



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 22, 2026 – 11:49 AM EDT

PDB ID : 2RMU / pdb\_00002rmu  
Title : THREE-DIMENSIONAL STRUCTURES OF DRUG-RESISTANT MUTANTS OF HUMAN RHINOVIRUS 14  
Authors : Badger, J.; Krishnaswamy, S.; Kremer, M.J.; Oliveira, M.A.; Rossmann, M.G.; Heinz, B.A.; Rueckert, R.R.; Dutko, F.J.; Mckinlay, M.A.  
Deposited on : 1988-10-03  
Resolution : 3.00 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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : **FAILED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

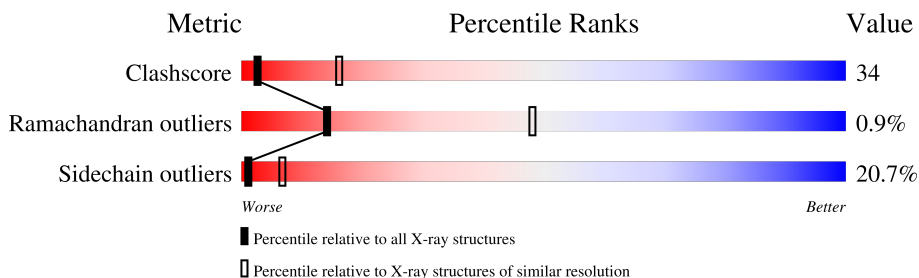
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	289	22% (green), 40% (yellow), 24% (orange), 8% (red), 6% (grey)
2	2	262	24% (green), 37% (yellow), 27% (orange), 9% (red), 3% (grey)
3	3	236	25% (green), 38% (yellow), 29% (orange), 9% (red), 1% (grey)
4	4	68	13% (green), 21% (yellow), 15% (orange), 10% (red), 41% (grey)

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6541 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 HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	273	2171	1374	375	414	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	188	LEU	VAL	conflict	UNP P03303

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	255	1952	1238	330	372	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	conflict	UNP P03303

- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	236	1849	1184	305	353	7	0	0	0

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	40	Total	C	N	O	S	0	0	0
			297	186	47	62	2			

- Molecule 5 is water.

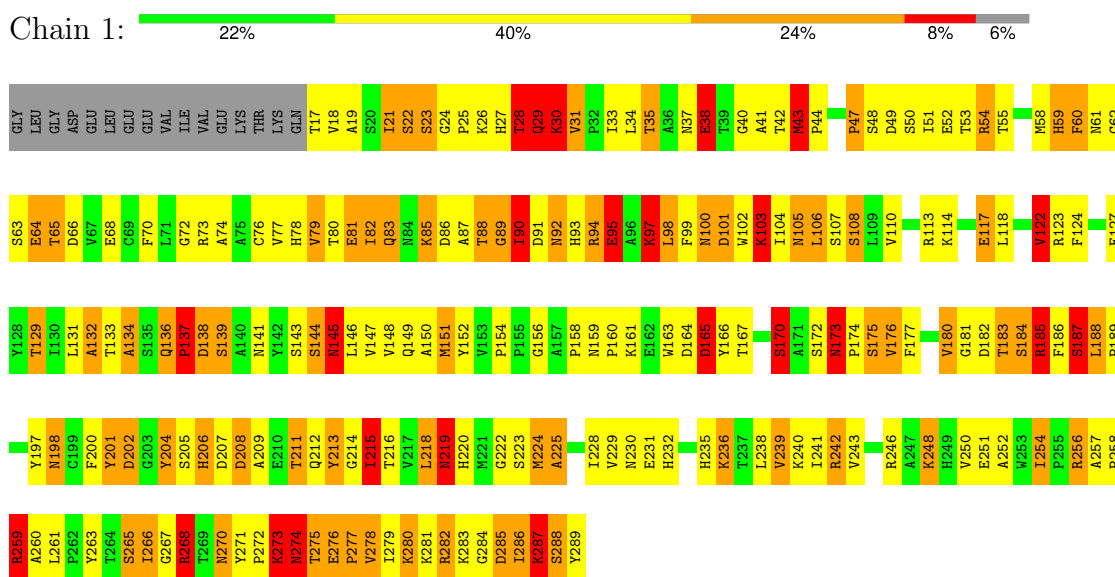
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	95	Total	O	0	0
			95	95		
5	2	85	Total	O	0	0
			85	85		
5	3	84	Total	O	0	0
			84	84		
5	4	8	Total	O	0	0
			8	8		

