



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:22 am BST

PDB ID : 6NMQ  
Title : Hypoxia-Inducible Factor (HIF) Prolyl Hydroxylase 2 (PHD2) in Complex with the Carboxamide Analog JNJ43058171  
Authors : Bembenek, S.D.; Mirzadegan, T.  
Deposited on : 2019-01-11  
Resolution : 1.58 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

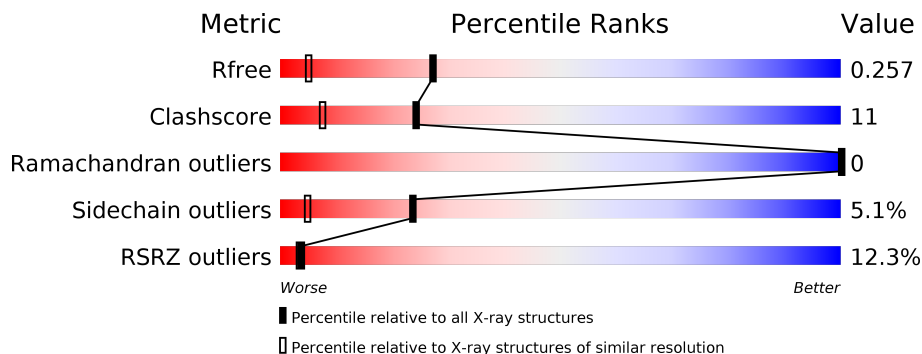
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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))
$R_{free}$	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 on 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  $\leq 5\%$ . 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	213	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1702 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.

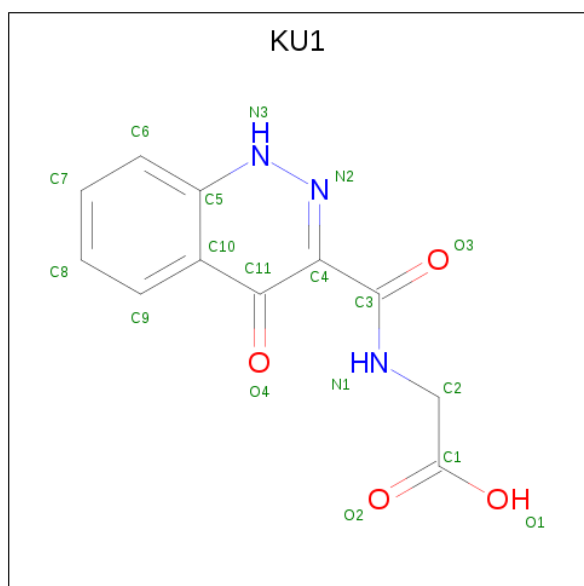
- Molecule 1 is a protein called Egl nine homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	187	1512	963	260	277	12	0	5	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is N-(4-oxo-1,4-dihydrocinnoline-3-carbonyl)glycine (three-letter code: KU1) (formula: C<sub>11</sub>H<sub>9</sub>N<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	11	3	4		

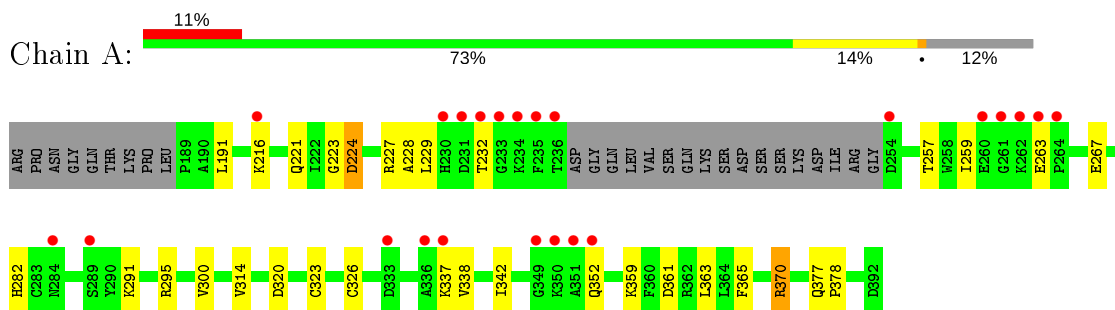
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	171	Total 171	O 171	0	0

### 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 the various outlier classes 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: Egl nine homolog 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.10Å 91.10Å 169.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 1.58 35.76 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-1.58) 99.9 (35.76-1.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.58Å)	Xtrriage
Refinement program	REFMAC 5.5.0104	Depositor
R, $R_{free}$	0.222 , 0.260 0.224 , 0.257	Depositor DCC
$R_{free}$ test set	1862 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: FE2, KU1

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	1.01	1/1564 (0.1%)	1.02	4/2113 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	CYS	CB-SG	-10.48	1.64	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	361	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	361	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	295	ARG	NE-CZ-NH2	-5.37	117.61	120.30

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	1512	0	1482	33	1
2	A	1	0	0	0	0
3	A	18	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	171	0	0	9	0
All	All	1702	0	1482	33	1

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 11.

