



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:44 pm GMT

PDB ID : 3GLK  
Title : The biotin carboxylase (BC) domain of human Acetyl-CoA Carboxylase 2 (ACC2)  
Authors : Price, A.; Kulathila, R.  
Deposited on : 2009-03-12  
Resolution : 2.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

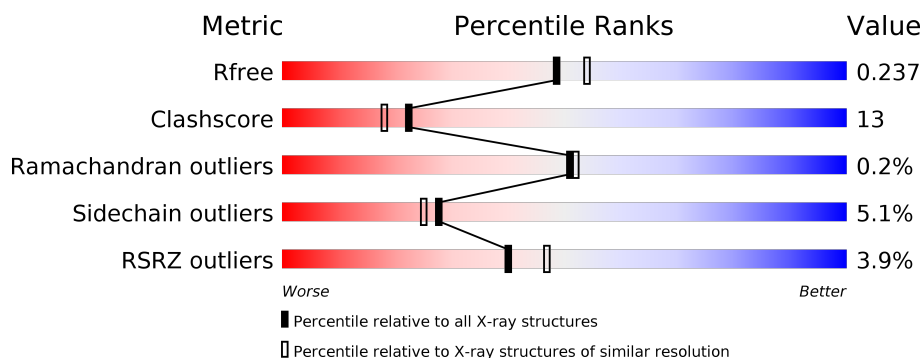
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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  $\geq 3$ , 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	540	<div> <div>3%</div> <div>66%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3935 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 Acetyl-CoA carboxylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3646	2330	621	677	18	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MET	-	EXPRESSION TAG	UNP O00763
A	222	GLY	-	EXPRESSION TAG	UNP O00763
A	223	SER	-	EXPRESSION TAG	UNP O00763
A	224	SER	-	EXPRESSION TAG	UNP O00763
A	225	HIS	-	EXPRESSION TAG	UNP O00763
A	226	HIS	-	EXPRESSION TAG	UNP O00763
A	227	HIS	-	EXPRESSION TAG	UNP O00763
A	228	HIS	-	EXPRESSION TAG	UNP O00763
A	229	HIS	-	EXPRESSION TAG	UNP O00763
A	230	HIS	-	EXPRESSION TAG	UNP O00763
A	231	GLU	-	EXPRESSION TAG	UNP O00763
A	232	ASN	-	EXPRESSION TAG	UNP O00763
A	233	LEU	-	EXPRESSION TAG	UNP O00763
A	234	TYR	-	EXPRESSION TAG	UNP O00763
A	235	PHE	-	EXPRESSION TAG	UNP O00763
A	236	GLN	-	EXPRESSION TAG	UNP O00763
A	237	GLY	-	EXPRESSION TAG	UNP O00763

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	289	Total	O	0	0
			289	289		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.54Å 97.54Å 127.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.28 – 2.10 34.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.6 (33.28-2.10) 94.7 (34.48-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 2.10Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.212 , 0.247 0.205 , 0.237	Depositor DCC
$R_{free}$ test set	2060 reflections (6.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 60.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.57	0/3723	0.68	1/5049 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	379	MET	C-N-CA	-5.26	108.55	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	TYR	Sidechain

### 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	3646	0	3607	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	289	0	0	18	0
All	All	3935	0	3607	95	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 13.

