



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DV2  
Title : The structure of biotin carboxylase, mutant E288K, complexed with ATP  
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Deposited on : 2000-01-19  
Resolution : 2.50 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  
<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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

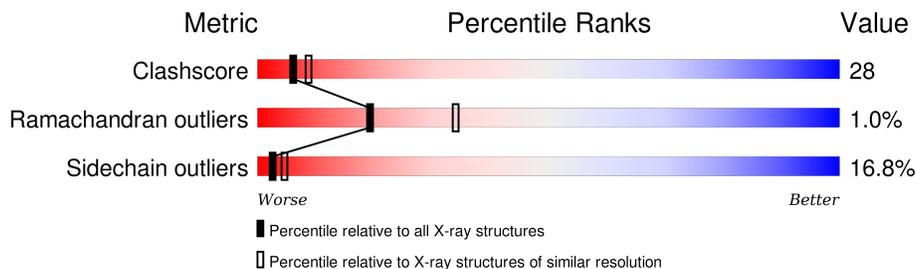
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	452	
1	B	452	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	1000	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7113 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.

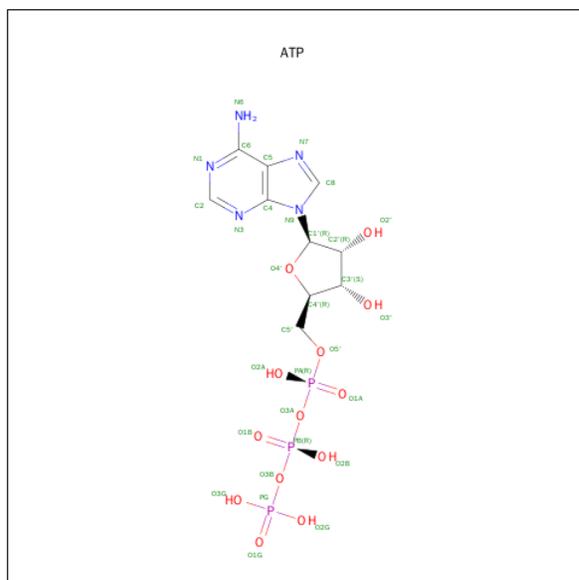
- Molecule 1 is a protein called BIOTIN CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	Total	C	N	O	S	0	1	0
			3469	2184	624	639	22			
1	B	448	Total	C	N	O	S	0	0	0
			3452	2175	619	636	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1A	HIS	-	INSERTED	UNP P24182
A	1B	SER	-	INSERTED	UNP P24182
A	1C	GLY	-	INSERTED	UNP P24182
B	1A	HIS	-	INSERTED	UNP P24182
B	1B	SER	-	INSERTED	UNP P24182
B	1C	GLY	-	INSERTED	UNP P24182
A	288	LYS	GLU	MUTATION	UNP P24182
B	288	LYS	GLU	MUTATION	UNP P24182

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0
2	B	1	31	10	5	13	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	82	82	82	0	0
3	B	48	48	48	0	0



Q294	S369
V295	H370
E296	I371
H297	
P298	P378
	Y380
E301	Y381
M302	
I303	M384
D307	K387
L308	
I309	C390
K310	
E311	D396
Q312	
L313	I399
R314	M400
I315	R401
	M402
Q319	K403
F320	
L321	L409
S322	
I323	T416
K324	
Q325	D419
E327	L420
	Q421
V330	I422
	R423
H333	I424
A334	M425
V335	M426
E336	D427
C337	E428
R338	M429
I339	F430
I340	Q431
A341	
E342	T435
D343	M436
P344	I437
H345	H438
T346	Y439
F347	L440
L348	E441
P349	K442
S350	K443
	L444
K353	G445
	L446
H358	Q447
	GLU
G364	LYS
V365	
R366	
M367	
E368	

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.30Å 115.50Å 122.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	92.6 (30.00-2.50)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.171 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.02	27/3537 (0.8%)	1.48	49/4771 (1.0%)
1	B	0.98	27/3516 (0.8%)	1.40	32/4744 (0.7%)
All	All	1.00	54/7053 (0.8%)	1.44	81/9515 (0.9%)

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	GLU	CD-OE2	7.32	1.33	1.25
1	A	342	GLU	CD-OE2	7.01	1.33	1.25
1	A	211	GLU	CD-OE2	6.79	1.33	1.25
1	B	342	GLU	CD-OE2	6.69	1.33	1.25
1	B	177	GLU	CD-OE2	6.62	1.32	1.25

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ARG	NE-CZ-NH1	15.59	128.09	120.30
1	B	97	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	A	270	ARG	NE-CZ-NH1	9.95	125.27	120.30
1	A	16	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	B	37	ARG	NE-CZ-NH1	9.18	124.89	120.30

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	3469	0	3498	188	0
1	B	3452	0	3481	207	0
2	A	31	0	12	10	0
2	B	31	0	12	8	0
3	A	82	0	0	3	0
3	B	48	0	0	4	0
All	All	7113	0	7003	394	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 28.

The worst 5 of 394 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:B:179:ALA:HB3	1:B:180:GLN:HE21	1.19	1.00
1:B:440:LEU:HG	1:B:444:LEU:HD22	1.40	0.97
1:B:131:VAL:HG22	1:B:285:TYR:HB3	1.45	0.95
1:A:117:VAL:HG21	1:A:197:MET:HE3	1.48	0.95
1:B:278:LEU:HD22	1:B:287:ILE:HD11	1.51	0.93

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	449/452 (99%)	406 (90%)	41 (9%)	2 (0%)	39	61
1	B	446/452 (99%)	407 (91%)	32 (7%)	7 (2%)	12	21
All	All	895/904 (99%)	813 (91%)	73 (8%)	9 (1%)	19	34

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	MET
1	B	181	SER
1	B	179	ALA
1	B	196	ASP
1	B	226	ALA

### 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	362/363 (100%)	307 (85%)	55 (15%)	3	6
1	B	360/363 (99%)	294 (82%)	66 (18%)	2	3
All	All	722/726 (99%)	601 (83%)	121 (17%)	2	4

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	B	120	ILE
1	B	324	LYS
1	B	4	LYS
1	B	82	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	ASN
1	B	209	HIS
1	B	370	HIS
1	A	447	GLN
1	B	404	ASN

### 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](#)

2 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	ATP	A	1000	-	24,33,33	1.96	1 (4%)	31,52,52	1.20	3 (9%)
2	ATP	B	1001	-	24,33,33	1.85	1 (4%)	31,52,52	1.25	4 (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	ATP	A	1000	-	-	0/18/38/38	0/3/3/3
2	ATP	B	1001	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	ATP	C2'-C3'	-8.57	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ATP	C2'-C3'	-8.05	1.31	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ATP	O3A-PA-O5'	-3.02	94.91	102.94
2	B	1001	ATP	O3A-PA-O5'	-2.78	95.55	102.94
2	B	1001	ATP	C1'-N9-C4	-2.58	123.04	126.94
2	A	1000	ATP	PA-O3A-PB	-2.38	126.05	132.73
2	A	1000	ATP	O4'-C4'-C3'	-2.18	100.75	105.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	ATP	10	0
2	B	1001	ATP	8	0

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.