



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:18 PM UTC

PDB ID : 1CIA / pdb_00001cia
Title : REPLACEMENT OF CATALYTIC HISTIDINE-195 OF CHLORAMPHENICOL ACETYLTRANSFERASE: EVIDENCE FOR A GENERAL BASE ROLE FOR GLUTAMATE
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Deposited on : 1993-07-19
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

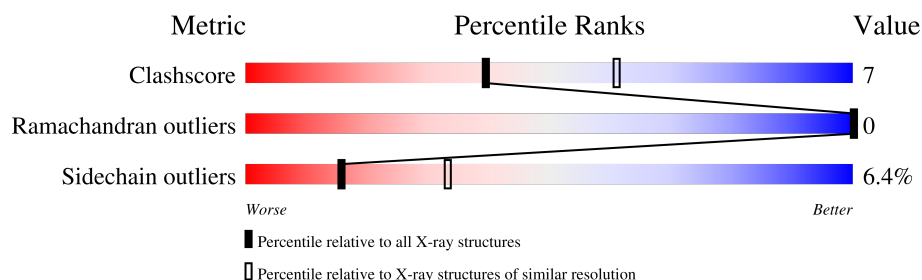
1 Overall quality at a glance

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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	213	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1815 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 CHLORAMPHENICOL ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1685	1105	265	306	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	GLN	HIS	conflict	UNP P00484

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		

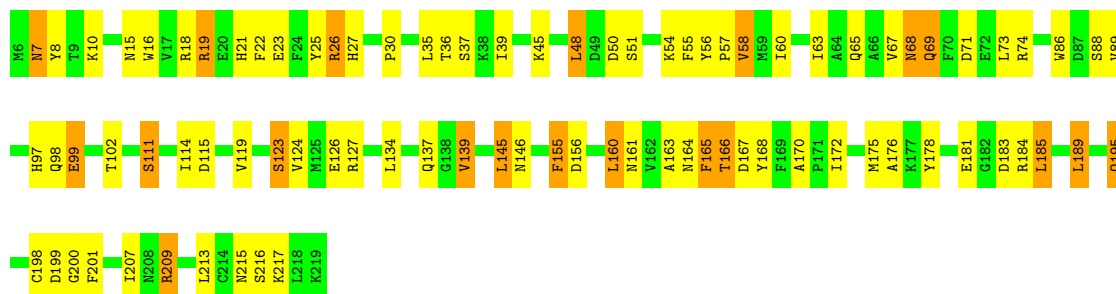
3 Residue-property plots

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: CHLORAMPHENICOL ACETYLTRANSFERASE

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	107.64Å 107.64Å 124.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.131 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1815	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BME, CO

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	1.44	5/1732 (0.3%)	2.25	81/2358 (3.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	PHE	N-CA	5.93	1.53	1.46
1	A	164	ASN	C-O	5.79	1.30	1.23
1	A	54	LYS	N-CA	5.55	1.52	1.45
1	A	166	THR	C-N	-5.47	1.26	1.33
1	A	98	GLN	C-N	-5.42	1.27	1.33

