Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 01:06 AM EDT

PDB ID	:	6OJO
Title	:	Dihydroneopterin aldolase (DHNA) from Yersinia pestis co-crystallized with pterine
Authors	:	Bourne, C.R.
Deposited on	:	2019-04-11
Resolution	:	1.89 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4241 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 7,8-dihydroneopterin aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			927	587	160	177	3			
1	B	116	Total	C	N	O	S	0	0	0
			917	581	158	175	3			
1	C	118	Total	C	N	O	S	0	2	0
			952	605	164	180	3			
1	D	118	Total	C	N	O	S	0	3	0
			960	611	165	181	3			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q8CZR7
A	-22	HIS	-	expression tag	UNP Q8CZR7
A	-21	HIS	-	expression tag	UNP Q8CZR7
A	-20	HIS	-	expression tag	UNP Q8CZR7
A	-19	HIS	-	expression tag	UNP Q8CZR7
A	-18	HIS	-	expression tag	UNP Q8CZR7
A	-17	HIS	-	expression tag	UNP Q8CZR7
A	-16	SER	-	expression tag	UNP Q8CZR7
A	-15	SER	-	expression tag	UNP Q8CZR7
A	-14	GLY	-	expression tag	UNP Q8CZR7
A	-13	VAL	-	expression tag	UNP Q8CZR7
A	-12	ASP	-	expression tag	UNP Q8CZR7
A	-11	LEU	-	expression tag	UNP Q8CZR7
A	-10	GLY	-	expression tag	UNP Q8CZR7
A	-9	THR	-	expression tag	UNP Q8CZR7
A	-8	GLU	-	expression tag	UNP Q8CZR7
A	-7	ASN	-	expression tag	UNP Q8CZR7
A	-6	LEU	-	expression tag	UNP Q8CZR7
A	-5	TYR	-	expression tag	UNP Q8CZR7
A	-4	PHE	-	expression tag	UNP Q8CZR7
A	-3	GLN	-	expression tag	UNP Q8CZR7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8CZR7
A	-1	ASN	-	expression tag	UNP Q8CZR7
A	0	ALA	-	expression tag	UNP Q8CZR7
B	-23	MET	-	expression tag	UNP Q8CZR7
B	-22	HIS	-	expression tag	UNP Q8CZR7
B	-21	HIS	-	expression tag	UNP Q8CZR7
B	-20	HIS	-	expression tag	UNP Q8CZR7
B	-19	HIS	-	expression tag	UNP Q8CZR7
B	-18	HIS	-	expression tag	UNP Q8CZR7
B	-17	HIS	-	expression tag	UNP Q8CZR7
B	-16	SER	-	expression tag	UNP Q8CZR7
B	-15	SER	-	expression tag	UNP Q8CZR7
B	-14	GLY	-	expression tag	UNP Q8CZR7
B	-13	VAL	-	expression tag	UNP Q8CZR7
B	-12	ASP	-	expression tag	UNP Q8CZR7
B	-11	LEU	-	expression tag	UNP Q8CZR7
B	-10	GLY	-	expression tag	UNP Q8CZR7
B	-9	THR	-	expression tag	UNP Q8CZR7
B	-8	GLU	-	expression tag	UNP Q8CZR7
B	-7	ASN	-	expression tag	UNP Q8CZR7
B	-6	LEU	-	expression tag	UNP Q8CZR7
B	-5	TYR	-	expression tag	UNP Q8CZR7
B	-4	PHE	-	expression tag	UNP Q8CZR7
B	-3	GLN	-	expression tag	UNP Q8CZR7
B	-2	SER	-	expression tag	UNP Q8CZR7
B	-1	ASN	-	expression tag	UNP Q8CZR7
B	0	ALA	-	expression tag	UNP Q8CZR7
C	-23	MET	-	expression tag	UNP Q8CZR7
