



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:39 PM GMT

PDB ID : 1UN0
Title : CRYSTAL STRUCTURE OF YEAST KARYOPHERIN (IMPORTIN) ALPHA IN COMPLEX WITH A NUP2P N-TERMINAL FRAGMENT
Authors : Matsuura, Y.; Lange, A.; Harreman, M.T.; Corbett, A.H.; Stewart, M.
Deposited on : 2003-09-03
Resolution : 2.60 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
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

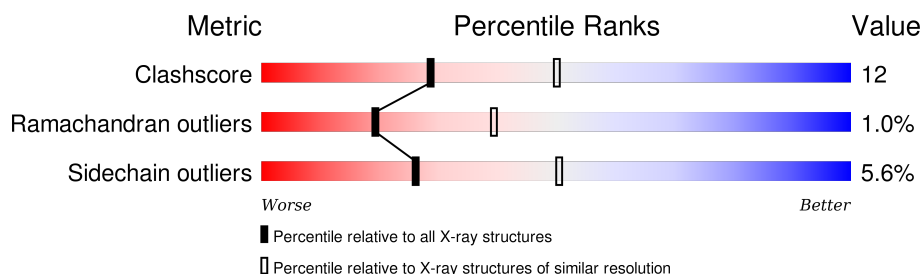
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	443	 77% 20% ..
1	B	443	 78% 18% ..
2	C	51	 12% 6% 6% 8% 69%
2	D	51	 14% 6% 8% 6% 69%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7231 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 ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	15	0	1
			3398	2139	574	668	17			
1	B	439	Total	C	N	O	S	16	0	0
			3397	2139	573	668	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	397	ASP	TYR	ENGINEERED MUTATION	UNP Q02821
B	397	ASP	TYR	ENGINEERED MUTATION	UNP Q02821

- Molecule 2 is a protein called NUCLEOPORIN NUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	16	Total	C	N	O	S	10	0	0
			139	87	32	17	3			
2	D	16	Total	C	N	O	S	10	0	0
			139	87	32	17	3			

- Molecule 3 is water.

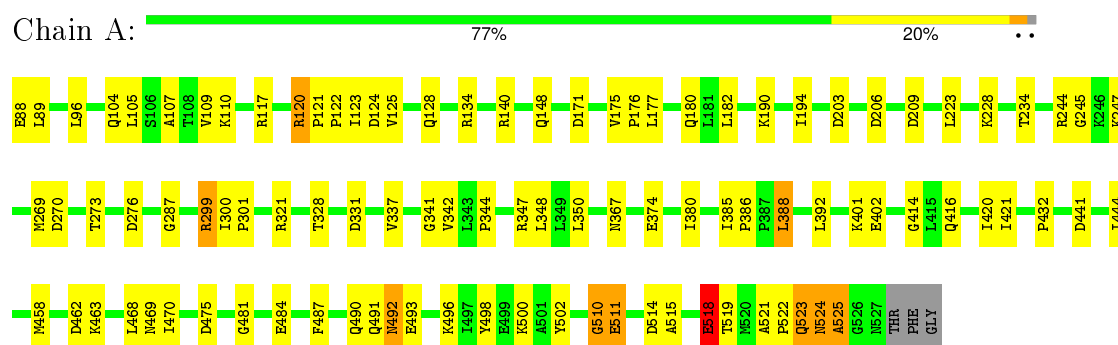
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	94	Total	O	0	0
			94	94		
3	C	7	Total	O	0	0
			7	7		
3	D	11	Total	O	0	0
			11	11		

3 Residue-property plots

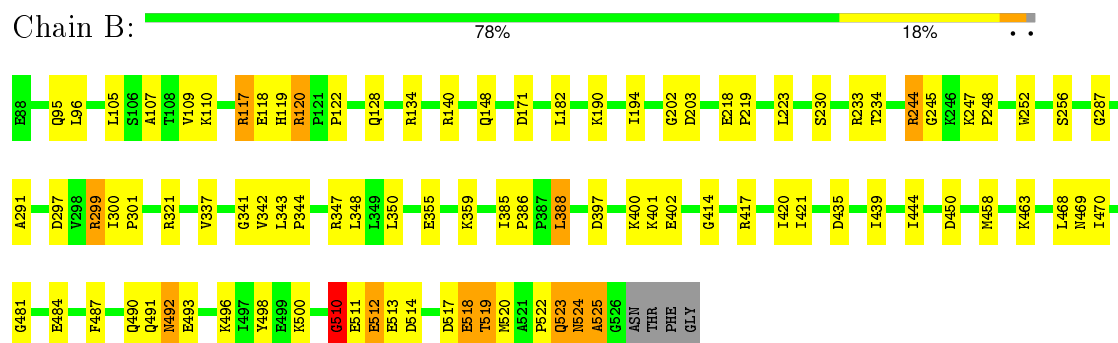
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

