



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:55 pm GMT

PDB ID : 2CLA  
Title : CRYSTAL STRUCTURE OF THE ASP-199-ASN MUTANT OF CHLORAMPHENICOL ACETYLTRANSFERASE TO 2.35 ANGSTROMS RESOLUTION. STRUCTURAL CONSEQUENCES OF DISRUPTION OF A BURIED SALT-BRIDGE  
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Deposited on : 1990-04-05  
Resolution : 2.35 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

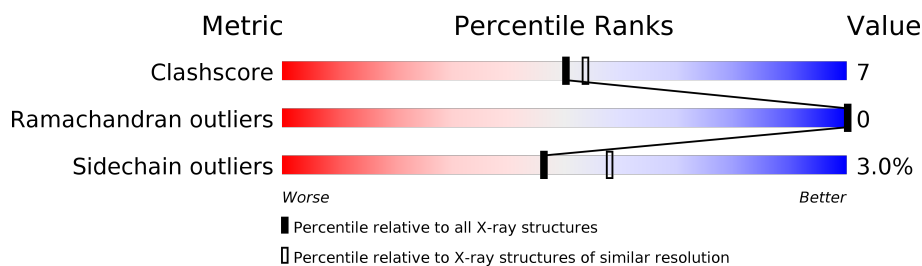
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	213	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1750 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
			1644	1074	267	293	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ASN	ASP	CONFLICT	UNP P00484

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	0
			104	104		

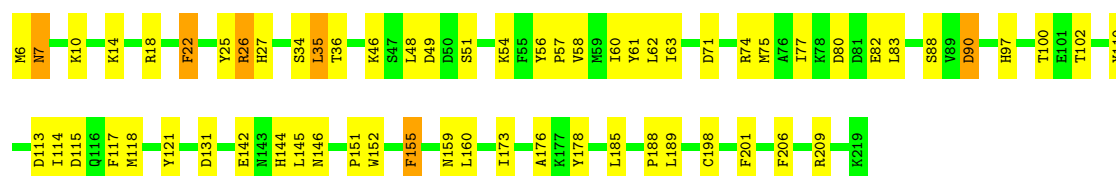
### 3 Residue-property plots [i](#)

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.

Note EDS was not executed.

#### • Molecule 1: CHLORAMPHENICOL ACETYLTRANSFERASE

Chain A:  70% 27%



## 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, $\alpha$ , $\beta$ , $\gamma$	107.70Å 107.70Å 124.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.35	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.35)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
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	1.12	1/1691 (0.1%)	1.91	47/2299 (2.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	ARG	CD-NE	-5.27	1.37	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	NE-CZ-NH2	-16.19	112.20	120.30
1	A	209	ARG	CD-NE-CZ	11.39	139.54	123.60
1	A	25	TYR	CB-CG-CD2	-10.91	114.45	121.00
1	A	178	TYR	CB-CG-CD1	10.44	127.26	121.00
1	A	36	THR	O-C-N	9.73	138.27	122.70
1	A	61	TYR	CB-CG-CD1	9.18	126.51	121.00
1	A	26	ARG	NE-CZ-NH1	8.99	124.79	120.30
1	A	178	TYR	CB-CG-CD2	-8.68	115.79	121.00
1	A	74	ARG	NH1-CZ-NH2	8.00	128.20	119.40
1	A	71	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	131	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	71	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	22	PHE	CB-CG-CD1	-7.22	115.75	120.80
1	A	121	TYR	CB-CG-CD1	6.64	124.98	121.00
1	A	113	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	A	18	ARG	CD-NE-CZ	6.31	132.44	123.60
1	A	88	SER	N-CA-CB	-6.28	101.09	110.50
1	A	110	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	A	117	PHE	CB-CG-CD1	-6.17	116.48	120.80
1	A	115	ASP	CB-CG-OD1	6.08	123.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	206	PHE	CB-CG-CD2	-5.97	116.62	120.80
1	A	90	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	61	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	61	TYR	CD1-CE1-CZ	-5.72	114.65	119.80
1	A	61	TYR	CG-CD1-CE1	5.71	125.87	121.30
1	A	146	ASN	CB-CG-OD1	-5.65	110.29	121.60
1	A	160	LEU	O-C-N	5.62	131.70	122.70
1	A	18	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	142	GLU	CA-CB-CG	5.52	125.54	113.40
1	A	27	HIS	CA-CB-CG	5.46	122.88	113.60
1	A	178	TYR	CG-CD2-CE2	5.44	125.65	121.30
1	A	146	ASN	OD1-CG-ND2	5.42	134.35	121.90
1	A	121	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	A	10	LYS	N-CA-CB	5.29	120.11	110.60
1	A	131	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	178	TYR	CZ-CE2-CD2	-5.27	115.06	119.80
1	A	189	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	A	198	CYS	O-C-N	5.25	131.09	122.70
1	A	75	MET	CG-SD-CE	5.22	108.56	100.20
1	A	201	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	A	14	LYS	C-N-CA	5.19	134.66	121.70
1	A	26	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	A	185	LEU	CB-CA-C	5.14	119.97	110.20
1	A	35	LEU	CA-CB-CG	5.08	127.00	115.30
1	A	7	ASN	CB-CG-OD1	-5.02	111.55	121.60
1	A	160	LEU	CB-CG-CD2	-5.00	102.49	111.00

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	1644	0	1519	21	2
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	104	0	0	1	2
All	All	1750	0	1519	21	2

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 (21) 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:48:LEU:HD21	1:A:58:VAL:HG21	1.79	0.64
1:A:176:ALA:HB3	1:A:188:PRO:HG2	1.85	0.58
1:A:34:SER:CB	1:A:159:ASN:HD22	2.16	0.56
1:A:34:SER:OG	1:A:159:ASN:ND2	2.37	0.54
1:A:90:ASP:O	1:A:144:HIS:HA	2.10	0.52
1:A:54:LYS:O	1:A:58:VAL:HG23	2.10	0.51
1:A:58:VAL:O	1:A:62:LEU:HG	2.11	0.51
1:A:22:PHE:O	1:A:26:ARG:HB2	2.13	0.49
1:A:46:LYS:CG	3:A:335:HOH:O	2.63	0.46
1:A:77:ILE:HA	1:A:82:GLU:O	2.16	0.45
1:A:151:PRO:HD2	1:A:152:TRP:CZ3	2.52	0.45
1:A:77:ILE:HD13	1:A:83:LEU:HA	1.98	0.45
1:A:56:TYR:N	1:A:57:PRO:HD2	2.32	0.45
1:A:114:ILE:O	1:A:118:MET:HG2	2.18	0.43
1:A:56:TYR:O	1:A:60:ILE:HG13	2.18	0.43
1:A:63:ILE:CG2	1:A:173:ILE:HD13	2.49	0.42
1:A:97:HIS:HB2	1:A:100:THR:HG22	2.02	0.42
1:A:80:ASP:C	1:A:82:GLU:N	2.71	0.41
1:A:155:PHE:CE2	1:A:176:ALA:HB2	2.55	0.41
1:A:46:LYS:O	1:A:49:ASP:HB2	2.20	0.41
1:A:100:THR:HG23	1:A:102:THR:OG1	2.21	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:MET:CG	3:A:504:HOH:O[12_555]	1.99	0.21
1:A:6:MET:CE	3:A:501:HOH:O[12_555]	2.18	0.02



## 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%)	201 (95%)	10 (5%)	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	165/198 (83%)	160 (97%)	5 (3%)	46	58

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	35	LEU
1	A	51	SER
1	A	145	LEU
1	A	155	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.