Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 01:20 pm GMT

PDB ID	:	6ZZH
Title	:	Structure of soluble SmhB crystal form 2 of the tripartite alpha-pore forming toxin, Smh, from Serratia marcescens.
Authors	:	Churchill-Angus, A.M.; Baker, P.J.
Deposited on	:	2020-08-04
Resolution	:	1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

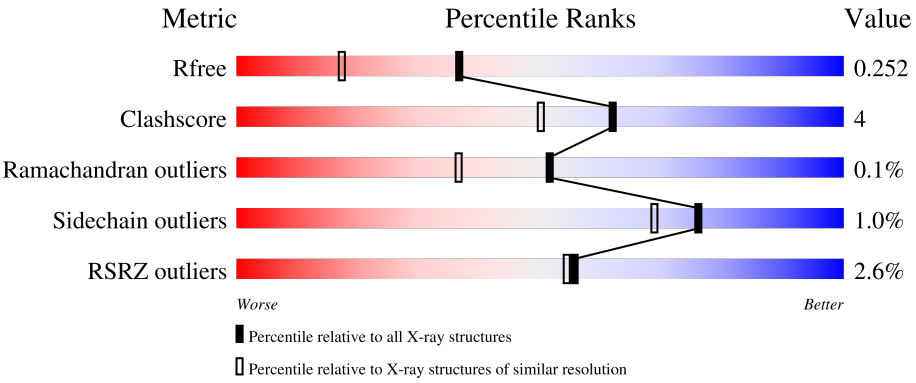
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

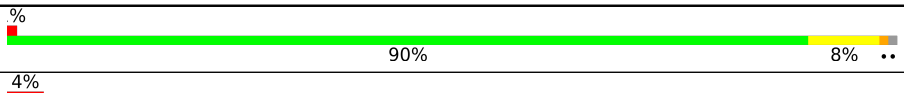
The reported resolution of this entry is 1.86 Å.

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 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 <=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	366	
1	BBB	366	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11247 atoms, of which 5560 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 SmhB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	361	Total	C	H	N	O	S	182	6	0
			5548	1714	2792	495	537	10			
1	BBB	360	Total	C	H	N	O	S	179	7	0
			5501	1698	2768	488	537	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	359	LEU	-	expression tag	UNP A0A1Q4NVM7
AAA	360	GLU	-	expression tag	UNP A0A1Q4NVM7
AAA	361	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	362	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	363	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	364	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	365	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	366	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	359	LEU	-	expression tag	UNP A0A1Q4NVM7
BBB	360	GLU	-	expression tag	UNP A0A1Q4NVM7
BBB	361	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	362	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	363	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	364	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	365	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	366	HIS	-	expression tag	UNP A0A1Q4NVM7

- Molecule 2 is water.

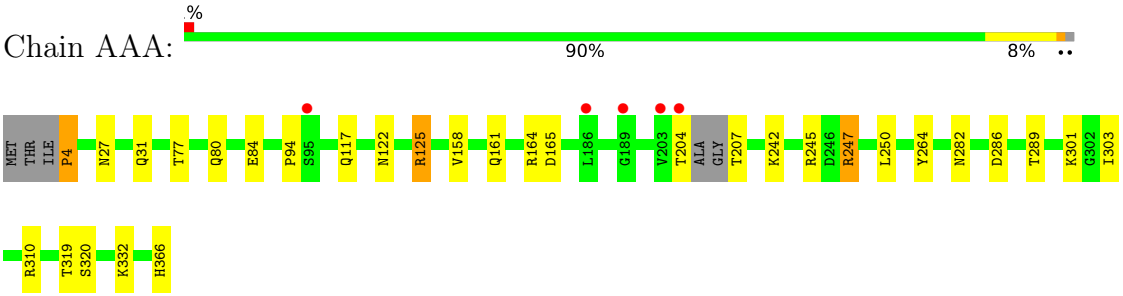
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	110	Total	O	0	0
			110	110		
2	BBB	88	Total	O	0	0
			88	88		

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.