### 3 Residue-property plots

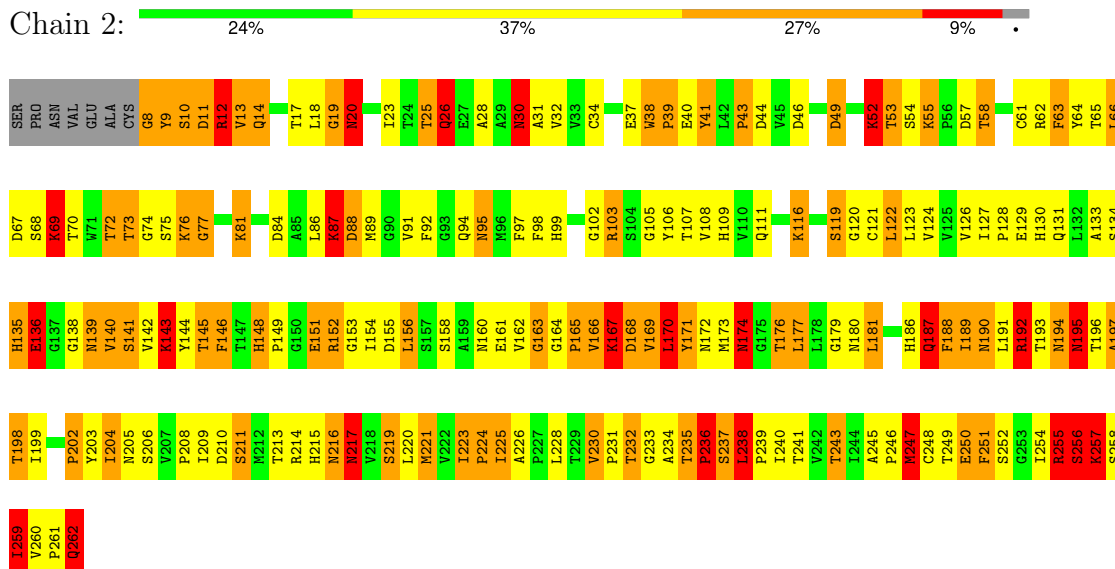
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

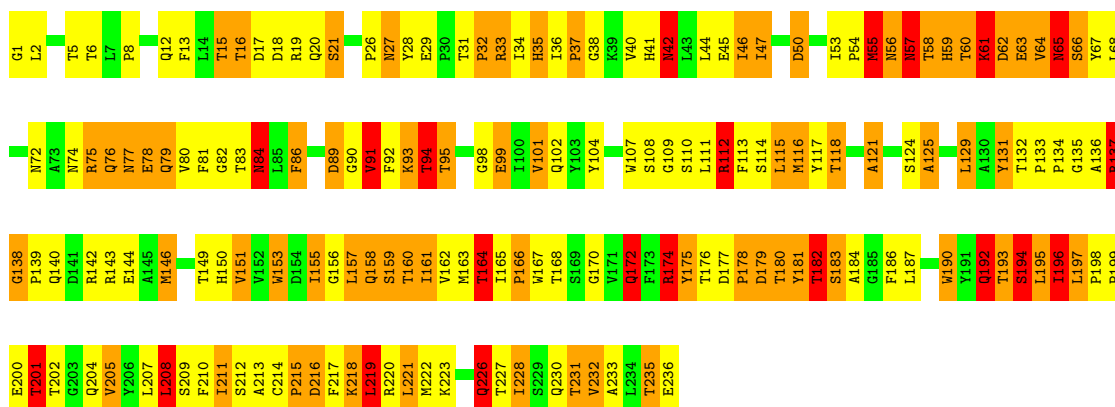
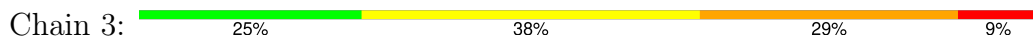
- Molecule 1: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)



