wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 04:38 am GMT

PDB ID	:	4CIH
Title	:	Structure of LntA-K180D-K181D from Listeria monocytogenes
Authors	:	Lebreton, A.; Job, V.; Ragon, M.; Le Monnier, A.; Dessen, A.; Cossart, P.; Bierne, H.
Deposited on	:	2013-12-09
Resolution	:	2.22 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:

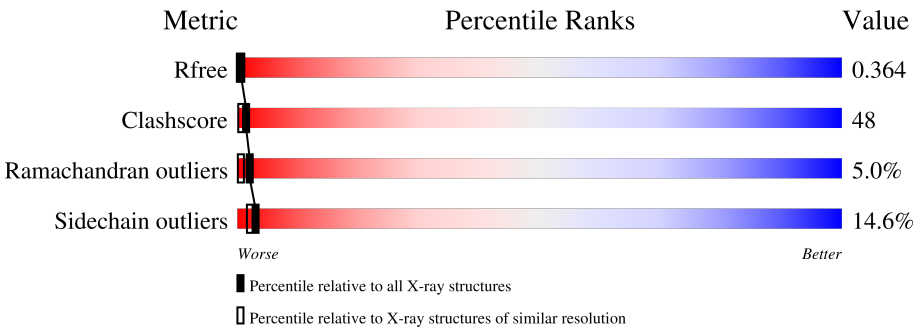
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)

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%

Mol	Chain	Length	Quality of chain
1	A	150	26% 59% 11% • •
1	B	150	27% 53% 17% • •
1	C	150	41% 48% 9% • •
1	D	150	34% 53% 9% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4806 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 LISTERIA NUCLEAR TARGETED PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	146	1188	754	198	234	2	0	0	0
1	B	146	1188	754	198	234	2	0	0	0
1	C	147	1196	758	199	237	2	0	0	0
1	D	146	1188	754	198	234	2	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	ASP	LYS	engineered mutation	UNP Q8Y9T5
A	181	ASP	LYS	engineered mutation	UNP Q8Y9T5
B	180	ASP	LYS	engineered mutation	UNP Q8Y9T5
B	181	ASP	LYS	engineered mutation	UNP Q8Y9T5
C	180	ASP	LYS	engineered mutation	UNP Q8Y9T5
C	181	ASP	LYS	engineered mutation	UNP Q8Y9T5
D	180	ASP	LYS	engineered mutation	UNP Q8Y9T5
D	181	ASP	LYS	engineered mutation	UNP Q8Y9T5

- Molecule 2 is water.

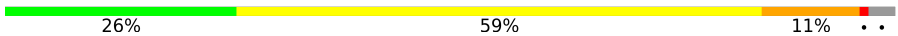
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	18	18	18	0	0
2	B	13	13	13	0	0
2	C	6	6	6	0	0
2	D	9	9	9	0	0

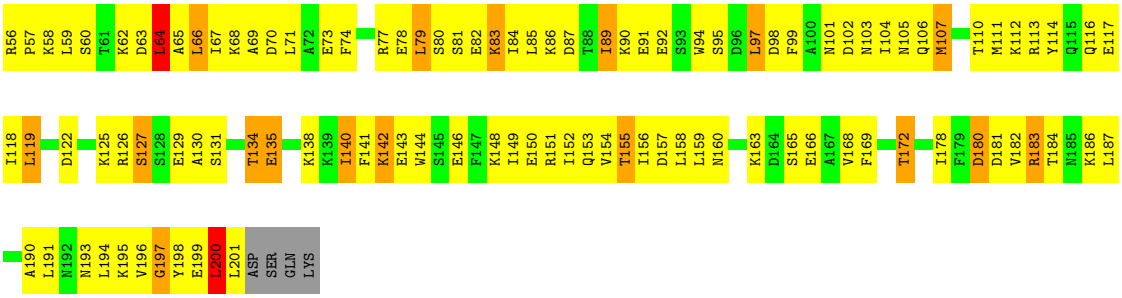
3 Residue-property plots (i)

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.

