



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 02:08 am BST

PDB ID : 4TW1
Title : Crystal structure of the octameric pore complex of the Staphylococcus aureus
Bi-component Toxin LukGH
Authors : Logan, D.T.; Hakansson, M.; Saline, M.; Kimbung, R.; Badarau, A.; Rouha,
H.; Nagy, E.
Deposited on : 2014-06-29
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

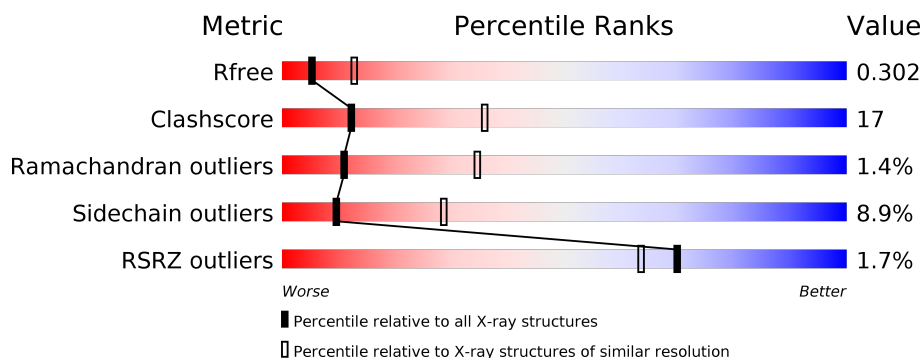
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	311	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>26%</div> <div>5%</div> <div>10%</div> </div> </div>
1	C	311	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>32%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	311	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>•</div> <div>7%</div> </div> </div>
1	G	311	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>30%</div> <div>•</div> <div>7%</div> </div> </div>
1	I	311	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>29%</div> <div>5%</div> <div>7%</div> </div> </div>
1	K	311	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>29%</div> <div>•</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	311	<div><div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>59%</div><div>31%</div><div>•</div><div>8%</div></div></div>
1	O	311	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>54%</div><div>34%</div><div>•</div><div>9%</div></div></div>
2	B	324	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>54%</div><div>28%</div><div>5%</div><div>13%</div></div></div>
2	D	324	<div><div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>51%</div><div>35%</div><div>•</div><div>11%</div></div></div>
2	F	324	<div><div><div></div><div></div><div></div><div></div></div><div><div></div><div>57%</div><div>28%</div><div>•</div><div>12%</div></div></div>
2	H	324	<div><div><div></div><div></div><div></div><div></div></div><div><div></div><div>55%</div><div>30%</div><div>•</div><div>11%</div></div></div>
2	J	324	<div><div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>54%</div><div>31%</div><div>•</div><div>11%</div></div></div>
2	L	324	<div><div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>52%</div><div>32%</div><div>•</div><div>•</div><div>11%</div></div></div>
2	N	324	<div><div><div></div><div></div><div></div><div></div></div><div><div></div><div>56%</div><div>30%</div><div>•</div><div>•</div><div>11%</div></div></div>
2	P	324	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>51%</div><div>32%</div><div>5%</div><div>•</div><div>12%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37620 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 Possible leukocidin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2289	1433	399	452	5			
1	C	281	Total	C	N	O	S	0	0	0
			2281	1425	398	453	5			
1	E	290	Total	C	N	O	S	0	0	0
			2356	1475	412	464	5			
1	G	290	Total	C	N	O	S	0	0	0
			2356	1475	412	464	5			
1	I	290	Total	C	N	O	S	0	0	0
			2356	1475	412	464	5			
1	K	281	Total	C	N	O	S	0	0	0
			2293	1438	398	452	5			
1	M	287	Total	C	N	O	S	0	0	0
			2332	1460	408	459	5			
1	O	283	Total	C	N	O	S	0	0	0
			2305	1447	400	453	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A8Z4S0
A	0	LEU	-	expression tag	UNP A8Z4S0
C	-1	SER	-	expression tag	UNP A8Z4S0
C	0	LEU	-	expression tag	UNP A8Z4S0
E	-1	SER	-	expression tag	UNP A8Z4S0
E	0	LEU	-	expression tag	UNP A8Z4S0
G	-1	SER	-	expression tag	UNP A8Z4S0
G	0	LEU	-	expression tag	UNP A8Z4S0
I	-1	SER	-	expression tag	UNP A8Z4S0
I	0	LEU	-	expression tag	UNP A8Z4S0
K	-1	SER	-	expression tag	UNP A8Z4S0
K	0	LEU	-	expression tag	UNP A8Z4S0
M	-1	SER	-	expression tag	UNP A8Z4S0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	LEU	-	expression tag	UNP A8Z4S0
O	-1	SER	-	expression tag	UNP A8Z4S0
O	0	LEU	-	expression tag	UNP A8Z4S0

