



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:59 PM UTC

PDB ID : 3BIL / pdb_00003bil
Title : Crystal structure of a probable LacI family transcriptional regulator from *Corynebacterium glutamicum*
Authors : Bonanno, J.B.; Freeman, J.; Bain, K.T.; Mendoza, M.; Ozyurt, S.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-11-30
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

<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

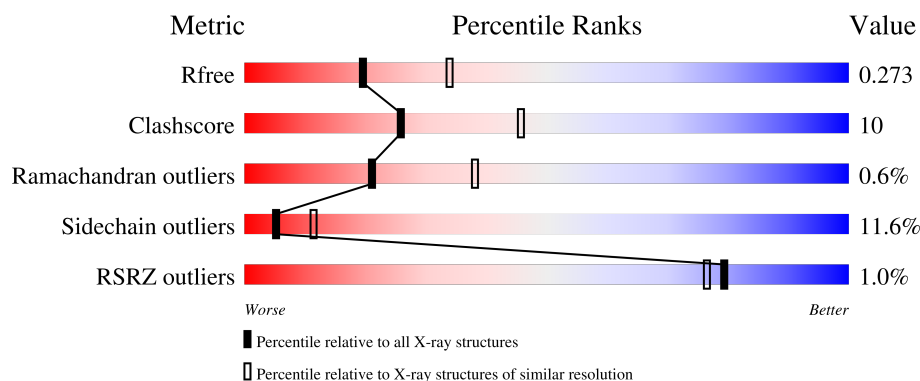
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	348	53% 17% 26%
1	B	348	59% 12% 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3842 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 Probable LacI-family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			1911	1202	319	380	10			
1	B	257	Total	C	N	O	S	0	1	0
			1911	1202	319	380	10			

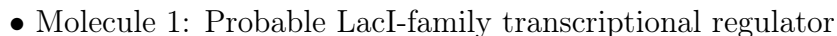
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q8NQQ9
A	1	SER	-	expression tag	UNP Q8NQQ9
A	2	LEU	-	expression tag	UNP Q8NQQ9
A	340	GLU	-	expression tag	UNP Q8NQQ9
A	341	GLY	-	expression tag	UNP Q8NQQ9
A	342	HIS	-	expression tag	UNP Q8NQQ9
A	343	HIS	-	expression tag	UNP Q8NQQ9
A	344	HIS	-	expression tag	UNP Q8NQQ9
A	345	HIS	-	expression tag	UNP Q8NQQ9
A	346	HIS	-	expression tag	UNP Q8NQQ9
A	347	HIS	-	expression tag	UNP Q8NQQ9
B	0	MET	-	expression tag	UNP Q8NQQ9
B	1	SER	-	expression tag	UNP Q8NQQ9
B	2	LEU	-	expression tag	UNP Q8NQQ9
B	340	GLU	-	expression tag	UNP Q8NQQ9
B	341	GLY	-	expression tag	UNP Q8NQQ9
B	342	HIS	-	expression tag	UNP Q8NQQ9
B	343	HIS	-	expression tag	UNP Q8NQQ9
B	344	HIS	-	expression tag	UNP Q8NQQ9
B	345	HIS	-	expression tag	UNP Q8NQQ9
B	346	HIS	-	expression tag	UNP Q8NQQ9
B	347	HIS	-	expression tag	UNP Q8NQQ9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	O	0	0
			11	11		
2	B	9	Total	O	0	0
			9	9		

- Molecule 1: Probable LacI-family transcriptional regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.21Å 54.34Å 78.65Å 90.00° 94.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.50) 99.7 (20.00-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.278 0.215 , 0.273	Depositor DCC
R_{free} test set	1117 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3842	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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	0.96	0/1942	1.12	7/2641 (0.3%)
1	B	0.97	1/1942 (0.1%)	1.13	4/2641 (0.2%)
All	All	0.97	1/3884 (0.0%)	1.13	11/5282 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	ILE	CA-CB	5.38	1.58	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	VAL	CB-CA-C	-6.20	103.92	112.04
1	A	330	GLU	N-CA-C	5.84	119.63	111.56
1	B	72	VAL	CB-CA-C	5.60	114.82	109.33
1	B	183	ALA	N-CA-C	-5.49	103.73	110.65
1	A	231	GLU	N-CA-C	-5.24	105.48	111.14
1	A	322	ILE	CA-C-N	-5.13	115.44	120.52
1	A	322	ILE	C-N-CA	-5.13	115.44	120.52
1	B	273	ILE	CB-CA-C	-5.12	103.20	110.83
1	B	228	VAL	N-CA-C	5.07	115.68	110.36
1	A	72	VAL	CB-CA-C	5.04	114.27	109.33
1	A	86	GLU	N-CA-C	5.00	117.62	111.82

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	1911	0	1914	47	0
1	B	1911	0	1914	32	0
2	A	11	0	0	2	0
2	B	9	0	0	0	0
All	All	3842	0	3828	73	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 10.