C	-22	HIS	-	expression tag	UNP Q8CZR7
C	-21	HIS	-	expression tag	UNP Q8CZR7
C	-20	HIS	-	expression tag	UNP Q8CZR7
C	-19	HIS	-	expression tag	UNP Q8CZR7
C	-18	HIS	-	expression tag	UNP Q8CZR7
C	-17	HIS	-	expression tag	UNP Q8CZR7
C	-16	SER	-	expression tag	UNP Q8CZR7
C	-15	SER	-	expression tag	UNP Q8CZR7
C	-14	GLY	-	expression tag	UNP Q8CZR7
C	-13	VAL	-	expression tag	UNP Q8CZR7
C	-12	ASP	-	expression tag	UNP Q8CZR7
C	-11	LEU	-	expression tag	UNP Q8CZR7
C	-10	GLY	-	expression tag	UNP Q8CZR7
C	-9	THR	-	expression tag	UNP Q8CZR7

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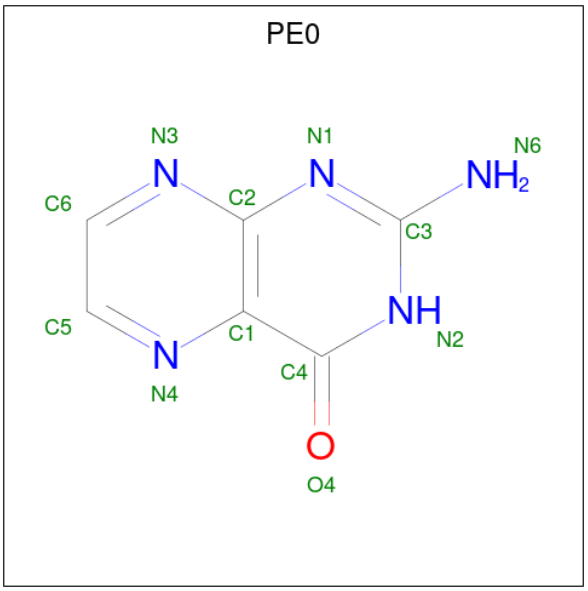
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP Q8CZR7
C	-7	ASN	-	expression tag	UNP Q8CZR7
C	-6	LEU	-	expression tag	UNP Q8CZR7
C	-5	TYR	-	expression tag	UNP Q8CZR7
C	-4	PHE	-	expression tag	UNP Q8CZR7
C	-3	GLN	-	expression tag	UNP Q8CZR7
C	-2	SER	-	expression tag	UNP Q8CZR7
C	-1	ASN	-	expression tag	UNP Q8CZR7
C	0	ALA	-	expression tag	UNP Q8CZR7
D	-23	MET	-	expression tag	UNP Q8CZR7
D	-22	HIS	-	expression tag	UNP Q8CZR7
D	-21	HIS	-	expression tag	UNP Q8CZR7
D	-20	HIS	-	expression tag	UNP Q8CZR7
D	-19	HIS	-	expression tag	UNP Q8CZR7
D	-18	HIS	-	expression tag	UNP Q8CZR7
D	-17	HIS	-	expression tag	UNP Q8CZR7
D	-16	SER	-	expression tag	UNP Q8CZR7
D	-15	SER	-	expression tag	UNP Q8CZR7
D	-14	GLY	-	expression tag	UNP Q8CZR7
D	-13	VAL	-	expression tag	UNP Q8CZR7
D	-12	ASP	-	expression tag	UNP Q8CZR7
D	-11	LEU	-	expression tag	UNP Q8CZR7
D	-10	GLY	-	expression tag	UNP Q8CZR7
D	-9	THR	-	expression tag	UNP Q8CZR7
D	-8	GLU	-	expression tag	UNP Q8CZR7
D	-7	ASN	-	expression tag	UNP Q8CZR7
D	-6	LEU	-	expression tag	UNP Q8CZR7
D	-5	TYR	-	expression tag	UNP Q8CZR7
D	-4	PHE	-	expression tag	UNP Q8CZR7
D	-3	GLN	-	expression tag	UNP Q8CZR7
D	-2	SER	-	expression tag	UNP Q8CZR7
D	-1	ASN	-	expression tag	UNP Q8CZR7
D	0	ALA	-	expression tag	UNP Q8CZR7

- Molecule 2 is PTERINE (three-letter code: PE0) (formula: $C_6H_5N_5O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 12 6 5 1	0	0
2	B	1	Total C N O 12 6 5 1	0	0
2	C	1	Total C N O 12 6 5 1	0	0
2	D	1	Total C N O 12 6 5 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	105	Total O 105 105	0	0
3	B	106	Total O 106 106	0	0
3	C	114	Total O 114 114	0	0
3	D	112	Total O 112 112	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.09Å 81.49Å 96.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.56 – 1.89	Depositor
