



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 09:36 pm GMT

PDB ID : 1DTZ
Title : STRUCTURE OF CAMEL APO-LACTOFERRIN DEMONSTRATES ITS DUAL ROLE IN SEQUESTERING AND TRANSPORTING FERRIC IONS SIMULTANEOUSLY: CRYSTAL STRUCTURE OF CAMEL APO-LACTOFERRIN AT 2.6Å RESOLUTION.
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Deposited on : 2000-01-13
Resolution : 2.65 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:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

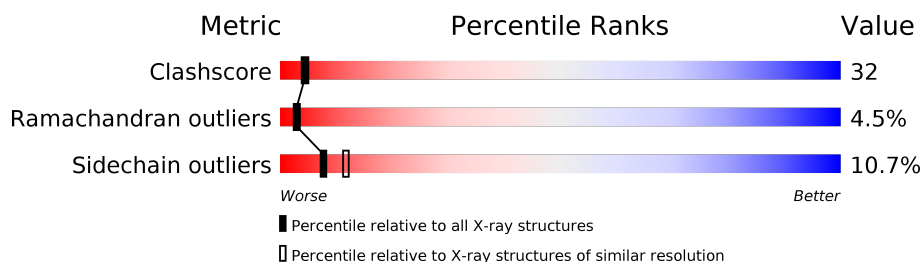
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)

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 $\leq 5\%$. 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	689	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5511 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 APO LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	689	Total	C	N	O	S	15	0	0
			5284	3318	934	994	38			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	LYS	SER	CONFLICT	UNP Q9TUM0
A	87	GLN	ASN	CONFLICT	UNP Q9TUM0
A	242	PHE	SER	CONFLICT	UNP Q9TUM0
A	312	LYS	SER	CONFLICT	UNP Q9TUM0
A	477	ASP	ASN	CONFLICT	UNP Q9TUM0
A	513	LEU	ASN	CONFLICT	UNP Q9TUM0
A	523	LEU	TYR	CONFLICT	UNP Q9TUM0
A	556	GLY	ASN	CONFLICT	UNP Q9TUM0
A	608	ARG	GLU	CONFLICT	UNP Q9TUM0
A	623	GLU	GLN	CONFLICT	UNP Q9TUM0
A	658	ASP	GLU	CONFLICT	UNP Q9TUM0

- Molecule 2 is water.

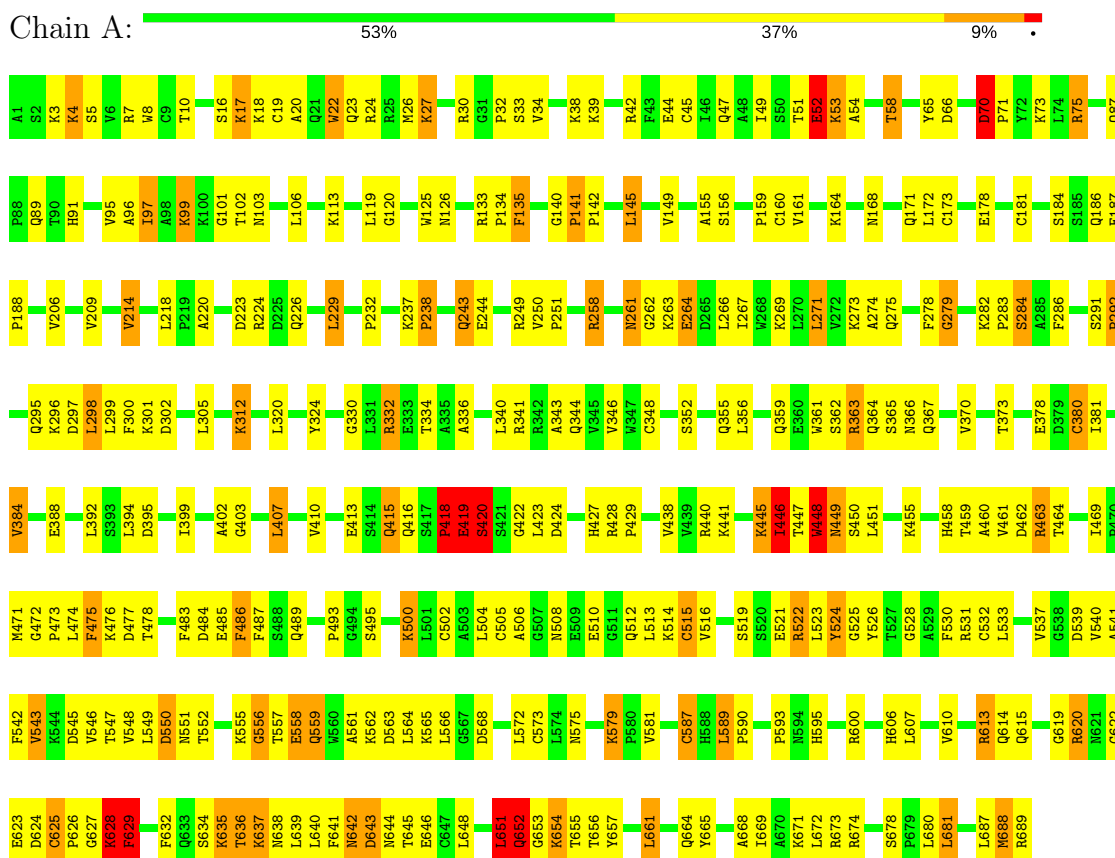
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	227	Total	O	0	0
			227	227		

