



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1J7N
Title : Anthrax Toxin Lethal factor
Authors : Pannifer, A.D.; Wong, T.Y.; Schwarzenbacher, R.; Renatus, M.; Petosa, C.;
Collier, R.J.; Bienkowska, J.; Lacy, D.B.; Park, S.; Leppla, S.H.; Hanna, P.;
Liddington, R.C.
Deposited on : 2001-05-17
Resolution : 2.30 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 (RC4), CSD as536be (2015)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

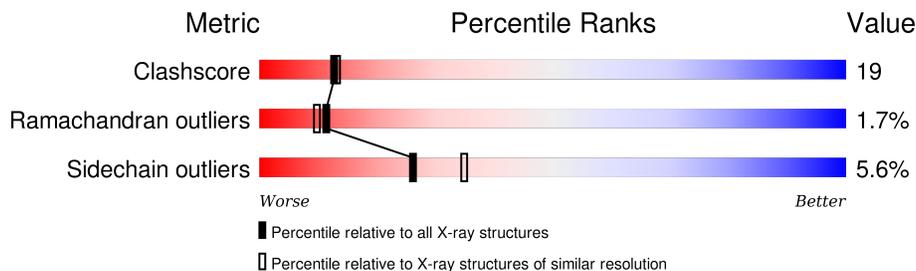
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	776	
1	B	776	

2 Entry composition [i](#)

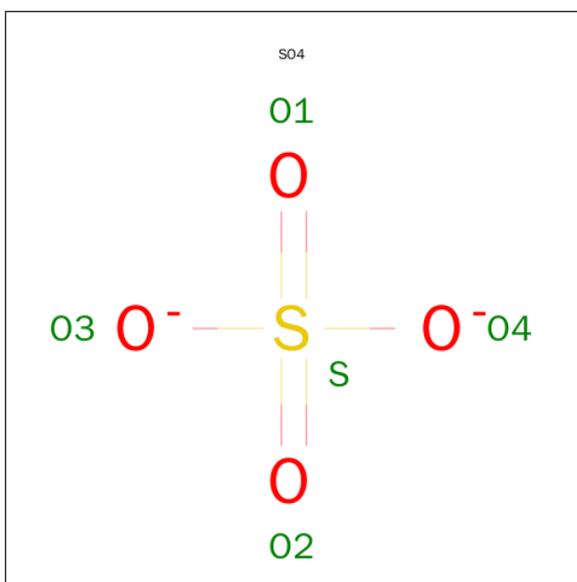
There are 4 unique types of molecules in this entry. The entry contains 12924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lethal Factor precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	725	Total 5947	C 3785	N 1003	O 1152	S 7	0	0	0
1	B	736	Total 6031	C 3832	N 1017	O 1175	S 7	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

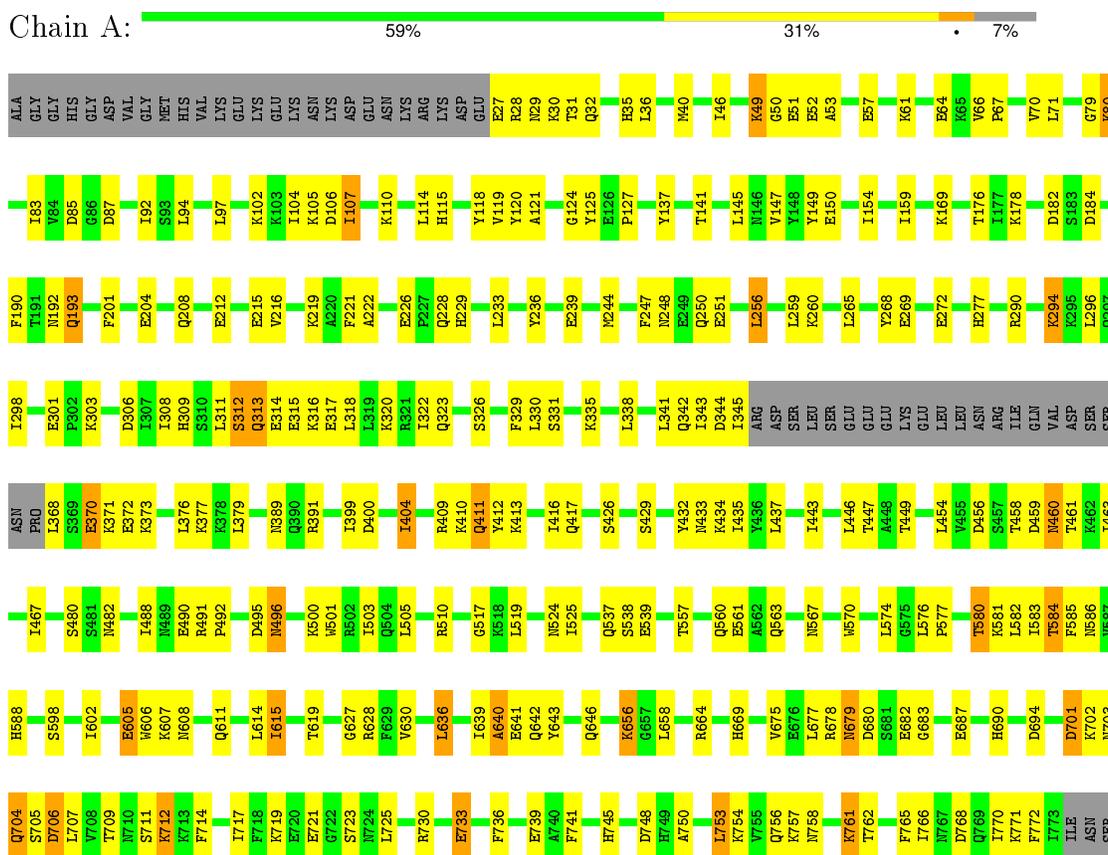
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	436	Total 436	O 436	0	0
4	B	498	Total 498	O 498	0	0

