



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 01:58 pm GMT

PDB ID : 3IB9
Title : Propionyl-CoA Carboxylase Beta Subunit, D422L
Authors : Diacovich, L.; Arabolaza, A.; Shillito, E.M.; Lin, T.-W.; Mitchell, D.L.; Pham, H.; Melgar, M.M.
Deposited on : 2009-07-15
Resolution : 2.00 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

<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
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

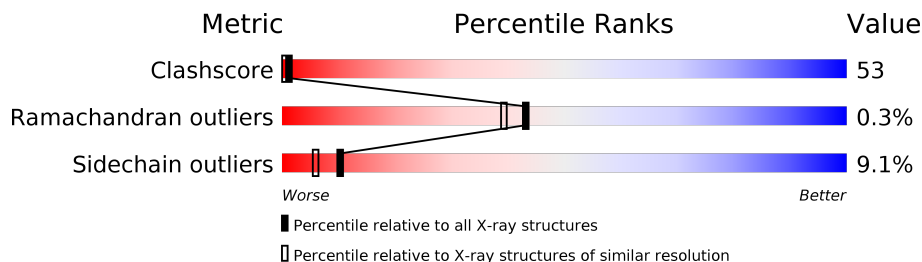
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	530	 42% 51% 5% •
1	B	530	 42% 51% 6% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8285 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.

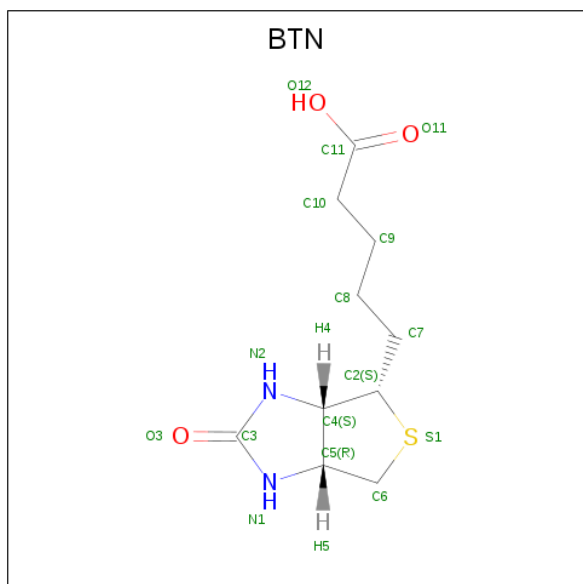
- Molecule 1 is a protein called Propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			3952	2483	698	758	13			
1	B	521	Total	C	N	O	S	0	0	0
			3952	2483	698	758	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	LEU	ASP	ENGINEERED	UNP Q9X4K7
B	422	LEU	ASP	ENGINEERED	UNP Q9X4K7

- Molecule 2 is BIOTIN (three-letter code: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

