



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2017 – 05:51 PM EDT

PDB ID : 1X89  
Title : Crystal structure of Siderocalin (NGAL, Lipocalin 2) complexed with Carboxymycobactin S  
Authors : Holmes, M.A.; Paulsene, W.; Jide, X.; Ratledge, C.; Strong, R.K.  
Deposited on : unknown  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

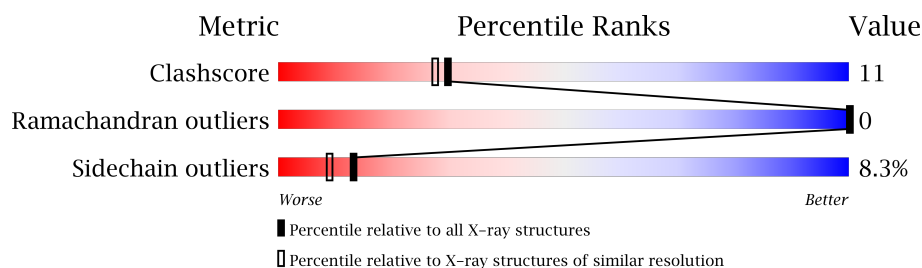
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	178	
1	B	178	
1	C	178	

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	CM1	A	200	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CM1	B	200	X	-	-	-
2	CM1	C	200	X	-	-	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4408 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.

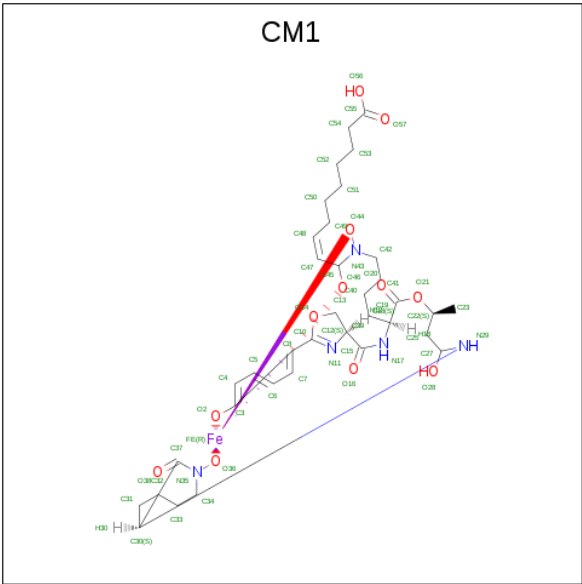
- Molecule 1 is a protein called Neutrophil gelatinase-associated lipocalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1412	915	234	259	4			
1	B	171	Total	C	N	O	S	0	0	0
			1339	876	220	239	4			
1	C	173	Total	C	N	O	S	0	0	0
			1400	909	235	252	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	SER	CYS	ENGINEERED	UNP P80188
B	87	SER	CYS	ENGINEERED	UNP P80188
C	87	SER	CYS	ENGINEERED	UNP P80188

- Molecule 2 is CARBOXYMYCOBACTIN S (three-letter code: CM1) (formula: C<sub>36</sub>H<sub>51</sub>FeN<sub>5</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			54	36	1	5	12		
2	B	1	Total	C	Fe	N	O	0	0
			54	36	1	5	12		
2	C	1	Total	C	Fe	N	O	0	0
			54	36	1	5	12		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	4	Total	O	0	0
			4	4		
3	C	57	Total	O	0	0
			57	57		

### 3 Residue-property plots [i](#)

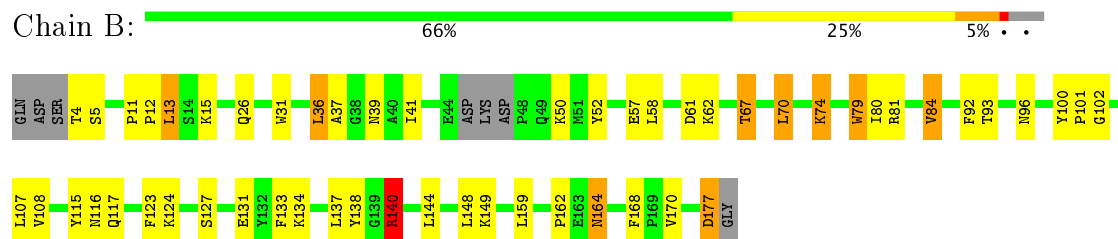
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

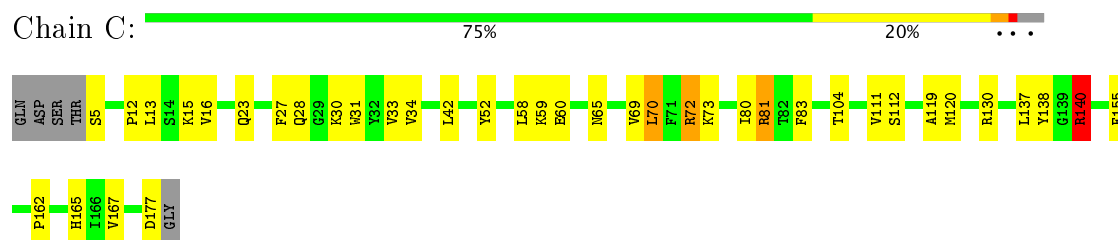
#### • Molecule 1: Neutrophil gelatinase-associated lipocalin



