



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 12:35 pm GMT

PDB ID : 2V5A
Title : CRYSTAL STRUCTURE OF BIOTIN CARBOXYLASE FROM E.COLI IN COMPLEX WITH POTENT INHIBITOR 3
Authors : Mochalkin, I.; Miller, J.R.
Deposited on : 2008-10-02
Resolution : 2.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk31020
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) : trunk31020

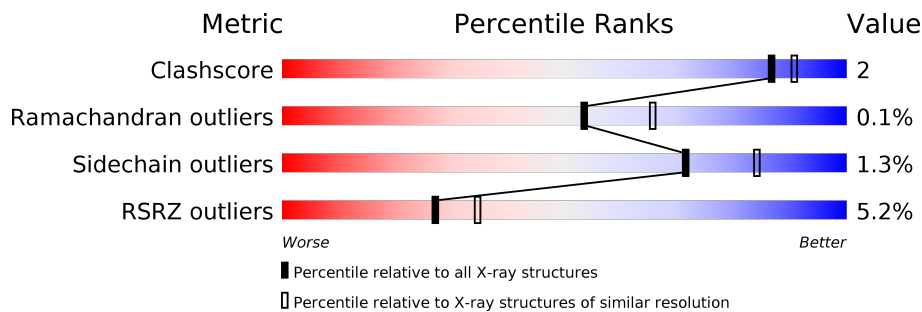
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	122126	5849 (2.34-2.30)
Ramachandran outliers	120053	5790 (2.34-2.30)
Sidechain outliers	120020	5789 (2.34-2.30)
RSRZ outliers	108989	5109 (2.34-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	449	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	B	449	<div> <div>10%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>

2 Entry composition [i](#)

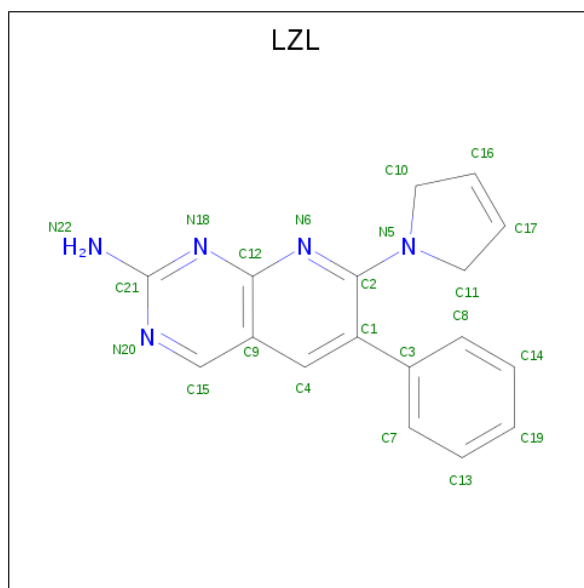
There are 4 unique types of molecules in this entry. The entry contains 7255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	447	Total	C	N	O	S	0	4	1
			3445	2170	615	638	22			
1	B	446	Total	C	N	O	S	0	6	1
			3447	2168	618	639	22			

- Molecule 2 is 7-(2,5-dihydropyrrol-1-yl)-6-phenyl-pyrido[6,5-d]pyrimidin-2-amine (three-letter code: LZL) (formula: C₁₇H₁₅N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			22	17	5		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

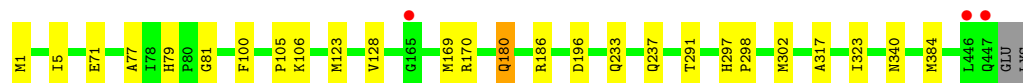
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	152	Total	O	0	0
			152	152		

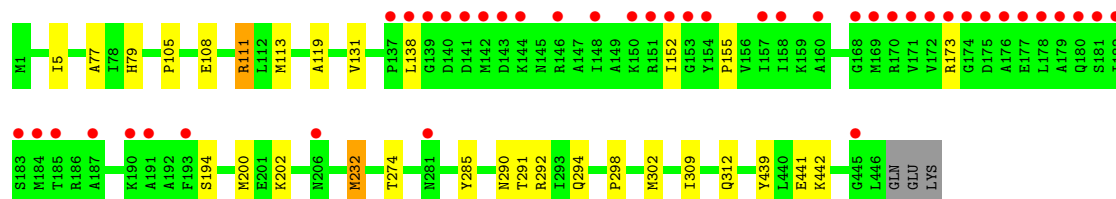
3 Residue-property plots [i](#)

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.

