



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:14 am GMT

PDB ID : 4Z7H  
Title : Crystal structure of human IRE1 cytoplasmic kinase-RNase region - complex with imidazopyridine compound 3  
Authors : Joshi, A.; Bayliss, R.  
Deposited on : 2015-04-07  
Resolution : 2.90 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 : trunk28620  
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) : recalc28949

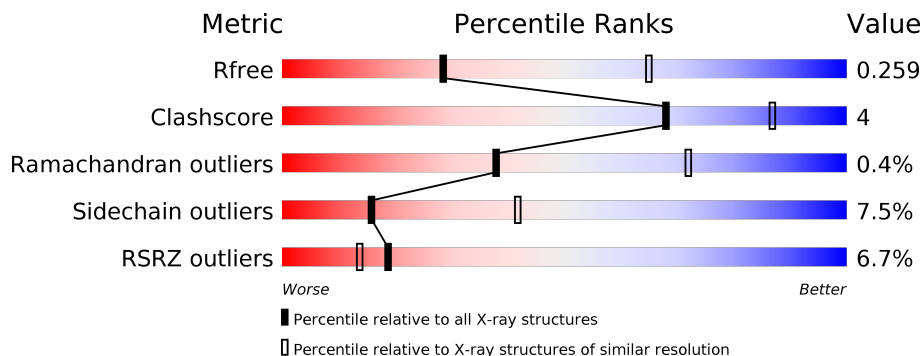
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	416	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	B	416	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	4L5	B	1001	-	-	-	X

## 2 Entry composition [i](#)

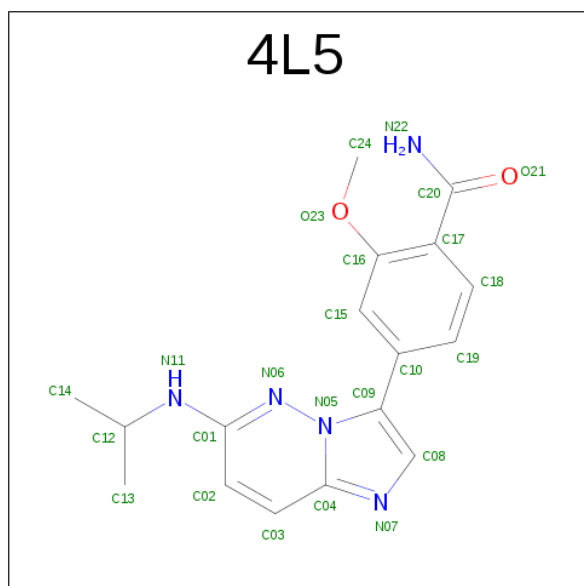
There are 4 unique types of molecules in this entry. The entry contains 6298 atoms, of which 38 are hydrogens and 0 are deuteriums.

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 Serine/threonine-protein kinase/endoribonuclease IRE1.

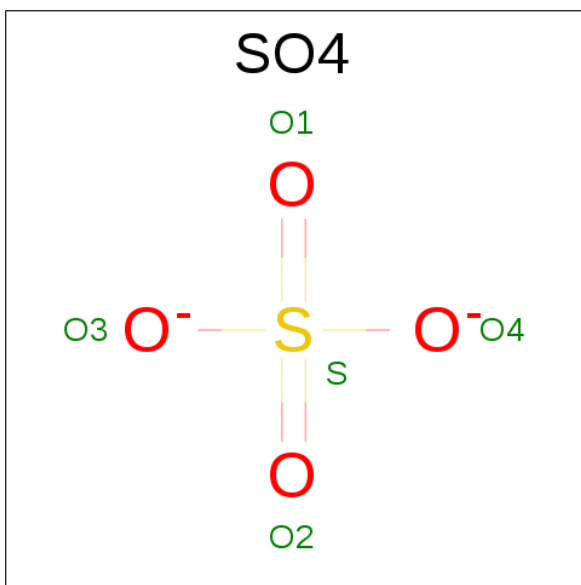
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3072	1962	536	555	19			
1	B	388	Total	C	N	O	S	0	0	0
			3114	1991	546	558	19			

- Molecule 2 is 2-methoxy-4-[6-(propan-2-ylamino)imidazo[1,2-b]pyridazin-3-yl]benzamide (three-letter code: 4L5) (formula: C<sub>17</sub>H<sub>19</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			43	17	19	5	2		
2	B	1	Total	C	H	N	O	0	0
			43	17	19	5	2		

