



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2023 – 01:14 AM EDT

PDB ID : 6D0C
Title : Crystal structure of HIF2a-B*:ARNT-B* complex
Authors : Du, X.
Deposited on : 2018-04-10
Resolution : 1.50 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

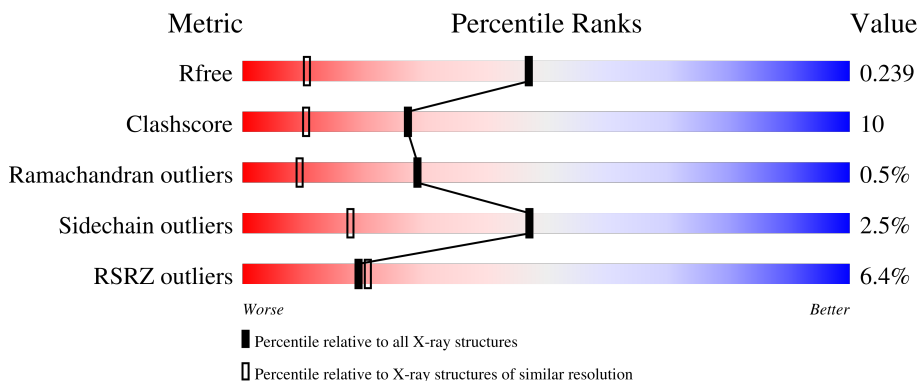
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 ≥ 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	117	 9% (red), 74% (green), 16% (yellow), 7% (grey)
2	B	121	 3% (red), 69% (green), 21% (yellow), 9% (grey)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1934 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
			Total	C	N	O	S			
1	A	109	889	566	144	170	9	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q99814
A	-1	GLU	-	expression tag	UNP Q99814
A	0	PHE	-	expression tag	UNP Q99814
A	1	LYS	-	expression tag	UNP Q99814
A	2	GLY	-	expression tag	UNP Q99814
A	247	GLU	ARG	engineered mutation	UNP Q99814

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	110	917	583	161	167	6	0	0	0

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 mutation	UNP P27540

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total 52	O 52	0	0
3	B	76	Total 76	O 76	0	0

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 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

Chain A: 



- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.60Å 82.83Å 41.32Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	24.88 – 1.50 24.88 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (24.88-1.50) 98.2 (24.88-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.240 0.204 , 0.239	Depositor DCC
R_{free} test set	1875 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1934	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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.

5 Model quality i

5.1 Standard geometry i

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	1.24	3/913 (0.3%)	1.29	7/1230 (0.6%)
2	B	1.28	2/939 (0.2%)	1.32	7/1269 (0.6%)
All	All	1.26	5/1852 (0.3%)	1.30	14/2499 (0.6%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	GLY	C-N	11.20	1.59	1.34
2	B	438	TRP	CD2-CE2	7.38	1.50	1.41
2	B	436	TRP	CD2-CE2	6.96	1.49	1.41
1	A	307	TYR	CE1-CZ	5.45	1.45	1.38
1	A	254	PHE	CG-CD2	5.35	1.46	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	409	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	A	2	GLY	O-C-N	-10.20	106.38	122.70
1	A	258	ASP	N-CA-CB	-9.28	93.90	110.60
1	A	258	ASP	CB-CG-OD2	-8.27	110.85	118.30
2	B	409	ARG	NE-CZ-NH2	-8.04	116.28	120.30
2	B	428	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	338	MET	CG-SD-CE	-7.01	88.98	100.20
1	A	319	LEU	CA-CB-CG	7.01	131.42	115.30
2	B	446	PHE	CB-CG-CD1	-6.80	116.04	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	439	MET	CG-SD-CE	-6.56	89.70	100.20
1	A	338	MET	CA-CB-CG	5.58	122.78	113.30
1	A	319	LEU	CB-CA-C	-5.24	100.24	110.20
2	B	409	ARG	CG-CD-NE	-5.23	100.81	111.80
2	B	379	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	GLY	Mainchain

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	889	0	852	20	0
2	B	917	0	891	17	0
3	A	52	0	0	5	0
3	B	76	0	0	12	0
All	All	1934	0	1743	36	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 10.

