

wwPDB X-ray Structure Validation Summary Report (i)

Oct 1, 2021 – 03:09 am BST

PDB ID : 7NLG

Title : S. cerevisiae Ty1 p22 restriction factor, Gag CA-CTD, AUG2 variant A273V

mutant

Authors : Cottee, M.A.; Taylor, I.A.

Deposited on : 2021-02-22

Resolution : 3.53 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*A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

EDS : 2.23.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

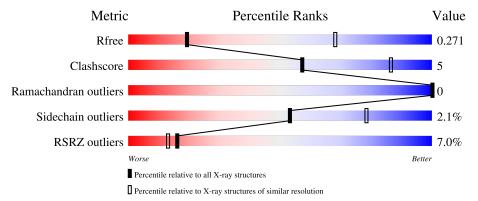
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 3.53 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 <=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	106	74%	9%	•	15%	
1	В	106	72%	13%		15%	
1	С	106	73%	12%		15%	



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2186 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 Ty1 Gag p22.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	90	Total	С	N	О	S	0	0	0
1	Α	90	726	453	130	140	3	0	U	U
1	D	90	Total	С	N	О	S	0	1	0
1	Ъ	90	734	461	130	140	3	0	1	0
1	C	90	Total	С	N	О	S	0	0	0
1		90	726	453	130	140	3	U		0

There are 30 discrepancies between the modelled and reference sequences:

A 356 PRO - expression tag UNP P084 A 357 LEU - expression tag UNP P084 A 358 GLU - expression tag UNP P084 A 359 HIS - expression tag UNP P084 A 360 HIS - expression tag UNP P084 A 361 HIS - expression tag UNP P084 A 363 HIS - expression tag UNP P084 A 364 HIS - expression tag UNP P084 B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 </th <th>Chain</th> <th>Residue</th> <th>Modelled</th> <th>Actual</th> <th>Comment</th> <th>Reference</th>	Chain	Residue	Modelled	Actual	Comment	Reference
A 357 LEU - expression tag UNP P084 A 358 GLU - expression tag UNP P084 A 359 HIS - expression tag UNP P084 A 360 HIS - expression tag UNP P084 A 361 HIS - expression tag UNP P084 A 363 HIS - expression tag UNP P084 A 364 HIS - expression tag UNP P084 B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 </td <td>A</td> <td>273</td> <td>VAL</td> <td>ALA</td> <td>engineered mutation</td> <td>UNP P08405</td>	A	273	VAL	ALA	engineered mutation	UNP P08405
A 358 GLU - expression tag UNP P084 A 359 HIS - expression tag UNP P084 A 360 HIS - expression tag UNP P084 A 361 HIS - expression tag UNP P084 A 362 HIS - expression tag UNP P084 A 363 HIS - expression tag UNP P084 B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 </td <td>A</td> <td>356</td> <td>PRO</td> <td>-</td> <td>expression tag</td> <td>UNP P08405</td>	A	356	PRO	-	expression tag	UNP P08405
A 359 HIS - expression tag UNP P084 A 360 HIS - expression tag UNP P084 A 361 HIS - expression tag UNP P084 A 362 HIS - expression tag UNP P084 A 363 HIS - expression tag UNP P084 A 364 HIS - expression tag UNP P084 B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 </td <td>A</td> <td>357</td> <td>LEU</td> <td>-</td> <td>expression tag</td> <td>UNP P08405</td>	A	357	LEU	-	expression tag	UNP P08405
A 360 HIS - expression tag UNP P084 A 361 HIS - expression tag UNP P084 A 362 HIS - expression tag UNP P084 A 363 HIS - expression tag UNP P084 A 364 HIS - expression tag UNP P084 B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 </td <td>A</td> <td>358</td> <td>GLU</td> <td>-</td> <td>expression tag</td> <td>UNP P08405</td>	A	358	GLU	-	expression tag	UNP P08405
A 361 HIS - expression tag UNP P084 A 362 HIS - expression tag UNP P084 A 363 HIS - expression tag UNP P084 A 364 HIS - expression tag UNP P084 B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 </td <td>A</td> <td>359</td> <td>HIS</td> <td>-</td> <td>expression tag</td> <td>UNP P08405</td>	A	359	HIS	-	expression tag	UNP P08405
A 362 HIS - expression tag UNP P084 A 363 HIS - expression tag UNP P084 A 364 HIS - expression tag UNP P084 B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084 </td <td>A</td> <td>360</td> <td>HIS</td> <td>-</td> <td>expression tag</td> <td>UNP P08405</td>	A	360	HIS	-	expression tag	UNP P08405
A 363 HIS - expression tag UNP P084 A 364 HIS - expression tag UNP P084 B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	A	361	HIS	-	expression tag	UNP P08405
A 364 HIS - expression tag UNP P084 B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	A	362	HIS	-	expression tag	UNP P08405
B 273 VAL ALA engineered mutation UNP P084 B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	A	363	HIS	-	expression tag	UNP P08405
B 356 PRO - expression tag UNP P084 B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	A	364	HIS	-	- expression tag	
B 357 LEU - expression tag UNP P084 B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	В	273	VAL	ALA	engineered mutation	UNP P08405
B 358 GLU - expression tag UNP P084 B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	В	356	PRO	-	expression tag	UNP P08405
B 359 HIS - expression tag UNP P084 B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	В	357	LEU	-	expression tag	UNP P08405
B 360 HIS - expression tag UNP P084 B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	В	358	GLU	-	expression tag	UNP P08405
B 361 HIS - expression tag UNP P084 B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	В	359	HIS	-	expression tag	UNP P08405
B 362 HIS - expression tag UNP P084 B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	В	360	HIS	-	expression tag	UNP P08405
B 363 HIS - expression tag UNP P084 B 364 HIS - expression tag UNP P084	В	361	HIS	-	expression tag	UNP P08405
B 364 HIS - expression tag UNP P084	В	362	HIS	-	expression tag	UNP P08405
	В	363	HIS	-	expression tag	UNP P08405
C SEC TIAL ALA LINE DOCA	В	364	HIS	-	expression tag	UNP P08405
C 273 VAL ALA engineered mutation UNP P084	С	273	VAL	ALA	engineered mutation	UNP P08405
C 356 PRO - expression tag UNP P084	С	356	PRO	-	expression tag	UNP P08405
C 357 LEU - expression tag UNP P084	С	357	LEU	-	<u> </u>	UNP P08405

