



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 07:02 PM EDT

PDB ID : 3K55 / pdb_00003k55
Title : Structure of beta hairpin deletion mutant of beta toxin from *Staphylococcus aureus*
Authors : Kruse, A.C.; Huseby, M.; Shi, K.; Digre, J.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on : 2009-10-06
Resolution : 3.35 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

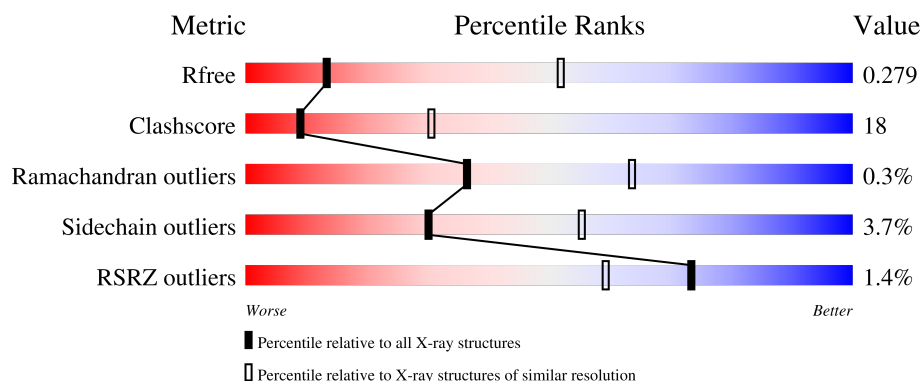
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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 $\leq 5\%$. 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	306	% 59% 29% • 8%
1	B	306	2% 56% 31% • 8%
1	C	306	3% 57% 32% • 8%
1	D	306	% 58% 31% • 8%
1	E	306	% 62% 27% • 8%

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Mol	Chain	Length	Quality of chain
1	F	306	2% 60% 29% 8%
1	G	306	61% 28% 8%
1	H	306	2% 60% 29% 8%
1	I	306	% 61% 28% 8%
1	J	306	3% 59% 31% 8%
1	K	306	57% 31% 8%
1	L	306	% 60% 30% 8%
1	M	306	60% 29% 8%
1	N	306	59% 30% 8%
1	O	306	% 56% 33% 8%
1	P	306	3% 57% 33% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35844 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 Beta-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	24	0	0
			2240	1413	383	439	5			
1	B	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	C	280	Total	C	N	O	S	16	0	0
			2240	1413	383	439	5			
1	D	280	Total	C	N	O	S	12	0	0
			2240	1413	383	439	5			
1	E	280	Total	C	N	O	S	24	0	0
			2240	1413	383	439	5			
1	F	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	G	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	H	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	I	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	J	280	Total	C	N	O	S	16	0	0
			2240	1413	383	439	5			
1	K	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	L	280	Total	C	N	O	S	24	0	0
			2240	1413	383	439	5			
1	M	280	Total	C	N	O	S	16	0	0
			2240	1413	383	439	5			
1	N	280	Total	C	N	O	S	12	0	0
			2240	1413	383	439	5			
1	O	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	P	280	Total	C	N	O	S	24	0	0
			2240	1413	383	439	5			