• Molecule 1: BIOTIN CARBOXYLASE



• Molecule 1: BIOTIN CARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.31Å 106.41Å 122.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.32 – 2.31 48.78 – 2.31	Depositor EDS
% Data completeness (in resolution range)	85.4 (80.32-2.31) 81.7 (48.78-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.237 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7255	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/3528	0.52	0/4761
1	B	0.36	0/3540	0.50	0/4777
All	All	0.37	0/7068	0.51	0/9538

There are no bond length outliers.

There are no bond angle outliers.

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	3445	0	3476	14	0
1	B	3447	0	3473	18	0
2	A	22	0	15	2	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
4	A	187	0	0	0	0
4	B	152	0	0	0	0
All	All	7255	0	6964	32	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 2.

All (32) 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:71:GLU:HG2	1:A:100:PHE:HZ	1.57	0.70
1:B:131:VAL:HG22	1:B:285:TYR:HB3	1.80	0.63
1:B:232:MET:HE2	1:B:232:MET:HA	1.82	0.60
1:A:79:HIS:HD1	1:A:81:GLY:H	1.50	0.59
1:A:71:GLU:HG2	1:A:100:PHE:CZ	2.41	0.55
1:A:340:ASN:HD22	1:A:384:MET:HA	1.71	0.55
1:B:105:PRO:HG2	1:B:291:THR:HB	1.90	0.54
1:B:292:ARG:NH1	3:B:1446:CL:CL	2.76	0.53
1:B:274:THR:HG21	1:B:294:GLN:HE22	1.74	0.52
1:B:155:PRO:HB3	1:B:173:ARG:HG2	1.92	0.52
1:A:298:PRO:O	1:A:302:MET:HG2	2.10	0.52
1:B:113:MET:HA	1:B:119:ALA:HB2	1.93	0.49
1:B:138:LEU:HD11	1:B:200:MET:HB2	1.93	0.49
1:B:152:ILE:HG23	1:B:202:LYS:HB2	1.95	0.48
1:B:298:PRO:O	1:B:302:MET:HG2	2.14	0.48
1:B:108:GLU:OE1	1:B:111:ARG:HD2	2.15	0.47
1:B:79:HIS:HE2	1:B:312:GLN:NE2	2.13	0.46
1:A:233:GLN:CD	2:A:1447:LZL:H19	2.35	0.46
1:B:274:THR:HG21	1:B:294:GLN:NE2	2.32	0.45
1:B:232:MET:HA	1:B:232:MET:CE	2.45	0.45
1:A:169:MET:CE	2:A:1447:LZL:H112	2.47	0.44
1:A:297:HIS:N	1:A:298:PRO:CD	2.81	0.44
1:B:309:ILE:HA	1:B:312:GLN:HE21	1.83	0.44
1:A:186:ARG:HG3	1:A:196:ASP:O	2.18	0.44
1:A:5:ILE:HG22	1:A:77:ALA:HB3	1.99	0.43
1:A:123:MET:HB3	1:A:128:VAL:HB	2.01	0.42
1:A:105:PRO:HG2	1:A:291:THR:HB	2.02	0.42
1:A:1:MET:HE3	1:A:317:ALA:HB2	2.02	0.41
1:B:5:ILE:HG22	1:B:77:ALA:HB3	2.02	0.41
1:A:180:GLN:HB3	1:A:180:GLN:HE21	1.65	0.41
1:B:232:MET:HE1	1:B:439:TYR:HD2	1.85	0.41
1:B:290:ASN:ND2	1:B:294:GLN:OE1	2.53	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	449/449 (100%)	441 (98%)	8 (2%)	0	100	100
1	B	450/449 (100%)	441 (98%)	8 (2%)	1 (0%)	49	61
All	All	899/898 (100%)	882 (98%)	16 (2%)	1 (0%)	53	65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	194	SER

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	362/361 (100%)	357 (99%)	5 (1%)	69	83
1	B	363/361 (101%)	359 (99%)	4 (1%)	76	87
All	All	725/722 (100%)	716 (99%)	9 (1%)	71	86

