wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 08:24 AM EST

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*
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:

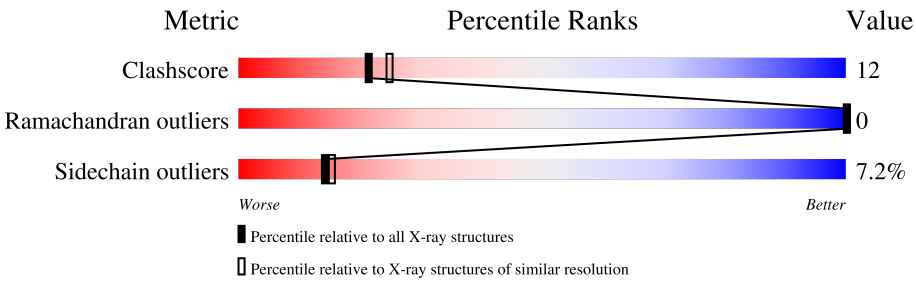
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 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 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 (i)

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
			Total	C	N	O	S			
1	A	132	1029	646	177	199	7	0	0	0
1	C	132	1029	646	177	199	7	0	0	0

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

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

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

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

- Molecule 4 is water.

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

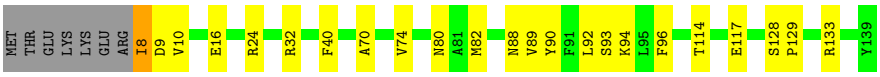
3 Residue-property plots (i)

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.

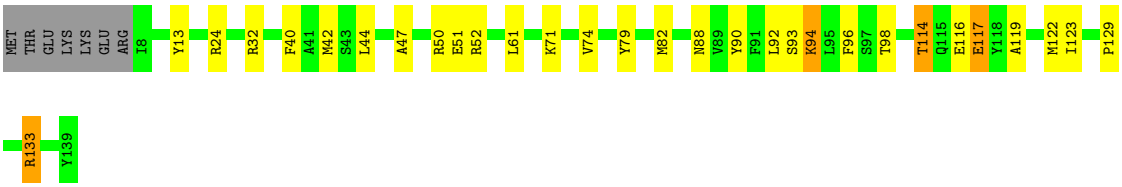
• Molecule 1: 4,5-DIOXYGENASE ALPHA CHAIN

Chain A: 78% 16% • 5%



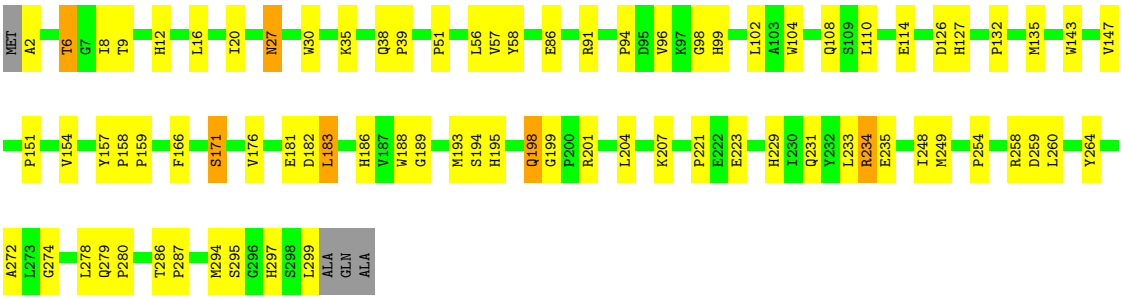
• Molecule 1: 4,5-DIOXYGENASE ALPHA CHAIN

Chain C: 73% 19% • 5%



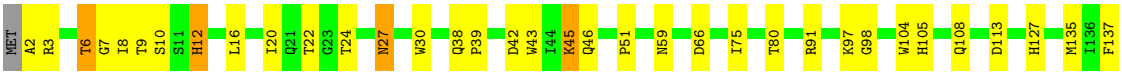
• Molecule 2: 4,5-DIOXYGENASE BETA CHAIN

Chain B: 72% 25% • •



• Molecule 2: 4,5-DIOXYGENASE BETA CHAIN

Chain D: 66% 30% • •



P140
V147
V154
V155
T156
Y157
P158
P159
K163
F166
S171
V176
F179
P180
E181
D182
L183
H186
V187
W188
G189
M193
S194
H195
Q196
L197
Q198
R201
A202
G203
L204
I205
N206
K207
E208
F209
D210
L211
I214
D215
K216
P221
E222
E223
L224
M227
P228
H229
L233
R234
S238
V241
V244
M249
K256
V257
R258
D259
L260
F263
Y264
H265
I266
P267
T271
G274
A275
M276
I277
L278
Q279
P280
E281
G285
T286
P287
R291
K292
V293
M294
H297
S298
L299
ALA
GLN
ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.40Å 66.50Å 119.80Å 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^2)	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(^{o})	Ideal(^{o})
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

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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%)	19	23
1	C	102/109 (94%)	96 (94%)	6 (6%)	19	23
2	B	253/255 (99%)	235 (93%)	18 (7%)	14	16
2	D	253/255 (99%)	232 (92%)	21 (8%)	11	11
All	All	710/728 (98%)	659 (93%)	51 (7%)	14	15

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

Mol	Chain	Res	Type
1	C	117	GLU
2	D	45	LYS
2	D	297	HIS
1	C	133	ARG
2	D	10	SER

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

Mol	Chain	Res	Type
2	D	198	GLN
2	D	279	GLN
2	D	229	HIS
2	B	198	GLN
2	D	122	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 monosaccharides 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 (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.