There are 512 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A7LAI8
A	-18	ARG	-	expression tag	UNP A7LAI8
A	-17	SER	-	expression tag	UNP A7LAI8
A	-16	SER	-	expression tag	UNP A7LAI8
A	-15	HIS	-	expression tag	UNP A7LAI8
A	-14	HIS	-	expression tag	UNP A7LAI8
A	-13	HIS	-	expression tag	UNP A7LAI8
A	-12	HIS	-	expression tag	UNP A7LAI8
A	-11	HIS	-	expression tag	UNP A7LAI8
A	-10	HIS	-	expression tag	UNP A7LAI8
A	-9	SER	-	expression tag	UNP A7LAI8
A	-8	SER	-	expression tag	UNP A7LAI8
A	-7	GLY	-	expression tag	UNP A7LAI8
A	-6	LEU	-	expression tag	UNP A7LAI8
A	-5	VAL	-	expression tag	UNP A7LAI8
A	-4	PRO	-	expression tag	UNP A7LAI8
A	-3	ARG	-	expression tag	UNP A7LAI8
A	-2	GLY	-	expression tag	UNP A7LAI8
A	-1	SER	-	expression tag	UNP A7LAI8
A	0	HIS	-	expression tag	UNP A7LAI8
A	1	MET	-	expression tag	UNP A7LAI8
A	?	-	ASP	deletion	UNP A7LAI8
A	?	-	VAL	deletion	UNP A7LAI8
A	?	-	TYR	deletion	UNP A7LAI8
A	?	-	ALA	deletion	UNP A7LAI8
A	?	-	PHE	deletion	UNP A7LAI8
A	?	-	PRO	deletion	UNP A7LAI8
A	?	-	TYR	deletion	UNP A7LAI8
A	?	-	TYR	deletion	UNP A7LAI8
A	?	-	TYR	deletion	UNP A7LAI8
A	?	-	VAL	deletion	UNP A7LAI8
A	?	-	TYR	deletion	UNP A7LAI8
B	-19	MET	-	expression tag	UNP A7LAI8
B	-18	ARG	-	expression tag	UNP A7LAI8
B	-17	SER	-	expression tag	UNP A7LAI8
B	-16	SER	-	expression tag	UNP A7LAI8
B	-15	HIS	-	expression tag	UNP A7LAI8
B	-14	HIS	-	expression tag	UNP A7LAI8
B	-13	HIS	-	expression tag	UNP A7LAI8
B	-12	HIS	-	expression tag	UNP A7LAI8
B	-11	HIS	-	expression tag	UNP A7LAI8
B	-10	HIS	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	expression tag	UNP A7LAI8
B	-8	SER	-	expression tag	UNP A7LAI8
B	-7	GLY	-	expression tag	UNP A7LAI8
B	-6	LEU	-	expression tag	UNP A7LAI8
B	-5	VAL	-	expression tag	UNP A7LAI8
B	-4	PRO	-	expression tag	UNP A7LAI8
B	-3	ARG	-	expression tag	UNP A7LAI8
B	-2	GLY	-	expression tag	UNP A7LAI8
B	-1	SER	-	expression tag	UNP A7LAI8
B	0	HIS	-	expression tag	UNP A7LAI8
B	1	MET	-	expression tag	UNP A7LAI8
B	?	-	ASP	deletion	UNP A7LAI8
B	?	-	VAL	deletion	UNP A7LAI8
B	?	-	TYR	deletion	UNP A7LAI8
B	?	-	ALA	deletion	UNP A7LAI8
B	?	-	PHE	deletion	UNP A7LAI8
B	?	-	PRO	deletion	UNP A7LAI8
B	?	-	TYR	deletion	UNP A7LAI8
B	?	-	TYR	deletion	UNP A7LAI8
B	?	-	TYR	deletion	UNP A7LAI8
B	?	-	TYR	deletion	UNP A7LAI8
B	?	-	VAL	deletion	UNP A7LAI8
B	?	-	TYR	deletion	UNP A7LAI8
C	-19	MET	-	expression tag	UNP A7LAI8
C	-18	ARG	-	expression tag	UNP A7LAI8
C	-17	SER	-	expression tag	UNP A7LAI8
C	-16	SER	-	expression tag	UNP A7LAI8
C	-15	HIS	-	expression tag	UNP A7LAI8
C	-14	HIS	-	expression tag	UNP A7LAI8
C	-13	HIS	-	expression tag	UNP A7LAI8
C	-12	HIS	-	expression tag	UNP A7LAI8
C	-11	HIS	-	expression tag	UNP A7LAI8
C	-10	HIS	-	expression tag	UNP A7LAI8
C	-9	SER	-	expression tag	UNP A7LAI8
C	-8	SER	-	expression tag	UNP A7LAI8
C	-7	GLY	-	expression tag	UNP A7LAI8
C	-6	LEU	-	expression tag	UNP A7LAI8
C	-5	VAL	-	expression tag	UNP A7LAI8
C	-4	PRO	-	expression tag	UNP A7LAI8
C	-3	ARG	-	expression tag	UNP A7LAI8
C	-2	GLY	-	expression tag	UNP A7LAI8
C	-1	SER	-	expression tag	UNP A7LAI8
C	0	HIS	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	expression tag	UNP A7LAI8
C	?	-	ASP	deletion	UNP A7LAI8
C	?	-	VAL	deletion	UNP A7LAI8
C	?	-	TYR	deletion	UNP A7LAI8
C	?	-	ALA	deletion	UNP A7LAI8
C	?	-	PHE	deletion	UNP A7LAI8
C	?	-	PRO	deletion	UNP A7LAI8
C	?	-	TYR	deletion	UNP A7LAI8
C	?	-	TYR	deletion	UNP A7LAI8
C	?	-	TYR	deletion	UNP A7LAI8
C	?	-	VAL	deletion	UNP A7LAI8
C	?	-	TYR	deletion	UNP A7LAI8
D	-19	MET	-	expression tag	UNP A7LAI8
D	-18	ARG	-	expression tag	UNP A7LAI8
D	-17	SER	-	expression tag	UNP A7LAI8
D	-16	SER	-	expression tag	UNP A7LAI8
D	-15	HIS	-	expression tag	UNP A7LAI8
D	-14	HIS	-	expression tag	UNP A7LAI8
D	-13	HIS	-	expression tag	UNP A7LAI8
D	-12	HIS	-	expression tag	UNP A7LAI8
D	-11	HIS	-	expression tag	UNP A7LAI8
D	-10	HIS	-	expression tag	UNP A7LAI8
D	-9	SER	-	expression tag	UNP A7LAI8
D	-8	SER	-	expression tag	UNP A7LAI8
D	-7	GLY	-	expression tag	UNP A7LAI8
D	-6	LEU	-	expression tag	UNP A7LAI8
D	-5	VAL	-	expression tag	UNP A7LAI8
D	-4	PRO	-	expression tag	UNP A7LAI8
D	-3	ARG	-	expression tag	UNP A7LAI8
D	-2	GLY	-	expression tag	UNP A7LAI8
D	-1	SER	-	expression tag	UNP A7LAI8
D	0	HIS	-	expression tag	UNP A7LAI8
D	1	MET	-	expression tag	UNP A7LAI8
D	?	-	ASP	deletion	UNP A7LAI8
D	?	-	VAL	deletion	UNP A7LAI8
D	?	-	TYR	deletion	UNP A7LAI8
D	?	-	ALA	deletion	UNP A7LAI8
D	?	-	PHE	deletion	UNP A7LAI8
D	?	-	PRO	deletion	UNP A7LAI8
D	?	-	TYR	deletion	UNP A7LAI8
D	?	-	TYR	deletion	UNP A7LAI8
D	?	-	TYR	deletion	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	VAL	deletion	UNP A7LAI8
