



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 1, 2018 – 07:47 PM EST

PDB ID : 5K7I  
Title : IRAK4 in complex with AZ3864  
Authors : Ferguson, A.D.  
Deposited on : 2016-05-26  
Resolution : 2.31 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

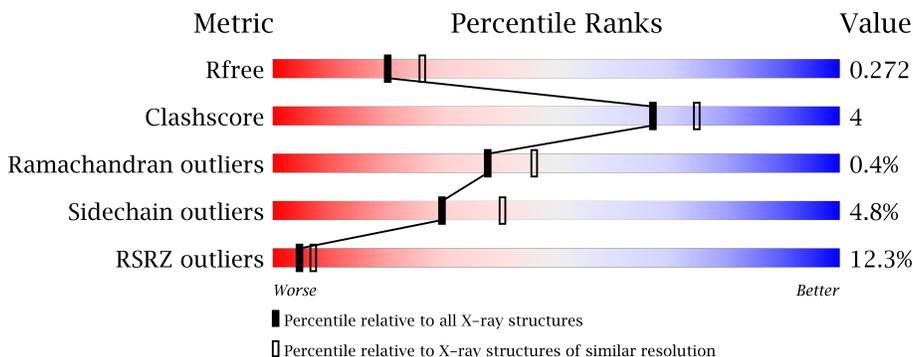
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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))
$R_{free}$	100719	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

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	301	
1	B	301	

## 2 Entry composition [i](#)

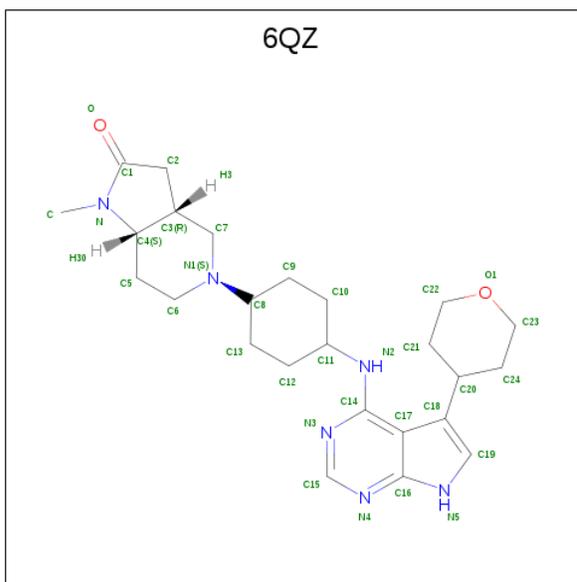
There are 4 unique types of molecules in this entry. The entry contains 4497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

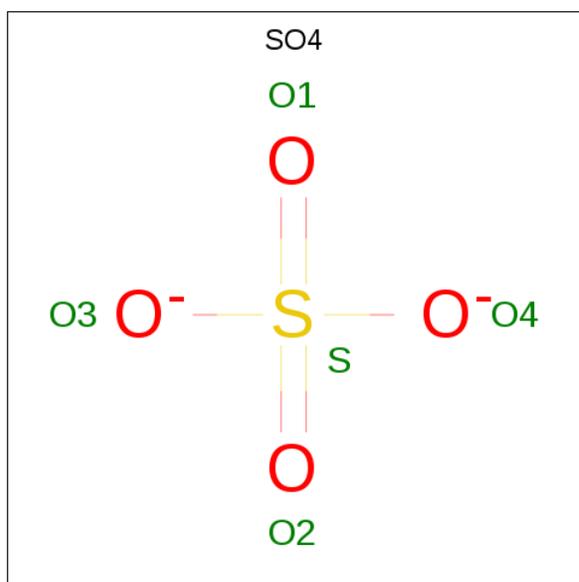
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	274	Total 2174	C 1370	N 368	O 420	P 2	S 14	0	0	0
1	B	273	Total 2175	C 1370	N 367	O 422	P 2	S 14	0	0	0

- Molecule 2 is (3 {a} {R},7 {a} {S})-1-methyl-5-[4-[[5-(oxan-4-yl)-7 {H}-pyrrolo[2,3-d]pyrimidin-4-yl]amino]cyclohexyl]-3,3 {a},4,6,7,7 {a}-hexahydropyrrolo[3,2-c]pyridin-2-one (three-letter code: 6QZ) (formula: C<sub>25</sub>H<sub>36</sub>N<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 33	C 25	N 6	O 2	0	0
2	B	1	Total 33	C 25	N 6	O 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	45	Total	O	0	0
			45	45		



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.54Å 110.53Å 142.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.21 – 2.31 71.21 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.1 (71.21-2.31) 99.1 (71.21-2.31)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.32Å)	Xtrriage
Refinement program	BUSTER-TNT 2.11.7	Depositor
R, $R_{free}$	0.219 , 0.257 0.233 , 0.272	Depositor DCC
$R_{free}$ test set	1491 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtrriage
Anisotropy	0.519	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.45 % 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 5.6884e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 6QZ, TPO, SO4, SEP

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	0.48	0/2188	0.65	0/2944
1	B	0.49	0/2188	0.67	0/2943
All	All	0.49	0/4376	0.66	0/5887

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	2174	0	2154	14	0
1	B	2175	0	2151	27	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0
3	B	5	0	0	0	0
4	A	32	0	0	1	0
4	B	45	0	0	0	0
All	All	4497	0	4305	39	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 4.