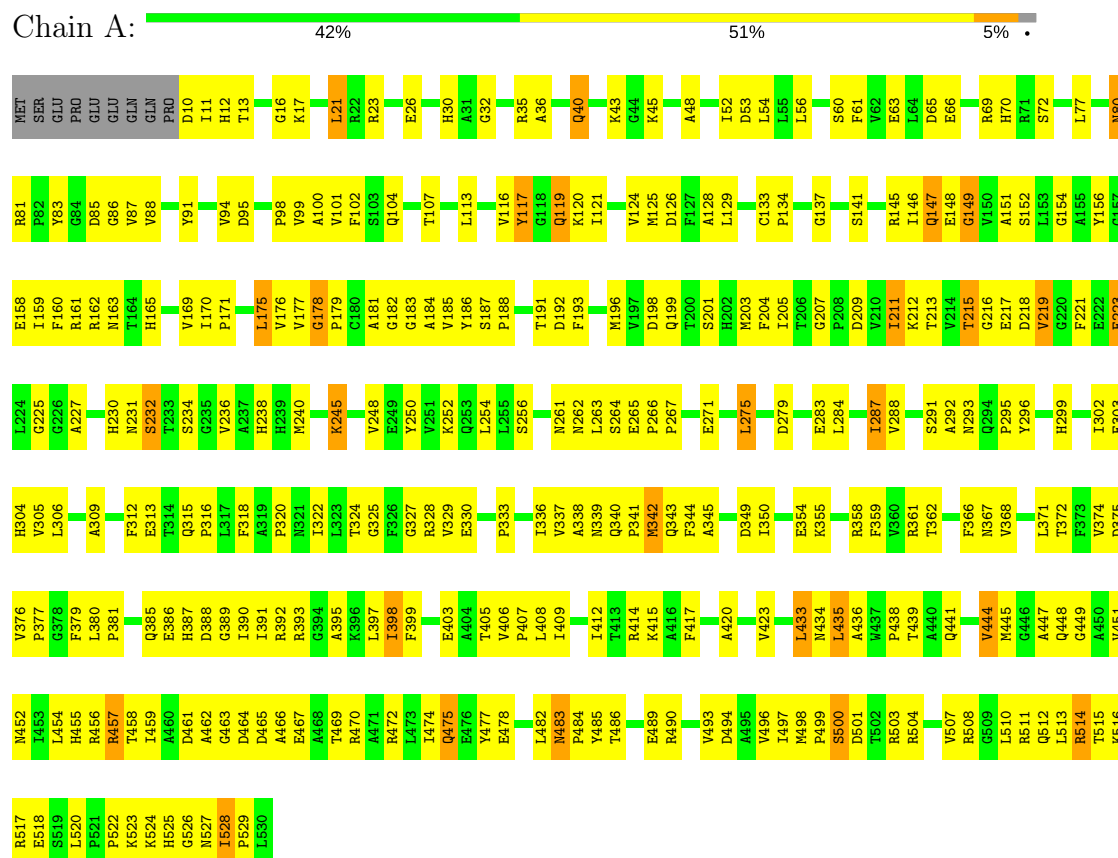
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	172	Total	O	0	0
			172	172		

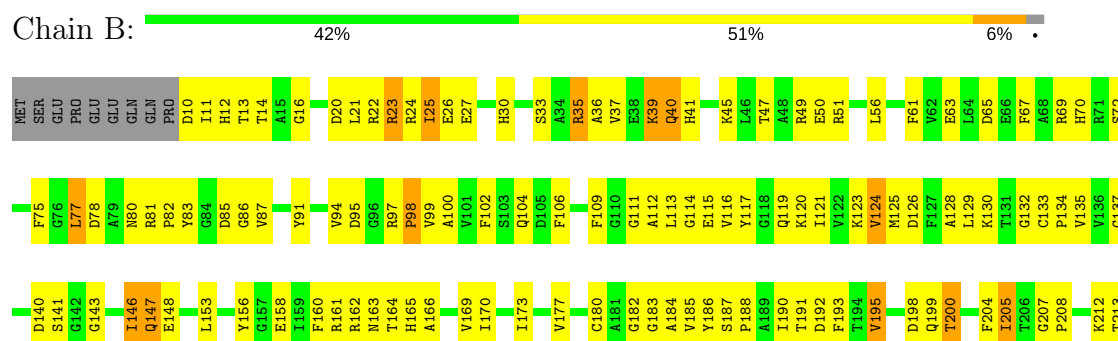
3 Residue-property plots

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. 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. 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: Propionyl-CoA carboxylase complex B subunit



• Molecule 1: Propionyl-CoA carboxylase complex B subunit



G509	T439	V368	M298	V214
L513	A440	L371	H299	T215
R514	Q441		S300	
	I442		V301	D218
L520	A443	V374	I302	V219
P521	V444	D375	E303	G220
P522	M445	V376	H304	F221
K523	G446	P377	V305	
	A447	G378	L306	G226
	Q448	F379	D307	A227
L528	G449	L380	D308	R228
P529	A450	P381	A309	T229
L530	V451		E310	H230
		R387	F311	N231
	L454		F312	S232
	H455	I390	E313	T233
	R456	I391	T314	S234
	R457	R392	Q315	G235
	T458	R393	P316	V236
	I459	G394	L317	A237
	A460	A395	F318	H238
	D461	K396	A319	H239
	A462	L397	P320	M240
	G463	I398	N321	A241
	D464	F399	I322	
	D465	A400	L323	K245
	A466	Y401	T324	D246
	E467	A402	G325	A247
	A468	E403	F326	
	T469	A404	G327	V251
	R470	T405	R328	K252
	A471	V406	Q253	G253
	R472	P407	E330	L254
	L473	L408	G331	L255
	I474	I409	R332	S256
	Q475			Y257
	E476	I412	I336	
	Y477	T413		N261
	E478	R414	N339	
		K415	Q340	P266
	L482	A416	P341	P267
	M483	F417	M342	A268
	P484	G418	Q343	F269
	Y485	G419	F344	P270
			A345	E271
	E489	V423	G346	
	V493	M424	C347	V277
	D494	G425	L348	
		S426	D349	E280
		K427	I350	
	I497	H428		E283
		L429	K355	L284
		G430		
	D501		R358	I287
	T502	L433	F359	V288
	R503	N434		
	R504	L435	C363	N293
	H505	A436	D364	
	I506	V437	Y296	
	V507	P438	N367	D297
	R508			