D	?	-	TYR	deletion	UNP A7LAI8
E	-19	MET	-	expression tag	UNP A7LAI8
E	-18	ARG	-	expression tag	UNP A7LAI8
E	-17	SER	-	expression tag	UNP A7LAI8
E	-16	SER	-	expression tag	UNP A7LAI8
E	-15	HIS	-	expression tag	UNP A7LAI8
E	-14	HIS	-	expression tag	UNP A7LAI8
E	-13	HIS	-	expression tag	UNP A7LAI8
E	-12	HIS	-	expression tag	UNP A7LAI8
E	-11	HIS	-	expression tag	UNP A7LAI8
E	-10	HIS	-	expression tag	UNP A7LAI8
E	-9	SER	-	expression tag	UNP A7LAI8
E	-8	SER	-	expression tag	UNP A7LAI8
E	-7	GLY	-	expression tag	UNP A7LAI8
E	-6	LEU	-	expression tag	UNP A7LAI8
E	-5	VAL	-	expression tag	UNP A7LAI8
E	-4	PRO	-	expression tag	UNP A7LAI8
E	-3	ARG	-	expression tag	UNP A7LAI8
E	-2	GLY	-	expression tag	UNP A7LAI8
E	-1	SER	-	expression tag	UNP A7LAI8
E	0	HIS	-	expression tag	UNP A7LAI8
E	1	MET	-	expression tag	UNP A7LAI8
E	?	-	ASP	deletion	UNP A7LAI8
E	?	-	VAL	deletion	UNP A7LAI8
E	?	-	TYR	deletion	UNP A7LAI8
E	?	-	ALA	deletion	UNP A7LAI8
E	?	-	PHE	deletion	UNP A7LAI8
E	?	-	PRO	deletion	UNP A7LAI8
E	?	-	TYR	deletion	UNP A7LAI8
E	?	-	TYR	deletion	UNP A7LAI8
E	?	-	TYR	deletion	UNP A7LAI8
E	?	-	VAL	deletion	UNP A7LAI8
E	?	-	TYR	deletion	UNP A7LAI8
F	-19	MET	-	expression tag	UNP A7LAI8
F	-18	ARG	-	expression tag	UNP A7LAI8
F	-17	SER	-	expression tag	UNP A7LAI8
F	-16	SER	-	expression tag	UNP A7LAI8
F	-15	HIS	-	expression tag	UNP A7LAI8
F	-14	HIS	-	expression tag	UNP A7LAI8
F	-13	HIS	-	expression tag	UNP A7LAI8
F	-12	HIS	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	HIS	-	expression tag	UNP A7LAI8
F	-10	HIS	-	expression tag	UNP A7LAI8
F	-9	SER	-	expression tag	UNP A7LAI8
F	-8	SER	-	expression tag	UNP A7LAI8
F	-7	GLY	-	expression tag	UNP A7LAI8
F	-6	LEU	-	expression tag	UNP A7LAI8
F	-5	VAL	-	expression tag	UNP A7LAI8
F	-4	PRO	-	expression tag	UNP A7LAI8
F	-3	ARG	-	expression tag	UNP A7LAI8
F	-2	GLY	-	expression tag	UNP A7LAI8
F	-1	SER	-	expression tag	UNP A7LAI8
F	0	HIS	-	expression tag	UNP A7LAI8
F	1	MET	-	expression tag	UNP A7LAI8
F	?	-	ASP	deletion	UNP A7LAI8
F	?	-	VAL	deletion	UNP A7LAI8
F	?	-	TYR	deletion	UNP A7LAI8
F	?	-	ALA	deletion	UNP A7LAI8
F	?	-	PHE	deletion	UNP A7LAI8
F	?	-	PRO	deletion	UNP A7LAI8
F	?	-	TYR	deletion	UNP A7LAI8
F	?	-	TYR	deletion	UNP A7LAI8
F	?	-	TYR	deletion	UNP A7LAI8
F	?	-	VAL	deletion	UNP A7LAI8
F	?	-	TYR	deletion	UNP A7LAI8
G	-19	MET	-	expression tag	UNP A7LAI8
G	-18	ARG	-	expression tag	UNP A7LAI8
G	-17	SER	-	expression tag	UNP A7LAI8
G	-16	SER	-	expression tag	UNP A7LAI8
G	-15	HIS	-	expression tag	UNP A7LAI8
G	-14	HIS	-	expression tag	UNP A7LAI8
G	-13	HIS	-	expression tag	UNP A7LAI8
G	-12	HIS	-	expression tag	UNP A7LAI8
G	-11	HIS	-	expression tag	UNP A7LAI8
G	-10	HIS	-	expression tag	UNP A7LAI8
G	-9	SER	-	expression tag	UNP A7LAI8
G	-8	SER	-	expression tag	UNP A7LAI8
G	-7	GLY	-	expression tag	UNP A7LAI8
G	-6	LEU	-	expression tag	UNP A7LAI8
G	-5	VAL	-	expression tag	UNP A7LAI8
G	-4	PRO	-	expression tag	UNP A7LAI8
G	-3	ARG	-	expression tag	UNP A7LAI8
G	-2	GLY	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	SER	-	expression tag	UNP A7LAI8
G	0	HIS	-	expression tag	UNP A7LAI8
G	1	MET	-	expression tag	UNP A7LAI8
G	?	-	ASP	deletion	UNP A7LAI8
G	?	-	VAL	deletion	UNP A7LAI8
G	?	-	TYR	deletion	UNP A7LAI8
G	?	-	ALA	deletion	UNP A7LAI8
G	?	-	PHE	deletion	UNP A7LAI8
G	?	-	PRO	deletion	UNP A7LAI8
G	?	-	TYR	deletion	UNP A7LAI8
G	?	-	TYR	deletion	UNP A7LAI8
G	?	-	TYR	deletion	UNP A7LAI8
G	?	-	VAL	deletion	UNP A7LAI8
G	?	-	TYR	deletion	UNP A7LAI8
H	-19	MET	-	expression tag	UNP A7LAI8
H	-18	ARG	-	expression tag	UNP A7LAI8
H	-17	SER	-	expression tag	UNP A7LAI8
H	-16	SER	-	expression tag	UNP A7LAI8
H	-15	HIS	-	expression tag	UNP A7LAI8
H	-14	HIS	-	expression tag	UNP A7LAI8
H	-13	HIS	-	expression tag	UNP A7LAI8
H	-12	HIS	-	expression tag	UNP A7LAI8
H	-11	HIS	-	expression tag	UNP A7LAI8
H	-10	HIS	-	expression tag	UNP A7LAI8
H	-9	SER	-	expression tag	UNP A7LAI8
H	-8	SER	-	expression tag	UNP A7LAI8
H	-7	GLY	-	expression tag	UNP A7LAI8
H	-6	LEU	-	expression tag	UNP A7LAI8
H	-5	VAL	-	expression tag	UNP A7LAI8
H	-4	PRO	-	expression tag	UNP A7LAI8
H	-3	ARG	-	expression tag	UNP A7LAI8
H	-2	GLY	-	expression tag	UNP A7LAI8
H	-1	SER	-	expression tag	UNP A7LAI8
H	0	HIS	-	expression tag	UNP A7LAI8
H	1	MET	-	expression tag	UNP A7LAI8
H	?	-	ASP	deletion	UNP A7LAI8
H	?	-	VAL	deletion	UNP A7LAI8
H	?	-	TYR	deletion	UNP A7LAI8
H	?	-	ALA	deletion	UNP A7LAI8
H	?	-	PHE	deletion	UNP A7LAI8
H	?	-	PRO	deletion	UNP A7LAI8
H	?	-	TYR	deletion	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	TYR	deletion	UNP A7LAI8
H	?	-	TYR	deletion	UNP A7LAI8
H	?	-	VAL	deletion	UNP A7LAI8
H	?	-	TYR	deletion	UNP A7LAI8
