



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4LPZ  
Title : ARNT transcription factor/coactivator complex  
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Deposited on : 2013-07-16  
Resolution : 3.15 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

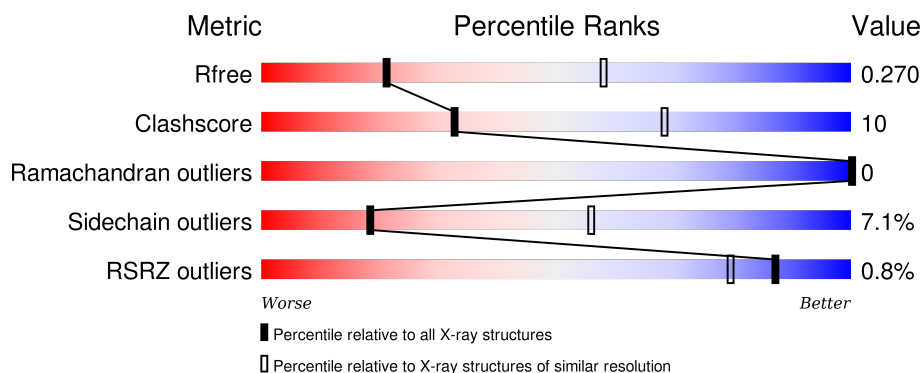
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	119	<div> <div>2%</div> <div>55%</div> <div>21%</div> <div>•</div> <div>19%</div> </div>
1	B	119	<div> <div>57%</div> <div>24%</div> <div>•</div> <div>18%</div> </div>
2	C	44	<div> <div>66%</div> <div>5%</div> <div>30%</div> </div>
2	D	44	<div> <div>52%</div> <div>14%</div> <div>5%</div> <div>30%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2108 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 Aryl hydrocarbon receptor nuclear translocator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	96	Total	C	N	O	S	0	0	0
			803	515	139	144	5			
1	B	97	Total	C	N	O	S	0	0	0
			811	521	140	145	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	GLY	-	EXPRESSION TAG	UNP P27540
A	353	ALA	-	EXPRESSION TAG	UNP P27540
A	354	MET	-	EXPRESSION TAG	UNP P27540
A	355	ASP	-	EXPRESSION TAG	UNP P27540
B	352	GLY	-	EXPRESSION TAG	UNP P27540
B	353	ALA	-	EXPRESSION TAG	UNP P27540
B	354	MET	-	EXPRESSION TAG	UNP P27540
B	355	ASP	-	EXPRESSION TAG	UNP P27540

- Molecule 2 is a protein called Transforming acidic coiled-coil-containing protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	31	Total	C	N	O	S	0	0	0
			249	156	44	48	1			
2	D	31	Total	C	N	O	S	0	0	0
			245	153	42	49	1			



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.85Å 59.82Å 73.51Å 90.00° 97.85° 90.00°	Depositor
Resolution (Å)	44.27 – 3.15 44.27 – 3.15	Depositor EDS
% Data completeness (in resolution range)	94.2 (44.27-3.15) 94.3 (44.27-3.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.244 , 0.272 0.242 , 0.270	Depositor DCC
$R_{free}$ test set	832 reflections (9.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.6	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.1	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 8344 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% 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 [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	0.28	0/821	0.46	0/1107
1	B	0.26	0/829	0.43	0/1118
2	C	0.24	0/249	0.42	0/332
2	D	0.24	0/244	0.53	0/325
All	All	0.27	0/2143	0.45	0/2882

There are no bond length outliers.

There are no bond angle outliers.