3 Residue-property plots [i](#)

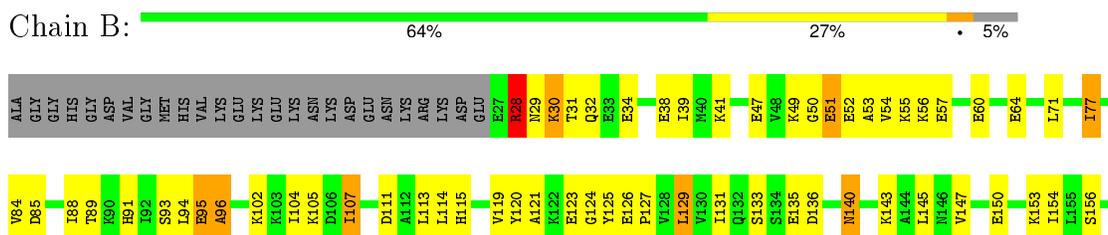
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Lethal Factor precursor



- Molecule 1: Lethal Factor precursor



S776	1666	T509	R391	E317	T176
R673	R510	R513	L392	L318	L177
V675	Y513	L514	L398	L319	K178
B676	E515	L514	P402	Q323	Q186
L677	M516	M516	V408	I324	K195
R678	G517	G518	Q411	S326	F201
H690	L519	L519	Y412	S327	L206
D693	I520	I520	R413	S331	E207
L700	Q522	Q522	R414	T332	E212
D701	R523	R523	D415	E333	V213
K702	K530	K530	I416	E334	E212
N703	I535	I535	D420	K335	V216
S705	R536	R536	H424	E336	F217
D706	Q537	Q537	Q425	K339	F221
L707	R544	R544	S426	K340	E226
K712	R544	R544	I427	L341	P227
K713	A547	A547	G428	Q342	Q228
I717	P551	P551	L431	D344	D231
G722	K554	K554	Y432	R346	V232
R730	Q563	Q563	N441	D347	L233
E733	L564	L564	N444	S348	L233
F741	Q568	Q568	N445	LEU	Q234
M744	K578	K578	L446	SER	L235
H745	Y579	Y579	T447	GLU	Y236
S746	F585	F585	A448	GLU	A237
D748	W606	W606	D456	GLU	P238
H749	K607	K607	S457	LYS	E239
A750	R611	R611	I464	LEU	A240
R751	D613	D613	S467	LEU	F241
R752	L614	L614	N464	ASN	M244
L753	L615	L615	I467	ARG	D245
A759	F629	F629	I468	ILE	M248
P760	T632	T632	R491	GLN	E249
K761	D633	D633	P492	VAL	E250
F765	I634	I634	D495	D663	E251
I766	I639	I639	M496	M366	E251
D768	I649	I649	L499	P367	L256
I770	I659	I659	K500	L368	L265
I773	I774	I774	H501	S369	L265
I774	I770	I770	R502	E370	Y278
I775	I773	I773	I503	K371	Q297
	N775	N775	Q504	E372	Q297
			L505	K373	Q297
				K377	K304
				K378	K304
				L379	S312
				I388	Q315
				N389	E314
				Q390	E315
					K316

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.20Å 137.46Å 98.55Å 90.00° 98.35° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	5.0 (15.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12924	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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: ZN, 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	0.34	0/6053	0.57	1/8153 (0.0%)
1	B	0.36	1/6139 (0.0%)	0.59	2/8272 (0.0%)
All	All	0.35	1/12192 (0.0%)	0.58	3/16425 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	615	ILE	CG1-CD1	-5.50	1.12	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	615	ILE	CB-CG1-CD1	8.66	138.14	113.90
1	A	615	ILE	CB-CG1-CD1	-7.22	93.67	113.90
1	B	629	PHE	N-CA-C	-5.57	95.95	111.00

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	5947	0	5938	247	0
1	B	6031	0	5992	221	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	436	0	0	16	0
4	B	498	0	0	17	0
All	All	12924	0	11930	461	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 19.

The worst 5 of 461 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:615:ILE:CG1	1:A:615:ILE:CD1	1.74	1.58
1:A:268:TYR:HB3	1:B:125:TYR:CE2	1.87	1.09
1:B:704:GLN:NE2	1:B:706:ASP:H	1.52	1.07
1:A:92:ILE:HD12	1:A:92:ILE:H	1.25	1.01
1:A:677:LEU:HD13	1:A:683:GLY:HA2	1.43	1.01

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	721/776 (93%)	670 (93%)	38 (5%)	13 (2%)	11 9
1	B	732/776 (94%)	685 (94%)	35 (5%)	12 (2%)	12 11
All	All	1453/1552 (94%)	1355 (93%)	73 (5%)	25 (2%)	11 10

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	313	GLN
1	A	640	ALA
1	B	28	ARG
1	B	96	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	660/710 (93%)	623 (94%)	37 (6%)	26	35
1	B	669/710 (94%)	631 (94%)	38 (6%)	25	34
All	All	1329/1420 (94%)	1254 (94%)	75 (6%)	26	35

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	712	LYS
1	B	102	LYS
1	B	615	ILE
1	A	733	GLU
1	B	51	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	767	ASN
1	B	193	GLN
1	B	638	ASN
1	B	164	ASN
1	B	214	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	SO4	A	777	-	4,4,4	0.08	0	6,6,6	0.12	0
2	SO4	B	777	-	4,4,4	0.19	0	6,6,6	0.08	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
2	SO4	A	777	-	-	0/0/0/0	0/0/0/0
2	SO4	B	777	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

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.