



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2016 – 08:34 AM EDT

PDB ID : 5IKY  
Title : Apo structure of Obc1, a bifunctional enzyme for quorum sensing-dependent oxalogenesis  
Authors : Oh, J.; Rhee, S.  
Deposited on : 2016-03-04  
Resolution : 2.50 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

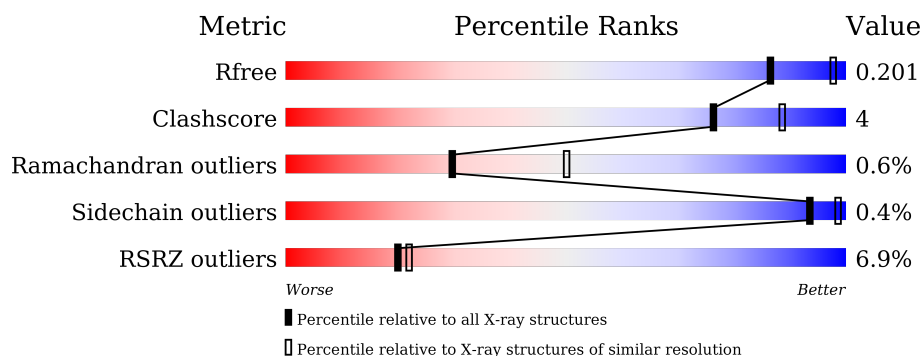
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	1125	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8036 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 Oxalate biosynthetic component 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1048	Total	C	N	O	S	0	0	0
			7835	4962	1403	1453	17			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

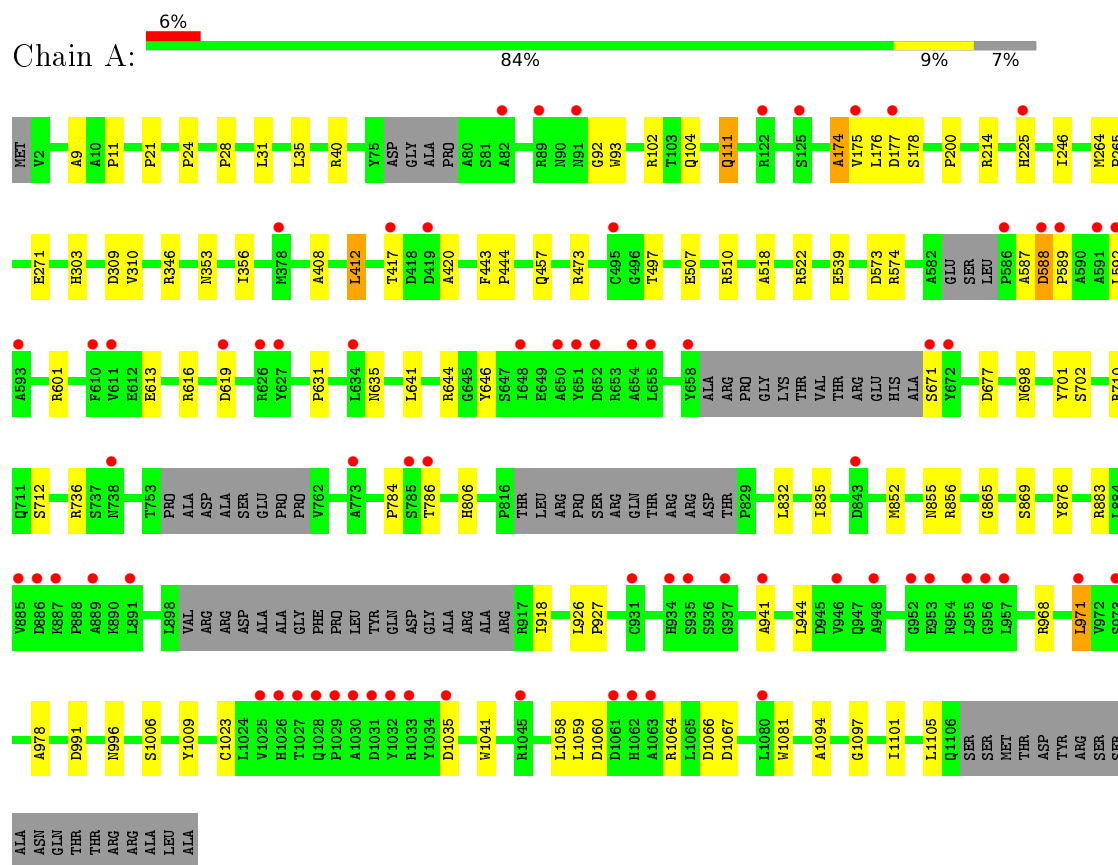
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	200	Total	O	0	0
			200	200		

### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

- Molecule 1: Oxalate biosynthetic component 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	230.81Å 230.81Å 253.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.77 – 2.50 38.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.77-2.50) 99.6 (38.77-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.198 , 0.227 0.197 , 0.201	Depositor DCC
$R_{free}$ test set	4570 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.22	0/8011	0.40	0/10954

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	7835	0	7516	59	0
2	A	1	0	0	0	0
3	A	200	0	0	3	0
All	All	8036	0	7516	59	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 4.

All (59) 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:111:GLN:HA	1:A:111:GLN:HE21	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:O	1:A:177:ASP:N	2.18	0.73
1:A:111:GLN:HA	1:A:111:GLN:NE2	2.04	0.71
1:A:698:ASN:HD21	1:A:702:SER:HB2	1.56	0.71
1:A:174:ALA:O	1:A:176:LEU:N	2.25	0.70
1:A:177:ASP:OD1	1:A:178:SER:N	2.26	0.69
1:A:35:LEU:O	1:A:40:ARG:NH2	2.25	0.68
1:A:613:GLU:OE2	1:A:616:ARG:NH1	2.27	0.67
1:A:111:GLN:CA	1:A:111:GLN:HE21	2.08	0.66
1:A:1064:ARG:NH1	3:A:1304:HOH:O	2.29	0.65
1:A:601:ARG:NH1	1:A:701:TYR:OH	2.29	0.65
1:A:677:ASP:O	1:A:736:ARG:NH2	2.31	0.64
1:A:303:HIS:O	1:A:574:ARG:NH2	2.34	0.61
1:A:539:GLU:OE1	1:A:712:SER:OG	2.21	0.59
1:A:1060:ASP:OD1	1:A:1064:ARG:N	2.31	0.57
1:A:309:ASP:OD1	1:A:522:ARG:NH2	2.36	0.57
1:A:876:TYR:HB2	1:A:944:LEU:HD22	1.88	0.56
1:A:588:ASP:H	1:A:589:PRO:HD2	1.72	0.54
1:A:1097:GLY:O	1:A:1101:ILE:HG13	2.08	0.54
1:A:996:ASN:ND2	1:A:1058:LEU:O	2.41	0.54
1:A:457:GLN:N	3:A:1310:HOH:O	2.42	0.53
1:A:786:THR:HG23	1:A:852:MET:HB2	1.91	0.53
1:A:225:HIS:HD2	1:A:473:ARG:NH1	2.07	0.53
1:A:507:GLU:OE2	1:A:510:ARG:NH1	2.43	0.52
1:A:806:HIS:HB2	1:A:832:LEU:HD22	1.91	0.52
1:A:28:PRO:HD2	1:A:31:LEU:HD12	1.93	0.51
1:A:856:ARG:HG2	1:A:978:ALA:HB2	1.92	0.51
1:A:1023:CYS:HB3	1:A:1059:LEU:HD11	1.93	0.51
1:A:855:ASN:ND2	1:A:869:SER:HB3	2.26	0.50
1:A:214:ARG:NH2	3:A:1313:HOH:O	2.46	0.49
1:A:619:ASP:OD2	1:A:671:SER:N	2.46	0.48
1:A:1066:ASP:OD1	1:A:1067:ASP:N	2.47	0.48
1:A:587:ALA:HB3	1:A:592:LEU:HD22	1.96	0.48
1:A:1035:ASP:HA	1:A:1081:TRP:HE1	1.79	0.47
1:A:710:ARG:NH2	1:A:1006:SER:O	2.32	0.47
1:A:518:ALA:O	1:A:522:ARG:HG3	2.14	0.47
1:A:1041:TRP:CE3	1:A:1105:LEU:HD11	2.50	0.47
1:A:92:GLY:HA3	1:A:104:GLN:OE1	2.15	0.46
1:A:926:LEU:O	1:A:968:ARG:NE	2.47	0.46
1:A:991:ASP:OD2	1:A:1009:TYR:OH	2.22	0.46
1:A:11:PRO:HD2	1:A:225:HIS:O	2.16	0.45
1:A:883:ARG:NH2	1:A:927:PRO:O	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LEU:HB3	1:A:646:TYR:HB2	1.98	0.44
1:A:93:TRP:CE2	1:A:102:ARG:HG3	2.53	0.44
1:A:784:PRO:HD3	1:A:835:ILE:HB	1.99	0.43
1:A:417:THR:HG23	1:A:420:ALA:H	1.83	0.43
1:A:1041:TRP:CZ3	1:A:1105:LEU:HD11	2.52	0.43
1:A:443:PHE:HA	1:A:444:PRO:HD2	1.88	0.43
1:A:214:ARG:HD2	1:A:271:GLU:OE2	2.18	0.43
1:A:353:ASN:OD1	1:A:356:ILE:HG12	2.20	0.42
1:A:264:MET:HB2	1:A:265:PRO:HD3	2.03	0.41
1:A:408:ALA:O	1:A:412:LEU:HD12	2.21	0.41
1:A:9:ALA:HB1	1:A:497:THR:HG21	2.02	0.41
1:A:310:VAL:HA	1:A:346:ARG:O	2.21	0.41
1:A:21:PRO:HG3	1:A:200:PRO:CB	2.51	0.41
1:A:941:ALA:HB1	1:A:971:LEU:HD11	2.02	0.41
1:A:573:ASP:OD1	1:A:644:ARG:NH2	2.55	0.40
1:A:24:PRO:HG2	1:A:246:ILE:HD11	2.03	0.40
1:A:631:PRO:O	1:A:635:ASN:ND2	2.52	0.40