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	9	Total	O	0	0
			9	9		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.68Å 81.96Å 168.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 2.90 46.36 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.36-2.90) 99.6 (46.36-2.90)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.200 , 0.225 0.225 , 0.259	Depositor DCC
$R_{free}$ test set	1259 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 72.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.041 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6298	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	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 27.84 % 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 2.0486e-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: SO4, 4L5

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	0/3145	0.69	0/4247
1	B	0.50	0/3189	0.71	1/4307 (0.0%)
All	All	0.49	0/6334	0.70	1/8554 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	890	ARG	C-N-CA	5.13	134.52	121.70

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	3072	0	3026	26	0
1	B	3114	0	3086	26	0
2	A	24	19	19	1	0
2	B	24	19	19	3	0
3	A	5	0	0	0	0
4	A	12	0	0	0	0
4	B	9	0	0	0	0
All	All	6260	38	6150	55	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 55 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:584:THR:HG22	1:B:601:ILE:HA	1.72	0.72
1:B:577:LEU:HB2	1:B:586:VAL:HG23	1.76	0.67
1:B:658:PHE:O	1:B:661:LEU:HB2	1.95	0.66
1:A:658:PHE:O	1:A:661:LEU:HB2	1.97	0.65
1:A:626:ILE:HD12	1:A:695:LEU:HD12	1.77	0.65

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	377/416 (91%)	346 (92%)	30 (8%)	1 (0%)	44	77
1	B	382/416 (92%)	349 (91%)	31 (8%)	2 (0%)	32	68
All	All	759/832 (91%)	695 (92%)	61 (8%)	3 (0%)	38	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	867	ARG
1	B	867	ARG
1	B	866	GLY

### 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	333/369 (90%)	311 (93%)	22 (7%)	19	49
1	B	338/369 (92%)	310 (92%)	28 (8%)	13	36
All	All	671/738 (91%)	621 (92%)	50 (8%)	16	42

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	585	ILE
1	B	709	ILE
1	B	907	LYS
1	B	590	MET
1	B	657	ASP

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	693	ASN
1	A	909	HIS
1	A	910	HIS
1	B	678	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	4L5	A	1001	-	23,26,26	2.22	8 (34%)	29,37,37	1.98	10 (34%)
3	SO4	A	1002	-	4,4,4	0.24	0	6,6,6	0.19	0
2	4L5	B	1001	-	23,26,26	2.19	8 (34%)	29,37,37	1.57	7 (24%)

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	4L5	A	1001	-	-	0/14/14/14	0/3/3/3
3	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	4L5	B	1001	-	-	0/14/14/14	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	4L5	C17-C20	2.13	1.52	1.50
2	A	1001	4L5	C17-C20	2.15	1.53	1.50
2	B	1001	4L5	C01-N11	2.61	1.41	1.36
2	B	1001	4L5	O23-C16	2.70	1.41	1.37
2	A	1001	4L5	O23-C16	3.04	1.41	1.37

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	4L5	C16-C17-C20	-4.36	121.81	125.04
2	B	1001	4L5	O21-C20-N22	-3.50	117.61	122.58
2	A	1001	4L5	O21-C20-N22	-3.49	117.62	122.58
2	A	1001	4L5	O23-C16-C15	-2.87	119.33	124.17
2	B	1001	4L5	O23-C16-C15	-2.62	119.76	124.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	4L5	1	0
2	B	1001	4L5	3	0

## 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	385/416 (92%)	0.55	34 (8%) 11 7	40, 79, 154, 179	0
1	B	388/416 (93%)	0.39	18 (4%) 33 28	41, 78, 138, 169	0
All	All	773/832 (92%)	0.47	52 (6%) 19 14	40, 79, 146, 179	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	855	ASP	6.3
1	B	731	VAL	6.3
1	B	581	ALA	6.2
1	A	581	ALA	5.6
1	A	884	THR	4.9

### 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](#)

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( $\text{\AA}^2$ )	Q<0.9
2	4L5	B	1001	24/24	0.96	0.31	2.63	68,77,94,94	0
2	4L5	A	1001	24/24	0.97	0.26	0.81	55,61,69,70	0
3	SO4	A	1002	5/5	0.85	0.16	-	128,128,129,130	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.