

# Full wwPDB X-ray Structure Validation Report (i)

#### May 1, 2021 – 05:40 PM EDT

PDB ID	:	5QU5
Title	:	Domain Swap in the first SH3 domain of human Nck1
Authors	:	Burger, D.; Ruf, A.; Benz, J.; Schlatter, D.; Rudolph, M.G.
Deposited on		
Resolution	:	1.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

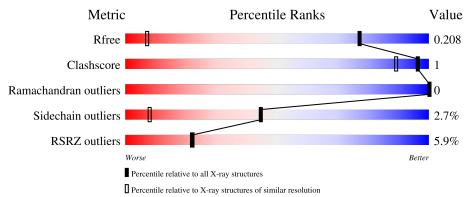
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)		
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.18

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.11 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1168 (1.14-1.10)
Clashscore	141614	1205 (1.14-1.10)
Ramachandran outliers	138981	1168 (1.14-1.10)
Sidechain outliers	138945	1165 (1.14-1.10)
RSRZ outliers	127900	1146 (1.14-1.10)

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	Qua	ality of chain	
1	А	99	2% 53%	6% •	40%
1	В	99	5%	•	40%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1207 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	59	Total	С	Ν	Ο	$\mathbf{S}$	0	2	0
		- 59	526	330	93	102	1	0	ა	U
1	В	50	Total	С	Ν	Ο	S	0	1	0
1	ГБ	B 59		330	91	98	2	0	4	0

• Molecule 1 is a protein called Cytoplasmic protein NCK1.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-36	MET	-	initiating methionine	UNP P16333
А	-35	GLY	-	expression tag	UNP P16333
А	-34	HIS	-	expression tag	UNP P16333
А	-33	HIS	-	expression tag	UNP P16333
А	-32	HIS	-	expression tag	UNP P16333
А	-31	HIS	-	expression tag	UNP P16333
А	-30	HIS	-	expression tag	UNP P16333
А	-29	HIS	-	expression tag	UNP P16333
А	-28	HIS	-	expression tag	UNP P16333
А	-27	HIS	-	expression tag	UNP P16333
A	-26	HIS	-	expression tag	UNP P16333
А	-25	HIS	-	expression tag	UNP P16333
A	-24	SER	-	expression tag	UNP P16333
А	-23	GLY	-	expression tag	UNP P16333
А	-22	GLY	-	expression tag	UNP P16333
A	-21	LEU	-	expression tag	UNP P16333
А	-20	ASN	-	expression tag	UNP P16333
А	-19	ASP	-	expression tag	UNP P16333
А	-18	ILE	-	expression tag	UNP P16333
А	-17	PHE	-	expression tag	UNP P16333
А	-16	GLU	-	expression tag	UNP P16333
А	-15	ALA	-	expression tag	UNP P16333
А	-14	GLN	-	expression tag	UNP P16333
А	-13	LYS	-	expression tag	UNP P16333
А	-12	ILE	-	expression tag	UNP P16333

There are 76 discrepancies between the modelled and reference sequences:

Continued on next page...



,	Reference
ag	UNP P16333
ag	UNP P16333
ag	UNP P16333

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$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Chain	Residue	Modelled	Actual	Comment	Reference
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	А	-11	GLU	-	expression tag	UNP P16333
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	А	-10	TRP	-	expression tag	UNP P16333
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	А	-9	HIS	-	expression tag	UNP P16333
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	А	-8	GLU	-	expression tag	UNP P16333
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	А	-7	GLY	-	expression tag	UNP P16333
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-6	SER	-	expression tag	UNP P16333
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	А	-5	GLU	-	expression tag	UNP P16333
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	A	-4	ASN	-	expression tag	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-3		-	expression tag	UNP P16333
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-2	TYR	-	expression tag	UNP P16333
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$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	1	SER	-		UNP P16333
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	В	-36		-	initiating methionine	UNP P16333
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B-32HIS-expression tagUNP P16333B-31HIS-expression tagUNP P16333B-30HIS-expression tagUNP P16333B-29HIS-expression tagUNP P16333B-28HIS-expression tagUNP P16333B-27HIS-expression tagUNP P16333B-26HIS-expression tagUNP P16333B-25HIS-expression tagUNP P16333B-24SER-expression tagUNP P16333B-23GLY-expression tagUNP P16333B-21LEU-expression tagUNP P16333B-20ASN-expression tagUNP P16333B-19ASP-expression tagUNP P16333B-16GLU-expression tagUNP P16333B-16GLU-expression tagUNP P16333B-14GLN-expression tagUNP P16333B-11GLU-expression tagUNP P16333B-11GLU-expression tagUNP P16333B-10TRP-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-10TRP-<	В	-34	HIS	-	expression tag	UNP P16333
B-31HIS-expression tagUNP P16333B-30HIS-expression tagUNP P16333B-29HIS-expression tagUNP P16333B-28HIS-expression tagUNP P16333B-27HIS-expression tagUNP P16333B-26HIS-expression tagUNP P16333B-26HIS-expression tagUNP P16333B-25HIS-expression tagUNP P16333B-24SER-expression tagUNP P16333B-23GLY-expression tagUNP P16333B-21LEU-expression tagUNP P16333B-20ASN-expression tagUNP P16333B-19ASP-expression tagUNP P16333B-18ILE-expression tagUNP P16333B-16GLU-expression tagUNP P16333B-16GLU-expression tagUNP P16333B-14GLN-expression tagUNP P16333B-11GLU-expression tagUNP P16333B-10TRP-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-10TRP-<	В	-33	HIS	-	expression tag	UNP P16333
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B-16GLU-expression tagUNP P16333B-15ALA-expression tagUNP P16333B-14GLN-expression tagUNP P16333B-13LYS-expression tagUNP P16333B-12ILE-expression tagUNP P16333B-11GLU-expression tagUNP P16333B-10TRP-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-8GLU-expression tagUNP P16333	В	-18	ILE	-	expression tag	
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B-14GLN-expression tagUNP P16333B-13LYS-expression tagUNP P16333B-12ILE-expression tagUNP P16333B-11GLU-expression tagUNP P16333B-10TRP-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-8GLU-expression tagUNP P16333	В	-16	GLU	-	expression tag	UNP P16333
B-13LYS-expression tagUNP P16333B-12ILE-expression tagUNP P16333B-11GLU-expression tagUNP P16333B-10TRP-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-8GLU-expression tagUNP P16333				-	- *	
B-12ILE-expression tagUNP P16333B-11GLU-expression tagUNP P16333B-10TRP-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-8GLU-expression tagUNP P16333				-	expression tag	
B-11GLU-expression tagUNP P16333B-10TRP-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-8GLU-expression tagUNP P16333	В			-	expression tag	
B-10TRP-expression tagUNP P16333B-9HIS-expression tagUNP P16333B-8GLU-expression tagUNP P16333				-		
B-9HIS-expression tagUNP P16333B-8GLU-expression tagUNP P16333	В	-11		-		
B -8 GLU - expression tag UNP P16333				-		
				-		
Continued on next page	В	-8	GLU	-		

