



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:04 pm BST

PDB ID : 3CQG  
Title : Nucleoporin Nup107/Nup133 interaction complex, delta finger mutant  
Authors : Jeudy, S.; Boehmer, T.; Berke, I.; Schwartz, T.U.  
Deposited on : 2008-04-02  
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)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

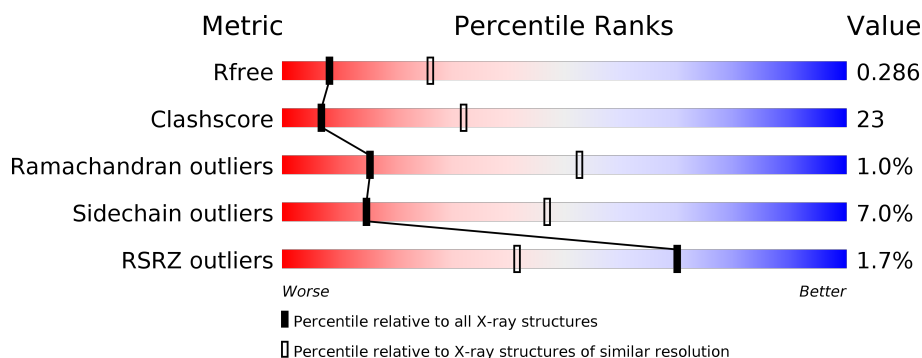
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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  $\leq 5\%$ . 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	246	<div> <div>54%</div> <div>36%</div> <div>• 9%</div> </div>
2	B	227	<div> <div>3%</div> <div>45%</div> <div>30%</div> <div>6%</div> <div>19%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3285 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 Nuclear pore complex protein Nup107.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1817	1160	311	333	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	656	GLY	-	EXPRESSION TAG	UNP P57740
A	657	SER	-	EXPRESSION TAG	UNP P57740
A	796	GLY	-	LINKER	UNP P57740
A	797	GLY	-	LINKER	UNP P57740
A	798	SER	-	LINKER	UNP P57740
A	799	GLY	-	LINKER	UNP P57740
A	800	GLY	-	LINKER	UNP P57740
A	801	SER	-	LINKER	UNP P57740

- Molecule 2 is a protein called Nuclear pore complex protein Nup133.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1434	911	237	280	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	930	MET	-	EXPRESSION TAG	UNP Q8WUM0
B	931	ALA	-	EXPRESSION TAG	UNP Q8WUM0
B	932	SER	-	EXPRESSION TAG	UNP Q8WUM0
B	933	HIS	-	EXPRESSION TAG	UNP Q8WUM0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	5	Total 5	O 5	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.66 Å 65.53 Å 193.23 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.00 – 3.00 46.27 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.4 (46.00-3.00) 97.4 (46.27-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 3.01 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.239 , 0.287 0.236 , 0.286	Depositor DCC
$R_{free}$ test set	1004 reflections (8.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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

### 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	0.40	0/1852	0.52	0/2495
2	B	0.35	0/1449	0.48	0/1955
All	All	0.38	0/3301	0.50	0/4450

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

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	1817	0	1797	74	0
2	B	1434	0	1397	76	0
3	A	29	0	0	1	0
3	B	5	0	0	0	0
All	All	3285	0	3194	148	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 23.

The worst 5 of 148 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:A:33:HOH:O	2:B:962:ARG:HG2	1.71	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1069:LEU:O	2:B:1073:ILE:HG23	1.71	0.88
2:B:1119:LEU:N	2:B:1120:PRO:CD	2.35	0.87
2:B:1097:LYS:O	2:B:1101:PHE:HD1	1.58	0.86
1:A:736:LEU:HD12	1:A:737:PRO:HD2	1.58	0.86

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	A	219/246 (89%)	203 (93%)	15 (7%)	1 (0%)	29	68
2	B	174/227 (77%)	155 (89%)	16 (9%)	3 (2%)	9	39
All	All	393/473 (83%)	358 (91%)	31 (8%)	4 (1%)	15	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1020	LEU
1	A	716	PRO
2	B	1019	ASN
2	B	1120	PRO

### 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	A	195/215 (91%)	188 (96%)	7 (4%)	35	70
2	B	149/203 (73%)	132 (89%)	17 (11%)	5	24
All	All	344/418 (82%)	320 (93%)	24 (7%)	15	47

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	991	LYS
2	B	1003	LEU
2	B	1083	TRP
2	B	992	ILE
2	B	994	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	862	HIS
1	A	886	HIS
2	B	958	ASN
1	A	844	HIS
1	A	914	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	225/246 (91%)	-0.26	0	100 100	44, 64, 92, 116	0
2	B	184/227 (81%)	0.00	7 (3%)	40 16	55, 89, 181, 193	0
All	All	409/473 (86%)	-0.14	7 (1%)	70 41	44, 73, 140, 193	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1083	TRP	4.5
2	B	1155	GLN	3.8
2	B	1127	GLN	3.2
2	B	1154	GLY	3.1
2	B	1101	PHE	2.2

### 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 carbohydrates 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.