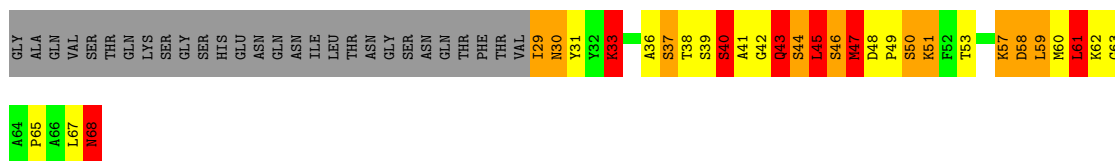
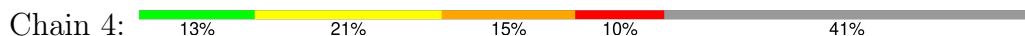
- Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)



● Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)



● Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4)



## 4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.15 (at 2.91Å)	Xtrriage
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Wilson B-factor (Å <sup>2</sup> )	14.2	Xtrriage
Anisotropy	0.000	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.14$	Xtrriage
Estimated twinning fraction	0.176 for l,-k,h	Xtrriage
Total number of atoms	6541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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	1	2.45	109/2229 (4.9%)	2.91	246/3032 (8.1%)
2	2	2.40	96/2001 (4.8%)	2.77	193/2735 (7.1%)
3	3	2.31	81/1898 (4.3%)	2.80	192/2597 (7.4%)
4	4	2.64	14/302 (4.6%)	3.14	33/406 (8.1%)
All	All	2.40	300/6430 (4.7%)	2.84	664/8770 (7.6%)

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	1	0	2
2	2	0	2
All	All	0	4

The worst 5 of 300 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	285	ASP	CA-CB	17.77	1.79	1.53
4	4	41	ALA	C-O	13.33	1.41	1.24
3	3	57	ASN	CA-CB	12.78	1.75	1.53
4	4	42	GLY	N-CA	12.59	1.63	1.45
1	1	187	SER	N-CA	11.77	1.60	1.46

The worst 5 of 664 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	50	ASP	CA-CB-CG	27.73	140.33	112.60
1	1	285	ASP	CA-CB-CG	-22.21	90.39	112.60
3	3	215	PRO	CA-C-N	20.36	149.20	120.29
3	3	215	PRO	C-N-CA	20.36	149.20	120.29
2	2	87	LYS	CA-CB-CG	19.05	152.21	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	259	ARG	Sidechain
1	1	268	ARG	Sidechain
2	2	12	ARG	Sidechain
2	2	255	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	1	2171	0	2108	162	0
2	2	1952	0	1926	139	0
3	3	1849	0	1832	157	0
4	4	297	0	294	38	0
5	1	95	0	0	11	0
5	2	85	0	0	7	0
5	3	84	0	0	6	0
5	4	8	0	0	1	0
All	All	6541	0	6160	420	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 34.

The worst 5 of 420 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)
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.58
4:4:33:LYS:CE	4:4:33:LYS:NZ	1.67	1.55
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.54
1:1:285:ASP:CB	1:1:285:ASP:CA	1.79	1.54
3:3:179:ASP:OD1	3:3:182:THR:HB	1.41	1.17

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	1	271/289 (94%)	254 (94%)	15 (6%)	2 (1%)	18	53
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	16	50
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	14	48
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	4	23
All	All	796/855 (93%)	738 (93%)	51 (6%)	7 (1%)	14	48

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	SER
3	3	57	ASN
3	3	77	ASN
1	1	165	ASP
2	2	255	ARG

### 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	1	239/253 (94%)	192 (80%)	47 (20%)	1	8
2	2	223/229 (97%)	176 (79%)	47 (21%)	1	6
3	3	209/209 (100%)	170 (81%)	39 (19%)	1	9
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	1
All	All	704/748 (94%)	558 (79%)	146 (21%)	1	7

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	164	THR
4	4	61	LEU
3	3	182	THR
3	3	226	GLN
2	2	20	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	74	ASN
3	3	84	ASN
3	3	226	GLN
2	2	111	GLN
2	2	94	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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.