



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:23 am GMT

PDB ID : 1W78
Title : E.COLI FOLC IN COMPLEX WITH DHPP AND ADP
Authors : Mathieu, M.; Debousker, G.; Vincent, S.; Viviani, F.; Bamas-Jacques, N.; Mikol, V.
Deposited on : 2004-08-31
Resolution : 1.82 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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

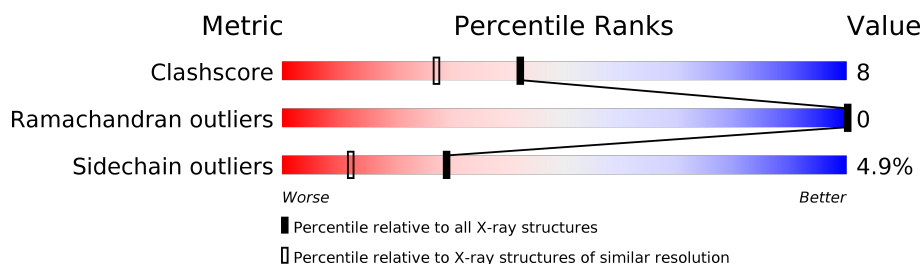
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)

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 ≥ 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	422	 85% 10% . .

2 Entry composition [i](#)

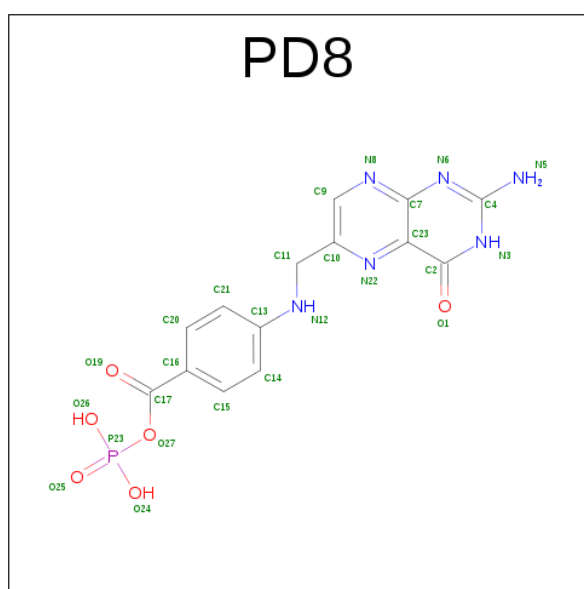
There are 6 unique types of molecules in this entry. The entry contains 3692 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FOLC BIFUNCTIONAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3141	1985	547	600	9			

- Molecule 2 is PHOSPHORYLATED DIHYDROPTEROATE (three-letter code: PD8) (formula: C₁₄H₁₃N₆O₆P).

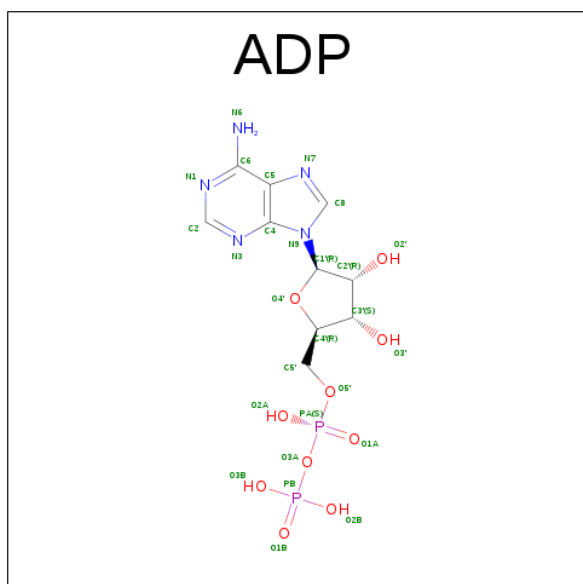


- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



- Molecule 6 is water.

