



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 10:47 am BST

PDB ID : 7AHL  
Title : ALPHA-HEMOLYSIN FROM STAPHYLOCOCCUS AUREUS  
Authors : Song, L.; Hobbaugh, M.; Shustak, C.; Cheley, S.; Bayley, H.; Gouaux, J.E.  
Deposited on : 1996-12-02  
Resolution : 1.89 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

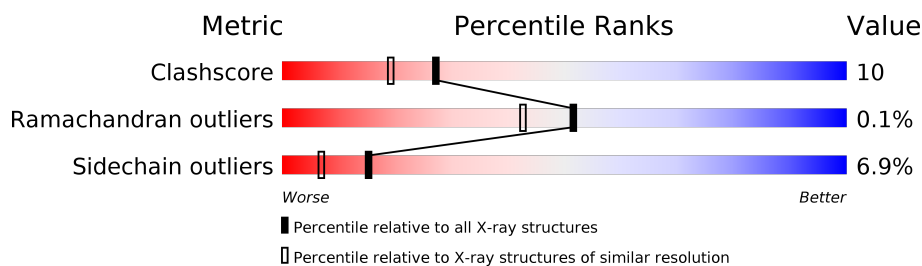
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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  $\geq 3$ , 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	293	
1	B	293	
1	C	293	
1	D	293	
1	E	293	
1	F	293	
1	G	293	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22778 atoms, of which 5571 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 ALPHA-HEMOLYSIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	H	N	O	S	0	0	0
			2891	1466	556	397	465	7			
1	B	293	Total	C	H	N	O	S	0	0	0
			2909	1472	564	401	465	7			
1	C	293	Total	C	H	N	O	S	0	0	0
			2909	1472	564	401	465	7			
1	D	293	Total	C	H	N	O	S	0	0	0
			2896	1466	559	399	465	7			
1	E	293	Total	C	H	N	O	S	0	0	0
			2911	1472	566	401	465	7			
1	F	293	Total	C	H	N	O	S	0	0	0
			2904	1469	563	400	465	7			
1	G	293	Total	C	H	N	O	S	0	0	0
			2904	1469	563	400	465	7			

- Molecule 2 is water.

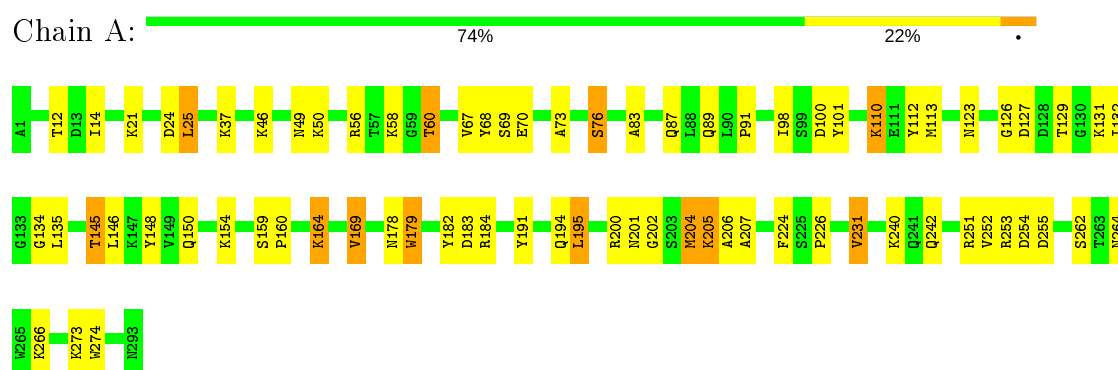
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	118	Total	H	O	0	0
			354	236	118		
2	B	128	Total	H	O	0	0
			384	256	128		
2	C	119	Total	H	O	0	0
			357	238	119		
2	D	122	Total	H	O	0	0
			366	244	122		
2	E	126	Total	H	O	0	0
			378	252	126		
2	F	92	Total	H	O	0	0
			276	184	92		
2	G	113	Total	H	O	0	0
			339	226	113		

