



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 06:45 pm GMT

PDB ID : 3CF3  
Title : Structure of P97/vcp in complex with ADP  
Authors : Davies, J.M.; Delabarre, B.; Brunger, A.T.; Weis, W.I.  
Deposited on : 2008-03-01  
Resolution : 4.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

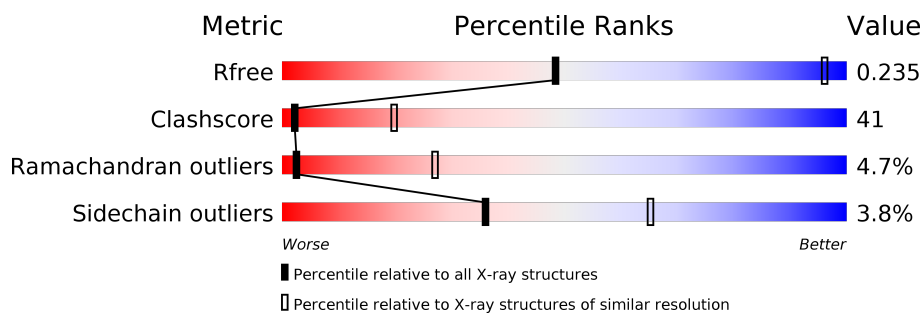
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.25 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))
$R_{free}$	111664	1027 (4.80-3.70)
Clashscore	122126	1097 (4.80-3.70)
Ramachandran outliers	120053	1047 (4.80-3.70)
Sidechain outliers	120020	1031 (4.80-3.70)

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. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	806	<div> <div>37%</div> <div>48%</div> <div>5%</div> <div>10%</div> </div>
1	B	806	<div> <div>37%</div> <div>49%</div> <div>•</div> <div>10%</div> </div>
1	C	806	<div> <div>37%</div> <div>47%</div> <div>5%</div> <div>10%</div> </div>

## 2 Entry composition [i](#)

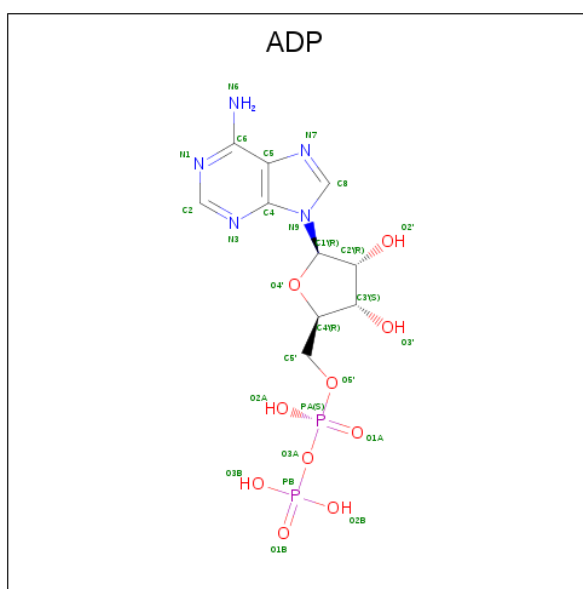
There are 2 unique types of molecules in this entry. The entry contains 17139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			
1	B	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			
1	C	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



- Molecule 1: Transitional endoplasmic reticulum ATPase

- Molecule 1: Transitional endoplasmic reticulum ATPase



SER	L213	L286	P350	I423	Y495	P571	P646	SER
GLY		R287		R424	P496	C572	L647	ALA
GLY	K217	K288	T353	K425	Y497	V573	P648	MET
GLY		A289	K426	K426	Y498	L574	D649	GLU
THR	E221	F290	P355	M427	H499	F575	E650	VAL
GLY	L222	E291	A356	D428	P500	F576	R653	GLU
GLY	L223	E292	L357	L429	D501	D577		GLU
SER	P223	A293	R358	I430	K502	E578	T656	ASP
GLY	L224	E294	L430	D431	F503	L579	L657	ASP
THR		K295	F360	L432	L504	D580	K658	PRO
THR	P227	N296	G361	E433	K505	S581	A659	THR
GLU	A228	A297	F362	T436	M508	I582	N660	GLU
ASP	L229	P298	R363	I437	T509	R586	L661	ASP
ASN	F230	A299	D364	D438	P510	G587	R662	ASN
ASP	K231	I300	R365	A439	S511	G588	K663	ASP
ASP	A232	I301		E440	K512	N589	S664	ASP
LEU	G234	F302	D369	E441	G513	I590	P665	ASP
LEU	V235	I303	V441	V441	V514	G591	V666	LEU
TYR	K236	D304	M442	M442	L515		A667	TYR
GLY	P237		A374	K443	L516	V600		
	P239	I309	R377	S444	F517	I604	V670	
		A310	L378	L445	G518	L605		
	Y244	P311	L379	M449	P519			
		K312	L381	A455	P520	M608	K677	
	G248	R313	Q382		G521	D609	N678	
	T249	E314	L383	Q458	C522	G610	T679	
	K250	R315	H384	S459	G523	M611	N680	
	K251	H317	T385	N460	K524	S612	F682	
	T252	G318	K386	P461	T525	T613	S683	
	L253	E319	N387	S462	L526	K614	G684	
	T254	V320	K388	A463	L527	K615	L687	
		E321	R389	L464	I531	V617	T688	
	A257	R322	L390	R465	A532	F618	E689	
	V258	A259	A391	T467	N533	I619	I690	
	E260			V394		T620	A694	
	E261		S326	V468	N538	G621		
	T262		Q327	V469	P539	A622	L697	
		F265	L328	E470	I540	T623	A698	
			L329	V471	S541	N624	I699	
	F266		T330	P472	I542		R700	
	F267		L331	Q473	K543		E701	
		L268	E402	V474	G544	I628	S702	
	T269		M332	T475	I547	D629	I703	
	N270		D333			P631	E704	
	G271		G334	I479	E556	I633	S705	
	P272		L335	H406		L634	E706	
	E273		K336	V407			I707	
	I274		Q337	G408		G637	ARG	
	M275		R338	A409		R638	ARG	
	S276		A339	D410		L639	GLU	
			H340	L411		D640	ALA	
	K277		V341	L414		Q641	GLY	
				C415		L642	ARG	
	G280		M344	S416		I643	GLN	
	E281		A345			Y644	THR	
	S282		A346			I645	SER	
	E283		T347				GLN	
	S284		N348				ASN	
	N285		R349				PRO	

