



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 02:59 AM BST

PDB ID : 6KTS  
Title : Structure of C34N126K/N36  
Authors : Yu, D.W.; Qin, B.  
Deposited on : 2019-08-28  
Resolution : 1.65 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
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) : 2.14.4.dev1

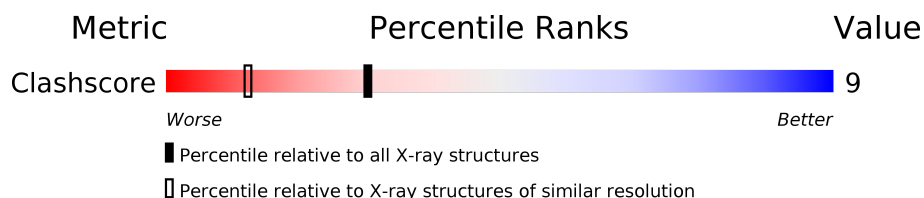
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1931 (1.66-1.66)

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 on 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	B	37	84% 16%
1	E	37	84% 16%
1	N	37	78% 22%
2	A	35	86% 14%
2	C	35	94% 6%
2	D	35	80% 20%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1987 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	N	37	Total	C	N	O	3	0	0
			293	186	56	51			
1	B	37	Total	C	N	O	3	0	0
			293	186	56	51			
1	E	37	Total	C	N	O	3	0	0
			293	186	56	51			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	545	ACE	-	acetylation	UNP C7F2J9
B	545	ACE	-	acetylation	UNP C7F2J9
E	545	ACE	-	acetylation	UNP C7F2J9

- Molecule 2 is a protein called Glycoprotein 41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	35	Total	C	N	O	S	3	0	0
			302	188	50	63	1			
2	A	35	Total	C	N	O	S	3	0	0
			302	188	50	63	1			
2	D	35	Total	C	N	O	S	3	0	0
			302	188	50	63	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	627	ACE	-	acetylation	UNP Q6TAN7
C	637	LYS	ASN	engineered mutation	UNP Q6TAN7
A	627	ACE	-	acetylation	UNP Q6TAN7
A	637	LYS	ASN	engineered mutation	UNP Q6TAN7
D	627	ACE	-	acetylation	UNP Q6TAN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	637	LYS	ASN	engineered mutation	UNP Q6TAN7

- Molecule 3 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	30	Total O 30 30	0	0
3	C	39	Total O 39 39	0	0
3	B	32	Total O 32 32	0	0
3	A	24	Total O 24 24	0	0
3	E	29	Total O 29 29	0	0
3	D	48	Total O 48 48	0	0

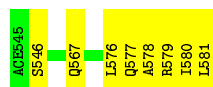
### 3 Residue-property plots [i](#)

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. 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: Envelope glycoprotein

Chain N:  78% 22%




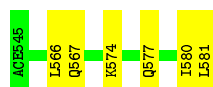
- Molecule 1: Envelope glycoprotein

Chain B:  84% 16%



- Molecule 1: Envelope glycoprotein

Chain E:  84% 16%




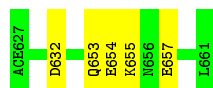
- Molecule 2: Glycoprotein 41

Chain C:  94% 6%




- Molecule 2: Glycoprotein 41

Chain A:  86% 14%



- Molecule 2: Glycoprotein 41

Chain D:  80% 20%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.86Å 50.81Å 56.11Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	44.11 – 1.65	Depositor
% Data completeness (in resolution range)	98.8 (44.11-1.65)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.206 , 0.226	Depositor
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.181	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.021 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.117 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.075 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.036 for -h,-k,l	Xtriage
Total number of atoms	1987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.32% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

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	B	1.44	4/293 (1.4%)	0.70	0/396
1	E	1.17	0/293	0.66	0/396
1	N	1.00	0/293	0.73	0/396
2	A	1.34	2/305 (0.7%)	0.76	1/411 (0.2%)
2	C	1.23	1/305 (0.3%)	0.69	0/411
2	D	1.31	1/305 (0.3%)	0.61	0/411
All	All	1.26	8/1794 (0.4%)	0.69	1/2421 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	627	ACE	C-N	-9.49	1.12	1.34
1	B	579	ARG	CZ-NH2	-8.72	1.21	1.33
1	B	579	ARG	NE-CZ	-7.88	1.22	1.33
1	B	579	ARG	CD-NE	-7.31	1.34	1.46
1	B	579	ARG	CZ-NH1	-6.79	1.24	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	654	GLU	OE1-CD-OE2	-5.54	116.66	123.30

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	B	293	0	313	5	1
1	E	293	0	313	12	0
1	N	293	0	313	10	0
2	A	302	0	282	2	0
2	C	302	0	282	1	0
2	D	302	0	281	5	0
3	A	24	0	0	1	0
3	B	32	0	0	1	1
3	C	39	0	0	1	1
3	D	48	0	0	3	2
3	E	29	0	0	3	1
3	N	30	0	0	7	0
All	All	1987	0	1784	33	3

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 9.

The worst 5 of 33 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:D:643:HIS:ND1	3:D:701:HOH:O	1.85	1.10
1:N:578:ALA:O	3:N:601:HOH:O	1.82	0.97
1:E:577:GLN:O	1:E:581:LEU:HD23	1.64	0.96
1:E:577:GLN:O	1:E:581:LEU:CD2	2.16	0.94
2:D:637:LYS:NZ	3:D:702:HOH:O	1.98	0.89

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:726:HOH:O	3:D:729:HOH:O[4_545]	2.04	0.16
3:B:618:HOH:O	3:E:615:HOH:O[1_554]	2.12	0.08
1:B:550:GLN:OE1	3:D:702:HOH:O[4_545]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	627:ACE	C	628:TRP	N	1.12

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

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

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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