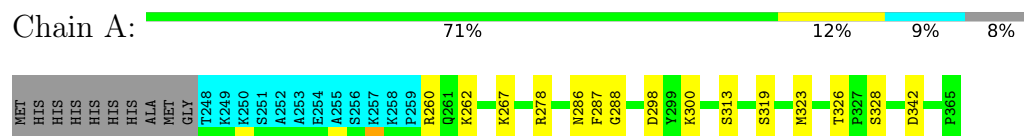


- Molecule 1: Nucleocapsid protein

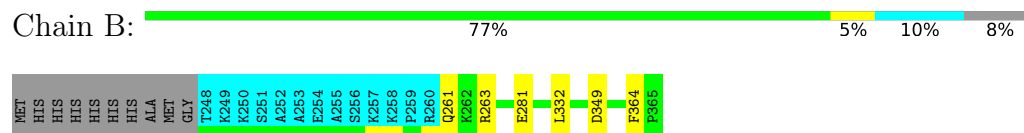


4.2.7 Score per residue for model 7

- Molecule 1: Nucleocapsid protein

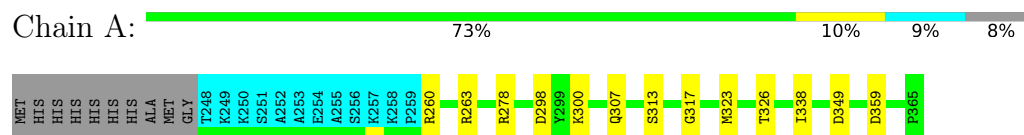


- Molecule 1: Nucleocapsid protein

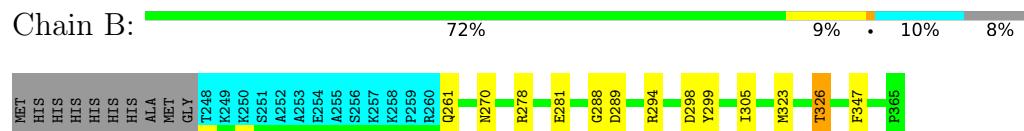


4.2.8 Score per residue for model 8

- Molecule 1: Nucleocapsid protein

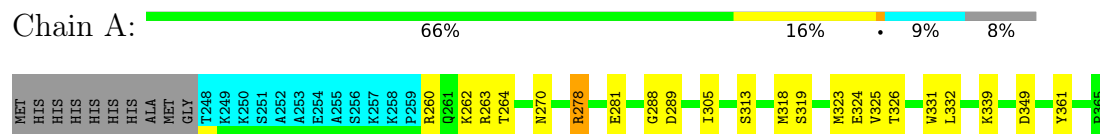


- Molecule 1: Nucleocapsid protein

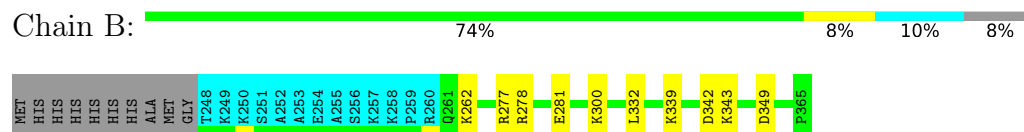


4.2.9 Score per residue for model 9

- Molecule 1: Nucleocapsid protein

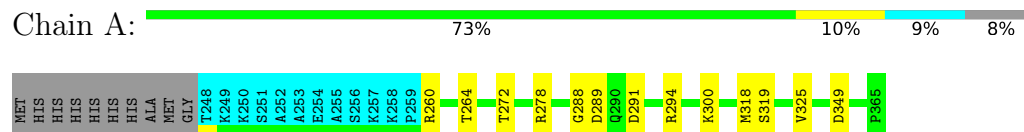


- Molecule 1: Nucleocapsid protein

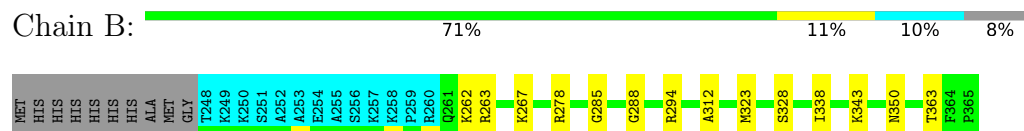


4.2.10 Score per residue for model 10

- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



4.2.11 Score per residue for model 11

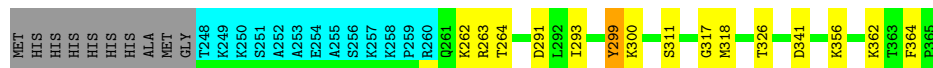
- Molecule 1: Nucleocapsid protein

Chain A: 