There are no symmetry-related clashes.

## 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	1034/1125 (92%)	993 (96%)	35 (3%)	6 (1%)	30 50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ALA
1	A	175	VAL
1	A	1094	ALA
1	A	588	ASP

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Mol	Chain	Res	Type
1	A	918	ILE
1	A	865	GLY

### 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	775/922 (84%)	772 (100%)	3 (0%)	<a href="#">93</a> <a href="#">98</a>

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	412	LEU
1	A	971	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	A	111	GLN
1	A	225	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](#)

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1048/1125 (93%)	0.27	72 (6%)	20 22	39, 75, 123, 171	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	672	TYR	6.1
1	A	1029	PRO	5.5
1	A	1027	THR	4.9
1	A	1026	HIS	4.2
1	A	589	PRO	4.2
1	A	586	PRO	3.9
1	A	588	ASP	3.8
1	A	1025	VAL	3.7
1	A	658	TYR	3.6
1	A	1031	ASP	3.6
1	A	1028	GLN	3.6
1	A	378	MET	3.3
1	A	650	ALA	3.3
1	A	651	TYR	3.3
1	A	956	GLY	3.2
1	A	1032	TYR	3.2
1	A	955	LEU	3.2
1	A	952	GLY	3.2
1	A	671	SER	3.1
1	A	495	CYS	3.1
1	A	1030	ALA	3.0
1	A	953	GLU	2.9
1	A	592	LEU	2.9
1	A	885	VAL	2.8
1	A	971	LEU	2.8
1	A	935	SER	2.8
1	A	1035	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	738	ASN	2.8
1	A	843	ASP	2.8
1	A	786	THR	2.7
1	A	1080	LEU	2.7
1	A	591	ALA	2.7
1	A	655	LEU	2.7
1	A	773	ALA	2.7
1	A	610	PHE	2.7
1	A	89	ARG	2.6
1	A	889	ALA	2.6
1	A	593	ALA	2.6
1	A	634	LEU	2.6
1	A	654	ALA	2.5
1	A	887	LYS	2.5
1	A	1063	ALA	2.5
1	A	1045	ARG	2.5
1	A	1033	ARG	2.5
1	A	125	SER	2.5
1	A	175	VAL	2.4
1	A	946	VAL	2.4
1	A	225	HIS	2.4
1	A	82	ALA	2.4
1	A	934	HIS	2.3
1	A	419	ASP	2.3
1	A	1061	ASP	2.3
1	A	611	VAL	2.3
1	A	785	SER	2.2
1	A	948	ALA	2.2
1	A	931	CYS	2.2
1	A	122	ARG	2.2
1	A	627	TYR	2.2
1	A	648	ILE	2.2
1	A	652	ASP	2.2
1	A	941	ALA	2.1
1	A	973	SER	2.1
1	A	177	ASP	2.1
1	A	886	ASP	2.1
1	A	626	ARG	2.1
1	A	937	GLY	2.1
1	A	1062	HIS	2.1
1	A	91	ASN	2.1
1	A	891	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	619	ASP	2.0
1	A	957	LEU	2.0
1	A	417	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	1201	1/1	0.96	0.26	0.54	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.