- Molecule 2 is a protein called Possible leukocidin subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	282	Total	C	N	O	0	0	0
			2320	1462	405	453			
2	D	289	Total	C	N	O	0	0	0
			2373	1496	413	464			
2	F	284	Total	C	N	O	0	0	0
			2340	1477	407	456			
2	H	288	Total	C	N	O	0	0	0
			2366	1492	412	462			
2	J	288	Total	C	N	O	0	0	0
			2366	1492	412	462			
2	L	288	Total	C	N	O	0	0	0
			2366	1492	412	462			
2	N	288	Total	C	N	O	0	0	0
			2366	1492	412	462			
2	P	286	Total	C	N	O	0	0	0
			2350	1482	409	459			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	15	Total	O	0	0
			15	15		
3	C	11	Total	O	0	0
			11	11		
3	D	8	Total	O	0	0
			8	8		
3	E	11	Total	O	0	0
			11	11		
3	F	17	Total	O	0	0
			17	17		
3	G	13	Total	O	0	0
			13	13		
3	H	18	Total	O	0	0
			18	18		

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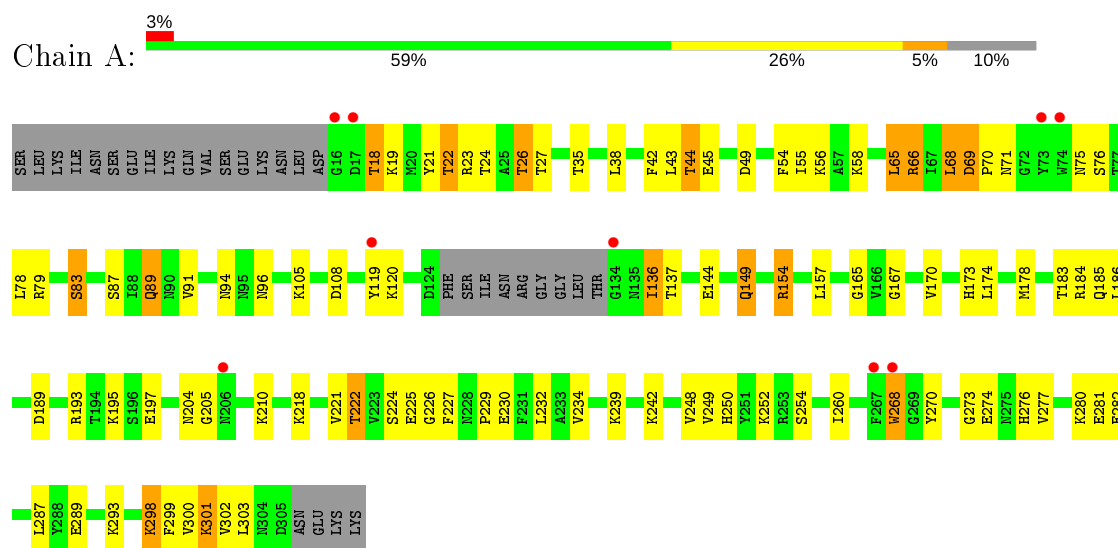
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	10	Total 10	O 10	0	0
3	J	17	Total 17	O 17	0	0
3	K	12	Total 12	O 12	0	0
3	L	16	Total 16	O 16	0	0
3	M	11	Total 11	O 11	0	0
3	N	9	Total 9	O 9	0	0
3	O	11	Total 11	O 11	0	0
3	P	17	Total 17	O 17	0	0

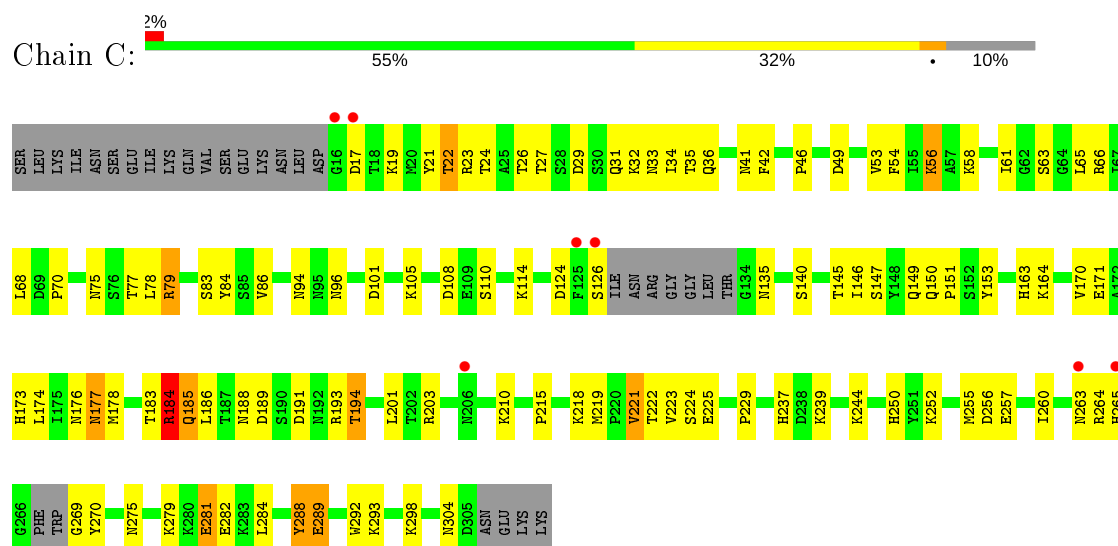
3 Residue-property plots [i](#)

