



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:17 PM GMT

PDB ID : 1X1Z
Title : Orotidine 5'-monophosphate decarboxylase (odcase) complexed with BMP
(produced from 6-cyanoump)
Authors : Fujihashi, M.; Bello, A.M.; Poduch, E.; Wei, L.; Annedi, S.C.; Pai, E.F.;
Kotra, L.P.
Deposited on : 2005-04-15
Resolution : 1.45 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

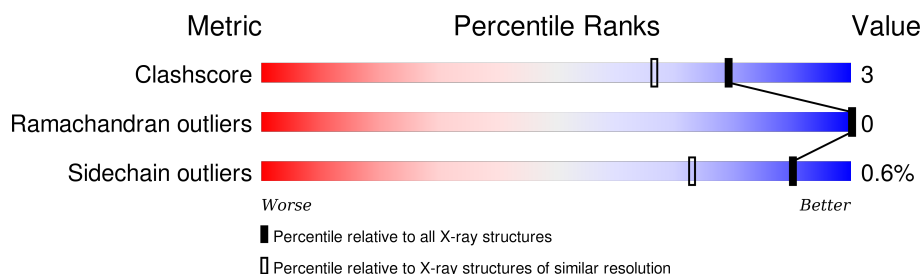
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)

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	252	
1	B	252	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3738 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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	15	0
			1696	1066	298	321	11			
1	B	215	Total	C	N	O	S	0	15	0
			1696	1066	298	321	11			

There are 54 discrepancies between the modelled and reference sequences:

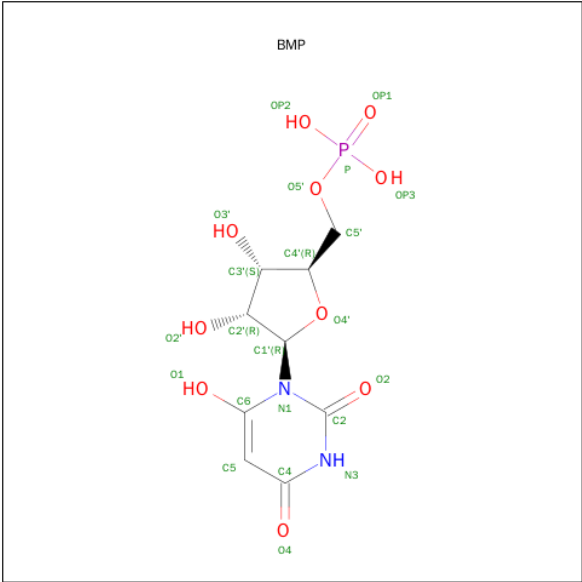
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP O26232
A	-1	SER	-	CLONING ARTIFACT	UNP O26232
A	0	HIS	-	CLONING ARTIFACT	UNP O26232
A	101	PRO	ARG	CONFLICT	UNP O26232
A	226	ARG	LEU	ENGINEERED	UNP O26232
A	227	ILE	ASN	ENGINEERED	UNP O26232
A	229	GLU	-	CLONING ARTIFACT	UNP O26232
A	230	ASP	-	CLONING ARTIFACT	UNP O26232
A	231	PRO	-	CLONING ARTIFACT	UNP O26232
A	232	ALA	-	CLONING ARTIFACT	UNP O26232
A	233	ALA	-	CLONING ARTIFACT	UNP O26232
A	234	ASN	-	CLONING ARTIFACT	UNP O26232
A	235	LYS	-	CLONING ARTIFACT	UNP O26232
A	236	ALA	-	CLONING ARTIFACT	UNP O26232
A	237	ARG	-	CLONING ARTIFACT	UNP O26232
A	238	LYS	-	CLONING ARTIFACT	UNP O26232
A	239	GLU	-	CLONING ARTIFACT	UNP O26232
A	240	ALA	-	CLONING ARTIFACT	UNP O26232
A	241	GLU	-	CLONING ARTIFACT	UNP O26232
A	242	LEU	-	CLONING ARTIFACT	UNP O26232
A	243	ALA	-	CLONING ARTIFACT	UNP O26232
A	244	ALA	-	CLONING ARTIFACT	UNP O26232
A	245	ALA	-	CLONING ARTIFACT	UNP O26232
A	246	THR	-	CLONING ARTIFACT	UNP O26232
A	247	ALA	-	CLONING ARTIFACT	UNP O26232

