



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2024 – 01:47 AM EDT

PDB ID : 1TD5
Title : Crystal Structure of the Ligand Binding Domain of E. coli IclR.
Authors : Walker, J.R.; Evdokimova, L.; Zhang, R.-G.; Bochkarev, A.; Joachimiak, A.; Arrowsmith, C.; Edwards, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2004-05-21
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

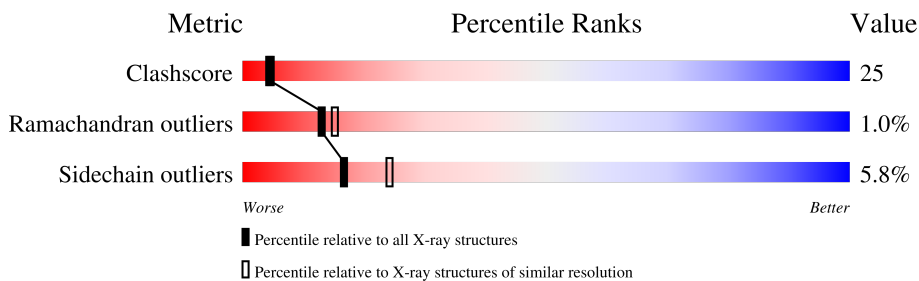
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	202	
1	B	202	
1	C	202	
1	D	202	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5834 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 Acetate operon repressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	Se	0	0	0
			1373	859	248	255	3	8			
1	B	179	Total	C	N	O	S	Se	0	0	0
			1373	859	248	255	3	8			
1	C	178	Total	C	N	O	S	Se	0	0	0
			1369	857	247	254	3	8			
1	D	180	Total	C	N	O	S	Se	0	0	0
			1384	865	252	256	3	8			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP P16528
A	-18	GLY	-	cloning artifact	UNP P16528
A	-17	SER	-	cloning artifact	UNP P16528
A	-16	SER	-	cloning artifact	UNP P16528
A	-15	HIS	-	cloning artifact	UNP P16528
A	-14	HIS	-	cloning artifact	UNP P16528
A	-13	HIS	-	cloning artifact	UNP P16528
A	-12	HIS	-	cloning artifact	UNP P16528
A	-11	HIS	-	cloning artifact	UNP P16528
A	-10	HIS	-	cloning artifact	UNP P16528
A	-9	SER	-	cloning artifact	UNP P16528
A	-8	SER	-	cloning artifact	UNP P16528
A	-7	GLY	-	cloning artifact	UNP P16528
A	-6	ARG	-	cloning artifact	UNP P16528
A	-5	GLU	-	cloning artifact	UNP P16528
A	-4	ASN	-	cloning artifact	UNP P16528
A	-3	LEU	-	cloning artifact	UNP P16528
A	-2	TYR	-	cloning artifact	UNP P16528
A	-1	PHE	-	cloning artifact	UNP P16528
A	0	GLN	-	cloning artifact	UNP P16528
A	1	GLY	-	cloning artifact	UNP P16528

