



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:13 AM UTC

PDB ID : 1QJM / pdb_00001qjm
Title : Crystal Structure of a Complex of Lactoferrin with a Lanthanide Ion (SM3+) at 3.4 Angstrom Resolution
Authors : Sharma, A.K.; Singh, T.P.
Deposited on : 1999-06-27
Resolution : 3.40 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

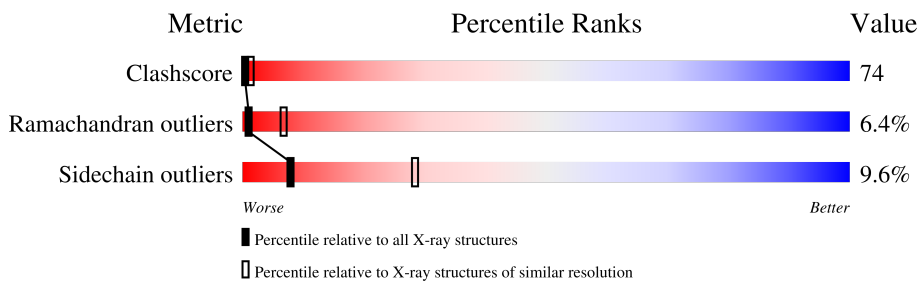
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	689	19% 58% 19% .

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
3	CO3	A	692	-	-	X	-
3	CO3	A	693	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5291 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
1	A	689	Total	C	N	O	S	0	0	0
			5281	3299	937	1008	37			

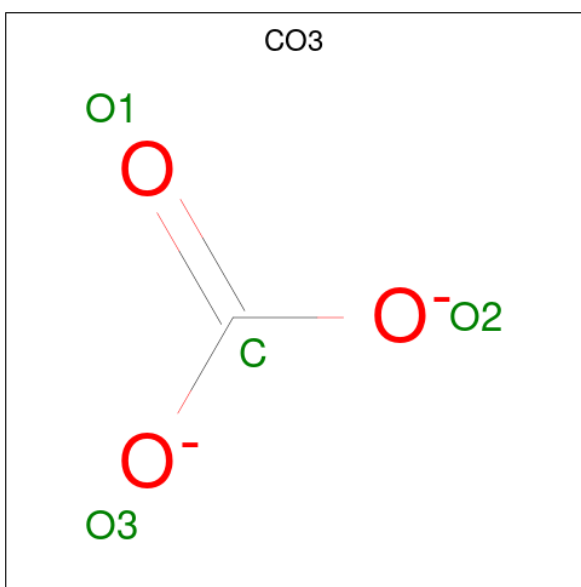
There are 6 discrepancies between the modelled and reference sequences:

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 O77811
A	296	GLN	LYS	conflict	UNP O77811

- Molecule 2 is SAMARIUM (III) ION (CCD ID: SM) (formula: Sm).