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	THR	CA-C-O	-10.60	110.35	120.95
1	A	166	THR	CA-C-N	10.34	137.28	122.08
1	A	166	THR	C-N-CA	10.34	137.28	122.08
1	A	160	LEU	CA-C-O	-9.08	110.64	120.36
1	A	27	HIS	CA-CB-CG	9.07	122.87	113.80
1	A	36	THR	O-C-N	8.40	133.13	123.31
1	A	145	LEU	CA-C-O	-8.05	112.03	121.44
1	A	58	VAL	CA-C-O	-7.68	113.03	121.17
1	A	181	GLU	N-CA-CB	7.63	123.31	110.87
1	A	185	LEU	CB-CA-C	7.43	122.90	110.79
1	A	168	TYR	O-C-N	7.28	132.30	123.13
1	A	8	TYR	CA-C-O	-7.17	113.78	121.45
1	A	19	ARG	CB-CG-CD	7.10	127.62	111.30
1	A	213	LEU	O-C-N	6.84	129.37	122.12
1	A	21	HIS	CA-CB-CG	-6.84	106.96	113.80
1	A	126	GLU	N-CA-C	-6.80	103.56	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	LYS	CA-CB-CG	6.79	127.68	114.10
1	A	102	THR	CA-C-O	-6.62	113.90	121.58
1	A	156	ASP	N-CA-C	-6.59	105.39	113.50
1	A	155	PHE	CA-CB-CG	6.57	120.37	113.80
1	A	98	GLN	CA-C-N	6.47	128.85	120.44
1	A	98	GLN	C-N-CA	6.47	128.85	120.44
1	A	161	ASN	CA-C-O	-6.47	113.66	120.58
1	A	15	ASN	CA-CB-CG	6.43	119.03	112.60
1	A	164	ASN	N-CA-CB	-6.40	100.03	110.59
1	A	198	CYS	N-CA-C	6.26	119.33	108.76
1	A	160	LEU	O-C-N	6.15	130.23	123.22
1	A	51	SER	O-C-N	6.14	129.87	122.75
1	A	139	VAL	CA-C-N	6.13	128.99	120.65
1	A	139	VAL	C-N-CA	6.13	128.99	120.65
1	A	156	ASP	CA-CB-CG	-6.10	106.50	112.60
1	A	167	ASP	CA-C-N	-6.08	114.47	123.11
1	A	167	ASP	C-N-CA	-6.08	114.47	123.11
1	A	86	TRP	CA-C-O	-6.07	114.13	121.05
1	A	165	PHE	CA-C-N	-6.07	112.09	121.56
1	A	165	PHE	C-N-CA	-6.07	112.09	121.56
1	A	50	ASP	CA-CB-CG	-6.03	106.57	112.60
1	A	200	GLY	O-C-N	6.02	127.97	122.19
1	A	127	ARG	CA-C-O	-5.98	112.02	119.38
1	A	156	ASP	O-C-N	5.98	130.50	122.49
1	A	86	TRP	O-C-N	5.93	130.01	123.01
1	A	111	SER	O-C-N	5.93	130.34	123.41
1	A	63	ILE	CA-C-O	-5.88	114.94	121.17
1	A	68	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	A	217	LYS	CA-C-O	-5.86	115.17	121.56
1	A	195	GLN	CG-CD-NE2	5.86	125.19	116.40
1	A	48	LEU	O-C-N	5.84	128.31	122.12
1	A	99	GLU	CA-C-O	-5.80	114.73	120.82
1	A	114	ILE	CA-C-O	-5.74	114.42	120.57
1	A	124	VAL	O-C-N	5.72	127.65	121.87
1	A	123	SER	CB-CA-C	5.71	119.84	110.88
1	A	216	SER	CA-C-O	-5.69	114.96	121.68
1	A	213	LEU	CA-C-O	-5.67	114.54	120.55
1	A	184	ARG	O-C-N	5.66	130.29	123.16
1	A	71	ASP	O-C-N	5.53	127.77	122.07
1	A	215	ASN	CA-C-O	-5.50	112.82	119.59
1	A	37	SER	N-CA-CB	-5.48	102.16	111.69
1	A	156	ASP	CA-C-O	-5.45	113.15	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	GLN	OE1-CD-NE2	-5.45	117.15	122.60
1	A	172	ILE	CA-C-O	-5.44	114.71	120.53
1	A	201	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	51	SER	N-CA-CB	-5.39	103.10	111.35
1	A	170	ALA	O-C-N	5.39	127.47	121.43
1	A	199	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	183	ASP	CA-CB-CG	-5.29	107.31	112.60
1	A	26	ARG	CD-NE-CZ	-5.27	117.03	124.40
1	A	55	PHE	N-CA-C	5.25	117.42	111.02
1	A	146	ASN	CA-C-O	-5.24	114.66	120.38
1	A	163	ALA	CA-C-O	-5.24	114.18	120.10
1	A	217	LYS	N-CA-CB	5.21	117.67	110.17
1	A	23	GLU	CB-CG-CD	5.21	121.46	112.60
1	A	195	GLN	CB-CG-CD	5.20	121.43	112.60
1	A	209	ARG	N-CA-CB	5.18	117.52	110.01
1	A	89	VAL	O-C-N	5.15	128.44	123.03
1	A	69	GLN	OE1-CD-NE2	5.14	127.74	122.60
1	A	134	LEU	CB-CA-C	5.14	119.58	110.85
1	A	97	HIS	CA-CB-CG	-5.11	108.69	113.80
1	A	98	GLN	CA-C-O	5.04	125.89	120.55
1	A	115	ASP	N-CA-CB	5.03	118.05	110.30
1	A	134	LEU	CA-C-N	5.03	129.34	123.16
1	A	134	LEU	C-N-CA	5.03	129.34	123.16