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	cloning artifact	UNP P16528
A	3	MSE	-	cloning artifact	UNP P16528
A	19	MSE	MET	modified residue	UNP P16528
A	28	MSE	MET	modified residue	UNP P16528
A	50	MSE	MET	modified residue	UNP P16528
A	52	MSE	MET	modified residue	UNP P16528
A	62	MSE	MET	modified residue	UNP P16528
A	164	MSE	MET	modified residue	UNP P16528
A	179	MSE	MET	modified residue	UNP P16528
A	181	GLY	-	cloning artifact	UNP P16528
A	182	SER	-	cloning artifact	UNP P16528
B	-19	MET	-	cloning artifact	UNP P16528
B	-18	GLY	-	cloning artifact	UNP P16528
B	-17	SER	-	cloning artifact	UNP P16528
B	-16	SER	-	cloning artifact	UNP P16528
B	-15	HIS	-	cloning artifact	UNP P16528
B	-14	HIS	-	cloning artifact	UNP P16528
B	-13	HIS	-	cloning artifact	UNP P16528
B	-12	HIS	-	cloning artifact	UNP P16528
B	-11	HIS	-	cloning artifact	UNP P16528
B	-10	HIS	-	cloning artifact	UNP P16528
B	-9	SER	-	cloning artifact	UNP P16528
B	-8	SER	-	cloning artifact	UNP P16528
B	-7	GLY	-	cloning artifact	UNP P16528
B	-6	ARG	-	cloning artifact	UNP P16528
B	-5	GLU	-	cloning artifact	UNP P16528
B	-4	ASN	-	cloning artifact	UNP P16528
B	-3	LEU	-	cloning artifact	UNP P16528
B	-2	TYR	-	cloning artifact	UNP P16528
B	-1	PHE	-	cloning artifact	UNP P16528
B	0	GLN	-	cloning artifact	UNP P16528
B	1	GLY	-	cloning artifact	UNP P16528
B	2	HIS	-	cloning artifact	UNP P16528
B	3	MSE	-	cloning artifact	UNP P16528
B	19	MSE	MET	modified residue	UNP P16528
B	28	MSE	MET	modified residue	UNP P16528
B	50	MSE	MET	modified residue	UNP P16528
B	52	MSE	MET	modified residue	UNP P16528
B	62	MSE	MET	modified residue	UNP P16528
B	164	MSE	MET	modified residue	UNP P16528
B	179	MSE	MET	modified residue	UNP P16528
B	181	GLY	-	cloning artifact	UNP P16528

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Chain	Residue	Modelled	Actual	Comment	Reference
B	182	SER	-	cloning artifact	UNP P16528
C	-19	MET	-	cloning artifact	UNP P16528
C	-18	GLY	-	cloning artifact	UNP P16528
C	-17	SER	-	cloning artifact	UNP P16528
C	-16	SER	-	cloning artifact	UNP P16528
C	-15	HIS	-	cloning artifact	UNP P16528
C	-14	HIS	-	cloning artifact	UNP P16528
C	-13	HIS	-	cloning artifact	UNP P16528
C	-12	HIS	-	cloning artifact	UNP P16528
C	-11	HIS	-	cloning artifact	UNP P16528
C	-10	HIS	-	cloning artifact	UNP P16528
C	-9	SER	-	cloning artifact	UNP P16528
C	-8	SER	-	cloning artifact	UNP P16528
C	-7	GLY	-	cloning artifact	UNP P16528
C	-6	ARG	-	cloning artifact	UNP P16528
C	-5	GLU	-	cloning artifact	UNP P16528
C	-4	ASN	-	cloning artifact	UNP P16528
C	-3	LEU	-	cloning artifact	UNP P16528
C	-2	TYR	-	cloning artifact	UNP P16528
C	-1	PHE	-	cloning artifact	UNP P16528
C	0	GLN	-	cloning artifact	UNP P16528
C	1	GLY	-	cloning artifact	UNP P16528
C	2	HIS	-	cloning artifact	UNP P16528
C	3	MSE	-	cloning artifact	UNP P16528
C	19	MSE	MET	modified residue	UNP P16528
C	28	MSE	MET	modified residue	UNP P16528
C	50	MSE	MET	modified residue	UNP P16528
C	52	MSE	MET	modified residue	UNP P16528
C	62	MSE	MET	modified residue	UNP P16528
C	164	MSE	MET	modified residue	UNP P16528
C	179	MSE	MET	modified residue	UNP P16528
C	181	GLY	-	cloning artifact	UNP P16528
C	182	SER	-	cloning artifact	UNP P16528
D	-19	MET	-	cloning artifact	UNP P16528
D	-18	GLY	-	cloning artifact	UNP P16528
D	-17	SER	-	cloning artifact	UNP P16528
D	-16	SER	-	cloning artifact	UNP P16528
D	-15	HIS	-	cloning artifact	UNP P16528
D	-14	HIS	-	cloning artifact	UNP P16528
D	-13	HIS	-	cloning artifact	UNP P16528
D	-12	HIS	-	cloning artifact	UNP P16528
D	-11	HIS	-	cloning artifact	UNP P16528

