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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 06:06 AM EDT

PDB ID	:	1BNC
Title	:	THREE-DIMENSIONAL STRUCTURE OF THE BIOTIN CARBOXYLASE SUBUNIT OF ACETYL-COA CARBOXYLASE
Authors	:	Waldrop, G.; Rayment, I.; Holden, H.M.
Deposited on	:	1994-07-06
Resolution	:	2.40 Å(reported)

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

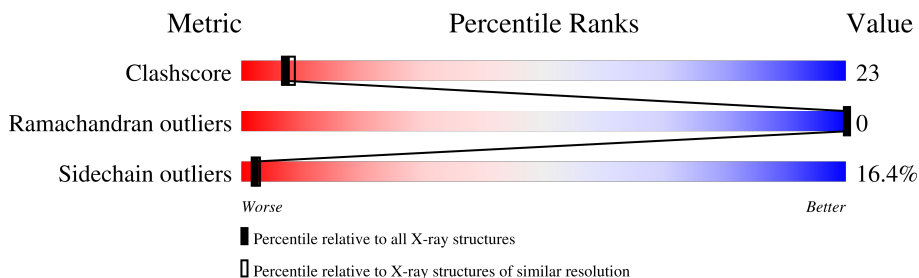|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 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	Percentile Ranks	Value
Clashscore		23
Ramachandran outliers		0
Sidechain outliers		16.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	48% 35% 11% · ·
1	B	449	48% 36% 10% · 6%

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	PO4	B	954	-	X	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6743 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	433	Total 3356	C 2119	N 599	O 617	S 21	0	0	0
1	B	424	Total 3261	C 2059	N 580	O 603	S 19	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O$_4$P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0

- Molecule 3 is water.

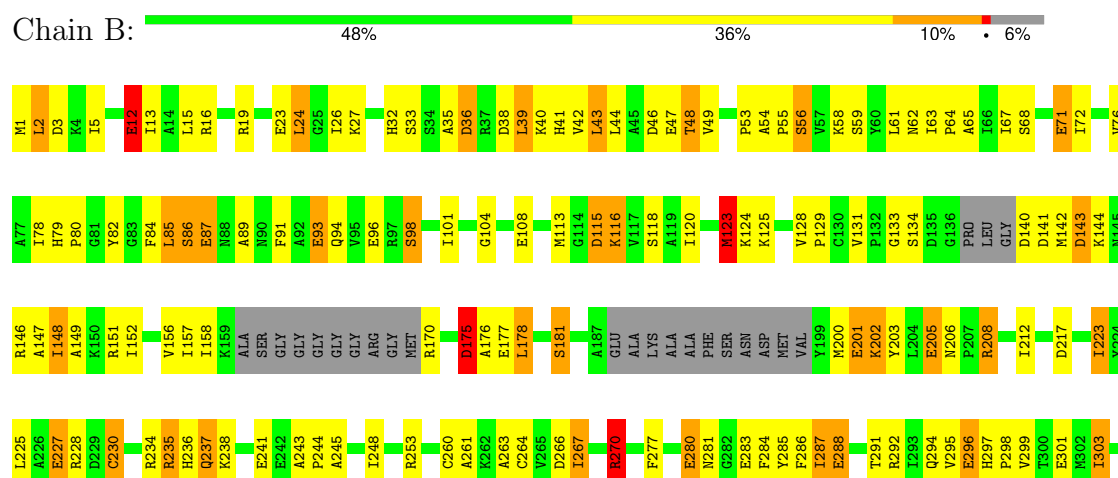| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total 66	O 66	0	0
3	B	50	Total 50	O 50	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Note EDS was not executed.

• Molecule 1: BIOTIN CARBOXYLASE

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D307 L308 I309 Q312 L313 R314 I315 A316 A317 G318 Q319 P320 L321 S322 I323 K324 Q325 E326 E327 R331 G332 H333 A334 V335 E336 C337 R338 I339 E342 D343 F347 L348 R356 F357 P360 E368 S369 H370 I371 Y372 Y375 D382 S383 M384 K387 E393 N394 R395