- Molecule 1: Nucleocapsid protein

Chain B: 



4.2.12 Score per residue for model 12

- Molecule 1: Nucleocapsid protein

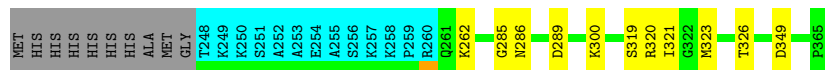
Chain A: 



P365

- Molecule 1: Nucleocapsid protein

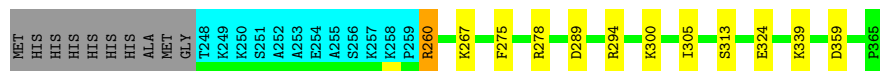
Chain B: 



4.2.13 Score per residue for model 13

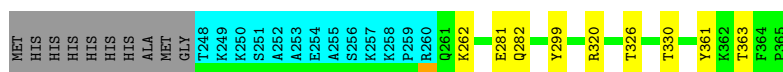
- Molecule 1: Nucleocapsid protein

Chain A: 



- Molecule 1: Nucleocapsid protein

Chain B: 



4.2.14 Score per residue for model 14

- Molecule 1: Nucleocapsid protein

Chain A: 71% 12% 9% 8%



- Molecule 1: Nucleocapsid protein

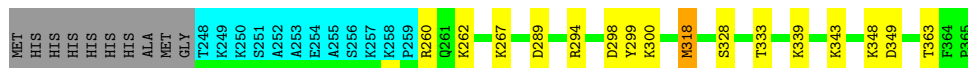
Chain B: 72% 9% 10% 8%



4.2.15 Score per residue for model 15

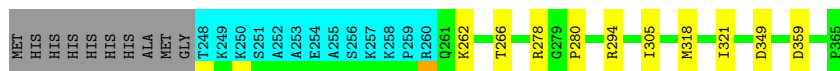
- Molecule 1: Nucleocapsid protein

Chain A: 70% 12% 9% 8%



- Molecule 1: Nucleocapsid protein

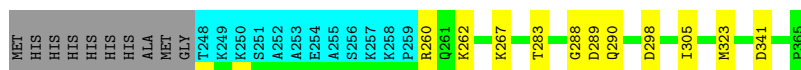
Chain B: 74% 8% 10% 8%



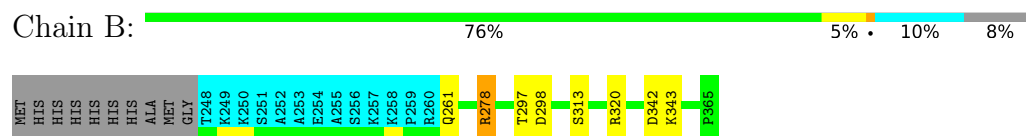
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Nucleocapsid protein