I	-19	MET	-	expression tag	UNP A7LAI8
I	-18	ARG	-	expression tag	UNP A7LAI8
I	-17	SER	-	expression tag	UNP A7LAI8
I	-16	SER	-	expression tag	UNP A7LAI8
I	-15	HIS	-	expression tag	UNP A7LAI8
I	-14	HIS	-	expression tag	UNP A7LAI8
I	-13	HIS	-	expression tag	UNP A7LAI8
I	-12	HIS	-	expression tag	UNP A7LAI8
I	-11	HIS	-	expression tag	UNP A7LAI8
I	-10	HIS	-	expression tag	UNP A7LAI8
I	-9	SER	-	expression tag	UNP A7LAI8
I	-8	SER	-	expression tag	UNP A7LAI8
I	-7	GLY	-	expression tag	UNP A7LAI8
I	-6	LEU	-	expression tag	UNP A7LAI8
I	-5	VAL	-	expression tag	UNP A7LAI8
I	-4	PRO	-	expression tag	UNP A7LAI8
I	-3	ARG	-	expression tag	UNP A7LAI8
I	-2	GLY	-	expression tag	UNP A7LAI8
I	-1	SER	-	expression tag	UNP A7LAI8
I	0	HIS	-	expression tag	UNP A7LAI8
I	1	MET	-	expression tag	UNP A7LAI8
I	?	-	ASP	deletion	UNP A7LAI8
I	?	-	VAL	deletion	UNP A7LAI8
I	?	-	TYR	deletion	UNP A7LAI8
I	?	-	ALA	deletion	UNP A7LAI8
I	?	-	PHE	deletion	UNP A7LAI8
I	?	-	PRO	deletion	UNP A7LAI8
I	?	-	TYR	deletion	UNP A7LAI8
I	?	-	TYR	deletion	UNP A7LAI8
I	?	-	TYR	deletion	UNP A7LAI8
I	?	-	VAL	deletion	UNP A7LAI8
I	?	-	TYR	deletion	UNP A7LAI8
J	-19	MET	-	expression tag	UNP A7LAI8
J	-18	ARG	-	expression tag	UNP A7LAI8
J	-17	SER	-	expression tag	UNP A7LAI8
J	-16	SER	-	expression tag	UNP A7LAI8
J	-15	HIS	-	expression tag	UNP A7LAI8
J	-14	HIS	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	HIS	-	expression tag	UNP A7LAI8
J	-12	HIS	-	expression tag	UNP A7LAI8
J	-11	HIS	-	expression tag	UNP A7LAI8
J	-10	HIS	-	expression tag	UNP A7LAI8
J	-9	SER	-	expression tag	UNP A7LAI8
J	-8	SER	-	expression tag	UNP A7LAI8
J	-7	GLY	-	expression tag	UNP A7LAI8
J	-6	LEU	-	expression tag	UNP A7LAI8
J	-5	VAL	-	expression tag	UNP A7LAI8
J	-4	PRO	-	expression tag	UNP A7LAI8
J	-3	ARG	-	expression tag	UNP A7LAI8
J	-2	GLY	-	expression tag	UNP A7LAI8
J	-1	SER	-	expression tag	UNP A7LAI8
J	0	HIS	-	expression tag	UNP A7LAI8
J	1	MET	-	expression tag	UNP A7LAI8
J	?	-	ASP	deletion	UNP A7LAI8
J	?	-	VAL	deletion	UNP A7LAI8
J	?	-	TYR	deletion	UNP A7LAI8
J	?	-	ALA	deletion	UNP A7LAI8
J	?	-	PHE	deletion	UNP A7LAI8
J	?	-	PRO	deletion	UNP A7LAI8
J	?	-	TYR	deletion	UNP A7LAI8
J	?	-	TYR	deletion	UNP A7LAI8
J	?	-	TYR	deletion	UNP A7LAI8
J	?	-	TYR	deletion	UNP A7LAI8
J	?	-	VAL	deletion	UNP A7LAI8
J	?	-	TYR	deletion	UNP A7LAI8
K	-19	MET	-	expression tag	UNP A7LAI8
K	-18	ARG	-	expression tag	UNP A7LAI8
K	-17	SER	-	expression tag	UNP A7LAI8
K	-16	SER	-	expression tag	UNP A7LAI8
K	-15	HIS	-	expression tag	UNP A7LAI8
K	-14	HIS	-	expression tag	UNP A7LAI8
K	-13	HIS	-	expression tag	UNP A7LAI8
K	-12	HIS	-	expression tag	UNP A7LAI8
K	-11	HIS	-	expression tag	UNP A7LAI8
K	-10	HIS	-	expression tag	UNP A7LAI8
K	-9	SER	-	expression tag	UNP A7LAI8
K	-8	SER	-	expression tag	UNP A7LAI8
K	-7	GLY	-	expression tag	UNP A7LAI8
K	-6	LEU	-	expression tag	UNP A7LAI8
K	-5	VAL	-	expression tag	UNP A7LAI8
K	-4	PRO	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	ARG	-	expression tag	UNP A7LAI8
K	-2	GLY	-	expression tag	UNP A7LAI8
K	-1	SER	-	expression tag	UNP A7LAI8
K	0	HIS	-	expression tag	UNP A7LAI8
K	1	MET	-	expression tag	UNP A7LAI8
K	?	-	ASP	deletion	UNP A7LAI8
K	?	-	VAL	deletion	UNP A7LAI8
K	?	-	TYR	deletion	UNP A7LAI8
K	?	-	ALA	deletion	UNP A7LAI8
K	?	-	PHE	deletion	UNP A7LAI8
K	?	-	PRO	deletion	UNP A7LAI8
K	?	-	TYR	deletion	UNP A7LAI8
K	?	-	TYR	deletion	UNP A7LAI8
K	?	-	TYR	deletion	UNP A7LAI8
K	?	-	VAL	deletion	UNP A7LAI8
K	?	-	TYR	deletion	UNP A7LAI8
L	-19	MET	-	expression tag	UNP A7LAI8
L	-18	ARG	-	expression tag	UNP A7LAI8
L	-17	SER	-	expression tag	UNP A7LAI8
L	-16	SER	-	expression tag	UNP A7LAI8
L	-15	HIS	-	expression tag	UNP A7LAI8
L	-14	HIS	-	expression tag	UNP A7LAI8
L	-13	HIS	-	expression tag	UNP A7LAI8
L	-12	HIS	-	expression tag	UNP A7LAI8
L	-11	HIS	-	expression tag	UNP A7LAI8
L	-10	HIS	-	expression tag	UNP A7LAI8
L	-9	SER	-	expression tag	UNP A7LAI8
L	-8	SER	-	expression tag	UNP A7LAI8
L	-7	GLY	-	expression tag	UNP A7LAI8
L	-6	LEU	-	expression tag	UNP A7LAI8
L	-5	VAL	-	expression tag	UNP A7LAI8
L	-4	PRO	-	expression tag	UNP A7LAI8
L	-3	ARG	-	expression tag	UNP A7LAI8
L	-2	GLY	-	expression tag	UNP A7LAI8
L	-1	SER	-	expression tag	UNP A7LAI8
L	0	HIS	-	expression tag	UNP A7LAI8
L	1	MET	-	expression tag	UNP A7LAI8
L	?	-	ASP	deletion	UNP A7LAI8
L	?	-	VAL	deletion	UNP A7LAI8
L	?	-	TYR	deletion	UNP A7LAI8
L	?	-	ALA	deletion	UNP A7LAI8
L	?	-	PHE	deletion	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	PRO	deletion	UNP A7LAI8
L	?	-	TYR	deletion	UNP A7LAI8
L	?	-	TYR	deletion	UNP A7LAI8
L	?	-	TYR	deletion	UNP A7LAI8
L	?	-	VAL	deletion	UNP A7LAI8
L	?	-	TYR	deletion	UNP A7LAI8