R401 M402 K403 N404 Q407 E408 L409 I410 I411 D412 K415 T416 N417 V418 D419 L420 Q421 I422 R423 D427 E428 N429 F430 Q431 Y439 L440 E441 K442 K443 L444 G445 L446 Q447 E448 LYS
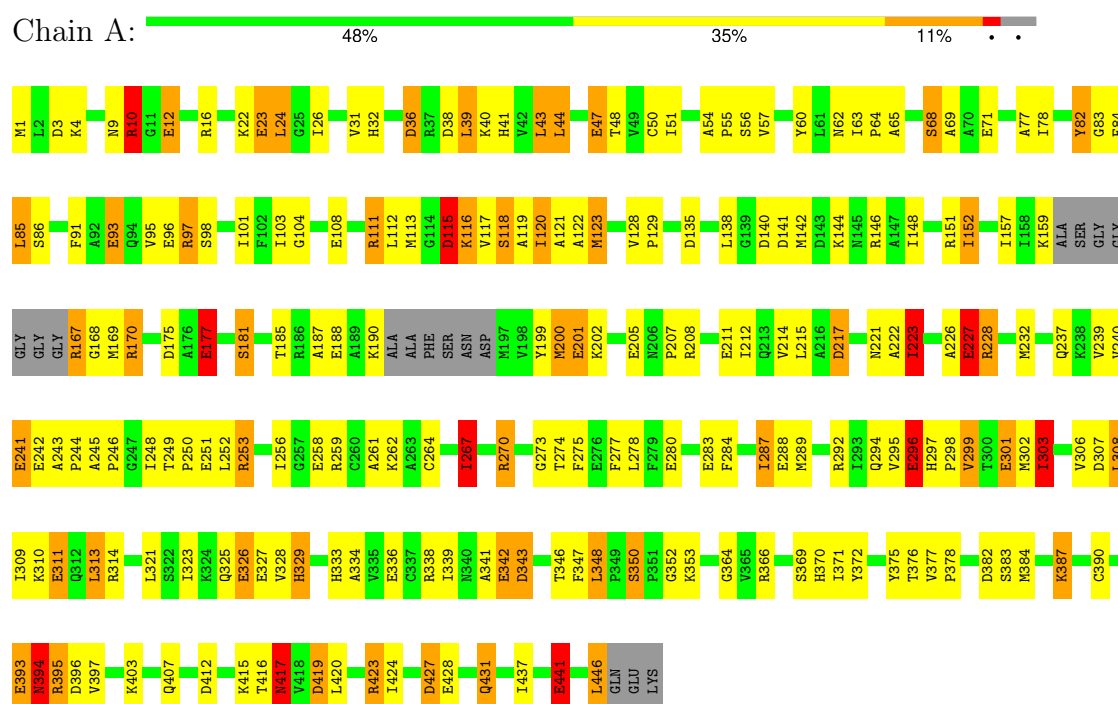
4 Data and refinement statistics ⓘ

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	61.90Å 96.10Å 180.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6743	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	1.08	29/3416 (0.8%)	1.41	48/4609 (1.0%)
1	B	1.05	24/3318 (0.7%)	1.35	33/4480 (0.7%)
All	All	1.06	53/6734 (0.8%)	1.38	81/9089 (0.9%)

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	GLU	CD-OE2	-8.70	1.16	1.25
1	A	47	GLU	CD-OE1	8.29	1.34	1.25
1	A	205	GLU	CD-OE1	7.98	1.34	1.25
1	A	188	GLU	CD-OE2	7.72	1.34	1.25
1	A	311	GLU	CD-OE1	7.66	1.34	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	A	417	ASN	N-CA-CB	-9.33	93.81	110.60
1	B	228	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	B	270	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	175	ASP	CB-CG-OD1	7.92	125.42	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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	3356	0	3391	138	0
1	B	3261	0	3260	163	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
3	A	66	0	0	1	0
3	B	50	0	0	5	0
All	All	6743	0	6651	300	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 23.

The worst 5 of 300 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:157:ILE:HD11	1:A:201:GLU:HB3	1.42	1.00
1:B:244:PRO:HD2	1:B:333:HIS:CD2	2.05	0.91
1:B:203:TYR:HE2	1:B:205:GLU:HG3	1.35	0.90
1:A:264:CYS:O	1:A:267:ILE:HG22	1.74	0.88
1:B:36:ASP:HB3	1:B:39:LEU:HD22	1.55	0.87

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	427/449 (95%)	404 (95%)	23 (5%)	0	100	100
1	B	416/449 (93%)	387 (93%)	29 (7%)	0	100	100
All	All	843/898 (94%)	791 (94%)	52 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	352/361 (98%)	294 (84%)	58 (16%)	2	2
1	B	338/361 (94%)	283 (84%)	55 (16%)	2	3
All	All	690/722 (96%)	577 (84%)	113 (16%)	2	2

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	LEU
1	B	444	LEU
1	B	76	VAL
1	B	415	LYS
1	B	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	417	ASN
1	B	447	GLN
1	B	431	GLN
1	B	145	ASN
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.

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5.5 Carbohydrates (i)

There are no monosaccharides 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	PO4	A	953	-	4,4,4	3.11	3 (75%)	6,6,6	0.51	0
2	PO4	B	954	-	4,4,4	3.04	4 (100%)	6,6,6	0.53	0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	953	PO4	P-O3	-4.59	1.41	1.54
2	B	954	PO4	P-O3	-3.98	1.43	1.54
2	A	953	PO4	P-O4	-3.18	1.45	1.54
2	B	954	PO4	P-O2	-2.98	1.46	1.54
2	B	954	PO4	P-O4	-2.65	1.46	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	953	PO4	1	0
2	B	954	PO4	2	0

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 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.