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

Mol	Chain	Res	Type
1	A	106	LYS
1	A	170	ARG
1	A	180	GLN
1	A	237	GLN
1	A	323	ILE

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Mol	Chain	Res	Type
1	B	111	ARG
1	B	232	MET
1	B	441	GLU
1	B	442	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	206	ASN
1	A	312	GLN
1	A	319	GLN
1	A	340	ASN
1	A	404	ASN
1	B	290	ASN
1	B	294	GLN
1	B	312	GLN
1	B	319	GLN
1	B	345	ASN
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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	LZL	A	1447	-	25,25,25	3.04	7 (28%)	31,35,35	2.65	14 (45%)

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	LZL	A	1447	-	-	0/8/15/15	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1447	LZL	C11-C17	-6.73	1.38	1.49
2	A	1447	LZL	C10-C16	-6.01	1.39	1.49
2	A	1447	LZL	C11-N5	-5.86	1.42	1.47
2	A	1447	LZL	C10-N5	-4.67	1.43	1.47
2	A	1447	LZL	C2-N6	4.10	1.36	1.31
2	A	1447	LZL	C9-C12	5.44	1.49	1.41
2	A	1447	LZL	C1-C2	5.61	1.50	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1447	LZL	C1-C2-N6	-5.52	118.78	124.08
2	A	1447	LZL	C11-C17-C16	-4.54	103.31	111.61
2	A	1447	LZL	C9-C12-N18	-3.95	118.99	122.47
2	A	1447	LZL	N20-C21-N18	-3.94	121.66	125.77
2	A	1447	LZL	C10-C16-C17	-3.56	105.10	111.61
2	A	1447	LZL	C9-C15-N20	-2.72	118.72	123.97
2	A	1447	LZL	C9-C12-N6	-2.35	120.40	122.47
2	A	1447	LZL	C7-C3-C1	-2.10	117.59	120.91
2	A	1447	LZL	N22-C21-N20	2.48	119.71	117.39
2	A	1447	LZL	C11-N5-C2	3.33	132.37	121.90
2	A	1447	LZL	C4-C1-C2	3.74	119.94	116.17
2	A	1447	LZL	C15-N20-C21	3.76	122.60	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1447	LZL	C21-N18-C12	4.05	119.88	115.16
2	A	1447	LZL	C17-C11-N5	5.12	105.20	101.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1447	LZL	2	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

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, 95th 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 ²)	Q<0.9
1	A	447/449 (99%)	-0.31	3 (0%) 87 91	20, 26, 35, 45	0
1	B	446/449 (99%)	0.25	43 (9%) 8 11	20, 27, 69, 73	0
All	All	893/898 (99%)	-0.03	46 (5%) 27 34	20, 26, 58, 73	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	GLY	7.3
1	B	183	SER	5.4
1	B	184	MET	5.3
1	B	154	TYR	5.0
1	B	146	ARG	4.8
1	B	181	SER	4.6
1	B	176	ALA	4.4
1	B	173	ARG	4.0
1	B	172	VAL	4.0
1	B	171	VAL	3.7
1	B	144	LYS	3.6
1	B	177	GLU	3.6
1	B	180	GLN	3.6
1	B	142	MET	3.5
1	B	139	GLY	3.4
1	B	178	LEU	3.4
1	B	143	ASP	3.4
1	B	179	ALA	3.3
1	B	168	GLY	3.3
1	B	150	LYS	3.3
1	B	191	ALA	3.3
1	A	446	LEU	3.3
1	B	193	PHE	3.2
1	B	152	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	148	ILE	2.9
1	B	157	ILE	2.9
1	B	185	THR	2.8
1	B	138	LEU	2.6
1	B	153	GLY	2.6
1	B	187	ALA	2.6
1	B	141	ASP	2.6
1	B	175	ASP	2.6
1	B	182	ILE	2.5
1	B	281	ASN	2.5
1	B	169	MET	2.5
1	B	137	PRO	2.4
1	A	165	GLY	2.4
1	B	190	LYS	2.3
1	B	445	GLY	2.3
1	B	158	ILE	2.2
1	A	447	GLN	2.2
1	B	151	ARG	2.2
1	B	140	ASP	2.2
1	B	160	ALA	2.2
1	B	206	ASN	2.1
1	B	170	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LZL	A	1447	22/22	0.94	0.12	27,27,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	B	1446	1/1	0.99	0.07	34,34,34,34	0
3	CL	A	1448	1/1	1.00	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.