

wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 02:00 AM EDT

PDB ID : 1L6Y

Title : Crystal Structure of Porphobilinogen Synthase Complexed with the Inhibitor

4-Oxosebacic Acid

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Deposited on : 2002-03-14

Resolution : 1.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

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)

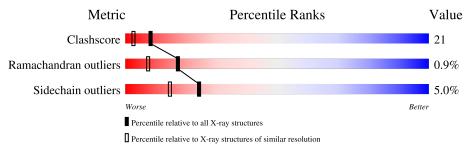
Validation Pipeline (wwPDB-VP) : 2.35

1 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 1.90 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of cha	in	
1	A	323	65%	33%	
1	В	323	55%	40%	5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	902	-	X	-	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5419 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 PORPHOBILINOGEN SYNTHASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	323	Total 2463	C 1538	N 429	O 476	S 20	0	0	0
1	В	323	Total 2463	C 1538	N 429	O 476	S 20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	CME	CYS	modified residue	UNP P0ACB2
В	133	CME	CYS	modified residue	UNP P0ACB2

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

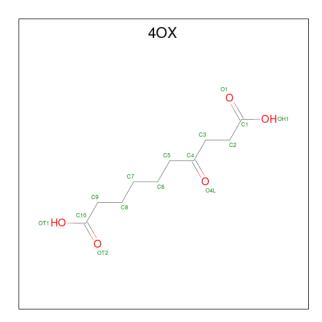
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0

• Molecule 4 is 4-OXODECANEDIOIC ACID (three-letter code: 4OX) (formula: $C_{10}H_{16}O_5$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
1	Λ	1	Total C O	0	0
4	Λ	1	14 10 4		U
4	D	1	Total C O	0	0
4	Ъ	1	14 10 4	0	0

 \bullet Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



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

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

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	216	Total O 216 216	0	0
6	В	215	Total O 215 215	0	0

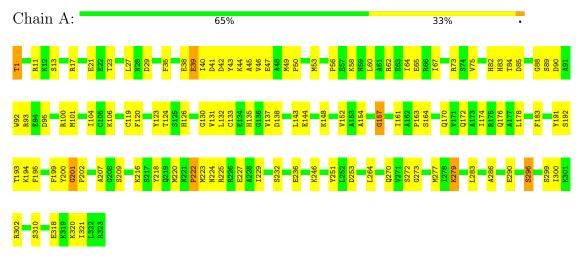


3 Residue-property plots (i)

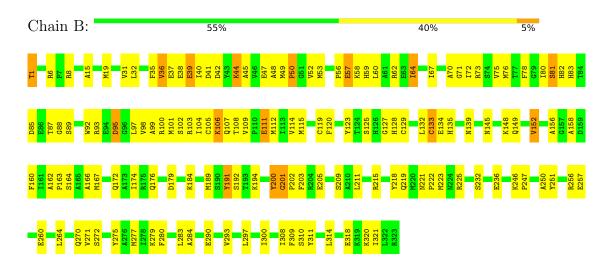
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: PORPHOBILINOGEN SYNTHASE



• Molecule 1: PORPHOBILINOGEN SYNTHASE





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants	129.00Å 129.00Å 142.80Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 - 1.90	Depositor
% Data completeness	99.8 (40.00-1.90)	Depositor
(in resolution range)	33.0 (40.00 1.30)	Берозгог
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5419	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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: ZN, GOL, MG, 4OX, CME

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			nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.90	1/2491 (0.0%)	1.01	5/3360 (0.1%)	
1	В	0.89	2/2491 (0.1%)	0.98	2/3360 (0.1%)	
All	All	0.90	3/4982 (0.1%)	1.00	7/6720 (0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers	
1	В	0	1	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	129	CYS	CB-SG	6.79	1.93	1.82
1	A	39	GLU	CB-CG	6.11	1.63	1.52
1	В	39	GLU	CB-CG	5.43	1.62	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	A	253	ASP	CB-CG-OD1	6.12	123.81	118.30
1	В	191	TYR	N-CA-C	-5.89	95.09	111.00
1	A	29	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	В	6	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	157	GLY	N-CA-C	5.03	125.68	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	В	200	TYR	Sidechain

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	2463	0	2418	92	1
1	В	2463	0	2418	119	2
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	A	14	0	14	0	0
4	В	14	0	14	4	0
5	A	24	0	32	0	0
5	В	6	0	8	1	0
6	A	216	0	0	9	1
6	В	215	0	0	12	0
All	All	5419	0	4904	208	4

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 21.