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.

• Molecule 1: Possible leukocidin subunit

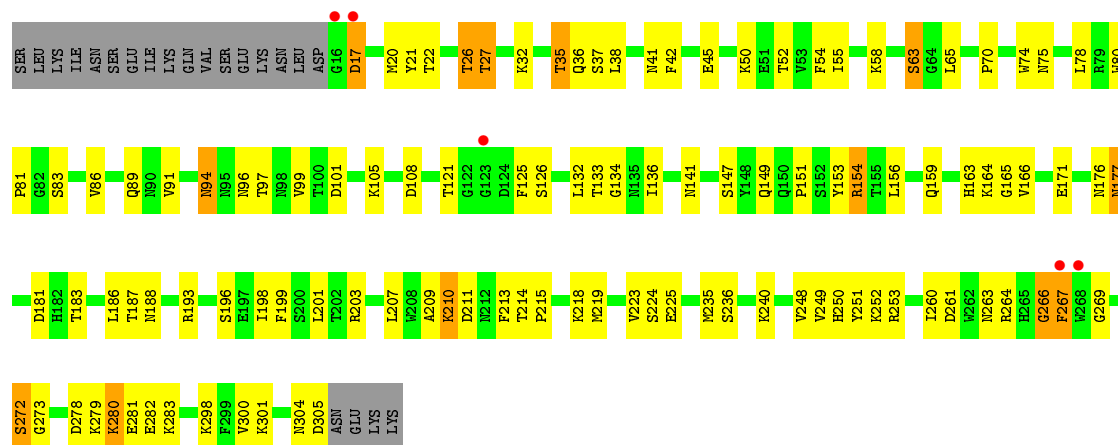


• Molecule 1: Possible leukocidin subunit

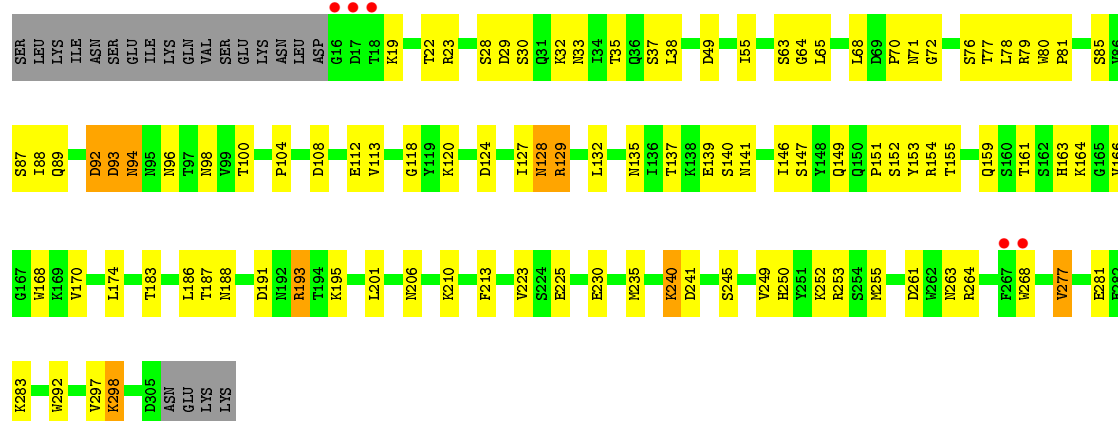