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	1685	0	1575	22	0
2	A	2	0	0	0	0
3	A	4	0	6	0	0
4	A	124	0	0	2	0
All	All	1815	0	1581	22	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 7.

All (22) 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:69:GLN:HE22	1:A:209:ARG:HE	0.93	0.92
1:A:69:GLN:NE2	1:A:209:ARG:HE	1.71	0.88
1:A:69:GLN:HE22	1:A:209:ARG:NE	1.73	0.85
1:A:175:MET:HG2	1:A:189:LEU:HD12	1.76	0.67
1:A:99:GLU:CD	1:A:99:GLU:H	2.12	0.57
1:A:165:PHE:O	1:A:166:THR:C	2.47	0.57
1:A:48:LEU:HD21	1:A:58:VAL:HG21	1.89	0.55
1:A:16:TRP:O	1:A:19:ARG:HG2	2.07	0.55
1:A:22:PHE:O	1:A:26:ARG:HB2	2.11	0.50
1:A:16:TRP:CE2	1:A:18:ARG:HB2	2.49	0.47
1:A:155:PHE:CE2	1:A:176:ALA:HB2	2.49	0.47
1:A:119:VAL:HG23	4:A:299:HOH:O	2.15	0.46
1:A:67:VAL:HG22	1:A:73:LEU:HD13	1.97	0.45
1:A:56:TYR:HB3	1:A:57:PRO:HD3	1.98	0.45
1:A:39:ILE:HD11	1:A:207:ILE:HG23	1.99	0.44
1:A:56:TYR:O	1:A:60:ILE:HG13	2.17	0.44
1:A:137:GLN:HG2	4:A:353:HOH:O	2.17	0.43
1:A:25:TYR:O	1:A:30:PRO:HA	2.18	0.43
1:A:178:TYR:CD1	1:A:185:LEU:HD11	2.54	0.43
1:A:68:ASN:HA	1:A:74:ARG:HD3	1.99	0.42
1:A:185:LEU:HD12	1:A:185:LEU:HA	1.94	0.40
1:A:7:ASN:N	1:A:7:ASN:HD22	2.20	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	211/213 (99%)	207 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	173/198 (87%)	162 (94%)	11 (6%)	16	33

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

Mol	Chain	Res	Type
1	A	7	ASN
1	A	35	LEU
1	A	45	LYS
1	A	88	SER
1	A	111	SER
1	A	123	SER
1	A	139	VAL
1	A	145	LEU
1	A	160	LEU
1	A	189	LEU
1	A	195	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	65	GLN
1	A	69	GLN
1	A	92	GLN
1	A	146	ASN
1	A	161	ASN

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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BME	A	536	-	3,3,3	0.94	0	2,2,2	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	A	536	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.