



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:33 PM UTC

PDB ID : 4N45 / pdb_00004n45
Title : Crystal structure of reduced form of thiolase from Clostridium acetobutylicum
Authors : Kim, S.; Ha, S.C.; Ahn, J.W.; Kim, E.J.; Lim, J.H.; Kim, K.J.
Deposited on : 2013-10-08
Resolution : 1.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

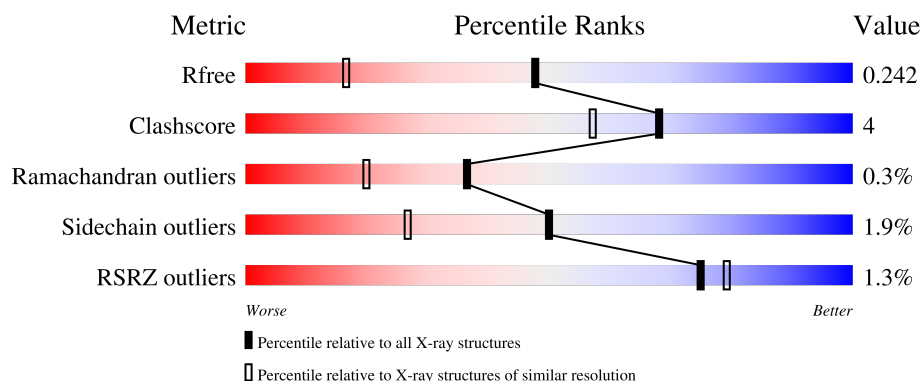
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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	400	% 89% 8% .
1	B	400	2% 88% 10% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6337 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 acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			2892	1824	501	553	14			
1	B	392	Total	C	N	O	S	0	0	0
			2892	1824	501	553	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	SER	CYS	engineered mutation	UNP F0K5D8
A	393	LEU	-	expression tag	UNP F0K5D8
A	394	GLU	-	expression tag	UNP F0K5D8
A	395	HIS	-	expression tag	UNP F0K5D8
A	396	HIS	-	expression tag	UNP F0K5D8
A	397	HIS	-	expression tag	UNP F0K5D8
A	398	HIS	-	expression tag	UNP F0K5D8
A	399	HIS	-	expression tag	UNP F0K5D8
A	400	HIS	-	expression tag	UNP F0K5D8
B	378	SER	CYS	engineered mutation	UNP F0K5D8
B	393	LEU	-	expression tag	UNP F0K5D8
B	394	GLU	-	expression tag	UNP F0K5D8
B	395	HIS	-	expression tag	UNP F0K5D8
B	396	HIS	-	expression tag	UNP F0K5D8
B	397	HIS	-	expression tag	UNP F0K5D8
B	398	HIS	-	expression tag	UNP F0K5D8
B	399	HIS	-	expression tag	UNP F0K5D8
B	400	HIS	-	expression tag	UNP F0K5D8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	303	Total	O	0	0
			303	303		

Continued on next page...

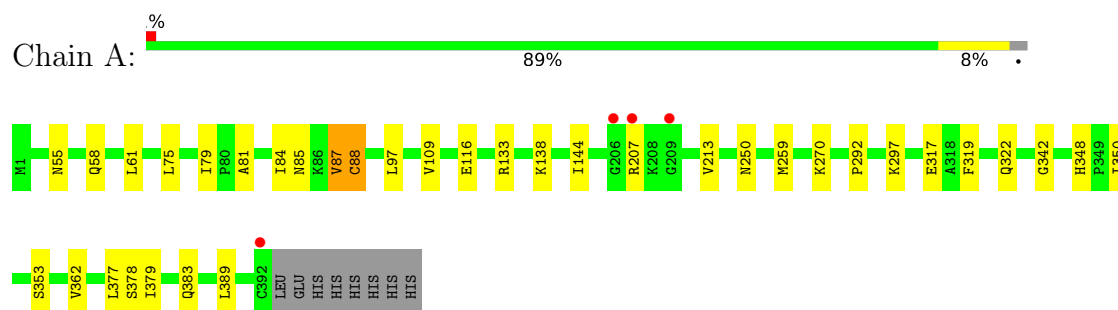
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	250	Total 250	O 250	0	0

