

wwPDB X-ray Structure Validation Summary Report (i)

Oct 22, 2023 – 05:55 PM EDT

PDB ID : 3CR9

Title : Crystal structure of the complex of Lactoferrin with 6-(Hydroxymethyl)oxan

e-2,3,4,5-tetrol at 3.49 A resolution

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Deposited on : 2008-04-05

Resolution : 3.49 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

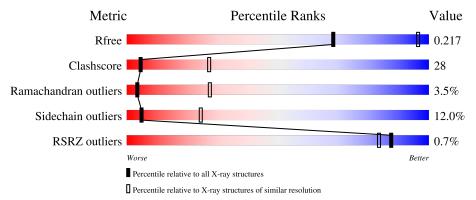
Validation Pipeline (wwPDB-VP) : 2.36

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 3.49 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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% 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.

Mol	Chain	Length	Quality o	f chain	
1	A	689	54%	38%	6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	A	692	-	-	-	X



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5295 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.

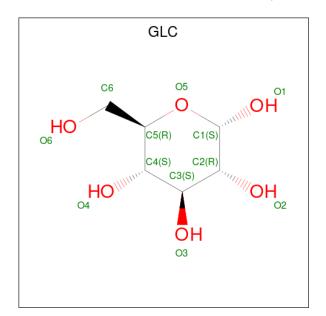
• Molecule 1 is a protein called Lactotransferrin.

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	SEE REMARK 999	UNP 077811
A	269	LYS	ARG	SEE REMARK 999	UNP 077811
A	290	GLY	LYS	SEE REMARK 999	UNP 077811
A	294	GLY	GLU	SEE REMARK 999	UNP 077811
A	295	GLU	ASN	SEE REMARK 999	UNP O77811
A	296	GLN	LYS	SEE REMARK 999	UNP 077811

• Molecule 2 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).





Mol	Chain	Residues	Atoms	5	ZeroOcc	AltConf
2	A	1	Total C 12 6	O 6	0	0

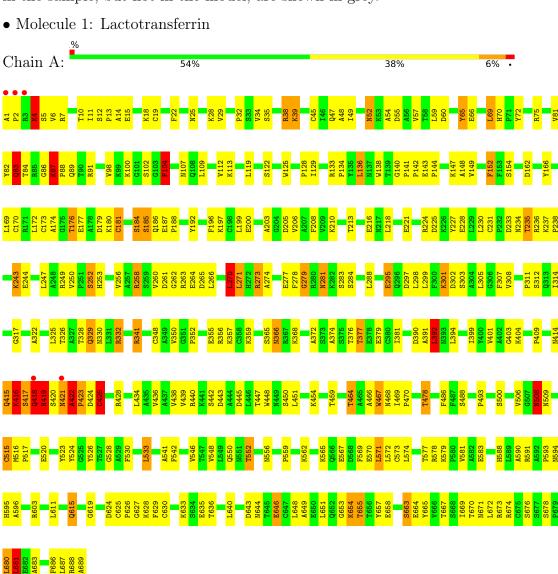
 \bullet Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Fe 2 2	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 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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	85.95Å 99.50Å 102.42Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 3.49	Depositor
resolution (A)	19.96 - 3.50	EDS
% Data completeness	81.4 (20.00-3.49)	Depositor
(in resolution range)	86.5 (19.96-3.50)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) > 1$	1.61 (at 3.52Å)	Xtriage
Refinement program	CNS 1.1	Depositor
P.P.	0.207 , 0.226	Depositor
R, R_{free}	0.195 , 0.217	DCC
R_{free} test set	530 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.22 , 45.2	EDS
L-test for twinning ²	$< L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5295	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: GLC, 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).

Mal	Chain	Bo	nd lengths	Во	ond angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.61	$2/5392 \ (0.0\%)$	1.01	$29/7298 \ (0.4\%)$

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}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	422	ALA	CA-CB	7.89	1.69	1.52
1	A	418	GLN	CA-C	6.00	1.68	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	104	PHE	CB-CG-CD2	-9.35	114.26	120.80
1	A	136	LEU	CA-CB-CG	8.75	135.43	115.30
1	A	508	ASN	N-CA-CB	8.53	125.96	110.60
1	A	646	GLU	CA-CB-CG	8.30	131.67	113.40
1	A	104	PHE	CB-CA-C	-8.30	93.80	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	GLN	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	5146	296	0
2	A	12	0	12	3	0
3	A	2	0	0	0	0
All	All	5295	0	5158	296	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 28.

The worst 5 of 296 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:66:GLU:HA	1:A:69:LEU:HD23	1.34	1.07
1:A:417:SER:OG	1:A:418:GLN:N	1.91	1.03
1:A:422:ALA:HB3	1:A:423:PRO:HD2	1.34	1.03
1:A:419:ASN:HD22	1:A:420:SER:N	1.57	1.01
1:A:422:ALA:HB3	1:A:423:PRO:CD	1.90	1.00

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%)	600 (87%)	63 (9%)	24 (4%)	3 27

5 of 24 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	177	GLU
1	A	416	LYS
1	A	421	ASN
1	A	422	ALA
1	A	423	PRO

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	Analysed Rotameric Outliers		Percentiles	
1	A	565/565~(100%)	497 (88%)	68 (12%)	5 24	

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	635	GLU
1	A	655	THR
1	A	680	LEU
1	A	252	SER
1	A	250	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	GLN
1	A	550	GLN
1	A	615	GLN
1	A	556	ASN
1	A	201	ASN

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths		$ ag{ths}$	В	ond ang	les
IVIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	A	692	-	12,12,12	0.40	0	17,17,17	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	692	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	692	GLC	O5-C5-C6-O6
2	A	692	GLC	C4-C5-C6-O6

There are no ring outliers.



1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	692	GLC	3	0

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)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	689/689 (100%)	-0.66	5 (0%) 87 83	4, 38, 67, 89	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	PRO	6.2
1	A	1	ALA	5.7
1	A	3	ARG	4.2
1	A	418	GLN	3.0
1	A	421	ASN	2.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	GLC	A	692	12/12	0.73	0.43	65,66,68,68	12
3	FE	A	691	1/1	0.94	0.13	23,23,23,23	0
3	FE	A	690	1/1	0.96	0.13	36,36,36,36	0



6.5 Other polymers (i)

There are no such residues in this entry.

