Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:30 PM GMT

PDB ID	:	1XKS
Title	:	The crystal structure of the N-terminal domain of Nup133 reveals a beta-propeller fold common to several nucleoporins
Authors	:	Berke, I.C.; Boehmer, T.; Blobel, G.; Schwartz, T.U.
Deposited on	:	2004-09-29
Resolution	:	2.35 Å(reported)

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

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MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.
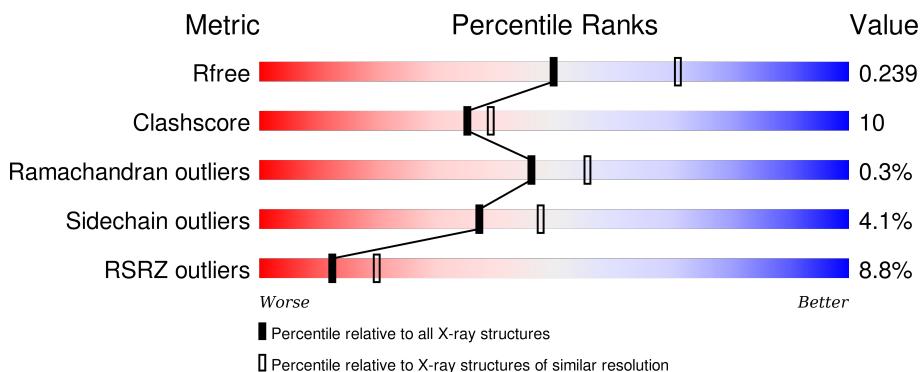
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 <=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	450	7% 64% 16% • 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2940 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 Nup133.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total 2845	C 1804	N 466	O 562	S 13	2	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	GLY	-	CLONING ARTIFACT	UNP Q8WUM0
A	66	SER	-	CLONING ARTIFACT	UNP Q8WUM0
A	345	LEU	PHE	ENGINEERED	UNP Q8WUM0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total 95	O 95	0	0

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.

• Molecule 1: Nuclear pore complex protein Nup133

Chain A:
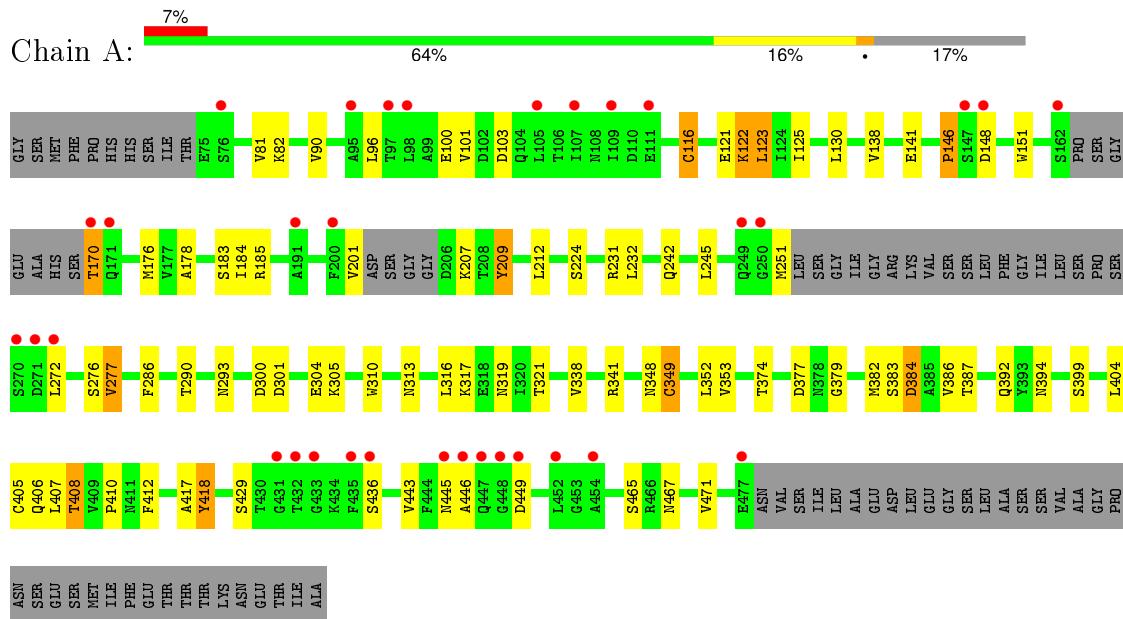
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.59Å 84.59Å 139.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.46 – 2.35 40.46 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.5 (40.46-2.35) 96.5 (40.46-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.93 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.236 0.202 , 0.239	Depositor DCC
R_{free} test set	2036 reflections (10.82%)	DCC
Wilson B-factor (Å²)	63.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.28 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	1 of 20856 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2940	wwPDB-VP
Average B, all atoms (Å²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	1.18	6/2902 (0.2%)	1.07	13/3950 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	TRP	CE3-CZ3	6.99	1.50	1.38
1	A	121	GLU	CG-CD	5.39	1.60	1.51
1	A	209	TYR	CE2-CZ	5.39	1.45	1.38
1	A	277	VAL	CB-CG1	5.37	1.64	1.52
1	A	418	TYR	CD1-CE1	5.25	1.47	1.39
1	A	116	CYS	CB-SG	5.16	1.91	1.82