All (73) 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:B:149:LEU:HB2	1:B:162:THR:HG22	1.50	0.93
1:B:122:VAL:O	1:B:145:MET:HE1	1.71	0.90
1:A:170:GLY:H	1:A:324:THR:HG22	1.43	0.82
1:B:170:GLY:H	1:B:324:THR:HG22	1.46	0.80
1:A:122:VAL:O	1:A:145:MET:HE1	1.82	0.79
1:A:99:ILE:CG2	1:B:99:ILE:HG23	2.14	0.77
1:A:99:ILE:CG2	1:B:99:ILE:CG2	2.62	0.77
1:A:90:THR:CG2	1:A:303:VAL:HG11	2.17	0.75
1:A:149:LEU:HB2	1:A:162:THR:HG22	1.69	0.73
1:B:170:GLY:H	1:B:324:THR:CG2	2.01	0.73
1:A:251:MET:HA	1:A:251:MET:HE2	1.75	0.66
1:A:192:PRO:HD3	1:A:223:GLY:O	1.95	0.65
1:A:99:ILE:HG23	1:B:99:ILE:CG2	2.27	0.65
1:B:278:HIS:HD1	1:B:280:LEU:H	1.46	0.64
1:A:298:LEU:HG	1:A:322:ILE:HG13	1.80	0.63
1:B:276:ASP:OD1	1:B:293:GLN:NE2	2.31	0.61
1:A:266:ILE:HD13	1:A:272:VAL:HG21	1.83	0.61
1:A:90:THR:CG2	1:A:303:VAL:CG1	2.79	0.60
1:A:328[B]:HIS:CE1	2:A:351:HOH:O	2.54	0.60
1:B:170:GLY:HA3	1:B:324:THR:HG23	1.82	0.60
1:B:143:GLN:O	1:B:145:MET:N	2.35	0.59
1:A:166:ASN:O	1:A:324:THR:HB	2.02	0.59
1:A:72:VAL:HG22	1:A:73:PRO:HD2	1.85	0.59
1:A:190:SER:HB3	1:A:221:LEU:HA	1.85	0.58
1:A:328[B]:HIS:NE2	2:A:351:HOH:O	2.32	0.58
1:B:251:MET:HA	1:B:251:MET:HE2	1.87	0.57
1:A:90:THR:HG21	1:A:303:VAL:CG1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:CD1	1:A:332:ILE:HD11	2.36	0.56
1:B:166:ASN:O	1:B:324:THR:HB	2.05	0.56
1:A:99:ILE:HG22	1:B:99:ILE:HG23	1.86	0.55
1:A:196:SER:O	1:A:200:GLU:HB2	2.07	0.55
1:A:277:THR:O	1:A:278:HIS:C	2.52	0.53
1:B:273:ILE:CD1	1:B:332:ILE:HD11	2.38	0.53
1:A:276:ASP:OD1	1:A:293:GLN:NE2	2.41	0.53
1:A:243:THR:OG1	1:A:271:SER:HB2	2.09	0.53
1:B:294:ASN:OD1	1:B:297:GLN:HB2	2.09	0.53
1:A:90:THR:HG22	1:A:303:VAL:HG11	1.89	0.52
1:A:170:GLY:H	1:A:324:THR:CG2	2.20	0.52
1:A:148:VAL:HG23	1:A:306:LEU:HD13	1.92	0.52
1:A:273:ILE:HD11	1:A:332:ILE:HD11	1.92	0.51
1:B:131:GLU:HG2	1:B:155:PRO:HD3	1.92	0.51
1:A:67:THR:HG21	1:B:116:PHE:CE1	2.46	0.51
1:A:170:GLY:N	1:A:324:THR:HG22	2.20	0.51
1:A:176:GLU:OE1	1:A:180:HIS:CE1	2.64	0.51
1:B:170:GLY:N	1:B:324:THR:CG2	2.73	0.50
1:A:126:ILE:HG13	1:A:306:LEU:HD22	1.94	0.50
1:A:265:VAL:HB	1:A:268:LYS:HB3	1.94	0.49
1:B:265:VAL:HB	1:B:268:LYS:HB3	1.95	0.48
1:B:266:ILE:HD13	1:B:272:VAL:HG21	1.95	0.48
1:A:143:GLN:O	1:A:145:MET:N	2.47	0.47
1:A:301:ARG:HG3	1:A:322:ILE:HD11	1.96	0.46
1:B:170:GLY:HA3	1:B:324:THR:CG2	2.46	0.45
1:B:273:ILE:HD13	1:B:332:ILE:HD11	1.98	0.45
1:A:271:SER:OG	1:A:333:ILE:HD12	2.18	0.44
1:B:140:LEU:HD23	1:B:140:LEU:HA	1.90	0.44
1:B:273:ILE:HD11	1:B:332:ILE:HD11	1.99	0.44
1:A:190:SER:HB3	1:A:220:PHE:O	2.18	0.44
1:B:231:GLU:HG3	1:B:235:LYS:HE2	2.00	0.44
1:A:131:GLU:OE1	1:A:199:ARG:NH2	2.37	0.43
1:A:273:ILE:HD13	1:A:332:ILE:HD11	2.01	0.43
1:A:127:CYS:O	1:A:149:LEU:HA	2.18	0.43
1:A:170:GLY:HA3	1:A:324:THR:CG2	2.49	0.43
1:A:170:GLY:HA3	1:A:324:THR:HG23	2.00	0.43
1:B:225:GLU:C	1:B:227:SER:N	2.75	0.43
1:B:283:LEU:O	1:B:284:GLN:O	2.38	0.42
1:A:131:GLU:C	1:A:133:CYS:H	2.28	0.41
1:B:245:PHE:C	1:B:245:PHE:HD2	2.29	0.41
1:A:281:PHE:HE2	1:B:280:LEU:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:O	1:B:284:GLN:C	2.63	0.41
1:B:70:VAL:HA	1:B:126:ILE:O	2.21	0.41
1:A:86:GLU:HG2	1:A:296:GLU:HG3	2.02	0.41
1:A:90:THR:HG22	1:A:303:VAL:CG1	2.50	0.40
1:A:166:ASN:HA	1:A:167:PRO:HD3	1.94	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	250/348 (72%)	236 (94%)	12 (5%)	2 (1%)	16	31
1	B	250/348 (72%)	236 (94%)	13 (5%)	1 (0%)	30	49
All	All	500/696 (72%)	472 (94%)	25 (5%)	3 (1%)	21	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	GLN
1	A	308	GLU
1	A	132	GLU

