



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2025 – 10:04 AM EDT

PDB ID : 9CCV / pdb\_00009ccv  
Title : Crystal structure of human respiratory syncytial virus NS1 bound to human MED25 ACID  
Authors : Kalita, P.; Borek, D.M.; Amarasinghe, G.K.; Leung, D.W.  
Deposited on : 2024-06-23  
Resolution : 2.53 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

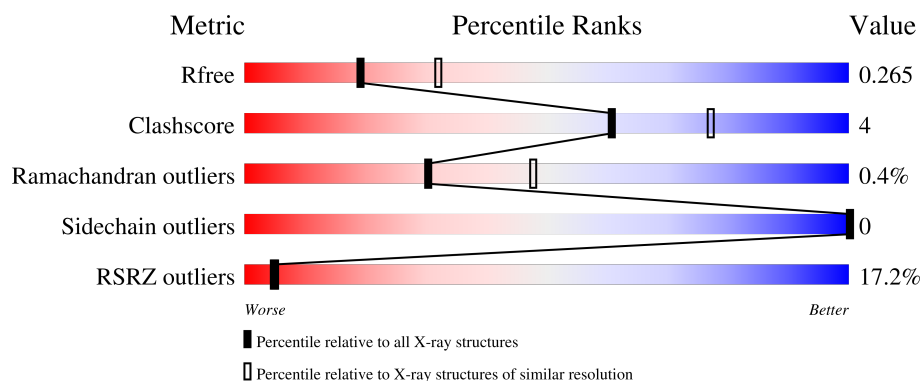
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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	6935 (2.54-2.50)
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)
RSRZ outliers	164620	6935 (2.54-2.50)

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  $\geq 3$ , 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	141	<div> <div>15%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
2	B	185	<div> <div>14%</div> <div> <div></div> <div>66%</div> <div>7%</div> <div>26%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2196 atoms, of which 0 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1036	658	171	197	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP E0WLW8
A	0	HIS	-	expression tag	UNP E0WLW8

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	136	Total	C	N	O	S	0	3	0
			1127	731	196	192	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	359	MET	-	initiating methionine	UNP Q71SY5
B	360	GLY	-	expression tag	UNP Q71SY5
B	361	SER	-	expression tag	UNP Q71SY5
B	362	SER	-	expression tag	UNP Q71SY5
B	363	HIS	-	expression tag	UNP Q71SY5
B	364	HIS	-	expression tag	UNP Q71SY5
B	365	HIS	-	expression tag	UNP Q71SY5
B	366	HIS	-	expression tag	UNP Q71SY5
B	367	HIS	-	expression tag	UNP Q71SY5
B	368	HIS	-	expression tag	UNP Q71SY5
B	369	SER	-	expression tag	UNP Q71SY5
B	370	SER	-	expression tag	UNP Q71SY5
B	371	GLY	-	expression tag	UNP Q71SY5
B	372	LEU	-	expression tag	UNP Q71SY5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	373	VAL	-	expression tag	UNP Q71SY5
B	374	PRO	-	expression tag	UNP Q71SY5
B	375	ARG	-	expression tag	UNP Q71SY5
B	376	GLY	-	expression tag	UNP Q71SY5
B	377	SER	-	expression tag	UNP Q71SY5
B	378	HIS	-	expression tag	UNP Q71SY5
B	379	ILE	-	expression tag	UNP Q71SY5
B	380	GLU	-	expression tag	UNP Q71SY5
B	381	ASN	-	expression tag	UNP Q71SY5
B	382	LEU	-	expression tag	UNP Q71SY5
B	383	TYR	-	expression tag	UNP Q71SY5
B	384	PHE	-	expression tag	UNP Q71SY5
B	385	GLN	-	expression tag	UNP Q71SY5
B	386	GLY	-	expression tag	UNP Q71SY5
B	387	HIS	-	expression tag	UNP Q71SY5
B	388	MET	-	expression tag	UNP Q71SY5