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	803	0	783	21	0
1	B	811	0	794	20	0
2	C	249	0	265	1	0
2	D	245	0	263	5	0
All	All	2108	0	2105	44	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 (44) 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:401:HIS:HB2	1:A:428:ARG:HB2	1.67	0.75
1:A:433:ASN:N	1:A:433:ASN:OD1	2.23	0.70
1:B:362:GLU:HB2	1:B:462:THR:HA	1.75	0.66
1:B:421:GLN:HA	1:B:421:GLN:NE2	2.13	0.64
1:B:401:HIS:HB2	1:B:428:ARG:HB2	1.80	0.63
1:B:414:GLN:HA	1:B:417:LYS:HE2	1.80	0.62
1:B:403:GLU:OE1	1:B:428:ARG:NH2	2.33	0.62
1:A:414:GLN:NE2	1:B:426:MET:O	2.33	0.62
1:A:418:LEU:HB3	1:A:421:GLN:HB2	1.84	0.60
2:C:614:ILE:HG13	2:D:614:ILE:HG22	1.84	0.59
1:B:366:ARG:O	1:B:374:THR:OG1	2.20	0.59
1:B:384:VAL:HG23	1:B:386:TYR:H	1.69	0.58
1:B:404:ASP:OD2	1:B:428:ARG:NH1	2.37	0.57
1:A:434:GLN:NE2	1:A:434:GLN:N	2.56	0.54
1:A:428:ARG:HD2	1:A:438:TRP:CZ2	2.42	0.53
1:B:421:GLN:HA	1:B:421:GLN:HE21	1.72	0.53
1:B:368:ASN:ND2	1:B:370:GLU:OE1	2.41	0.53
2:D:614:ILE:HG13	2:D:615:ASP:N	2.23	0.52
2:D:610:LYS:O	2:D:614:ILE:HG23	2.09	0.52
1:A:363:PHE:CD1	1:A:383:THR:HG21	2.44	0.52
1:B:426:MET:HE2	1:B:440:ARG:HG3	1.91	0.51
1:A:429:PHE:HB2	1:A:439:MET:HG3	1.93	0.51
1:A:363:PHE:HD1	1:A:383:THR:HG21	1.75	0.50
2:D:616:GLU:OE1	2:D:619:ARG:NH1	2.45	0.49
1:A:369:ILE:HD12	1:A:369:ILE:H	1.79	0.48
1:A:368:ASN:OD1	1:A:372:ILE:HG12	2.13	0.48
1:A:390:GLU:OE1	1:A:432:LYS:NZ	2.46	0.48
1:A:366:ARG:O	1:A:374:THR:OG1	2.28	0.47
1:A:370:GLU:HG2	1:A:370:GLU:H	1.48	0.47
1:B:401:HIS:CD2	1:B:428:ARG:HD2	2.51	0.46
1:A:432:LYS:O	1:A:434:GLN:NE2	2.49	0.46
1:B:366:ARG:HD2	1:B:374:THR:OG1	2.16	0.45
1:B:419:LYS:HE3	1:B:454:ILE:HG13	1.98	0.45
1:A:378:HIS:CE1	1:A:379:ARG:HG3	2.51	0.45
1:A:440:ARG:HB3	1:A:462:THR:HB	1.99	0.45
1:B:376:VAL:HG11	1:B:391:LEU:HD12	1.99	0.44
1:B:366:ARG:HB3	1:B:375:PHE:HB3	2.00	0.44
1:A:458:ILE:HG13	1:A:458:ILE:O	2.17	0.43
1:B:421:GLN:CA	1:B:421:GLN:HE21	2.30	0.43
2:D:621:CYS:HA	2:D:624:LEU:HD12	2.01	0.42
1:A:379:ARG:O	1:A:383:THR:HG22	2.20	0.42
1:A:438:TRP:CZ2	1:B:418:LEU:HD21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASN:HB3	1:A:398:GLU:HG3	2.01	0.41
1:B:412:PHE:O	1:B:416:VAL:HG23	2.21	0.40

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	92/119 (77%)	89 (97%)	3 (3%)	0	100	100
1	B	93/119 (78%)	89 (96%)	4 (4%)	0	100	100
2	C	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
2	D	29/44 (66%)	27 (93%)	2 (7%)	0	100	100
All	All	243/326 (74%)	233 (96%)	10 (4%)	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	91/112 (81%)	83 (91%)	8 (9%)	12	43
1	B	92/112 (82%)	87 (95%)	5 (5%)	27	67
2	C	28/39 (72%)	27 (96%)	1 (4%)	42	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	28/39 (72%)	25 (89%)	3 (11%)	8	32
All	All	239/302 (79%)	222 (93%)	17 (7%)	18	56

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	GLU
1	A	384	VAL
1	A	404	ASP
1	A	424	SER
1	A	432	LYS
1	A	433	ASN
1	A	434	GLN
1	A	458	ILE
1	B	361	THR
1	B	362	GLU
1	B	392	LEU
1	B	430	ARG
1	B	441	THR
2	C	596	LEU
2	D	603	LEU
2	D	614	ILE
2	D	624	LEU

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	434	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 [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	96/119 (80%)	0.26	2 (2%) 67 50	48, 64, 83, 95	0
1	B	97/119 (81%)	0.12	0 100 100	46, 63, 84, 97	0
2	C	31/44 (70%)	-0.04	0 100 100	54, 62, 72, 84	0
2	D	31/44 (70%)	-0.02	0 100 100	50, 60, 76, 78	0
All	All	255/326 (78%)	0.14	2 (0%) 87 79	46, 63, 83, 97	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	PHE	2.7
1	A	457	ILE	2.4

### 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.