



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:06 PM GMT

PDB ID : 1IQA  
Title : CRYSTAL STRUCTURE OF THE EXTRACELLULAR DOMAIN OF  
MOUSE RANK LIGAND  
Authors : Ito, S.; Wakabayashi, K.; Ubukata, O.; Hayashi, S.; Okada, F.; Hata, T.  
Deposited on : 2001-07-11  
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure 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/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

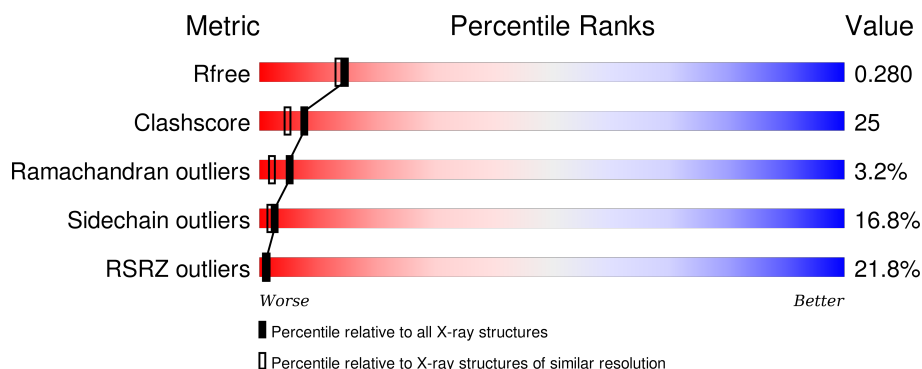
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	160	<div> <div>12%</div> <div>68%</div> <div>25%</div> <div>• • •</div> </div>
1	B	160	<div> <div>29%</div> <div>43%</div> <div>44%</div> <div>11%</div> <div>•</div> </div>
1	C	160	<div> <div>22%</div> <div>54%</div> <div>31%</div> <div>11%</div> <div>• •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3768 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 RECEPTOR ACTIVATOR OF NUCLEAR FACTOR KAPPA B LIGAND.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	Se	0	0	0
			1233	787	210	232	1	3			
1	B	156	Total	C	N	O	S	Se	0	0	0
			1233	787	210	232	1	3			
1	C	156	Total	C	N	O	S	Se	0	0	0
			1233	787	210	232	1	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	MSE	MET	MODIFIED RESIDUE	UNP O35235
A	238	MSE	MET	MODIFIED RESIDUE	UNP O35235
A	255	MSE	MET	MODIFIED RESIDUE	UNP O35235
B	198	MSE	MET	MODIFIED RESIDUE	UNP O35235
B	238	MSE	MET	MODIFIED RESIDUE	UNP O35235
B	255	MSE	MET	MODIFIED RESIDUE	UNP O35235
C	198	MSE	MET	MODIFIED RESIDUE	UNP O35235
C	238	MSE	MET	MODIFIED RESIDUE	UNP O35235
C	255	MSE	MET	MODIFIED RESIDUE	UNP O35235

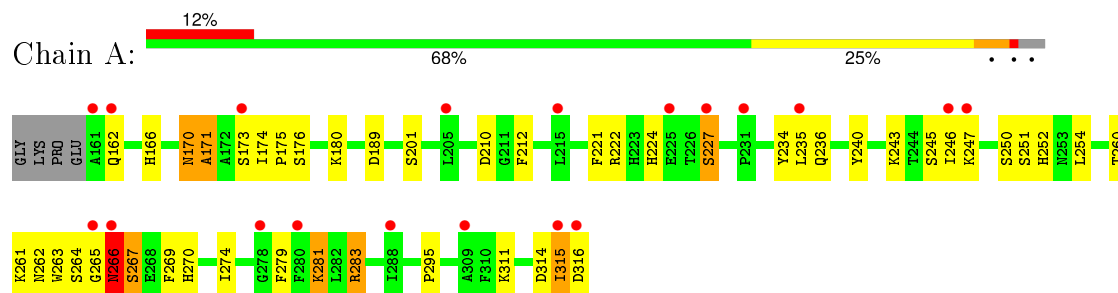
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	14	Total	O	0	0
			14	14		
2	C	17	Total	O	0	0
			17	17		

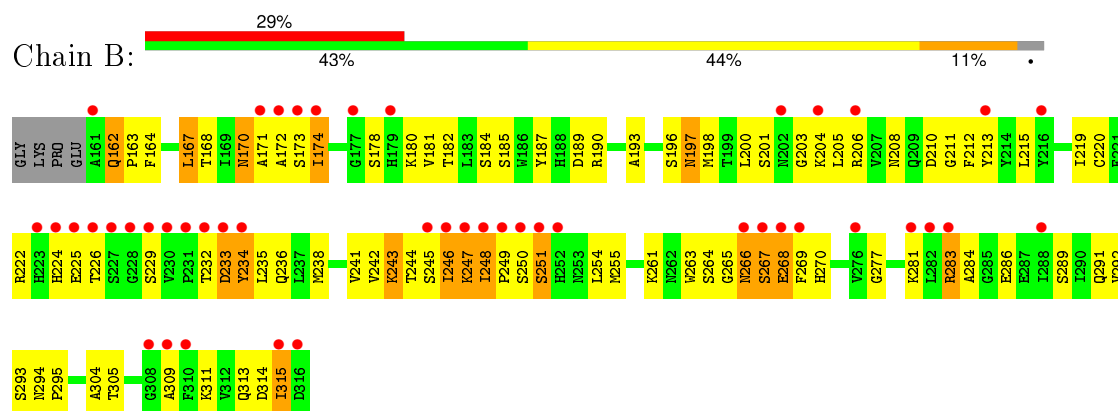
### 3 Residue-property plots [i](#)

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.

