



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:35 pm GMT

PDB ID : 2HJW
Title : Crystal Structure of the BC domain of ACC2
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Deposited on : 2006-07-02
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
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

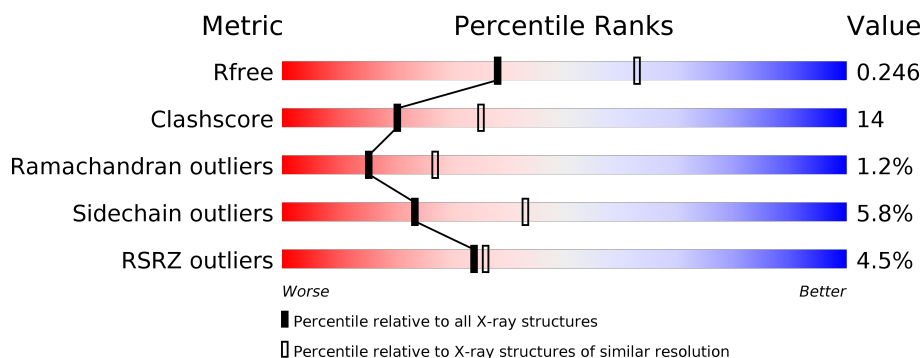
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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. 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	573	<div> <div>4%</div> <div>61%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3958 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
1	A	494	Total	C	N	O	S	0	0	0
			3871	2468	671	714	18			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	MET	-	CLONING ARTIFACT	UNP Q6KE87
A	212	ARG	-	CLONING ARTIFACT	UNP Q6KE87
A	213	GLY	-	CLONING ARTIFACT	UNP Q6KE87
A	214	SER	-	CLONING ARTIFACT	UNP Q6KE87
A	215	GLY	-	CLONING ARTIFACT	UNP Q6KE87
A	216	SER	-	CLONING ARTIFACT	UNP Q6KE87
A	776	LEU	-	EXPRESSION TAG	UNP Q6KE87
A	777	GLU	-	EXPRESSION TAG	UNP Q6KE87
A	778	HIS	-	EXPRESSION TAG	UNP Q6KE87
A	779	HIS	-	EXPRESSION TAG	UNP Q6KE87
A	780	HIS	-	EXPRESSION TAG	UNP Q6KE87
A	781	HIS	-	EXPRESSION TAG	UNP Q6KE87
A	782	HIS	-	EXPRESSION TAG	UNP Q6KE87
A	783	HIS	-	EXPRESSION TAG	UNP Q6KE87

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	87	Total	O	0	0
			87	87		

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: Acetyl-CoA carboxylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	75.80Å 75.80Å 189.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.86 – 2.50 38.35 – 2.49	Depositor EDS
% Data completeness (in resolution range)	86.5 (19.86-2.50) 86.1 (38.35-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.248 0.211 , 0.246	Depositor DCC
R_{free} test set	932 reflections (4.79%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3958	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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](#)

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	0/3961	0.57	0/5376

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	3871	0	3826	108	0
2	A	87	0	0	1	0
All	All	3958	0	3826	108	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 14.

