



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:20 AM GMT

PDB ID : 3UN9  
Title : Crystal structure of an immune receptor  
Authors : Hong, M.; Yoon, S.I.; Wilson, I.A.  
Deposited on : 2011-11-15  
Resolution : 2.65 Å(reported)

This is a wwPDB validation summary 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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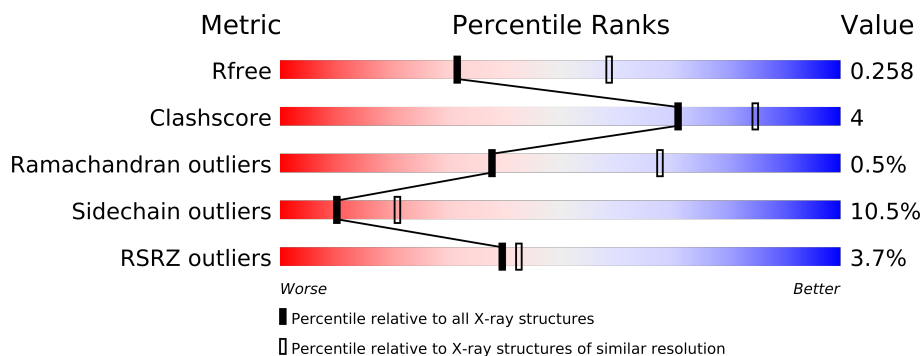
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.65 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	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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	372	
1	B	372	
1	C	372	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PT	A	1001	-	X
2	PT	A	1002	-	X
2	PT	B	1001	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6679 atoms, of which 0 are hydrogen 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 NLR family member X1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	17	0	0
			2277	1426	424	421	6			
1	B	294	Total	C	N	O	S	11	2	0
			2293	1436	425	426	6			
1	C	279	Total	C	N	O	S	0	1	0
			2097	1317	381	393	6			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	625	MET	-	EXPRESSION TAG	UNP Q86UT6
A	626	LEU	-	EXPRESSION TAG	UNP Q86UT6
A	627	LEU	-	EXPRESSION TAG	UNP Q86UT6
A	628	VAL	-	EXPRESSION TAG	UNP Q86UT6
A	976	PRO	-	EXPRESSION TAG	UNP Q86UT6
A	977	SER	-	EXPRESSION TAG	UNP Q86UT6
A	978	GLY	-	EXPRESSION TAG	UNP Q86UT6
A	979	SER	-	EXPRESSION TAG	UNP Q86UT6
A	980	TRP	-	EXPRESSION TAG	UNP Q86UT6
A	981	SER	-	EXPRESSION TAG	UNP Q86UT6
A	982	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	983	PRO	-	EXPRESSION TAG	UNP Q86UT6
A	984	GLN	-	EXPRESSION TAG	UNP Q86UT6
A	985	PHE	-	EXPRESSION TAG	UNP Q86UT6
A	986	GLU	-	EXPRESSION TAG	UNP Q86UT6
A	987	LYS	-	EXPRESSION TAG	UNP Q86UT6
A	988	GLY	-	EXPRESSION TAG	UNP Q86UT6
A	989	ALA	-	EXPRESSION TAG	UNP Q86UT6
A	990	GLY	-	EXPRESSION TAG	UNP Q86UT6
A	991	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	992	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	993	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	994	HIS	-	EXPRESSION TAG	UNP Q86UT6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	995	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	996	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	625	MET	-	EXPRESSION TAG	UNP Q86UT6
B	626	LEU	-	EXPRESSION TAG	UNP Q86UT6
B	627	LEU	-	EXPRESSION TAG	UNP Q86UT6
B	628	VAL	-	EXPRESSION TAG	UNP Q86UT6
B	976	PRO	-	EXPRESSION TAG	UNP Q86UT6
B	977	SER	-	EXPRESSION TAG	UNP Q86UT6
B	978	GLY	-	EXPRESSION TAG	UNP Q86UT6
B	979	SER	-	EXPRESSION TAG	UNP Q86UT6
B	980	TRP	-	EXPRESSION TAG	UNP Q86UT6
B	981	SER	-	EXPRESSION TAG	UNP Q86UT6
B	982	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	983	PRO	-	EXPRESSION TAG	UNP Q86UT6
B	984	GLN	-	EXPRESSION TAG	UNP Q86UT6
B	985	PHE	-	EXPRESSION TAG	UNP Q86UT6
B	986	GLU	-	EXPRESSION TAG	UNP Q86UT6
B	987	LYS	-	EXPRESSION TAG	UNP Q86UT6
B	988	GLY	-	EXPRESSION TAG	UNP Q86UT6
B	989	ALA	-	EXPRESSION TAG	UNP Q86UT6
B	990	GLY	-	EXPRESSION TAG	UNP Q86UT6
B	991	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	992	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	993	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	994	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	995	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	996	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	625	MET	-	EXPRESSION TAG	UNP Q86UT6
C	626	LEU	-	EXPRESSION TAG	UNP Q86UT6
C	627	LEU	-	EXPRESSION TAG	UNP Q86UT6
C	628	VAL	-	EXPRESSION TAG	UNP Q86UT6
C	976	PRO	-	EXPRESSION TAG	UNP Q86UT6
C	977	SER	-	EXPRESSION TAG	UNP Q86UT6
C	978	GLY	-	EXPRESSION TAG	UNP Q86UT6
C	979	SER	-	EXPRESSION TAG	UNP Q86UT6
C	980	TRP	-	EXPRESSION TAG	UNP Q86UT6
C	981	SER	-	EXPRESSION TAG	UNP Q86UT6
C	982	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	983	PRO	-	EXPRESSION TAG	UNP Q86UT6
C	984	GLN	-	EXPRESSION TAG	UNP Q86UT6
C	985	PHE	-	EXPRESSION TAG	UNP Q86UT6
C	986	GLU	-	EXPRESSION TAG	UNP Q86UT6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	987	LYS	-	EXPRESSION TAG	UNP Q86UT6
C	988	GLY	-	EXPRESSION TAG	UNP Q86UT6
C	989	ALA	-	EXPRESSION TAG	UNP Q86UT6
C	990	GLY	-	EXPRESSION TAG	UNP Q86UT6
C	991	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	992	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	993	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	994	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	995	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	996	HIS	-	EXPRESSION TAG	UNP Q86UT6

- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Pt 1 1	0	0
2	A	2	Total Pt 2 2	0	0
2	C	1	Total Pt 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0



HS  
STH

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.01Å 123.47Å 145.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.24 – 2.65 77.24 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.8 (77.24-2.65) 97.9 (77.24-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.267 0.217 , 0.258	Depositor DCC
$R_{free}$ test set	1311 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25759 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 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: PT

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	0.80	2/2308 (0.1%)	0.85	1/3131 (0.0%)
1	B	0.73	2/2330 (0.1%)	0.76	2/3160 (0.1%)
1	C	0.93	9/2127 (0.4%)	0.80	0/2889
All	All	0.82	13/6765 (0.2%)	0.80	3/9180 (0.0%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	871	TYR	CE2-CZ	-11.47	1.23	1.38
1	C	871	TYR	CE1-CZ	-9.55	1.26	1.38
1	C	871	TYR	CG-CD1	-9.39	1.26	1.39
1	C	871	TYR	CG-CD2	-9.20	1.27	1.39
1	C	681	PHE	CE2-CZ	-8.96	1.20	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	895	ARG	N-CA-CB	-6.57	98.77	110.60
1	B	670	LEU	CA-CB-CG	5.59	128.16	115.30
1	B	737	LEU	CB-CG-CD2	-5.20	102.16	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	2277	0	21	7	0
1	B	2293	0	19	11	0
1	C	2097	0	0	13	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	6679	0	40	30	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.

The worst 5 of 30 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:880:ARG:NH1	1:C:898:VAL:O	2.13	0.80
1:B:938:ARG:NH1	1:B:938:ARG:CG	2.59	0.66
1:A:880:ARG:NH1	1:A:898:VAL:O	2.30	0.65
1:C:791:LEU:O	1:C:792:THR:CB	2.43	0.65
1:B:880:ARG:NH1	1:B:898:VAL:O	2.33	0.62

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	288/372 (77%)	275 (96%)	13 (4%)	0	100	100
1	B	290/372 (78%)	280 (97%)	9 (3%)	1 (0%)	50	80
1	C	270/372 (73%)	251 (93%)	16 (6%)	3 (1%)	21	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	848/1116 (76%)	806 (95%)	38 (4%)	4 (0%)	38 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	930	GLN
1	B	925	ASP
1	C	908	GLU
1	C	933	LEU

### 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	244/303 (80%)	221 (91%)	23 (9%)	13 26
1	B	247/303 (82%)	221 (90%)	26 (10%)	10 21
1	C	217/303 (72%)	191 (88%)	26 (12%)	7 16
All	All	708/909 (78%)	633 (89%)	75 (11%)	10 20

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	826	LEU
1	B	911	SER
1	C	917	VAL
1	B	836	GLN
1	B	878	GLU

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	668	GLN

### 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	294/372 (79%)	-0.01	5 (1%) 67 71	40, 68, 105, 128	4 (1%)
1	B	294/372 (79%)	0.22	11 (3%) 39 42	50, 83, 123, 144	3 (1%)
1	C	279/372 (75%)	0.17	16 (5%) 23 24	44, 68, 144, 217	0
All	All	867/1116 (77%)	0.13	32 (3%) 39 42	40, 72, 128, 217	7 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	667	ARG	5.6
1	C	913	ILE	5.4
1	B	762	LEU	5.0
1	B	668	GLN	5.0
1	C	918	GLN	4.9

### 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	PT	A	1002	1/1	0.41	27.59	45,45,45,45	1
2	PT	B	1001	1/1	0.34	10.94	82,82,82,82	1
2	PT	A	1001	1/1	0.23	3.77	85,85,85,85	1
2	PT	C	1001	1/1	0.23	0.80	69,69,69,69	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.