



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 09:33 AM EST

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

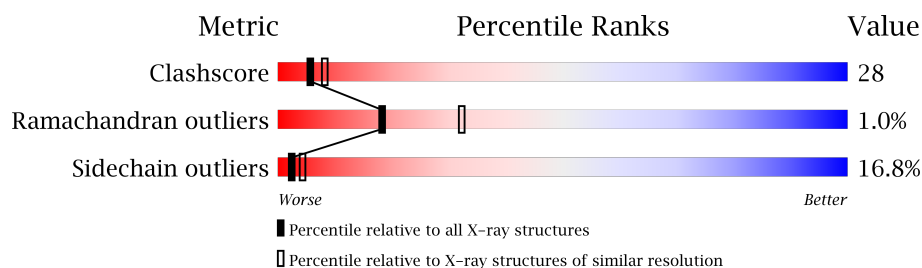
1 Overall quality at a glance

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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (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 ≥ 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.

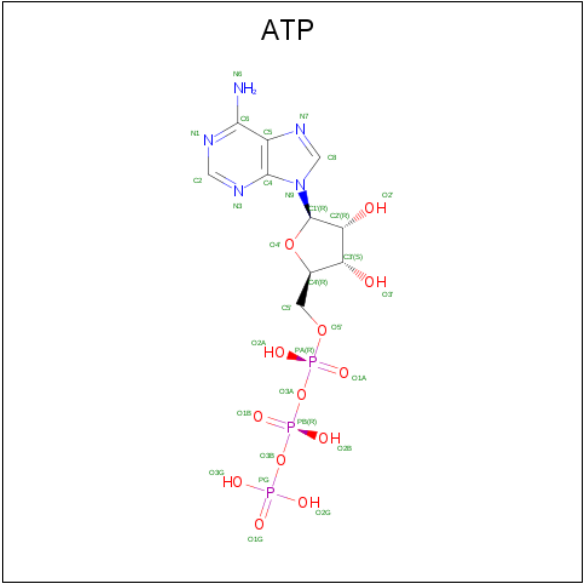
- Molecule 1 is a protein called BIOTIN CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	ENGINEERED MUTATION	UNP P24182
B	288	LYS	GLU	ENGINEERED MUTATION	UNP P24182

