



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 03:35 AM EDT

PDB ID : 6URC
Title : Crystal structure of IRE1a in complex with compound 18
Authors : Wallweber, H.H.; Wang, W.
Deposited on : 2019-10-23
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7116 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	400	Total	C	N	O	S	0	0	0
			3226	2053	570	583	20			
1	B	398	Total	C	N	O	S	0	0	0
			3211	2043	568	580	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	978	GLY	-	expression tag	UNP O75460
A	979	ASN	-	expression tag	UNP O75460
A	980	SER	-	expression tag	UNP O75460
B	978	GLY	-	expression tag	UNP O75460
B	979	ASN	-	expression tag	UNP O75460
B	980	SER	-	expression tag	UNP O75460

- Molecule 2 is 2-chloro-N-(6-methyl-5-{[3-(2-{{(3S)-piperidin-3-yl}amino}pyrimidin-4-yl)pyridin-2-yl]oxy}naphthalen-1-yl)benzene-1-sulfonamide (three-letter code: QFV) (formula: C₃₁H₂₉ClN₆O₃S) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	297	Total 297	O 297	0	0
4	B	292	Total 292	O 292	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.12Å 84.66Å 175.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.10 – 2.20	Depositor
% Data completeness (in resolution range)	99.7 (44.10-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.274	Depositor
Wilson B-factor (Å ²)	19.0	Xtrriage
Anisotropy	0.173	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7116	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 56.19 % 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 2.8380e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 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
3	GOL	A	1002	-	5,5,5	0.29	0	5,5,5	0.38	0
2	QFV	A	1001	-	46,47,47	0.81	2 (4%)	61,67,67	1.94	13 (21%)
2	QFV	B	1001	-	46,47,47	0.80	1 (2%)	61,67,67	1.95	14 (22%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1002	-	-	2/4/4/4	-
2	QFV	A	1001	-	-	7/23/31/31	0/6/6/6
2	QFV	B	1001	-	-	8/23/31/31	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	QFV	C19-N21	2.55	1.37	1.34
2	A	1001	QFV	C19-N21	2.42	1.37	1.34
2	A	1001	QFV	C19-N18	-2.02	1.31	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	QFV	C17-N18-C19	5.79	120.58	115.45
2	B	1001	QFV	C17-N18-C19	5.68	120.49	115.45
2	A	1001	QFV	C15-N20-C19	5.67	121.36	116.69
2	B	1001	QFV	C7-O8-C9	5.34	122.36	116.88
2	A	1001	QFV	C7-O8-C9	5.23	122.24	116.88
2	B	1001	QFV	C15-N20-C19	5.18	120.96	116.69
2	A	1001	QFV	N18-C19-N20	-4.71	122.08	126.55
2	B	1001	QFV	N18-C19-N20	-4.49	122.30	126.55
2	B	1001	QFV	O8-C9-C10	4.24	120.83	116.61
2	A	1001	QFV	O8-C9-C10	3.92	120.51	116.61
2	A	1001	QFV	C16-C17-N18	-3.83	119.20	123.96
2	B	1001	QFV	C16-C17-N18	-3.82	119.22	123.96
2	B	1001	QFV	C16-C15-N20	-3.29	117.70	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	QFV	C16-C15-N20	-3.27	117.73	121.97
2	B	1001	QFV	C42-C37-S34	-2.76	121.44	123.25
2	A	1001	QFV	C13-N14-C9	2.59	122.62	116.43
2	B	1001	QFV	O8-C7-C2	2.56	123.93	118.35
2	B	1001	QFV	C13-N14-C9	2.55	122.52	116.43
2	B	1001	QFV	C1-C2-C7	2.48	123.18	120.52
2	A	1001	QFV	C2-C7-C6	-2.31	119.51	122.48
2	A	1001	QFV	C24-C22-N21	-2.27	107.06	110.60
2	B	1001	QFV	C17-C16-C15	2.24	119.33	117.22
2	A	1001	QFV	O8-C7-C2	2.23	123.21	118.35
2	A	1001	QFV	C12-C13-N14	-2.14	119.93	123.43
2	A	1001	QFV	C1-C2-C7	2.12	122.80	120.52
2	B	1001	QFV	C2-C7-C6	-2.06	119.83	122.48
2	B	1001	QFV	C19-N21-C22	-2.04	120.87	124.31

There are no chirality outliers.

All (17) torsion outliers are listed below:

