



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:50 PM GMT

PDB ID : 2QX5
Title : Structure of nucleoporin Nic96
Authors : Jeudy, S.; Schwartz, T.U.
Deposited on : 2007-08-10
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

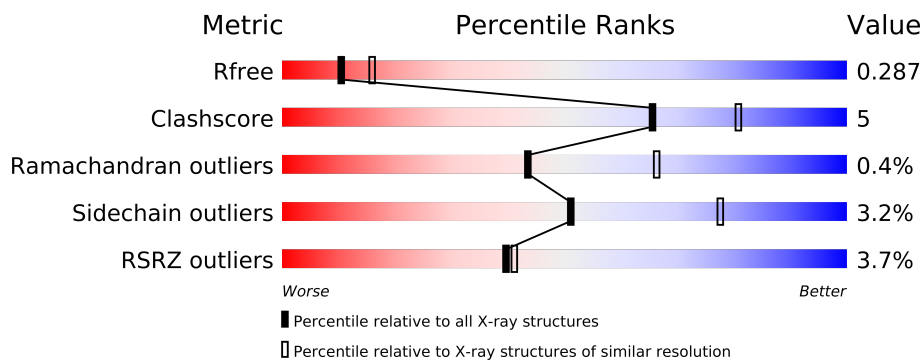
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	661	
1	B	661	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9160 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Nucleoporin NIC96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4521	2910	752	842	17			
1	B	569	Total	C	N	O	S	0	0	0
			4514	2896	754	847	17			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	PRO	-	EXPRESSION TAG	UNP P34077
A	180	GLY	-	EXPRESSION TAG	UNP P34077
A	181	SER	-	EXPRESSION TAG	UNP P34077
A	182	GLU	-	EXPRESSION TAG	UNP P34077
A	183	PHE	-	EXPRESSION TAG	UNP P34077
A	184	GLU	-	EXPRESSION TAG	UNP P34077
A	185	LEU	-	EXPRESSION TAG	UNP P34077
B	179	PRO	-	EXPRESSION TAG	UNP P34077
B	180	GLY	-	EXPRESSION TAG	UNP P34077
B	181	SER	-	EXPRESSION TAG	UNP P34077
B	182	GLU	-	EXPRESSION TAG	UNP P34077
B	183	PHE	-	EXPRESSION TAG	UNP P34077
B	184	GLU	-	EXPRESSION TAG	UNP P34077
B	185	LEU	-	EXPRESSION TAG	UNP P34077

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0
3	B	60	Total 60	O 60	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.12Å 82.48Å 113.03Å 90.00° 91.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 32.08 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.50) 98.3 (32.08-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.41 (at 2.39Å)	Xtriage
Refinement program	phenix	Depositor
R, R_{free}	0.233 , 0.285 0.237 , 0.287	Depositor DCC
R_{free} test set	3106 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	8 of 61613 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9160	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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 52.13 % 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 5.0839e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.35	0/4597	0.50	0/6227
1	B	0.35	0/4590	0.51	0/6222
All	All	0.35	0/9187	0.50	0/12449

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	315	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4521	0	0	22	0
1	B	4514	0	0	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	63	0	0	3	0
3	B	60	0	0	2	0
All	All	9160	0	0	47	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (47) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:374:TYR:CD2	1:B:374:TYR:C	2.45	0.87
1:A:374:TYR:C	1:A:374:TYR:CD2	2.50	0.83
1:B:405:ASP:OD1	1:B:406:PRO:CD	2.34	0.76
1:A:357:LYS:O	1:A:360:ILE:CG1	2.34	0.76
1:B:533:ARG:CB	1:B:533:ARG:NH1	2.50	0.75
1:B:405:ASP:O	1:B:408:ARG:N	2.26	0.68
1:B:405:ASP:C	1:B:405:ASP:OD1	2.34	0.66
1:A:533:ARG:CB	1:A:533:ARG:NH1	2.58	0.66
1:B:315:LYS:O	1:B:317:ASP:N	2.30	0.64
1:B:533:ARG:NH1	1:B:533:ARG:CG	2.60	0.62
1:A:342:ARG:NH1	1:A:434:ASP:OD1	2.33	0.61
1:B:317:ASP:OD1	1:B:317:ASP:N	2.33	0.60
1:B:405:ASP:O	1:B:407:TYR:N	2.36	0.59
1:A:826:ARG:NH1	1:A:826:ARG:CG	2.68	0.56
1:B:740:GLU:CG	1:B:747:PHE:CE2	2.89	0.56
1:B:342:ARG:NH1	1:B:434:ASP:OD1	2.41	0.53
1:B:413:LYS:NZ	1:B:422:ARG:O	2.42	0.52
1:B:826:ARG:CG	1:B:826:ARG:NH1	2.72	0.51
1:B:793:LYS:NZ	3:B:869:HOH:O	2.45	0.49
1:B:220:PHE:CD1	1:B:555:GLU:CG	2.97	0.48
1:A:443:ILE:CG2	1:A:444:LYS:N	2.76	0.47
1:A:405:ASP:C	1:A:405:ASP:OD1	2.53	0.47
1:A:444:LYS:N	1:A:457:TYR:O	2.48	0.47
1:A:832:LEU:O	1:A:835:ILE:CG2	2.63	0.47
1:A:315:LYS:O	1:A:316:ALA:CB	2.62	0.47
1:B:668:SER:OG	1:B:724:ARG:NH2	2.48	0.46
1:B:227:GLN:NE2	1:B:607:ARG:CD	2.79	0.46
1:A:306:LYS:NZ	3:A:867:HOH:O	2.48	0.46
1:B:733:GLN:CG	3:B:871:HOH:O	2.64	0.45
1:B:223:ASN:OD1	1:B:226:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:295:ASN:O	1:B:296:GLU:C	2.55	0.45
1:A:515:LEU:O	1:A:515:LEU:CD1	2.65	0.44
1:B:735:THR:O	1:B:739:MET:N	2.52	0.43
1:A:747:PHE:CD1	1:A:747:PHE:N	2.87	0.42
1:A:356:ASN:O	1:A:357:LYS:C	2.58	0.42
1:B:405:ASP:O	1:B:406:PRO:C	2.58	0.42
1:A:766:ASN:ND2	3:A:869:HOH:O	2.52	0.42
1:A:435:TRP:CE2	1:A:439:HIS:CE1	3.08	0.42
1:A:608:GLN:N	1:A:609:PRO:CD	2.82	0.42
1:B:766:ASN:O	1:B:770:ASN:ND2	2.53	0.41
1:A:632:ASP:CB	3:A:909:HOH:O	2.68	0.41
1:B:257:TRP:O	1:B:261:GLU:N	2.52	0.41
1:A:439:HIS:CD2	1:A:457:TYR:OH	2.74	0.41
1:A:815:ILE:CG1	1:A:816:TYR:N	2.84	0.41
1:A:356:ASN:O	1:A:358:ALA:N	2.55	0.40
1:B:780:SER:O	1:B:784:ASN:ND2	2.54	0.40
1:A:357:LYS:O	1:A:360:ILE:CG2	2.68	0.40

