



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:32 AM GMT

PDB ID : 3F1P  
Title : Crystal structure of a high affinity heterodimer of HIF2 alpha and ARNT C-terminal PAS domains  
Authors : Scheuermann, T.H.; Tomchick, D.R.; Machius, M.; Guo, Y.; Bruick, R.K.; Gardner, K.H.  
Deposited on : 2008-10-28  
Resolution : 1.17 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

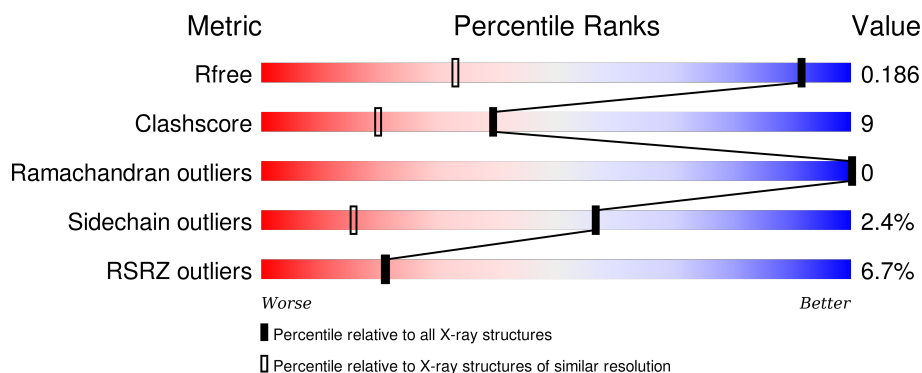
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.17 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))
$R_{free}$	91344	1018 (1.22-1.14)
Clashscore	102246	1094 (1.22-1.14)
Ramachandran outliers	100387	1047 (1.22-1.14)
Sidechain outliers	100360	1046 (1.22-1.14)
RSRZ outliers	91569	1020 (1.22-1.14)

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	117	<div> <div>8%</div> <div>79%</div> <div>15%</div> <div>• • •</div> </div>
2	B	121	<div> <div>5%</div> <div>79%</div> <div>12%</div> <div>• 8%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4275 atoms, of which 1974 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	114	Total	C	H	N	O	S	0	18	0
			1983	637	973	168	194	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	GLY	-	EXPRESSION TAG	UNP Q99814
A	235	GLU	-	EXPRESSION TAG	UNP Q99814
A	236	PHE	-	EXPRESSION TAG	UNP Q99814
A	237	LYS	-	EXPRESSION TAG	UNP Q99814
A	238	GLY	-	EXPRESSION TAG	UNP Q99814
A	247	GLU	ARG	ENGINEERED	UNP Q99814

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	111	Total	C	H	N	O	S	0	23	0
			2029	647	1001	179	194	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	350	GLY	-	EXPRESSION TAG	UNP P27540
B	351	GLU	-	EXPRESSION TAG	UNP P27540
B	352	PHE	-	EXPRESSION TAG	UNP P27540
B	353	LYS	-	EXPRESSION TAG	UNP P27540
B	354	GLY	-	EXPRESSION TAG	UNP P27540
B	355	LEU	-	EXPRESSION TAG	UNP P27540
B	362	ARG	GLU	ENGINEERED	UNP P27540

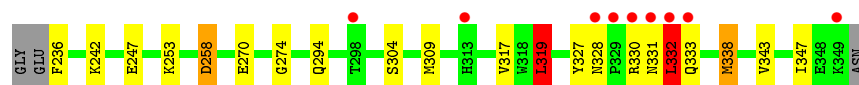
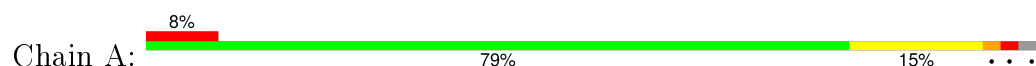
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total 127	O 127	0	2
3	B	132	Total 136	O 136	0	4

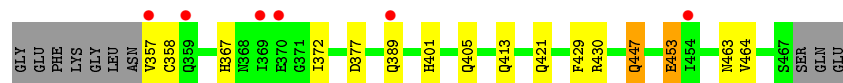
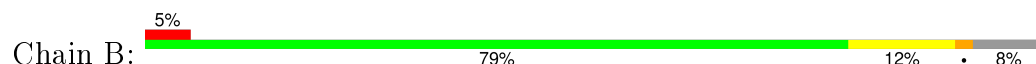
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Endothelial PAS domain-containing protein 1



