



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:14 AM GMT

PDB ID : 1BXX  
Title : MU2 ADAPTIN SUBUNIT (AP50) OF AP2 ADAPTOR (SECOND DOMAIN), COMPLEXED WITH TGN38 INTERNALIZATION PEPTIDE DYQRLN  
Authors : Owen, D.J.; Evans, P.R.  
Deposited on : 1998-10-08  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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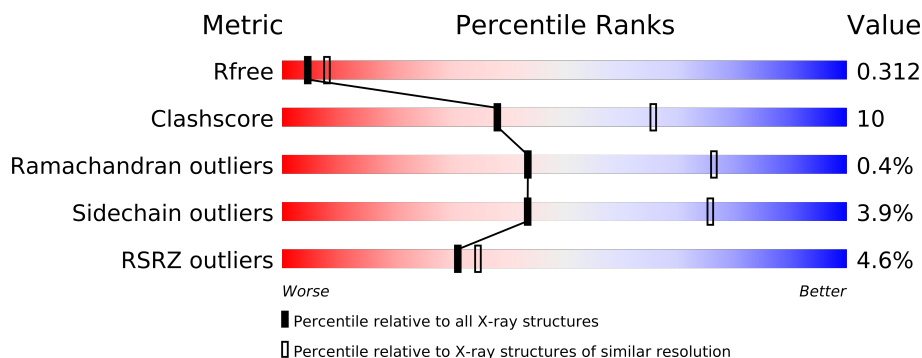
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	285	
2	P	6	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2142 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (AP50).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2036	1312	349	361	14			

- Molecule 2 is a protein called PROTEIN (TGN38 PEPTIDE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	0	0	0
			57	34	11	12			

- Molecule 3 is water.

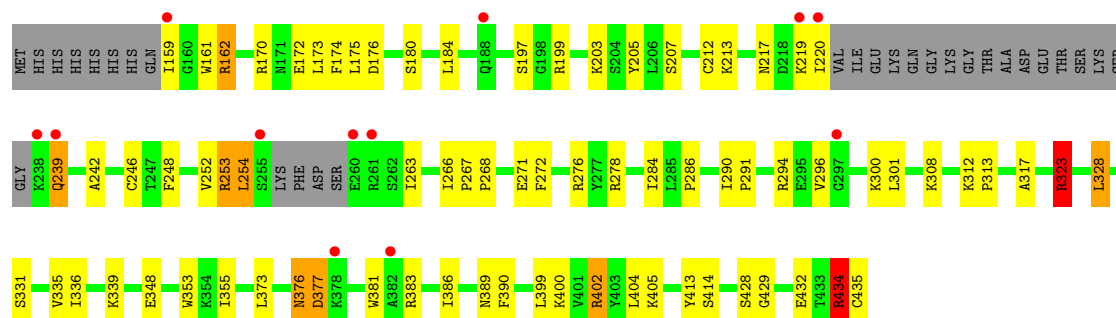
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	P	2	Total	O	0	0
			2	2		

### 3 Residue-property plots

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: PROTEIN (AP50)

Chain A: 



- Molecule 2: PROTEIN (TGN38 PEPTIDE)