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	A	557/661 (84%)	537 (96%)	17 (3%)	3 (0%)	38	60
1	B	557/661 (84%)	533 (96%)	22 (4%)	2 (0%)	43	66
All	All	1114/1322 (84%)	1070 (96%)	39 (4%)	5 (0%)	43	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	835	ILE
1	A	317	ASP
1	A	499	SER

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Mol	Chain	Res	Type
1	B	268	ILE
1	A	359	ASN

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	A	490/598 (82%)	473 (96%)	17 (4%)	48	74
1	B	489/598 (82%)	475 (97%)	14 (3%)	55	81
All	All	979/1196 (82%)	948 (97%)	31 (3%)	51	77

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	342	ARG
1	A	374	TYR
1	A	405	ASP
1	A	418	CYS
1	A	444	LYS
1	A	475	SER
1	A	506	LEU
1	A	533	ARG
1	A	542	THR
1	A	580	VAL
1	A	589	LEU
1	A	681	SER
1	A	688	LEU
1	A	742	LEU
1	A	814	MET
1	A	826	ARG
1	B	280	GLN
1	B	312	LYS
1	B	317	ASP
1	B	319	SER
1	B	342	ARG
1	B	374	TYR

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Mol	Chain	Res	Type
1	B	405	ASP
1	B	506	LEU
1	B	515	LEU
1	B	533	ARG
1	B	589	LEU
1	B	742	LEU
1	B	826	ARG
1	B	828	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	569/661 (86%)	0.05	17 (2%)	48 50	31, 56, 100, 135	0
1	B	569/661 (86%)	0.11	25 (4%)	33 34	33, 58, 106, 143	0
All	All	1138/1322 (86%)	0.08	42 (3%)	39 41	31, 58, 102, 143	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	833	ILE	5.3
1	A	265	SER	3.5
1	A	315	LYS	3.4
1	B	364	GLU	3.4
1	B	265	SER	3.3
1	B	267	ASP	3.2
1	B	837	VAL	3.2
1	A	456	ARG	3.1
1	B	316	ALA	3.1
1	A	264	LYS	3.0
1	B	229	ASN	3.0
1	B	365	GLN	2.9
1	B	515	LEU	2.8
1	A	204	GLU	2.7
1	B	754	ARG	2.7
1	B	366	SER	2.7
1	B	614	ARG	2.7
1	B	677	PRO	2.6
1	A	246	ASN	2.5
1	A	245	ALA	2.5
1	A	231	ASN	2.5
1	B	634	ASP	2.5
1	A	753	ALA	2.4
1	A	833	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	346	ILE	2.4
1	B	368	LEU	2.4
1	B	220	PHE	2.3
1	A	357	LYS	2.3
1	B	422	ARG	2.3
1	A	317	ASP	2.3
1	A	420	LEU	2.2
1	B	412	TYR	2.2
1	B	834	ASN	2.2
1	B	318	LYS	2.2
1	A	201	ASN	2.2
1	B	317	ASP	2.2
1	A	556	TYR	2.1
1	A	370	TYR	2.1
1	A	774	LEU	2.0
1	B	322	ILE	2.0
1	B	629	ARG	2.0
1	B	836	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CL	B	844	1/1	0.17	-0.56	57,57,57,57	0
2	CL	A	854	1/1	0.14	-0.98	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.