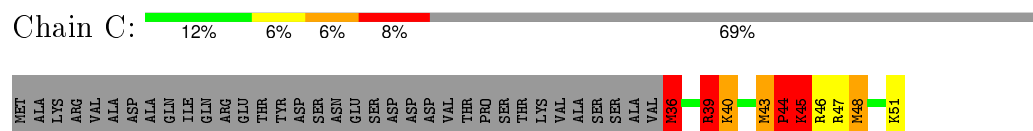
• Molecule 1: IMPORTIN ALPHA SUBUNIT



• Molecule 1: IMPORTIN ALPHA SUBUNIT



• Molecule 2: NUCLEOPORIN NUP2



• Molecule 2: NUCLEOPORIN NUP2



MET	ALA	LYS	ARG	VAL	ALA	ASP	ALA	GLN	ILE	GLN	ARG	GLU	THR	TYR	ASP	SER	ASN	GLU	SER	ASP	ASP	ASP	VAL	THR	PRO	SER	THR	LYS	VAL	ALA	SER	SER	ALA	VAL	R36	R39	R40	M43	P44	R45	R46	R47	R48	R51
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.81Å 140.08Å 63.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	97.8 (20.00-2.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7231	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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	0.86	3/3450 (0.1%)	1.14	23/4694 (0.5%)
1	B	0.67	3/3448 (0.1%)	1.16	20/4689 (0.4%)
2	C	4.12	5/140 (3.6%)	3.00	11/180 (6.1%)
2	D	2.31	4/140 (2.9%)	3.33	11/180 (6.1%)
All	All	1.00	15/7178 (0.2%)	1.28	65/9743 (0.7%)

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	A	0	2
1	B	0	2
2	D	0	1
All	All	0	5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	36	MET	CG-SD	-39.76	0.77	1.81
1	A	510	GLY	C-N	-27.88	0.69	1.34
1	A	511	GLU	CA-C	22.28	2.10	1.52
1	A	511	GLU	C-N	-19.98	0.88	1.34
2	C	45	LYS	CD-CE	19.33	1.99	1.51

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	GLY	O-C-N	-32.17	71.23	122.70
2	D	43	MET	C-N-CD	-26.49	62.33	120.60
1	A	510	GLY	O-C-N	-26.47	80.34	122.70
2	C	43	MET	C-N-CD	-24.97	65.67	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	510	GLY	CA-C-N	20.33	161.92	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	510	GLY	Mainchain
1	A	511	GLU	Peptide
1	B	510	GLY	Mainchain,Peptide
2	D	44	PRO	Peptide

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	3398	0	3427	71	0
1	B	3397	0	3427	64	0
2	C	139	0	160	20	0
2	D	139	0	156	21	0
3	A	46	0	0	6	0
3	B	94	0	0	9	0
3	C	7	0	0	2	0
3	D	11	0	0	10	0
All	All	7231	0	7170	163	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 12.

The worst 5 of 163 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:43:MET:O	2:D:44:PRO:O	1.58	1.21
2:D:43:MET:O	2:D:44:PRO:C	1.84	1.11
2:C:43:MET:O	2:C:44:PRO:O	1.74	1.03
2:C:44:PRO:O	2:C:45:LYS:O	1.77	1.01
1:A:492:ASN:HD22	1:A:493:GLU:N	1.59	0.99

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	438/443 (99%)	415 (95%)	21 (5%)	2 (0%)	34	60
1	B	435/443 (98%)	413 (95%)	18 (4%)	4 (1%)	21	42
2	C	14/51 (28%)	11 (79%)	1 (7%)	2 (14%)	0	0
2	D	14/51 (28%)	11 (79%)	2 (14%)	1 (7%)	1	1
All	All	901/988 (91%)	850 (94%)	42 (5%)	9 (1%)	19	39

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	GLN
1	A	525	ALA
1	B	523	GLN
1	B	525	ALA
2	C	44	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	376/379 (99%)	358 (95%)	18 (5%)	31	58
1	B	376/379 (99%)	360 (96%)	16 (4%)	35	64
2	C	14/44 (32%)	9 (64%)	5 (36%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	14/44 (32%)	9 (64%)	5 (36%)	0	0
All	All	780/846 (92%)	736 (94%)	44 (6%)	26	50

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	120	ARG
1	B	402	GLU
2	D	40	LYS
1	B	299	ARG
1	B	348	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	ASN
1	A	492	ASN
1	B	469	ASN
1	A	227	ASN
1	B	227	ASN

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.