



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 03:21 pm GMT

PDB ID : 9F83
Title : SARS-CoV-2 Nucleocapsid N-terminal domain (NTD) mutant D63G
Authors : Dhamotharan, K.; Schlundt, A.; Guenther, S.
Deposited on : 2024-05-06
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

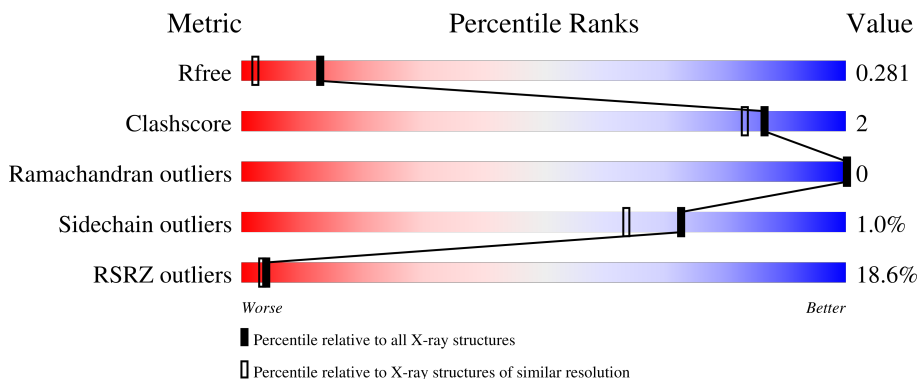
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	136	
1	B	136	
1	C	136	
1	D	136	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8009 atoms, of which 3716 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	122	1872	599	928	172	172	1	24	0	0
1	B	123	1893	608	937	173	174	1	25	0	0
1	C	119	1823	582	903	168	169	1	24	0	0
1	D	125	1919	616	948	175	179	1	25	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	expression tag	UNP P0DTC9
A	40	SER	-	expression tag	UNP P0DTC9
A	63	GLY	ASP	variant	UNP P0DTC9
B	39	GLY	-	expression tag	UNP P0DTC9
B	40	SER	-	expression tag	UNP P0DTC9
B	63	GLY	ASP	variant	UNP P0DTC9
C	39	GLY	-	expression tag	UNP P0DTC9
C	40	SER	-	expression tag	UNP P0DTC9
C	63	GLY	ASP	variant	UNP P0DTC9
D	39	GLY	-	expression tag	UNP P0DTC9
D	40	SER	-	expression tag	UNP P0DTC9
D	63	GLY	ASP	variant	UNP P0DTC9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	135	Total	O	0	0
			135	135		
2	B	141	Total	O	0	0
			141	141		

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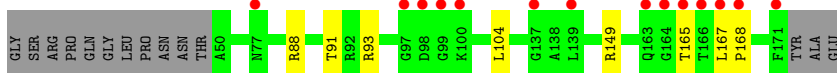
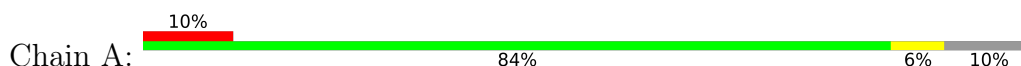
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	89	Total O 89 89	0	0
2	D	137	Total O 137 137	0	0

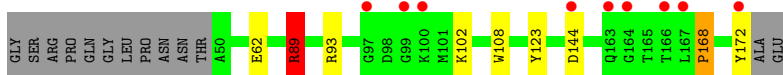
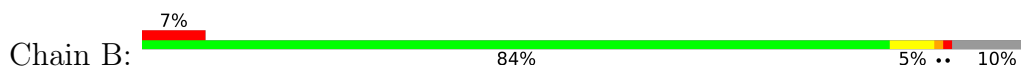
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