### 3 Residue-property plots

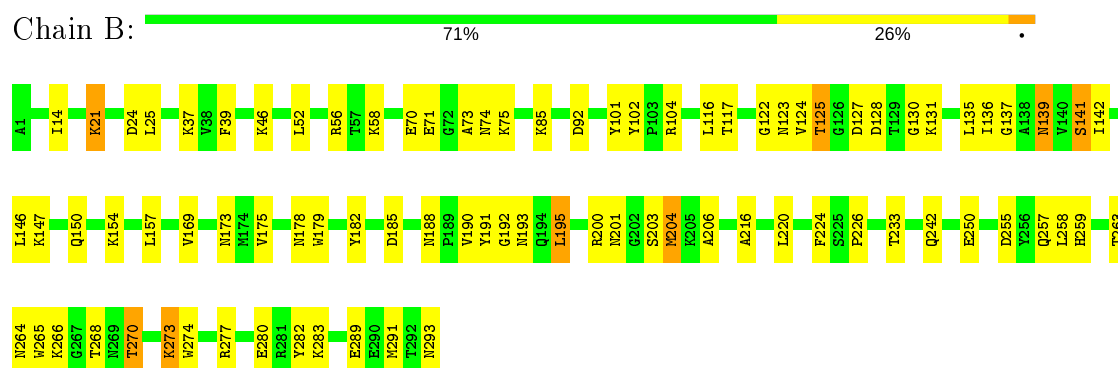
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

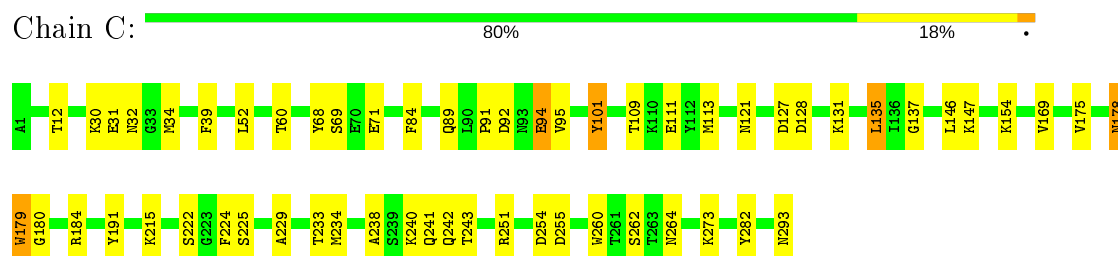
#### • Molecule 1: ALPHA-HEMOLYSIN



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#### • Molecule 1: ALPHA-HEMOLYSIN

[illegible]

T142	T143	T144	T145	K154	L157	K164	V169	M178	D183	R184	Y191	L195	R200	R201	G202	S203	M204	F224	S225	P226	T233	Q242	T243	T248	T249	E250	R251	D254	D255	H259	T260	T261	S262	R266	G267	T268	H269	T270	Y282	M293
A1	T12	D13	L25	R30	F39	K50	K51	L52	K58	A62	V65	R66	V67	E71	K75	L78	K85	R86	Q87	P91	D92	H93	E94	V95	Y101	D108	M113	L116	T117	G122	M123	V124	T125	G136	D127	K131	L135	S141		

D254	H259	W260	S262	T263	N264	T268	K273	W274	R277	Y282	T283	I284	N293	V140	S141	I142	T145	Y148	T155	I156	L157	P160	V165	V169	Q177	N178	D183	R184	N188	Y191	I192	K198	T199	R200	N201	M204	D208	N209	F210	S222	G223	F224	S225	P226	T233	R236	K240	O241	Q242	T243	I248	Y249	E250	P251
A1	I5	N6	I7	S16	N17	D24	L25	M34	K37	V38	L52	I55	R56	T57	K58	I61	E71	N74	K75	S76	K85	N93	Y101	Y102	T109	K110	E111	L116	T117	N121	G122	N123	Y124	T125	G126	D127	K131	I132	G133	G134	C137													

