



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2017 – 11:22 AM EDT

PDB ID : 1X71
Title : Crystal structure of Siderocalin (NGAL, Lipocalin 2) complexed with
TRENCA-3,2-HOPO, a cepabactin analogue
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

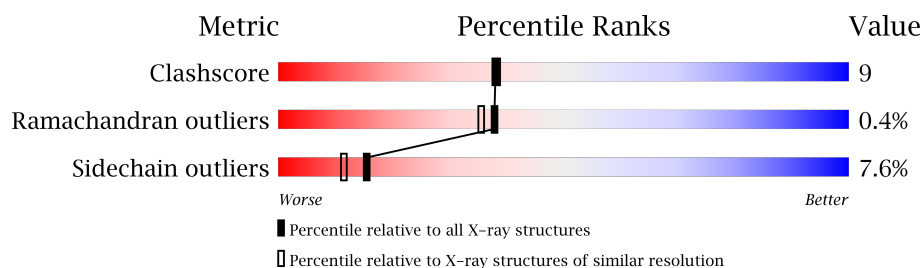
1 Overall quality at a glance

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 ≥ 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	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4298 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	175	Total	C	N	O	S	0	0	0
			1391	901	230	256	4			
1	B	171	Total	C	N	O	S	0	0	0
			1337	869	223	241	4			
1	C	174	Total	C	N	O	S	0	0	0
			1396	902	232	258	4			

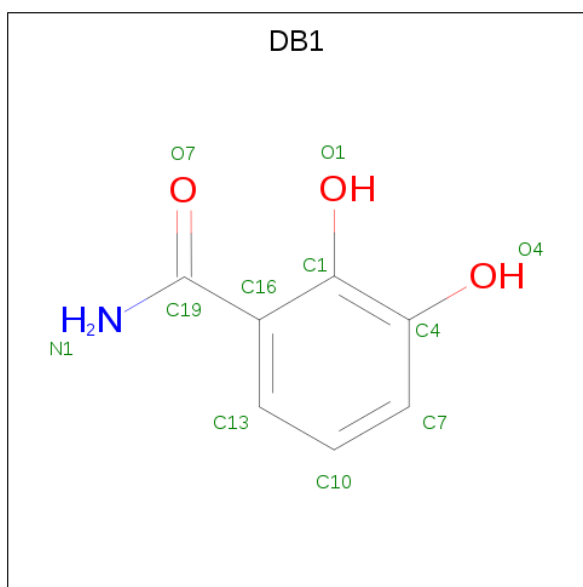
There are 3 discrepancies between the modelled and reference sequences:

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 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 2,3-DIHYDROXYBENZAMIDE (three-letter code: DB1) (formula: C₇H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		
3	C	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	8	Total	O	0	0
			8	8		
4	C	70	Total	O	0	0
			70	70		

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, α , β , γ	114.40 Å 114.40 Å 119.00 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}	0.05	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4298	wwPDB-VP
Average B, all atoms (Å ²)	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: DB1, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	0/1426	1.14	8/1936 (0.4%)
1	B	0.90	0/1371	1.22	4/1862 (0.2%)
1	C	1.22	5/1431 (0.3%)	1.14	5/1942 (0.3%)
All	All	1.08	5/4228 (0.1%)	1.16	17/5740 (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	B	0	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	GLU	CD-OE2	5.87	1.32	1.25
1	C	83	PHE	CE1-CZ	5.62	1.48	1.37
1	C	28	GLN	CB-CG	-5.14	1.38	1.52
1	C	111	VAL	CB-CG2	5.04	1.63	1.52
1	C	83	PHE	CG-CD1	5.03	1.46	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ARG	NE-CZ-NH1	-22.52	109.04	120.30
1	B	81	ARG	NE-CZ-NH2	21.40	131.00	120.30
1	C	140	ARG	NE-CZ-NH1	15.52	128.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	C	140	ARG	NE-CZ-NH2	-10.12	115.24	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	32	TYR	Sidechain
1	C	138	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	1391	0	1362	15	0
1	B	1337	0	1298	36	0
1	C	1396	0	1370	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	22	0	10	2	0
3	B	22	0	10	1	0
3	C	11	0	5	0	0
4	A	38	0	0	0	0
4	B	8	0	0	0	0
4	C	70	0	0	0	0
All	All	4298	0	4055	72	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 9.

The worst 5 of 72 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:59:LYS:HE3	1:A:65:ASN:HD22	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:THR:HG23	1:C:80:ILE:HD11	1.56	0.85
1:C:12:PRO:HD2	1:C:15:LYS:CE	2.11	0.79
1:A:31:TRP:CZ3	1:A:140:ARG:HD2	2.19	0.77
1:A:140:ARG:HG2	1:C:23:GLN:NE2	2.01	0.76

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	173/178 (97%)	167 (96%)	5 (3%)	1 (1%)	28	24
1	B	167/178 (94%)	157 (94%)	9 (5%)	1 (1%)	28	24
1	C	172/178 (97%)	166 (96%)	6 (4%)	0	100	100
All	All	512/534 (96%)	490 (96%)	20 (4%)	2 (0%)	38	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	THR
1	A	46	LYS

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	152/163 (93%)	144 (95%)	8 (5%)	26	24
1	B	143/163 (88%)	130 (91%)	13 (9%)	11	7
1	C	154/163 (94%)	141 (92%)	13 (8%)	13	8
All	All	449/489 (92%)	415 (92%)	34 (8%)	15	11

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	SER
1	B	151	ASN
1	C	137	LEU
1	B	137	LEU
1	A	140	ARG

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	151	ASN
1	C	116	ASN
1	C	65	ASN
1	B	65	ASN
1	B	164	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	DB1	A	201	2	11,11,11	2.26	3 (27%)	15,15,15	1.31	2 (13%)
3	DB1	A	202	2	11,11,11	3.16	6 (54%)	15,15,15	1.35	3 (20%)
3	DB1	B	201	2	11,11,11	5.57	4 (36%)	15,15,15	2.21	6 (40%)
3	DB1	B	203	2	11,11,11	3.19	5 (45%)	15,15,15	1.09	1 (6%)
3	DB1	C	201	2	11,11,11	2.60	3 (27%)	15,15,15	1.47	3 (20%)

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
3	DB1	A	201	2	-	0/4/4/4	0/1/1/1
3	DB1	A	202	2	-	0/4/4/4	0/1/1/1
3	DB1	B	201	2	-	0/4/4/4	0/1/1/1
3	DB1	B	203	2	-	0/4/4/4	0/1/1/1
3	DB1	C	201	2	-	0/4/4/4	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	203	DB1	O1-C1	-3.28	1.29	1.37
3	C	201	DB1	C16-C1	2.13	1.45	1.41
3	A	201	DB1	C13-C16	2.20	1.43	1.39
3	A	202	DB1	C10-C13	2.22	1.43	1.38
3	B	203	DB1	C13-C16	2.35	1.43	1.39

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	DB1	C7-C4-C1	-3.57	116.25	120.08
3	B	201	DB1	O7-C19-C16	-2.84	116.89	120.28
3	B	201	DB1	C16-C19-N1	-2.39	114.50	118.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	DB1	O1-C1-C4	-2.13	114.06	119.66
3	C	201	DB1	O1-C1-C4	-2.13	114.06	119.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	DB1	2	0
3	B	201	DB1	1	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.