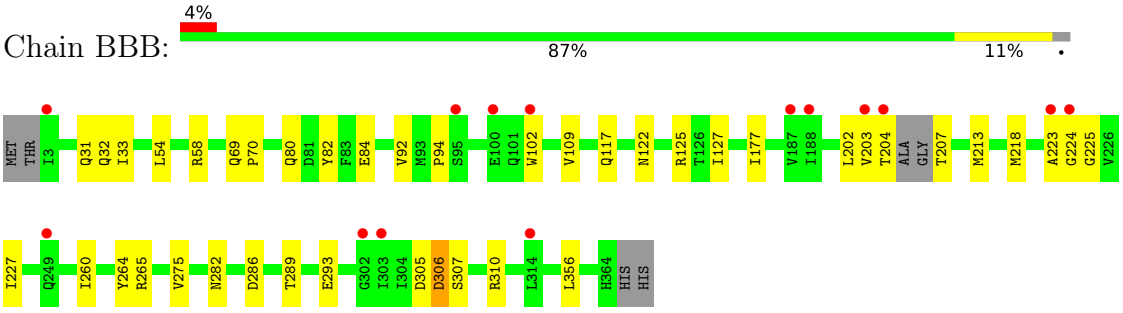
• Molecule 1: SmhB

Chain AAA:



• Molecule 1: SmhB

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.93Å 49.73Å 99.50Å 90.00° 118.43° 90.00°	Depositor
Resolution (Å)	87.50 – 1.86 87.50 – 1.86	Depositor EDS
% Data completeness (in resolution range)	72.2 (87.50-1.86) 72.2 (87.50-1.86)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.213 , 0.247 0.216 , 0.252	Depositor DCC
R_{free} test set	2522 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.019 for h,-k,-h-l 0.000 for -h-l,-k,l 0.025 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11247	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	AAA	0.76	0/2801	0.90	3/3797 (0.1%)
1	BBB	0.72	0/2781	0.87	1/3772 (0.0%)
All	All	0.74	0/5582	0.88	4/7569 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	4	PRO	CA-N-CD	-7.52	100.97	111.50
1	AAA	366	HIS	CA-C-O	-6.37	106.73	120.10
1	AAA	125	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	BBB	265	ARG	NE-CZ-NH2	-5.39	117.60	120.30

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	AAA	2756	2792	2782	21	0
1	BBB	2733	2768	2759	29	0
2	AAA	110	0	0	2	0
2	BBB	88	0	0	1	0
All	All	5687	5560	5541	48	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 4.

