



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:49 AM GMT

PDB ID : 1L6M
Title : Neutrophil Gelatinase-associatedLipocalin is a Novel Bacteriostatic Agent that Interferes with Siderophore-mediated Iron Acquisition
Authors : Goetz, D.H.; Borregaard, N.; Bluhm, M.E.; Raymond, K.N.; Strong, R.K.
Deposited on : 2002-03-11
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

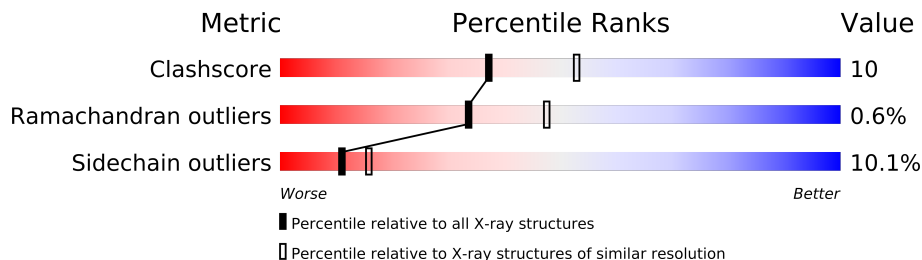
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	180	
1	B	180	
1	C	180	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4318 atoms, of which 0 are hydrogen and 0 are deuterium.

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	2	0
			1418	917	234	263	4			
1	B	169	Total	C	N	O	S	0	1	0
			1351	876	228	243	4			
1	C	172	Total	C	N	O	S	0	0	0
			1364	887	226	247	4			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP P80188
A	0	SER	-	CLONING ARTIFACT	UNP P80188
A	87	SER	CYS	ENGINEERED	UNP P80188
B	-1	GLY	-	CLONING ARTIFACT	UNP P80188
B	0	SER	-	CLONING ARTIFACT	UNP P80188
B	87	SER	CYS	ENGINEERED	UNP P80188
C	-1	GLY	-	CLONING ARTIFACT	UNP P80188
C	0	SER	-	CLONING ARTIFACT	UNP P80188
C	87	SER	CYS	ENGINEERED	UNP P80188

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

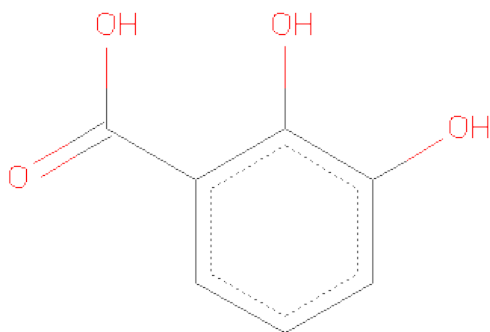
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



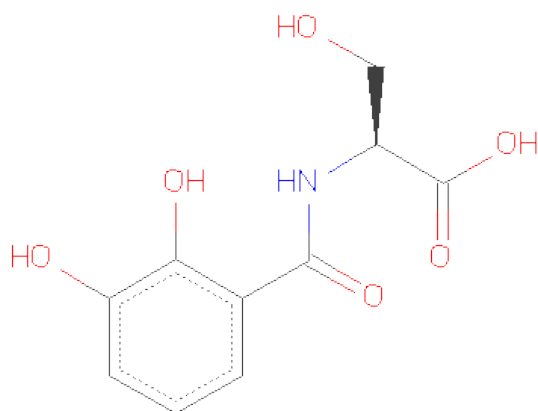
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2,3-DIHYDROXY-BENZOICACID (three-letter code: DBH) (formula: C₇H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	7	4		
4	A	1	Total	C	O	0	0
			11	7	4		
4	B	1	Total	C	O	0	0
			11	7	4		
4	B	1	Total	C	O	0	0
			11	7	4		
4	C	1	Total	C	O	0	0
			11	7	4		

- Molecule 5 is 2-(2,3-DIHYDROXY-BENZOYLAMINO)-3-HYDROXY-PROPIONICACID (three-letter code: DBS) (formula: C₁₀H₁₁NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	10	1	6		
5	B	1	Total	C	N	O	0	0
			17	10	1	6		
5	C	1	Total	C	N	O	0	0
			17	10	1	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	26	Total	O	0	0
			26	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	8	Total	O	0	0
			8	8		
6	C	27	Total	O	0	0
			27	27		