• Molecule 1: Possible leukocidin subunit

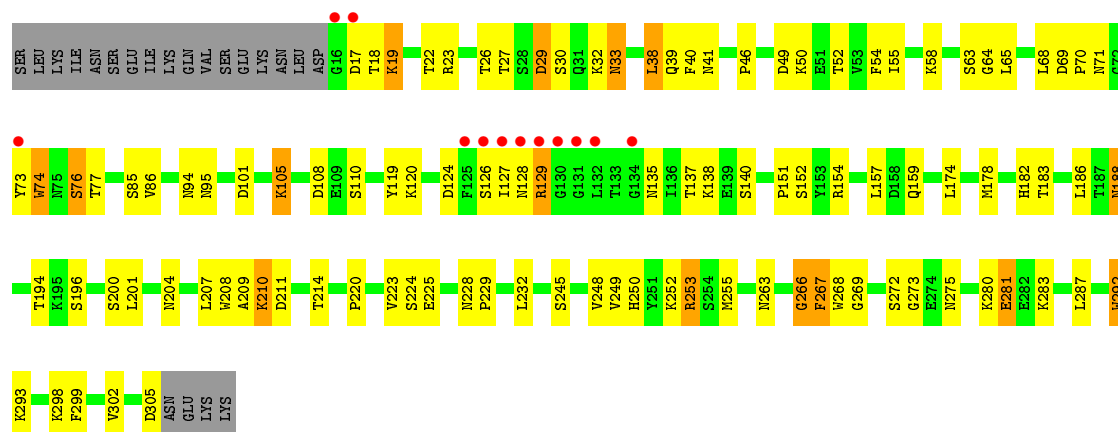




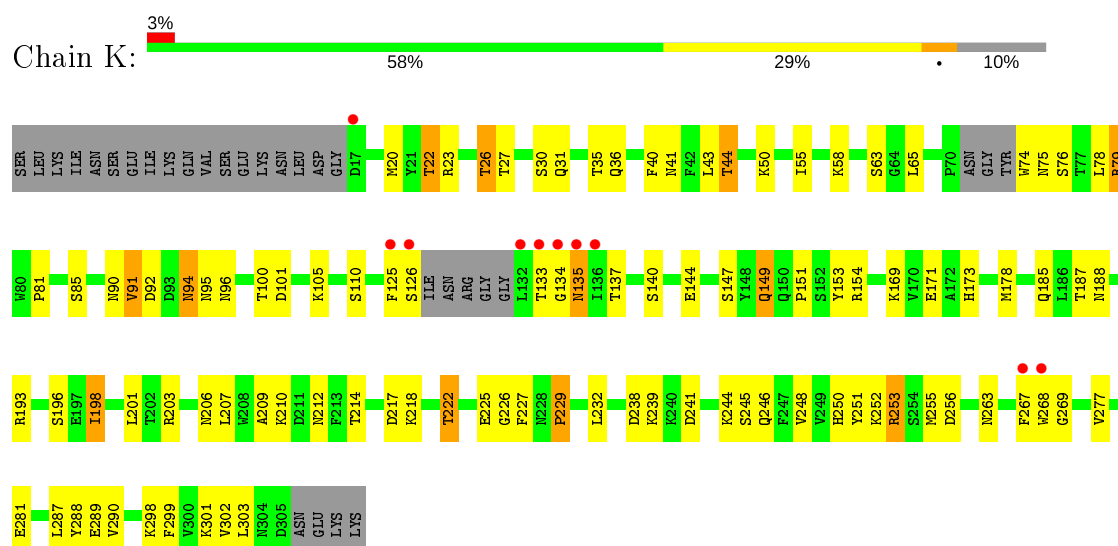
- Molecule 1: Possible leukocidin subunit



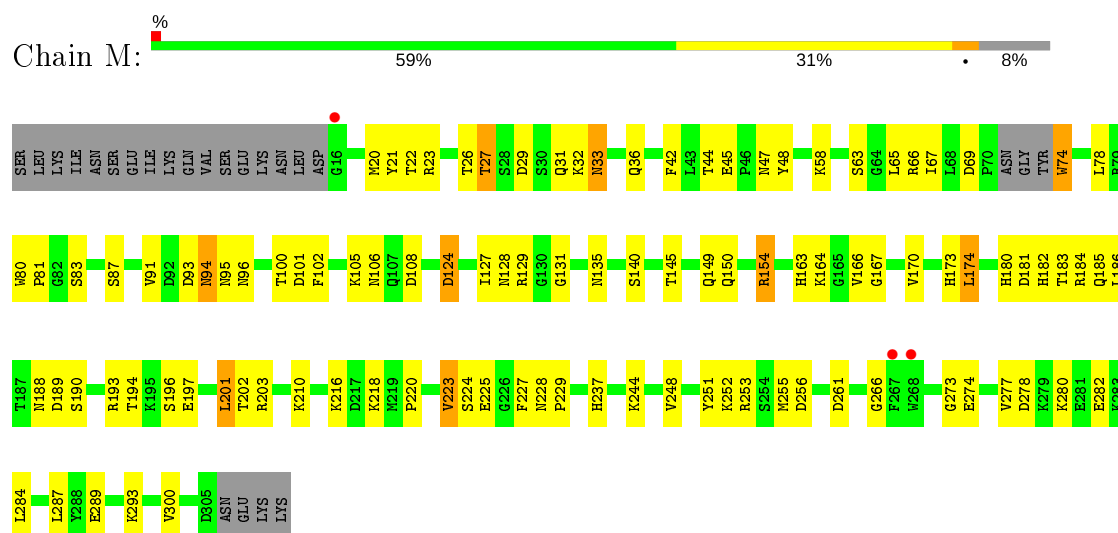
- Molecule 1: Possible leukocidin subunit