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	212/282 (75%)	183 (86%)	29 (14%)	3	7
1	B	212/282 (75%)	192 (91%)	20 (9%)	8	18
All	All	424/564 (75%)	375 (88%)	49 (12%)	5	11

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	72	VAL
1	A	86	GLU
1	A	89	SER
1	A	101	THR
1	A	115	GLU
1	A	119	SER
1	A	122	VAL
1	A	138	GLU
1	A	145	MET
1	A	147	VAL
1	A	150	VAL
1	A	160	ILE
1	A	197	THR
1	A	199	ARG
1	A	200	GLU
1	A	213	LYS
1	A	227	SER
1	A	231	GLU
1	A	245	PHE
1	A	275	PHE
1	A	277	THR
1	A	295	VAL
1	A	298	LEU
1	A	300	GLN
1	A	301	ARG
1	A	304	SER
1	A	324	THR
1	A	330	GLU
1	B	70	VAL
1	B	72	VAL
1	B	101	THR
1	B	113	SER
1	B	150	VAL
1	B	153	GLU

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Mol	Chain	Res	Type
1	B	157	ASP
1	B	159	THR
1	B	189	LEU
1	B	197	THR
1	B	200	GLU
1	B	227	SER
1	B	235	LYS
1	B	245	PHE
1	B	288	LEU
1	B	295	VAL
1	B	297	GLN
1	B	304	SER
1	B	320	THR
1	B	324	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	120	HIS
1	A	168	GLN
1	A	211	ASN
1	A	297	GLN
1	A	334	ASN
1	B	120	HIS
1	B	180	HIS
1	B	211	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 oligosaccharides 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	257/348 (73%)	0.00	2 (0%) 82 80	16, 45, 78, 88	1 (0%)
1	B	257/348 (73%)	0.06	3 (1%) 76 73	16, 45, 81, 95	1 (0%)
All	All	514/696 (73%)	0.03	5 (0%) 79 76	16, 45, 78, 95	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	ASP	2.9
1	A	157	ASP	2.8
1	B	309	LEU	2.2
1	A	302	ALA	2.1
1	B	146	PRO	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.