



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 10:06 PM EST

PDB ID : 5GXW  
Title : Importin and NuMA complex  
Authors : Chang, C.-C.; Huang, T.-L.; Hsia, K.-C.  
Deposited on : unknown  
Resolution : 2.39 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

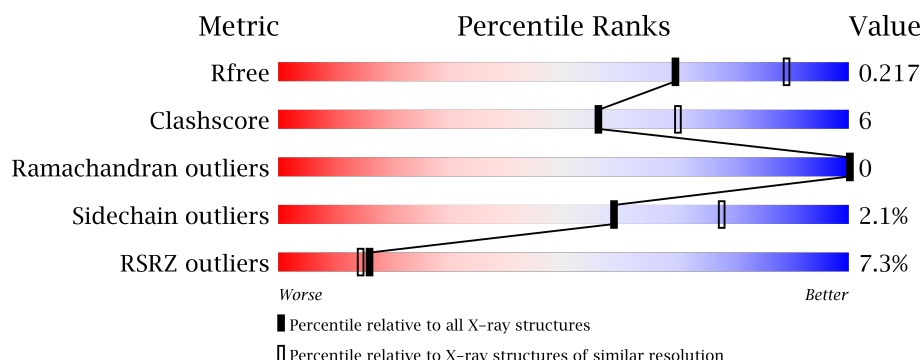
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. 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	428	
2	B	27	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3722 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 Importin subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3262	2075	554	623	10			

- Molecule 2 is a protein called Peptide from Nuclear mitotic apparatus protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	S	0	0	0
			214	129	44	40	1			

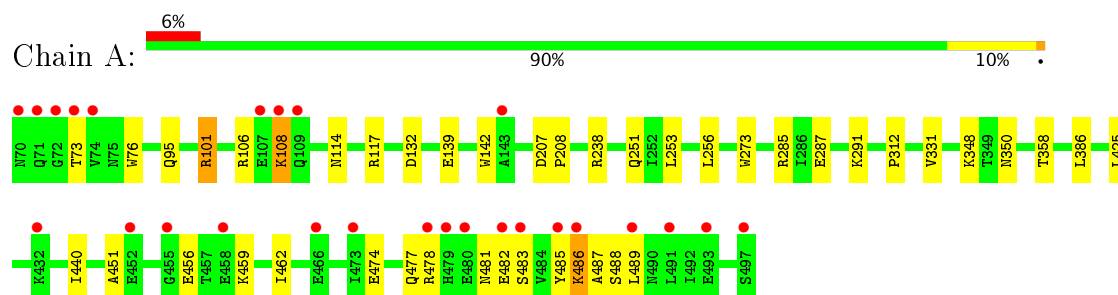
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total	O	0	0
			233	233		
3	B	13	Total	O	0	0
			13	13		

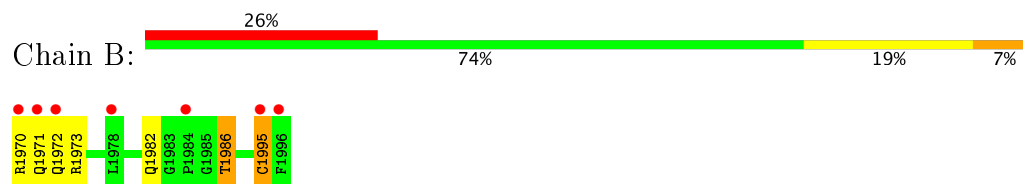
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Importin subunit alpha-1



- Molecule 2: Peptide from Nuclear mitotic apparatus protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.06 Å 89.66 Å 101.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.82 – 2.39 19.82 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.82-2.39) 97.9 (19.82-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 2.41 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.183 , 0.218 0.179 , 0.217	Depositor DCC
$R_{free}$ test set	2000 reflections (7.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3722	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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	0.42	0/3320	0.59	0/4523
2	B	0.54	0/218	0.63	0/289
All	All	0.43	0/3538	0.59	0/4812

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	3262	0	3334	36	0
2	B	214	0	215	7	0
3	A	233	0	0	4	1
3	B	13	0	0	2	0
All	All	3722	0	3549	41	1

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 6.

