



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:37 PM GMT

PDB ID : 1BOU  
Title : THREE-DIMENSIONAL STRUCTURE OF LIGAB  
Authors : Sugimoto, K.; Senda, T.; Fukuda, M.; Mitsui, Y.  
Deposited on : 1998-08-06  
Resolution : 2.20 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](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.

---

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

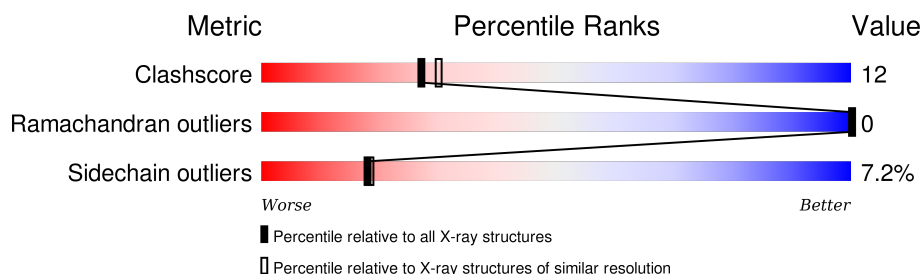
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	139	 78% 16% • 5%
1	C	139	 73% 19% • 5%
2	B	302	 72% 25% • •
2	D	302	 66% 30% • •

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6886 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 4,5-DIOXYGENASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1029	646	177	199	7			
1	C	132	Total	C	N	O	S	0	0	0
			1029	646	177	199	7			

- Molecule 2 is a protein called 4,5-DIOXYGENASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2313	1482	385	430	16			
2	D	298	Total	C	N	O	S	0	0	0
			2313	1482	385	430	16			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	76	Total	O	0	0
			76	76		
4	C	24	Total	O	0	0
			24	24		
4	D	61	Total	O	0	0
			61	61		

### 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.

Note EDS was not executed.

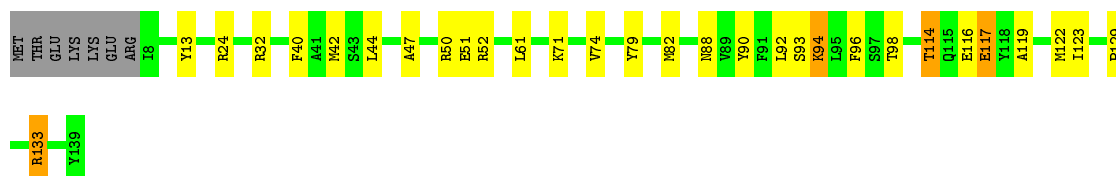
#### • Molecule 1: 4,5-DIOXYGENASE ALPHA CHAIN

Chain A: 



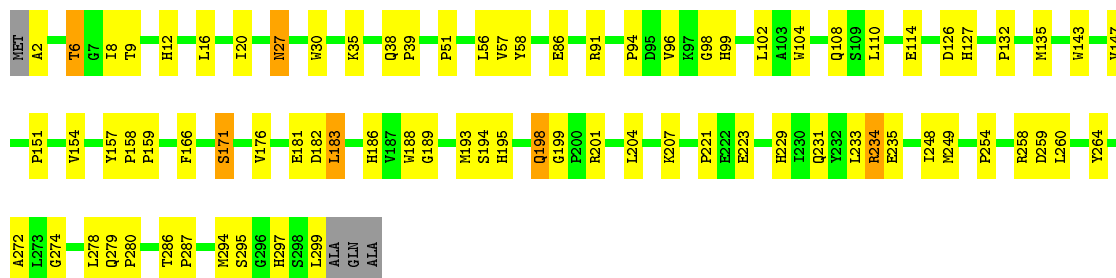
#### • Molecule 1: 4,5-DIOXYGENASE ALPHA CHAIN

Chain C: 



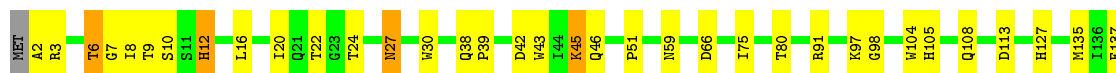
#### • Molecule 2: 4,5-DIOXYGENASE BETA CHAIN

Chain B: 



#### • Molecule 2: 4,5-DIOXYGENASE BETA CHAIN

Chain D: 



P238	P140
H229	V147
L233	V154
R234	V155
S238	T156
V241	Y157
V244	P158
M249	P159
K256	K163
V257	F166
R258	S171
D259	V176
L260	F179
F263	P180
Y264	E181
H265	D182
I266	L183
P267	H186
T271	V187
G274	W188
A275	G189
M276	M193
L277	S194
L278	H195
Q279	Q196
P280	L197
E281	Q198
G285	R201
L286	A202
P287	G203
R291	L204
K292	I205
V293	M206
M294	K207
H297	E208
S298	F209
L299	D210
ALA	L211
GLN	T214
ALA	D215
	K216
	P221
	E222
	E223
	L224
	M227

## 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, $\alpha$ , $\beta$ , $\gamma$	65.40 Å 66.50 Å 119.80 Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	60.00 – 2.20	Depositor
% Data completeness (in resolution range)	86.5 (60.00-2.20)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.149 , 0.206	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6886	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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: FE

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	0.37	0/1049	0.50	0/1408
1	C	0.36	0/1049	0.48	0/1408
2	B	0.36	0/2383	0.62	1/3253 (0.0%)
2	D	0.35	0/2383	0.60	0/3253
All	All	0.36	0/6864	0.58	1/9322 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	272	ALA	N-CA-C	-5.31	96.66	111.00

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	1029	0	986	17	0
1	C	1029	0	986	28	0
2	B	2313	0	2252	58	0
2	D	2313	0	2252	70	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	39	0	0	0	0
4	B	76	0	0	0	0
4	C	24	0	0	0	0
4	D	61	0	0	0	0
All	All	6886	0	6476	158	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 12.

The worst 5 of 158 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)
2:D:27:ASN:HD21	2:D:30:TRP:H	1.09	0.99
2:D:27:ASN:ND2	2:D:30:TRP:H	1.73	0.85
2:B:27:ASN:HD21	2:B:30:TRP:H	1.20	0.85
2:B:2:ALA:HB2	2:B:181:GLU:O	1.76	0.85
2:D:20:ILE:HD11	2:D:135:MET:HE2	1.60	0.84

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	130/139 (94%)	127 (98%)	3 (2%)	0	100	100
1	C	130/139 (94%)	128 (98%)	2 (2%)	0	100	100
2	B	296/302 (98%)	284 (96%)	12 (4%)	0	100	100
2	D	296/302 (98%)	284 (96%)	12 (4%)	0	100	100
All	All	852/882 (97%)	823 (97%)	29 (3%)	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	102/109 (94%)	96 (94%)	6 (6%)	24	27
1	C	102/109 (94%)	96 (94%)	6 (6%)	24	27
2	B	253/255 (99%)	235 (93%)	18 (7%)	18	19
2	D	253/255 (99%)	232 (92%)	21 (8%)	14	13
All	All	710/728 (98%)	659 (93%)	51 (7%)	18	18

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	297	HIS
1	C	117	GLU
2	D	256	LYS
1	C	52	ARG
1	C	133	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	198	GLN
2	B	279	GLN
2	D	198	GLN
2	B	99	HIS
2	B	121	ASN

### 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](#)

Of 2 ligands modelled in this entry, 2 are 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 [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 ⓘ

### 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.