The worst 5 of 39 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:265:MET:CE	1:B:326:LYS:HG3	2.21	0.71
1:B:265:MET:HE2	1:B:326:LYS:HG3	1.76	0.66
1:A:265:MET:CE	1:A:326:LYS:HG3	2.26	0.65
1:A:265:MET:HE1	1:A:326:LYS:HG3	1.79	0.63
1:B:201:TYR:HE2	1:B:214:LYS:HD2	1.64	0.62

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	264/301 (88%)	256 (97%)	7 (3%)	1 (0%)	38	46
1	B	261/301 (87%)	253 (97%)	7 (3%)	1 (0%)	38	46
All	All	525/602 (87%)	509 (97%)	14 (3%)	2 (0%)	38	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	GLU
1	A	181	ASP

### 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	238/260 (92%)	230 (97%)	8 (3%)	42	57
1	B	239/260 (92%)	224 (94%)	15 (6%)	21	27
All	All	477/520 (92%)	454 (95%)	23 (5%)	30	40

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	185	ILE
1	B	214	LYS
1	B	410	ILE
1	B	200	VAL
1	B	225	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	A	394	GLN
1	B	293	GLN
1	B	394	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	TPO	A	345	1	9,10,11	1.60	2 (22%)	10,14,16	1.12	1 (10%)
1	SEP	A	346	1	9,9,10	1.37	1 (11%)	9,12,14	1.45	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	B	345	1	9,10,11	1.56	2 (22%)	10,14,16	1.11	1 (10%)
1	SEP	B	346	1	9,9,10	1.35	1 (11%)	9,12,14	1.51	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	345	1	-	1/8/11/13	0/0/0/0
1	SEP	A	346	1	-	0/5/8/10	0/0/0/0
1	TPO	B	345	1	-	1/8/11/13	0/0/0/0
1	SEP	B	346	1	-	0/5/8/10	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	CB-CA	2.51	1.58	1.53
1	A	345	TPO	CA-C	2.91	1.54	1.50
1	A	345	TPO	CB-CA	2.95	1.59	1.53
1	B	345	TPO	CA-C	2.98	1.54	1.50
1	B	346	SEP	CA-C	3.12	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	TPO	O3P-P-OG1	2.32	116.54	106.00
1	B	345	TPO	O3P-P-OG1	2.34	116.64	106.00
1	A	346	SEP	OG-P-O1P	2.69	114.01	106.47
1	B	346	SEP	OG-P-O1P	2.71	114.08	106.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	OG1-CB-CA-N
1	B	345	TPO	OG1-CB-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	345	TPO	1	0
1	B	345	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	6QZ	A	501	-	37,38,38	1.03	1 (2%)	42,55,55	1.18	3 (7%)
3	SO4	B	501	-	4,4,4	0.28	0	6,6,6	0.14	0
2	6QZ	B	502	-	37,38,38	0.79	1 (2%)	42,55,55	1.30	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6QZ	A	501	-	-	0/10/55/55	0/6/6/6
3	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	6QZ	B	502	-	-	0/10/55/55	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	6QZ	C18-C17	3.25	1.44	1.40
2	A	501	6QZ	C18-C17	5.09	1.46	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	501	6QZ	C24-C20-C18	-2.17	108.38	112.39
2	A	501	6QZ	C9-C8-N1	2.30	119.14	112.61
2	B	502	6QZ	C13-C8-N1	2.44	119.56	112.61
2	B	502	6QZ	C7-C3-C4	3.13	118.32	111.33
2	A	501	6QZ	C6-C5-C4	5.44	118.46	109.91

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 [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	272/301 (90%)	0.97	40 (14%) 3   4	44, 77, 148, 170	0
1	B	271/301 (90%)	0.84	27 (9%) 8   11	47, 79, 123, 156	0
All	All	543/602 (90%)	0.90	67 (12%) 5   7	44, 78, 142, 170	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	ASN	8.7
1	A	171	TYR	8.0
1	A	197	PHE	6.3
1	A	239	LYS	6.0
1	A	236	VAL	5.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	B	346	10/11	0.71	0.24	-	147,158,168,170	0
1	TPO	A	345	11/12	0.86	0.17	-	117,124,130,133	0
1	SEP	A	346	10/11	0.80	0.26	-	130,137,150,151	0
1	TPO	B	345	11/12	0.77	0.20	-	134,143,148,151	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	501	5/5	0.83	0.21	0.81	121,121,123,125	0
2	6QZ	B	502	33/33	0.95	0.17	-0.25	40,52,58,59	0
2	6QZ	A	501	33/33	0.90	0.16	-0.49	54,63,81,84	0

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

There are no such residues in this entry.