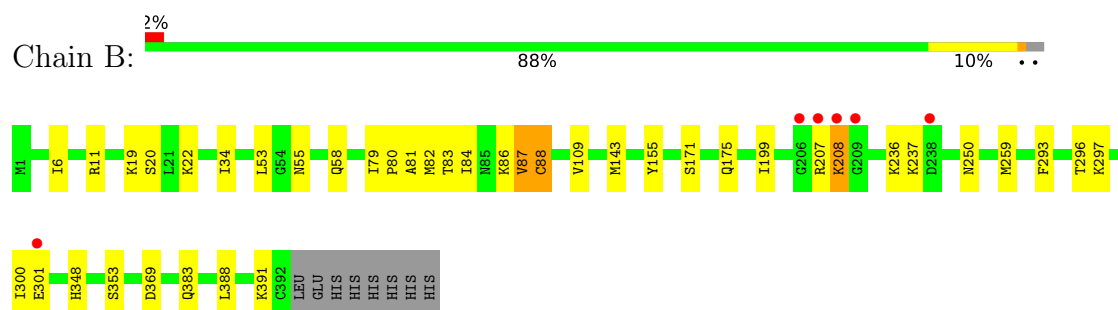
3 Residue-property plots [i](#)

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 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 acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	203.68Å 54.14Å 73.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 50.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-1.60) 91.9 (50.00-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.234 0.203 , 0.242	Depositor DCC
R_{free} test set	4925 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6337	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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

5.1 Standard geometry

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	1.25	4/2933 (0.1%)	1.13	5/3958 (0.1%)
1	B	1.21	8/2933 (0.3%)	1.13	1/3958 (0.0%)
All	All	1.23	12/5866 (0.2%)	1.13	6/7916 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	ILE	CA-C	6.89	1.60	1.52
1	A	144	ILE	C-O	6.06	1.30	1.24
1	B	86	LYS	C-O	-5.92	1.15	1.23
1	B	388	LEU	CA-C	5.72	1.59	1.52
1	A	213	VAL	C-O	-5.70	1.18	1.24
1	B	19	LYS	C-O	-5.59	1.17	1.24
1	B	143	MET	N-CA	5.51	1.52	1.46
1	A	138	LYS	C-O	-5.50	1.17	1.24
1	B	6	ILE	C-O	5.44	1.30	1.23
1	B	20	SER	C-O	-5.20	1.18	1.24
1	B	83	THR	C-O	-5.15	1.17	1.24
1	A	116	GLU	C-O	-5.11	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	LYS	CA-C-N	-8.64	111.84	120.31
1	A	270	LYS	C-N-CA	-8.64	111.84	120.31
1	A	350	ILE	N-CA-C	6.32	117.00	110.36
1	B	88	CYS	CA-CB-SG	-6.21	100.13	114.40
1	A	88	CYS	CA-CB-SG	-5.26	102.30	114.40
1	A	378	SER	CA-CB-OG	5.05	121.21	111.10

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	2892	0	2963	26	0
1	B	2892	0	2963	24	0
2	A	303	0	0	2	0
2	B	250	0	0	2	0
All	All	6337	0	5926	42	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 4.