Chain A: 74% 9% 9% 8%

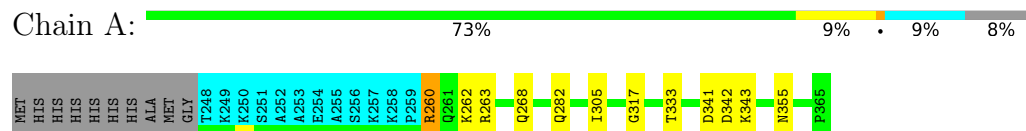


- Molecule 1: Nucleocapsid protein

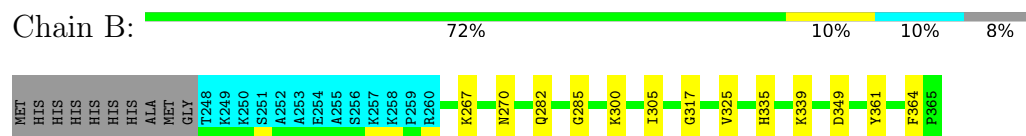


4.2.17 Score per residue for model 17

- Molecule 1: Nucleocapsid protein

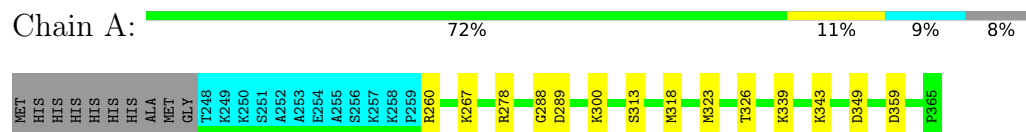


- Molecule 1: Nucleocapsid protein

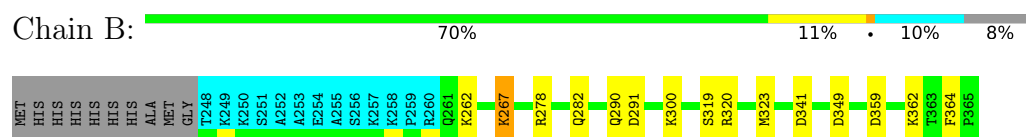


4.2.18 Score per residue for model 18

- Molecule 1: Nucleocapsid protein

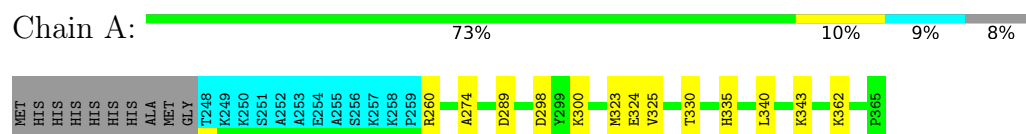


- Molecule 1: Nucleocapsid protein

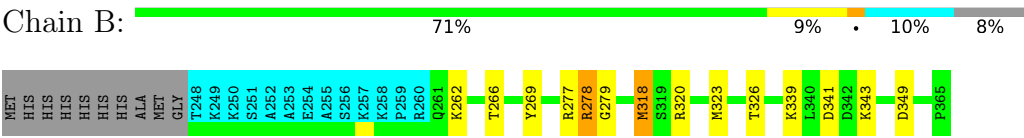


4.2.19 Score per residue for model 19

- Molecule 1: Nucleocapsid protein

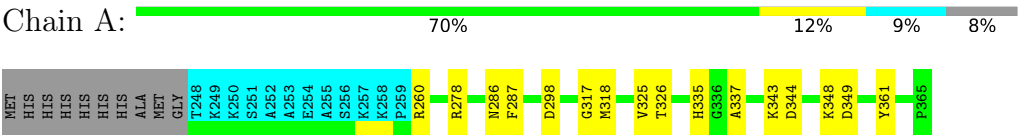


- Molecule 1: Nucleocapsid protein

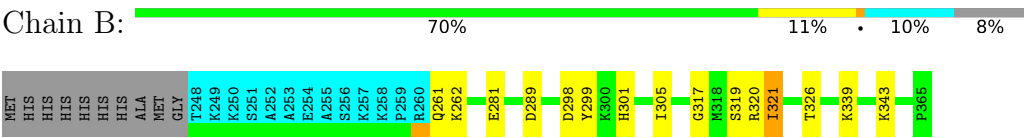


4.2.20 Score per residue for model 20

- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



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

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	0.67±0.01	0±0/878 (0.0± 0.0%)	1.37±0.03	2±2/1186 (0.2± 0.2%)
1	B	0.67±0.01	0±0/867 (0.0± 0.0%)	1.40±0.04	2±2/1172 (0.2± 0.1%)
All	All	0.67	0/34900 (0.0%)	1.39	93/47160 (0.2%)

