



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 20, 2024 – 03:13 pm GMT

PDB ID : 7A27
Title : Structure of soluble SmhA crystal form 2 of the tripartite alpha-pore forming toxin, Smh, from *Serratia marcescens*.
Authors : Churchill-Angus, A.M.; Baker, P.J.
Deposited on : 2020-08-16
Resolution : 2.57 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

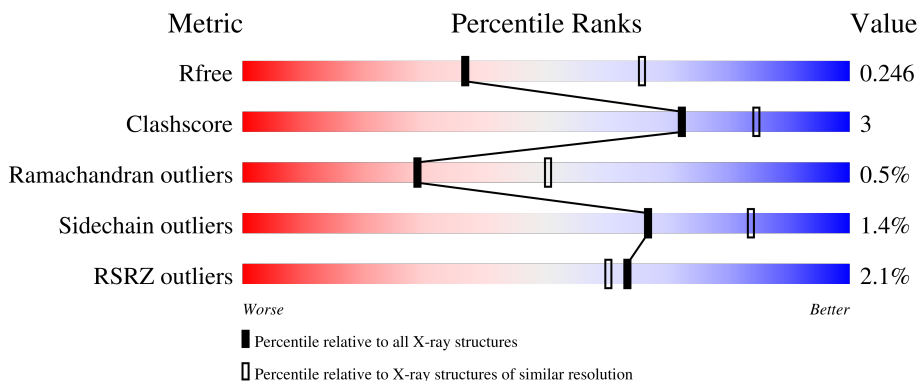
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



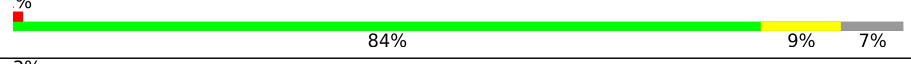

The reported resolution of this entry is 2.57 Å.

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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	AAA	373	 3% 82% 10% 8%
1	BBB	373	 % 85% 8% 7%
1	CCC	373	 % 84% 9% 7%
1	GGG	373	 3% 87% 7% 6%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 20988 atoms, of which 10544 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 SmhA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	GGG	349	5261	1642	2650	447	514	8	177	0	0
1	AAA	345	5192	1621	2619	441	503	8	172	0	0
1	BBB	346	5225	1629	2635	444	509	8	177	0	0
1	CCC	347	5236	1632	2640	445	511	8	178	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
GGG	366	LEU	-	expression tag	UNP A0A1Q4NVM5
GGG	367	GLU	-	expression tag	UNP A0A1Q4NVM5
GGG	368	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	369	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	370	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	371	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	372	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	373	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	366	LEU	-	expression tag	UNP A0A1Q4NVM5
AAA	367	GLU	-	expression tag	UNP A0A1Q4NVM5
AAA	368	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	369	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	370	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	371	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	372	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	373	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	366	LEU	-	expression tag	UNP A0A1Q4NVM5
BBB	367	GLU	-	expression tag	UNP A0A1Q4NVM5
BBB	368	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	369	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	370	HIS	-	expression tag	UNP A0A1Q4NVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	371	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	372	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	373	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	366	LEU	-	expression tag	UNP A0A1Q4NVM5
CCC	367	GLU	-	expression tag	UNP A0A1Q4NVM5
CCC	368	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	369	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	370	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	371	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	372	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	373	HIS	-	expression tag	UNP A0A1Q4NVM5

