



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 12:10 AM UTC

PDB ID : 9NW4 / pdb\_00009nw4  
Title : Structure of CISV1 antibody bound to PvCSP repeat peptide  
Authors : Hurlburt, N.K.; Pancera, M.  
Deposited on : 2025-03-21  
Resolution : 1.82 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

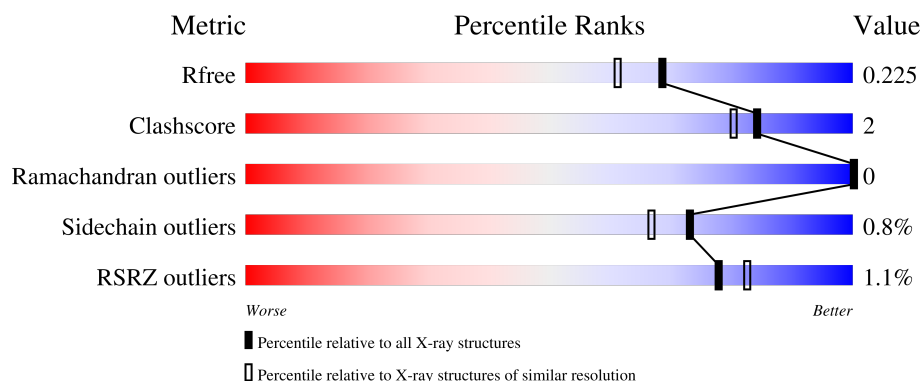
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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))
$R_{free}$	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	229	<div> <div>0%</div> <div>87%</div> <div>7%</div> </div>
1	H	229	<div> <div>2%</div> <div>90%</div> <div>7%</div> </div>
2	B	220	<div> <div>94%</div> <div>5%</div> </div>
2	L	220	<div> <div>94%</div> <div>5%</div> </div>
3	C	18	<div> <div>6%</div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain	
			6%	44%
3	P	18		

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7687 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 CISV1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	9	0
			1621	1025	273	317	6			
1	H	212	Total	C	N	O	S	0	5	0
			1604	1011	270	317	6			

- Molecule 2 is a protein called CISV1 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	6	0
			1728	1082	288	351	7			
2	L	218	Total	C	N	O	S	0	8	0
			1742	1091	291	355	5			

- Molecule 3 is a protein called PvCSPvk210 peptide from Circumsporozoite protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			61	34	13	14			
3	P	10	Total	C	N	O	0	0	0
			65	36	14	15			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	232	Total	O	0	0
			232	232		
4	B	217	Total	O	0	0
			217	217		
4	C	14	Total	O	0	0
			14	14		
4	H	198	Total	O	0	0
			198	198		

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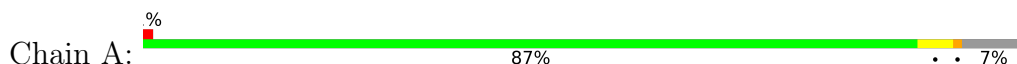
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	192	Total 192	O 192	0	0
4	P	13	Total 13	O 13	0	0

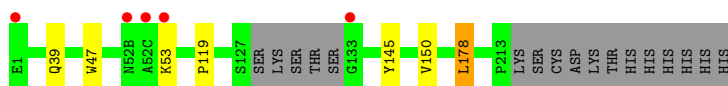
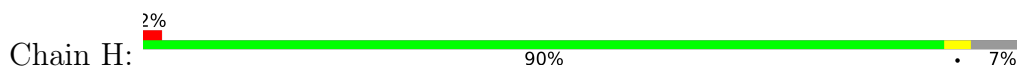
### 3 Residue-property plots [i](#)