All (95) 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:642:PRO:N	2:A:766:HOH:O	2.08	0.86
1:A:374:PRO:HG2	1:A:379:MET:SD	2.19	0.82
1:A:712:GLU:HB2	2:A:761:HOH:O	1.83	0.79
1:A:499:ARG:HD2	1:A:520:ASP:OD1	1.82	0.79
1:A:416:LEU:N	1:A:416:LEU:HD23	1.97	0.78
1:A:415:ASP:C	1:A:416:LEU:O	2.24	0.70
1:A:686:VAL:HG22	1:A:699:GLN:HG2	1.76	0.67
1:A:385:LYS:HD3	1:A:490:PHE:CZ	2.29	0.66
1:A:502:GLU:HB3	1:A:565:THR:HG23	1.77	0.65
1:A:667:GLY:HA2	2:A:841:HOH:O	1.96	0.65
1:A:475:ILE:HG12	2:A:81:HOH:O	1.97	0.64
1:A:241:ASP:N	2:A:61:HOH:O	2.31	0.63
1:A:594:MET:HG3	1:A:681:TRP:CH2	2.33	0.63
1:A:594:MET:HG3	1:A:681:TRP:HH2	1.64	0.63
1:A:725:SER:HB3	1:A:734:VAL:HG11	1.80	0.63
1:A:484:ILE:HG12	1:A:487:SER:HB2	1.81	0.62
1:A:528:GLN:N	2:A:789:HOH:O	2.31	0.62
1:A:385:LYS:HD3	1:A:490:PHE:HZ	1.65	0.60
1:A:457:GLU:HB2	1:A:484:ILE:HD11	1.85	0.58
1:A:452:MET:SD	1:A:494:LEU:HD21	2.44	0.57
1:A:415:ASP:O	1:A:416:LEU:O	2.22	0.57
1:A:377:GLU:HA	1:A:380:TRP:CE3	2.39	0.56
1:A:466:LYS:HE3	1:A:494:LEU:CD1	2.35	0.56
1:A:544:PHE:HA	1:A:547:MET:CE	2.36	0.56
1:A:358:PRO:O	1:A:361:PRO:HD2	2.06	0.56
1:A:325:ASN:HA	1:A:328:ASN:OD1	2.06	0.55
1:A:521:CYS:SG	1:A:524:GLN:HG2	2.46	0.55
1:A:504:GLN:OE1	1:A:519:ARG:HG3	2.07	0.55
1:A:502:GLU:HB3	1:A:565:THR:CG2	2.37	0.55
1:A:543:ILE:HG22	1:A:547:MET:CE	2.37	0.54
1:A:375:PRO:HB2	1:A:377:GLU:OE2	2.07	0.54
1:A:362:GLU:OE1	1:A:380:TRP:HZ2	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LEU:HD21	1:A:579:LEU:HD11	1.89	0.54
1:A:676:SER:O	1:A:678:LYS:HE2	2.07	0.53
1:A:374:PRO:HG2	1:A:379:MET:CG	2.39	0.53
1:A:731:ARG:N	2:A:100:HOH:O	2.42	0.52
1:A:567:GLU:CD	2:A:105:HOH:O	2.48	0.52
1:A:385:LYS:HE3	2:A:94:HOH:O	2.09	0.52
1:A:523:ILE:HD12	1:A:531:VAL:HG21	1.91	0.52
1:A:377:GLU:CD	1:A:377:GLU:H	2.13	0.51
1:A:723:GLU:O	1:A:726:ILE:HG12	2.10	0.51
1:A:409:VAL:CG1	1:A:410:GLU:N	2.73	0.51
1:A:411:TRP:CE3	1:A:413:GLU:HG3	2.46	0.51
1:A:529:LYS:HD2	1:A:532:GLU:OE2	2.10	0.50
1:A:290:GLU:HG3	1:A:291:ARG:HG2	1.93	0.49
1:A:496:GLN:HA	2:A:833:HOH:O	2.12	0.49
1:A:499:ARG:NH1	1:A:520:ASP:OD2	2.45	0.49
1:A:567:GLU:CG	2:A:105:HOH:O	2.61	0.49
1:A:402:TRP:HB2	1:A:491:LEU:O	2.13	0.48
1:A:544:PHE:HA	1:A:547:MET:HE3	1.96	0.48
1:A:333:GLU:H	1:A:333:GLU:CD	2.18	0.47
1:A:468:GLU:HB2	2:A:146:HOH:O	2.14	0.47
1:A:528:GLN:HA	2:A:173:HOH:O	2.14	0.47
1:A:584:ARG:HH12	1:A:586:GLN:HG3	1.80	0.47
1:A:501:LEU:HD21	1:A:538:ILE:HG21	1.97	0.47
1:A:502:GLU:HG2	1:A:567:GLU:OE1	2.14	0.47
1:A:435:LYS:NZ	2:A:72:HOH:O	2.48	0.46
1:A:544:PHE:HA	1:A:547:MET:HE2	1.98	0.46
1:A:473:PHE:N	1:A:474:PRO:HD2	2.30	0.46
1:A:413:GLU:O	1:A:414:ASP:O	2.33	0.45
1:A:543:ILE:HG22	1:A:547:MET:HE2	1.97	0.45
1:A:391:VAL:HG13	1:A:422:ILE:HD13	1.99	0.45
1:A:466:LYS:HE3	1:A:494:LEU:HD11	1.98	0.45
1:A:379:MET:HE3	1:A:583:PRO:HG2	1.98	0.44
1:A:493:LYS:HG3	1:A:494:LEU:O	2.17	0.44
1:A:379:MET:CE	1:A:583:PRO:CG	2.95	0.44
1:A:528:GLN:N	2:A:173:HOH:O	2.49	0.44
1:A:415:ASP:N	1:A:415:ASP:OD2	2.30	0.44
1:A:569:LEU:HD22	1:A:579:LEU:HG	2.00	0.44
1:A:744:GLU:HG3	2:A:814:HOH:O	2.18	0.44
1:A:543:ILE:HG22	1:A:547:MET:HE1	1.98	0.43
1:A:329:TYR:O	1:A:335:ILE:HD11	2.18	0.43
1:A:247:PRO:O	1:A:251:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LEU:CD2	1:A:579:LEU:HD11	2.48	0.43
1:A:357:ASN:HA	1:A:358:PRO:HD3	1.87	0.43
1:A:499:ARG:HH11	1:A:520:ASP:CG	2.21	0.43
1:A:569:LEU:O	1:A:576:PHE:HA	2.19	0.43
1:A:485:PRO:HB3	2:A:39:HOH:O	2.19	0.43
1:A:251:VAL:HG21	1:A:259:VAL:HA	2.01	0.42
1:A:325:ASN:HD22	1:A:325:ASN:N	2.17	0.42
1:A:589:HIS:N	1:A:590:PRO:CD	2.82	0.42
1:A:416:LEU:HD22	1:A:416:LEU:HA	1.82	0.42
1:A:414:ASP:C	1:A:416:LEU:H	2.21	0.42
1:A:523:ILE:HD12	1:A:531:VAL:CG2	2.50	0.42
1:A:677:SER:OG	1:A:720:ALA:HA	2.20	0.42
1:A:300:THR:HB	1:A:302:GLU:OE2	2.20	0.42
1:A:377:GLU:HG3	1:A:421:ARG:NH1	2.35	0.42
1:A:567:GLU:HG3	2:A:105:HOH:O	2.20	0.41
1:A:569:LEU:CD2	1:A:579:LEU:HG	2.49	0.41
1:A:581:LEU:C	1:A:581:LEU:HD12	2.41	0.41
1:A:594:MET:HE2	1:A:594:MET:HB3	1.87	0.41
1:A:436:ASP:H	1:A:439:GLU:HG2	1.84	0.41
1:A:303:ASP:OD1	1:A:667:GLY:N	2.54	0.40
1:A:379:MET:HE2	1:A:583:PRO:CG	2.52	0.40
1:A:648:VAL:HA	1:A:705:SER:O	2.21	0.40