% Data completeness (in resolution range)	98.9 (41.56-1.89)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.69 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.184 , 0.206	Depositor
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.134	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4241	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9545e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 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	PE0	A	200	-	13,13,13	1.48	3 (23%)	15,18,18	2.41	7 (46%)
2	PE0	D	200	-	13,13,13	1.48	3 (23%)	15,18,18	2.40	7 (46%)
2	PE0	C	200	-	13,13,13	1.49	3 (23%)	15,18,18	2.41	7 (46%)
2	PE0	B	200	-	13,13,13	1.48	3 (23%)	15,18,18	2.41	7 (46%)

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	PE0	A	200	-	-	-	0/2/2/2
2	PE0	D	200	-	-	-	0/2/2/2
2	PE0	C	200	-	-	-	0/2/2/2
2	PE0	B	200	-	-	-	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	200	PE0	C1-C4	3.00	1.46	1.41
2	C	200	PE0	C1-C4	2.98	1.46	1.41
2	B	200	PE0	C1-C4	2.97	1.46	1.41
2	D	200	PE0	C1-C4	2.96	1.46	1.41
2	C	200	PE0	C1-N4	2.80	1.37	1.33
2	C	200	PE0	C4-N2	2.80	1.37	1.33
2	D	200	PE0	C4-N2	2.80	1.37	1.33
2	B	200	PE0	C4-N2	2.77	1.37	1.33
2	B	200	PE0	C1-N4	2.76	1.37	1.33
2	A	200	PE0	C4-N2	2.74	1.37	1.33
2	A	200	PE0	C1-N4	2.74	1.37	1.33
2	D	200	PE0	C1-N4	2.74	1.37	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	200	PE0	C1-C4-N2	-4.63	117.10	123.43
2	A	200	PE0	C1-C4-N2	-4.61	117.12	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	200	PE0	C1-C4-N2	-4.58	117.17	123.43
2	D	200	PE0	C1-C4-N2	-4.57	117.18	123.43
2	C	200	PE0	C3-N1-C2	3.79	119.69	115.36
2	B	200	PE0	C3-N1-C2	3.79	119.68	115.36
2	A	200	PE0	C3-N1-C2	3.78	119.68	115.36
2	D	200	PE0	C3-N1-C2	3.77	119.66	115.36
2	A	200	PE0	C3-N2-C4	3.76	121.91	115.93
2	B	200	PE0	N1-C3-N2	-3.76	122.20	127.22
2	A	200	PE0	N1-C3-N2	-3.75	122.22	127.22
2	C	200	PE0	C3-N2-C4	3.75	121.88	115.93
2	C	200	PE0	N1-C3-N2	-3.74	122.23	127.22
2	B	200	PE0	C3-N2-C4	3.74	121.87	115.93
2	D	200	PE0	N1-C3-N2	-3.71	122.27	127.22
2	D	200	PE0	C3-N2-C4	3.70	121.81	115.93
2	D	200	PE0	C2-C1-C4	-3.05	117.93	119.95
2	B	200	PE0	C2-C1-C4	-3.02	117.95	119.95
2	A	200	PE0	C2-C1-C4	-2.98	117.98	119.95
2	C	200	PE0	C2-C1-C4	-2.95	118.00	119.95
2	B	200	PE0	C4-C1-N4	2.36	121.18	118.24
2	D	200	PE0	C4-C1-N4	2.35	121.17	118.24
2	A	200	PE0	C4-C1-N4	2.35	121.17	118.24
2	C	200	PE0	C4-C1-N4	2.33	121.14	118.24
2	A	200	PE0	N3-C2-N1	2.10	118.21	115.82
2	C	200	PE0	N3-C2-N1	2.07	118.19	115.82
2	D	200	PE0	N3-C2-N1	2.07	118.19	115.82
2	B	200	PE0	N3-C2-N1	2.07	118.18	115.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.