



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2021 – 08:23 AM EDT

PDB ID : 1RUJ  
Title : RHINOVIRUS 14 MUTANT WITH SER 1 223 REPLACED BY GLY (S1223G)  
Authors : Hadfield, A.; Oliveira, M.A.; Kim, K.H.; Minor, I.; Kremer, M.J.; Heinz, B.A.; Shepard, D.; Pevear, D.C.; Rueckert, R.R.; Rossmann, M.G.  
Deposited on : 1995-06-09  
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

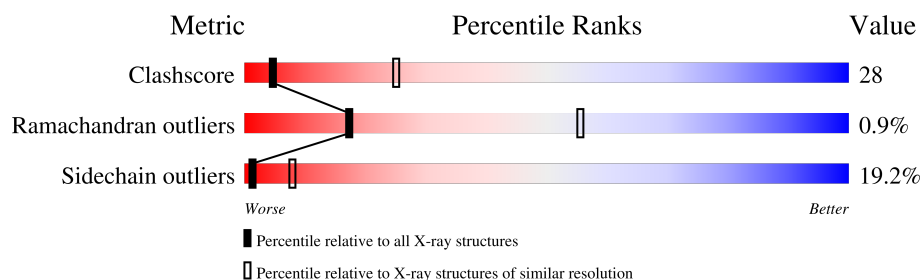
# 1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 was not executed.

Mol	Chain	Length	Quality of chain
1	1	289	
2	2	262	
3	3	236	
4	4	68	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6266 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 RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	273	Total	C	N	O	S	0	0	0
			2168	1372	375	413	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	223	GLY	SER	engineered mutation	UNP P03303

- Molecule 2 is a protein called RHINOVIRUS 14.

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

There is a discrepancy between the modelled and reference sequences:

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

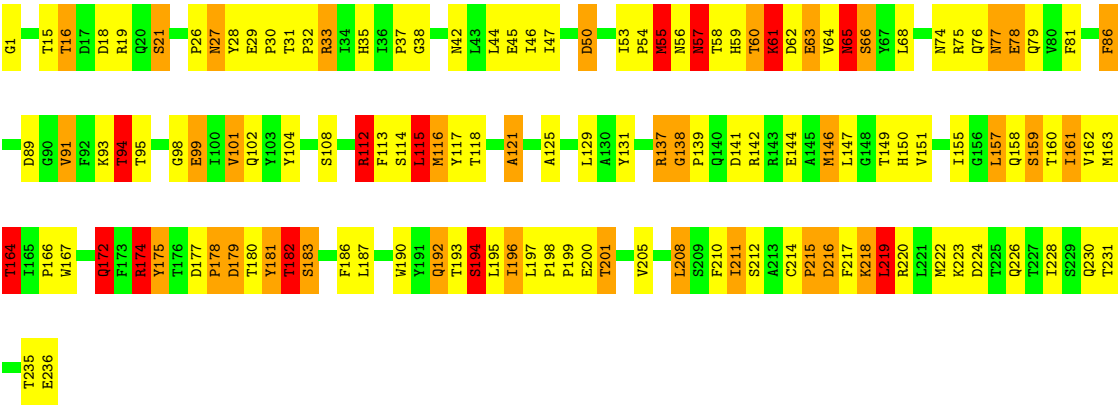
- Molecule 3 is a protein called RHINOVIRUS 14.

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

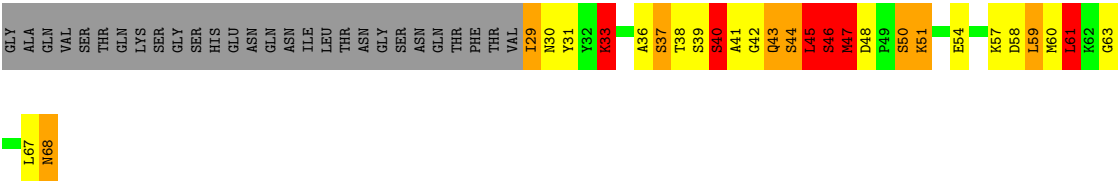
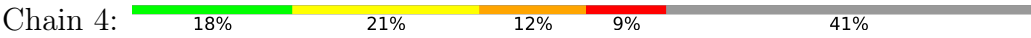
- Molecule 4 is a protein called RHINOVIRUS 14.

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





● Molecule 4: RHINOVIRUS 14



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - 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
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program		Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	1.0	wwPDB-VP

## 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	1	1.97	44/2226 (2.0%)	2.46	136/3028 (4.5%)
2	2	1.85	32/2001 (1.6%)	2.17	78/2735 (2.9%)
3	3	1.77	21/1898 (1.1%)	2.18	75/2597 (2.9%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.89	110/6427 (1.7%)	2.29	310/8766 (3.5%)

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 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	170	SER	CB-OG	-14.31	1.23	1.42
1	1	285	ASP	CA-CB	11.82	1.79	1.53
4	4	42	GLY	N-CA	11.70	1.63	1.46
4	4	40	SER	CB-OG	10.74	1.56	1.42
2	2	256	SER	CB-OG	10.20	1.55	1.42

The worst 5 of 310 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	246	ARG	NE-CZ-NH1	22.45	131.52	120.30
1	1	256	ARG	NE-CZ-NH2	20.38	130.49	120.30
1	1	123	ARG	NE-CZ-NH1	19.14	129.87	120.30
2	2	255	ARG	NE-CZ-NH2	-18.62	110.99	120.30
2	2	87	LYS	CA-CB-CG	17.62	152.17	113.40

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	2168	0	2102	146	0
2	2	1952	0	1926	113	0
3	3	1849	0	1831	130	0
4	4	297	0	294	28	0
All	All	6266	0	6153	349	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 28.

The worst 5 of 349 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)
4:4:33:LYS:CE	4:4:33:LYS:NZ	1.67	1.57
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.55
1:1:285:ASP:CB	1:1:285:ASP:CA	1.80	1.54
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.53
3:3:179:ASP:OD2	3:3:182:THR:HB	1.41	1.19

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	1	271/289 (94%)	254 (94%)	15 (6%)	2 (1%)	22	60
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	19	57
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	17	55
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	5	27
All	All	796/855 (93%)	738 (93%)	51 (6%)	7 (1%)	17	55

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 ⓘ

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	238/252 (94%)	195 (82%)	43 (18%)	1	9
2	2	223/229 (97%)	181 (81%)	42 (19%)	1	8
3	3	209/209 (100%)	172 (82%)	37 (18%)	2	9
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	0
All	All	703/747 (94%)	568 (81%)	135 (19%)	1	8

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	218	LYS
3	3	226	GLN
4	4	51	LYS
2	2	52	LYS
2	2	49	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	262	GLN
3	3	102	GLN
3	3	226	GLN
3	3	140	GLN
1	1	219	ASN

### 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 monosaccharides 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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.