All (108) 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:267:ASN:HD22	1:A:268:ASN:H	0.93	0.93
1:A:267:ASN:ND2	1:A:268:ASN:H	1.69	0.90
1:A:385:LYS:HG2	1:A:490:PHE:CZ	2.06	0.90
1:A:254:PHE:HA	1:A:615:ARG:HH12	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HD22	1:A:268:ASN:N	1.69	0.89
1:A:273:VAL:HG21	1:A:669:VAL:HG11	1.54	0.87
1:A:709:ASN:ND2	1:A:712:GLU:H	1.79	0.81
1:A:325:ASN:HA	1:A:328:ASN:OD1	1.87	0.74
1:A:254:PHE:HA	1:A:615:ARG:NH1	2.05	0.69
1:A:621:LEU:HD21	1:A:627:PRO:HG3	1.75	0.68
1:A:262:LYS:HG2	1:A:344:VAL:HA	1.76	0.67
1:A:280:ARG:HB3	1:A:290:GLU:HG2	1.77	0.67
1:A:464:ILE:O	1:A:465:ARG:HD3	1.95	0.67
1:A:708:GLU:CD	1:A:708:GLU:H	1.97	0.66
1:A:615:ARG:HE	1:A:630:VAL:HG13	1.62	0.65
1:A:325:ASN:N	1:A:325:ASN:HD22	1.94	0.64
1:A:569:LEU:O	1:A:576:PHE:HA	1.98	0.63
1:A:478:ARG:HA	1:A:481:GLN:HE21	1.64	0.63
1:A:465:ARG:HG3	1:A:476:LEU:HD22	1.80	0.63
1:A:473:PHE:HB3	1:A:474:PRO:HD3	1.81	0.62
1:A:739:ASN:O	1:A:743:THR:HG23	1.99	0.62
1:A:572:GLN:CD	1:A:572:GLN:H	2.01	0.62
1:A:709:ASN:HD22	1:A:709:ASN:C	2.07	0.58
1:A:264:LEU:HB2	1:A:344:VAL:HG11	1.85	0.58
1:A:724:LEU:HD22	1:A:730:PHE:CG	2.39	0.57
1:A:581:LEU:C	1:A:581:LEU:HD23	2.25	0.57
1:A:296:VAL:HA	1:A:316:HIS:O	2.05	0.56
1:A:589:HIS:ND1	1:A:590:PRO:HD3	2.20	0.56
1:A:276:MET:CE	1:A:295:PHE:HB3	2.36	0.56
1:A:477:PHE:O	1:A:481:GLN:HG3	2.06	0.55
1:A:361:PRO:HB3	1:A:371:PHE:CD2	2.41	0.55
1:A:436:ASP:OD1	1:A:438:ASP:HB2	2.07	0.55
1:A:385:LYS:HD2	1:A:389:THR:OG1	2.07	0.55
1:A:655:SER:O	1:A:733:THR:HG21	2.08	0.54
1:A:276:MET:HE1	1:A:314:ALA:HB2	1.90	0.53
1:A:530:ILE:HG22	1:A:531:VAL:HG23	1.91	0.53
1:A:452:MET:SD	1:A:494:LEU:HD13	2.49	0.52
1:A:305:LYS:HA	1:A:305:LYS:HE3	1.91	0.52
1:A:709:ASN:HD21	1:A:712:GLU:H	1.57	0.51
1:A:296:VAL:HG22	1:A:316:HIS:HB2	1.93	0.51
1:A:310:TYR:HA	1:A:313:MET:HE3	1.92	0.51
1:A:508:ASP:OD2	1:A:512:ASN:HB2	2.10	0.51
1:A:519:ARG:NH2	1:A:586:GLN:OE1	2.44	0.51
1:A:753:THR:O	1:A:756:LEU:HD13	2.11	0.51
1:A:378:ALA:N	1:A:421:ARG:HH11	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:ARG:HB3	1:A:729:ASP:OD1	2.11	0.50
1:A:276:MET:HE3	1:A:295:PHE:HB3	1.94	0.50
1:A:262:LYS:CG	1:A:344:VAL:HA	2.43	0.49
1:A:584:ARG:HH12	1:A:586:GLN:HA	1.77	0.49
1:A:728:GLY:O	1:A:731:ARG:HG2	2.12	0.49
1:A:332:VAL:O	1:A:336:VAL:HG23	2.12	0.49
1:A:669:VAL:HG13	1:A:669:VAL:O	2.12	0.49
1:A:538:ILE:HD11	1:A:751:ILE:HA	1.94	0.49
1:A:561:VAL:O	1:A:562:SER:HB3	2.13	0.49
1:A:584:ARG:HH11	1:A:584:ARG:HG3	1.78	0.48
1:A:439:GLU:HA	1:A:442:GLU:HB2	1.96	0.48
1:A:744:GLU:HG2	1:A:748:ASN:HD21	1.79	0.47
1:A:751:ILE:HG23	1:A:752:ASP:N	2.29	0.47
1:A:523:ILE:HD12	1:A:523:ILE:N	2.29	0.47
1:A:755:TRP:HA	1:A:758:TYR:CE1	2.50	0.47
1:A:435:LYS:HE3	1:A:439:GLU:OE2	2.14	0.47
1:A:589:HIS:CG	1:A:590:PRO:HD3	2.50	0.47
1:A:725:SER:HA	1:A:730:PHE:O	2.15	0.47
1:A:729:ASP:N	1:A:729:ASP:OD1	2.47	0.46
1:A:419:GLY:O	1:A:420:LYS:HB3	2.16	0.46
1:A:375:PRO:HD3	1:A:561:VAL:HB	1.98	0.46
1:A:594:MET:HE1	1:A:681:TRP:HE1	1.81	0.46
1:A:436:ASP:OD1	1:A:439:GLU:HG2	2.16	0.46
1:A:709:ASN:HD22	1:A:712:GLU:H	1.56	0.46
1:A:402:TRP:HB2	1:A:491:LEU:O	2.16	0.46
1:A:286:MET:HA	1:A:286:MET:CE	2.46	0.45
1:A:264:LEU:HD12	1:A:265:ILE:N	2.31	0.45
1:A:360:LEU:HB3	1:A:361:PRO:CD	2.47	0.45
1:A:377:GLU:C	1:A:421:ARG:HH11	2.21	0.45
1:A:680:VAL:HG11	1:A:720:ALA:CB	2.47	0.45
1:A:724:LEU:HD22	1:A:730:PHE:CD1	2.52	0.44
1:A:683:TYR:CE1	1:A:702:HIS:HB2	2.52	0.44
1:A:273:VAL:CG2	1:A:669:VAL:HG11	2.38	0.44
1:A:736:TYR:CE2	1:A:737:LEU:HG	2.52	0.44
1:A:325:ASN:N	1:A:325:ASN:ND2	2.63	0.44
1:A:378:ALA:N	1:A:421:ARG:NH1	2.65	0.44
1:A:284:TYR:O	1:A:288:ARG:HA	2.18	0.44
1:A:465:ARG:CG	1:A:476:LEU:HD22	2.45	0.44
1:A:340:LYS:O	1:A:343:PRO:HB3	2.18	0.43
1:A:334:LEU:O	1:A:338:ILE:HG13	2.18	0.43
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:THR:O	1:A:735:GLU:HB2	2.19	0.43
1:A:724:LEU:HD13	1:A:734:VAL:HG11	2.01	0.43
1:A:553:ARG:HG3	1:A:553:ARG:HH11	1.84	0.42
1:A:676:SER:HB3	1:A:719:VAL:HG12	2.00	0.42
1:A:652:ARG:HG3	1:A:702:HIS:CE1	2.54	0.42
1:A:377:GLU:HB2	1:A:421:ARG:NH1	2.35	0.42
1:A:630:VAL:HG12	2:A:58:HOH:O	2.19	0.42
1:A:589:HIS:N	1:A:590:PRO:CD	2.82	0.42
1:A:710:ARG:O	1:A:714:ILE:HG13	2.19	0.42
1:A:267:ASN:ND2	1:A:268:ASN:N	2.46	0.41
1:A:543:ILE:HG22	1:A:547:MET:HE2	2.02	0.41
1:A:251:VAL:HG21	1:A:259:VAL:HA	2.01	0.41
1:A:596:ALA:O	1:A:598:VAL:HG23	2.19	0.41
1:A:584:ARG:NH1	1:A:584:ARG:HG3	2.34	0.41
1:A:523:ILE:HG22	1:A:530:ILE:HB	2.02	0.41
1:A:594:MET:HE1	1:A:704:PHE:HB3	2.02	0.41
1:A:740:LEU:HD23	1:A:740:LEU:C	2.41	0.41
1:A:385:LYS:HE2	1:A:490:PHE:CE1	2.56	0.40
1:A:594:MET:CE	1:A:681:TRP:HE1	2.35	0.40
1:A:244:VAL:HG21	1:A:250:PHE:HB2	2.03	0.40
1:A:496:GLN:O	1:A:497:HIS:C	2.60	0.40
1:A:600:LEU:HB2	1:A:601:PRO:HD3	2.02	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	486/573 (85%)	451 (93%)	29 (6%)	6 (1%)	15 27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	573	ASP
1	A	497	HIS
1	A	562	SER
1	A	420	LYS
1	A	574	GLY
1	A	422	ILE