Continued on next page...



Continued from previous page...

Chain	Residue	Modelled	Actual Comment		Reference
С	358	GLU	-	expression tag	UNP P08405
С	359	HIS	-	expression tag	UNP P08405
С	360	HIS	-	expression tag	UNP P08405
С	361	HIS	-	expression tag	UNP P08405
С	362	HIS	-	expression tag	UNP P08405
С	363	HIS	-	expression tag	UNP P08405
С	364	HIS	-	expression tag	UNP P08405



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: Ty1 Gag p22

Chain A:

74%

9%

15%

Molecule 1: Ty1 Gag p22

Chain B:

72%

13%

15%

Molecule 1: Ty1 Gag p22

Chain C:

73%

12%

15%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	279.87Å 279.87Å 39.92Å	Domositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	91.61 - 3.53	Depositor
Resolution (A)	91.61 - 3.53	EDS
% Data completeness	99.7 (91.61-3.53)	Depositor
(in resolution range)	99.7 (91.61-3.53)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.83 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.14_3260, REFMAC 5.8.0258	Depositor
D.D.	0.225 , 0.272	Depositor
R, R_{free}	0.225 , 0.271	DCC
R_{free} test set	630 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	154.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2186	wwPDB-VP
Average B, all atoms (Å ²)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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	Mol Chain		lengths	Bond	angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.24	0/737	0.39	0/998
1	В	0.25	0/749	0.40	0/1014
1	С	0.23	0/737	0.39	0/998
All	All	0.24	0/2223	0.39	0/3010

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	726	0	710	8	0
1	В	734	0	719	9	0
1	С	726	0	710	7	0
All	All	2186	0	2139	21	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 5.

The worst 5 of 21 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\mathring{\mathbf{A}}) \end{aligned}$
1:B:265:GLU:HG3	1:B:300:ASN:HD22	1.68	0.58

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:B:273:VAL:O	1:B:315:ARG:NH1	2.37	0.56
1:A:273:VAL:O	1:A:315:ARG:NH1	2.40	0.53
1:C:265:GLU:HG3	1:C:300:ASN:HD22	1.75	0.50
1:B:277:TYR:HB3	1:B:317:LEU:HD12	1.93	0.50

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	Perce	$_{ m ntiles}$
1	A	88/106 (83%)	82 (93%)	6 (7%)	0	100	100
1	В	89/106 (84%)	83 (93%)	6 (7%)	0	100	100
1	С	88/106 (83%)	82 (93%)	6 (7%)	0	100	100
All	All	265/318 (83%)	247 (93%)	18 (7%)	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 side chain 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	80/95 (84%)	77 (96%)	3 (4%)	33 65
1	В	81/95 (85%)	80 (99%)	1 (1%)	71 87
1	C	80/95 (84%)	79 (99%)	1 (1%)	69 86

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	241/285 (85%)	236 (98%)	5 (2%)	53 78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	ASP
1	A	323	PHE
1	A	332	LEU
1	В	295	ASP
1	С	295	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	303	HIS
1	В	300	ASN
1	С	300	ASN
1	С	311	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 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 (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^{th} 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	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	90/106 (84%)	0.49	8 (8%) 9 8	113, 160, 226, 284	0
1	В	90/106 (84%)	0.26	1 (1%) 80 69	118, 161, 217, 256	0
1	С	90/106 (84%)	0.61	10 (11%) 5 5	162, 220, 271, 347	0
All	All	270/318 (84%)	0.45	19 (7%) 16 13	113, 181, 264, 347	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	330	ARG	6.9
1	A	320	GLU	5.9
1	С	320	GLU	5.8
1	С	334	MET	5.6
1	A	330	ARG	4.2

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.

