



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:53 PM GMT

PDB ID : 4G3V  
Title : Crystal structure of A. Aeolicus nlh2 gaf domain in an inactive state  
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Deposited on : 2012-07-15  
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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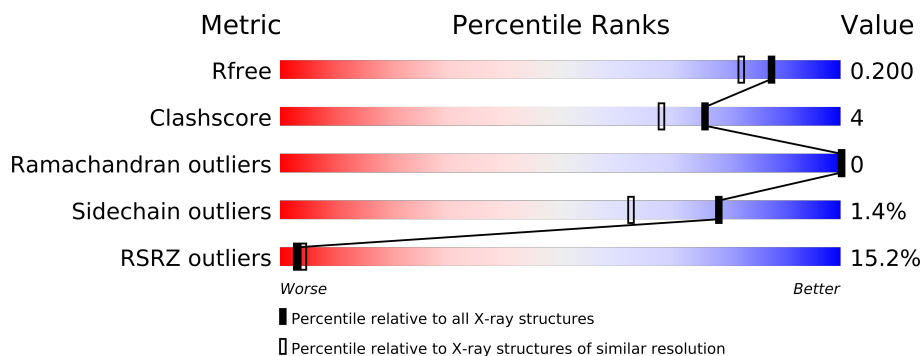
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	172	
1	B	172	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5497 atoms, of which 2727 are hydrogens and 0 are deuterium.

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 Transcriptional regulator nlh2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	162	Total	C	H	N	O	S	0	3	0
			2671	852	1370	216	231	2			
1	B	162	Total	C	H	N	O	S	0	2	0
			2653	847	1357	216	231	2			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	3	Total	Cl	0	0
			3	3		

- Molecule 3 is water.

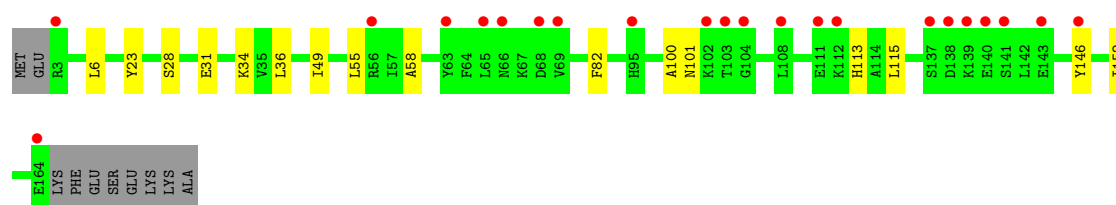
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	96	Total	O	0	0
			96	96		
3	B	73	Total	O	0	0
			73	73		

### 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.

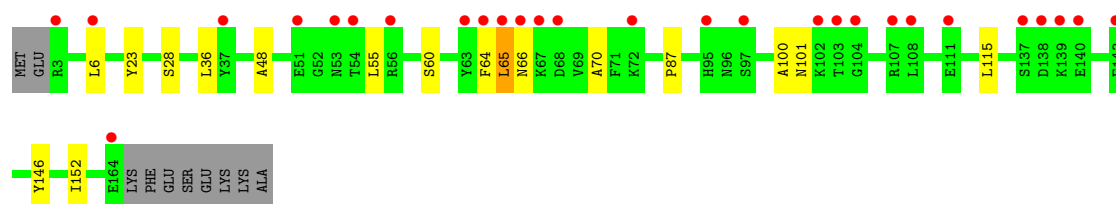
- Molecule 1: Transcriptional regulator nlh2

Chain A: 



- Molecule 1: Transcriptional regulator nlh2

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.45Å 65.45Å 128.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.16 – 1.70 19.16 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.16-1.70) 99.7 (19.16-1.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.163 , 0.206 0.157 , 0.200	Depositor DCC
$R_{free}$ test set	1946 reflections (5.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 62.8	EDS
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35725 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.45 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1427e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.40	0/1332	0.52	0/1788
1	B	0.39	0/1324	0.49	0/1777
All	All	0.40	0/2656	0.50	0/3565