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.26Å 125.26Å 73.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	22.00 – 2.70 22.89 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.4 (22.00-2.70) 98.4 (22.89-2.68)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.67Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.263 , 0.325 0.270 , 0.312	Depositor DCC
$R_{free}$ test set	932 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.5	EDS
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 18413 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.63	0/2077	1.72	35/2797 (1.3%)
2	P	0.71	0/57	2.17	3/74 (4.1%)
All	All	0.63	0/2134	1.74	38/2871 (1.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ARG	NE-CZ-NH1	17.63	129.12	120.30
1	A	434	ARG	NE-CZ-NH2	-14.85	112.88	120.30
1	A	294	ARG	CD-NE-CZ	12.00	140.40	123.60
1	A	323	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	A	294	ARG	NE-CZ-NH2	-10.85	114.87	120.30
1	A	402	ARG	NE-CZ-NH2	10.50	125.55	120.30
1	A	278	ARG	NE-CZ-NH2	9.50	125.05	120.30
2	P	4	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	A	278	ARG	NE-CZ-NH1	-8.90	115.85	120.30
1	A	199	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	P	4	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	205	TYR	CB-CG-CD2	8.30	125.98	121.00
1	A	162	ARG	CD-NE-CZ	7.53	134.14	123.60
1	A	205	TYR	CB-CG-CD1	-7.51	116.50	121.00
1	A	199	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	162	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	253	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	323	ARG	NH1-CZ-NH2	6.86	126.95	119.40
1	A	432	GLU	OE1-CD-OE2	6.71	131.36	123.30
1	A	429	GLY	N-CA-C	-6.69	96.37	113.10
1	A	170	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	172	GLU	N-CA-CB	-6.20	99.45	110.60
1	A	323	ARG	CB-CA-C	6.14	122.69	110.40
1	A	176	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	317	ALA	N-CA-CB	6.03	118.54	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ARG	N-CA-CB	-5.91	99.95	110.60
1	A	389	ASN	N-CA-CB	5.72	120.90	110.60
1	A	336	ILE	N-CA-CB	5.66	123.81	110.80
1	A	266	ILE	N-CA-C	-5.55	96.00	111.00
1	A	434	ARG	CD-NE-CZ	5.25	130.95	123.60
2	P	4	ARG	CD-NE-CZ	5.23	130.92	123.60
1	A	276	ARG	N-CA-CB	-5.19	101.25	110.60
1	A	239	GLN	CB-CG-CD	5.15	124.99	111.60
1	A	414	SER	O-C-N	-5.14	114.47	122.70
1	A	335	VAL	CB-CA-C	-5.14	101.63	111.40
1	A	301	LEU	N-CA-CB	5.09	120.59	110.40
1	A	246	CYS	CA-CB-SG	5.04	123.08	114.00
1	A	197	SER	N-CA-CB	5.03	118.04	110.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2036	0	2094	41	0
2	P	57	0	53	1	0
3	A	47	0	0	1	0
3	P	2	0	0	0	0
All	All	2142	0	2147	42	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:ILE:HG12	1:A:242:ALA:HA	1.54	0.89
1:A:328:LEU:HD12	1:A:328:LEU:H	1.45	0.82
1:A:434:ARG:HD3	3:A:16:HOH:O	1.85	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:GLN:HB2	1:A:402:ARG:NH2	2.06	0.71
1:A:239:GLN:HB2	1:A:402:ARG:HH22	1.55	0.69
1:A:175:LEU:HD11	1:A:404:LEU:HD22	1.79	0.64
1:A:328:LEU:CD1	1:A:328:LEU:H	2.11	0.62
1:A:173:LEU:CD1	1:A:404:LEU:HD23	2.30	0.62
1:A:252:VAL:HG13	1:A:263:ILE:HG23	1.82	0.61
1:A:328:LEU:HD12	1:A:328:LEU:N	2.16	0.61
1:A:217:ASN:HB3	1:A:402:ARG:HH21	1.67	0.59
1:A:331:SER:HB3	1:A:373:LEU:HG	1.85	0.58
1:A:399:LEU:HD23	1:A:400:LYS:N	2.19	0.57
1:A:248:PHE:CE1	1:A:263:ILE:HG12	2.40	0.57
1:A:323:ARG:HH22	1:A:348:GLU:HB3	1.69	0.56
1:A:254:LEU:H	1:A:254:LEU:HD22	1.70	0.56
1:A:284:ILE:O	1:A:286:PRO:HD3	2.06	0.55
1:A:248:PHE:HE1	1:A:263:ILE:HG12	1.72	0.54
1:A:161:TRP:HH2	1:A:253:ARG:HH21	1.56	0.53
1:A:173:LEU:HD13	1:A:404:LEU:HD23	1.90	0.52
1:A:376:ASN:HD22	1:A:377:ASP:N	2.07	0.52
1:A:212:CYS:HA	1:A:405:LYS:O	2.09	0.51
1:A:174:PHE:HB2	1:A:203:LYS:HB2	1.93	0.49
1:A:376:ASN:HD22	1:A:376:ASN:C	2.17	0.48
1:A:207:SER:HB2	1:A:413:TYR:CE1	2.48	0.48
1:A:159:ILE:HG22	1:A:162:ARG:H	1.79	0.48
1:A:213:LYS:HB2	1:A:405:LYS:HB2	1.96	0.47
1:A:252:VAL:CG1	1:A:263:ILE:HG23	2.44	0.46
1:A:290:ILE:HD13	1:A:308:LYS:HE2	1.98	0.46
1:A:390:PHE:CE2	1:A:428:SER:HB3	2.52	0.45
1:A:219:LYS:O	1:A:220:ILE:HB	2.16	0.45
1:A:296:VAL:HB	1:A:300:LYS:HB2	1.99	0.44
1:A:312:LYS:HA	1:A:313:PRO:HD3	1.86	0.43
1:A:268:PRO:HD2	1:A:272:PHE:CE1	2.54	0.43
1:A:353:TRP:CE2	1:A:355:ILE:HD11	2.54	0.42
1:A:381:TRP:CE3	1:A:383:ARG:HG2	2.54	0.42
2:P:5:LEU:O	2:P:6:ASN:C	2.58	0.42
1:A:203:LYS:HG2	1:A:271:GLU:HB2	2.02	0.41
1:A:267:PRO:HA	1:A:268:PRO:HD3	1.92	0.41
1:A:268:PRO:HD2	1:A:272:PHE:CD1	2.56	0.41
1:A:399:LEU:C	1:A:399:LEU:HD23	2.41	0.40
1:A:291:PRO:HB3	1:A:386:ILE:HD12	2.03	0.40

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	250/285 (88%)	230 (92%)	19 (8%)	1 (0%)	43	76
2	P	4/6 (67%)	4 (100%)	0	0	100	100
All	All	254/291 (87%)	234 (92%)	19 (8%)	1 (0%)	43	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	LEU

### 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	225/257 (88%)	216 (96%)	9 (4%)	42	75
2	P	6/6 (100%)	6 (100%)	0	100	100
All	All	231/263 (88%)	222 (96%)	9 (4%)	43	76

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

Mol	Chain	Res	Type
1	A	180	SER
1	A	184	LEU
1	A	323	ARG
1	A	328	LEU
1	A	339	LYS
1	A	376	ASN
1	A	377	ASP
1	A	434	ARG

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Mol	Chain	Res	Type
1	A	435	CYS

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	376	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	256/285 (89%)	0.12	12 (4%) 30 34	48, 72, 119, 140	0
2	P	6/6 (100%)	-0.27	0 100 100	58, 79, 80, 102	0
All	All	262/291 (90%)	0.11	12 (4%) 31 35	48, 72, 117, 140	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	5.7
1	A	378	LYS	4.2
1	A	260	GLU	3.8
1	A	382	ALA	3.6
1	A	238	LYS	3.4
1	A	239	GLN	3.4
1	A	297	GLY	2.7
1	A	255	SER	2.6
1	A	219	LYS	2.5
1	A	261	ARG	2.4
1	A	188	GLN	2.1
1	A	159	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.