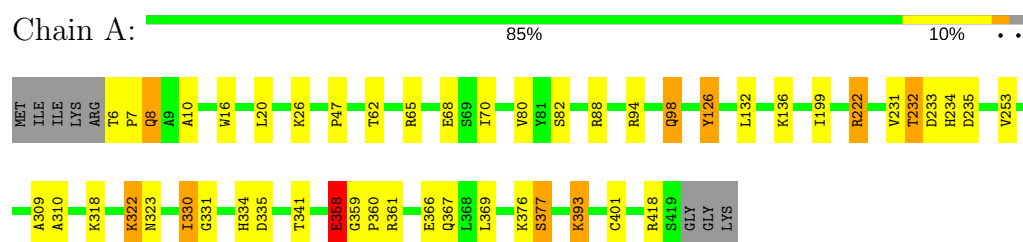
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	490	Total 490	O 490	0	0

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: FOLC BIFUNCTIONAL PROTEIN



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	64.37Å 80.62Å 92.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.82	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-1.82)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BUSTER	Depositor
R, R_{free}	0.165 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3692	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: MG, KCX, SO4, ADP, PD8

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	0.57	0/3195	0.75	1/4354 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	GLU	C-N-CA	-5.14	111.50	122.30

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	3141	0	3113	49	0
2	A	27	0	11	1	0
3	A	2	0	0	0	0
4	A	5	0	0	0	0
5	A	27	0	12	0	0
6	A	490	0	0	12	1
All	All	3692	0	3136	50	1

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 8.

All (50) 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:232:THR:HG22	1:A:235:ASP:H	1.37	0.89
1:A:232:THR:HG23	1:A:234:HIS:H	1.41	0.83
1:A:65:ARG:HH21	1:A:94:ARG:NH1	1.77	0.83
1:A:232:THR:CG2	1:A:234:HIS:H	1.98	0.77
1:A:70:ILE:HG21	1:A:265:LEU:CD2	2.15	0.77
1:A:70:ILE:HG21	1:A:265:LEU:HD21	1.74	0.68
1:A:322:LYS:HD3	1:A:322:LYS:H	1.57	0.68
1:A:322:LYS:CD	1:A:322:LYS:H	2.09	0.65
1:A:98:GLN:HE21	1:A:98:GLN:HA	1.61	0.64
1:A:222:ARG:HD3	6:A:2321:HOH:O	1.99	0.62
1:A:222:ARG:NH1	6:A:2314:HOH:O	2.33	0.60
1:A:358:GLU:H	1:A:358:GLU:CD	2.06	0.59
1:A:232:THR:HG22	1:A:235:ASP:N	2.15	0.58
1:A:199:ILE:HG13	1:A:264:ALA:HA	1.86	0.57
1:A:231:VAL:HG12	1:A:232:THR:N	2.23	0.54
1:A:65:ARG:HE	1:A:94:ARG:NH2	2.06	0.53
1:A:8:GLN:HB2	6:A:2008:HOH:O	2.08	0.53
1:A:70:ILE:CG2	1:A:265:LEU:HD21	2.39	0.52
1:A:10:ALA:HB1	6:A:2007:HOH:O	2.09	0.52
1:A:6:THR:N	6:A:2002:HOH:O	2.43	0.51
1:A:88:ARG:HD3	6:A:2151:HOH:O	2.10	0.51
1:A:232:THR:HG21	1:A:234:HIS:CE1	2.47	0.50
1:A:65:ARG:HH21	1:A:94:ARG:CZ	2.25	0.49
1:A:232:THR:HG23	1:A:233:ASP:N	2.27	0.49
1:A:7:PRO:HB2	1:A:16:TRP:CE2	2.49	0.48
1:A:318:LYS:HE3	6:A:2430:HOH:O	2.14	0.48
1:A:334:HIS:NE2	1:A:367:GLN:OE1	2.43	0.47
1:A:401:CYS:HB2	6:A:2473:HOH:O	2.15	0.46
1:A:82:SER:HB3	6:A:2216:HOH:O	2.16	0.45
1:A:62:THR:HB	1:A:253:VAL:HB	1.98	0.45
1:A:322:LYS:N	1:A:322:LYS:CD	2.79	0.44
2:A:1421:PD8:H21	2:A:1421:PD8:H111	1.69	0.44
1:A:306:ASN:ND2	1:A:309:ALA:H	2.15	0.44
1:A:366:GLU:CD	1:A:366:GLU:H	2.21	0.44
1:A:70:ILE:HG21	1:A:265:LEU:HD22	1.97	0.44
1:A:47:PRO:HG3	1:A:132:LEU:HD22	2.00	0.44
1:A:359:GLY:HA2	1:A:360:PRO:HD3	1.67	0.43
1:A:369:LEU:HA	1:A:369:LEU:HD23	1.82	0.43
1:A:310:ALA:HB2	1:A:341:THR:HG23	2.00	0.43
1:A:231:VAL:CG1	1:A:232:THR:N	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:HIS:HE2	1:A:367:GLN:CD	2.20	0.43
1:A:68:GLU:HB2	1:A:80:VAL:HG21	1.99	0.43
1:A:369:LEU:HD12	1:A:377:SER:HB3	2.01	0.42
1:A:418:ARG:NH1	6:A:2482:HOH:O	2.51	0.42
1:A:94:ARG:HD2	6:A:2140:HOH:O	2.20	0.41
1:A:393:LYS:HE3	1:A:393:LYS:HB3	1.52	0.41
1:A:322:LYS:O	1:A:323:ASN:HB2	2.21	0.41
1:A:305:HIS:HE1	6:A:2256:HOH:O	2.03	0.41
1:A:330:ILE:HG13	1:A:331:GLY:N	2.35	0.41
1:A:20:LEU:CD2	1:A:126:TYR:CD1	3.05	0.40