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(°)	Ideal(°)	Models	
								Worst	Total
1	B	341	ASP	CA-CB-CG	7.56	120.16	112.60	1	1
1	A	274	ALA	N-CA-C	7.01	122.12	113.50	19	1
1	B	305	ILE	N-CA-C	-6.99	104.95	111.45	5	5
1	B	364	PHE	CA-CB-CG	6.79	120.58	113.80	18	5
1	A	305	ILE	N-CA-C	-6.78	105.14	111.45	17	8
1	B	341	ASP	CA-C-N	6.74	134.41	121.54	3	2
1	B	341	ASP	C-N-CA	6.74	134.41	121.54	3	2
1	A	364	PHE	CA-CB-CG	6.32	120.12	113.80	1	3
1	B	278	ARG	CA-C-N	6.14	131.50	121.87	19	1
1	B	278	ARG	C-N-CA	6.14	131.50	121.87	19	1
1	B	289	ASP	CA-CB-CG	6.09	118.69	112.60	4	1
1	A	291	ASP	CA-C-N	6.03	128.64	120.44	10	1
1	A	291	ASP	C-N-CA	6.03	128.64	120.44	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	289	ASP	CA-C-N	6.00	128.56	120.65	20	1
1	B	289	ASP	C-N-CA	6.00	128.56	120.65	20	1
1	B	321	ILE	CA-C-N	5.93	127.09	121.46	15	1
1	B	321	ILE	C-N-CA	5.93	127.09	121.46	15	1
1	A	335	HIS	CA-CB-CG	5.87	119.67	113.80	19	1
1	A	337	ALA	CA-C-N	5.78	130.55	122.23	20	1
1	A	337	ALA	C-N-CA	5.78	130.55	122.23	20	1
1	A	289	ASP	CA-CB-CG	5.77	118.37	112.60	5	6
1	B	321	ILE	CA-CB-CG1	5.75	120.17	110.40	20	1
1	A	340	LEU	CA-C-N	5.74	130.68	122.08	19	1
1	A	340	LEU	C-N-CA	5.74	130.68	122.08	19	1
1	A	331	TRP	CA-C-N	5.73	130.05	122.42	9	1
1	A	331	TRP	C-N-CA	5.73	130.05	122.42	9	1
1	B	340	LEU	CA-C-N	5.70	128.23	120.54	5	1
1	B	340	LEU	C-N-CA	5.70	128.23	120.54	5	1
1	B	342	ASP	CA-CB-CG	5.68	118.28	112.60	9	1
1	B	285	GLY	CA-C-N	5.63	132.30	121.54	12	1
1	B	285	GLY	C-N-CA	5.63	132.30	121.54	12	1
1	B	318	MET	CA-C-N	5.63	131.80	122.73	19	1
1	B	318	MET	C-N-CA	5.63	131.80	122.73	19	1
1	B	311	SER	CA-C-N	5.62	128.09	120.38	11	1
1	B	311	SER	C-N-CA	5.62	128.09	120.38	11	1
1	B	359	ASP	CA-CB-CG	5.62	118.22	112.60	15	1
1	A	318	MET	CA-C-N	5.60	132.23	121.54	12	1
1	A	318	MET	C-N-CA	5.60	132.23	121.54	12	1
1	A	335	HIS	CB-CG-CD2	-5.56	123.97	131.20	19	1
1	A	275	PHE	CA-C-N	5.55	128.13	120.92	13	1
1	A	275	PHE	C-N-CA	5.55	128.13	120.92	13	1
1	B	342	ASP	N-CA-C	5.54	122.60	110.80	3	1
1	A	325	VAL	CB-CA-C	5.52	118.27	111.25	19	2
1	A	318	MET	N-CA-C	5.49	119.45	112.87	18	1
1	B	312	ALA	CA-C-N	5.48	127.62	120.28	10	1
1	B	312	ALA	C-N-CA	5.48	127.62	120.28	10	1
1	A	260	ARG	CA-C-N	5.44	128.33	120.38	13	1
1	A	260	ARG	C-N-CA	5.44	128.33	120.38	13	1
1	B	335	HIS	CB-CG-CD2	-5.28	124.34	131.20	6	2
1	B	347	PHE	CA-CB-CG	5.25	119.05	113.80	8	1
1	B	301	HIS	CB-CG-CD2	-5.22	124.41	131.20	20	1
1	B	325	VAL	CB-CA-C	5.22	117.65	111.59	3	1
1	B	326	THR	CB-CA-C	5.20	116.87	108.91	8	1
1	A	330	THR	CB-CA-C	5.19	118.59	110.19	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	271	VAL	CA-C-N	5.13	127.67	120.28	11	1
1	A	271	VAL	C-N-CA	5.13	127.67	120.28	11	1
1	B	270	ASN	CA-C-N	5.12	127.75	120.53	2	2
1	B	270	ASN	C-N-CA	5.12	127.75	120.53	2	2
1	B	350	ASN	CA-CB-CG	5.10	117.70	112.60	10	1
1	A	341	ASP	CA-CB-CG	-5.09	107.51	112.60	17	1
1	A	287	PHE	CA-CB-CG	5.08	118.88	113.80	7	1
1	A	291	ASP	CA-CB-CG	5.03	117.63	112.60	4	1
1	B	281	GLU	CB-CA-C	5.03	118.26	109.65	9	1
1	B	281	GLU	CA-C-N	5.01	127.69	120.38	4	1
1	B	281	GLU	C-N-CA	5.01	127.69	120.38	4	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	278	ARG	Sidechain	4
1	B	294	ARG	Sidechain	4
1	B	299	TYR	Sidechain	4
1	B	263	ARG	Sidechain	2
1	A	260	ARG	Sidechain	2
1	B	320	ARG	Sidechain	2
1	A	263	ARG	Sidechain	2
1	A	278	ARG	Sidechain	2
1	B	361	TYR	Sidechain	2
1	A	277	ARG	Sidechain	1
1	A	361	TYR	Sidechain	1
1	A	299	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	855	828	828	0±1
All	All	33980	32860	32860	9

