wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:10 AM GMT

PDB ID	:	3O44
Title	:	Crystal Structure of the Vibrio cholerae Cytolysin (HlyA) Heptameric Pore
Authors	:	De, S.; Olson, R.
Deposited on	:	2010-07-26
Resolution	:	2.88 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

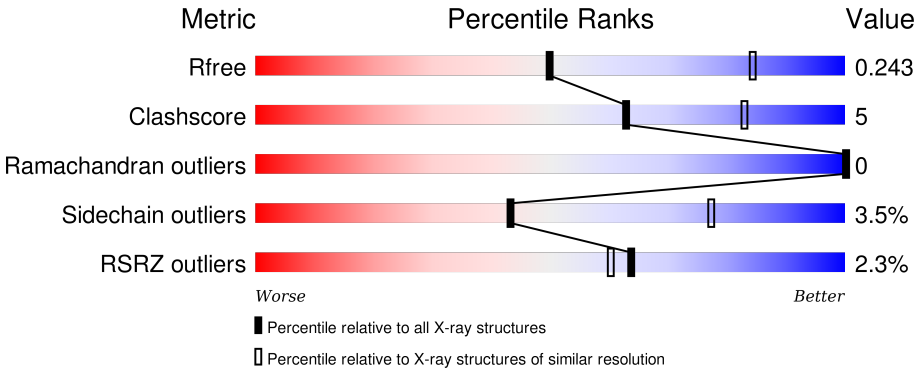
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.88 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}	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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 <=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	593	83% 14%
1	B	593	85% 12%
1	C	593	86% 11%
1	D	593	84% 13%
1	E	593	85% 12%

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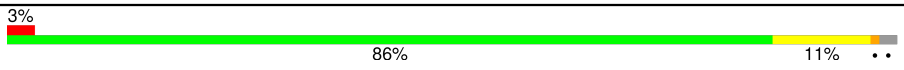
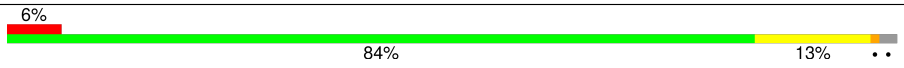
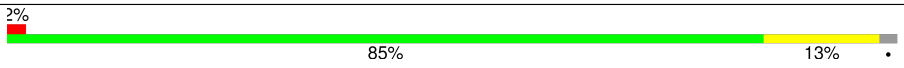
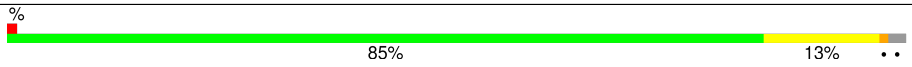
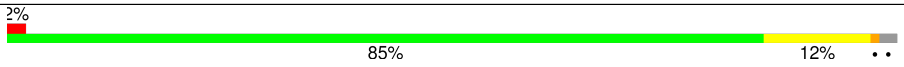
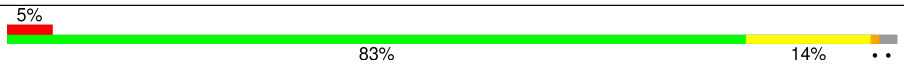
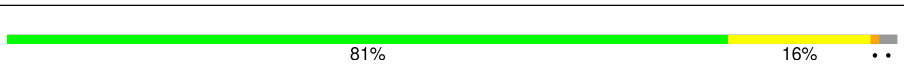
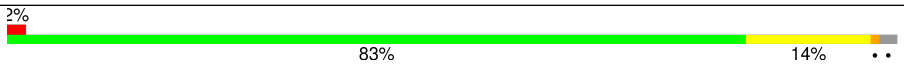
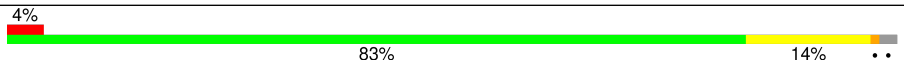
Mol	Chain	Length	Quality of chain
1	F	593	
1	G	593	
1	H	593	
1	I	593	
1	J	593	
1	K	593	
1	L	593	
1	M	593	
1	N	593	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 62948 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 Hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4464	2784	779	892	9			
1	B	581	Total	C	N	O	S	0	0	0
			4457	2783	778	887	9			
1	C	581	Total	C	N	O	S	0	0	0
			4431	2759	776	887	9			
1	D	581	Total	C	N	O	S	0	0	0
			4471	2794	778	890	9			
1	E	581	Total	C	N	O	S	0	0	0
			4460	2784	777	890	9			
1	F	581	Total	C	N	O	S	0	0	0
			4412	2746	768	889	9			
1	G	581	Total	C	N	O	S	0	0	0
			4436	2764	777	886	9			
1	H	581	Total	C	N	O	S	0	0	0
			4468	2791	774	894	9			
1	I	581	Total	C	N	O	S	0	0	0
			4479	2797	780	893	9			
1	J	581	Total	C	N	O	S	0	0	0
			4487	2804	782	892	9			
1	K	581	Total	C	N	O	S	0	0	0
			4417	2755	772	881	9			
1	L	581	Total	C	N	O	S	0	0	0
			4449	2773	779	888	9			
1	M	581	Total	C	N	O	S	0	0	0
			4447	2773	777	888	9			
1	N	581	Total	C	N	O	S	0	0	0
			4420	2759	769	883	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	606	ASN	HIS	CONFLICT	UNP C2C744