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	168.49Å 168.49Å 80.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 29.60 – 1.90	Depositor EDS
% Data completeness (in resolution range)	75.7 (50.00-2.00) 70.8 (29.60-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-3.70 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.274 0.317 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8285	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.06% 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: BTN, SO4

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	0.23	0/4032	0.49	2/5478 (0.0%)
1	B	0.24	0/4032	0.49	0/5478
All	All	0.24	0/8064	0.49	2/10956 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	GLY	C-N-CD	-5.88	107.67	120.60
1	A	149	GLY	N-CA-C	5.04	125.69	113.10

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	3952	0	3887	461	0
1	B	3952	0	3887	432	0
2	A	16	0	15	2	0
2	B	16	0	15	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	167	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	172	0	0	13	0
All	All	8285	0	7804	842	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 53.

The worst 5 of 842 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:87:VAL:HB	1:A:117:TYR:CE2	1.33	1.57
1:A:456:ARG:NH1	1:A:457:ARG:HH22	1.30	1.29
1:A:87:VAL:HB	1:A:117:TYR:CD2	1.68	1.26
1:B:113:LEU:HD13	1:B:156:TYR:CE1	1.72	1.25
1:A:456:ARG:NH1	1:A:457:ARG:NH2	1.91	1.18

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	519/530 (98%)	459 (88%)	58 (11%)	2 (0%)	36	31
1	B	519/530 (98%)	458 (88%)	60 (12%)	1 (0%)	49	46
All	All	1038/1060 (98%)	917 (88%)	118 (11%)	3 (0%)	43	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	GLY
1	A	514	ARG
1	B	98	PRO

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	412/421 (98%)	374 (91%)	38 (9%)	10	6
1	B	412/421 (98%)	375 (91%)	37 (9%)	10	6
All	All	824/842 (98%)	749 (91%)	75 (9%)	10	6

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
1	B	39	LYS
1	B	458	THR
1	A	483	ASN
1	B	23	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	ASN
1	A	527	ASN
1	B	483	ASN
1	A	505	HIS
1	B	30	HIS

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](#)

4 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
3	SO4	A	531	-	4,4,4	0.34	0	6,6,6	0.14	0
2	BTN	A	5600	-	14,17,17	4.41	8 (57%)	19,23,23	4.01	8 (42%)
3	SO4	B	531	-	4,4,4	0.30	0	6,6,6	0.13	0
2	BTN	B	5601	-	14,17,17	4.04	8 (57%)	19,23,23	4.25	8 (42%)

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
3	SO4	A	531	-	-	0/0/0/0	0/0/0/0
2	BTN	A	5600	-	-	0/5/28/28	0/2/2/2
3	SO4	B	531	-	-	0/0/0/0	0/0/0/0
2	BTN	B	5601	-	-	0/5/28/28	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5600	BTN	C3-N1	-5.66	1.27	1.35
2	B	5601	BTN	C3-N1	-5.47	1.27	1.35
2	B	5601	BTN	C5-C4	-2.09	1.51	1.56
2	A	5600	BTN	C5-C4	-2.08	1.51	1.56
2	B	5601	BTN	O3-C3	2.66	1.29	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5601	BTN	C4-N2-C3	-8.63	105.05	112.68
2	A	5600	BTN	C4-N2-C3	-8.24	105.39	112.68
2	B	5601	BTN	O3-C3-N2	-8.15	114.86	125.92
2	A	5600	BTN	O3-C3-N2	-7.11	116.28	125.92
2	A	5600	BTN	C6-C5-N1	-6.97	106.10	113.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5600	BTN	2	0
2	B	5601	BTN	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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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