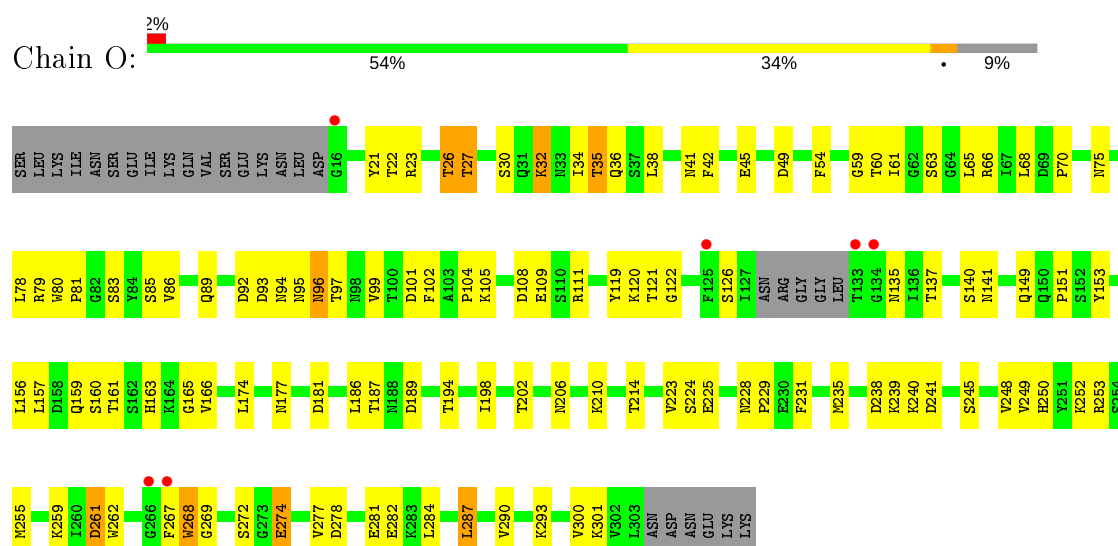
- Molecule 1: Possible leukocidin subunit



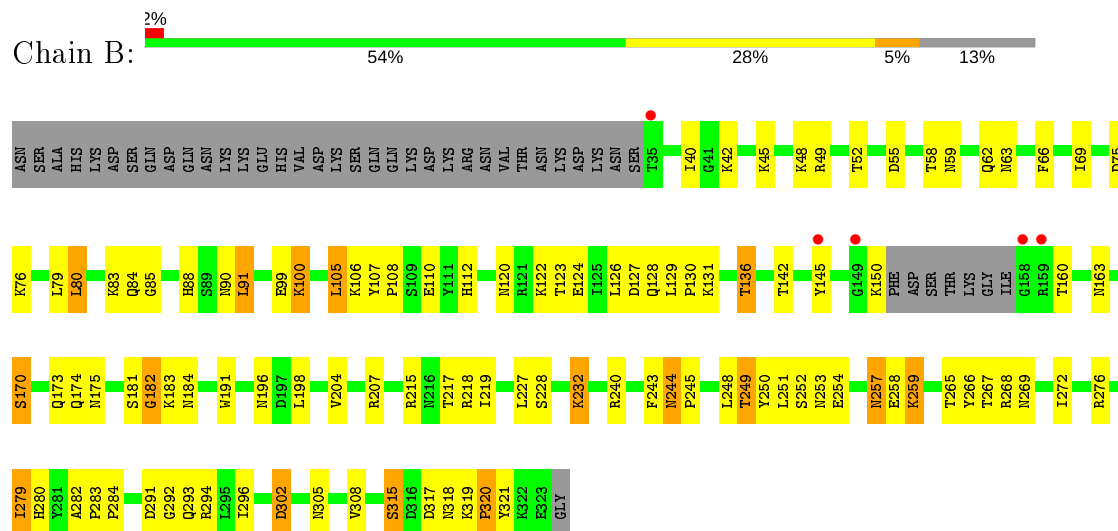
- Molecule 1: Possible leukocidin subunit



