



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7WWP  
Title : Crystal structure of human Npl4  
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Deposited on : 2022-02-14  
Resolution : 2.99 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

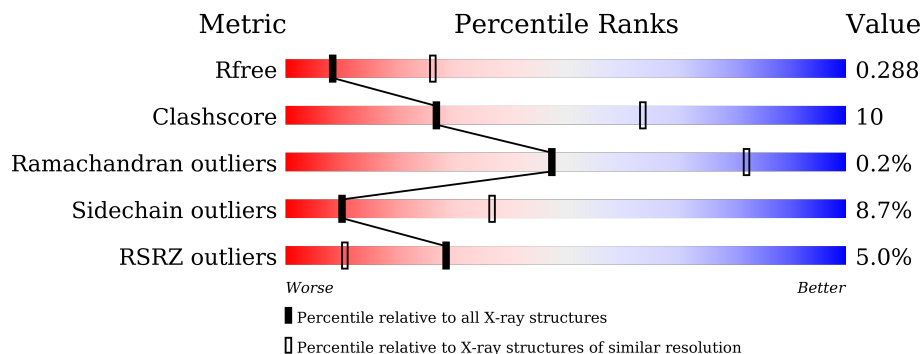
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	473	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3358 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 protein localization protein 4 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3357	2132	568	643	14	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	561	LEU	-	expression tag	UNP Q8TAT6
A	562	GLU	-	expression tag	UNP Q8TAT6
A	563	ALA	-	expression tag	UNP Q8TAT6

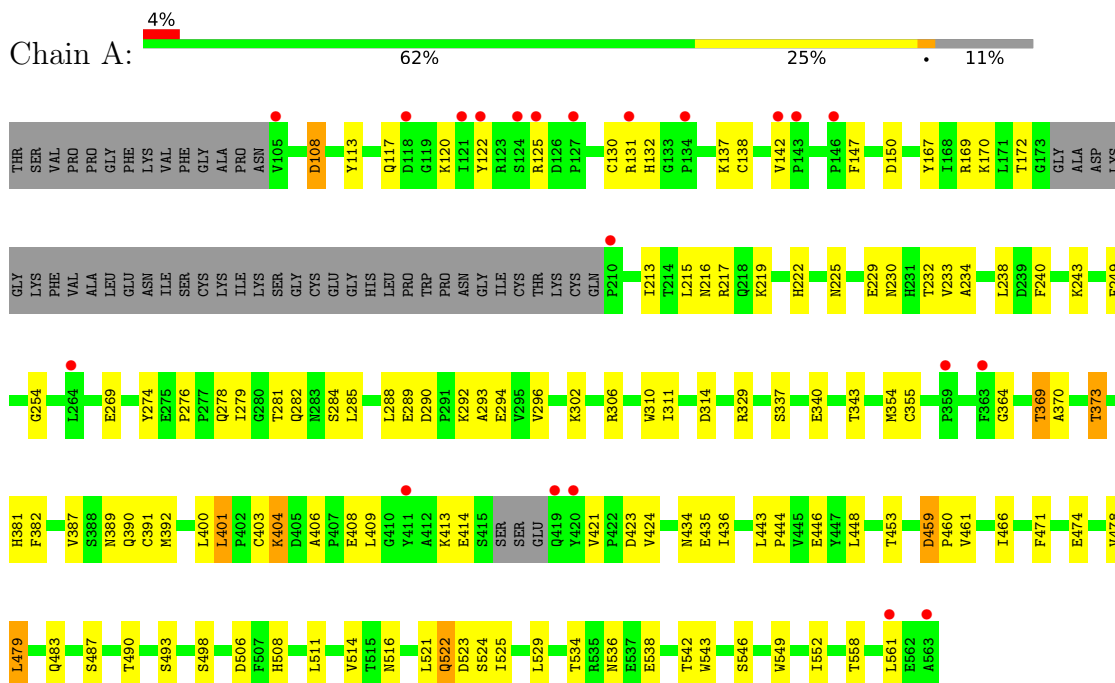
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Nuclear protein localization protein 4 homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.32Å 136.32Å 126.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.44 – 2.99 46.44 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.44-2.99) 99.3 (46.44-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.231 , 0.290 0.230 , 0.288	Depositor DCC
$R_{free}$ test set	736 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.9	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3358	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.46	0/3439	0.65	0/4672

