



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:19 PM GMT

PDB ID : 1OHK
Title : HUMAN DIHYDROFOLATE REDUCTASE, ORTHORHOMBIC (P21 21 21)
CRYSTAL FORM
Authors : Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.
Deposited on : 1997-09-17
Resolution : 2.50 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

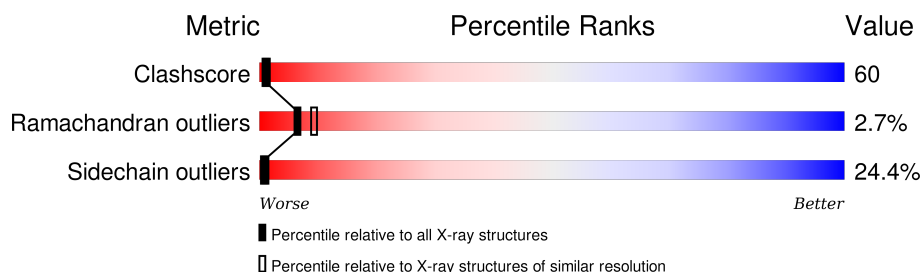
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 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	186	<div> <div></div> <div>16%</div> <div>41%</div> <div>32%</div> <div>11%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1638 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 DIHYDROFOLATE REDUCTASE.

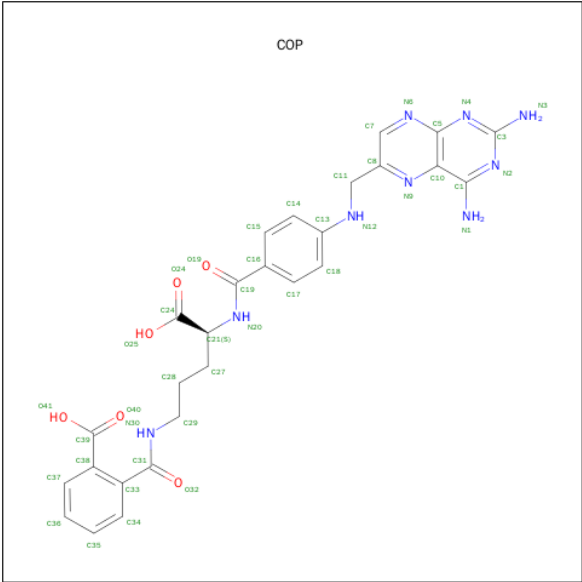
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1502	963	253	279	7			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is N-(4-CARBOXY-4-{4-[(2,4-DIAMINO-PTERIDIN-6-YLMETHYL)-AMINO]-BENZOYLAMINO}-BUTYL)-PHTHALAMIC ACID (three-letter code: COP) (formula: $C_{27}H_{27}N_9O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			70	47	11	12		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		

i

Note EDS was not executed.

Chain A:

16% 41% 32% 11%

G129 H130 L131 K132 K133 F134 V135 T136 R137 L138 M139 D140 D141 F142 E143 S144 D145 T146 F147 F148 P149 E150 H151 D152 L153 E154 K155 Y156 K157 L158 L159 P160 E161 Y162 P163 G164 V165 L166 S167 D168 W169 Q170 E171 E172 L175 K176 Y177 K178 F179 E180 W181 Y182 E183 K184 M185 D186
 R65 P66 L67 K68 G69 A70 I71 M72 L73 V74 L75 W76 E77 F78 L79 K80 P81 P82 P83 Q84 G85 A86 H87 P88 L89 S90 R91 S92 L93 D94 K98 L99 T100 E101 Q102 P103 E104 L105 V109 D110 M111 Y112 M113 L114 V115 G116 G117 S118 S119 V120 Y121 K122 E123 A124 M125 L126 H127 P128
 V1 G2 S3 L4 M5 C6 I7 V8 A9 Y10 S11 Q12 M13 M14 G15 L16 G17 K18 M19 G20 D21 L22 P23 G24 P25 P26 L27 R28 T29 E30 F31 R32 Y33 R36 R37 T40 V43 E44 G45 K46 L49 V50 I51 M52 G53 K54 K55 T56 W57 P58 S59 P61 E62 K63 M64