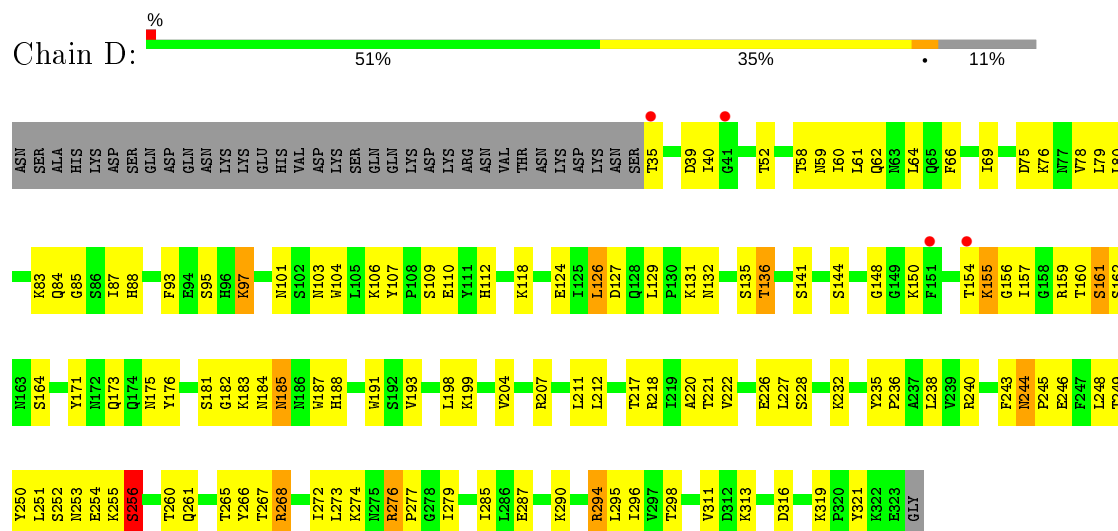
- Molecule 1: Possible leukocidin subunit



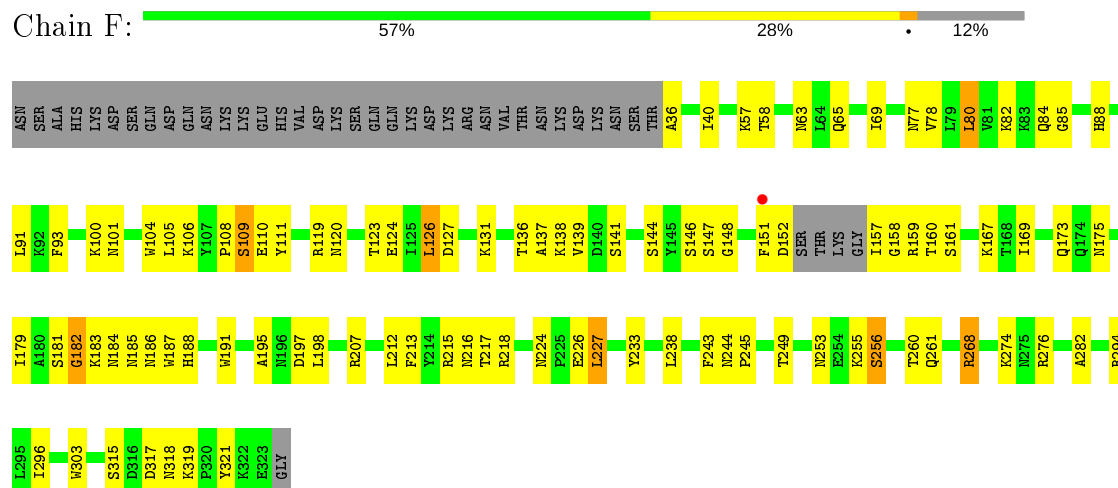
- Molecule 2: Possible leukocidin subunit



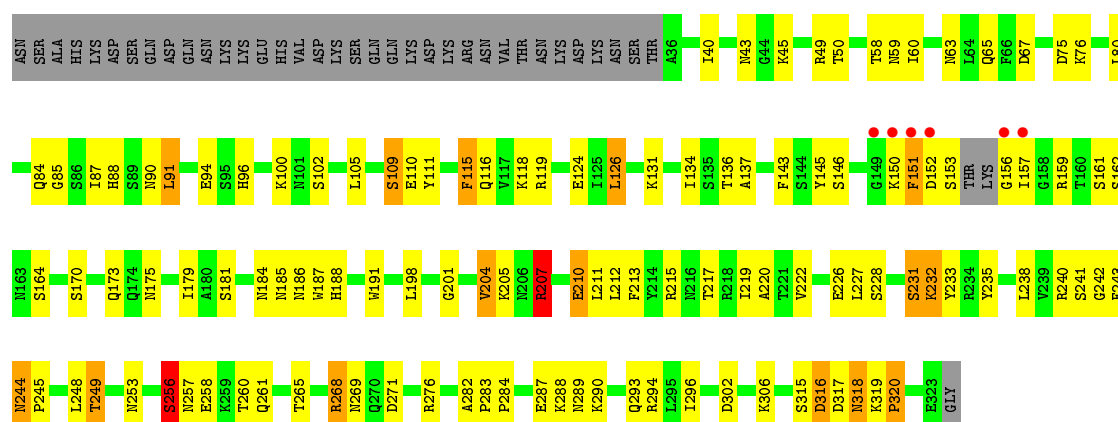
- Molecule 2: Possible leukocidin subunit