All (33) 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:A:224:ASP:HB2	4:A:502:HOH:O	1.55	1.05
1:A:224:ASP:CB	4:A:502:HOH:O	2.10	0.98
1:A:370[B]:ARG:CG	1:A:370[B]:ARG:HH21	1.81	0.94
1:A:314:VAL:HG11	1:A:370[B]:ARG:HD3	1.49	0.94
1:A:320:ASP:O	4:A:501:HOH:O	1.88	0.90
1:A:370[B]:ARG:HG3	1:A:370[B]:ARG:HH21	1.39	0.85
1:A:224:ASP:OD2	4:A:502:HOH:O	1.99	0.79
1:A:370[B]:ARG:HG3	1:A:370[B]:ARG:NH2	1.97	0.78
1:A:267:GLU:OE1	4:A:503:HOH:O	2.02	0.78
1:A:263[A]:GLU:OE1	4:A:504:HOH:O	2.02	0.76
1:A:370[B]:ARG:HG2	4:A:616:HOH:O	1.93	0.69
1:A:314:VAL:HG21	1:A:370[B]:ARG:CD	2.27	0.65
1:A:326[B]:CYS:SG	1:A:365:PHE:CD2	2.91	0.63
1:A:377[A]:GLN:HA	1:A:377[A]:GLN:NE2	2.17	0.60
1:A:359:LYS:HB3	1:A:359:LYS:NZ	2.16	0.60
1:A:224:ASP:OD1	1:A:227:ARG:NH2	2.30	0.59
1:A:314:VAL:HG21	1:A:370[B]:ARG:HD2	1.84	0.59
1:A:326[B]:CYS:SG	1:A:365:PHE:CE2	2.97	0.58
1:A:370[B]:ARG:HG2	1:A:370[B]:ARG:HH21	1.67	0.58
1:A:228:ALA:O	1:A:232:THR:HG23	2.04	0.57
1:A:314:VAL:CG1	1:A:370[B]:ARG:HD3	2.29	0.56
1:A:229:LEU:HD11	1:A:259:ILE:HD11	1.88	0.55
1:A:377[A]:GLN:HA	1:A:377[A]:GLN:HE21	1.71	0.55
1:A:314:VAL:HG21	1:A:370[B]:ARG:HD3	1.90	0.54
1:A:221:GLN:NE2	4:A:503:HOH:O	2.38	0.52
1:A:359:LYS:NZ	1:A:359:LYS:CB	2.73	0.51
1:A:191:LEU:HD13	1:A:282:HIS:CD2	2.46	0.50
1:A:359:LYS:HB3	1:A:359:LYS:HZ3	1.76	0.49
1:A:223:GLY:HA3	4:A:589:HOH:O	2.13	0.48
1:A:229:LEU:CD1	1:A:259:ILE:HD11	2.47	0.44
1:A:326[A]:CYS:SG	1:A:363:LEU:HD11	2.57	0.44
1:A:314:VAL:HG21	1:A:370[A]:ARG:HG2	2.01	0.43

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:THR:HG22	1:A:300:VAL:HB	2.00	0.43

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASP:OD2	1:A:224:ASP:OD2[12_555]	2.01	0.19

### 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	188/213 (88%)	184 (98%)	4 (2%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

#### 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	162/180 (90%)	153 (94%)	9 (6%)	<a href="#">21</a> <a href="#">4</a>

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	291	LYS
1	A	337	LYS
1	A	338	VAL
1	A	342	ILE
1	A	352	GLN
1	A	370[A]	ARG
1	A	370[B]	ARG
1	A	378	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	KU1	A	402	2	14,19,19	1.64	2 (14%)	19,26,26	3.01	7 (36%)

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
3	KU1	A	402	2	-	4/7/9/9	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	KU1	C4-C3	-4.94	1.43	1.50
3	A	402	KU1	C7-C6	2.37	1.42	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	KU1	C4-C11-C10	-8.43	112.10	120.95
3	A	402	KU1	C4-C3-N1	6.15	121.71	115.60
3	A	402	KU1	O3-C3-C4	-4.47	114.02	120.68
3	A	402	KU1	C4-N2-N3	3.94	124.73	120.43
3	A	402	KU1	C9-C10-C11	2.73	122.38	119.19
3	A	402	KU1	C8-C7-C6	-2.35	117.15	120.44
3	A	402	KU1	C7-C8-C9	2.25	123.60	120.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	KU1	O3-C3-C4-N2
3	A	402	KU1	N1-C3-C4-C11
3	A	402	KU1	N1-C3-C4-N2
3	A	402	KU1	O3-C3-C4-C11

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	187/213 (87%)	0.60	23 (12%) <b>4</b> <b>3</b>	10, 18, 39, 63	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	GLY	10.2
1	A	351	ALA	7.7
1	A	235	PHE	5.9
1	A	231	ASP	5.1
1	A	236	THR	5.1
1	A	234	LYS	4.8
1	A	262	LYS	4.4
1	A	260	GLU	3.5
1	A	264	PRO	3.2
1	A	232	THR	3.2
1	A	230	HIS	3.1
1	A	350	LYS	2.6
1	A	336	ALA	2.6
1	A	349	GLY	2.6
1	A	337	LYS	2.6
1	A	216	LYS	2.5
1	A	254	ASP	2.4
1	A	261	GLY	2.3
1	A	352	GLN	2.3
1	A	289	SER	2.3
1	A	333	ASP	2.2
1	A	284	ASN	2.2
1	A	263[A]	GLU	2.0

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	KU1	A	402	18/18	0.94	0.09	12,19,21,22	0
2	FE2	A	401	1/1	1.00	0.10	9,9,9,9	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.