- Molecule 2: Aryl hydrocarbon receptor nuclear translocator



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.92Å 82.56Å 41.03Å 90.00° 106.02° 90.00°	Depositor
Resolution (Å)	26.93 – 1.17 26.93 – 1.17	Depositor EDS
% Data completeness (in resolution range)	95.1 (26.93-1.17) 95.1 (26.93-1.17)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.17Å)	Xtriage
Refinement program	PHENIX 1.3	Depositor
R, $R_{free}$	0.141 , 0.167 0.165 , 0.186	Depositor DCC
$R_{free}$ test set	1520 reflections (2.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.2	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 75657 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4275	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	1.03	0/1126	1.11	6/1519 (0.4%)
2	B	1.01	4/1157 (0.3%)	1.02	7/1561 (0.4%)
All	All	1.02	4/2283 (0.2%)	1.07	13/3080 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	421	GLN	CG-CD	5.56	1.63	1.51
2	B	463	ASN	CB-CG	5.30	1.63	1.51
2	B	453[A]	GLU	CD-OE2	5.07	1.31	1.25
2	B	453[B]	GLU	CD-OE2	5.07	1.31	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	LEU	CB-CG-CD2	13.20	133.44	111.00
1	A	258	ASP	CB-CG-OD1	-11.07	108.34	118.30
1	A	332	LEU	CA-CB-CG	10.62	139.73	115.30
2	B	430	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	258	ASP	CB-CG-OD2	6.90	124.51	118.30
2	B	377	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	319[A]	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	319[B]	LEU	CA-CB-CG	5.85	128.76	115.30
2	B	429	PHE	CB-CG-CD2	5.63	124.74	120.80
2	B	453[A]	GLU	OE1-CD-OE2	5.58	129.99	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	453[B]	GLU	OE1-CD-OE2	5.58	129.99	123.30
2	B	377	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	B	377	ASP	N-CA-CB	-5.06	101.49	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	327	TYR	Peptide

## 5.2 Too-close contacts

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	1010	973	914	26	15
2	B	1028	1001	902	9	0
3	A	127	0	0	4	0
3	B	136	0	0	11	0
All	All	2301	1974	1816	36	15

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 9.

All (36) 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:338[B]:MET:SD	3:B:163:HOH:O	2.16	1.04
1:A:338[C]:MET:CE	3:B:163:HOH:O	2.18	0.92
1:A:338[C]:MET:HE1	3:B:163:HOH:O	1.75	0.85
1:A:304[B]:SER:O	3:A:126:HOH:O	1.97	0.81
1:A:319[B]:LEU:CD1	1:A:343[B]:VAL:HG22	2.11	0.79
1:A:328:ASN:ND2	3:B:205:HOH:O	2.13	0.79
1:A:319[B]:LEU:HD11	1:A:343[B]:VAL:HG22	1.70	0.71
1:A:338[C]:MET:HE2	1:A:338[C]:MET:HA	1.74	0.70
1:A:317[B]:VAL:CG1	1:A:343[B]:VAL:HG13	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338[C]:MET:CE	1:A:338[C]:MET:HA	2.27	0.65
1:A:236:PHE:N	3:A:217:HOH:O	2.31	0.63
1:A:338[C]:MET:HE3	3:B:163:HOH:O	1.87	0.62
2:B:357:VAL:HG23	3:B:203:HOH:O	2.02	0.60
1:A:328:ASN:ND2	1:A:330:ARG:HH11	2.02	0.58
1:A:294:GLN:HG3	3:A:100:HOH:O	2.05	0.56
1:A:328:ASN:CG	3:B:205:HOH:O	2.42	0.54
2:B:447[B]:GLN:NE2	2:B:453[B]:GLU:O	2.35	0.54
1:A:270:GLU:HG2	3:A:204:HOH:O	2.09	0.52
1:A:338[C]:MET:CA	1:A:338[C]:MET:CE	2.88	0.52
1:A:317[B]:VAL:HG11	1:A:343[B]:VAL:HG13	1.94	0.49
2:B:401:HIS:O	2:B:405[B]:GLN:HG3	2.14	0.48
1:A:247:GLU:HG3	1:A:338[C]:MET:CE	2.45	0.47
2:B:357:VAL:HG22	2:B:358:CYS:N	2.30	0.46
2:B:357:VAL:CG2	3:B:203:HOH:O	2.62	0.46
1:A:309:MET:HB2	1:A:319[A]:LEU:HD11	1.97	0.45
1:A:253:LYS:HE3	1:A:274:GLY:O	2.17	0.45
1:A:328:ASN:OD1	1:A:330:ARG:HG3	2.17	0.43
1:A:242:LYS:HB3	1:A:343[A]:VAL:HG22	2.00	0.43
1:A:338[C]:MET:HB2	1:A:338[C]:MET:HE3	1.60	0.43
1:A:319[B]:LEU:HD11	1:A:343[B]:VAL:CG2	2.46	0.42
1:A:317[B]:VAL:HG23	1:A:347:ILE:HG12	2.03	0.41
2:B:389[A]:GLN:HG2	3:B:228:HOH:O	2.20	0.40
2:B:367:HIS:HA	2:B:372:ILE:O	2.21	0.40
2:B:413:GLN:NE2	3:B:103:HOH:O	2.55	0.40