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Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLU	-	CLONING ARTIFACT	UNP O26232
A	249	GLN	-	CLONING ARTIFACT	UNP O26232
B	998	GLY	-	CLONING ARTIFACT	UNP O26232
B	999	SER	-	CLONING ARTIFACT	UNP O26232
B	1000	HIS	-	CLONING ARTIFACT	UNP O26232
B	1101	PRO	ARG	CONFLICT	UNP O26232
B	1226	ARG	LEU	ENGINEERED	UNP O26232
B	1227	ILE	ASN	ENGINEERED	UNP O26232
B	1229	GLU	-	CLONING ARTIFACT	UNP O26232
B	1230	ASP	-	CLONING ARTIFACT	UNP O26232
B	1231	PRO	-	CLONING ARTIFACT	UNP O26232
B	1232	ALA	-	CLONING ARTIFACT	UNP O26232
B	1233	ALA	-	CLONING ARTIFACT	UNP O26232
B	1234	ASN	-	CLONING ARTIFACT	UNP O26232
B	1235	LYS	-	CLONING ARTIFACT	UNP O26232
B	1236	ALA	-	CLONING ARTIFACT	UNP O26232
B	1237	ARG	-	CLONING ARTIFACT	UNP O26232
B	1238	LYS	-	CLONING ARTIFACT	UNP O26232
B	1239	GLU	-	CLONING ARTIFACT	UNP O26232
B	1240	ALA	-	CLONING ARTIFACT	UNP O26232
B	1241	GLU	-	CLONING ARTIFACT	UNP O26232
B	1242	LEU	-	CLONING ARTIFACT	UNP O26232
B	1243	ALA	-	CLONING ARTIFACT	UNP O26232
B	1244	ALA	-	CLONING ARTIFACT	UNP O26232
B	1245	ALA	-	CLONING ARTIFACT	UNP O26232
B	1246	THR	-	CLONING ARTIFACT	UNP O26232
B	1247	ALA	-	CLONING ARTIFACT	UNP O26232
B	1248	GLU	-	CLONING ARTIFACT	UNP O26232
B	1249	GLN	-	CLONING ARTIFACT	UNP O26232

- Molecule 2 is 6-HYDROXYURIDINE-5'-PHOSPHATE (three-letter code: BMP) (formula: $C_9H_{13}N_2O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	2	Total	C	N	O	P	0	0
			44	18	4	20	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

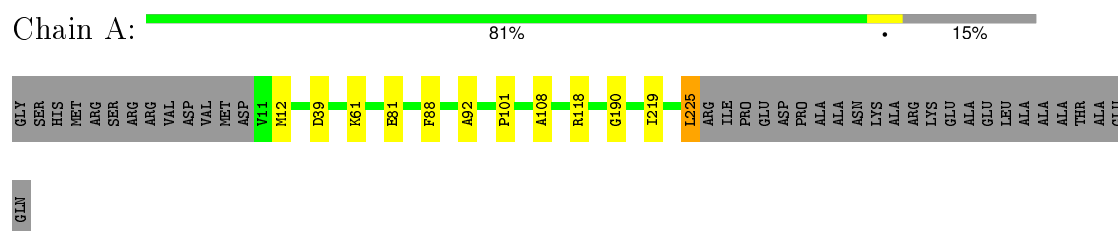
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		
4	B	141	Total	O	0	0
			141	141		

3 Residue-property plots [i](#)

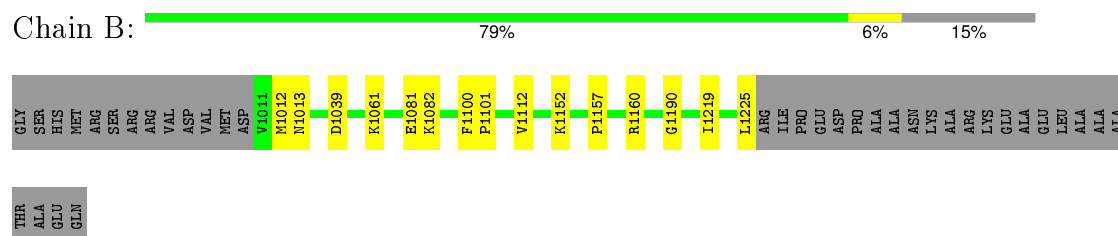
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: Orotidine 5'-phosphate decarboxylase



