WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2023 – 04:46 AM EDT

PDB ID	:	1I6Q
Title	:	Formation of a protein intermediate and its trapping by the simultaneous crystallization process: Crystal structure of an iron-saturated intermediate in the FE3+ binding pathway of camel lactoferrin at 2.7 resolution
Authors	:	Khan, J.A.; Kumar, P.; Srinivasan, A.; Singh, T.P.
Deposited on	:	2001-03-03
Resolution	:	2.70 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:

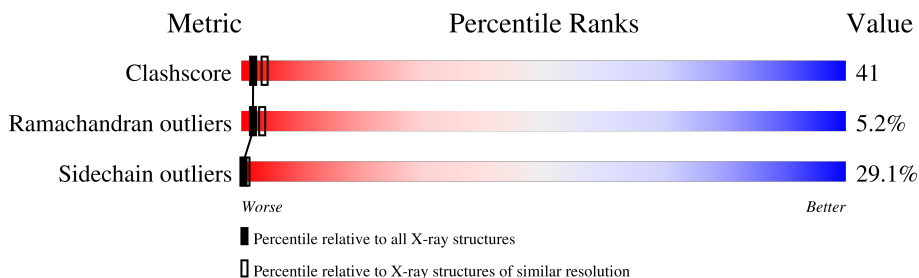|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.70 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		41
Ramachandran outliers		5.2%
Sidechain outliers		29.1%

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	27% 43% 21% 8%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5527 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 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	SEE REMARK 999	UNP Q9TUM0
A	87	GLN	ASN	SEE REMARK 999	UNP Q9TUM0
A	242	PHE	SER	SEE REMARK 999	UNP Q9TUM0
A	312	LYS	SER	SEE REMARK 999	UNP Q9TUM0
A	477	ASP	ASN	SEE REMARK 999	UNP Q9TUM0
A	513	LEU	ASN	SEE REMARK 999	UNP Q9TUM0
A	523	LEU	TYR	SEE REMARK 999	UNP Q9TUM0
A	556	GLY	ASN	SEE REMARK 999	UNP Q9TUM0
A	608	ARG	GLU	SEE REMARK 999	UNP Q9TUM0
A	623	GLU	GLN	SEE REMARK 999	UNP Q9TUM0
A	658	ASP	GLU	SEE REMARK 999	UNP Q9TUM0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	2	2	2	0	0

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).

CO3

O1

O⁻O2

C

O3

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 1	O 3	0	0
3	A	1	Total 4	C 1	O 3	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	233	Total 233	O 233	0	0

3 Residue-property plots ⓘ

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: LACTOFERRIN

Chain A:
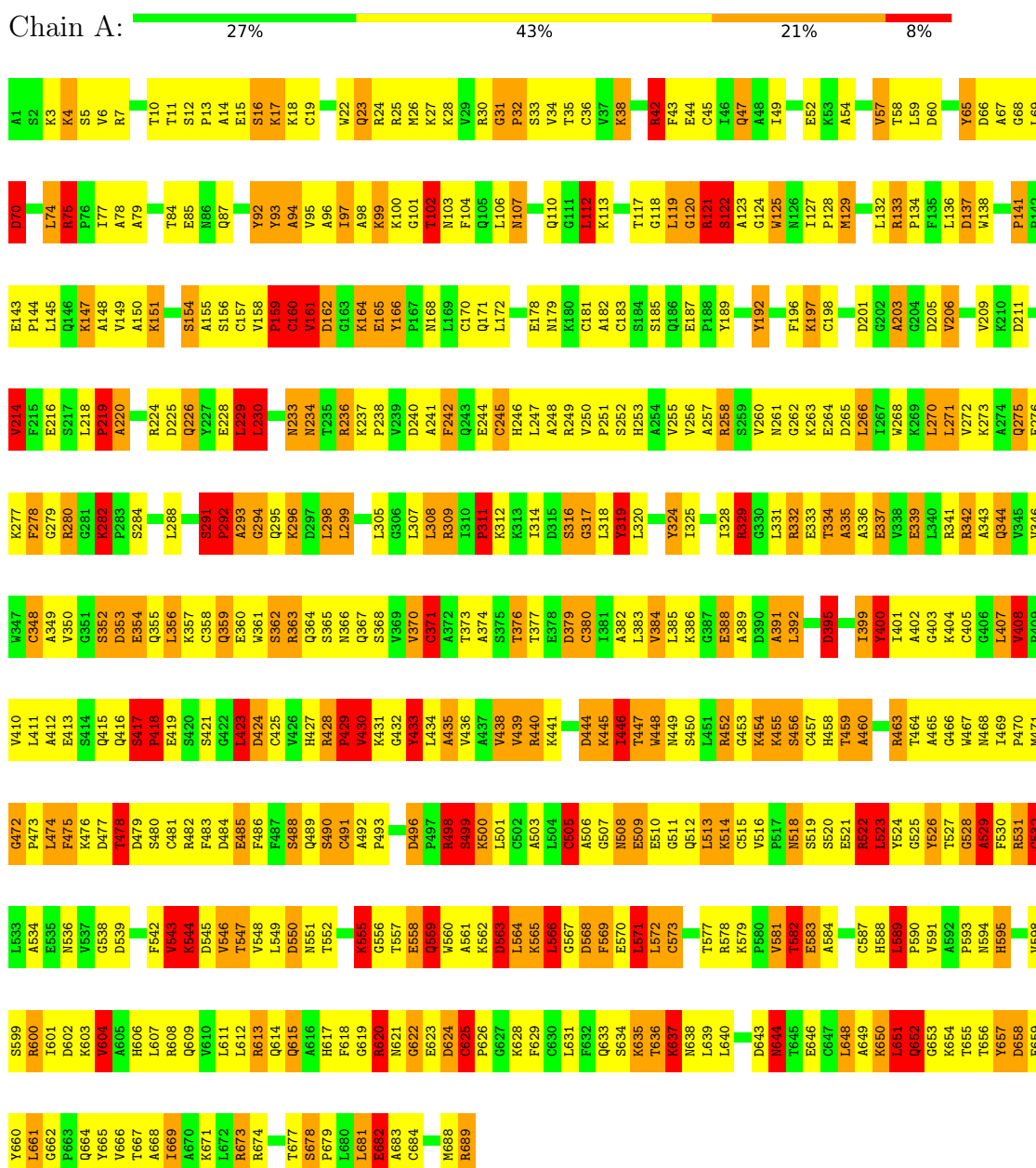
4 Data and refinement statistics (i)