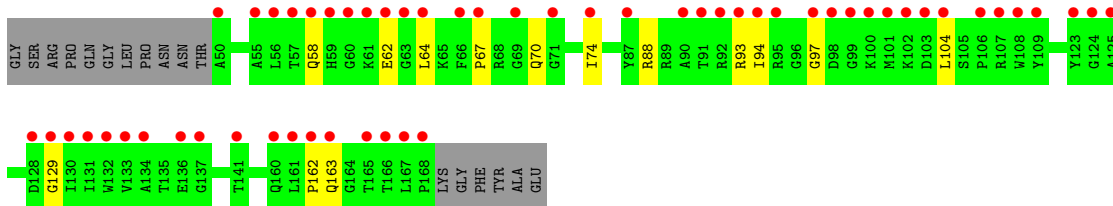
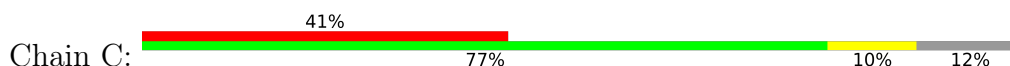
- Molecule 1: Nucleoprotein



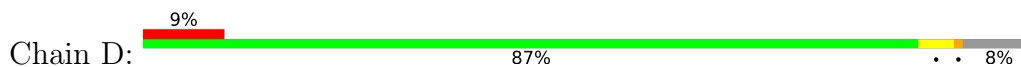
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.01Å 55.66Å 84.89Å 90.00° 95.15° 90.00°	Depositor
Resolution (Å)	50.48 – 1.70 50.48 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.48-1.70) 96.4 (50.48-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0425, BUSTER 2.10.4	Depositor
R, R_{free}	0.229 , 0.280 0.230 , 0.281	Depositor DCC
R_{free} test set	2859 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8009	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4933e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 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 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	0.73	0/971	1.09	3/1319 (0.2%)
1	B	0.76	0/984	1.24	7/1337 (0.5%)
1	C	0.61	0/946	1.05	0/1287
1	D	0.77	0/999	1.11	2/1356 (0.1%)
All	All	0.72	0/3900	1.13	12/5299 (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 outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	6