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	36.90 Å 69.19 Å 69.95 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	94.7 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1638	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: COP, NDP

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	1.19	2/1537 (0.1%)	2.79	135/2073 (6.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLU	CD-OE1	-5.74	1.19	1.25
1	A	112	VAL	N-CA	-5.36	1.35	1.46

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	NE-CZ-NH2	-16.87	111.87	120.30
1	A	28	ARG	NE-CZ-NH1	16.22	128.41	120.30
1	A	137	ARG	NE-CZ-NH2	-14.92	112.84	120.30
1	A	44	GLU	O-C-N	14.46	147.78	123.20
1	A	36	ARG	CD-NE-CZ	14.26	143.57	123.60

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	1502	0	1510	190	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	25	16	0
3	A	70	0	33	8	0
4	A	18	0	0	1	5
All	All	1638	0	1568	190	5

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 60.

The worst 5 of 190 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:28:ARG:HD3	3:A:188[A]:COP:O40	1.15	1.32
1:A:102:GLN:NE2	1:A:102:GLN:HA	1.36	1.25
1:A:102:GLN:CA	1:A:102:GLN:HE21	1.38	1.19
1:A:166:LEU:H	1:A:166:LEU:HD12	1.04	1.10
1:A:54:LYS:N	2:A:187:NDP:H52A	1.65	1.10

All (5) 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)
4:A:195:HOH:O	4:A:201:HOH:O[2_555]	1.65	0.55
1:A:157:LYS:NZ	4:A:194:HOH:O[2_554]	1.68	0.52
4:A:196:HOH:O	4:A:202:HOH:O[2_555]	1.76	0.44
1:A:157:LYS:CD	4:A:194:HOH:O[2_554]	1.96	0.24
1:A:157:LYS:CE	4:A:194:HOH:O[2_554]	1.99	0.21

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	184/186 (99%)	161 (88%)	18 (10%)	5 (3%)	6 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ALA
1	A	152	ASP
1	A	40	THR
1	A	103	PRO
1	A	163	PRO

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	168/168 (100%)	127 (76%)	41 (24%)	1 1

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	128	PRO
1	A	171	GLU
1	A	112	VAL
1	A	122	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	102	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are 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$
2	NDP	A	187	-	42,52,52	2.69	14 (33%)	55,80,80	2.81	25 (45%)
3	COP	A	188[A]	-	37,45,45	1.99	6 (16%)	43,62,62	2.50	18 (41%)
3	COP	A	188[B]	-	37,45,45	1.74	6 (16%)	43,62,62	2.85	19 (44%)
3	COP	A	188[C]	-	37,45,45	1.74	6 (16%)	43,62,62	2.53	19 (44%)

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	NDP	A	187	-	-	0/30/77/77	0/5/5/5
3	COP	A	188[A]	-	-	0/24/32/32	0/4/4/4
3	COP	A	188[B]	-	-	0/24/32/32	0/4/4/4
3	COP	A	188[C]	-	-	0/24/32/32	0/4/4/4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C4B	-9.71	1.22	1.45
2	A	187	NDP	O3B-C3B	-8.01	1.23	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188[C]	COP	C5-N6	-4.36	1.30	1.37
3	A	188[B]	COP	C5-N6	-4.36	1.30	1.37
3	A	188[A]	COP	C5-N6	-4.36	1.30	1.37

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[B]	COP	C27-C28-C29	-9.18	83.84	112.13
2	A	187	NDP	C1B-N9A-C4A	-5.72	118.32	126.94
2	A	187	NDP	O3B-C3B-C4B	-5.18	95.50	111.05
3	A	188[C]	COP	C11-N12-C13	-4.28	110.52	122.15
3	A	188[B]	COP	C11-N12-C13	-4.28	110.52	122.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NDP	16	0
3	A	188[A]	COP	6	0
3	A	188[B]	COP	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.