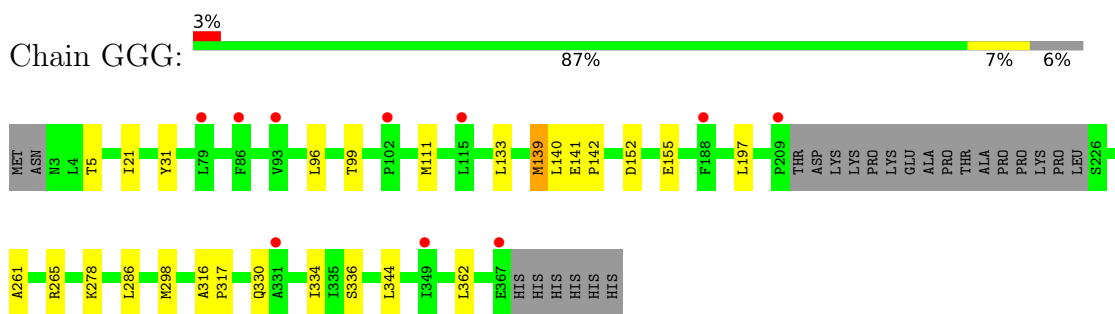
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	GGG	21	Total O 21 21	0	0
2	AAA	7	Total O 7 7	0	0
2	BBB	22	Total O 22 22	0	0
2	CCC	24	Total O 24 24	0	0

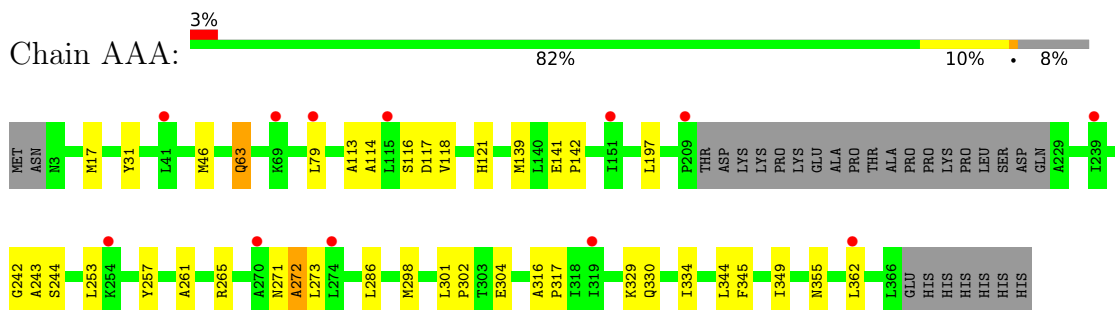
3 Residue-property plots [i](#)

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.

