

Full wwPDB X-ray Structure Validation Report (i)

Mar 28, 2022 – 01:06 pm BST

PDB ID : 7P8X

Title: Crystal Structure of leukotoxin LukE from Staphylococcus aureus in complex

with a doubly sulfated CCR2 N-terminal peptide

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Deposited on : 2021-07-23

Resolution : 1.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.27

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

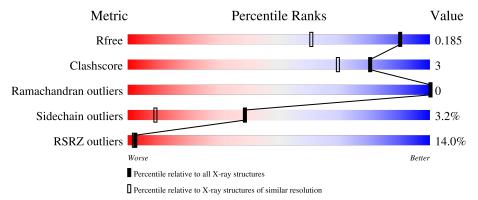
Validation Pipeline (wwPDB-VP) : 2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.40 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 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% 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	308	12%	6% • 8%
2	M	6	50%	33%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2749 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 Leucotoxin LukEv.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	282	Total	С	N	O	S	0	20	0
_			2368	1497	405	464	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP Q2FXB0
A	312	LYS	-	expression tag	UNP Q2FXB0
A	313	HIS	-	expression tag	UNP Q2FXB0
A	314	HIS	-	expression tag	UNP Q2FXB0
A	315	HIS	-	expression tag	UNP Q2FXB0
A	316	HIS	-	expression tag	UNP Q2FXB0
A	317	HIS	-	expression tag	UNP Q2FXB0
A	318	HIS	-	expression tag	UNP Q2FXB0

• Molecule 2 is a protein called C-C chemokine receptor type 2.

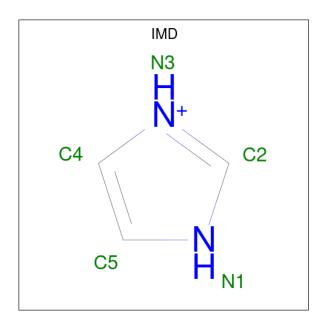
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	M	6	Total 71		- 1	O 23	S 3	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	24	ACE	-	acetylation	UNP P41597

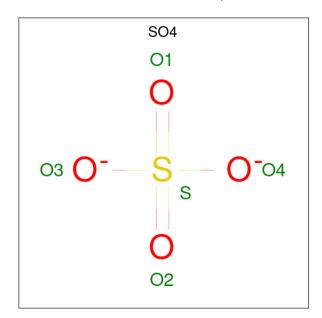
• Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	C 3	N 2	0	0

 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



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

 \bullet Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	289	Total O 289 289	0	0
5	M	6	Total O 6 6	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 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.



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	63.30Å 72.41Å 79.00Å	Donositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	40.81 - 1.40	Depositor	
rtesolution (A)	40.81 - 1.40	EDS	
% Data completeness	99.0 (40.81-1.40)	Depositor	
(in resolution range)	99.0 (40.81-1.40)	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.64 (at 1.40Å)	Xtriage	
Refinement program	BUSTER 2.10.4	Depositor	
R, R_{free}	0.186 , 0.198	Depositor	
it, it free	0.178 , 0.185	DCC	
R_{free} test set	3616 reflections (5.06%)	wwPDB-VP	
Wilson B-factor (Å ²)	21.7	Xtriage	
Anisotropy	0.416	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS	
L-test for twinning ²	$ < L > = 0.50, < L^2 > = 0.33$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.97	EDS	
Total number of atoms	2749	wwPDB-VP	
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.09% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, TYS, ACE, 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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.54	0/2439	0.73	0/3297	
2	M	0.39	0/18	0.70	0/20	
All	All	0.54	0/2457	0.73	0/3317	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2368	0	2315	13	0
2	M	71	0	34	0	0
3	A	5	0	5	1	0
4	A	10	0	0	0	0
5	A	289	0	0	2	0
5	M	6	0	0	0	0
All	All	2749	0	2354	13	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 3.

All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:29:ASN:HB2	1:A:44:ARG:HH22	1.36	0.90
1:A:125:LEU:HD21	1:A:149:SER:HB2	1.80	0.63
1:A:203:HIS:HD2	3:A:401:IMD:HN1	1.47	0.63
1:A:29:ASN:HB2	1:A:44:ARG:NH2	2.17	0.50
1:A:114:THR:HG23	5:A:505:HOH:O	2.14	0.47
1:A:182:LYS:HD2	5:A:505:HOH:O	2.14	0.46
1:A:130:ILE:HG12	1:A:135:VAL:HG22	2.00	0.44
1:A:42:ILE:CD1	1:A:65[A]:LYS:HD2	2.48	0.43
1:A:178:LYS:HB3	1:A:178:LYS:HE2	1.65	0.43
1:A:195:THR:HG23	1:A:196:PRO:HD2	2.00	0.42
1:A:274:PRO:HD2	1:A:275:ARG:HH21	1.85	0.42
1:A:86:THR:HA	1:A:103:ILE:O	2.20	0.42
1:A:42:ILE:HD12	1:A:65[A]:LYS:HD2	2.04	0.40

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	voured Allowed		Percentiles		
1	A	300/308 (97%)	291 (97%)	9 (3%)	0	100	100	
2	M	2/6~(33%)	2 (100%)	0	0	100	100	
All	All	302/314 (96%)	293 (97%)	9 (3%)	0	100	100	

There are no Ramachandran outliers to report.