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	HIS	-	cloning artifact	UNP P16528
D	-9	SER	-	cloning artifact	UNP P16528
D	-8	SER	-	cloning artifact	UNP P16528
D	-7	GLY	-	cloning artifact	UNP P16528
D	-6	ARG	-	cloning artifact	UNP P16528
D	-5	GLU	-	cloning artifact	UNP P16528
D	-4	ASN	-	cloning artifact	UNP P16528
D	-3	LEU	-	cloning artifact	UNP P16528
D	-2	TYR	-	cloning artifact	UNP P16528
D	-1	PHE	-	cloning artifact	UNP P16528
D	0	GLN	-	cloning artifact	UNP P16528
D	1	GLY	-	cloning artifact	UNP P16528
D	2	HIS	-	cloning artifact	UNP P16528
D	3	MSE	-	cloning artifact	UNP P16528
D	19	MSE	MET	modified residue	UNP P16528
D	28	MSE	MET	modified residue	UNP P16528
D	50	MSE	MET	modified residue	UNP P16528
D	52	MSE	MET	modified residue	UNP P16528
D	62	MSE	MET	modified residue	UNP P16528
D	164	MSE	MET	modified residue	UNP P16528
D	179	MSE	MET	modified residue	UNP P16528
D	181	GLY	-	cloning artifact	UNP P16528
D	182	SER	-	cloning artifact	UNP P16528

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	109	Total O 109 109	0	0
2	C	58	Total O 58 58	0	0
2	D	103	Total O 103 103	0	0

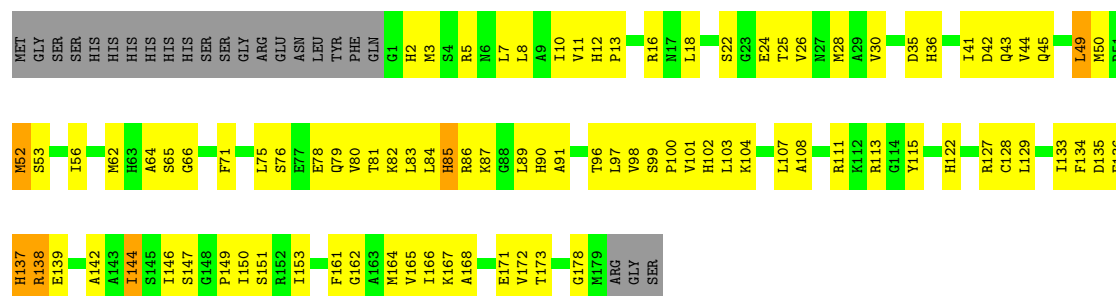
3 Residue-property plots

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.

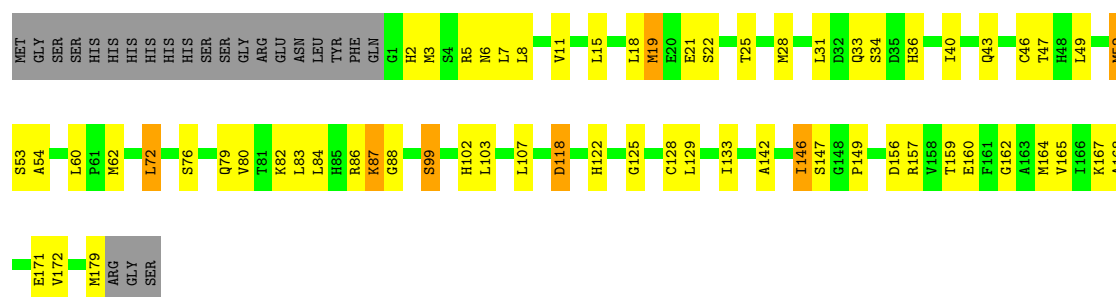
- Molecule 1: Acetate operon repressor

Chain A: 