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Chain	Residue	Modelled	Actual	Comment	Reference
B	606	ASN	HIS	CONFLICT	UNP C2C744
C	606	ASN	HIS	CONFLICT	UNP C2C744
D	606	ASN	HIS	CONFLICT	UNP C2C744
E	606	ASN	HIS	CONFLICT	UNP C2C744
F	606	ASN	HIS	CONFLICT	UNP C2C744
G	606	ASN	HIS	CONFLICT	UNP C2C744
H	606	ASN	HIS	CONFLICT	UNP C2C744
I	606	ASN	HIS	CONFLICT	UNP C2C744
J	606	ASN	HIS	CONFLICT	UNP C2C744
K	606	ASN	HIS	CONFLICT	UNP C2C744
L	606	ASN	HIS	CONFLICT	UNP C2C744
M	606	ASN	HIS	CONFLICT	UNP C2C744
N	606	ASN	HIS	CONFLICT	UNP C2C744

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	58	Total O 58 58	0	0
2	B	62	Total O 62 62	0	0
2	C	57	Total O 57 57	0	0
2	D	65	Total O 65 65	0	0
2	E	44	Total O 44 44	0	0
2	F	26	Total O 26 26	0	0
2	G	50	Total O 50 50	0	0
2	H	48	Total O 48 48	0	0
2	I	61	Total O 61 61	0	0
2	J	32	Total O 32 32	0	0
2	K	25	Total O 25 25	0	0
2	L	43	Total O 43 43	0	0
2	M	43	Total O 43 43	0	0

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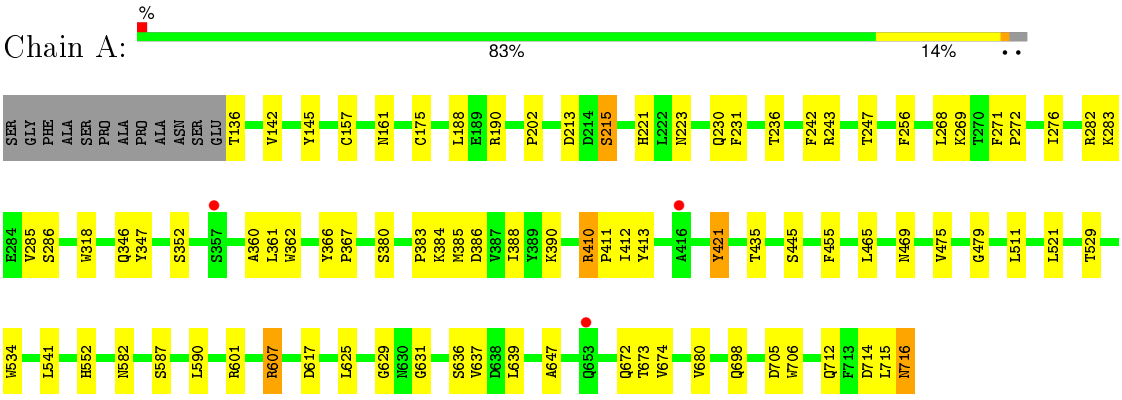
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	36	Total	O	0	0
			36	36		

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.

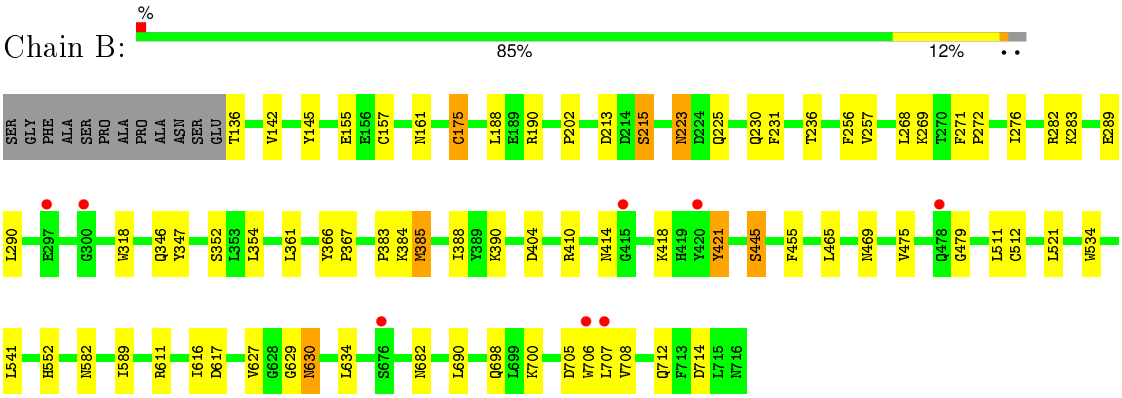
- Molecule 1: Hemolysin

Chain A:



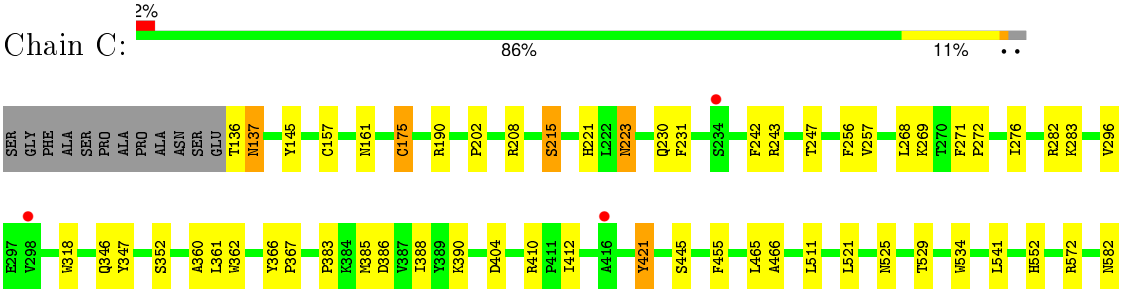
- Molecule 1: Hemolysin

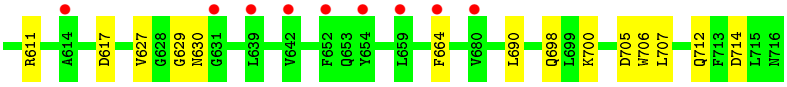
Chain B:



- Molecule 1: Hemolysin

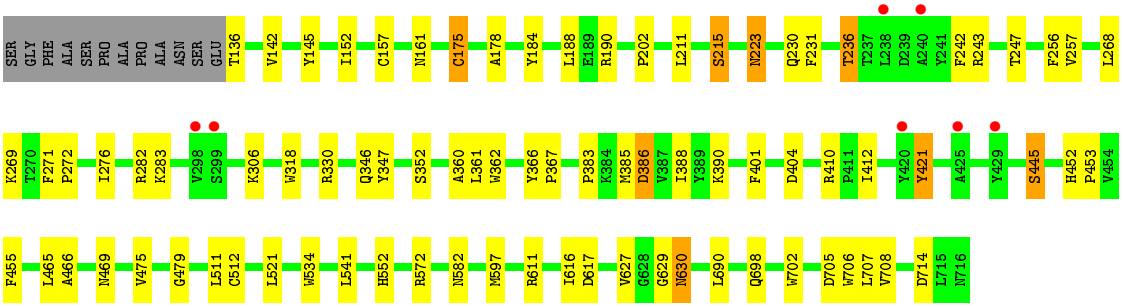
Chain C:





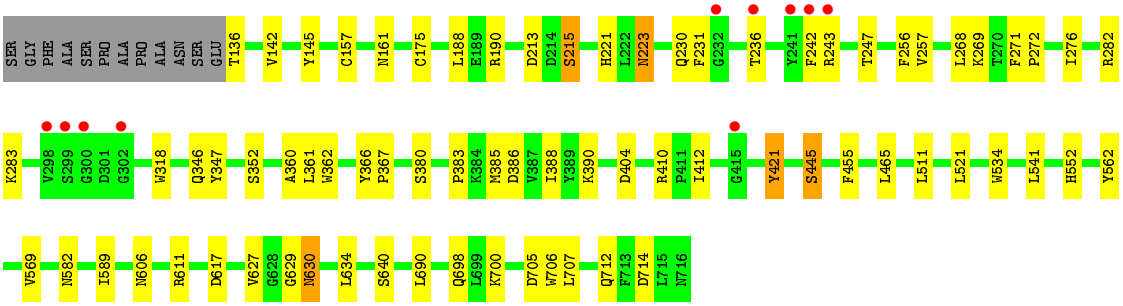
• Molecule 1: Hemolysin

Chain D:



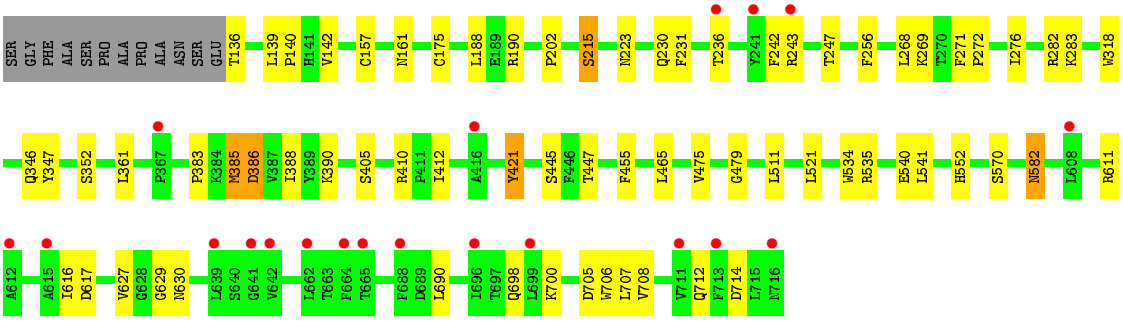
• Molecule 1: Hemolysin

Chain E:



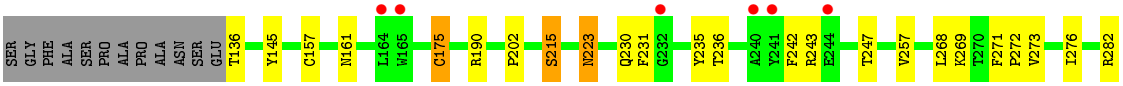
• Molecule 1: Hemolysin

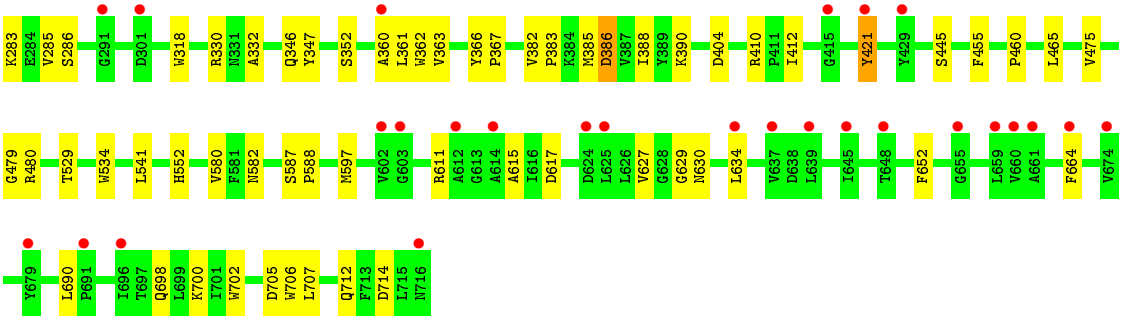
Chain F:



• Molecule 1: Hemolysin

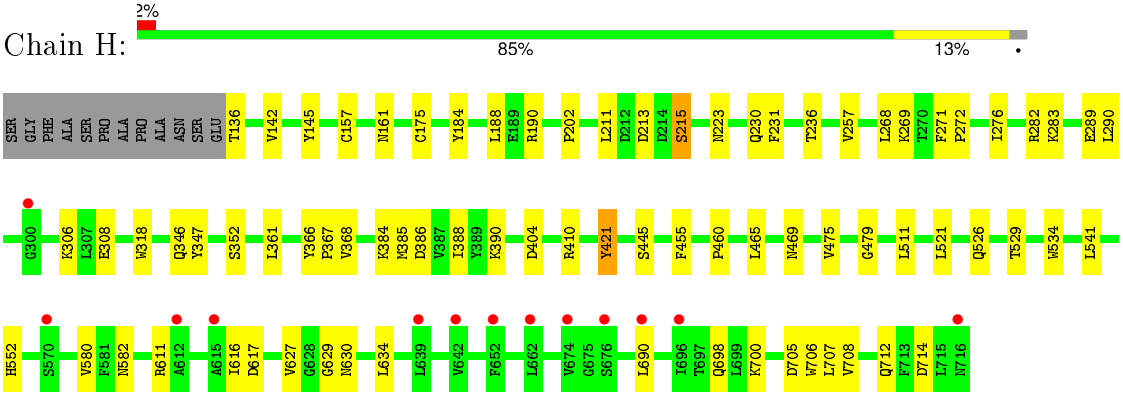
Chain G:





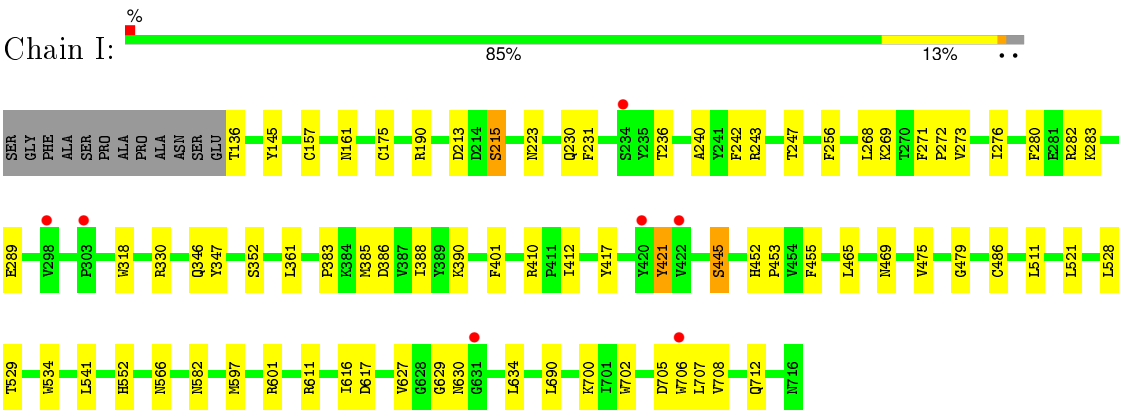
• Molecule 1: Hemolysin

Chain H:



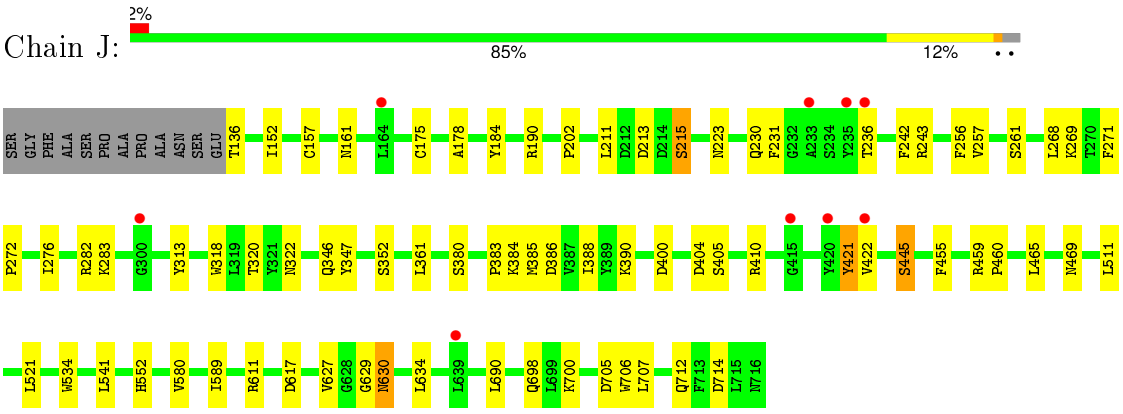
• Molecule 1: Hemolysin

Chain I:



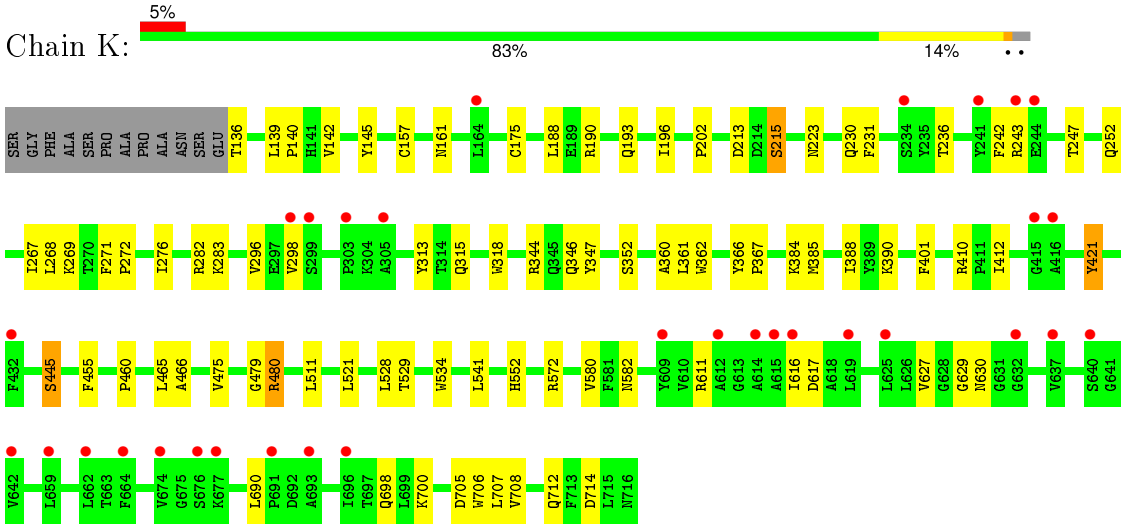
• Molecule 1: Hemolysin

Chain J:



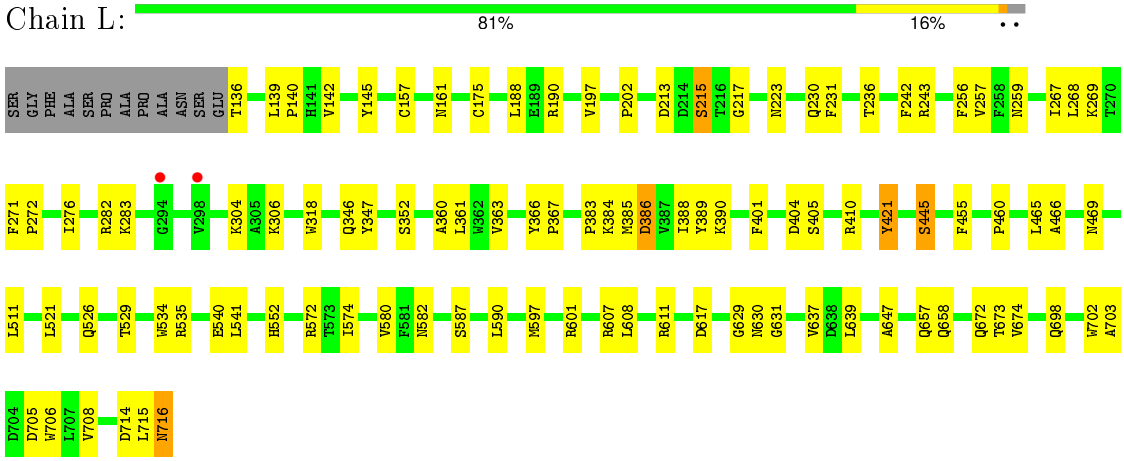
• Molecule 1: Hemolysin

Chain K:



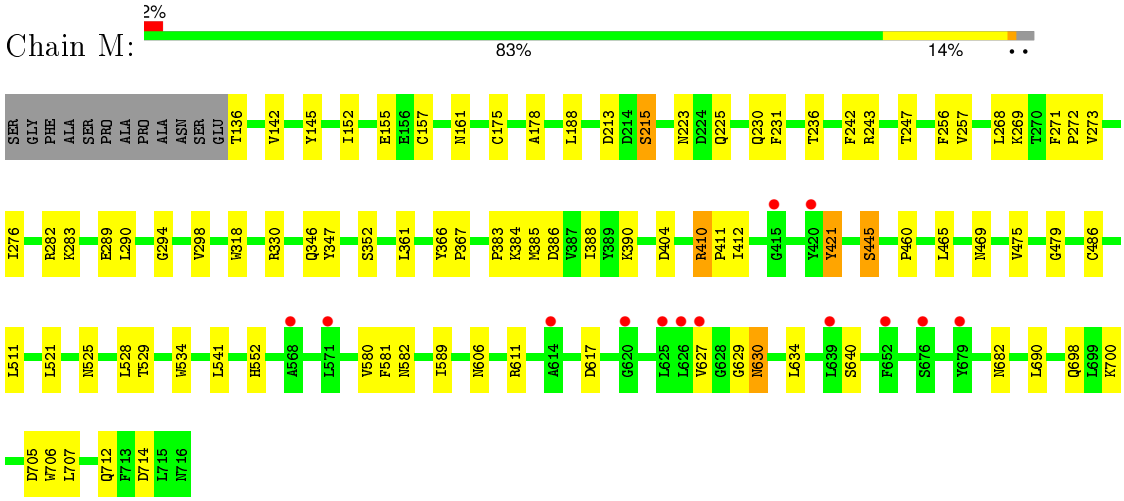
• Molecule 1: Hemolysin

Chain L:

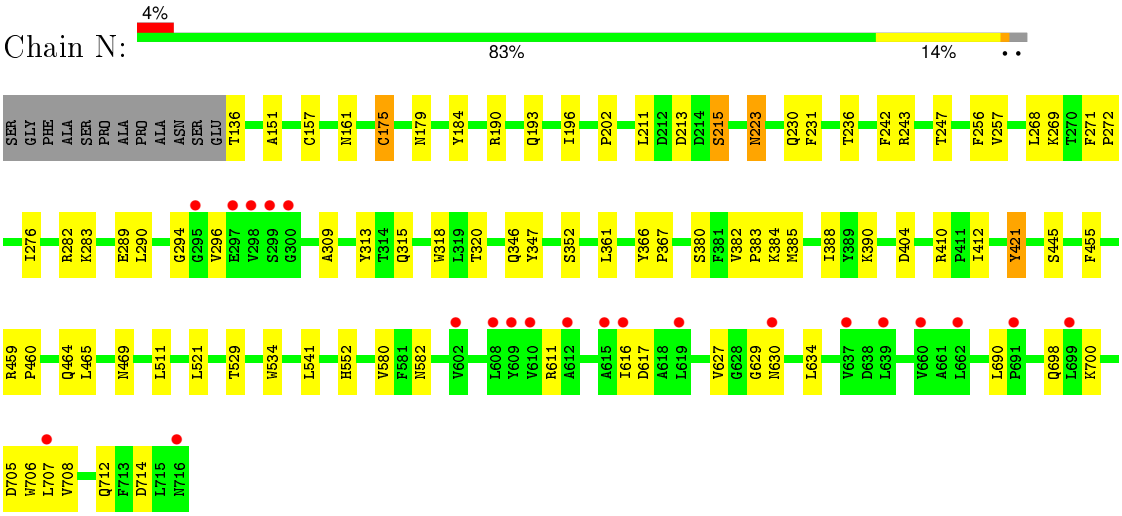


• Molecule 1: Hemolysin

Chain M:



• Molecule 1: Hemolysin


Chain N:
4%
83%
14%
SER GLY PHE ALA SER PRO ALA PRO ALA ASN SER GLU T136 A151 C157 N161 C175 N179 Y184 R190 Q193 I196 P202 L211 D212 D213 D214 S215 N223 Q230 F231 T236 F242 R243 T247 F256 V257 L268 K269 T270 F271 P272
I276 R282 K283 E289 L290 G294 G295 V296 E297 V298 S299 G300 A309 Y313 T314 Q315 W318 L319 T320 Q346 Y347 S352 L361 Y366 P367 S380 F381 V382 P383 K384 M385 I388 Y389 K390 D404 R410 P411 I412 Y421 S445 F455
R459 P460 Q464 L465 N469 L511 L521 T529 W534 L541 H552 V580 F581 N582 V602 L608 Y609 V610 R611 A612 A615 I616 D617 A618 L619 V627 G628 G629 N630 L634 V637 D638 L639 V660 A661 L662 L690 P691 Q698 L699 K700
D705 W706 L707 V708 Q712 F713 D714 L715 N716

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	172.35Å 182.86Å 430.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.96 – 2.88 86.18 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.8 (43.96-2.88) 98.4 (86.18-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.218 , 0.249 0.212 , 0.243	Depositor DCC
R_{free} test set	15094 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 299067 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	62948	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.44	0/4557	0.57	0/6204
1	B	0.43	0/4551	0.56	0/6198
1	C	0.44	0/4523	0.55	0/6164
1	D	0.45	0/4567	0.56	0/6221
1	E	0.43	0/4555	0.55	0/6205
1	F	0.42	0/4503	0.56	0/6139
1	G	0.45	0/4528	0.56	0/6168
1	H	0.40	0/4564	0.55	0/6219
1	I	0.44	0/4575	0.56	0/6233
1	J	0.42	0/4583	0.55	0/6240
1	K	0.43	0/4509	0.56	0/6146
1	L	0.43	0/4541	0.58	0/6183
1	M	0.43	0/4539	0.57	0/6183
1	N	0.42	0/4513	0.56	0/6153
All	All	0.43	0/63608	0.56	0/86656

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

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	4464	0	4169	57	0
1	B	4457	0	4163	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4431	0	4100	50	0
1	D	4471	0	4172	57	1
1	E	4460	0	4146	46	0
1	F	4412	0	4065	47	0
1	G	4436	0	4120	55	1
1	H	4468	0	4156	51	0
1	I	4479	0	4178	55	0
1	J	4487	0	4205	50	0
1	K	4417	0	4093	58	0
1	L	4449	0	4145	67	0
1	M	4447	0	4147	61	0
1	N	4420	0	4094	61	0
2	A	58	0	0	1	0
2	B	62	0	0	1	0
2	C	57	0	0	1	0
2	D	65	0	0	2	0
2	E	44	0	0	0	0
2	F	26	0	0	2	0
2	G	50	0	0	0	0
2	H	48	0	0	0	0
2	I	61	0	0	1	0
2	J	32	0	0	0	0
2	K	25	0	0	0	0
2	L	43	0	0	1	0
2	M	43	0	0	2	0
2	N	36	0	0	1	0
All	All	62948	0	57953	639	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 5.