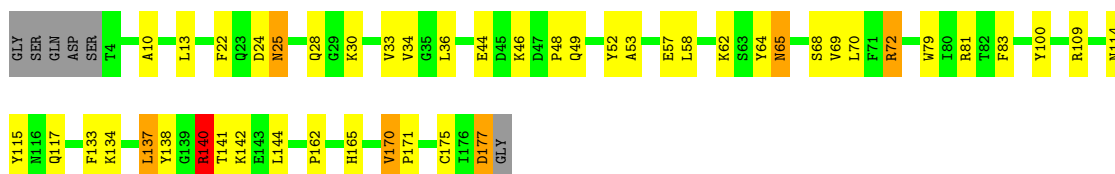
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

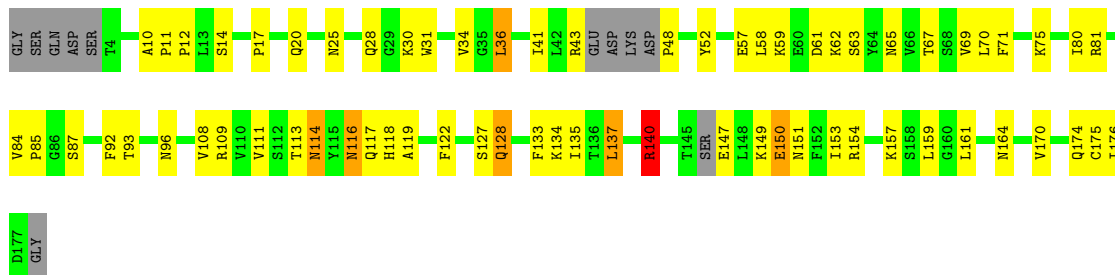
• Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain A: 



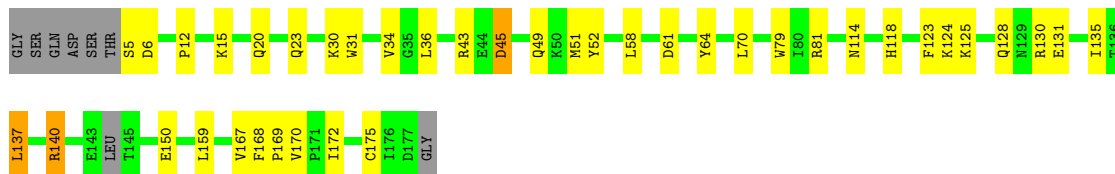
• Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain B: 



• Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.08Å 115.08Å 115.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.40	Depositor
% Data completeness (in resolution range)	96.5 (19.76-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.232 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4318	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: DBH, DBS, FE, SO4

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	1.13	1/1455 (0.1%)	1.16	5/1974 (0.3%)
1	B	0.94	0/1384	1.01	1/1874 (0.1%)
1	C	1.12	1/1400 (0.1%)	1.11	5/1900 (0.3%)
All	All	1.07	2/4239 (0.0%)	1.10	11/5748 (0.2%)

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
1	B	0	1
1	C	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	PHE	CE1-CZ	5.73	1.48	1.37
1	C	150	GLU	CG-CD	5.40	1.60	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	C	140	ARG	NE-CZ-NH1	11.74	126.17	120.30
1	C	140	ARG	NE-CZ-NH2	-11.70	114.45	120.30
1	A	140	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	A	115	TYR	CB-CG-CD2	6.34	124.80	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TYR	Sidechain
1	A	64	TYR	Sidechain
1	B	48	PRO	Mainchain
1	C	43	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1418	0	1386	30	0
1	B	1351	0	1318	38	0
1	C	1364	0	1326	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	0	0
3	C	10	0	0	0	0
4	A	22	0	7	5	0
4	B	22	0	7	0	0
4	C	11	0	4	0	0
5	A	17	0	9	0	0
5	B	17	0	9	0	0
5	C	17	0	9	2	0
6	A	26	0	0	0	0
6	B	8	0	0	1	0
6	C	27	0	0	0	0
All	All	4318	0	4075	84	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 84 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:122:PHE:HD2	1:B:135:ILE:HD11	1.17	1.06
1:B:34:VAL:HG23	1:B:137:LEU:HD13	1.44	0.95
1:A:141:THR:HB	1:C:20:GLN:HE21	1.34	0.92
1:C:5:SER:HA	1:C:130:ARG:HH22	1.39	0.88
1:B:122:PHE:CD2	1:B:135:ILE:HD11	2.09	0.83