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:282:GLN:CD	1:B:282:GLN:H	0.43	2.21	18	1
1:B:291:ASP:HB3	1:B:299:TYR:CE1	0.42	2.49	11	1
1:B:282:GLN:H	1:B:282:GLN:CD	0.42	2.23	17	1
1:A:358:ILE:HD11	1:B:321:ILE:HG22	0.41	1.93	12	1
1:A:282:GLN:CD	1:A:282:GLN:H	0.41	2.22	17	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%)	9	53
1	B	104/128 (81%)	94±3 (90±3%)	9±2 (9±2%)	2±1 (2±1%)	11	57
All	All	4180/5120 (82%)	3748 (90%)	365 (9%)	67 (2%)	10	55

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

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Mol	Chain	Res	Type	Models (Total)
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	318	MET	2
1	B	280	PRO	2
1	A	267	LYS	2
1	B	285	GLY	2
1	B	320	ARG	2
1	A	301	HIS	1
1	A	296	GLY	1
1	B	278	ARG	1
1	A	278	ARG	1
1	B	286	ASN	1
1	A	285	GLY	1
1	B	263	ARG	1
1	A	318	MET	1
1	B	261	GLN	1
1	B	267	LYS	1
1	B	290	GLN	1
1	B	279	GLY	1

6.3.2 Protein sidechains ⓘ

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 (89±3%)	10±3 (11±3%)	8	51
1	B	88/106 (83%)	80±2 (91±3%)	8±2 (9±3%)	11	57
All	All	3540/4240 (83%)	3180 (90%)	360 (10%)	9	53

All 94 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	16
1	A	278	ARG	12

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Mol	Chain	Res	Type	Models (Total)
1	A	323	MET	12
1	B	262	LYS	12
1	B	323	MET	11
1	A	300	LYS	11
1	A	262	LYS	10
1	A	298	ASP	10
1	B	349	ASP	10
1	A	343	LYS	10
1	A	324	GLU	9
1	A	326	THR	9
1	B	278	ARG	9
1	B	326	THR	9
1	B	343	LYS	9
1	B	281	GLU	8
1	A	349	ASP	8
1	B	300	LYS	7
1	A	313	SER	7
1	B	267	LYS	6
1	A	267	LYS	6
1	B	298	ASP	6
1	A	289	ASP	6
1	A	318	MET	6
1	B	339	LYS	5
1	A	359	ASP	5
1	A	339	LYS	5
1	A	325	VAL	4
1	B	313	SER	4
1	B	363	THR	4
1	A	281	GLU	4
1	B	261	GLN	4
1	B	320	ARG	4
1	A	263	ARG	3
1	A	264	THR	3
1	B	325	VAL	3
1	B	362	LYS	3
1	A	344	ASP	3
1	B	289	ASP	3
1	B	341	ASP	3
1	A	307	GLN	3
1	A	328	SER	3
1	B	263	ARG	3
1	A	341	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	B	318	MET	3
1	B	266	THR	3
1	B	282	GLN	2
1	B	291	ASP	2
1	B	359	ASP	2
1	A	261	GLN	2
1	A	335	HIS	2
1	A	362	LYS	2
1	A	286	ASN	2
1	B	332	LEU	2
1	B	277	ARG	2
1	B	328	SER	2
1	A	266	THR	2
1	A	268	GLN	2
1	A	355	ASN	2
1	A	333	THR	2
1	A	348	LYS	2
1	A	277	ARG	1
1	A	321	ILE	1
1	B	275	PHE	1
1	B	344	ASP	1
1	A	319	SER	1
1	B	286	ASN	1
1	B	324	GLU	1
1	B	342	ASP	1
1	B	348	LYS	1
1	A	364	PHE	1
1	B	307	GLN	1
1	B	333	THR	1
1	A	338	ILE	1
1	A	270	ASN	1
1	A	332	LEU	1
1	A	272	THR	1
1	B	338	ILE	1
1	B	264	THR	1
1	B	293	ILE	1
1	B	356	LYS	1
1	B	330	THR	1
1	B	353	LEU	1
1	A	363	THR	1
1	A	283	THR	1
1	A	290	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	B	297	THR	1
1	B	270	ASN	1
1	B	335	HIS	1
1	B	364	PHE	1
1	B	269	TYR	1
1	A	287	PHE	1
1	A	361	TYR	1
1	B	321	ILE	1

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 oligosaccharides 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