All (42) 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:362:VAL:HG12	1:A:389:LEU:CD1	2.20	0.71
1:A:84:ILE:CD1	1:B:84:ILE:HD12	2.25	0.67
1:A:79:ILE:HD11	2:A:629:HOH:O	1.93	0.67
1:A:362:VAL:HG12	1:A:389:LEU:HD13	1.75	0.66
1:B:22:LYS:HE2	2:B:651:HOH:O	1.98	0.63
1:A:84:ILE:HD12	1:B:84:ILE:HD12	1.84	0.59
1:A:250:ASN:HD22	1:A:348:HIS:H	1.51	0.59
1:A:383:GLN:HE22	1:B:81:ALA:H	1.52	0.58
1:A:362:VAL:CG1	1:A:389:LEU:CD1	2.82	0.57
1:A:133:ARG:HD2	2:A:689:HOH:O	2.07	0.55
1:A:133:ARG:HH11	1:A:133:ARG:HG2	1.72	0.54
1:B:293:PHE:CZ	1:B:297:LYS:HD2	2.43	0.53
1:A:81:ALA:H	1:B:383:GLN:HE22	1.56	0.53
1:B:250:ASN:HD22	1:B:348:HIS:H	1.56	0.52
1:A:250:ASN:ND2	1:A:348:HIS:H	2.07	0.52
1:A:85:ASN:HD22	1:B:58:GLN:NE2	2.08	0.52
1:B:55:ASN:HD22	1:B:58:GLN:HG2	1.74	0.52
1:A:88:CYS:HG	1:A:348:HIS:CE1	2.29	0.51
1:B:171:SER:O	1:B:175:GLN:HG3	2.11	0.51
1:B:296:THR:HG22	1:B:300:ILE:HD12	1.93	0.50
1:B:34:ILE:HD11	1:B:53:LEU:HD11	1.94	0.49
1:A:55:ASN:HD22	1:A:58:GLN:HG2	1.78	0.48
1:B:109:VAL:HG22	1:B:259:MET:HE3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASN:ND2	1:A:58:GLN:HG2	2.29	0.47
1:A:97:LEU:HD21	1:B:82:MET:HE1	1.96	0.47
1:B:293:PHE:O	1:B:297:LYS:HG3	2.14	0.47
1:B:301:GLU:HG3	2:B:681:HOH:O	2.14	0.47
1:B:207:ARG:HB2	1:B:208:LYS:HD2	1.96	0.47
1:B:55:ASN:ND2	1:B:58:GLN:HG2	2.30	0.46
1:B:250:ASN:ND2	1:B:348:HIS:H	2.14	0.45
1:A:317:GLU:CD	1:A:342:GLY:HA3	2.41	0.45
1:A:109:VAL:HG22	1:A:259:MET:HE3	1.99	0.44
1:B:11:ARG:O	1:B:199:ILE:HA	2.18	0.44
1:A:379:ILE:HB	1:A:383:GLN:HB2	2.00	0.43
1:B:369:ASP:HA	1:B:391:LYS:HE2	1.99	0.43
1:A:319:PHE:H	1:A:322:GLN:HE21	1.65	0.43
1:A:55:ASN:HD21	1:A:61:LEU:HD12	1.81	0.43
1:A:362:VAL:CG1	1:A:389:LEU:HD13	2.45	0.42
1:B:88:CYS:HG	1:B:348:HIS:CE1	2.37	0.42
1:A:292:PRO:HG3	1:A:377:LEU:C	2.45	0.41
1:A:383:GLN:NE2	1:B:80:PRO:HA	2.36	0.40
1:A:85:ASN:HD22	1:B:58:GLN:HE22	1.68	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	390/400 (98%)	375 (96%)	14 (4%)	1 (0%)	36	20
1	B	390/400 (98%)	378 (97%)	11 (3%)	1 (0%)	36	20
All	All	780/800 (98%)	753 (96%)	25 (3%)	2 (0%)	36	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	B	87	VAL

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	294/302 (97%)	289 (98%)	5 (2%)	53	30
1	B	294/302 (97%)	288 (98%)	6 (2%)	48	24
All	All	588/604 (97%)	577 (98%)	11 (2%)	50	27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	87	VAL
1	A	207	ARG
1	A	297	LYS
1	A	353	SER
1	B	87	VAL
1	B	155	TYR
1	B	208	LYS
1	B	236	LYS
1	B	237	LYS
1	B	353	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	58	GLN
1	A	153	ASN
1	A	194	GLN
1	A	250	ASN
1	A	322	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	383	GLN
1	B	55	ASN
1	B	58	GLN
1	B	153	ASN
1	B	194	GLN
1	B	250	ASN
1	B	316	ASN
1	B	383	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 oligosaccharides 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 [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	392/400 (98%)	-0.18	4 (1%) 79 83	11, 17, 30, 60	0
1	B	392/400 (98%)	0.05	6 (1%) 72 76	11, 19, 35, 73	0
All	All	784/800 (98%)	-0.06	10 (1%) 75 79	11, 18, 33, 73	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	GLY	3.2
1	A	209	GLY	3.0
1	B	207	ARG	2.8
1	B	208	LYS	2.5
1	B	209	GLY	2.5
1	B	301	GLU	2.4
1	A	206	GLY	2.4
1	A	207	ARG	2.2
1	B	238	ASP	2.1
1	A	392	CYS	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 oligosaccharides 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.