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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.20 Å   114.20 Å   119.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.220 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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: CM1

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	1.29	6/1449 (0.4%)	1.22	9/1964 (0.5%)
1	B	0.93	0/1375	0.94	2/1866 (0.1%)
1	C	1.41	11/1437 (0.8%)	1.30	8/1945 (0.4%)
All	All	1.23	17/4261 (0.4%)	1.16	19/5775 (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	C	0	1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	VAL	CB-CG2	6.23	1.66	1.52
1	A	56	TYR	CE2-CZ	6.08	1.46	1.38
1	C	16	VAL	CB-CG2	6.03	1.65	1.52
1	A	78	TYR	CD2-CE2	5.90	1.48	1.39
1	C	155	PHE	CE1-CZ	5.67	1.48	1.37

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	ARG	NE-CZ-NH1	21.06	130.83	120.30
1	A	140	ARG	NE-CZ-NH1	18.59	129.60	120.30
1	C	140	ARG	NE-CZ-NH2	-17.91	111.35	120.30
1	A	140	ARG	NE-CZ-NH2	-14.70	112.95	120.30
1	C	140	ARG	CD-NE-CZ	9.61	137.05	123.60



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	138	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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	1412	0	1397	30	0
1	B	1339	0	1309	39	0
1	C	1400	0	1395	21	0
2	A	54	0	43	4	0
2	B	54	0	43	4	0
2	C	54	0	43	5	0
3	A	34	0	0	0	0
3	B	4	0	0	0	0
3	C	57	0	0	0	0
All	All	4408	0	4230	91	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 11.

The worst 5 of 91 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)
2:C:200:CM1:C50	2:C:200:CM1:C49	1.74	1.54
1:A:81:ARG:HD2	1:A:100:TYR:OH	1.65	0.96
1:C:5:SER:HA	1:C:130:ARG:HH12	1.29	0.94
1:B:164:ASN:H	1:B:164:ASN:HD22	0.95	0.92
1:B:164:ASN:HD22	1:B:164:ASN:N	1.71	0.88

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	172/178 (97%)	164 (95%)	8 (5%)	0	100	100
1	B	167/178 (94%)	160 (96%)	7 (4%)	0	100	100
1	C	171/178 (96%)	163 (95%)	8 (5%)	0	100	100
All	All	510/534 (96%)	487 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	157/163 (96%)	144 (92%)	13 (8%)	13	9
1	B	144/163 (88%)	129 (90%)	15 (10%)	8	5
1	C	155/163 (95%)	145 (94%)	10 (6%)	20	16
All	All	456/489 (93%)	418 (92%)	38 (8%)	13	9

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	58	LEU
1	B	79	TRP
1	C	80	ILE
1	B	70	LEU
1	B	84	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	GLN
1	C	151	ASN
1	C	26	GLN
1	A	116	ASN
1	B	164	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	$\# Z  > 2$
2	CM1	A	200	-	46,59,59	2.90	25 (54%)	49,82,82	3.53	21 (42%)
2	CM1	B	200	-	46,59,59	3.07	24 (52%)	49,82,82	3.44	22 (44%)
2	CM1	C	200	-	46,59,59	2.89	22 (47%)	49,82,82	3.50	21 (42%)

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	CM1	A	200	-	2/2/14/18	0/43/94/94	0/1/6/6
2	CM1	B	200	-	2/2/14/18	0/43/94/94	0/1/6/6
2	CM1	C	200	-	2/2/14/18	0/43/94/94	0/1/6/6

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	200	CM1	O28-C27	-7.19	1.20	1.40
2	A	200	CM1	O28-C27	-6.85	1.21	1.40
2	B	200	CM1	O28-C27	-5.54	1.25	1.40
2	A	200	CM1	C12-C15	-4.36	1.43	1.52
2	B	200	CM1	C52-C51	-4.28	1.27	1.51

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	200	CM1	C31-C30-C37	-6.58	103.20	111.68
2	A	200	CM1	C31-C30-C37	-6.48	103.33	111.68
2	B	200	CM1	C3-C8-C10	-5.84	115.35	122.70
2	A	200	CM1	C33-C34-N35	-5.63	103.82	112.51
2	A	200	CM1	C3-C8-C10	-5.39	115.91	122.70

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	200	CM1	C27
2	C	200	CM1	C45
2	B	200	CM1	C27
2	B	200	CM1	C45
2	A	200	CM1	C27

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	200	CM1	4	0
2	B	200	CM1	4	0
2	C	200	CM1	5	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.