- Molecule 2: Possible leukocidin subunit



Chain N: 56% 30% .. 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.50Å 198.56Å 179.53Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	48.00 – 2.80 48.19 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.00-2.80) 96.1 (48.19-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.238 , 0.292 0.248 , 0.302	Depositor DCC
R_{free} test set	2207 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	37620	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.68	0/2345	0.88	1/3170 (0.0%)
1	C	0.67	0/2334	0.82	0/3152
1	E	0.66	0/2414	0.84	1/3264 (0.0%)
1	G	0.68	0/2414	0.86	1/3264 (0.0%)
1	I	0.70	1/2414 (0.0%)	0.88	3/3264 (0.1%)
1	K	0.68	0/2348	0.90	3/3173 (0.1%)
1	M	0.67	0/2388	0.85	0/3227
1	O	0.70	0/2362	0.87	2/3193 (0.1%)
2	B	0.68	0/2371	0.91	2/3202 (0.1%)
2	D	0.71	0/2426	0.88	0/3277
2	F	0.66	0/2392	0.88	1/3230 (0.0%)
2	H	0.68	1/2419 (0.0%)	0.88	2/3267 (0.1%)
2	J	0.69	0/2419	0.91	1/3267 (0.0%)
2	L	0.71	0/2419	0.88	0/3267
2	N	0.68	0/2419	0.86	2/3267 (0.1%)
2	P	0.67	0/2402	0.89	2/3243 (0.1%)
All	All	0.68	2/38286 (0.0%)	0.88	21/51727 (0.0%)

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	E	0	1
1	G	0	2
1	I	0	1
1	K	0	1
2	F	0	1
2	L	0	2
2	N	0	1
2	P	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	292	TRP	CB-CG	-5.77	1.39	1.50
2	H	75	ASP	CB-CG	-5.14	1.41	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	49	ASP	CB-CG-OD1	6.84	124.46	118.30
1	E	253	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	O	287	LEU	CA-CB-CG	6.09	129.31	115.30
2	N	268	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	J	297	ASP	CB-CG-OD1	5.86	123.57	118.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	94	ASN	Peptide
2	F	36	ALA	Peptide
1	G	128	ASN	Peptide
1	G	93	ASP	Peptide
1	I	94	ASN	Peptide

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	2289	0	2171	70	0
1	C	2281	0	2165	80	0
1	E	2356	0	2240	75	0
1	G	2356	0	2240	65	0
1	I	2356	0	2240	84	0
1	K	2293	0	2181	66	0
1	M	2332	0	2221	87	0
1	O	2305	0	2193	77	0
2	B	2320	0	2268	102	0
2	D	2373	0	2321	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2340	0	2285	93	0
2	H	2366	0	2314	90	0
2	J	2366	0	2314	93	0
2	L	2366	0	2314	102	0
2	N	2366	0	2314	97	0
2	P	2350	0	2293	100	0
3	A	9	0	0	2	0
3	B	15	0	0	4	0
3	C	11	0	0	0	0
3	D	8	0	0	1	0
3	E	11	0	0	2	0
3	F	17	0	0	2	0
3	G	13	0	0	0	0
3	H	18	0	0	1	0
3	I	10	0	0	0	0
3	J	17	0	0	2	0
3	K	12	0	0	1	0
3	L	16	0	0	1	0
3	M	11	0	0	1	0
3	N	9	0	0	1	0
3	O	11	0	0	0	0
3	P	17	0	0	3	0
All	All	37620	0	36074	1246	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 17.

The worst 5 of 1246 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:B:100:LYS:HD2	2:B:100:LYS:H	1.08	1.16
1:E:183:THR:HG21	3:E:409:HOH:O	1.47	1.13
2:F:88:HIS:HB3	1:G:159:GLN:HG2	1.32	1.12
2:B:170:SER:HB3	3:B:413:HOH:O	1.53	1.09
1:M:26:THR:HG23	2:N:186:ASN:HD22	1.16	1.09

