



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:10 PM GMT

PDB ID : 4WYK  
Title : Structure of the LRR and NTF2-like domains of NXF1 complexed with NXT1  
Authors : Aibara, S.; Valkov, E.; Stewart, M.  
Deposited on : 2014-11-17  
Resolution : 3.40 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  
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

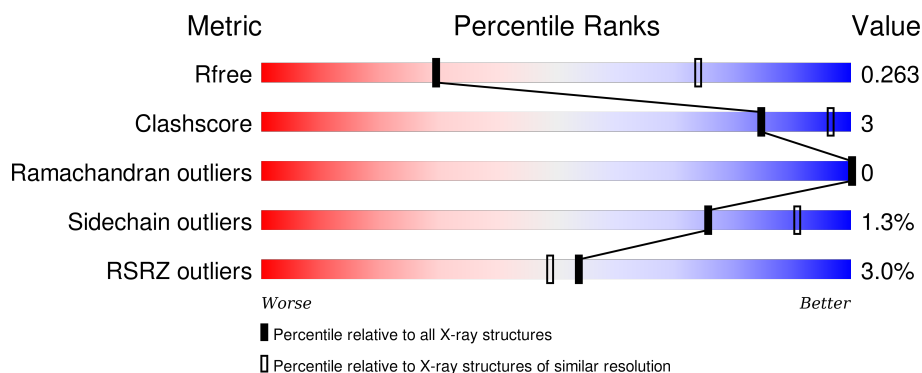
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	461	<div> <div>2%</div> <div>69%</div> <div>5%</div> <div>25%</div> </div>
1	C	461	<div> <div>4%</div> <div>67%</div> <div>7%</div> <div>25%</div> </div>
2	B	139	<div> <div>89%</div> <div>10%</div> </div>
2	D	139	<div> <div>%</div> <div>92%</div> <div>7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15326 atoms, of which 7647 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 RNA export factor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	H	N	O	S	0	0	0
			5500	1727	2767	477	519	10			
1	C	346	Total	C	H	N	O	S	0	0	0
			5528	1736	2780	480	522	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	SER	-	expression tag	UNP Q9UBU9
C	95	SER	-	expression tag	UNP Q9UBU9

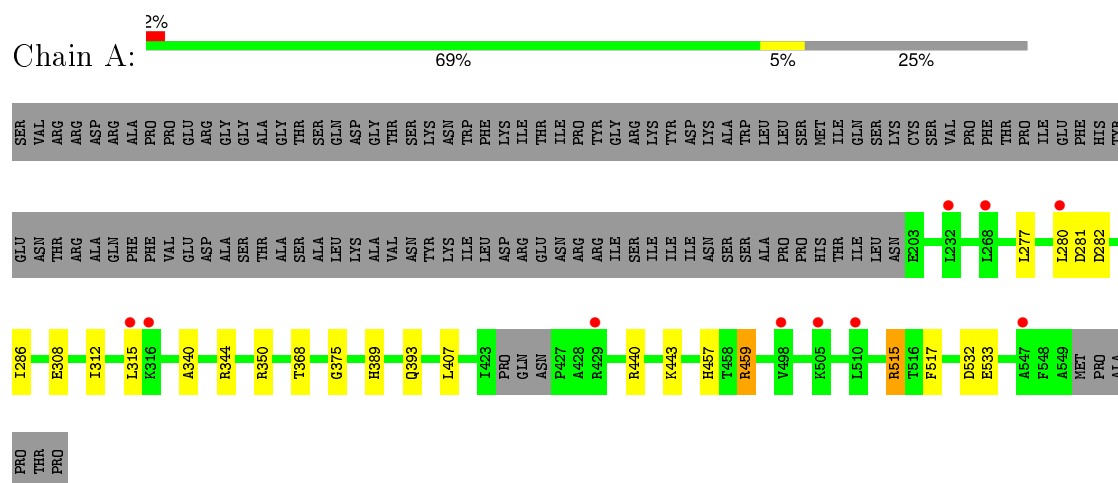
- Molecule 2 is a protein called NTF2-related export protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	138	Total	C	H	N	O	S	0	0	0
			2149	693	1050	185	214	7			
2	D	138	Total	C	H	N	O	S	0	0	0
			2149	693	1050	185	214	7			