M178	M179	G180	P181	R184	M188	Y191	G192	L195	R200	M204	M209	S222	G223	F224	T230	V231	M234	K237	A238	Q242	D254	D255	H259	T261	S262	W265	K273	Y282	K283	E290	M291	T292	M293	A1	D4	T12	L25	Y40	M49	K50	K51	L52	T60	V67	M74	P81	D92	N93	E94	V95	D100	Y101	Y102	L116	T117	M123	Y124	T125	G126	D127	K131	L135	L136	G137	A138	T142	Y148	V149	Q150	P151	K154	T155	K164	V160
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.92Å 136.76Å 135.12Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	8.00 – 1.89	Depositor
% Data completeness (in resolution range)	93.3 (8.00-1.89)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.199 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 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	0.49	0/2387	0.75	1/3232 (0.0%)
1	B	0.50	0/2397	0.74	0/3243
1	C	0.50	0/2397	0.75	0/3243
1	D	0.48	0/2389	0.74	0/3235
1	E	0.51	0/2397	0.75	1/3243 (0.0%)
1	F	0.47	0/2393	0.73	1/3239 (0.0%)
1	G	0.49	0/2393	0.77	1/3239 (0.0%)
All	All	0.49	0/16753	0.75	4/22674 (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	B	0	1
1	F	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	52	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	251	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	G	52	LEU	CA-CB-CG	5.13	127.10	115.30
1	F	251	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	TYR	Sidechain
1	F	102	TYR	Sidechain
1	G	102	TYR	Sidechain

## 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	2335	556	2248	60	0
1	B	2345	564	2270	62	0
1	C	2345	564	2270	45	0
1	D	2337	559	2248	66	0
1	E	2345	566	2270	55	0
1	F	2341	563	2259	59	0
1	G	2341	563	2259	50	0
2	A	118	236	0	5	1
2	B	128	256	0	4	0
2	C	119	238	0	5	0
2	D	122	244	0	4	0
2	E	126	252	0	6	0
2	F	92	184	0	2	0
2	G	113	226	0	7	0
All	All	17207	5571	15824	325	1

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 10.

The worst 5 of 325 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:113:MET:HG3	1:A:145:THR:HG23	1.50	0.92
1:F:260:TRP:NE1	1:F:262:SER:HA	1.92	0.84
1:E:282:TYR:CD2	1:E:293:ASN:HB3	2.14	0.82
1:B:125:THR:HG23	1:C:135:LEU:HD22	1.61	0.82
1:E:260:TRP:NE1	1:E:262:SER:HA	1.96	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:338:HOH:H1	2:A:338:HOH:H1[2_656]	1.34	0.26

## 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	291/293 (99%)	272 (94%)	19 (6%)	0	100	100
1	B	291/293 (99%)	274 (94%)	16 (6%)	1 (0%)	41	31
1	C	291/293 (99%)	273 (94%)	18 (6%)	0	100	100
1	D	291/293 (99%)	272 (94%)	17 (6%)	2 (1%)	22	12
1	E	291/293 (99%)	273 (94%)	18 (6%)	0	100	100
1	F	291/293 (99%)	271 (93%)	20 (7%)	0	100	100
1	G	291/293 (99%)	274 (94%)	17 (6%)	0	100	100
All	All	2037/2051 (99%)	1909 (94%)	125 (6%)	3 (0%)	51	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	262	SER
1	B	73	ALA
1	D	92	ASP

### 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	257/259 (99%)	238 (93%)	19 (7%)	13	6
1	B	259/259 (100%)	239 (92%)	20 (8%)	13	5
1	C	259/259 (100%)	243 (94%)	16 (6%)	18	9
1	D	257/259 (99%)	238 (93%)	19 (7%)	13	6
1	E	259/259 (100%)	241 (93%)	18 (7%)	15	7
1	F	258/259 (100%)	243 (94%)	15 (6%)	20	10
1	G	258/259 (100%)	240 (93%)	18 (7%)	15	7
All	All	1807/1813 (100%)	1682 (93%)	125 (7%)	15	7

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	25	LEU
1	D	230	THR
1	G	125	THR
1	D	71	GLU
1	D	120	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	241	GLN
1	D	123	ASN
1	G	93	ASN
1	C	264	ASN
1	D	89	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.