All (1) 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)
6:A:2373:HOH:O	6:A:2478:HOH:O[4_556]	2.12	0.08

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	411/422 (97%)	403 (98%)	8 (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	327/333 (98%)	311 (95%)	16 (5%)	29	12

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	26	LYS
1	A	98	GLN
1	A	126	TYR
1	A	136	LYS
1	A	222	ARG
1	A	232	THR
1	A	306	ASN
1	A	322	LYS
1	A	330	ILE
1	A	335	ASP
1	A	358	GLU
1	A	361	ARG
1	A	376	LYS
1	A	377	SER
1	A	393	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	98	GLN
1	A	234	HIS
1	A	306	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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$
1	KCX	A	188	1	8,11,12	0.98	1 (12%)	6,12,14	1.59	1 (16%)

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
1	KCX	A	188	1	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	KCX	CA-C	2.35	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	KCX	CE-NZ-CX	3.05	127.08	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
2	PD8	A	1421	3	28,29,29	2.07	5 (17%)	37,42,42	2.47	12 (32%)
4	SO4	A	1424	-	4,4,4	0.59	0	6,6,6	0.77	0
5	ADP	A	1425	3	25,29,29	1.29	2 (8%)	24,45,45	3.18	3 (12%)

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
2	PD8	A	1421	3	-	0/14/14/14	0/3/3/3
4	SO4	A	1424	-	-	0/0/0/0	0/0/0/0
5	ADP	A	1425	3	-	0/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1425	ADP	C6-N6	2.23	1.43	1.34
2	A	1421	PD8	C21-C13	3.49	1.45	1.39
2	A	1421	PD8	C2-C23	3.80	1.48	1.41
5	A	1425	ADP	PB-O3A	4.34	1.67	1.60
2	A	1421	PD8	C2-N3	4.56	1.41	1.33
2	A	1421	PD8	C9-N8	4.59	1.39	1.31
2	A	1421	PD8	O27-C17	5.17	1.42	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1425	ADP	N3-C2-N1	-13.90	116.76	128.86
2	A	1421	PD8	C23-C2-N3	-7.62	112.64	123.48
2	A	1421	PD8	C23-C7-N8	-4.06	114.56	121.77
2	A	1421	PD8	C9-C10-N22	-3.59	118.44	120.80
2	A	1421	PD8	C10-C9-N8	-3.11	119.94	123.09
2	A	1421	PD8	N6-C4-N3	-2.33	124.06	127.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1421	PD8	O24-P23-O27	2.01	112.31	105.57
2	A	1421	PD8	N5-C4-N6	2.15	121.72	117.75
2	A	1421	PD8	C4-N6-C7	2.28	117.82	115.16
2	A	1421	PD8	C10-N22-C23	2.32	121.22	118.44
5	A	1425	ADP	C5-C6-N6	3.18	126.95	120.47
5	A	1425	ADP	C2-N1-C6	3.99	125.76	118.77
2	A	1421	PD8	N8-C7-N6	4.78	122.21	116.04
2	A	1421	PD8	C2-N3-C4	4.89	123.10	116.06
2	A	1421	PD8	O27-C17-O19	5.60	126.63	122.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1421	PD8	1	0

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.