The worst 5 of 639 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:C:283:LYS:HB2	1:C:318:TRP:HB2	1.36	1.04
1:K:480:ARG:HH11	1:K:480:ARG:HB3	1.22	1.02
1:N:283:LYS:HB2	1:N:318:TRP:HB2	1.41	1.02
1:F:283:LYS:HB2	1:F:318:TRP:HB2	1.43	1.01
1:K:283:LYS:HB2	1:K:318:TRP:HB2	1.42	1.01

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)
1:D:236:THR:OG1	1:G:235:TYR:CE2[4_456]	1.90	0.30

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	579/593 (98%)	557 (96%)	22 (4%)	0	100	100
1	B	579/593 (98%)	556 (96%)	23 (4%)	0	100	100
1	C	579/593 (98%)	554 (96%)	25 (4%)	0	100	100
1	D	579/593 (98%)	556 (96%)	23 (4%)	0	100	100
1	E	579/593 (98%)	553 (96%)	26 (4%)	0	100	100
1	F	579/593 (98%)	555 (96%)	24 (4%)	0	100	100
1	G	579/593 (98%)	556 (96%)	23 (4%)	0	100	100
1	H	579/593 (98%)	555 (96%)	24 (4%)	0	100	100
1	I	579/593 (98%)	552 (95%)	27 (5%)	0	100	100
1	J	579/593 (98%)	554 (96%)	25 (4%)	0	100	100
1	K	579/593 (98%)	553 (96%)	26 (4%)	0	100	100
1	L	579/593 (98%)	555 (96%)	24 (4%)	0	100	100
1	M	579/593 (98%)	554 (96%)	25 (4%)	0	100	100
1	N	579/593 (98%)	559 (96%)	20 (4%)	0	100	100
All	All	8106/8302 (98%)	7769 (96%)	337 (4%)	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	464/495 (94%)	446 (96%)	18 (4%)	39	74
1	B	462/495 (93%)	446 (96%)	16 (4%)	43	77
1	C	456/495 (92%)	440 (96%)	16 (4%)	43	77
1	D	464/495 (94%)	448 (97%)	16 (3%)	44	78
1	E	461/495 (93%)	445 (96%)	16 (4%)	43	77
1	F	453/495 (92%)	436 (96%)	17 (4%)	40	75
1	G	457/495 (92%)	440 (96%)	17 (4%)	41	75
1	H	464/495 (94%)	450 (97%)	14 (3%)	48	81
1	I	466/495 (94%)	451 (97%)	15 (3%)	46	80
1	J	468/495 (94%)	451 (96%)	17 (4%)	42	76
1	K	453/495 (92%)	437 (96%)	16 (4%)	43	77
1	L	460/495 (93%)	442 (96%)	18 (4%)	39	74
1	M	461/495 (93%)	444 (96%)	17 (4%)	41	75
1	N	454/495 (92%)	440 (97%)	14 (3%)	47	80
All	All	6443/6930 (93%)	6216 (96%)	227 (4%)	43	77

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	215	SER
1	H	445	SER
1	M	445	SER
1	G	276	ILE
1	G	630	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	179	ASN

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Mol	Chain	Res	Type
1	H	346	GLN
1	M	427	GLN
1	G	315	GLN
1	G	426	HIS

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

There are no ligands in this entry.

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, 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>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	581/593 (97%)	0.03	3 (0%)	91	90	29, 48, 92, 128	0
1	B	581/593 (97%)	0.10	8 (1%)	78	76	29, 50, 93, 132	0
1	C	581/593 (97%)	0.17	12 (2%)	67	63	28, 51, 94, 129	0
1	D	581/593 (97%)	0.23	7 (1%)	81	79	29, 49, 93, 128	0
1	E	581/593 (97%)	0.11	10 (1%)	73	71	31, 50, 94, 131	0
1	F	581/593 (97%)	0.18	20 (3%)	49	42	31, 53, 96, 130	0
1	G	581/593 (97%)	0.36	33 (5%)	27	21	31, 53, 96, 127	0
1	H	581/593 (97%)	0.17	13 (2%)	65	62	29, 51, 94, 132	0
1	I	581/593 (97%)	0.19	7 (1%)	81	79	29, 49, 89, 129	0
1	J	581/593 (97%)	0.08	9 (1%)	76	74	31, 51, 94, 128	0
1	K	581/593 (97%)	0.28	32 (5%)	29	23	33, 53, 96, 130	0
1	L	581/593 (97%)	-0.07	2 (0%)	94	94	31, 51, 93, 128	0
1	M	581/593 (97%)	0.08	13 (2%)	65	62	31, 52, 92, 127	0
1	N	581/593 (97%)	0.22	22 (3%)	44	38	31, 52, 96, 132	0
All	All	8134/8302 (97%)	0.15	191 (2%)	64	60	28, 51, 94, 132	0

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	300	GLY	5.0
1	G	716	ASN	4.9
1	G	679	TYR	4.8
1	I	298	VAL	4.6
1	F	416	ALA	4.5

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.