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-7	GLY	-	expression tag	UNP P16333
В	-6	SER	-	expression tag	UNP P16333
В	-5	GLU	-	expression tag	UNP P16333
В	-4	ASN	-	expression tag	UNP P16333
В	-3	LEU	-	expression tag	UNP P16333
В	-2	TYR	-	expression tag	UNP P16333
В	-1	PHE	-	expression tag	UNP P16333
В	0	GLN	-	expression tag	UNP P16333
В	1	SER	-	expression tag	UNP P16333

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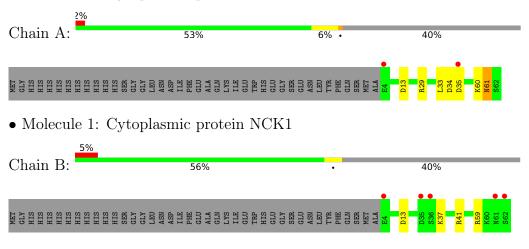
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	72	Total         O           73         73	0	1
2	В	85	Total O 87 87	0	2



# 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: Cytoplasmic protein NCK1



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	40.20Å 55.17Å 55.23Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	39.03 - 1.11	Depositor
Resolution (A)	32.49 - 1.11	EDS
% Data completeness	57.2(39.03-1.11)	Depositor
(in resolution range)	57.2(32.49-1.11)	EDS
R <sub>merge</sub>	0.08	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.07 (at 1.11 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
B B.	0.152 , $0.208$	Depositor
$R, R_{free}$	0.153 , $0.208$	DCC
$R_{free}$ test set	1391 reflections $(4.90\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	14.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32 , $40.7$	EDS
L-test for $twinning^2$	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	1207	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 50.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4876e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	1.10	1/535~(0.2%)	1.11	2/716~(0.3%)
1	В	1.08	0/543	1.10	2/729~(0.3%)
All	All	1.09	1/1078~(0.1%)	1.11	4/1445~(0.3%)

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	А	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	33	LEU	C-O	5.10	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	13	ASP	CB-CG-OD1	6.86	124.47	118.30
1	А	29	ARG	NE-CZ-NH2	6.59	123.59	120.30
1	А	13	ASP	CB-CG-OD1	6.45	124.10	118.30
1	В	41	ARG	NE-CZ-NH2	-5.53	117.53	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	61[B]	ASN	Mainchain



### 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	А	526	0	513	2	0
1	В	521	0	521	1	0
2	А	73	0	0	0	0
2	В	87	0	0	0	0
All	All	1207	0	1034	2	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 1.

All (2) 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)
1:A:35:ASP:HB2	1:B:59:ARG:HH22	1.81	0.46
1:A:34:ASP:C	1:A:34:ASP:OD1	2.59	0.40

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	А	59/99~(60%)	56~(95%)	3~(5%)	0	100 100
1	В	61/99~(62%)	60~(98%)	1 (2%)	0	100 100
All	All	120/198~(61%)	116 (97%)	4(3%)	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 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	А	59/90~(66%)	55~(93%)	4 (7%)	16 1
1	В	60/90~(67%)	59~(98%)	1 (2%)	60 22
All	All	119/180~(66%)	114 (96%)	5 (4%)	44 3

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

Mol	Chain	Res	Type
1	А	60[A]	LYS
1	А	60[B]	LYS
1	А	61[A]	ASN
1	А	61[B]	ASN
1	В	37	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

#### 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.



# $6 \quad \text{Fit of model and data} \quad (i)$

### 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	$\langle RSRZ \rangle$	# <b>RS</b>	SRZ>	>2	$\mathbf{OWAB}(\mathbf{A}^2)$	$Q{<}0.9$
1	А	59/99~(59%)	0.06	2(3%)	45	44	11, 15, 39, 56	0
1	В	59/99~(59%)	0.26	5 (8%)	10	12	10, 16, 37, 55	0
All	All	118/198~(59%)	0.16	7 (5%)	22	22	10, 16, 39, 56	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	4	GLU	5.0
1	А	4	GLU	4.7
1	В	61	ASN	3.3
1	В	62	SER	3.1
1	А	35	ASP	2.6
1	В	36	SER	2.5
1	В	35	ASP	2.1

### 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.