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.97Å 178.93Å 320.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.25 29.94 – 4.25	Depositor EDS
% Data completeness (in resolution range)	86.4 (40.00-4.25) 92.9 (29.94-4.25)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 4.26Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.198 , 0.226 0.210 , 0.235	Depositor DCC
$R_{free}$ test set	4669 reflections (7.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	143.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 188.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.38	0/5751	0.87	9/7767 (0.1%)
1	B	0.37	0/5751	0.87	9/7767 (0.1%)
1	C	0.38	0/5751	0.88	9/7767 (0.1%)
All	All	0.38	0/17253	0.87	27/23301 (0.1%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	ARG	NE-CZ-NH2	-29.67	105.46	120.30
1	A	338	ARG	NE-CZ-NH1	-29.13	105.74	120.30
1	B	287	ARG	NE-CZ-NH2	-28.38	106.11	120.30
1	A	338	ARG	NE-CZ-NH2	27.38	133.99	120.30
1	B	287	ARG	NE-CZ-NH1	27.28	133.94	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5659	0	5731	495	0
1	B	5659	0	5731	491	0
1	C	5659	0	5731	466	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	54	0	24	6	0
2	B	54	0	24	4	0
2	C	54	0	24	3	0
All	All	17139	0	17265	1421	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 41.

The worst 5 of 1421 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:206:ILE:CD1	1:A:213:LEU:HD11	1.25	1.64
1:B:206:ILE:CD1	1:B:213:LEU:HD11	1.24	1.61
1:C:206:ILE:CD1	1:C:213:LEU:HD11	1.25	1.59
1:A:206:ILE:HD11	1:A:213:LEU:CD1	1.55	1.34
1:C:206:ILE:HD11	1:C:213:LEU:CD1	1.55	1.34

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	719/806 (89%)	566 (79%)	119 (17%)	34 (5%)	2	27
1	B	719/806 (89%)	564 (78%)	123 (17%)	32 (4%)	3	28
1	C	719/806 (89%)	561 (78%)	122 (17%)	36 (5%)	2	26
All	All	2157/2418 (89%)	1691 (78%)	364 (17%)	102 (5%)	2	27

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	85	ASN
1	A	140	LEU
1	A	185	GLU
1	A	312	LYS

### 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	615/678 (91%)	590 (96%)	25 (4%)	33	63
1	B	615/678 (91%)	593 (96%)	22 (4%)	38	66
1	C	615/678 (91%)	592 (96%)	23 (4%)	37	66
All	All	1845/2034 (91%)	1775 (96%)	70 (4%)	36	65

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	287	ARG
1	B	440	GLU
1	C	579	LEU
1	B	314	GLU
1	B	340	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	285	ASN
1	B	348	ASN
1	C	616	ASN
1	B	327	GLN
1	B	401	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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$
2	ADP	A	807	-	25,29,29	1.67	5 (20%)	25,45,45	3.11	6 (24%)
2	ADP	A	900	-	25,29,29	1.73	5 (20%)	25,45,45	2.88	1 (4%)
2	ADP	B	807	-	25,29,29	1.68	5 (20%)	25,45,45	2.90	3 (12%)
2	ADP	B	900	-	25,29,29	1.46	3 (12%)	25,45,45	2.67	3 (12%)
2	ADP	C	807	-	25,29,29	1.58	4 (16%)	25,45,45	2.93	4 (16%)
2	ADP	C	900	-	25,29,29	1.62	3 (12%)	25,45,45	2.93	3 (12%)

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
2	ADP	A	807	-	-	0/12/32/32	0/3/3/3
2	ADP	A	900	-	-	0/12/32/32	0/3/3/3
2	ADP	B	807	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	900	-	-	0/12/32/32	0/3/3/3
2	ADP	C	807	-	-	0/12/32/32	0/3/3/3
2	ADP	C	900	-	-	0/12/32/32	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	807	ADP	PB-O3A	-4.10	1.53	1.60
2	C	807	ADP	C5-N7	-3.13	1.28	1.39
2	C	900	ADP	C5-N7	-2.89	1.29	1.39
2	A	900	ADP	C5-N7	-2.62	1.30	1.39
2	A	807	ADP	C5-N7	-2.55	1.30	1.39

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	807	ADP	N3-C2-N1	-13.99	116.89	128.86
2	C	900	ADP	N3-C2-N1	-13.60	117.22	128.86
2	A	900	ADP	N3-C2-N1	-13.46	117.35	128.86
2	B	807	ADP	N3-C2-N1	-13.34	117.45	128.86
2	C	807	ADP	N3-C2-N1	-13.33	117.45	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	807	ADP	4	0
2	A	900	ADP	2	0
2	B	807	ADP	3	0
2	B	900	ADP	1	0
2	C	807	ADP	1	0
2	C	900	ADP	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.