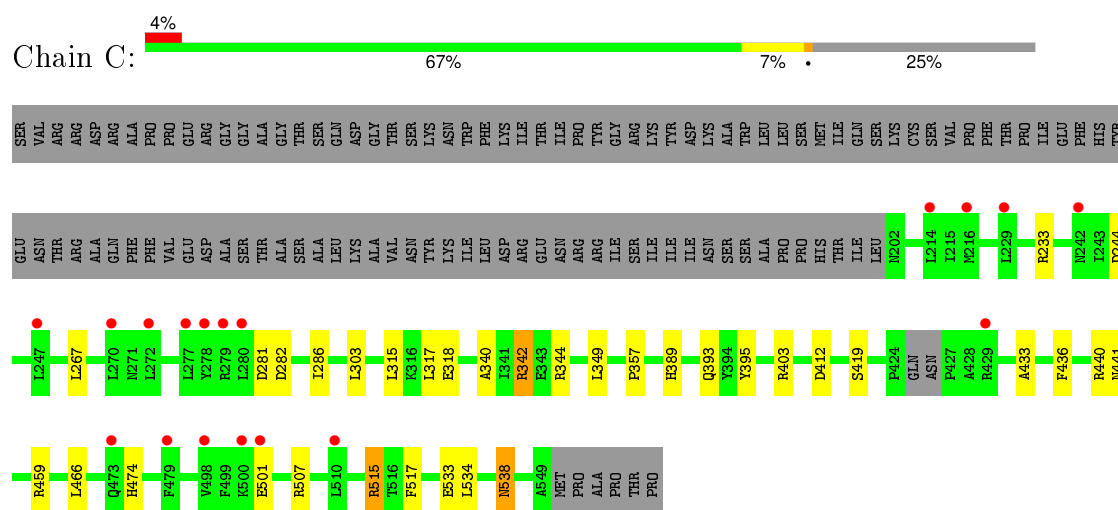
### 3 Residue-property plots

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.

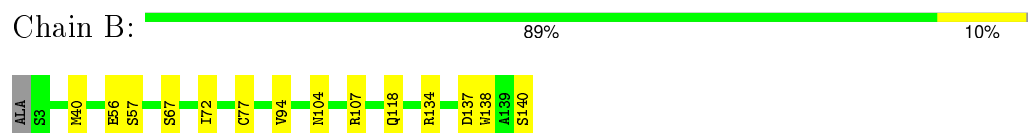
#### • Molecule 1: Nuclear RNA export factor 1



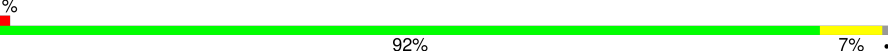
#### • Molecule 1: Nuclear RNA export factor 1



#### • Molecule 2: NTF2-related export protein 1



- Molecule 2: NTF2-related export protein 1

Chain D:  % 92% 7% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.05Å 83.97Å 108.23Å 108.69° 99.76° 97.51°	Depositor
Resolution (Å)	46.41 – 3.40 46.41 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (46.41-3.40) 82.6 (46.41-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.213 , 0.266 0.222 , 0.263	Depositor DCC
$R_{free}$ test set	1016 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.3	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.1	EDS
Estimated twinning fraction	0.033 for -h,-k,h+k+l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 19891 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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, 0.375 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	0.26	0/2779	0.46	0/3754
1	C	0.26	0/2795	0.46	0/3777
2	B	0.27	0/1123	0.45	0/1524
2	D	0.27	0/1123	0.43	0/1524
All	All	0.26	0/7820	0.45	0/10579

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 [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	2733	2767	2767	17	0
1	C	2748	2780	2780	19	0
2	B	1099	1050	1050	10	0
2	D	1099	1050	1050	7	0
All	All	7679	7647	7647	44	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 3.

