WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID	:	1BSL
Title	:	STRUCTURE OF ALKANAL MONOOXYGENASE BETA CHAIN
Authors	:	Rayment, I.; Holden, H.M.; Thoden, J.B.; Baldwin, T.O.
Deposited on	:	1996-10-22
Resolution	:	1.95 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:

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 1.95 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	Percentile Ranks	Value
Clashscore		25
Ramachandran outliers		0.6%
Sidechain outliers		11.9%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
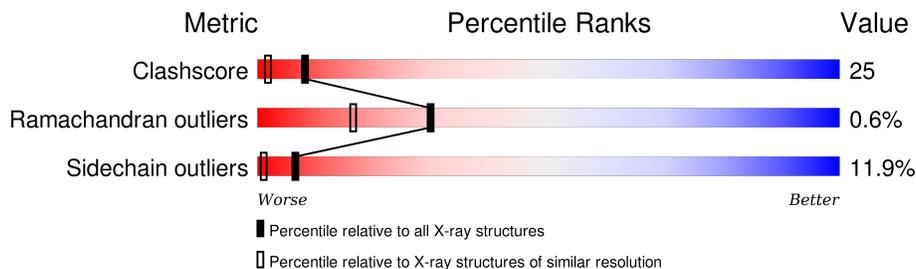
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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 <=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	324	56%　　　29%　　　13%　　・
1	B	324	44%　　　45%　　　10%

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2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6116 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 BACTERIAL LUCIFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total 2559	C 1612	N 441	O 491	S 15	0	2	0
1	B	324	Total 2568	C 1616	N 440	O 497	S 15	0	3	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	586	Total 586	O 586	0	0
2	B	403	Total 403	O 403	0	0

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 (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: BACTERIAL LUCIFERASE
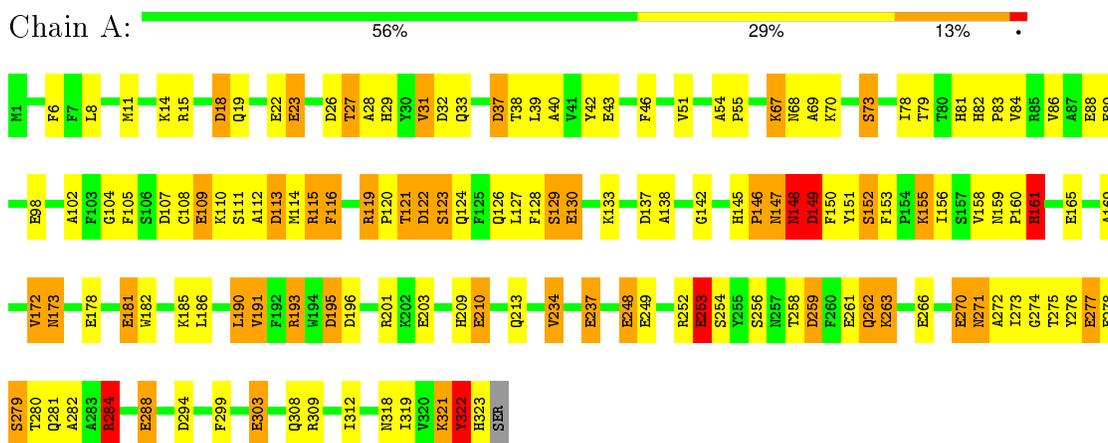
- Molecule 1: BACTERIAL LUCIFERASE
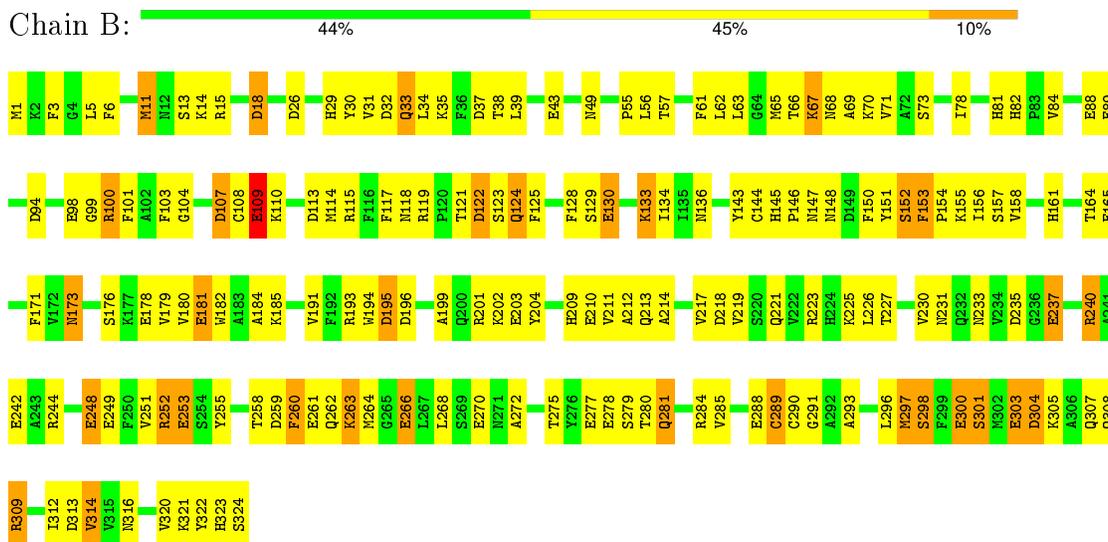
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.80Å 62.00Å 218.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.95)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6116	wwPDB-VP
Average B, all atoms (Å²)	35.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1.19	22/2629 (0.8%)	1.63	52/3556 (1.5%)
1	B	1.21	24/2640 (0.9%)	1.68	56/3570 (1.6%)
All	All	1.20	46/5269 (0.9%)	1.66	108/7126 (1.5%)