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	3357	0	3222	67	0
2	A	1	0	0	0	0
All	All	3358	0	3222	67	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 (67) 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:514:VAL:HG13	1:A:522:GLN:HA	1.54	0.88
1:A:225:ASN:HD22	1:A:453:THR:HG22	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HB	1:A:424:VAL:HG12	1.58	0.85
1:A:404:LYS:HD3	1:A:404:LYS:H	1.45	0.82
1:A:534:THR:HG22	1:A:536:ASN:HB2	1.67	0.74
1:A:120:LYS:HB2	1:A:122:TYR:HE1	1.54	0.71
1:A:310:TRP:NE1	1:A:369:THR:HB	2.08	0.68
1:A:514:VAL:HG22	1:A:525:ILE:HG12	1.76	0.68
1:A:389:ASN:HA	1:A:392:MET:HG3	1.76	0.67
1:A:120:LYS:HB2	1:A:122:TYR:CE1	2.31	0.65
1:A:125:ARG:NH1	1:A:132:HIS:O	2.30	0.65
1:A:558:THR:HA	1:A:561:LEU:HB2	1.77	0.64
1:A:302:LYS:HB2	1:A:529:LEU:HD23	1.81	0.63
1:A:329:ARG:HG3	1:A:373:THR:HG21	1.81	0.62
1:A:408:GLU:HG2	1:A:409:LEU:HG	1.82	0.62
1:A:401:LEU:HD21	1:A:413:LYS:HE2	1.80	0.62
1:A:249:PHE:HB2	1:A:285:LEU:HD22	1.80	0.61
1:A:108:ASP:OD2	1:A:306:ARG:NH1	2.30	0.61
1:A:230:ASN:OD1	1:A:233:VAL:HG23	2.01	0.61
1:A:413:LYS:HB2	1:A:421:VAL:HG21	1.82	0.60
1:A:225:ASN:ND2	1:A:453:THR:HG22	2.16	0.59
1:A:138:CYS:O	1:A:142:VAL:HG23	2.01	0.59
1:A:538:GLU:O	1:A:542:THR:HG23	2.02	0.59
1:A:254:GLY:HA3	1:A:269:GLU:O	2.05	0.57
1:A:314:ASP:O	1:A:373:THR:HG23	2.05	0.56
1:A:506:ASP:OD1	1:A:508:HIS:N	2.39	0.55
1:A:222:HIS:NE2	1:A:364:GLY:HA3	2.22	0.54
1:A:391:CYS:HB2	1:A:448:LEU:HD22	1.89	0.54
1:A:292:LYS:O	1:A:296:VAL:HG23	2.08	0.53
1:A:117:GLN:O	1:A:169:ARG:NH1	2.36	0.53
1:A:525:ILE:HB	1:A:529:LEU:HD13	1.91	0.51
1:A:290:ASP:HB3	1:A:293:ALA:HB2	1.92	0.51
1:A:137:LYS:HB2	1:A:142:VAL:HG22	1.92	0.51
1:A:215:LEU:HA	1:A:390:GLN:OE1	2.11	0.50
1:A:232:THR:HG21	1:A:466:ILE:HD12	1.94	0.49
1:A:243:LYS:HB3	1:A:243:LYS:HE3	1.66	0.48
1:A:534:THR:CG2	1:A:536:ASN:HB2	2.41	0.48
1:A:404:LYS:H	1:A:404:LYS:CD	2.21	0.48
1:A:337:SER:HB2	1:A:340:GLU:HG3	1.97	0.47
1:A:471:PHE:CE2	1:A:483:GLN:HG2	2.50	0.46
1:A:543:TRP:O	1:A:546:SER:HB3	2.15	0.46
1:A:147:PHE:CE1	1:A:170:LYS:HA	2.49	0.46
1:A:479:LEU:N	1:A:479:LEU:HD23	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:VAL:CG2	1:A:525:ILE:HG12	2.45	0.45
1:A:403:CYS:HB3	1:A:406:ALA:HB3	1.98	0.45
1:A:170:LYS:O	1:A:172:THR:N	2.50	0.45
1:A:296:VAL:HG22	1:A:511:LEU:HD21	1.99	0.45
1:A:219:LYS:H	1:A:219:LYS:HG2	1.63	0.45
1:A:478:VAL:HB	1:A:479:LEU:HD23	1.98	0.45
1:A:229:GLU:HB3	1:A:461:VAL:O	2.17	0.44
1:A:238:LEU:HD11	1:A:382:PHE:CZ	2.53	0.44
1:A:276:PRO:O	1:A:278:GLN:HG2	2.17	0.44
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.85	0.44
1:A:413:LYS:CB	1:A:421:VAL:HG21	2.48	0.43
1:A:443:LEU:HD12	1:A:444:PRO:HD2	2.00	0.42
1:A:521:LEU:HD11	1:A:552:ILE:HG13	2.02	0.42
1:A:523:ASP:OD1	1:A:524:SER:N	2.52	0.42
1:A:281:THR:HG1	1:A:284:SER:HG	1.66	0.41
1:A:311:ILE:HA	1:A:370:ALA:O	2.20	0.41
1:A:459:ASP:HA	1:A:460:PRO:HD3	1.89	0.41
1:A:240:PHE:CE2	1:A:479:LEU:HD21	2.55	0.41
1:A:274:TYR:CZ	1:A:296:VAL:HG21	2.55	0.41
1:A:549:TRP:CZ3	1:A:552:ILE:HG21	2.56	0.41
1:A:167:TYR:O	1:A:170:LYS:HB3	2.21	0.40
1:A:474:GLU:CD	1:A:474:GLU:H	2.23	0.40
1:A:279:ILE:HG13	1:A:288:LEU:HD13	2.03	0.40
1:A:234:ALA:HB1	1:A:382:PHE:CZ	2.56	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	414/473 (88%)	382 (92%)	31 (8%)	1 (0%)	47 82



