



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:31 AM UTC

PDB ID : 9I64 / pdb\_00009i64  
Title : Crystal structure of Casdatifan bound to HIF2a-B\*:ARNT-B\* complex  
Authors : Walker, N.P.; Lawson, K.V.  
Deposited on : 2025-01-29  
Resolution : 1.56 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](mailto: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	:	4-5-2 with Phenix2.0
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	2.0
EDS	:	NOT EXECUTED
Buster-report	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

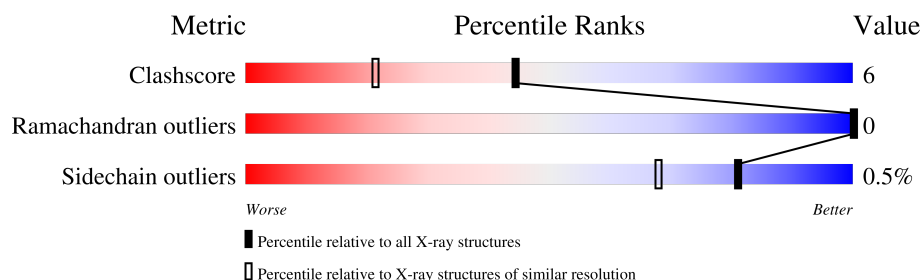
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.56 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))
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	112	 96% 5% 9%
2	B	116	 84% 5% 9%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2129 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 Endothelial PAS domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	19	3	0
			914	575	154	175	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	SER	-	expression tag	UNP Q99814
A	247	GLU	ARG	conflict	UNP Q99814

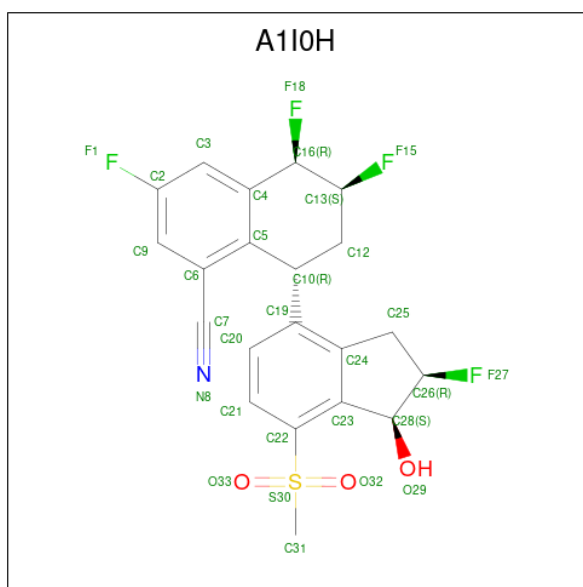
- Molecule 2 is a protein called Aryl hydrocarbon receptor nuclear translocator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	105	Total	C	N	O	S	18	11	0
			977	618	175	178	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	362	ARG	GLU	conflict	UNP P27540

- Molecule 3 is (5 {R},6 {S},8 {R})-3,5,6-tris(fluoranyl)-8-[(1 {S},2 {R})-2-fluoranyl-7-methylsulfonyl-1-oxidanyl-2,3-dihydro-1 {H}-inden-4-yl]-5,6,7,8-tetrahydronaphthalene-1-carbonitrile (CCD ID: A1I0H) (formula: C<sub>21</sub>H<sub>17</sub>F<sub>4</sub>NO<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	
			30	21	4	1	3	1	

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total 113	O 113	0	1
6	B	90	Total 91	O 91	0	1

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.


Note EDS was not executed.

- Molecule 1: Endothelial PAS domain-containing protein 1

Chain A:  96% . .



- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

Chain B:  84% 5% . 9%



## 4 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.69Å 61.15Å 91.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.70 – 1.56	Depositor
% Data completeness (in resolution range)	99.5 (45.70-1.56)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.191 , 0.214	Depositor
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.171	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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, 0.333 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: A1I0H, FMT, MG

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	0.46	0/934	0.83	1/1260 (0.1%)
2	B	0.46	0/999	0.81	2/1348 (0.1%)
All	All	0.46	0/1933	0.82	3/2608 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ASP	CA-CB-CG	7.53	120.13	112.60
2	B	377	ASP	CA-CB-CG	5.67	118.27	112.60
2	B	377	ASP	CB-CA-C	5.23	118.59	109.65

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	914	0	877	7	0
2	B	977	0	944	22	0
3	A	30	0	0	0	0
4	A	3	0	1	0	0
5	B	1	0	0	0	0
6	A	113	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	91	0	0	2	0
All	All	2129	0	1822	22	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 6.