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ASP	CB-CG-OD2	8.03	125.53	118.30
1	A	386	VAL	CB-CA-C	-6.06	99.88	111.40
1	A	300	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	382	MET	CG-SD-CE	-5.89	90.78	100.20
1	A	301	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	301	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	341	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	185	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	146	PRO	N-CD-CG	-5.41	95.09	103.20
1	A	349	CYS	CA-CB-SG	-5.38	104.32	114.00
1	A	379	GLY	N-CA-C	-5.07	100.44	113.10
1	A	392	GLN	CB-CA-C	-5.03	100.34	110.40
1	A	300	ASP	CB-CG-OD2	-5.03	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2845	0	2760	55	0
2	A	95	0	0	7	0
All	All	2940	0	2760	55	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 10.

All (55) 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:176:MET:HE2	1:A:212:LEU:HD11	1.46	0.95
1:A:138:VAL:HG11	1:A:170:THR:HG22	1.54	0.90
1:A:176:MET:CE	1:A:212:LEU:HD11	2.02	0.89
1:A:406:GLN:HG2	2:A:560:HOH:O	1.77	0.85
1:A:293:ASN:HB2	1:A:310:TRP:O	1.81	0.79
1:A:176:MET:HE3	1:A:232:LEU:HD13	1.68	0.74
1:A:408:THR:HG22	1:A:418:TYR:HB2	1.69	0.74
1:A:100:GLU:O	1:A:103:ASP:N	2.21	0.72
1:A:184:ILE:HD11	1:A:201:VAL:HG23	1.72	0.71
1:A:176:MET:HE2	1:A:212:LEU:CD1	2.21	0.70
1:A:138:VAL:CG1	1:A:170:THR:HG22	2.22	0.69
1:A:293:ASN:CB	1:A:310:TRP:O	2.42	0.68
1:A:313:ASN:O	1:A:317:LYS:HB2	1.96	0.65
1:A:316:LEU:HA	1:A:319:ASN:HD22	1.62	0.65
1:A:251:MET:HG3	1:A:272:LEU:HB2	1.78	0.64
1:A:305:LYS:HE3	2:A:575:HOH:O	1.97	0.64
1:A:176:MET:HE3	1:A:232:LEU:CD1	2.30	0.60
1:A:90:VAL:HG23	2:A:605:HOH:O	2.02	0.58
1:A:349:CYS:HA	1:A:412:PHE:CE2	2.38	0.58
1:A:429:SER:HB2	1:A:436:SER:CB	2.33	0.58
1:A:384:ASP:OD1	1:A:384:ASP:N	2.38	0.57
1:A:184:ILE:HD11	1:A:201:VAL:CG2	2.34	0.57
1:A:276:SER:HB2	2:A:556:HOH:O	2.06	0.56
1:A:176:MET:CE	1:A:232:LEU:CD1	2.85	0.55
1:A:122:LYS:HG2	1:A:141:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:THR:OG1	1:A:387:THR:OG1	2.24	0.54
1:A:443:VAL:HG13	1:A:445:ASN:CG	2.30	0.52
1:A:176:MET:HE1	1:A:212:LEU:HD11	1.89	0.50
1:A:353:VAL:HG22	1:A:374:THR:HG22	1.91	0.50
1:A:176:MET:HE1	1:A:232:LEU:HD12	1.94	0.49
1:A:176:MET:CE	1:A:232:LEU:HD12	2.42	0.49
1:A:418:TYR:CD1	1:A:418:TYR:N	2.80	0.49
1:A:429:SER:HB2	1:A:436:SER:OG	2.12	0.48