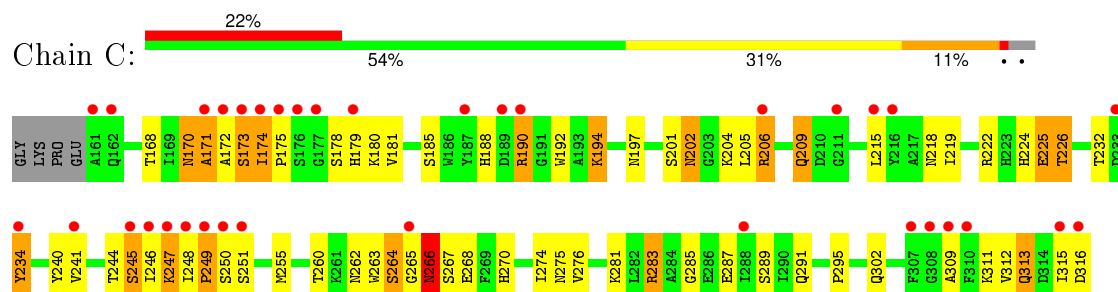
#### • Molecule 1: RECEPTOR ACTIVATOR OF NUCLEAR FACTOR KAPPA B LIGAND



#### • Molecule 1: RECEPTOR ACTIVATOR OF NUCLEAR FACTOR KAPPA B LIGAND



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.68Å 78.98Å 100.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 24.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (15.00-2.20) 96.5 (24.48-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.05 (at 2.19Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.226 , 0.274 0.234 , 0.280	Depositor DCC
$R_{free}$ test set	2035 reflections (7.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 70.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25967 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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

### 5.1 Standard geometry

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	0.99	0/1265	0.98	1/1709 (0.1%)
1	B	0.71	0/1265	0.82	0/1709
1	C	0.77	0/1265	0.89	0/1709
All	All	0.83	0/3795	0.90	1/5127 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	166	HIS	N-CA-C	-5.14	97.13	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	1233	0	1182	46	0
1	B	1233	0	1182	90	0
1	C	1233	0	1182	55	0
2	A	38	0	0	2	0
2	B	14	0	0	2	0
2	C	17	0	0	3	0
All	All	3768	0	3546	183	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 25.

The worst 5 of 183 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:B:283:ARG:HG3	1:B:283:ARG:HH11	1.16	1.07
1:C:283:ARG:HG3	1:C:283:ARG:HH11	1.21	1.04
1:B:219:ILE:HD13	1:B:305:THR:HG23	1.45	0.98
1:C:224:HIS:CD2	1:C:226:THR:HB	2.03	0.93
1:A:281:LYS:HD2	1:A:315:ILE:HD13	1.51	0.92

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	154/160 (96%)	142 (92%)	8 (5%)	4 (3%)	7	3
1	B	154/160 (96%)	140 (91%)	8 (5%)	6 (4%)	4	1
1	C	154/160 (96%)	141 (92%)	8 (5%)	5 (3%)	5	2
All	All	462/480 (96%)	423 (92%)	24 (5%)	15 (3%)	5	2

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	ALA
1	B	246	ILE
1	B	265	GLY
1	B	266	ASN
1	C	171	ALA

### 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	135/135 (100%)	119 (88%)	16 (12%)	6	5
1	B	135/135 (100%)	109 (81%)	26 (19%)	2	1
1	C	135/135 (100%)	109 (81%)	26 (19%)	2	1
All	All	405/405 (100%)	337 (83%)	68 (17%)	2	2

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	232	THR
1	B	283	ARG
1	C	266	ASN
1	B	233	ASP
1	B	247	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	209	GLN
1	B	270	HIS
1	C	224	HIS
1	B	197	ASN
1	C	236	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [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, 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	153/160 (95%)	0.40	19 (12%) 5 5	21, 35, 67, 87	0
1	B	153/160 (95%)	1.84	46 (30%) 1 0	32, 64, 104, 121	0
1	C	153/160 (95%)	1.24	35 (22%) 1 1	29, 51, 86, 100	0
All	All	459/480 (95%)	1.16	100 (21%) 1 1	21, 49, 95, 121	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	THR	14.0
1	B	231	PRO	10.8
1	B	229	SER	9.1
1	B	230	VAL	8.6
1	B	246	ILE	8.2

### 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.