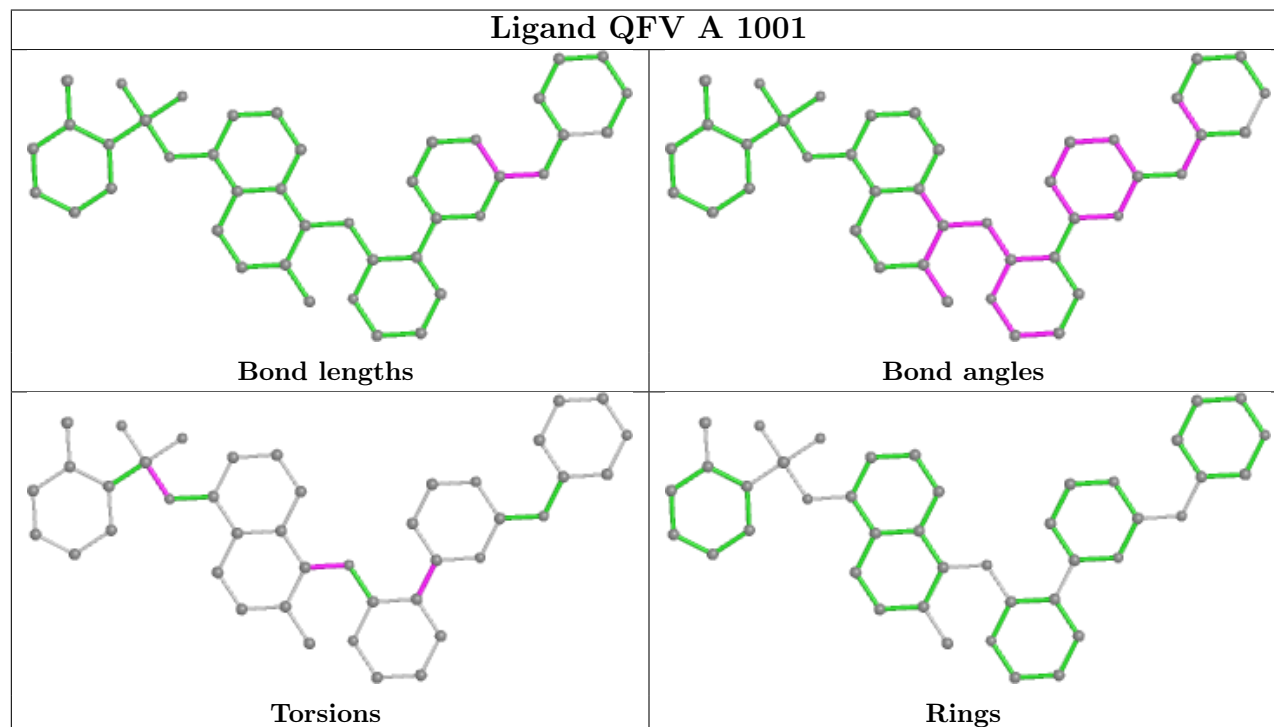
Mol	Chain	Res	Type	Atoms
2	B	1001	QFV	C5-C32-N33-S34
2	B	1001	QFV	C31-C32-N33-S34
3	A	1002	GOL	C1-C2-C3-O3
3	A	1002	GOL	O2-C2-C3-O3
2	B	1001	QFV	C32-N33-S34-O36
2	B	1001	QFV	C32-N33-S34-O35
2	A	1001	QFV	C32-N33-S34-O36
2	A	1001	QFV	C6-C7-O8-C9
2	B	1001	QFV	C32-N33-S34-C37
2	A	1001	QFV	C11-C10-C15-N20
2	B	1001	QFV	C11-C10-C15-N20
2	A	1001	QFV	C11-C10-C15-C16
2	A	1001	QFV	C32-N33-S34-O35
2	B	1001	QFV	C11-C10-C15-C16
2	B	1001	QFV	C6-C7-O8-C9
2	A	1001	QFV	C9-C10-C15-C16
2	A	1001	QFV	C32-N33-S34-C37

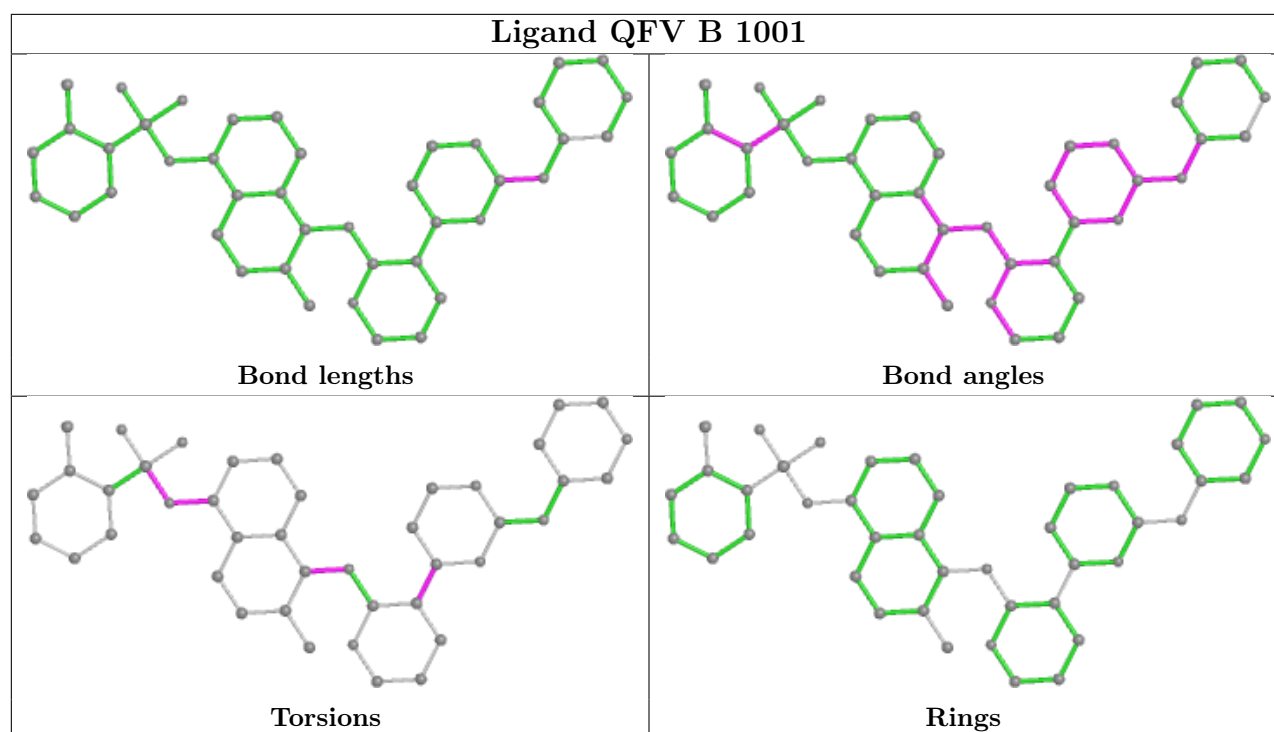
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.