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	GLU

### 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	369/420 (88%)	337 (91%)	32 (9%)	10 37

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASP
1	A	113	TYR
1	A	130	CYS
1	A	131	ARG
1	A	150	ASP
1	A	216	ASN
1	A	217	ARG
1	A	282	GLN
1	A	289	GLU
1	A	294	GLU
1	A	343	THR
1	A	354	MET
1	A	355	CYS
1	A	369	THR
1	A	373	THR
1	A	381	HIS
1	A	387	VAL
1	A	401	LEU
1	A	404	LYS
1	A	414	GLU
1	A	423	ASP
1	A	434	ASN
1	A	436	ILE
1	A	446	GLU

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Mol	Chain	Res	Type
1	A	459	ASP
1	A	479	LEU
1	A	487	SER
1	A	490	THR
1	A	493	SER
1	A	498	SER
1	A	516	ASN
1	A	522	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	225	ASN
1	A	381	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

No monomer is involved in short contacts.

## 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 [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, 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	420/473 (88%)	0.36	21 (5%) 28 10	35, 62, 117, 163	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	PRO	6.3
1	A	122	TYR	5.0
1	A	121	ILE	4.3
1	A	419	GLN	4.2
1	A	411	TYR	3.5
1	A	105	VAL	3.5
1	A	118	ASP	3.5
1	A	561	LEU	3.2
1	A	363	PHE	3.0
1	A	142	VAL	3.0
1	A	264	LEU	2.9
1	A	210	PRO	2.7
1	A	124	SER	2.7
1	A	146	PRO	2.6
1	A	359	PRO	2.6
1	A	563	ALA	2.6
1	A	125	ARG	2.5
1	A	420	TYR	2.5
1	A	131	ARG	2.3
1	A	143	PRO	2.3
1	A	134	PRO	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	901	1/1	0.98	0.07	106,106,106,106	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.