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

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



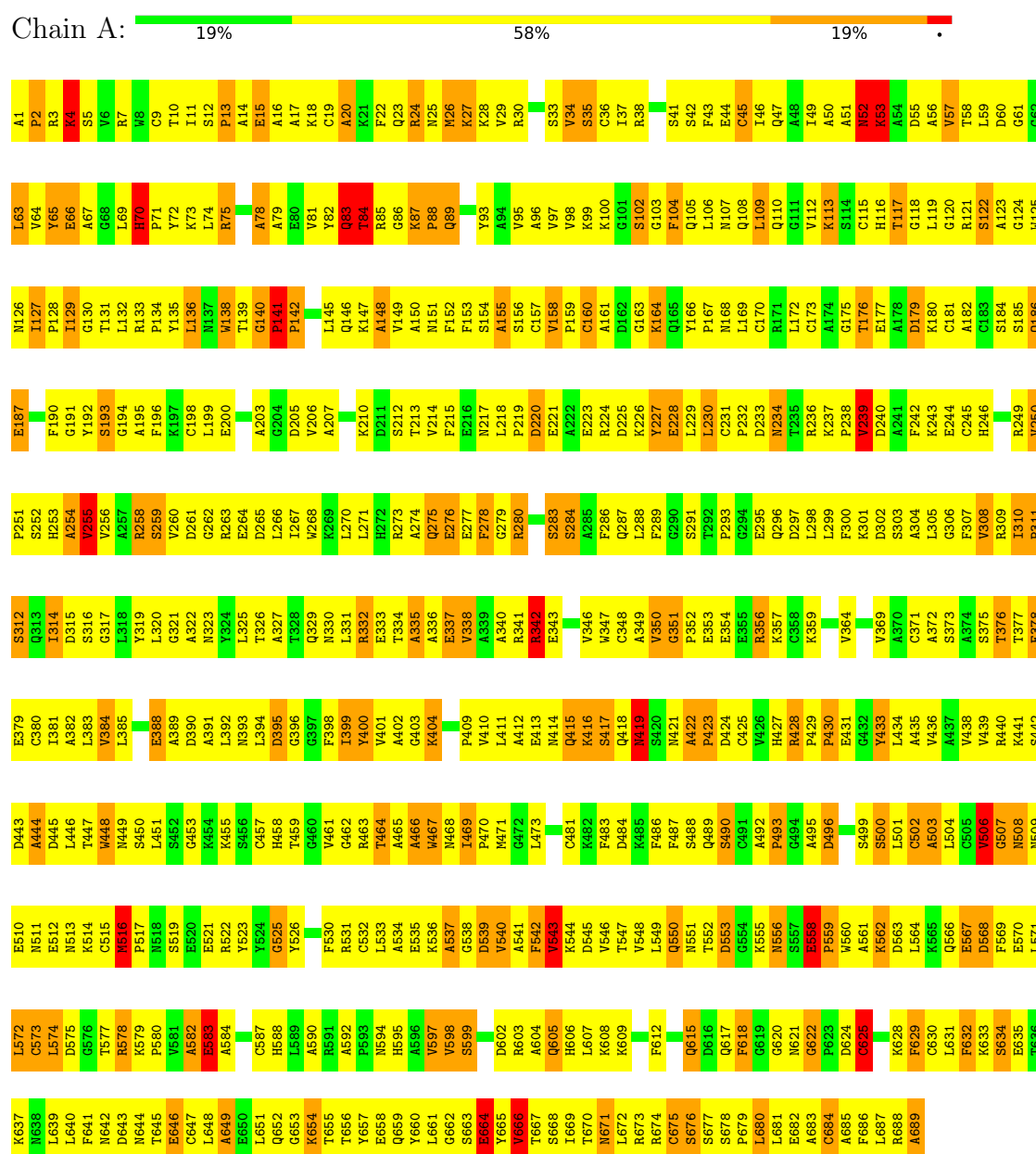
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	A	1	Total	C	O	0	0
			4	1	3		

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.49Å 103.19Å 113.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 3.40	Depositor
% Data completeness (in resolution range)	85.0 (17.00-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.219 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5291	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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: CO3, SM

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	1.39	24/5392 (0.4%)	1.66	125/7298 (1.7%)

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	0	2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	689	ALA	C-OXT	24.16	1.71	1.23
1	A	516	MET	SD-CE	7.49	1.98	1.79
1	A	195	ALA	CA-CB	-6.91	1.42	1.53
1	A	346	VAL	CA-CB	6.65	1.61	1.54
1	A	618	PHE	CA-C	6.39	1.62	1.52

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	VAL	N-CA-C	12.46	124.01	112.17
1	A	388	GLU	N-CA-C	-11.90	98.48	113.23
1	A	516	MET	CA-C-N	-11.81	104.30	120.96
1	A	516	MET	C-N-CA	-11.81	104.30	120.96
1	A	187	GLU	CA-C-N	11.78	133.13	119.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	433	TYR	Sidechain
1	A	65	TYR	Sidechain

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	5145	775	0
2	A	2	0	0	0	0
3	A	8	0	0	10	0
All	All	5291	0	5145	775	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 74.

The worst 5 of 775 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:288:LEU:HD23	1:A:289:PHE:CE1	1.77	1.17
1:A:561:ALA:HA	1:A:564:LEU:HD12	1.34	1.05
1:A:484:ASP:HA	1:A:501:LEU:HD21	1.31	1.04
1:A:463:ARG:HB3	3:A:693:CO3:O2	1.58	1.03
1:A:580:PRO:HD2	1:A:583:GLU:HG3	1.41	1.02

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%)	518 (75%)	125 (18%)	44 (6%)	1 7

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	52	ASN
1	A	70	HIS
1	A	139	THR
1	A	141	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	Rotameric	Outliers	Percentiles
1	A	565/565 (100%)	511 (90%)	54 (10%)	8 28

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	VAL
1	A	506	VAL
1	A	625	CYS
1	A	375	SER
1	A	415	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	566	GLN
1	A	617	GLN
1	A	652	GLN
1	A	615	GLN
1	A	360	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	693	2	3,3,3	1.10	0	2,3,3	1.13	0
3	CO3	A	692	2	3,3,3	1.52	1 (33%)	2,3,3	4.37	1 (50%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	692	CO3	O3-C	-2.29	1.13	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	692	CO3	O3-C-O1	-6.17	103.90	119.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	693	CO3	6	0
3	A	692	CO3	4	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

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.