All (22) 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)
2:B:440[B]:ARG:NH1	6:B:603[B]:HOH:O	1.80	1.09
2:B:362[B]:ARG:HB3	2:B:462[B]:THR:HG22	1.36	1.01
1:A:338[B]:MET:CE	2:B:460[B]:THR:HG22	1.93	0.98
1:A:338[B]:MET:HE2	2:B:460[B]:THR:CG2	1.98	0.94
2:B:440[A]:ARG:NH1	6:B:603[A]:HOH:O	1.94	0.88
2:B:421[B]:GLN:HE21	2:B:421[B]:GLN:H	1.20	0.86
1:A:338[B]:MET:HE2	2:B:460[B]:THR:HG22	1.58	0.78
2:B:362[B]:ARG:CB	2:B:462[B]:THR:HG22	2.15	0.77
1:A:338[B]:MET:CE	2:B:460[B]:THR:CG2	2.61	0.76
2:B:362[B]:ARG:CZ	2:B:462[B]:THR:HG21	2.16	0.75
2:B:362[B]:ARG:NE	2:B:462[B]:THR:CG2	2.50	0.74
1:A:338[B]:MET:HE1	2:B:460[B]:THR:HG22	1.73	0.70
2:B:362[B]:ARG:NH2	2:B:462[B]:THR:HG21	2.06	0.70
2:B:421[B]:GLN:HE21	2:B:421[B]:GLN:N	1.95	0.64
2:B:362[B]:ARG:CZ	2:B:462[B]:THR:CG2	2.82	0.58
2:B:362[B]:ARG:HB3	2:B:462[B]:THR:CG2	2.24	0.57
1:A:338[B]:MET:HE2	2:B:460[B]:THR:HG21	1.85	0.56
2:B:362[B]:ARG:CB	2:B:462[B]:THR:CG2	2.85	0.55
2:B:421[B]:GLN:H	2:B:421[B]:GLN:NE2	1.99	0.47
2:B:362[B]:ARG:NE	2:B:462[B]:THR:HG22	2.27	0.47
1:A:338[B]:MET:HE1	2:B:364:ILE:HG12	1.97	0.46
2:B:362[B]:ARG:HE	2:B:462[B]:THR:HG22	1.82	0.44

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	111/112 (99%)	108 (97%)	3 (3%)	0	100	100
2	B	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
All	All	225/228 (99%)	220 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	103/102 (101%)	103 (100%)	0	100	100
2	B	111/111 (100%)	110 (99%)	1 (1%)	70	51
All	All	214/213 (100%)	213 (100%)	1 (0%)	81	68

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	377	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	313	HIS
2	B	378	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

Mogul was not executed - this section is therefore empty.

## 5.5 Carbohydrates [i](#)

Mogul was not executed - this section is therefore empty.

## 5.6 Ligand geometry [i](#)

Mogul was not executed - this section is therefore empty.

## 5.7 Other polymers [i](#)

Mogul was not executed - this section is therefore empty.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

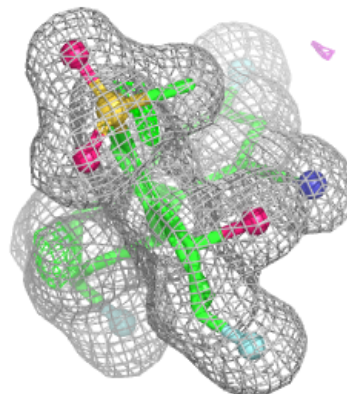
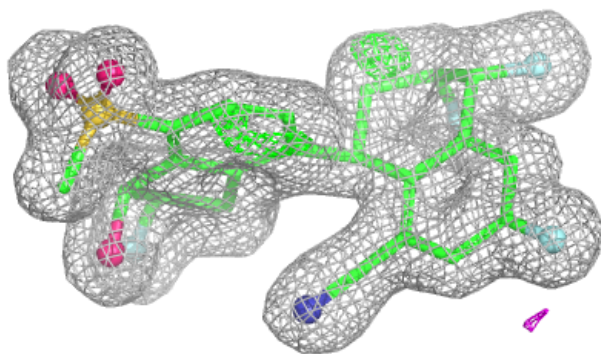
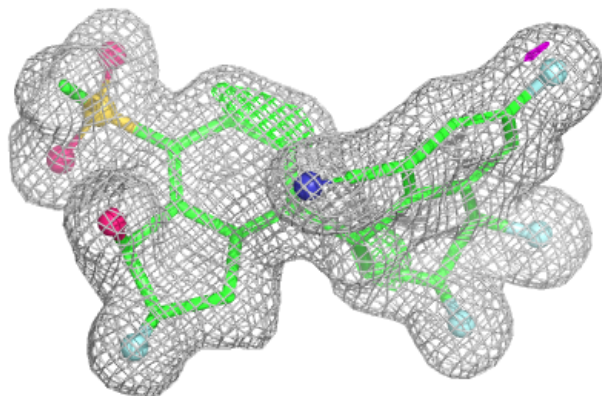
### 6.4 Ligands

EDS was not executed - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around A1I0H A 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.