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	174/180 (97%)	165 (95%)	8 (5%)	1 (1%)	33	47
1	B	164/180 (91%)	153 (93%)	10 (6%)	1 (1%)	33	47
1	C	168/180 (93%)	158 (94%)	9 (5%)	1 (1%)	33	47
All	All	506/540 (94%)	476 (94%)	27 (5%)	3 (1%)	33	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	CYS
1	B	175	CYS
1	C	175	CYS

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	157/164 (96%)	141 (90%)	16 (10%)	11	15
1	B	145/164 (88%)	124 (86%)	21 (14%)	5	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	147/164 (90%)	138 (94%)	9 (6%)	26	40
All	All	449/492 (91%)	403 (90%)	46 (10%)	11	15

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	ARG
1	B	70	LEU
1	C	81	ARG
1	B	57	GLU
1	B	63	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	114	ASN
1	B	116	ASN
1	C	20	GLN
1	B	49	GLN
1	B	164	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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
4	DBH	A	201	2	11,11,11	2.76	3 (27%)	15,15,15	1.71	3 (20%)
4	DBH	A	202	2	11,11,11	2.42	5 (45%)	15,15,15	1.38	0
5	DBS	A	203	2	17,17,17	1.94	2 (11%)	23,23,23	1.52	6 (26%)
3	SO4	A	230	-	4,4,4	0.39	0	6,6,6	0.16	0
4	DBH	B	301	2,4	11,11,11	2.44	3 (27%)	15,15,15	1.51	3 (20%)
4	DBH	B	302	2,4	11,11,11	2.49	5 (45%)	15,15,15	1.52	3 (20%)
5	DBS	B	303	2	17,17,17	1.93	3 (17%)	23,23,23	1.29	3 (13%)
3	SO4	C	330	-	4,4,4	0.28	0	6,6,6	0.10	0
4	DBH	C	401	2	11,11,11	2.64	6 (54%)	15,15,15	1.66	4 (26%)
5	DBS	C	403	2	17,17,17	2.13	4 (23%)	23,23,23	1.80	8 (34%)
3	SO4	C	430	-	4,4,4	0.34	0	6,6,6	0.31	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
4	DBH	A	201	2	-	0/4/4/4	0/1/1/1
4	DBH	A	202	2	-	0/4/4/4	0/1/1/1
5	DBS	A	203	2	-	0/14/14/14	0/1/1/1
3	SO4	A	230	-	-	0/0/0/0	0/0/0/0
4	DBH	B	301	2,4	-	0/4/4/4	0/1/1/1
4	DBH	B	302	2,4	-	0/4/4/4	0/1/1/1
5	DBS	B	303	2	-	0/14/14/14	0/1/1/1
3	SO4	C	330	-	-	0/0/0/0	0/0/0/0
4	DBH	C	401	2	-	0/4/4/4	0/1/1/1
5	DBS	C	403	2	-	0/14/14/14	0/1/1/1
3	SO4	C	430	-	-	0/0/0/0	0/0/0/0

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	DBH	C6-C3	6.55	1.47	1.39
5	A	203	DBS	C4-C1	6.47	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	303	DBS	C4-C1	6.22	1.47	1.39
5	C	403	DBS	C4-C1	6.07	1.47	1.39
4	A	202	DBH	C15-C18	5.56	1.49	1.39

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	DBH	C3-C18-C21	4.07	124.06	119.93
4	C	401	DBH	C3-C18-C21	3.62	123.60	119.93
5	C	403	DBS	C28-C22-N1	-3.61	103.71	110.62
5	C	403	DBS	O4-C4-C7	3.33	128.49	119.37
5	C	403	DBS	C16-C1-C4	-3.19	117.77	120.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.