1:A:290:THR:HG23	2:A:550:HOH:O	2.12	0.47
1:A:148:ASP:HB2	2:A:604:HOH:O	2.15	0.47
1:A:123:LEU:HD22	1:A:125:ILE:HG13	1.96	0.47
1:A:245:LEU:HD22	1:A:304:GLU:CD	2.34	0.47
1:A:352:LEU:O	1:A:374:THR:HA	2.15	0.46
1:A:184:ILE:CD1	1:A:201:VAL:HG23	2.45	0.45
1:A:449:ASP:HB2	1:A:467:ASN:ND2	2.31	0.45
1:A:407:LEU:HD11	1:A:417:ALA:HB1	2.00	0.44
1:A:404:LEU:O	1:A:405:CYS:HB2	2.18	0.44
1:A:277:VAL:HB	1:A:286:PHE:CZ	2.54	0.42
1:A:81:VAL:CG1	1:A:471:VAL:HG11	2.49	0.42
1:A:176:MET:CE	1:A:232:LEU:HD13	2.43	0.42
1:A:348:ASN:HB2	1:A:412:PHE:O	2.20	0.42
1:A:178:ALA:HA	1:A:183:SER:O	2.19	0.42
1:A:146:PRO:HA	2:A:566:HOH:O	2.19	0.42
1:A:321:THR:HG22	1:A:338:VAL:HG11	2.02	0.41
1:A:408:THR:HG23	1:A:410:PRO:HD3	2.03	0.41
1:A:116:CYS:HB3	1:A:123:LEU:HD21	2.01	0.41
1:A:445:ASN:OD1	1:A:446:ALA:N	2.54	0.41
1:A:231:ARG:O	1:A:242:GLN:HA	2.21	0.41
1:A:209:TYR:HA	1:A:224:SER:HA	2.03	0.40
1:A:443:VAL:CG1	1:A:445:ASN:OD1	2.69	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	A	366/450 (81%)	347 (95%)	18 (5%)	1 (0%)	46 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	VAL

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	314/387 (81%)	301 (96%)	13 (4%)	37 48

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	96	LEU
1	A	122	LYS
1	A	123	LEU
1	A	130	LEU
1	A	170	THR
1	A	207	LYS
1	A	383	SER
1	A	384	ASP
1	A	394	ASN
1	A	399	SER
1	A	408	THR
1	A	465	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	ASN

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 (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, 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	374/450 (83%)	0.56	33 (8%)	12	20	34, 63, 115, 166	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	GLY	5.8
1	A	445	ASN	4.3
1	A	170	THR	4.1
1	A	448	GLY	4.0
1	A	272	LEU	3.7
1	A	446	ALA	3.5
1	A	435	PHE	3.5
1	A	97	THR	3.4
1	A	111	GLU	3.4
1	A	107	ILE	3.3
1	A	271	ASP	3.3
1	A	436	SER	3.1
1	A	171	GLN	2.9
1	A	191	ALA	2.9
1	A	452	LEU	2.7
1	A	109	ILE	2.7
1	A	200	PHE	2.7
1	A	454	ALA	2.7
1	A	432	THR	2.7
1	A	477	GLU	2.6
1	A	98	LEU	2.6
1	A	147	SER	2.4
1	A	447	GLN	2.4
1	A	249	GLN	2.3
1	A	95	ALA	2.3
1	A	105	LEU	2.2
1	A	270	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	449	ASP	2.2
1	A	431	GLY	2.2
1	A	250	GLY	2.1
1	A	76	SER	2.0
1	A	162	SER	2.0
1	A	148	ASP	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.