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

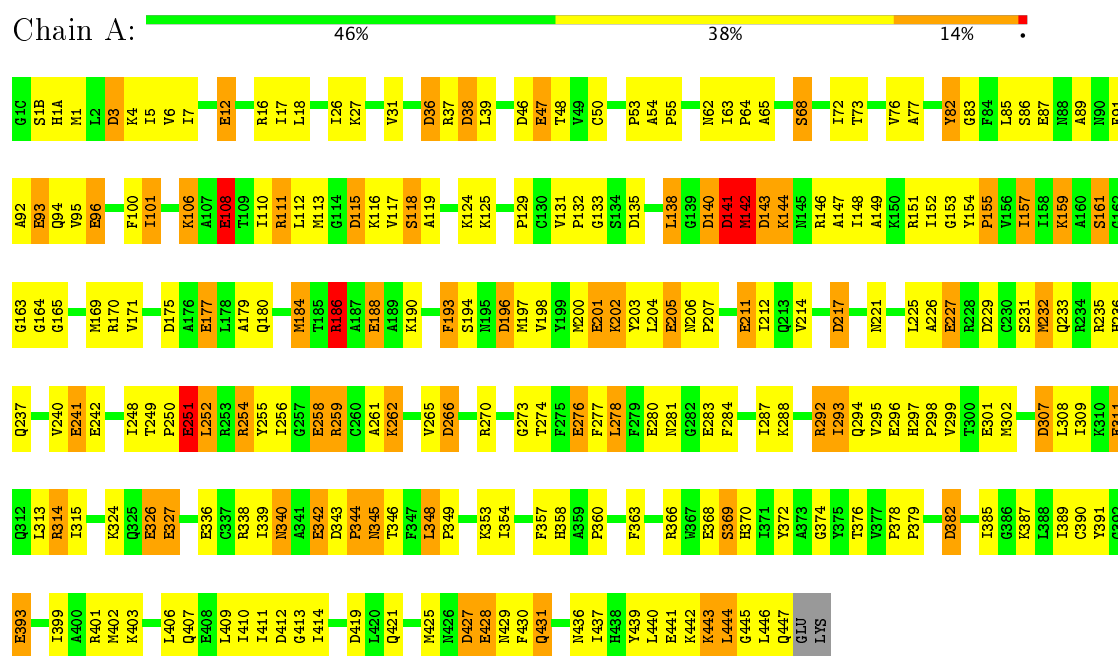


3 Residue-property plots

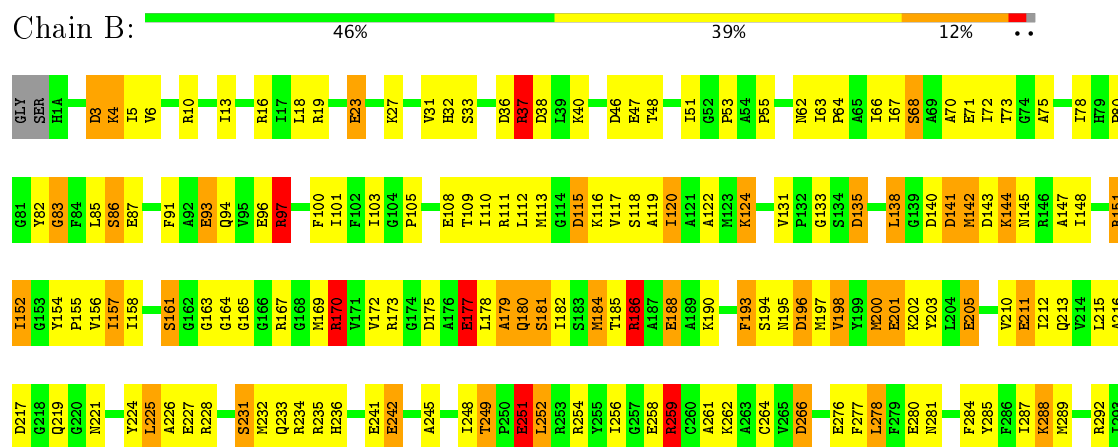
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: BIOTIN CARBOXYLASE



• Molecule 1: BIOTIN CARBOXYLASE



S369	Q294	H370	Y295	P378	E301	D307	L308	K387	L309	C390	D396	I399	A400	R401	M402	K403	L409	T416	D419	L420	Q421	I422	R423	I424	M425	N426	D427	E428	M429	F430	Q431	T435	M436	L437	H438	Y439	I440	E441	K442	K443	L444	G445	L446	Q447	GLU	LYS	E368
H371	E296	H297	P298	Y380	Y381	M384	K390	C390	D396	I399	A400	R401	M402	K403	L409	T416	D419	L420	Q421	I422	R423	I424	M425	N426	D427	E428	M429	F430	Q431	T435	M436	L437	H438	Y439	I440	E441	K442	K443	L444	G445	L446	Q447	GLU	LYS	E368		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.30 Å 115.50 Å 122.40 Å 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 5E	Depositor
R, R_{free}	0.171 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7113	wwPDB-VP
Average B, all atoms (Å ²)	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%)	38	59
1	B	446/452 (99%)	407 (91%)	32 (7%)	7 (2%)	11	19
All	All	895/904 (99%)	813 (91%)	73 (8%)	9 (1%)	18	32

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 ⓘ

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 ⓘ

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 ⓘ

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	-	27,33,33	2.05	3 (11%)	25,52,52	1.01	1 (4%)
2	ATP	B	1001	-	27,33,33	1.93	3 (11%)	25,52,52	1.10	2 (8%)

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	ATP	C2'-C3'	-8.83	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ATP	C2'-C3'	-8.29	1.31	1.53
2	A	1000	ATP	PG-O3B	-3.52	1.54	1.60
2	B	1001	ATP	PG-O3B	-3.14	1.55	1.60
2	A	1000	ATP	C2'-C1'	-2.60	1.49	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ATP	O4'-C4'-C3'	-2.22	100.75	105.17
2	B	1001	ATP	C1'-N9-C4	-2.08	123.04	126.64
2	B	1001	ATP	C2'-C3'-C4'	3.20	108.85	102.62

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.