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1301	1370	0	11	0
1	B	1296	1357	0	10	0
2	A	3	0	0	1	0
2	B	1	0	0	0	0
3	A	96	0	0	1	0
3	B	73	0	0	0	0
All	All	2770	2727	0	21	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:113:HIS:NE2	2:A:202:CL:CL	2.78	0.53
1:B:87:PRO:HG3	1:B:146:TYR:OH	2.11	0.51
1:A:36:LEU:HD21	1:A:152:ILE:CD1	2.45	0.47
1:A:49:ILE:HD12	1:A:58:ALA:CB	2.45	0.46
1:B:36:LEU:HD21	1:B:152:ILE:CD1	2.45	0.46
1:B:36:LEU:HD21	1:B:152:ILE:HD13	1.99	0.45
1:A:100:ALA:O	1:A:101:ASN:C	2.56	0.44
1:A:36:LEU:HD21	1:A:152:ILE:HD13	2.00	0.44
1:B:48:ALA:HB1	1:B:55:LEU:HG	2.00	0.44
1:A:49:ILE:HD12	1:A:58:ALA:HB2	2.00	0.43
1:A:115:LEU:HD23	1:A:115:LEU:C	2.39	0.43
1:B:55:LEU:O	1:B:70:ALA:HA	2.19	0.42
1:A:31:GLU:HA	1:A:34[A]:LYS:HE3	2.00	0.42
1:B:115:LEU:C	1:B:115:LEU:HD23	2.40	0.42
1:A:55:LEU:HG	1:A:82:PHE:CD2	2.55	0.42
1:B:60:SER:HB2	1:B:64:PHE:HB2	2.01	0.41
1:B:23:TYR:HB2	1:B:28:SER:HG	1.84	0.41
1:A:23:TYR:HB2	1:A:28:SER:HG	1.84	0.41
1:B:65:LEU:HD12	1:B:66:ASN:N	2.35	0.41
1:B:100:ALA:O	1:B:101:ASN:C	2.59	0.41
1:A:34[B]:LYS:NZ	3:A:346:HOH:O	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	163/172 (95%)	162 (99%)	1 (1%)	0	100	100
1	B	162/172 (94%)	160 (99%)	2 (1%)	0	100	100
All	All	325/344 (94%)	322 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	142/148 (96%)	140 (99%)	2 (1%)	78	62
1	B	141/148 (95%)	139 (99%)	2 (1%)	78	62
All	All	283/296 (96%)	279 (99%)	4 (1%)	78	62

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	146	TYR
1	B	6	LEU
1	B	65	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	150	ASN
1	B	92	ASN
1	B	147	GLN
1	B	150	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 4 ligands modelled in this entry, 4 are 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.

## 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	162/172 (94%)	0.53	22 (13%) 4 5	22, 37, 71, 92	0
1	B	162/172 (94%)	0.72	28 (17%) 2 3	22, 41, 87, 115	0
All	All	324/344 (94%)	0.63	50 (15%) 3 4	22, 39, 85, 115	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	LYS	6.6
1	B	53	ASN	6.4
1	B	65	LEU	6.0
1	B	104	GLY	5.9
1	A	63	TYR	5.5
1	B	68	ASP	4.9
1	B	63	TYR	4.6
1	B	139	LYS	4.4
1	A	108	LEU	4.3
1	B	102	LYS	4.2
1	A	137	SER	3.9
1	A	68	ASP	3.9
1	B	72	LYS	3.9
1	B	3	ARG	3.8
1	B	137	SER	3.6
1	A	65	LEU	3.6
1	B	67	LYS	3.5
1	A	3	ARG	3.4
1	A	140	GLU	3.3
1	B	138	ASP	3.3
1	B	54	THR	3.2
1	A	164	GLU	3.2
1	A	102	LYS	3.1
1	A	143	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	66	ASN	3.1
1	A	111	GLU	3.0
1	A	104	GLY	3.0
1	B	140	GLU	3.0
1	B	164	GLU	2.8
1	B	95	HIS	2.8
1	B	37	TYR	2.7
1	A	95	HIS	2.7
1	A	138	ASP	2.7
1	A	69	VAL	2.6
1	A	56	ARG	2.6
1	B	66	ASN	2.6
1	B	6	LEU	2.5
1	A	103	THR	2.5
1	B	107	ARG	2.5
1	B	51	GLU	2.5
1	B	56	ARG	2.4
1	B	97	SER	2.4
1	A	112	LYS	2.3
1	B	103	THR	2.3
1	B	111	GLU	2.3
1	B	64	PHE	2.2
1	B	143	GLU	2.1
1	B	108	LEU	2.1
1	A	146	TYR	2.1
1	A	141	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	201	1/1	0.09	0.01	37,37,37,37	0
2	CL	A	202	1/1	0.16	-0.06	79,79,79,79	0
2	CL	A	203	1/1	0.09	-0.47	49,49,49,49	0
2	CL	B	201	1/1	0.04	-5.53	42,42,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.