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	175.91Å 80.62Å 56.29Å 90.00° 92.37° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.1 (25.00-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.188 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5527	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE, CO3

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	1.28	18/5392 (0.3%)	2.33	250/7293 (3.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	16

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	GLU	CB-CG	-43.78	0.69	1.52
1	A	430	VAL	C-N	-34.30	0.55	1.34
1	A	526	TYR	N-CA	23.48	1.93	1.46
1	A	526	TYR	CA-C	-19.58	1.02	1.52
1	A	572	LEU	C-N	-17.49	0.93	1.34

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	571	LEU	CB-CG-CD2	-37.35	47.50	111.00
1	A	572	LEU	CB-CG-CD1	-22.51	72.73	111.00
1	A	569	PHE	O-C-N	-21.23	88.74	122.70
1	A	329	ARG	CD-NE-CZ	20.57	152.40	123.60
1	A	280	ARG	NE-CZ-NH1	18.16	129.38	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	70	ASP	CA

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	LYS	Mainchain
1	A	319	TYR	Sidechain
1	A	379	ASP	Mainchain
1	A	70	ASP	Sidechain
1	A	94	ALA	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	5237	433	0
2	A	2	0	0	0	0
3	A	8	0	0	0	0
4	A	233	0	0	8	0
All	All	5527	0	5237	433	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 41.

The worst 5 of 433 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:92:TYR:CB	1:A:92:TYR:CA	1.80	1.58
1:A:526:TYR:N	1:A:526:TYR:CA	1.93	1.31
1:A:343:ALA:O	1:A:606:HIS:NE2	1.66	1.29
1:A:423:LEU:HD12	1:A:423:LEU:O	1.25	1.27
1:A:233:ASN:O	1:A:234:ASN:HB2	1.50	1.11

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	562 (82%)	89 (13%)	36 (5%)	2	3

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ARG
1	A	159	PRO
1	A	160	CYS
1	A	220	ALA
1	A	335	ALA

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%)	404 (71%)	166 (29%)	0	1

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
1	A	612	LEU
1	A	524	TYR
1	A	563	ASP
1	A	637	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	ASN
1	A	644	ASN
1	A	518	ASN
1	A	652	GLN
1	A	615	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	CO3	A	692	-	2,3,3	0.96	0	2,3,3	1.73	0
3	CO3	A	693	2	2,3,3	0.96	0	2,3,3	2.90	2 (100%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	693	CO3	O3-C-O1	-3.43	110.64	119.55
3	A	693	CO3	O2-C-O1	2.25	125.39	119.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	569:PHE	C	570:GLU	N	0.94
1	A	572:LEU	C	573:CYS	N	0.93
1	A	430:VAL	C	431:LYS	N	0.55

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.