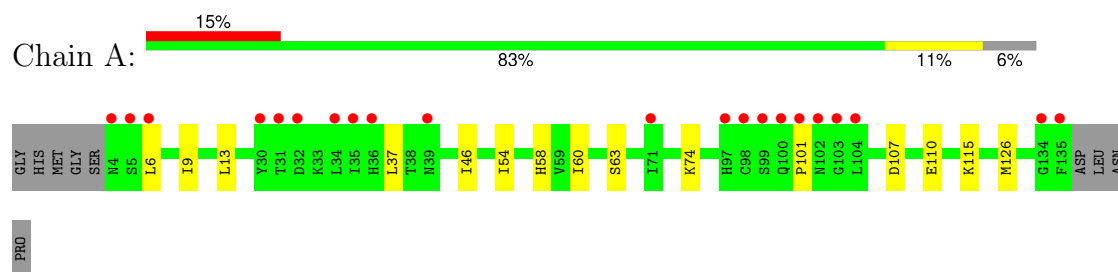
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	10	Total O 10 10	0	0

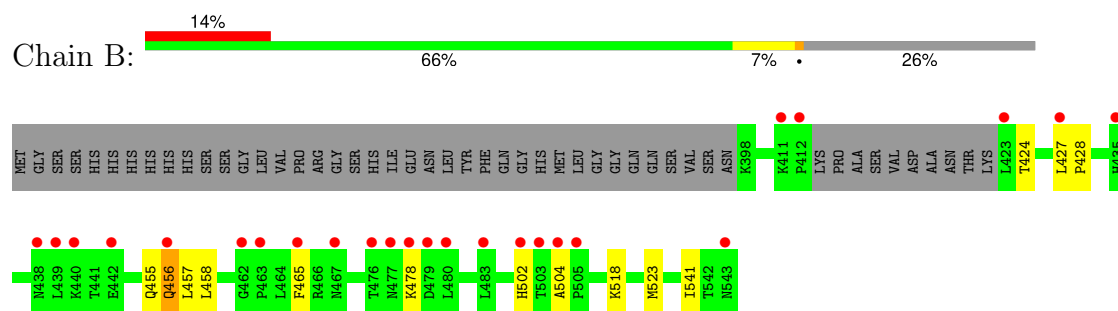
### 3 Residue-property plots [i](#)

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: Non-structural protein 1



- Molecule 2: Mediator of RNA polymerase II transcription subunit 25



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.95Å 104.95Å 63.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 2.53 48.23 – 2.53	Depositor EDS
% Data completeness (in resolution range)	87.9 (48.23-2.53) 87.9 (48.23-2.53)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, $R_{free}$	0.242 , 0.262 0.245 , 0.265	Depositor DCC
$R_{free}$ test set	605 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.25	0/1052	0.52	0/1425
2	B	0.26	0/1154	0.48	0/1559
All	All	0.26	0/2206	0.50	0/2984

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1036	0	1052	10	0
2	B	1127	0	1154	12	0
3	A	23	0	0	0	0
3	B	10	0	0	0	0
All	All	2196	0	2206	18	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 4.

The worst 5 of 18 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:A:126:MET:HA	2:B:541:ILE:HD12	1.76	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:HD12	1:A:37:LEU:HD23	1.89	0.53
2:B:456[A]:GLN:NE2	2:B:456[A]:GLN:H	2.08	0.52
2:B:455[B]:GLN:O	2:B:456[B]:GLN:C	2.48	0.51
1:A:54:ILE:HD12	2:B:523:MET:SD	2.53	0.49

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	130/141 (92%)	124 (95%)	6 (5%)	0	100	100
2	B	135/185 (73%)	131 (97%)	2 (2%)	2 (2%)	8	15
All	All	265/326 (81%)	255 (96%)	8 (3%)	2 (1%)	30	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	456[A]	GLN
2	B	456[B]	GLN

### 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.

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	123/130 (95%)	123 (100%)	0	100	100
2	B	126/164 (77%)	126 (100%)	0	100	100
All	All	249/294 (85%)	249 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	127	ASN
2	B	443	GLN
2	B	543	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	132/141 (93%)	0.80	21 (15%)	6 6	11, 44, 83, 96	0
2	B	136/185 (73%)	1.15	25 (18%)	4 4	14, 40, 79, 91	3 (2%)
All	All	268/326 (82%)	0.97	46 (17%)	5 5	11, 40, 80, 96	3 (1%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	465	PHE	7.5
1	A	104	LEU	6.0
2	B	412	PRO	5.7
2	B	505	PRO	5.5
2	B	423	LEU	4.9

### 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.