



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:44 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 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/ValidationPDFNotes.html>

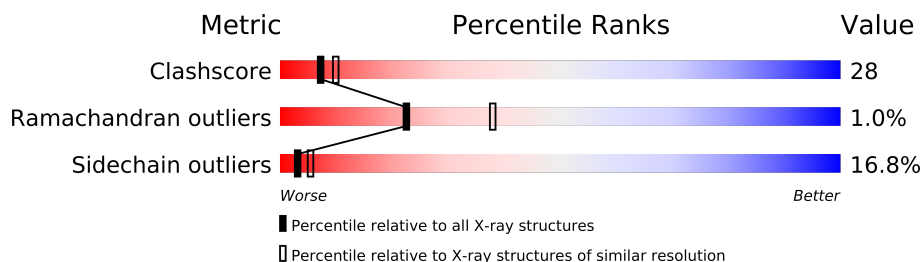
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
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 2.50 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2 Entry composition

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

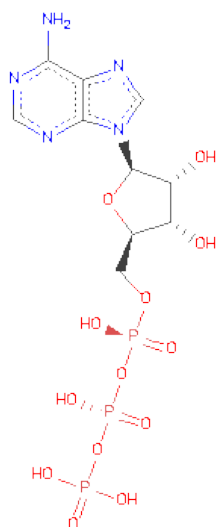
- Molecule 1 is a protein called BIOTIN CARBOXYLASE.

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
A	288	LYS	GLU	MUTATION	UNP P24182
B	1A	HIS	-	INSERTED	UNP P24182
B	1B	SER	-	INSERTED	UNP P24182
B	1C	GLY	-	INSERTED	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
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is water.

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

S369	Q294	H370	V295	E296	H297	P298	E301	M302	I303	D307	L308	I309	K310	E311	Q312	L313	R314	I315	Q319	P320	L321	S322	I323	K324	Q325	E326	E327	V330	H333	A334	V335	E336	C337	R338	I339	N340	A341	E342	D343	P344	R345	T346	F347	L348	P349	S350	K353	H358	G364	V365	R366	W367	E368
P378	P379	Y380	Y381	M384	K387	C390	D396	I399	M400	R401	M402	K403	L409	T416	D419	L420	Q421	I422	R423	I424	M425	M426	D427	E428	M429	F430	Q431	T435	M436	I437	H438	Y439	L440	E441	K442	K443	L444	G445	L446	Q447	GLU	LYS											

4 Data and refinement statistics

Xtriage (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, α , β , γ	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.	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 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 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	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

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 28.

The worst 5 of 394 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	449/452 (99%)	406 (90%)	41 (9%)	2 (0%)	43	66
1	B	446/452 (99%)	407 (91%)	32 (7%)	7 (2%)	14	23
All	All	895/904 (99%)	813 (91%)	73 (8%)	9 (1%)	22	38

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%)	4	7
1	B	360/363 (99%)	294 (82%)	66 (18%)	2	4
All	All	722/726 (99%)	601 (83%)	121 (17%)	3	5

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 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 ⓘ

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	-	33,33,33	1.98	4 (12%)	52,52,52	1.44	5 (9%)
2	ATP	B	1001	-	33,33,33	1.86	5 (15%)	52,52,52	1.42	6 (11%)

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	-	-	0/22/38/38	0/1/3/3
2	ATP	B	1001	-	-	0/22/38/38	0/1/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	ATP	C2'-C3'	-8.38	1.30	1.53
2	B	1001	ATP	C2'-C3'	-7.87	1.31	1.53
2	A	1000	ATP	PA-O3A	-3.98	1.52	1.59
2	B	1001	ATP	PB-O3A	3.40	1.66	1.59
2	A	1000	ATP	PG-O3B	-3.36	1.54	1.60

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ATP	C3'-C2'-C1'	4.85	108.50	100.91
2	B	1001	ATP	C3'-C2'-C1'	4.75	108.34	100.91
2	B	1001	ATP	O4'-C1'-N9	4.57	112.69	108.44
2	A	1000	ATP	O3A-PB-O3B	-4.39	92.73	101.66
2	B	1001	ATP	C2'-C3'-C4'	3.11	108.85	102.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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.