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	267/271 (98%)	258 (97%)	9 (3%)	37 8	
2	M	2/2~(100%)	2 (100%)	0	100 100	
All	All	269/273~(98%)	260 (97%)	9 (3%)	39 9	

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	115	LYS
1	A	130	ILE
1	A	152[A]	SER
1	A	152[B]	SER
1	A	195	THR
1	A	199	LYS
1	A	275	ARG
1	A	278	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	203	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	Trino	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TYS	M	26[B]	2	15,16,17	1.00	0	18,22,24	1.24	1 (5%)
2	TYS	M	28	2	15,16,17	1.38	2 (13%)	18,22,24	1.08	2 (11%)
2	TYS	M	26[A]	2	15,16,17	2.41	3 (20%)	18,22,24	2.05	5 (27%)

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	TYS	M	26[B]	2	-	0/10/11/13	0/1/1/1
2	TYS	M	28	2	-	2/10/11/13	0/1/1/1
2	TYS	M	26[A]	2	-	4/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
2	M	26[A]	TYS	OH-S	-7.77	1.46	1.58
2	M	28	TYS	OH-S	-3.56	1.52	1.58
2	M	26[A]	TYS	OH-CZ	-2.99	1.37	1.42
2	M	28	TYS	CE2-CZ	2.52	1.43	1.38
2	M	26[A]	TYS	CB-CA	2.02	1.58	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
2	M	26[A]	TYS	CB-CA-C	5.82	122.37	111.47
2	M	26[A]	TYS	CG-CB-CA	-4.01	105.98	114.10
2	M	26[B]	TYS	O3-S-O2	2.92	118.66	108.49
2	M	26[A]	TYS	CD2-CE2-CZ	2.27	122.52	119.73
2	M	28	TYS	CB-CA-C	-2.25	107.24	111.47
2	M	28	TYS	CD2-CE2-CZ	-2.23	117.01	119.73
2	M	26[A]	TYS	CE2-CZ-CE1	-2.21	116.78	120.18
2	M	26[A]	TYS	OH-S-O2	2.19	114.10	107.71

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	26[A]	TYS	CZ-OH-S-O1

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Mol	Chain	Res	Type	Atoms
2	M	26[A]	TYS	N-CA-CB-CG
2	M	28	TYS	CA-CB-CG-CD2
2	M	28	TYS	CA-CB-CG-CD1
2	M	26[A]	TYS	CZ-OH-S-O3
2	M	26[A]	TYS	CZ-OH-S-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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 Chair		Dec	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IMD	A	401	-	3,5,5	0.37	0	$4,\!5,\!5$	0.69	0
4	SO4	A	402	-	4,4,4	0.13	0	6,6,6	0.09	0
4	SO4	A	403	-	4,4,4	0.10	0	6,6,6	0.09	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
3	IMD	A	401	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	IMD	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	282/308 (91%)	0.84	37 (13%) 3 3	17, 28, 59, 80	1 (0%)
2	M	3/6 (50%)	11.05	3 (100%) 0 0	39, 39, 41, 42	3 (100%)
All	All	$285/314 \ (90\%)$	0.94	40 (14%) 2 2	17, 28, 59, 80	4 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	29	GLY	20.5
1	A	28	ALA	14.6
1	A	216	THR	13.0
1	A	214	GLY	11.1
1	A	275	ARG	10.3
1	A	213	ASN	10.3
1	A	215	PRO	9.2
1	A	274	PRO	8.5
2	M	27	ASP	8.3
1	A	276	THR	8.0
1	A	277	GLY	7.9
1	A	155	GLY	7.6
1	A	30	THR	7.5
1	A	29	ASN	7.3
1	A	156	ASN	6.8
1	A	197	ASP	6.4
1	A	196	PRO	6.4
1	A	95	GLY	6.3
1	A	217	GLY	5.8
1	A	273	PHE	5.5
1	A	309	GLY	4.9
1	A	278	ILE	4.9
1	A	198	GLY	4.8
1	A	195	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	98	LEU	4.5
1	A	157	GLY	4.4
2	M	25	ASP	4.3
1	A	94	SER	4.2
1	A	199	LYS	3.2
1	A	272	LEU	3.1
1	A	154	GLY	2.9
1	A	212	PRO	2.9
1	A	279	TYR	2.8
1	A	93	GLY	2.6
1	A	211	SER	2.5
1	A	194	VAL	2.3
1	A	203	HIS	2.3
1	A	151	PRO	2.2
1	A	259	ILE	2.2
1	A	96	TYR	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	TYS	M	28	16/17	0.88	0.22	28,33,38,39	16
2	TYS	M	26[B]	16/17	0.92	0.17	29,31,38,40	16
2	TYS	M	26[A]	16/17	0.92	0.17	29,33,39,40	16

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	IMD	A	401	5/5	0.68	0.16	61,62,62,62	0
4	SO4	A	403	5/5	0.72	0.32	89,90,90,90	5
4	SO4	A	402	5/5	0.77	0.27	92,92,92,92	5

6.5 Other polymers (i)

There are no such residues in this entry.

