wwPDB X-ray Structure Validation Summary Report (i)

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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 2.6A RESOLUTION.
Authors	:	Khan, J.A.; Kumar, P.; Paramasivam, M.; Srinivasan, A.; Yadav, R.S.; Sahani, M.S.; Singh, T.P.
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
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:

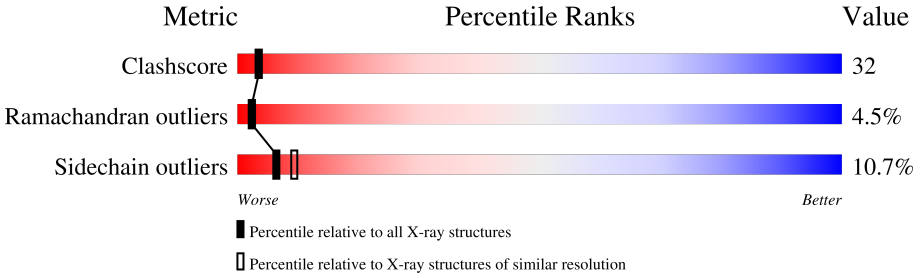
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.65 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	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (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 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	689	53% 37% 9% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	689	5284	3318	934	994	38	15	0	0

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
			Total	O		
2	A	227	227	227	0	0

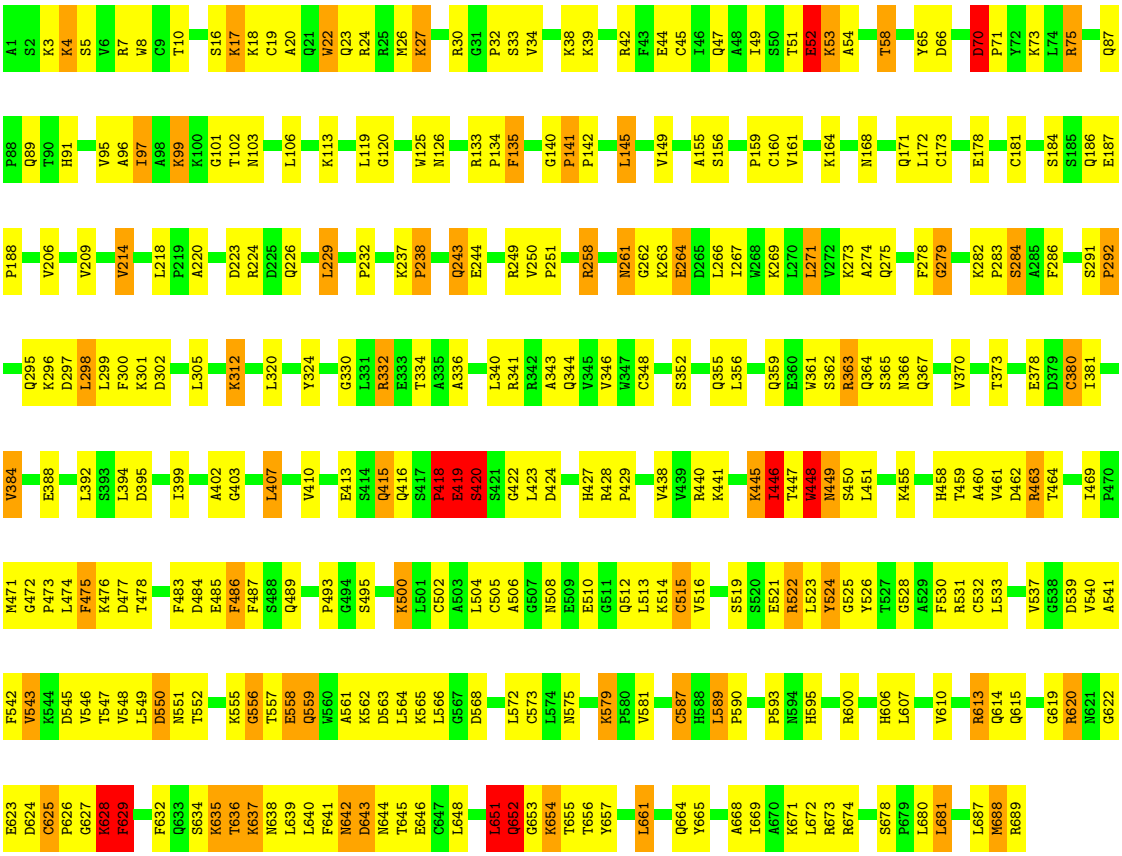
3 Residue-property plots (i)

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: APO LACTOFERRIN

Chain A: 53% 37% 9% •



4 Data and refinement statistics (i)

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(^{o})	Ideal(^{o})
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	Peptide,Mainchain
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:H	1:A:312:LYS:HE3	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%)	2 2

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 (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	570/570 (100%)	509 (89%)	61 (11%)	6 9

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

Mol	Chain	Res	Type
1	A	380	CYS
1	A	642	ASN
1	A	445	LYS
1	A	629	PHE
1	A	688	MET

Sometimes 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	449	ASN
1	A	551	ASN
1	A	508	ASN
1	A	559	GLN

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Mol	Chain	Res	Type
1	A	186	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)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	419:GLU	C	420:SER	N	1.18
1	A	418:PRO	C	419:GLU	N	1.15
1	A	448:TRP	C	449:ASN	N	1.03
1	A	651:LEU	C	652:GLN	N	0.99
1	A	628:LYS	C	629:PHE	N	0.98

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.