The worst 5 of 208 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:236:GLU:HG3	1:A:264:LEU:HD12	1.48	0.92
1:A:132:LEU:O	1:A:133:CME:HE3	1.75	0.84
1:A:236:GLU:HG3	1:A:264:LEU:CD1	2.08	0.84
1:B:172:GLN:O	1:B:176:GLN:HG3	1.84	0.78
1:B:103:ARG:HD3	6:B:629:HOH:O	1.83	0.77

All (4) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
6:A:610:HOH:O	6:A:610:HOH:O[8_666]	1.48	0.72
1:B:39:GLU:OE2	1:B:39:GLU:OE2[8_665]	1.78	0.42
1:A:39:GLU:OE2	1:A:39:GLU:OE2[8_666]	1.94	0.26
1:B:83:HIS:NE2	1:B:83:HIS:NE2[8_665]	2.01	0.19

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	320/323~(99%)	297 (93%)	21 (7%)	2 (1%)	25 15
1	В	320/323~(99%)	299 (93%)	17 (5%)	4 (1%)	12 4
All	All	640/646~(99%)	596 (93%)	38 (6%)	6 (1%)	17 7

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	57	GLU
1	A	50	PRO
1	В	134	GLU
1	A	201	GLY
1	В	50	PRO

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	251/257 (98%)	239 (95%)	12 (5%)	25 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	В	251/257 (98%)	238 (95%)	13 (5%)	23 14
All	All	502/514 (98%)	477 (95%)	25 (5%)	24 15

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	42	ASP
1	В	72	ILE
1	В	321	ILE
1	В	64	ILE
1	В	81	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	172	GLN
1	В	219	GLN
1	В	270	GLN
1	В	69	ASN
1	В	82	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	Chain	Chain	Chain	Res	Link	\mathbf{B}	ond leng	${ m gths}$	В	ond ang	gles	l
	IVIOI	туре	nes		LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	ĺ			
ĺ	1	CME	A	133	1	8,9,10	0.82	0	5,9,11	0.96	0	ĺ			



	Mol T	Type	Chain	Res	Link	B	ond leng	${ m gths}$	Bond angles		
		Type				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	1	CME	В	133	1	8,9,10	0.77	0	5,9,11	1.33	1 (20%)

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	CME	A	133	1	-	1/5/8/10	-
1	CME	В	133	1	-	1/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	В	133	CME	CB-SG-SD	2.76	110.97	103.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	133	CME	CZ-CE-SD-SG
1	В	133	CME	CZ-CE-SD-SG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	133	CME	3	0
1	В	133	CME	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	Tuno	pe Chain Res L		Link	Во	ond leng	$ ag{ths}$	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	902	-	5,5,5	1.56	2 (40%)	5,5,5	1.03	0
5	GOL	A	904	-	5,5,5	1.75	2 (40%)	5,5,5	1.32	0
4	4OX	A	350	1	13,13,14	1.37	1 (7%)	14,14,16	0.90	0
4	4OX	В	350	1	13,13,14	1.02	0	14,14,16	1.43	3 (21%)
5	GOL	A	901	-	5,5,5	2.12	2 (40%)	5,5,5	1.37	1 (20%)
5	GOL	A	905	-	5,5,5	1.87	2 (40%)	5,5,5	1.02	0
5	GOL	В	903	-	5,5,5	1.37	0	5,5,5	0.83	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
5	GOL	A	902	-	-	4/4/4/4	-
5	GOL	A	904	-	-	3/4/4/4	-
4	4OX	A	350	1	-	6/11/11/13	-
4	4OX	В	350	1	-	8/11/11/13	-
5	GOL	A	901	-	-	2/4/4/4	-
5	GOL	A	905	-	-	3/4/4/4	-
5	GOL	В	903	-	-	4/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
4	A	350	4OX	C9-C10	3.53	1.58	1.50
5	A	901	GOL	C3-C2	3.03	1.64	1.51
5	A	901	GOL	C1-C2	2.78	1.63	1.51
5	A	905	GOL	C1-C2	2.46	1.61	1.51
5	A	904	GOL	C1-C2	2.38	1.61	1.51

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
4	В	350	4OX	C8-C9-C10	-2.41	108.39	114.47
4	В	350	4OX	C3-C2-C1	-2.30	108.68	114.47
4	В	350	4OX	OT2-C10-C9	-2.17	116.10	123.08
5	A	901	GOL	C3-C2-C1	2.16	120.12	111.70

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	GOL	C1-C2-C3-O3
5	A	902	GOL	C1-C2-C3-O3
5	A	902	GOL	O2-C2-C3-O3
5	A	904	GOL	C1-C2-C3-O3
5	A	905	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	350	4OX	4	0
5	В	903	GOL	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