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	447/540 (83%)	429 (96%)	17 (4%)	1 (0%)	51	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	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	391/450 (87%)	371 (95%)	20 (5%)	28 25

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	ASP
1	A	281	ARG
1	A	286	MET
1	A	325	ASN
1	A	341	ARG
1	A	372	LEU
1	A	377	GLU
1	A	415	ASP
1	A	416	LEU
1	A	423	SER
1	A	468	GLU
1	A	484	ILE
1	A	581	LEU
1	A	586	GLN
1	A	668	THR
1	A	673	ASN
1	A	677	SER
1	A	724	LEU
1	A	726	ILE
1	A	745	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	ASN

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Mol	Chain	Res	Type
1	A	509	GLN
1	A	699	GLN
1	A	747	GLN

### 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](#)

There are no ligands in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	465/540 (86%)	0.06	18 (3%)	40 47	15, 27, 51, 70	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	LEU	6.3
1	A	380	TRP	6.3
1	A	731	ARG	5.0
1	A	686	VAL	4.3
1	A	379	MET	3.8
1	A	415	ASP	3.8
1	A	699	GLN	3.7
1	A	412	THR	3.6
1	A	427	ASP	3.5
1	A	673	ASN	3.3
1	A	667	GLY	3.3
1	A	410	GLU	3.0
1	A	700	PHE	2.9
1	A	413	GLU	2.9
1	A	426	GLU	2.4
1	A	475	ILE	2.1
1	A	446	ARG	2.1
1	A	636	GLU	2.0

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

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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.