M	-19	MET	-	expression tag	UNP A7LAI8
M	-18	ARG	-	expression tag	UNP A7LAI8
M	-17	SER	-	expression tag	UNP A7LAI8
M	-16	SER	-	expression tag	UNP A7LAI8
M	-15	HIS	-	expression tag	UNP A7LAI8
M	-14	HIS	-	expression tag	UNP A7LAI8
M	-13	HIS	-	expression tag	UNP A7LAI8
M	-12	HIS	-	expression tag	UNP A7LAI8
M	-11	HIS	-	expression tag	UNP A7LAI8
M	-10	HIS	-	expression tag	UNP A7LAI8
M	-9	SER	-	expression tag	UNP A7LAI8
M	-8	SER	-	expression tag	UNP A7LAI8
M	-7	GLY	-	expression tag	UNP A7LAI8
M	-6	LEU	-	expression tag	UNP A7LAI8
M	-5	VAL	-	expression tag	UNP A7LAI8
M	-4	PRO	-	expression tag	UNP A7LAI8
M	-3	ARG	-	expression tag	UNP A7LAI8
M	-2	GLY	-	expression tag	UNP A7LAI8
M	-1	SER	-	expression tag	UNP A7LAI8
M	0	HIS	-	expression tag	UNP A7LAI8
M	1	MET	-	expression tag	UNP A7LAI8
M	?	-	ASP	deletion	UNP A7LAI8
M	?	-	VAL	deletion	UNP A7LAI8
M	?	-	TYR	deletion	UNP A7LAI8
M	?	-	ALA	deletion	UNP A7LAI8
M	?	-	PHE	deletion	UNP A7LAI8
M	?	-	PRO	deletion	UNP A7LAI8
M	?	-	TYR	deletion	UNP A7LAI8
M	?	-	TYR	deletion	UNP A7LAI8
M	?	-	TYR	deletion	UNP A7LAI8
M	?	-	VAL	deletion	UNP A7LAI8
M	?	-	TYR	deletion	UNP A7LAI8
N	-19	MET	-	expression tag	UNP A7LAI8
N	-18	ARG	-	expression tag	UNP A7LAI8
N	-17	SER	-	expression tag	UNP A7LAI8
N	-16	SER	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-15	HIS	-	expression tag	UNP A7LAI8
N	-14	HIS	-	expression tag	UNP A7LAI8
N	-13	HIS	-	expression tag	UNP A7LAI8
N	-12	HIS	-	expression tag	UNP A7LAI8
N	-11	HIS	-	expression tag	UNP A7LAI8
N	-10	HIS	-	expression tag	UNP A7LAI8
N	-9	SER	-	expression tag	UNP A7LAI8
N	-8	SER	-	expression tag	UNP A7LAI8
N	-7	GLY	-	expression tag	UNP A7LAI8
N	-6	LEU	-	expression tag	UNP A7LAI8
N	-5	VAL	-	expression tag	UNP A7LAI8
N	-4	PRO	-	expression tag	UNP A7LAI8
N	-3	ARG	-	expression tag	UNP A7LAI8
N	-2	GLY	-	expression tag	UNP A7LAI8
N	-1	SER	-	expression tag	UNP A7LAI8
N	0	HIS	-	expression tag	UNP A7LAI8
N	1	MET	-	expression tag	UNP A7LAI8
N	?	-	ASP	deletion	UNP A7LAI8
N	?	-	VAL	deletion	UNP A7LAI8
N	?	-	TYR	deletion	UNP A7LAI8
N	?	-	ALA	deletion	UNP A7LAI8
N	?	-	PHE	deletion	UNP A7LAI8
N	?	-	PRO	deletion	UNP A7LAI8
N	?	-	TYR	deletion	UNP A7LAI8
N	?	-	TYR	deletion	UNP A7LAI8
N	?	-	TYR	deletion	UNP A7LAI8
N	?	-	VAL	deletion	UNP A7LAI8
N	?	-	TYR	deletion	UNP A7LAI8
O	-19	MET	-	expression tag	UNP A7LAI8
O	-18	ARG	-	expression tag	UNP A7LAI8
O	-17	SER	-	expression tag	UNP A7LAI8
O	-16	SER	-	expression tag	UNP A7LAI8
O	-15	HIS	-	expression tag	UNP A7LAI8
O	-14	HIS	-	expression tag	UNP A7LAI8
O	-13	HIS	-	expression tag	UNP A7LAI8
O	-12	HIS	-	expression tag	UNP A7LAI8
O	-11	HIS	-	expression tag	UNP A7LAI8
O	-10	HIS	-	expression tag	UNP A7LAI8
O	-9	SER	-	expression tag	UNP A7LAI8
O	-8	SER	-	expression tag	UNP A7LAI8
O	-7	GLY	-	expression tag	UNP A7LAI8
O	-6	LEU	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	VAL	-	expression tag	UNP A7LAI8
O	-4	PRO	-	expression tag	UNP A7LAI8
O	-3	ARG	-	expression tag	UNP A7LAI8
O	-2	GLY	-	expression tag	UNP A7LAI8
O	-1	SER	-	expression tag	UNP A7LAI8
O	0	HIS	-	expression tag	UNP A7LAI8
O	1	MET	-	expression tag	UNP A7LAI8
O	?	-	ASP	deletion	UNP A7LAI8
O	?	-	VAL	deletion	UNP A7LAI8
O	?	-	TYR	deletion	UNP A7LAI8
O	?	-	ALA	deletion	UNP A7LAI8
O	?	-	PHE	deletion	UNP A7LAI8
O	?	-	PRO	deletion	UNP A7LAI8
O	?	-	TYR	deletion	UNP A7LAI8
O	?	-	TYR	deletion	UNP A7LAI8
O	?	-	TYR	deletion	UNP A7LAI8
O	?	-	TYR	deletion	UNP A7LAI8
O	?	-	VAL	deletion	UNP A7LAI8
O	?	-	TYR	deletion	UNP A7LAI8
P	-19	MET	-	expression tag	UNP A7LAI8
P	-18	ARG	-	expression tag	UNP A7LAI8
P	-17	SER	-	expression tag	UNP A7LAI8
P	-16	SER	-	expression tag	UNP A7LAI8
P	-15	HIS	-	expression tag	UNP A7LAI8
P	-14	HIS	-	expression tag	UNP A7LAI8
P	-13	HIS	-	expression tag	UNP A7LAI8
P	-12	HIS	-	expression tag	UNP A7LAI8
P	-11	HIS	-	expression tag	UNP A7LAI8
P	-10	HIS	-	expression tag	UNP A7LAI8
P	-9	SER	-	expression tag	UNP A7LAI8
P	-8	SER	-	expression tag	UNP A7LAI8
P	-7	GLY	-	expression tag	UNP A7LAI8
P	-6	LEU	-	expression tag	UNP A7LAI8
P	-5	VAL	-	expression tag	UNP A7LAI8
P	-4	PRO	-	expression tag	UNP A7LAI8
P	-3	ARG	-	expression tag	UNP A7LAI8
P	-2	GLY	-	expression tag	UNP A7LAI8
P	-1	SER	-	expression tag	UNP A7LAI8
P	0	HIS	-	expression tag	UNP A7LAI8
P	1	MET	-	expression tag	UNP A7LAI8
P	?	-	ASP	deletion	UNP A7LAI8
P	?	-	VAL	deletion	UNP A7LAI8
P	?	-	TYR	deletion	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
P	?	-	ALA	deletion	UNP A7LAI8
P	?	-	PHE	deletion	UNP A7LAI8
P	?	-	PRO	deletion	UNP A7LAI8
P	?	-	TYR	deletion	UNP A7LAI8
P	?	-	TYR	deletion	UNP A7LAI8
P	?	-	TYR	deletion	UNP A7LAI8
P	?	-	VAL	deletion	UNP A7LAI8
P	?	-	TYR	deletion	UNP A7LAI8

