



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1J7N / pdb_00001j7n
Title : Anthrax Toxin Lethal factor
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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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

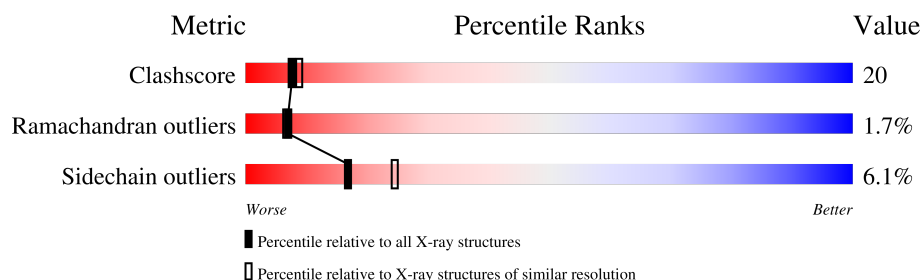
1 Overall quality at a glance

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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 $\leq 5\%$.

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
1	A	725	Total	C	N	O	S	0	0	0
			5947	3785	1003	1152	7			
1	B	736	Total	C	N	O	S	0	0	0
			6031	3832	1017	1175	7			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is water.

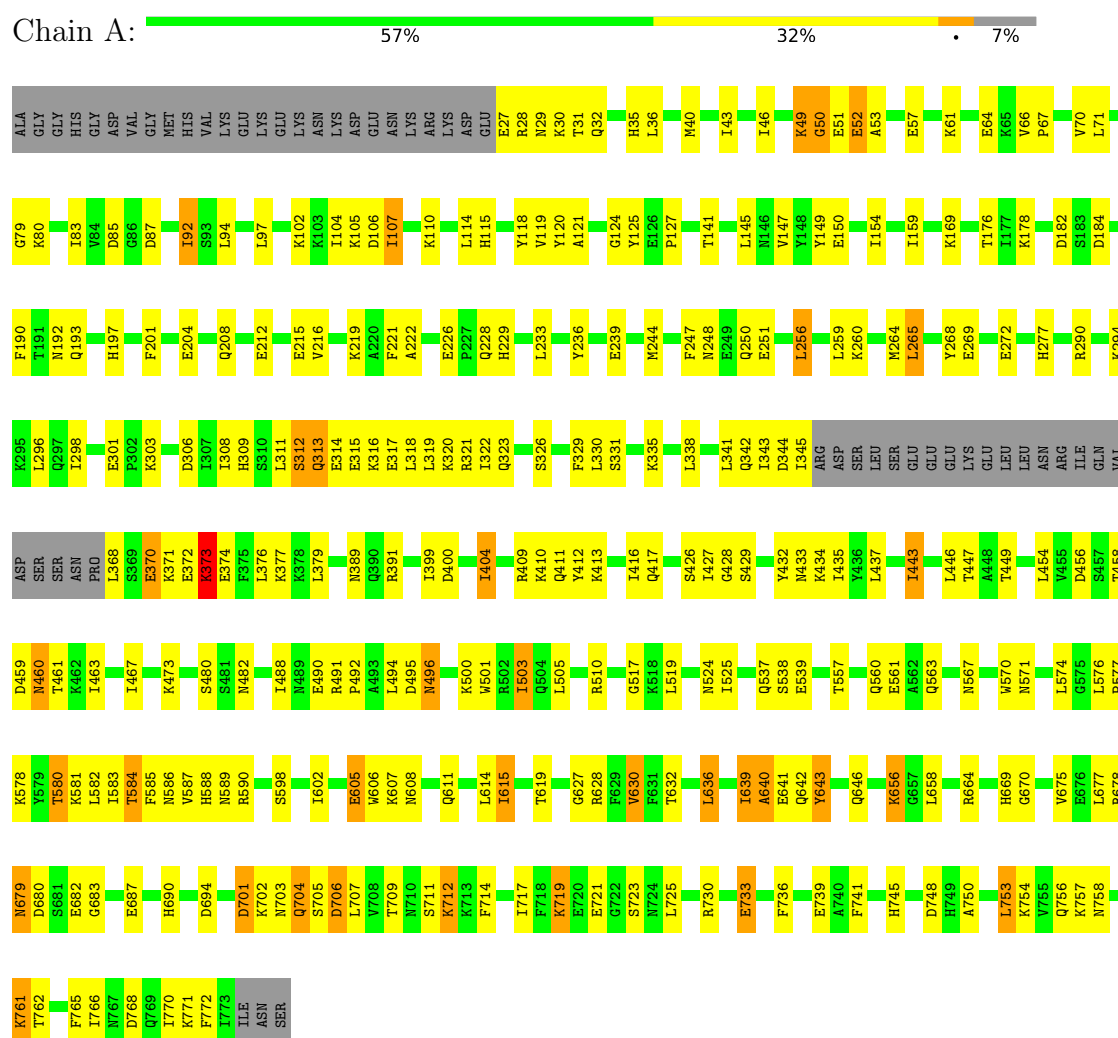
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	436	Total 436	O 436	0	0
4	B	498	Total 498	O 498	0	0

3 Residue-property plots

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.