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: CISV1 Fab Heavy Chain



- Molecule 1: CISV1 Fab Heavy Chain



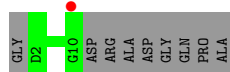
- Molecule 2: CISV1 Fab Light Chain



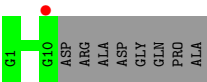
- Molecule 2: CISV1 Fab Light Chain



- Molecule 3: PvCSPvk210 peptide from Circumsporozoite protein



- Molecule 3: PvCSPvk210 peptide from Circumsporozoite protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.50Å 66.96Å 142.81Å 90.00° 96.19° 90.00°	Depositor
Resolution (Å)	48.76 – 1.82 48.76 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.76-1.82) 99.0 (48.76-1.82)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 1.82Å)	Xtriage
Refinement program	PDB-REDO, PHENIX 1.20.1	Depositor
R, $R_{free}$	0.183 , 0.215 0.198 , 0.225	Depositor DCC
$R_{free}$ test set	4376 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.85 % 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 2.9832e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 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 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	0.58	0/1669	0.81	0/2268
1	H	0.59	0/1640	0.81	0/2233
2	B	0.66	1/1770 (0.1%)	0.86	2/2404 (0.1%)
2	L	0.63	0/1781	0.85	1/2420 (0.0%)
3	C	0.63	0/61	0.78	0/81
3	P	0.57	0/65	0.90	0/86
All	All	0.62	1/6986 (0.0%)	0.83	3/9492 (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 outliers	#Planarity outliers
2	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	MET	SD-CE	-7.37	1.61	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	60	ASP	CA-CB-CG	5.72	118.32	112.60
2	B	60	ASP	CA-CB-CG	5.50	118.10	112.60
2	B	170	ASP	CA-CB-CG	5.19	117.79	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	211	ARG	Sidechain

## 5.2 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 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	1621	0	1614	11	0
1	H	1604	0	1576	5	0
2	B	1728	0	1676	8	0
2	L	1742	0	1689	9	0
3	C	61	0	51	0	0
3	P	65	0	57	0	0
4	A	232	0	0	3	0
4	B	217	0	0	0	0
4	C	14	0	0	0	0
4	H	198	0	0	1	0
4	L	192	0	0	5	0
4	P	13	0	0	0	0
All	All	7687	0	6663	31	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.

The worst 5 of 31 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)
2:L:210:ASN:HB3	4:L:350:HOH:O	1.88	0.74
1:A:147:PRO:O	1:A:200:HIS:HE1	1.78	0.67
1:A:53[A]:LYS:HD2	4:A:455:HOH:O	1.99	0.63
1:A:200:HIS:HD2	1:A:203:SER:OG	1.81	0.63
2:B:13:VAL:HG22	2:B:78:LEU:HD22	1.83	0.59

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 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 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	217/229 (95%)	214 (99%)	3 (1%)	0	100	100
1	H	213/229 (93%)	210 (99%)	3 (1%)	0	100	100
2	B	223/220 (101%)	220 (99%)	3 (1%)	0	100	100
2	L	224/220 (102%)	220 (98%)	4 (2%)	0	100	100
3	C	7/18 (39%)	7 (100%)	0	0	100	100
3	P	8/18 (44%)	8 (100%)	0	0	100	100
All	All	892/934 (96%)	879 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 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 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	184/192 (96%)	179 (97%)	5 (3%)	39	22
1	H	180/192 (94%)	178 (99%)	2 (1%)	65	56
2	B	199/194 (103%)	199 (100%)	0	100	100
2	L	200/194 (103%)	200 (100%)	0	100	100
3	C	5/10 (50%)	5 (100%)	0	100	100
3	P	5/10 (50%)	5 (100%)	0	100	100
All	All	773/792 (98%)	766 (99%)	7 (1%)	73	62

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LEU
1	A	212	GLU
1	H	178	LEU
1	H	53	LYS
1	A	149	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	147	GLN
2	B	199	GLN
2	L	152	ASN
2	L	138	ASN
2	L	147	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 [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	212/229 (92%)	-0.17	3 (1%) 73 79	6, 14, 27, 62	9 (4%)
1	H	212/229 (92%)	-0.09	5 (2%) 59 66	5, 14, 29, 54	5 (2%)
2	B	219/220 (99%)	-0.20	0 100 100	6, 14, 29, 39	6 (2%)
2	L	218/220 (99%)	-0.20	0 100 100	7, 14, 28, 36	8 (3%)
3	C	9/18 (50%)	0.47	1 (11%) 10 11	8, 10, 21, 22	0
3	P	10/18 (55%)	0.25	1 (10%) 12 14	10, 13, 23, 30	0
All	All	880/934 (94%)	-0.15	10 (1%) 78 82	5, 14, 28, 62	28 (3%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	133	GLY	4.5
1	A	132	SER	4.1
1	H	53	LYS	3.2
1	A	133	GLY	3.1
1	A	214	LYS	3.0

### 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 oligosaccharides 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.