• Molecule 1: LISTERIA NUCLEAR TARGETED PROTEIN A

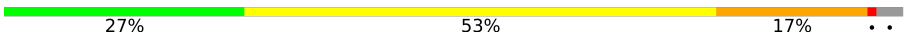
Chain A:

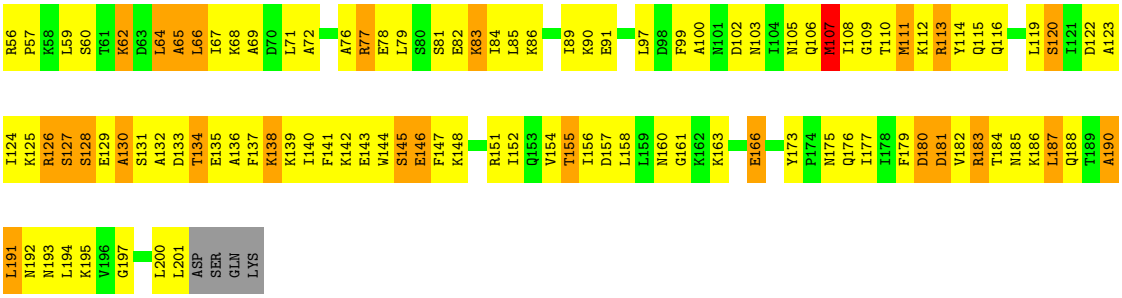




• Molecule 1: LISTERIA NUCLEAR TARGETED PROTEIN A

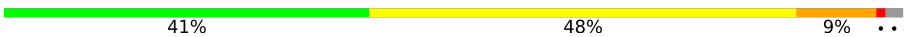
Chain B:

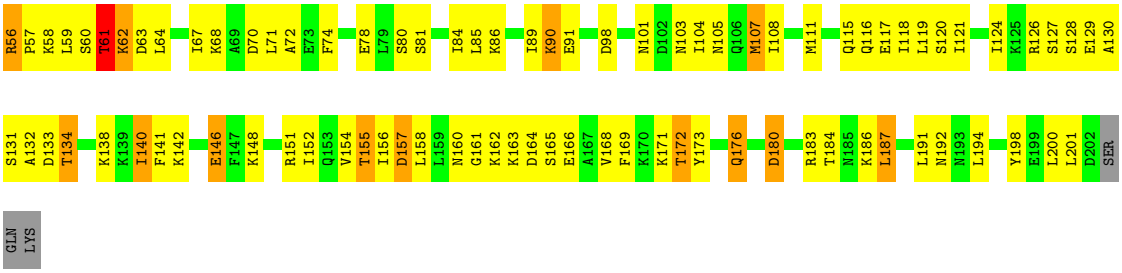




• Molecule 1: LISTERIA NUCLEAR TARGETED PROTEIN A

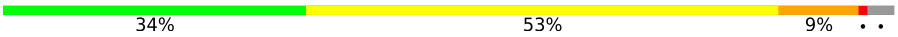
Chain C:

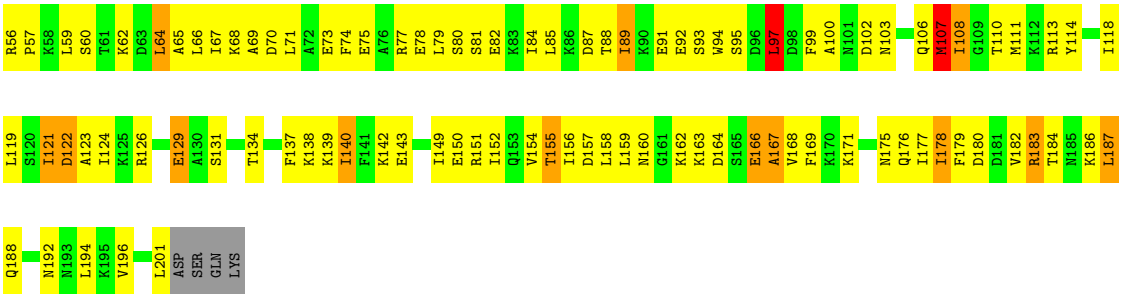




• Molecule 1: LISTERIA NUCLEAR TARGETED PROTEIN A

Chain D:


34%
53%
9%


R56 P57 K58 L59 S60 T61 K62 D63 L64 A65 L66 I67 K68 A69 D70 L71 A72 E73 F74 E75 A76 R77 E78 L79 S80 S81 E82 K83 I84 L85 K86 D87 T88 I89 K90 E91 E92 S93 W94 S95 D96 I97 D98 F99 A100 N101 D102 N103 Q106 M107 I108 G109 T110 M111 K112 R113 Y114 I118
L119 S120 I121 D122 A123 I124 K125 R126 E129 A130 S131 T134 F137 K138 K139 I140 F141 K142 E143 I149 E150 R151 I152 Q153 V154 T155 I156 D157 L158 L159 N160 G161 K162 K163 D164 S165 E166 A167 V168 F169 K170 K171 N175 Q176 I177 I178 F179 D180 D181 V182 R183 T184 N185 K186 L187
Q188 N192 N193 L194 K195 V196 L201 ASP SER GLN LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	141.19Å 141.19Å 60.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.06 – 2.22 47.06 – 2.22	Depositor EDS
% Data completeness (in resolution range)	93.9 (47.06-2.22) 94.6 (47.06-2.22)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.278 , 0.309 0.330 , 0.364	Depositor DCC
R_{free} test set	5622 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
Reported twinning fraction	0.511 for H, K, L 0.489 for -H, K, -L	Depositor
Outliers	1 of 56078 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	4806	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.61	0/1201	1.07	6/1608 (0.4%)
1	B	0.59	0/1201	1.01	3/1608 (0.2%)
1	C	0.55	0/1209	0.95	1/1619 (0.1%)
1	D	0.59	0/1201	0.95	3/1608 (0.2%)
All	All	0.59	0/4812	1.00	13/6443 (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	1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	LEU	CA-CB-CG	10.31	139.02	115.30
1	B	56	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	97	LEU	CA-CB-CG	6.48	130.19	115.30
1	C	107	MSE	CA-CB-CG	-6.01	103.09	113.30
1	A	107	MSE	N-CA-CB	-5.98	99.84	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	ALA	Peptide

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	1188	0	1211	134	0
1	B	1188	0	1211	146	0
1	C	1196	0	1215	109	0
1	D	1188	0	1211	111	0
2	A	18	0	0	5	0
2	B	13	0	0	1	0
2	C	6	0	0	1	0
2	D	9	0	0	0	0
All	All	4806	0	4848	457	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 48.

The worst 5 of 457 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:D:180:ASP:O	1:D:184:THR:HG23	1.54	1.07
1:D:59:LEU:HD12	1:D:123:ALA:HB1	1.37	1.02
1:B:197:GLY:O	1:C:91:GLU:OE2	1.80	1.00
1:B:110:THR:HG22	1:B:114:TYR:CE2	1.95	1.00
1:B:127:SER:OG	1:B:135:GLU:OE1	1.79	0.99

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	144/150 (96%)	106 (74%)	31 (22%)	7 (5%)	2	0
1	B	144/150 (96%)	114 (79%)	18 (12%)	12 (8%)	1	0
1	C	145/150 (97%)	125 (86%)	19 (13%)	1 (1%)	22	21
1	D	144/150 (96%)	116 (81%)	19 (13%)	9 (6%)	1	0
All	All	577/600 (96%)	461 (80%)	87 (15%)	29 (5%)	2	0

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	180	ASP
1	B	127	SER
1	B	128	SER
1	B	130	ALA

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	132/134 (98%)	109 (83%)	23 (17%)	2	1
1	B	132/134 (98%)	113 (86%)	19 (14%)	3	2
1	C	133/134 (99%)	113 (85%)	20 (15%)	3	2
1	D	132/134 (98%)	117 (89%)	15 (11%)	5	4
All	All	529/536 (99%)	452 (85%)	77 (15%)	3	2

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	172	THR
1	D	155	THR
1	C	180	ASP
1	D	88	THR
1	D	183	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	105	ASN
1	B	185	ASN
1	D	176	GLN
1	D	175	ASN
1	A	116	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.