- Molecule 1: Orotidine 5'-phosphate decarboxylase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.10 Å 73.57 Å 59.40 Å 90.00° 119.28° 90.00°	Depositor
Resolution (Å)	17.62 – 1.45	Depositor
% Data completeness (in resolution range)	97.5 (17.62-1.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.162 , 0.180	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3738	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: GOL, BMP

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	0.64	0/1779	0.78	0/2400
1	B	0.64	0/1779	0.79	2/2400 (0.1%)
All	All	0.64	0/3558	0.79	2/4800 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1160	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	1157	PRO	N-CA-C	5.03	125.17	112.10

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	1696	0	1668	12	0
1	B	1696	0	1668	10	0
2	A	44	0	20	0	0
3	A	18	0	24	0	0
3	B	6	0	8	0	0
4	A	137	0	0	3	0
4	B	141	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3738	0	3388	24	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 3.

The worst 5 of 24 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:B:1013:ASN:HB3	1:B:1219:ILE:HD12	1.49	0.91
1:A:118:ARG:HG3	1:A:118:ARG:HH11	1.47	0.80
1:A:92:ALA:O	1:A:118:ARG:NH1	2.20	0.73
1:A:88:PHE:HA	1:A:118:ARG:HH12	1.55	0.71
1:A:118:ARG:NH1	1:A:118:ARG:HG3	2.06	0.70

There are no symmetry-related clashes.

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	228/252 (90%)	222 (97%)	6 (3%)	0	100	100
1	B	228/252 (90%)	223 (98%)	5 (2%)	0	100	100
All	All	456/504 (90%)	445 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	182/197 (92%)	180 (99%)	2 (1%)	80	52
1	B	182/197 (92%)	182 (100%)	0	100	100
All	All	364/394 (92%)	362 (100%)	2 (0%)	90	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	225	LEU

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

Mol	Chain	Res	Type
1	B	1013	ASN
1	B	1173	GLN

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](#)

6 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	BMP	A	301	-	16,23,23	1.84	3 (18%)	19,35,35	3.39	3 (15%)
2	BMP	A	302	-	16,23,23	1.77	2 (12%)	19,35,35	3.59	3 (15%)
3	GOL	A	311	-	5,5,5	0.51	0	5,5,5	0.76	0
3	GOL	A	312	-	5,5,5	0.62	0	5,5,5	0.83	0
3	GOL	A	314	-	5,5,5	0.44	0	5,5,5	0.52	0
3	GOL	B	313	-	5,5,5	0.39	0	5,5,5	0.54	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
2	BMP	A	301	-	-	0/6/26/26	0/2/2/2
2	BMP	A	302	-	-	0/6/26/26	0/2/2/2
3	GOL	A	311	-	-	0/4/4/4	0/0/0/0
3	GOL	A	312	-	-	0/4/4/4	0/0/0/0
3	GOL	A	314	-	-	0/4/4/4	0/0/0/0
3	GOL	B	313	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	BMP	O4'-C1'	2.04	1.43	1.41
2	A	301	BMP	C6-N1	3.90	1.44	1.38
2	A	302	BMP	C6-N1	4.28	1.44	1.38
2	A	302	BMP	C4-N3	4.65	1.41	1.33
2	A	301	BMP	C4-N3	5.01	1.42	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	BMP	C5-C4-N3	-7.15	115.39	124.05
2	A	301	BMP	C5-C4-N3	-6.74	115.88	124.05
2	A	301	BMP	C4-C5-C6	2.34	119.83	116.06
2	A	302	BMP	C4-C5-C6	2.50	120.09	116.06
2	A	301	BMP	C4-N3-C2	12.40	126.42	114.14

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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