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0

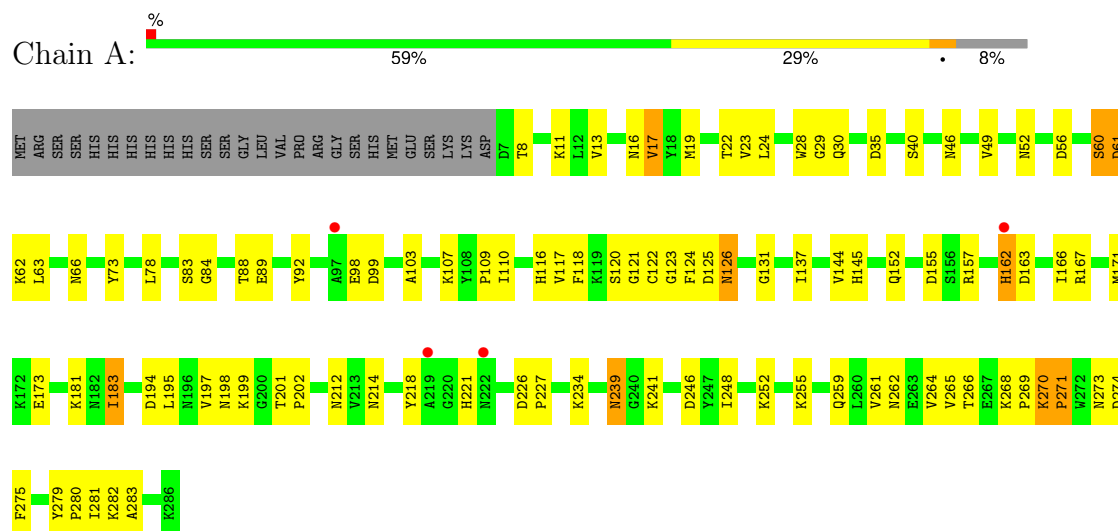
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Na 1 1	0	0

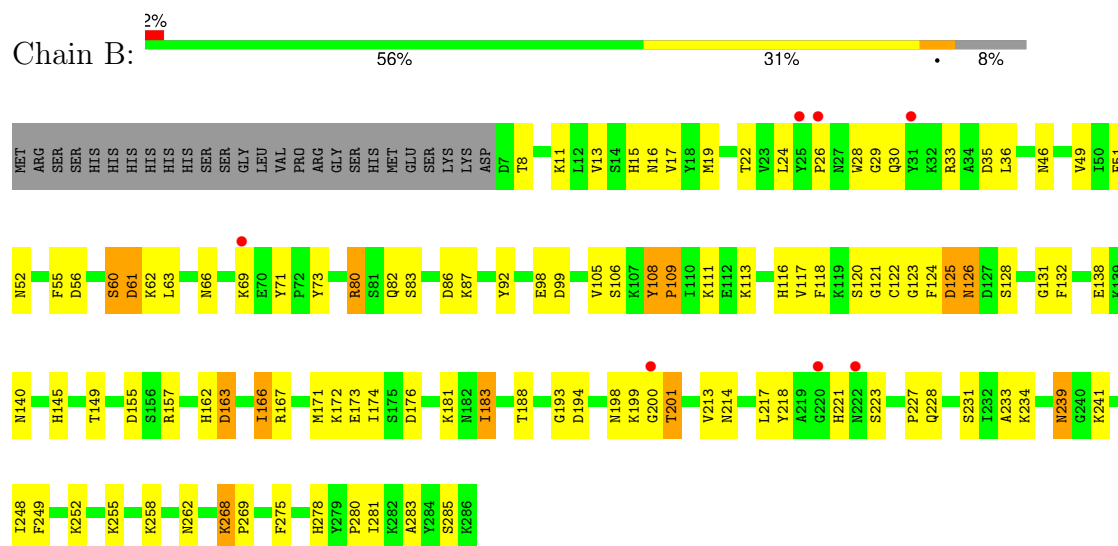
3 Residue-property plots [i](#)

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.