All (15) 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:332:LEU:N	1:A:332:LEU:CD2[2_556]	0.20	2.00
1:A:332:LEU:CA	1:A:332:LEU:CG[2_556]	0.24	1.96
1:A:332:LEU:C	1:A:332:LEU:CD1[2_556]	0.45	1.75
1:A:332:LEU:CD1	1:A:333:GLN:N[2_556]	0.88	1.32
1:A:332:LEU:C	1:A:332:LEU:CG[2_556]	1.34	0.86
1:A:332:LEU:CA	1:A:332:LEU:CD2[2_556]	1.38	0.82
1:A:331:ASN:C	1:A:332:LEU:CD2[2_556]	1.49	0.71
1:A:332:LEU:CD2	1:A:332:LEU:H[2_556]	0.90	0.70
1:A:332:LEU:O	1:A:332:LEU:CD1[2_556]	1.52	0.68
1:A:332:LEU:CG	1:A:332:LEU:HA[2_556]	0.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:CA	1:A:332:LEU:CB[2_556]	1.61	0.59
1:A:332:LEU:N	1:A:332:LEU:CG[2_556]	1.68	0.52
1:A:332:LEU:CA	1:A:332:LEU:CD1[2_556]	1.78	0.42
1:A:332:LEU:CD1	1:A:333:GLN:H[2_556]	1.53	0.07
1:A:332:LEU:O	1:A:332:LEU:CG[2_556]	2.19	0.01

## 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	134/117 (114%)	131 (98%)	3 (2%)	0	100	100
2	B	133/121 (110%)	133 (100%)	0	0	100	100
All	All	267/238 (112%)	264 (99%)	3 (1%)	0	100	100

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	124/105 (118%)	117 (94%)	7 (6%)	26	2
2	B	131/114 (115%)	128 (98%)	3 (2%)	58	18
All	All	255/219 (116%)	245 (96%)	10 (4%)	57	6

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	ASP
1	A	319[A]	LEU
1	A	319[B]	LEU
1	A	332	LEU
1	A	338[A]	MET
1	A	338[B]	MET
1	A	338[C]	MET
2	B	447[A]	GLN
2	B	447[B]	GLN
2	B	447[C]	GLN

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

Mol	Chain	Res	Type
1	A	294	GLN
2	B	413	GLN
2	B	434	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](#)

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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	114/117 (97%)	0.45	9 (7%)	15 15	9, 16, 30, 42	1 (0%)
2	B	111/121 (91%)	0.49	6 (5%)	29 28	9, 13, 25, 41	0
All	All	225/238 (94%)	0.47	15 (6%)	21 21	9, 15, 27, 42	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	LEU	9.3
2	B	357	VAL	9.1
1	A	349	LYS	5.6
1	A	333	GLN	4.3
1	A	329	PRO	4.0
1	A	330	ARG	3.6
2	B	369	ILE	3.4
1	A	331	ASN	3.1
2	B	454[A]	ILE	3.1
2	B	389[A]	GLN	3.0
1	A	328	ASN	2.8
2	B	359	GLN	2.8
1	A	313	HIS	2.7
1	A	298	THR	2.3
2	B	370	GLU	2.1

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.