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	412/478 (86%)	388 (94%)	24 (6%)	23	43

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	281	ARG
1	A	289	ASN
1	A	305	LYS
1	A	325	ASN
1	A	410	GLU
1	A	445	GLU
1	A	465	ARG
1	A	479	GLN
1	A	496	GLN
1	A	497	HIS
1	A	521	CYS
1	A	572	GLN
1	A	573	ASP
1	A	582	ASN
1	A	590	PRO
1	A	615	ARG
1	A	708	GLU
1	A	709	ASN
1	A	711	GLU
1	A	724	LEU

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Mol	Chain	Res	Type
1	A	729	ASP
1	A	749	ASN
1	A	752	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	289	ASN
1	A	325	ASN
1	A	327	ASN
1	A	367	ASN
1	A	481	GLN
1	A	496	GLN
1	A	512	ASN
1	A	524	GLN
1	A	572	GLN
1	A	699	GLN
1	A	709	ASN
1	A	716	ASN
1	A	739	ASN
1	A	747	GLN
1	A	748	ASN
1	A	749	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.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	494/573 (86%)	0.29	22 (4%) 34 36	26, 47, 73, 96	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	ARG	5.0
1	A	239	HIS	4.0
1	A	759	LEU	3.9
1	A	686	VAL	3.7
1	A	420	LYS	3.5
1	A	497	HIS	3.3
1	A	242	PHE	3.0
1	A	307	ASN	3.0
1	A	304	LEU	3.0
1	A	730	PHE	2.7
1	A	526	ARG	2.6
1	A	758	TYR	2.5
1	A	411	TRP	2.3
1	A	305	LYS	2.2
1	A	306	ALA	2.2
1	A	731	ARG	2.2
1	A	525	ARG	2.2
1	A	496	GLN	2.2
1	A	527	HIS	2.1
1	A	672	LEU	2.1
1	A	727	ARG	2.1
1	A	755	TRP	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.