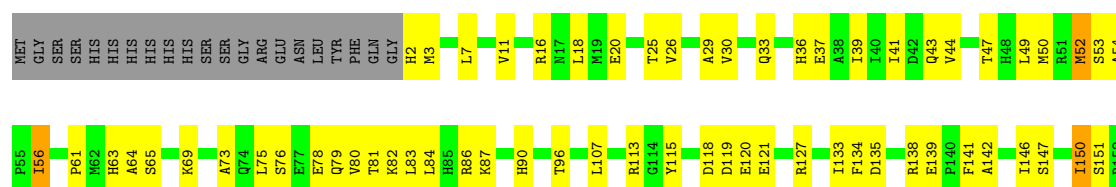
- Molecule 1: Acetate operon repressor

Chain B: 



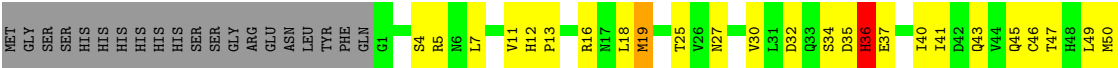
- Molecule 1: Acetate operon repressor

Chain C: 





● Molecule 1: Acetate operon repressor



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	54.10Å 82.91Å 157.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.30	Depositor
% Data completeness (in resolution range)	96.1 (19.91-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5834	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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	0.60	0/1389	0.74	0/1860
1	B	0.72	0/1389	0.76	0/1860
1	C	0.57	0/1385	0.70	0/1855
1	D	0.70	0/1400	0.77	0/1874
All	All	0.65	0/5563	0.74	0/7449

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	1373	0	1382	86	0
1	B	1373	0	1382	69	0
1	C	1369	0	1376	72	0
1	D	1384	0	1395	67	0
2	A	65	0	0	3	0
2	B	109	0	0	5	0
2	C	58	0	0	0	0
2	D	103	0	0	3	0
All	All	5834	0	5535	281	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 25.

The worst 5 of 281 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:25:THR:HG21	1:A:52:MSE:HE2	1.32	1.09
1:B:52:MSE:HG2	1:B:147:SER:HB2	1.44	0.96
1:A:76:SER:H	1:A:79:GLN:NE2	1.65	0.94
1:C:52:MSE:HG2	1:C:147:SER:HB2	1.50	0.93
1:D:25:THR:HG21	1:D:52:MSE:HE2	1.47	0.93

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	177/202 (88%)	165 (93%)	10 (6%)	2 (1%)	12	13
1	B	177/202 (88%)	169 (96%)	6 (3%)	2 (1%)	12	13
1	C	176/202 (87%)	158 (90%)	17 (10%)	1 (1%)	22	27
1	D	178/202 (88%)	167 (94%)	9 (5%)	2 (1%)	12	13
All	All	708/808 (88%)	659 (93%)	42 (6%)	7 (1%)	13	15

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	34	SER
1	B	88	GLY
1	C	75	LEU
1	D	36	HIS
1	A	178	GLY

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	146/158 (92%)	134 (92%)	12 (8%)	9	12
1	B	146/158 (92%)	137 (94%)	9 (6%)	15	22
1	C	146/158 (92%)	138 (94%)	8 (6%)	18	26
1	D	147/158 (93%)	142 (97%)	5 (3%)	32	47
All	All	585/632 (93%)	551 (94%)	34 (6%)	17	24

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	165	VAL
1	D	19	MSE
1	D	52	MSE
1	B	2	HIS
1	A	165	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	36	HIS
1	C	122	HIS
1	C	74	GLN
1	D	6	ASN
1	A	122	HIS

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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.