• Molecule 1: Beta-hemolysin

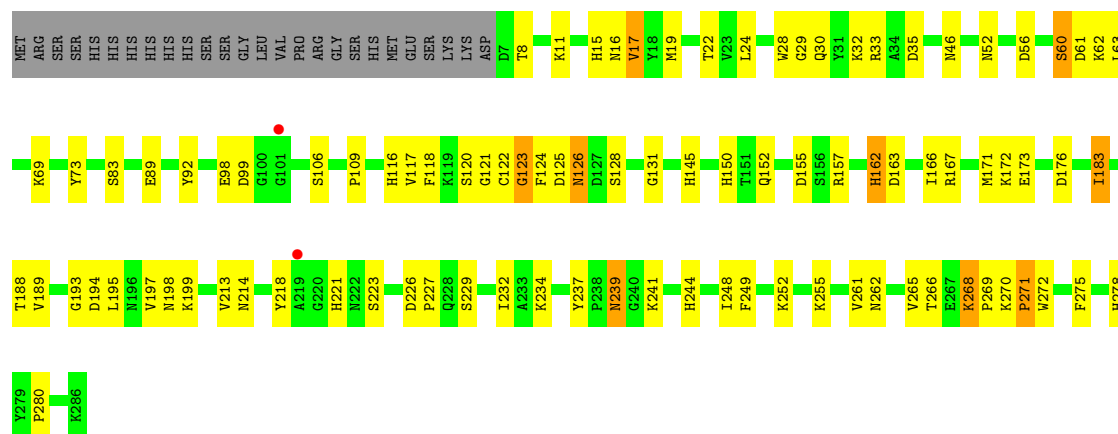


• Molecule 1: Beta-hemolysin

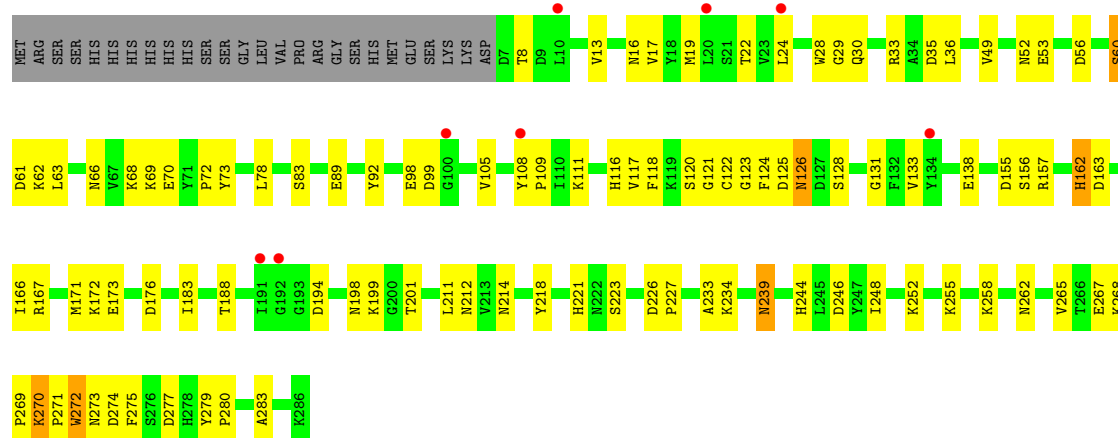


• Molecule 1: Beta-hemolysin

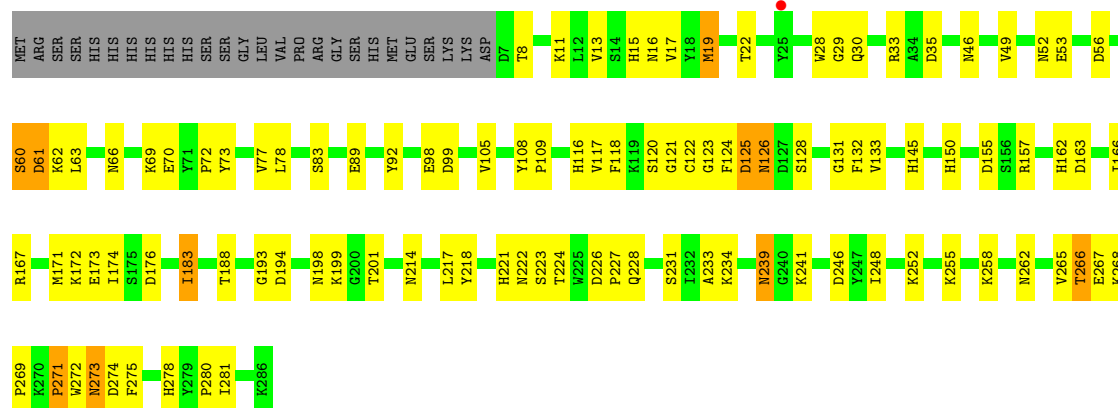




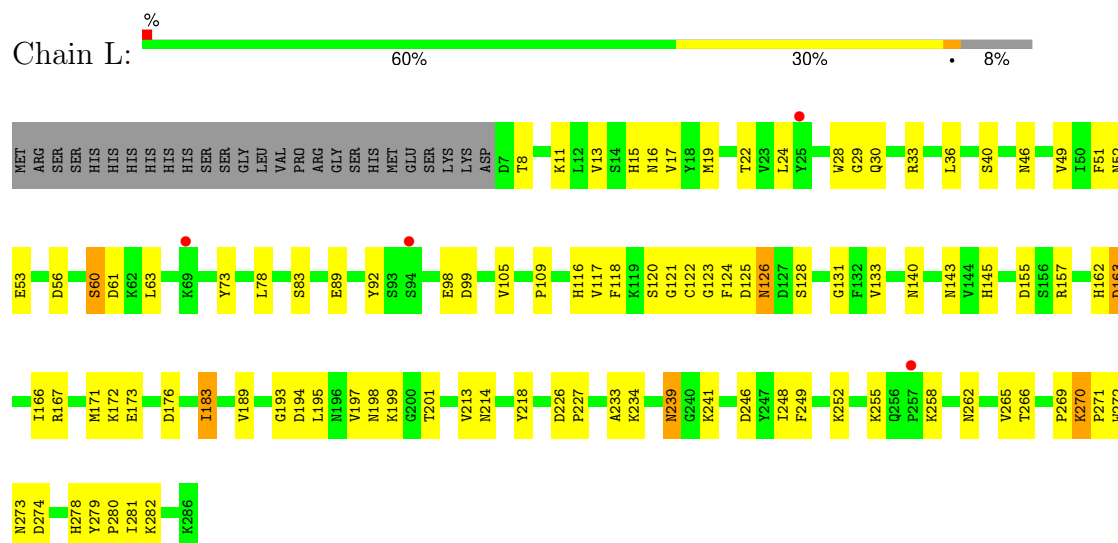
• Molecule 1: Beta-hemolysin



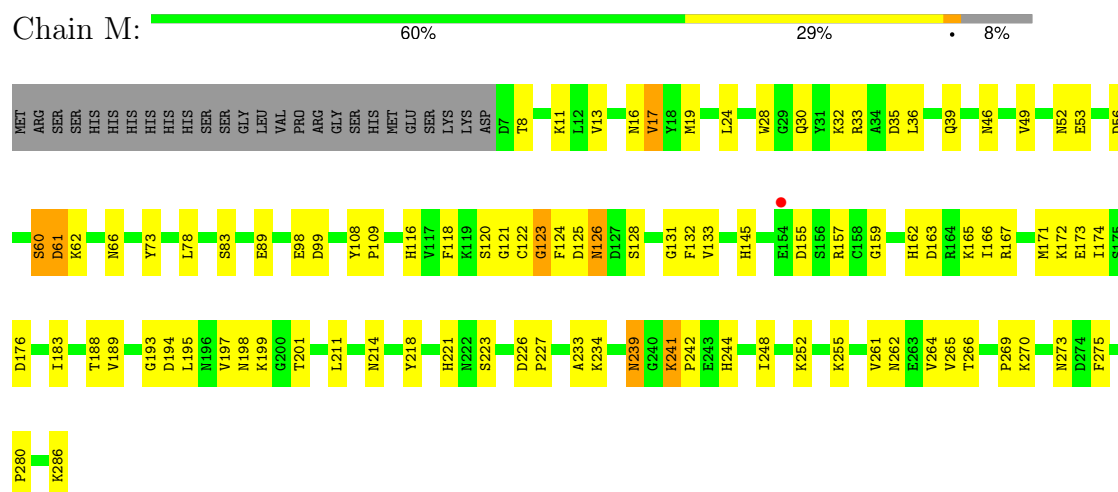
• Molecule 1: Beta-hemolysin



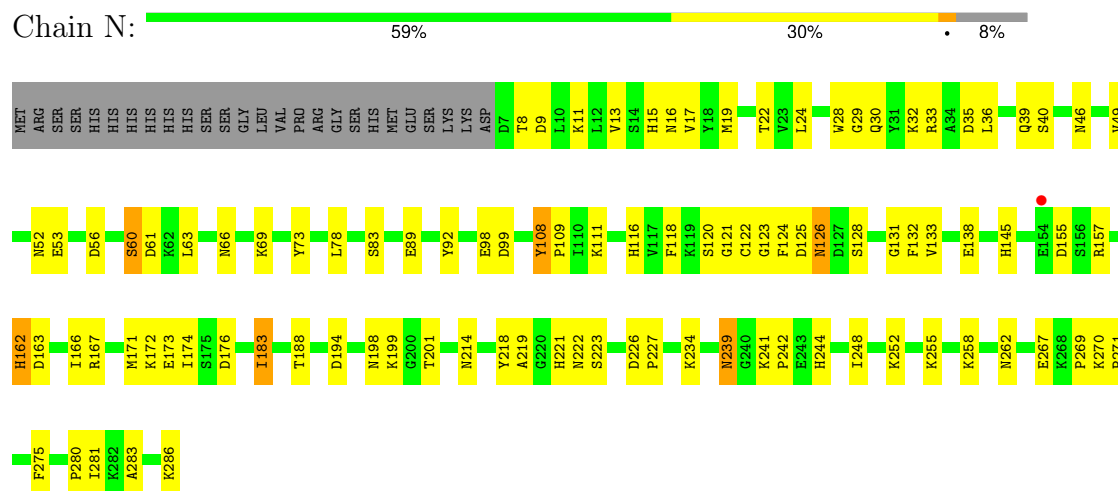
• Molecule 1: Beta-hemolysin



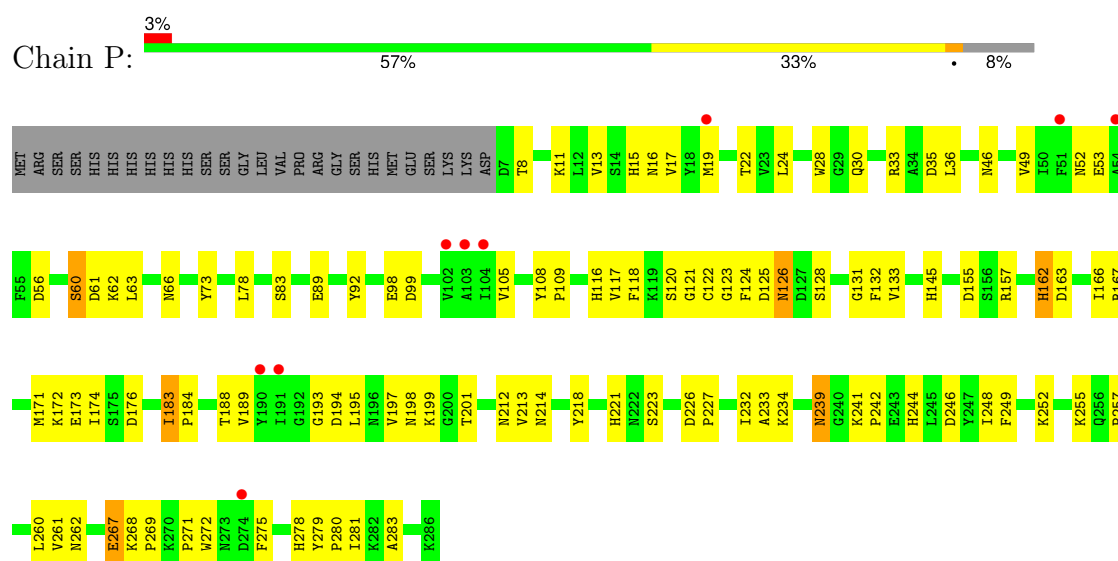
• Molecule 1: Beta-hemolysin



• Molecule 1: Beta-hemolysin



• Molecule 1: Beta-hemolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.38Å 134.47Å 156.99Å 90.00° 116.89° 90.00°	Depositor
Resolution (Å)	31.31 – 3.35 31.31 – 3.35	Depositor EDS
% Data completeness (in resolution range)	95.5 (31.31-3.35) 95.5 (31.31-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.241 , 0.281 0.241 , 0.279	Depositor DCC
R_{free} test set	4182 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	35844	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA

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	1.01	2/2294 (0.1%)	1.16	11/3100 (0.4%)
1	B	1.01	0/2294	1.17	15/3100 (0.5%)
1	C	0.91	0/2294	1.09	4/3100 (0.1%)
1	D	0.88	0/2294	1.09	6/3100 (0.2%)
1	E	0.67	0/2294	0.97	7/3100 (0.2%)
1	F	0.61	0/2294	0.90	1/3100 (0.0%)
1	G	0.65	0/2294	0.94	6/3100 (0.2%)
1	H	0.63	0/2294	0.91	1/3100 (0.0%)
1	I	0.70	0/2294	0.98	9/3100 (0.3%)
1	J	0.61	0/2294	0.92	2/3100 (0.1%)
1	K	0.73	0/2294	1.04	8/3100 (0.3%)
1	L	0.62	1/2294 (0.0%)	0.93	5/3100 (0.2%)
1	M	0.64	0/2294	0.94	7/3100 (0.2%)
1	N	0.57	0/2294	0.92	2/3100 (0.1%)
1	O	0.51	0/2294	0.86	1/3100 (0.0%)
1	P	0.43	0/2294	0.85	2/3100 (0.1%)
All	All	0.72	3/36704 (0.0%)	0.98	87/49600 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	265	VAL	CA-CB	-5.95	1.47	1.54
1	A	137	ILE	CA-CB	-5.33	1.47	1.54
1	A	103	ALA	CA-CB	-5.29	1.44	1.53

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	33	ARG	NE-CZ-NH2	14.40	132.16	119.20
1	K	33	ARG	NE-CZ-NH1	-11.92	109.58	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	LYS	CA-C-N	10.27	130.92	119.83
1	A	268	LYS	C-N-CA	10.27	130.92	119.83
1	K	33	ARG	CD-NE-CZ	10.07	138.50	124.40

There are no chirality outliers.