All (44) 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:515:ARG:NH1	1:A:532:ASP:OD2	2.21	0.73
1:A:281:ASP:OD1	1:A:282:ASP:N	2.32	0.63
2:D:100:LYS:NZ	2:D:104:ASN:O	2.21	0.62
1:A:389:HIS:NE2	1:A:393:GLN:OE1	2.34	0.61
1:C:389:HIS:NE2	1:C:393:GLN:OE1	2.35	0.59
1:A:407:LEU:O	1:A:459:ARG:NH1	2.36	0.58
1:C:533:GLU:OE1	1:C:534:LEU:N	2.40	0.55
1:A:280:LEU:HD13	1:A:312:ILE:HD11	1.89	0.54
2:D:107:ARG:NH2	2:D:140:SER:OG	2.42	0.53
1:A:515:ARG:HD3	1:A:517:PHE:CZ	2.47	0.50
1:C:281:ASP:OD1	1:C:282:ASP:N	2.46	0.48
1:C:340:ALA:O	1:C:344:ARG:NH1	2.45	0.48
1:A:368:THR:O	2:B:104:ASN:ND2	2.42	0.47
1:C:286:ILE:HG23	1:C:315:LEU:HD23	1.96	0.46
1:C:433:ALA:HA	1:C:436:PHE:HB2	1.96	0.46
2:B:107:ARG:NH2	2:B:137:ASP:O	2.49	0.46
2:B:40:MET:SD	2:B:118:GLN:NE2	2.89	0.46
1:C:533:GLU:HG2	2:D:94:VAL:HG11	1.98	0.46
1:C:318:GLU:O	1:C:349:LEU:N	2.45	0.46
1:A:440:ARG:NH1	2:B:77:CYS:O	2.48	0.46
1:C:403:ARG:NH1	1:C:466:LEU:O	2.49	0.45
2:D:53:SER:O	2:D:57:SER:OG	2.30	0.45
1:A:443:LYS:HZ1	2:B:72:ILE:HB	1.81	0.45
1:C:412:ASP:HA	1:C:459:ARG:HD2	1.99	0.45
1:C:538:ASN:N	1:C:538:ASN:OD1	2.49	0.44
1:A:375:GLY:O	2:B:134:ARG:NH2	2.51	0.44
1:C:315:LEU:CD1	1:C:317:LEU:HG	2.48	0.44
1:C:501:GLU:HB2	1:C:507:ARG:HA	1.98	0.44
2:D:76:ASP:OD1	2:D:77:CYS:N	2.51	0.44
1:C:233:ARG:NE	1:C:244:ASP:OD1	2.50	0.43
1:A:286:ILE:HG23	1:A:315:LEU:HD23	2.00	0.43
1:A:457:HIS:O	1:A:457:HIS:ND1	2.51	0.43
2:B:107:ARG:NH2	2:B:140:SER:OG	2.51	0.43
1:A:280:LEU:HD12	1:A:308:GLU:HB3	2.01	0.43
1:A:280:LEU:HD13	1:A:312:ILE:CD1	2.49	0.43
1:C:342:ARG:NH2	1:C:357:PRO:O	2.53	0.41
1:A:375:GLY:HA2	2:B:138:TRP:CH2	2.54	0.41
1:A:533:GLU:HG2	2:B:94:VAL:HG21	2.03	0.41
2:B:56:GLU:OE1	2:B:57:SER:N	2.53	0.41
1:A:340:ALA:O	1:A:344:ARG:NH1	2.53	0.41
1:C:515:ARG:HG2	1:C:517:PHE:CE2	2.56	0.41
1:C:395:TYR:CE1	1:C:474:HIS:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ARG:NH1	2:D:77:CYS:O	2.53	0.40
1:C:441:ASN:ND2	2:D:74:VAL:HG12	2.37	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	340/461 (74%)	337 (99%)	3 (1%)	0	100	100
1	C	342/461 (74%)	340 (99%)	2 (1%)	0	100	100
2	B	136/139 (98%)	131 (96%)	5 (4%)	0	100	100
2	D	136/139 (98%)	132 (97%)	4 (3%)	0	100	100
All	All	954/1200 (80%)	940 (98%)	14 (2%)	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	309/411 (75%)	305 (99%)	4 (1%)	76	91
1	C	311/411 (76%)	305 (98%)	6 (2%)	65	87
2	B	123/123 (100%)	122 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	123/123 (100%)	123 (100%)	0	100	100
All	All	866/1068 (81%)	855 (99%)	11 (1%)	76	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	LEU
1	A	350	ARG
1	A	459	ARG
1	A	515	ARG
2	B	67	SER
1	C	267	LEU
1	C	303	LEU
1	C	342	ARG
1	C	419	SER
1	C	515	ARG
1	C	538	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 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	344/461 (74%)	0.36	10 (2%) 55 50	50, 91, 134, 151	0
1	C	346/461 (75%)	0.42	18 (5%) 31 28	45, 100, 153, 186	0
2	B	138/139 (99%)	0.11	0 100 100	46, 72, 120, 160	0
2	D	138/139 (99%)	0.07	1 (0%) 89 85	43, 71, 123, 146	0
All	All	966/1200 (80%)	0.30	29 (3%) 54 49	43, 89, 144, 186	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	LEU	4.2
1	C	510	LEU	4.1
1	C	279	ARG	3.8
1	A	547	ALA	3.8
1	A	429	ARG	3.3
1	C	429	ARG	3.2
1	A	280	LEU	3.1
1	C	473	GLN	3.0
1	C	278	TYR	3.0
1	C	216	MET	2.6
1	C	247	LEU	2.6
1	C	277	LEU	2.6
1	C	479	PHE	2.5
1	C	500	LYS	2.5
1	A	268	LEU	2.5
1	A	315	LEU	2.5
1	A	316	LYS	2.4
1	C	270	LEU	2.4
1	C	501	GLU	2.3
1	A	510	LEU	2.3
1	C	229	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	498	VAL	2.1
1	C	242	ASN	2.1
1	A	505	LYS	2.1
1	A	232	LEU	2.1
2	D	119	ALA	2.1
1	C	214	LEU	2.1
1	C	272	LEU	2.0
1	A	498	VAL	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.