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	277/311 (89%)	248 (90%)	28 (10%)	1 (0%)	34	66
1	C	275/311 (88%)	247 (90%)	25 (9%)	3 (1%)	14	41
1	E	288/311 (93%)	260 (90%)	22 (8%)	6 (2%)	7	23
1	G	288/311 (93%)	251 (87%)	33 (12%)	4 (1%)	11	34
1	I	288/311 (93%)	262 (91%)	21 (7%)	5 (2%)	9	29
1	K	275/311 (88%)	241 (88%)	29 (10%)	5 (2%)	8	28
1	M	283/311 (91%)	245 (87%)	31 (11%)	7 (2%)	5	19
1	O	279/311 (90%)	249 (89%)	25 (9%)	5 (2%)	8	28
2	B	278/324 (86%)	257 (92%)	19 (7%)	2 (1%)	22	53
2	D	287/324 (89%)	258 (90%)	25 (9%)	4 (1%)	11	34
2	F	280/324 (86%)	261 (93%)	17 (6%)	2 (1%)	22	53
2	H	286/324 (88%)	261 (91%)	20 (7%)	5 (2%)	9	29
2	J	286/324 (88%)	263 (92%)	20 (7%)	3 (1%)	15	44
2	L	286/324 (88%)	259 (91%)	24 (8%)	3 (1%)	15	44
2	N	286/324 (88%)	266 (93%)	17 (6%)	3 (1%)	15	44
2	P	282/324 (87%)	259 (92%)	17 (6%)	6 (2%)	7	23
All	All	4524/5080 (89%)	4087 (90%)	373 (8%)	64 (1%)	11	34

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	320	PRO
1	E	210	LYS
1	E	267	PHE
1	G	94	ASN
2	H	37	PRO

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	255/283 (90%)	222 (87%)	33 (13%)	4	13
1	C	255/283 (90%)	232 (91%)	23 (9%)	9	28
1	E	262/283 (93%)	240 (92%)	22 (8%)	11	31
1	G	262/283 (93%)	238 (91%)	24 (9%)	9	27
1	I	262/283 (93%)	235 (90%)	27 (10%)	7	21
1	K	257/283 (91%)	230 (90%)	27 (10%)	7	20
1	M	260/283 (92%)	241 (93%)	19 (7%)	14	38
1	O	257/283 (91%)	234 (91%)	23 (9%)	9	28
2	B	261/301 (87%)	243 (93%)	18 (7%)	15	41
2	D	267/301 (89%)	243 (91%)	24 (9%)	9	28
2	F	263/301 (87%)	244 (93%)	19 (7%)	14	38
2	H	266/301 (88%)	252 (95%)	14 (5%)	22	54
2	J	266/301 (88%)	239 (90%)	27 (10%)	7	22
2	L	266/301 (88%)	242 (91%)	24 (9%)	9	28
2	N	266/301 (88%)	249 (94%)	17 (6%)	17	45
2	P	264/301 (88%)	233 (88%)	31 (12%)	5	16
All	All	4189/4672 (90%)	3817 (91%)	372 (9%)	9	28

5 of 372 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	146	SER
2	J	113	LYS
2	P	91	LEU
2	H	295	LEU
1	I	110	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	208	ASN
1	I	263	ASN
2	P	173	GLN
2	H	224	ASN
1	I	71	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](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	281/311 (90%)	-0.19	9 (3%) 47 37	17, 32, 79, 101	0
1	C	281/311 (90%)	-0.11	7 (2%) 57 47	16, 37, 77, 101	0
1	E	290/311 (93%)	-0.14	5 (1%) 70 63	17, 37, 72, 100	0
1	G	290/311 (93%)	-0.26	5 (1%) 70 63	13, 34, 75, 101	0
1	I	290/311 (93%)	-0.24	12 (4%) 37 27	13, 30, 81, 123	0
1	K	281/311 (90%)	-0.23	10 (3%) 42 32	17, 33, 70, 98	0
1	M	287/311 (92%)	-0.28	3 (1%) 82 77	13, 31, 67, 98	0
1	O	283/311 (90%)	-0.27	6 (2%) 63 54	17, 32, 77, 98	0
2	B	282/324 (87%)	-0.28	5 (1%) 68 61	16, 31, 58, 95	0
2	D	289/324 (89%)	-0.30	4 (1%) 75 70	18, 33, 61, 97	0
2	F	284/324 (87%)	-0.39	1 (0%) 92 91	14, 31, 57, 104	0
2	H	288/324 (88%)	-0.39	0 100 100	15, 28, 62, 86	0
2	J	288/324 (88%)	-0.34	2 (0%) 87 84	16, 29, 58, 98	0
2	L	288/324 (88%)	-0.35	3 (1%) 82 77	14, 27, 52, 110	0
2	N	288/324 (88%)	-0.39	0 100 100	15, 29, 55, 76	0
2	P	286/324 (88%)	-0.35	6 (2%) 63 54	16, 29, 62, 108	0
All	All	4576/5080 (90%)	-0.28	78 (1%) 70 63	13, 31, 69, 123	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	16	GLY	5.5
1	M	267	PHE	4.7
1	C	126	SER	4.7
2	L	154	THR	4.5
1	I	134	GLY	4.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.