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	0
All	All	1	1

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	LYS	CE-NZ	11.16	1.76	1.49
1	A	88	GLU	CD-OE1	11.10	1.37	1.25
1	B	261	GLU	CD-OE1	9.22	1.35	1.25
1	A	270	GLU	CD-OE1	8.89	1.35	1.25
1	A	109	GLU	CD-OE2	8.60	1.35	1.25

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	100	ARG	NE-CZ-NH2	-13.51	113.54	120.30
1	B	100	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	A	201	ARG	NE-CZ-NH2	-12.43	114.09	120.30
1	A	201	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	A	318	ASN	CB-CA-C	10.50	131.41	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	69	ALA	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	322	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	2559	0	2435	108	0
1	B	2568	0	2446	151	0
2	A	586	0	0	20	1
2	B	403	0	0	23	1
All	All	6116	0	4881	246	1

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 25.

The worst 5 of 246 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:67:LYS:NZ	1:B:67:LYS:CE	1.76	1.46
1:A:146:PRO:HG3	1:A:153:PHE:CE2	1.88	1.08
1:A:146:PRO:HD3	1:A:153:PHE:CE1	1.97	0.99
1:B:148:ASN:HD22	1:B:150:PHE:N	1.64	0.94
1:A:148:ASN:ND2	1:A:150:PHE:H	1.65	0.93

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
2:A:860:HOH:O	2:B:699:HOH:O[1_645]	0.36	1.84

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	323/324 (100%)	309 (96%)	13 (4%)	1 (0%)	46	35
1	B	325/324 (100%)	305 (94%)	17 (5%)	3 (1%)	21	9
All	All	648/648 (100%)	614 (95%)	30 (5%)	4 (1%)	30	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	B	260	PHE
1	B	68	ASN
1	B	320	VAL

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	275/274 (100%)	237 (86%)	38 (14%)	4	1
1	B	277/274 (101%)	249 (90%)	28 (10%)	9	2
All	All	552/548 (101%)	486 (88%)	66 (12%)	6	1

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	GLU
1	A	303	GLU

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Mol	Chain	Res	Type
1	B	288	GLU
1	A	256	SER
1	A	263	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	GLN
1	B	9	ASN
1	B	173	ASN
1	A	173	ASN
1	B	221	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)

There are no ligands in this entry.

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 will therefore be empty.

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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