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ARG	NE-CZ-NH1	13.83	127.22	120.30
1	B	89	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	B	89	ARG	CD-NE-CZ	11.00	139.01	123.60
1	B	123	TYR	CB-CG-CD2	6.38	124.83	121.00
1	A	149	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	D	95	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	123	TYR	CB-CG-CD1	-5.69	117.58	121.00
1	B	172	TYR	CA-C-O	-5.57	108.39	120.10
1	D	89	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	104	LEU	CB-CG-CD1	5.31	120.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	PRO	N-CA-CB	5.06	109.37	103.30
1	A	168	PRO	N-CA-CB	5.06	109.37	103.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	ARG	Sidechain
1	B	89	ARG	Sidechain
1	C	163	GLN	Peptide
1	C	88	ARG	Sidechain
1	C	93	ARG	Sidechain
1	D	92	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	944	928	925	3	0
1	B	956	937	934	3	0
1	C	920	903	900	6	0
1	D	971	948	945	3	0
2	A	135	0	0	1	0
2	B	141	0	0	0	0
2	C	89	0	0	2	0
2	D	137	0	0	1	0
All	All	4293	3716	3704	15	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLN:NE2	1:C:62:GLU:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLY:N	2:C:202:HOH:O	2.36	0.54
1:D:160:GLN:HE21	1:D:160:GLN:HA	1.73	0.53
1:D:164:GLY:N	2:D:201:HOH:O	2.39	0.48
1:B:93:ARG:HH11	1:B:93:ARG:HG2	1.80	0.47
1:C:94:ILE:CG2	1:C:104:LEU:HD11	2.46	0.46
1:B:89:ARG:HD3	1:B:108:TRP:CZ2	2.51	0.45
1:A:165:THR:O	1:A:167:LEU:HD12	2.18	0.43
1:B:62:GLU:HG2	1:B:168:PRO:HB3	2.00	0.43
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.82	0.43
1:C:67:PRO:HG2	1:C:70:GLN:OE1	2.19	0.42
1:D:93:ARG:HG2	1:D:103:ASP:OD1	2.18	0.42
1:C:74:ILE:HD11	1:C:162:PRO:HA	2.03	0.41
1:A:91:THR:HG21	2:A:318:HOH:O	2.20	0.41
1:C:129:GLY:N	2:C:204:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	120/136 (88%)	117 (98%)	3 (2%)	0	100	100
1	B	121/136 (89%)	118 (98%)	3 (2%)	0	100	100
1	C	117/136 (86%)	113 (97%)	4 (3%)	0	100	100
1	D	123/136 (90%)	119 (97%)	4 (3%)	0	100	100
All	All	481/544 (88%)	467 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	95/106 (90%)	95 (100%)	0	100	100
1	B	96/106 (91%)	94 (98%)	2 (2%)	48	32
1	C	93/106 (88%)	92 (99%)	1 (1%)	70	60
1	D	97/106 (92%)	96 (99%)	1 (1%)	73	64
All	All	381/424 (90%)	377 (99%)	4 (1%)	73	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	LYS
1	B	144	ASP
1	C	64	LEU
1	D	160	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	145	HIS
1	D	145	HIS
1	D	160	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	122/136 (89%)	0.68	14 (11%) 11 10	16, 32, 74, 93	0
1	B	123/136 (90%)	0.42	9 (7%) 22 23	16, 27, 65, 95	0
1	C	119/136 (87%)	1.93	56 (47%) 0 0	22, 45, 118, 164	0
1	D	125/136 (91%)	0.50	12 (9%) 15 15	15, 28, 84, 151	0
All	All	489/544 (89%)	0.87	91 (18%) 4 3	15, 32, 93, 164	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	LEU	6.6
1	C	108	TRP	6.2
1	B	172	TYR	5.7
1	C	168	PRO	5.4
1	A	166	THR	5.2
1	C	107	ARG	5.0
1	D	97	GLY	4.7
1	B	166	THR	4.6
1	C	94	ILE	4.4
1	C	104	LEU	4.3
1	A	99	GLY	4.2
1	A	168	PRO	4.1
1	C	59	HIS	4.1
1	C	56	LEU	4.1
1	C	123	TYR	4.1
1	C	58	GLN	4.0
1	A	164	GLY	4.0
1	C	167	LEU	4.0
1	C	129	GLY	3.9
1	C	137	GLY	3.8
1	B	97	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	131	ILE	3.7
1	C	93	ARG	3.7
1	C	92	ARG	3.7
1	C	103	ASP	3.6
1	C	106	PRO	3.6
1	A	139	LEU	3.6
1	C	132	TRP	3.6
1	C	99	GLY	3.6
1	A	97	GLY	3.5
1	C	165	THR	3.5
1	C	67	PRO	3.3
1	D	94	ILE	3.3
1	C	60	GLY	3.3
1	C	161	LEU	3.3
1	C	134	ALA	3.3
1	C	69	GLY	3.2
1	C	101	MET	3.1
1	C	66	PHE	2.9
1	C	125	ALA	2.9
1	C	57	THR	2.8
1	B	164	GLY	2.8
1	D	99	GLY	2.8
1	D	152	ALA	2.8
1	C	166	THR	2.8
1	C	133	VAL	2.8
1	C	62	GLU	2.8
1	C	124	GLY	2.7
1	B	100	LYS	2.6
1	D	137	GLY	2.6
1	C	95	ARG	2.6
1	A	165	THR	2.6
1	A	167	LEU	2.6
1	C	63	GLY	2.6
1	C	55	ALA	2.6
1	D	68	ARG	2.5
1	C	136	GLU	2.5
1	C	91	THR	2.5
1	D	96	GLY	2.5
1	D	136	GLU	2.5
1	D	61	LYS	2.4
1	B	99	GLY	2.4
1	D	95	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	141	THR	2.4
1	B	144	ASP	2.4
1	A	100	LYS	2.4
1	C	61	LYS	2.4
1	A	163	GLN	2.4
1	C	130	ILE	2.3
1	C	71	GLY	2.3
1	C	50	ALA	2.3
1	C	97	GLY	2.3
1	C	100	LYS	2.3
1	A	98	ASP	2.3
1	C	162	PRO	2.2
1	B	163	GLN	2.2
1	C	90	ALA	2.2
1	A	171	PHE	2.2
1	A	137	GLY	2.1
1	C	163	GLN	2.1
1	A	77	ASN	2.1
1	B	167	LEU	2.1
1	C	109	TYR	2.1
1	C	128	ASP	2.1
1	C	160	GLN	2.1
1	C	87	TYR	2.1
1	C	74	ILE	2.0
1	C	102	LYS	2.0
1	D	93	ARG	2.0
1	D	101	MET	2.0
1	C	98	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.