Note EDS was not executed.

- Molecule 1: Lethal Factor precursor



- Molecule 1: Lethal Factor precursor



H744	D495	S612	D496	K373	Q297	L155	I177	ALA
H745	M496	D613	M496	K377	Q304	S156	V84	GLY
S746	L499	L614	L499	K378	K304	Q165	D85	GLY
D748	K500	K616	K500	L379	S312	P166	I88	GLY
H749	W501	F629	W501	I388	Q313	T176	T89	ASP
A750	R502	F629	R502	N389	E314	I177	K90	VAL
E751	I503	T632	I503	Q390	E315	K178	T89	VAL
R752	Q504	T632	Q504	N391	K316	I192	K90	MET
L753	L505	T634	L505	L392	E317	Q186	S93	HIS
A759	S506	T634	S506	L392	L318	Q186	S93	HIS
P760	T509	L639	T509	L398	L319	T191	E95	LYS
K761	R510	Y643	R510	P402	I322	K195	A96	GLU
F765	Y513	Y643	Y513	V408	Q323	K195	E99	LYS
I766	L514	T649	L514	V408	I324	F201	E99	LYS
N767	E515	Y659	E515	Q411	D325	F201	K102	ASN
D768	M516	Y659	M516	Y412	S262	V203	K103	LYS
Q769	G517	E662	G517	Y412	S326	V203	K103	ASP
I770	R518	E662	R518	R414	S327	L206	I104	GLU
I773	L519	T666	L519	D415	S331	E207	K105	ASN
I774	T520	T666	T520	I416	T332	E212	D106	LYS
N775	L521	K673	L521	I416	E333	V213	I107	ARG
S776	R523	G674	R523	D420	E334	E213	D111	LYS
	T535	V675	T535	H424	K335	V216	A112	ASP
	K536	E676	K536	Q425	E336	F217	A112	GLU
	Q537	L677	Q537	S426	E336	F217	L113	
	R544	R678	R544	I427	K339	F221	L114	
	A547	H690	A547	Q428	K340	E226	V119	
	P551	D693	P551	L431	L341	P227	Y120	
	K554	D694	K554	Y432	Q342	Q228	A121	
	Q563	L700	Q563	Y438	I343	G124	K122	
	L564	D701	L564	M441	D344	Y125	E33	
	Q704	D701	Q704	N444	I345	E126	E34	
	S705	K702	S705	N445	LEU	P127	E38	
	D706	N703	D706	L446	SER	V128	I39	
	L707	S705	L707	T447	GLU	L129	M40	
		S705		A448	GLU	V130	K41	
				N571	LYS	I131	H42	
				K578	GLU	Q132	E47	
				Y579	LEU	S133	V48	
				S457	LEU	S134	K49	
				N464	ASN	E135	G50	
				F585	ARG	D136	E51	
				V586	ILE	M140	A53	
				V587	GLN	D245	V54	
				H588	VAL	N248	K55	
				N589	D363	E249	K56	
				R590	N366	Q250	E57	
				W606	P367	E251	E60	
				K607	L368	L256	L63	
				Q611	S369	L285	E64	
					E370	Y278	L71	
					K371		K153	
					P492		I154	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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.	Xtriage
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: SO4, ZN

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	0.40	1/6053 (0.0%)	0.90	20/8153 (0.2%)
1	B	0.43	1/6139 (0.0%)	0.91	20/8272 (0.2%)
All	All	0.41	2/12192 (0.0%)	0.90	40/16425 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	615	ILE	CG1-CD1	-10.06	1.12	1.51
1	A	615	ILE	CG1-CD1	5.90	1.74	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	615	ILE	CB-CG1-CD1	11.59	138.14	113.80
1	A	615	ILE	CB-CG1-CD1	-9.59	93.67	113.80
1	B	590	ARG	N-CA-C	8.96	123.32	112.38
1	A	639	ILE	N-CA-C	8.36	118.39	110.53
1	B	629	PHE	N-CA-C	-7.84	95.95	108.73

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	256	0
1	B	6031	0	5992	235	0
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	484	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 20.

The worst 5 of 484 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:CD1	1:A:615:ILE:CG1	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%)	6 6
1	B	732/776 (94%)	685 (94%)	35 (5%)	12 (2%)	7 7
All	All	1453/1552 (94%)	1355 (93%)	73 (5%)	25 (2%)	7 7

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 ⓘ

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%)	622 (94%)	38 (6%)	18	26
1	B	669/710 (94%)	626 (94%)	43 (6%)	16	23
All	All	1329/1420 (94%)	1248 (94%)	81 (6%)	17	24

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	314	GLU
1	B	520	ILE
1	B	323	GLN
1	B	447	THR
1	B	678	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	440	ASN
1	B	586	ASN
1	B	445	ASN
1	B	524	ASN
1	B	620	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	B	777	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	A	777	-	4,4,4	0.32	0	6,6,6	0.18	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 [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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.