All (41) 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:477:GLN:HE21	1:A:489:LEU:HA	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1970:ARG:HG2	2:B:1971:GLN:H	1.35	0.90
1:A:95:GLN:NE2	3:A:501:HOH:O	2.08	0.86
2:B:1972:GLN:O	3:B:2001:HOH:O	1.95	0.85
1:A:459:LYS:NZ	3:A:502:HOH:O	2.18	0.69
2:B:1982:GLN:HA	2:B:1986:THR:HG21	1.78	0.65
1:A:474:GLU:CD	1:A:478:ARG:HH22	2.03	0.62
1:A:486:LYS:HD2	1:A:487:ALA:N	2.18	0.58
1:A:459:LYS:HA	1:A:462:ILE:HD12	1.85	0.57
1:A:348:LYS:HG3	1:A:350:ASN:OD1	2.05	0.56
1:A:106:ARG:HD2	1:A:108:LYS:HE2	1.88	0.55
1:A:348:LYS:HZ2	1:A:350:ASN:H	1.56	0.54
1:A:477:GLN:HG2	1:A:489:LEU:HG	1.90	0.53
1:A:477:GLN:HA	1:A:488:SER:OG	2.09	0.53
1:A:207:ASP:OD1	1:A:251:GLN:NE2	2.42	0.53
1:A:482:GLU:O	1:A:486:LYS:HG3	2.08	0.53
2:B:1970:ARG:HG2	2:B:1971:GLN:N	2.17	0.52
1:A:238:ARG:NH2	2:B:1986:THR:HG23	2.25	0.51
1:A:474:GLU:O	1:A:478:ARG:NH2	2.44	0.51
1:A:108:LYS:HD3	1:A:108:LYS:H	1.74	0.50
1:A:207:ASP:HB2	1:A:208:PRO:HD3	1.95	0.49
1:A:73:THR:HA	1:A:76:TRP:NE1	2.27	0.49
1:A:483:SER:O	1:A:486:LYS:HE3	2.13	0.49
1:A:101:ARG:HD3	1:A:139:GLU:OE1	2.13	0.48
1:A:488:SER:OG	1:A:489:LEU:N	2.46	0.48
1:A:451:ALA:HB1	1:A:456:GLU:HB2	1.95	0.47
1:A:386:LEU:HD21	1:A:425:LEU:HD13	1.95	0.47
1:A:101:ARG:HD2	1:A:142:TRP:CE3	2.50	0.46
2:B:1973:ARG:HA	3:B:2001:HOH:O	2.15	0.46
1:A:142:TRP:CZ2	2:B:1995:CYS:HA	2.50	0.46
1:A:425:LEU:HG	1:A:440:ILE:HG23	1.98	0.45
1:A:482:GLU:HA	1:A:485:TYR:CE2	2.53	0.44
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.89	0.43
1:A:459:LYS:HD2	1:A:459:LYS:HA	1.72	0.43
1:A:273:TRP:CD2	1:A:312:PRO:HB3	2.54	0.43
1:A:114:ASN:OD1	1:A:117:ARG:NH1	2.53	0.42
1:A:483:SER:HA	1:A:486:LYS:HE3	2.00	0.42
1:A:287:GLU:O	1:A:291:LYS:HB2	2.20	0.41
1:A:285:ARG:HD2	3:A:584:HOH:O	2.21	0.41
1:A:358:THR:HA	3:A:561:HOH:O	2.20	0.41
1:A:481:ASN:OD1	1:A:483:SER:N	2.54	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:659:HOH:O	3:A:687:HOH:O[3_557]	2.01	0.19

## 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	426/428 (100%)	415 (97%)	11 (3%)	0	100	100
2	B	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
All	All	451/455 (99%)	438 (97%)	13 (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	A	359/359 (100%)	353 (98%)	6 (2%)	66	82
2	B	24/24 (100%)	22 (92%)	2 (8%)	13	20
All	All	383/383 (100%)	375 (98%)	8 (2%)	59	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ARG

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Mol	Chain	Res	Type
1	A	108	LYS
1	A	132	ASP
1	A	256	LEU
1	A	331	VAL
1	A	486	LYS
2	B	1986	THR
2	B	1995	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	477	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 carbohydrates 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 ⓘ

### 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, 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	428/428 (100%)	0.11	26 (6%)	22 20	25, 36, 80, 104	0
2	B	27/27 (100%)	1.15	7 (25%)	1 1	32, 45, 79, 93	0
All	All	455/455 (100%)	0.17	33 (7%)	16 14	25, 37, 80, 104	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	GLN	9.6
1	A	70	ASN	9.1
2	B	1995	CYS	8.7
2	B	1996	PHE	7.6
1	A	497	SER	6.5
1	A	72	GLY	5.6
1	A	485	TYR	5.3
1	A	478	ARG	5.0
1	A	489	LEU	4.8
2	B	1970	ARG	4.5
1	A	455	GLY	4.3
1	A	74	VAL	4.0
1	A	493	GLU	4.0
1	A	482	GLU	3.8
2	B	1972	GLN	3.7
1	A	107	GLU	3.7
1	A	108	LYS	3.7
1	A	432	LYS	3.5
1	A	73	THR	3.0
1	A	483	SER	3.0
2	B	1971	GLN	3.0
1	A	452	GLU	2.9
2	B	1978	LEU	2.8
1	A	109	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	458	GLU	2.7
1	A	473	ILE	2.7
1	A	480	GLU	2.6
1	A	143	ALA	2.6
1	A	479	HIS	2.4
1	A	486	LYS	2.3
2	B	1984	PRO	2.2
1	A	466	GLU	2.1
1	A	491	LEU	2.0

## 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.