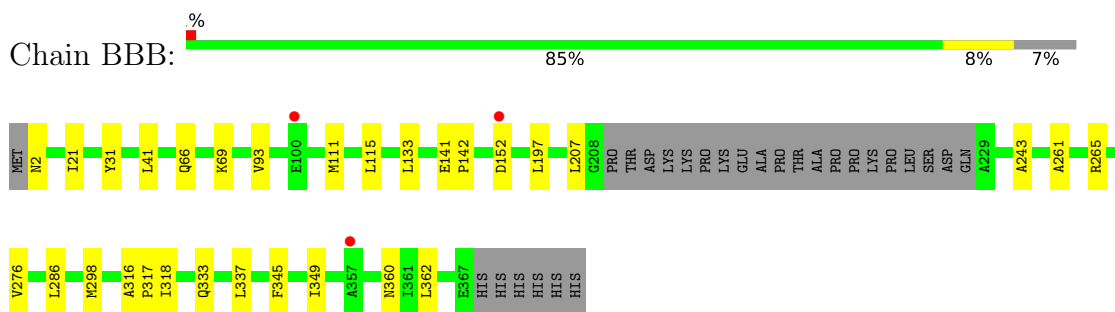
- Molecule 1: SmhA



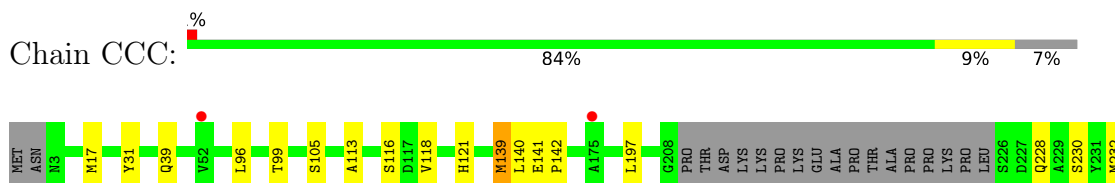
- Molecule 1: SmhA



- Molecule 1: SmhA



- Molecule 1: SmhA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.24Å 92.58Å 221.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.55 – 2.57 110.55 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (110.55-2.57) 99.7 (110.55-2.57)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.236 , 0.247 0.235 , 0.246	Depositor DCC
R_{free} test set	2611 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtrriage
Anisotropy	1.005	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20988	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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 [i](#)

5.1 Standard geometry [i](#)

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	AAA	0.70	0/2604	0.86	0/3536
1	BBB	0.75	0/2620	0.84	0/3556
1	CCC	0.74	0/2626	0.85	0/3564
1	GGG	0.72	0/2642	0.85	0/3587
All	All	0.73	0/10492	0.85	0/14243

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 [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	AAA	2573	2619	2609	22	0
1	BBB	2590	2635	2630	17	0
1	CCC	2596	2640	2635	22	0
1	GGG	2611	2650	2645	13	0
2	AAA	7	0	0	0	0
2	BBB	22	0	0	0	0
2	CCC	24	0	0	1	0
2	GGG	21	0	0	0	0
All	All	10444	10544	10519	71	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 3.

The worst 5 of 71 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:CCC:230:SER:HB3	1:CCC:232:MET:CE	2.15	0.75
1:GGG:155:GLU:OE2	1:GGG:278:LYS:HE2	1.90	0.72
1:CCC:239:ILE:HB	1:CCC:242:GLY:HA3	1.76	0.66
1:AAA:118:VAL:HG22	1:CCC:118:VAL:HG22	1.79	0.64
1:CCC:316:ALA:HB3	1:CCC:317:PRO:HD3	1.82	0.62

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	AAA	341/373 (91%)	324 (95%)	15 (4%)	2 (1%)	25	45
1	BBB	342/373 (92%)	327 (96%)	14 (4%)	1 (0%)	41	62
1	CCC	343/373 (92%)	329 (96%)	12 (4%)	2 (1%)	25	45
1	GGG	345/373 (92%)	329 (95%)	14 (4%)	2 (1%)	25	45
All	All	1371/1492 (92%)	1309 (96%)	55 (4%)	7 (0%)	29	50

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	243	ALA
1	CCC	240	SER
1	GGG	5	THR
1	AAA	272	ALA
1	CCC	244	SER

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	AAA	265/294 (90%)	260 (98%)	5 (2%)	57 77
1	BBB	269/294 (92%)	267 (99%)	2 (1%)	84 93
1	CCC	270/294 (92%)	266 (98%)	4 (2%)	65 82
1	GGG	271/294 (92%)	267 (98%)	4 (2%)	65 82
All	All	1075/1176 (91%)	1060 (99%)	15 (1%)	67 84

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	344	LEU
1	CCC	240	SER
1	AAA	355	ASN
1	CCC	366	LEU
1	CCC	105	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	345/373 (92%)	0.55	12 (3%) 44 39	60, 80, 109, 132	0
1	BBB	346/373 (92%)	0.32	3 (0%) 84 83	51, 76, 111, 136	0
1	CCC	347/373 (93%)	0.24	4 (1%) 79 77	59, 77, 105, 131	0
1	GGG	349/373 (93%)	0.50	10 (2%) 51 47	60, 76, 102, 146	0
All	All	1387/1492 (92%)	0.40	29 (2%) 63 60	51, 77, 109, 146	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	326	ALA	3.8
1	AAA	41	LEU	3.8
1	BBB	357	ALA	3.2
1	AAA	254	LYS	3.1
1	CCC	52	VAL	2.8

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.