There are no planarity outliers.

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	2240	0	2169	78	1
1	B	2240	0	2169	107	3
1	C	2240	0	2169	112	0
1	D	2240	0	2169	132	2
1	E	2240	0	2169	94	2
1	F	2240	0	2169	79	0
1	G	2240	0	2169	77	2
1	H	2240	0	2169	83	0
1	I	2240	0	2169	83	0
1	J	2240	0	2169	152	0
1	K	2240	0	2169	114	0
1	L	2240	0	2169	89	1
1	M	2240	0	2169	73	1
1	N	2240	0	2169	76	0
1	O	2240	0	2169	115	0
1	P	2240	0	2169	94	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	L	1	0	0	0	0
3	C	1	0	0	0	0
All	All	35844	0	34704	1283	6

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 18.

The worst 5 of 1283 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:K:272:TRP:CH2	1:L:28:TRP:HA	1.31	1.62
1:J:68:LYS:CE	1:O:83:SER:HA	1.54	1.38
1:K:272:TRP:CH2	1:L:28:TRP:CA	2.06	1.35
1:K:272:TRP:CZ2	1:L:28:TRP:C	2.18	1.22
1:D:284:TYR:HD2	1:J:157:ARG:NH2	1.40	1.20

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ASP:OD1	1:G:92:TYR:OH[2_645]	1.84	0.36
1:B:92:TYR:OH	1:D:61:ASP:OD2[2_555]	1.86	0.34
1:E:92:TYR:OH	1:G:61:ASP:OD2[2_645]	2.05	0.15
1:A:89:GLU:OE1	1:B:87:LYS:NZ[2_545]	2.09	0.11
1:B:61:ASP:OD1	1:D:82:GLN:N[2_555]	2.10	0.10

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	278/306 (91%)	261 (94%)	15 (5%)	2 (1%)	18	46
1	B	278/306 (91%)	260 (94%)	17 (6%)	1 (0%)	30	58
1	C	278/306 (91%)	257 (92%)	18 (6%)	3 (1%)	11	36
1	D	278/306 (91%)	259 (93%)	19 (7%)	0	100	100
1	E	278/306 (91%)	255 (92%)	23 (8%)	0	100	100
1	F	278/306 (91%)	258 (93%)	20 (7%)	0	100	100
1	G	278/306 (91%)	259 (93%)	19 (7%)	0	100	100
1	H	278/306 (91%)	256 (92%)	21 (8%)	1 (0%)	30	58
1	I	278/306 (91%)	257 (92%)	19 (7%)	2 (1%)	18	46
1	J	278/306 (91%)	256 (92%)	21 (8%)	1 (0%)	30	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	278/306 (91%)	256 (92%)	21 (8%)	1 (0%)	30	58
1	L	278/306 (91%)	259 (93%)	18 (6%)	1 (0%)	30	58
1	M	278/306 (91%)	259 (93%)	18 (6%)	1 (0%)	30	58
1	N	278/306 (91%)	257 (92%)	21 (8%)	0	100	100
1	O	278/306 (91%)	258 (93%)	19 (7%)	1 (0%)	30	58
1	P	278/306 (91%)	257 (92%)	21 (8%)	0	100	100
All	All	4448/4896 (91%)	4124 (93%)	310 (7%)	14 (0%)	36	63

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	270	LYS
1	K	271	PRO
1	C	271	PRO
1	C	40	SER
1	I	271	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	250/274 (91%)	239 (96%)	11 (4%)	25	51
1	B	250/274 (91%)	239 (96%)	11 (4%)	25	51
1	C	250/274 (91%)	243 (97%)	7 (3%)	38	60
1	D	250/274 (91%)	240 (96%)	10 (4%)	28	53
1	E	250/274 (91%)	239 (96%)	11 (4%)	25	51
1	F	250/274 (91%)	241 (96%)	9 (4%)	31	56
1	G	250/274 (91%)	241 (96%)	9 (4%)	31	56
1	H	250/274 (91%)	242 (97%)	8 (3%)	34	58
1	I	250/274 (91%)	242 (97%)	8 (3%)	34	58
1	J	250/274 (91%)	242 (97%)	8 (3%)	34	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	250/274 (91%)	239 (96%)	11 (4%)	25	51
1	L	250/274 (91%)	239 (96%)	11 (4%)	25	51
1	M	250/274 (91%)	243 (97%)	7 (3%)	38	60
1	N	250/274 (91%)	241 (96%)	9 (4%)	31	56
1	O	250/274 (91%)	242 (97%)	8 (3%)	34	58
1	P	250/274 (91%)	241 (96%)	9 (4%)	31	56
All	All	4000/4384 (91%)	3853 (96%)	147 (4%)	30	55

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	61	ASP
1	P	162	HIS
1	M	239	ASN
1	O	60	SER
1	E	239	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 185 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	221	HIS
1	M	74	GLN
1	K	74	GLN
1	L	52	ASN
1	M	262	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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	280/306 (91%)	0.00	4 (1%) 73 59	23, 55, 104, 194	6 (2%)
1	B	280/306 (91%)	0.01	7 (2%) 58 43	28, 54, 121, 196	5 (1%)
1	C	280/306 (91%)	0.10	8 (2%) 53 39	30, 64, 118, 193	4 (1%)
1	D	280/306 (91%)	0.02	2 (0%) 84 73	33, 66, 135, 234	3 (1%)
1	E	280/306 (91%)	0.08	2 (0%) 84 73	47, 93, 146, 213	6 (2%)
1	F	280/306 (91%)	0.12	5 (1%) 67 51	29, 107, 165, 221	5 (1%)
1	G	280/306 (91%)	0.09	0 100 100	58, 100, 166, 232	5 (1%)
1	H	280/306 (91%)	0.16	6 (2%) 63 47	64, 108, 191, 245	5 (1%)
1	I	280/306 (91%)	0.04	2 (0%) 84 73	39, 96, 169, 224	5 (1%)
1	J	280/306 (91%)	0.51	8 (2%) 53 39	45, 130, 205, 260	4 (1%)
1	K	280/306 (91%)	0.07	1 (0%) 88 81	40, 91, 147, 214	5 (1%)
1	L	280/306 (91%)	0.12	4 (1%) 73 59	44, 117, 196, 267	6 (2%)
1	M	280/306 (91%)	0.16	1 (0%) 88 81	66, 111, 171, 222	4 (1%)
1	N	280/306 (91%)	0.09	1 (0%) 88 81	28, 115, 165, 232	3 (1%)
1	O	280/306 (91%)	0.28	4 (1%) 73 59	43, 157, 228, 279	5 (1%)
1	P	280/306 (91%)	0.48	9 (3%) 50 36	88, 216, 285, 318	6 (2%)
All	All	4480/4896 (91%)	0.14	64 (1%) 73 59	23, 100, 209, 318	77 (1%)

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	129	ASN	7.0
1	P	54	ALA	4.4
1	D	69	LYS	4.1
1	N	154	GLU	4.1
1	P	191	ILE	3.5

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 oligosaccharides 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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	C	287	1/1	0.89	0.24	38,38,38,38	0
2	CL	D	287	1/1	0.91	0.10	56,56,56,56	0
2	CL	B	287	1/1	0.94	0.17	57,57,57,57	0
2	CL	L	287	1/1	0.95	0.11	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.