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 the various outlier classes 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: APO LACTOFERRIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.84Å 80.92Å 56.35Å 90.00° 92.35° 90.00°	Depositor
Resolution (Å)	11.94 – 2.65	Depositor
% Data completeness (in resolution range)	98.0 (11.94-2.65)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.198 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5511	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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	0.65	10/5392 (0.2%)	1.30	23/7293 (0.3%)

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	1	8

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	652	GLN	C-N	-21.05	0.95	1.33
1	A	628	LYS	C-N	-15.52	0.98	1.34
1	A	651	LEU	C-N	-15.17	0.99	1.34
1	A	448	TRP	C-N	-13.23	1.03	1.34
1	A	449	ASN	CA-CB	8.75	1.75	1.53

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	629	PHE	CB-CG-CD1	-35.15	96.20	120.80
1	A	629	PHE	CB-CG-CD2	33.32	144.12	120.80
1	A	651	LEU	O-C-N	-32.47	70.75	122.70
1	A	652	GLN	O-C-N	-32.21	68.45	123.20
1	A	652	GLN	CA-C-N	25.35	166.90	116.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	418	PRO	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	GLU	Peptide
1	A	420	SER	Mainchain
1	A	448	TRP	Mainchain,Peptide
1	A	628	LYS	Peptide
1	A	651	LEU	Mainchain

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	5284	0	5230	336	0
2	A	227	0	0	15	0
All	All	5511	0	5230	336	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 32.

The worst 5 of 336 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:449:ASN:CB	1:A:449:ASN:CA	1.75	1.63
1:A:312:LYS:HE3	1:A:312:LYS:H	1.08	1.18
1:A:429:PRO:CB	1:A:652:GLN:HE22	1.61	1.12
1:A:429:PRO:HB3	1:A:652:GLN:HE22	1.06	1.10
1:A:615:GLN:NE2	1:A:648:LEU:H	1.59	1.01

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	687/689 (100%)	578 (84%)	78 (11%)	31 (4%)	3 3

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	PRO
1	A	418	PRO
1	A	446	ILE
1	A	550	ASP
1	A	587	CYS

5.3.2 Protein sidechains ⓘ

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	570/570 (100%)	509 (89%)	61 (11%)	8 12

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	ARG
1	A	420	SER
1	A	661	LEU
1	A	380	CYS
1	A	388	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	415	GLN
1	A	642	ASN
1	A	364	GLN

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Mol	Chain	Res	Type
1	A	367	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.