

wwPDB X-ray Structure Validation Summary Report (i)

Dec 11, 2022 – 02:49 AM EST

PDB ID : 1B7U

Title: Structure of Mare Apolactoferrin: the N and C Lobes are in the Closed Form

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Deposited on : 1999-01-01

Resolution : 3.80 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 (1)) 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)

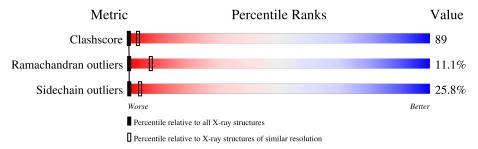
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.80 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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.

Mo	Chain	Length		Quality of chain		
1	A	689	16%	57%	23%	.



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5281 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 Lactotransferrin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	689	Total 5281	C 3299	N 937	O 1008	S 37	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLU	ASP	conflict	UNP O77811
A	269	LYS	ARG	conflict	UNP O77811
A	290	GLY	LYS	conflict	UNP O77811
A	294	GLY	GLU	conflict	UNP O77811
A	295	GLU	ASN	conflict	UNP 077811
A	296	GLN	LYS	conflict	UNP O77811

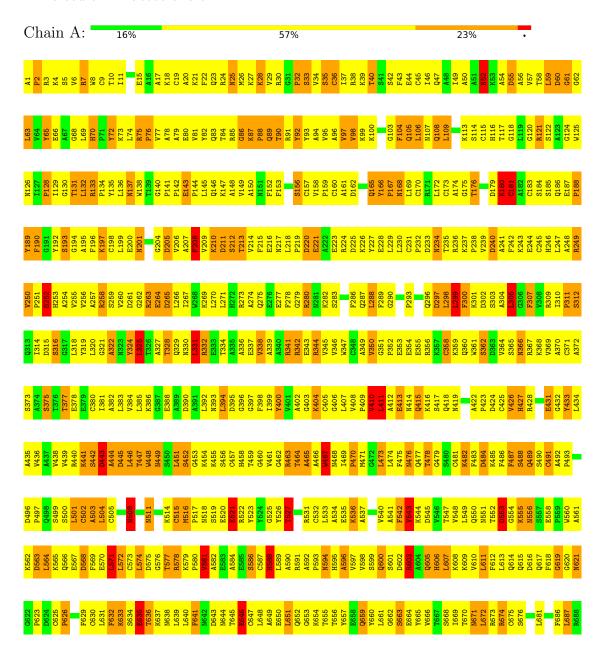


3 Residue-property plots (i)

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: Lactotransferrin









4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	100.40Å 77.40Å 102.60Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	32.00 - 3.80	Depositor	
% Data completeness	99.2 (32.00-3.80)	Depositor	
(in resolution range)	33.2 (82.00 8.00)	Берозпот	
R_{merge}	0.15	Depositor	
R_{sym}	0.15	Depositor	
Refinement program	X-PLOR 3.851	Depositor	
R, R_{free}	0.200 , 0.300	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	5281	wwPDB-VP	
Average B, all atoms (Å ²)	44.0	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	Bo	nd lengths	Bond angles		
	MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
	1	A	0.73	$2/5392 \ (0.0\%)$	1.09	$25/7298 \; (0.3\%)$

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
1	A	689	ALA	C-OXT	7.41	1.37	1.23
1	A	467	TRP	CB-CG	-5.18	1.41	1.50

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	A	180	LYS	CB-CA-C	17.81	146.03	110.40
1	A	410	VAL	CB-CA-C	13.43	136.92	111.40
1	A	7	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	A	571	LEU	CA-CB-CG	7.39	132.30	115.30
1	A	491	CYS	CA-CB-SG	-7.12	101.18	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	LYS	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	5281	0	5149	924	0
All	All	5281	0	5149	924	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 89.

The worst 5 of 924 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:258:ARG:NH2	1:A:261:ASP:O	1.64	1.30
1:A:179:ASP:O	1:A:180:LYS:O	1.56	1.21
1:A:299:LEU:HB2	1:A:300:PHE:CE1	1.79	1.18
1:A:75:ARG:HH12	1:A:312:SER:HA	1.03	1.16
1:A:579:LYS:HD2	1:A:587:CYS:HB2	1.27	1.16

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%)	468 (68%)	143 (21%)	76 (11%)	0 7

5 of 76 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	52	ASN
1	A	122	SER
1	A	167	PRO
1	A	168	ASN
1	A	180	LYS

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	565/565 (100%)	419 (74%)	146 (26%)	0 4

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563	ASP
1	A	674	ARG
1	A	572	LEU
1	A	621	ASN
1	A	252	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	ASN
1	A	595	HIS
1	A	550	GLN
1	A	606	HIS
1	A	165	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)

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.