All (48) 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:AAA:94:PRO:HD2	1:BBB:92:VAL:HG11	1.56	0.87
1:AAA:117:GLN:NE2	1:AAA:286:ASP:OD1	2.14	0.79
1:BBB:80:GLN:O	1:BBB:84:GLU:HG2	1.84	0.77
1:BBB:117:GLN:NE2	1:BBB:286:ASP:OD1	2.17	0.76
1:BBB:58:ARG:HD3	2:BBB:436:HOH:O	1.91	0.71
1:BBB:305:ASP:OD1	1:BBB:306:ASP:N	2.22	0.70
1:BBB:54:LEU:HD13	1:BBB:213:MET:HE1	1.74	0.69
1:BBB:305:ASP:OD2	1:BBB:307:SER:OG	2.13	0.64
1:AAA:204:THR:HG1	1:AAA:207:THR:N	1.95	0.64
1:BBB:204:THR:HA	1:BBB:207:THR:HG22	1.83	0.61
1:BBB:227:ILE:HD12	1:BBB:356:LEU:HD22	1.82	0.60
1:AAA:94:PRO:O	1:AAA:310:ARG:NH1	2.34	0.59
1:AAA:319:THR:HG22	1:AAA:320:SER:N	2.18	0.58
1:BBB:213:MET:HE1	1:BBB:260:ILE:HG23	1.89	0.55
1:BBB:102:TRP:HZ2	1:BBB:310:ARG:HG2	1.71	0.54
1:AAA:301:LYS:HD2	1:AAA:303:ILE:HD12	1.88	0.54
1:AAA:158:VAL:CG1	1:AAA:250:LEU:HD11	2.39	0.52
1:AAA:4:PRO:N	2:AAA:410:HOH:O	2.44	0.51
1:BBB:223:ALA:O	1:BBB:225:GLY:N	2.42	0.51
1:BBB:227:ILE:CD1	1:BBB:356:LEU:HD22	2.40	0.51
1:AAA:319:THR:HG22	1:AAA:320:SER:H	1.76	0.50
1:BBB:82:TYR:CE1	1:BBB:109:VAL:HG13	2.46	0.50
1:AAA:165:ASP:OD2	1:AAA:247:ARG:NH1	2.43	0.49
1:AAA:94:PRO:HD2	1:BBB:92:VAL:CG1	2.36	0.49
1:BBB:33:ILE:HD12	1:BBB:33:ILE:N	2.28	0.48
1:AAA:164:ARG:NH1	2:AAA:401:HOH:O	2.12	0.48
1:AAA:301:LYS:HD2	1:AAA:303:ILE:CD1	2.44	0.48
1:BBB:204:THR:HA	1:BBB:207:THR:CG2	2.43	0.48
1:BBB:92:VAL:O	1:BBB:94:PRO:HD3	2.15	0.47
1:BBB:202:LEU:O	1:BBB:203:VAL:HG13	2.15	0.47
1:AAA:161:GLN:OE1	1:AAA:164:ARG:NH1	2.49	0.46
1:BBB:32:GLN:HG2	1:BBB:213:MET:HE2	1.98	0.46
1:BBB:31:GLN:O	1:BBB:33:ILE:HD12	2.17	0.45
1:BBB:122:ASN:OD1	1:BBB:125:ARG:NH1	2.50	0.45
1:BBB:127[B]:ILE:HG22	1:BBB:275:VAL:HG22	1.99	0.44
1:AAA:80:GLN:O	1:AAA:84:GLU:HG3	2.17	0.44
1:BBB:54:LEU:CD1	1:BBB:213:MET:HE1	2.46	0.44
1:BBB:54:LEU:CD1	1:BBB:213:MET:CE	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:242:LYS:HD2	1:AAA:245:ARG:HH11	1.82	0.43
1:BBB:69:GLN:N	1:BBB:70:PRO:CD	2.82	0.42
1:AAA:117:GLN:OE1	1:AAA:289:THR:HG21	2.18	0.42
1:AAA:158:VAL:HG11	1:AAA:250:LEU:HD11	2.01	0.42
1:BBB:223:ALA:C	1:BBB:225:GLY:H	2.23	0.42
1:BBB:177:ILE:HG23	1:BBB:218:MET:HB2	2.02	0.42
1:BBB:289:THR:HG22	1:BBB:293:GLU:OE2	2.20	0.41
1:AAA:27:ASN:O	1:AAA:31:GLN:HG3	2.21	0.41
1:AAA:77:THR:OG1	1:AAA:332:LYS:NZ	2.52	0.41
1:AAA:122[A]:ASN:OD1	1:AAA:125:ARG:NH1	2.53	0.41

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	363/366 (99%)	358 (99%)	5 (1%)	0	100 100
1	BBB	363/366 (99%)	354 (98%)	8 (2%)	1 (0%)	41 26
All	All	726/732 (99%)	712 (98%)	13 (2%)	1 (0%)	51 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	224	GLY

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	300/298 (101%)	297 (99%)	3 (1%)	76	69
1	BBB	298/298 (100%)	295 (99%)	3 (1%)	76	69
All	All	598/596 (100%)	592 (99%)	6 (1%)	76	69

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	247	ARG
1	AAA	264	TYR
1	AAA	282	ASN
1	BBB	264	TYR
1	BBB	282	ASN
1	BBB	306	ASP

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

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	AAA	361/366 (98%)	-0.07	5 (1%) 75 76	13, 25, 50, 75	0
1	BBB	360/366 (98%)	0.10	14 (3%) 39 38	16, 30, 67, 90	0
All	All	721/732 (98%)	0.01	19 (2%) 56 54	13, 27, 61, 90	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	224	GLY	5.9
1	BBB	314	LEU	4.2
1	BBB	204	THR	4.2
1	BBB	302	GLY	4.1
1	BBB	3	ILE	3.7
1	BBB	249	GLN	3.5
1	BBB	95	SER	3.3
1	BBB	188	ILE	3.3
1	BBB	223	ALA	3.3
1	BBB	203	VAL	3.0
1	AAA	189	GLY	2.9
1	BBB	303	ILE	2.7
1	AAA	203	VAL	2.6
1	BBB	102	TRP	2.5
1	AAA	186	LEU	2.5
1	BBB	187	VAL	2.4
1	BBB	100	GLU	2.1
1	AAA	95	SER	2.0
1	AAA	204	THR	2.0

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 (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.