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:328:ASN:HB3	1:A:329:PRO:CD	1.67	1.22
1:A:328:ASN:CB	1:A:329:PRO:HD3	1.81	1.08
1:A:328:ASN:HB3	1:A:329:PRO:HD3	1.03	1.02
2:B:398:GLU:OE1	3:B:501:HOH:O	1.84	0.96
1:A:317:VAL:HG11	1:A:343:VAL:HG13	1.53	0.88
2:B:460:THR:HG22	3:B:503:HOH:O	1.83	0.78
2:B:428:ARG:HG2	3:B:558:HOH:O	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:CG1	1:A:343:VAL:HG13	2.19	0.73
1:A:342[B]:TYR:HE2	3:A:404:HOH:O	1.71	0.72
2:B:467:SER:C	3:B:565:HOH:O	2.30	0.69
2:B:378:HIS:HE1	3:B:529:HOH:O	1.81	0.63
1:A:270:GLU:HG3	3:A:448:HOH:O	2.02	0.58
1:A:317:VAL:HG11	1:A:343:VAL:CG1	2.29	0.58
2:B:440:ARG:NH1	3:B:505:HOH:O	2.38	0.56
2:B:366:ARG:HB3	2:B:375:PHE:HB3	1.86	0.56
1:A:346:GLU:HG2	3:A:436:HOH:O	2.05	0.56
2:B:392:LEU:HD11	3:B:559:HOH:O	2.07	0.54
1:A:319:LEU:CD2	1:A:343:VAL:HG22	2.37	0.54
1:A:328:ASN:HB2	1:A:335:GLN:NE2	2.22	0.53
2:B:410:ASP:OD2	3:B:502:HOH:O	2.19	0.53
1:A:342[B]:TYR:CE2	3:A:404:HOH:O	2.54	0.52
1:A:328:ASN:CG	1:A:329:PRO:HD3	2.29	0.52
1:A:270:GLU:CG	3:A:448:HOH:O	2.58	0.51
2:B:460:THR:CG2	3:B:503:HOH:O	2.51	0.51
1:A:294:GLN:O	1:A:298:THR:HG23	2.12	0.50
2:B:394:LYS:HD3	3:B:501:HOH:O	2.13	0.49
2:B:423:LEU:HD23	2:B:423:LEU:C	2.34	0.48
2:B:462:THR:OG1	3:B:503:HOH:O	2.20	0.48
1:A:328:ASN:CB	1:A:329:PRO:CD	2.48	0.47
1:A:1:LYS:NZ	1:A:263:GLU:OE2	2.41	0.46
1:A:326:ILE:HD12	1:A:336:CYS:SG	2.56	0.46
2:B:401:HIS:HB2	2:B:428:ARG:HB2	1.99	0.44
2:B:410:ASP:HB2	3:B:502:HOH:O	2.17	0.43
1:A:317:VAL:HG12	1:A:318:TRP:O	2.18	0.43
1:A:310:LEU:HD22	2:B:402:PRO:HB3	2.02	0.42
2:B:376:VAL:HG11	2:B:391:LEU:HD12	2.02	0.41

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	106/117 (91%)	103 (97%)	2 (2%)	1 (1%)	17	3
2	B	108/121 (89%)	108 (100%)	0	0	100	100
All	All	214/238 (90%)	211 (99%)	2 (1%)	1 (0%)	29	9

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ASN

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	99/105 (94%)	97 (98%)	2 (2%)	55	25
2	B	105/114 (92%)	102 (97%)	3 (3%)	42	13
All	All	204/219 (93%)	199 (98%)	5 (2%)	47	18

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	GLU
1	A	269	PRO
2	B	359	GLN
2	B	377	ASP
2	B	447	GLN

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	335	GLN
2	B	378	HIS
2	B	447	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 monosaccharides 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 [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, 95th 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 ²)	Q<0.9
1	A	109/117 (93%)	0.58	10 (9%) 9 9	12, 24, 40, 58	0
2	B	110/121 (90%)	0.22	4 (3%) 42 47	13, 19, 31, 50	0
All	All	219/238 (92%)	0.40	14 (6%) 19 20	12, 21, 39, 58	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	ILE	4.2
1	A	298	THR	3.8
1	A	342[A]	TYR	3.3
2	B	359	GLN	3.1
1	A	0	PHE	3.0
1	A	335	GLN	3.0
2	B	358	CYS	2.9
1	A	328	ASN	2.9
1	A	313	HIS	2.8
2	B	454	ILE	2.7
1	A	329	PRO	2.6
1	A	346	GLU	2.6
2	B	369	ILE	2.4
1	A	334	PRO	2.2

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.