



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:27 PM UTC

PDB ID : 7A0G / pdb_00007a0g
Title : Structure of the SmhB pore of the tripartite alpha-pore forming toxin, Smh, from *Serratia marcescens*.
Authors : Churchill-Angus, A.M.; Baker, P.J.
Deposited on : 2020-08-08
Resolution : 6.98 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

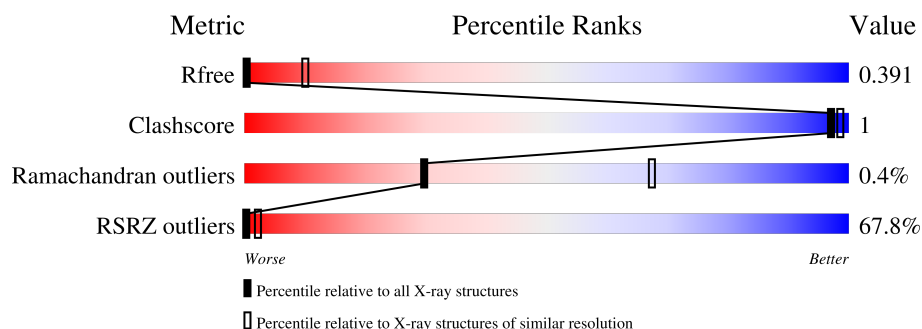
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.98 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	1166 (9.70-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1053 (9.70-4.00)
RSRZ outliers	180081	1159 (9.70-4.00)

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	366	63% 87% 10%
1	BBB	366	59% 86% 13%
1	CCC	366	64% 87% 10%
1	DDD	366	61% 85% 13%
1	EEE	366	61% 88% 10%
1	FFF	366	57% 83% 14%
1	GGG	366	56% 88% 10%

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Mol	Chain	Length	Quality of chain
1	HHH	366	60% 87% 10%
1	III	366	55% 84% 14%
1	JJJ	366	62% 85% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27767 atoms, of which 11987 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	329	Total	C	H	N	O	261	0	0
			2830	950	1222	329	329			
1	BBB	320	Total	C	H	N	O	254	0	0
			2751	924	1187	320	320			
1	CCC	329	Total	C	H	N	O	262	0	0
			2829	950	1221	329	329			
1	DDD	318	Total	C	H	N	O	254	0	0
			2735	919	1180	318	318			
1	EEE	329	Total	C	H	N	O	259	1	0
			2834	951	1225	329	329			
1	FFF	313	Total	C	H	N	O	249	0	0
			2691	904	1161	313	313			
1	GGG	329	Total	C	H	N	O	261	0	0
			2830	950	1222	329	329			
1	HHH	328	Total	C	H	N	O	260	0	0
			2822	947	1219	328	328			
1	III	313	Total	C	H	N	O	250	0	0
			2694	905	1163	313	313			
1	JJJ	320	Total	C	H	N	O	254	0	0
			2751	924	1187	320	320			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	368	LEU	-	expression tag	UNP A0A1Q4NVM7
AAA	369	GLU	-	expression tag	UNP A0A1Q4NVM7
AAA	370	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	371	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	372	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	373	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	374	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	375	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	368	LEU	-	expression tag	UNP A0A1Q4NVM7

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	369	GLU	-	expression tag	UNP A0A1Q4NVM7
BBB	370	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	371	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	372	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	373	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	374	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	375	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	368	LEU	-	expression tag	UNP A0A1Q4NVM7
CCC	369	GLU	-	expression tag	UNP A0A1Q4NVM7
CCC	370	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	371	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	372	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	373	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	374	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	375	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	368	LEU	-	expression tag	UNP A0A1Q4NVM7
DDD	369	GLU	-	expression tag	UNP A0A1Q4NVM7
DDD	370	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	371	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	372	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	373	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	374	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	375	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	368	LEU	-	expression tag	UNP A0A1Q4NVM7
EEE	369	GLU	-	expression tag	UNP A0A1Q4NVM7
EEE	370	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	371	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	372	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	373	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	374	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	375	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	368	LEU	-	expression tag	UNP A0A1Q4NVM7
FFF	369	GLU	-	expression tag	UNP A0A1Q4NVM7
FFF	370	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	371	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	372	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	373	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	374	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	375	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	368	LEU	-	expression tag	UNP A0A1Q4NVM7
GGG	369	GLU	-	expression tag	UNP A0A1Q4NVM7
GGG	370	HIS	-	expression tag	UNP A0A1Q4NVM7

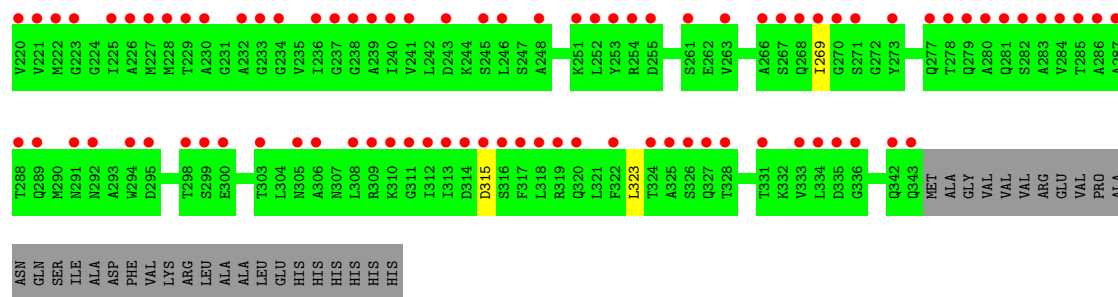
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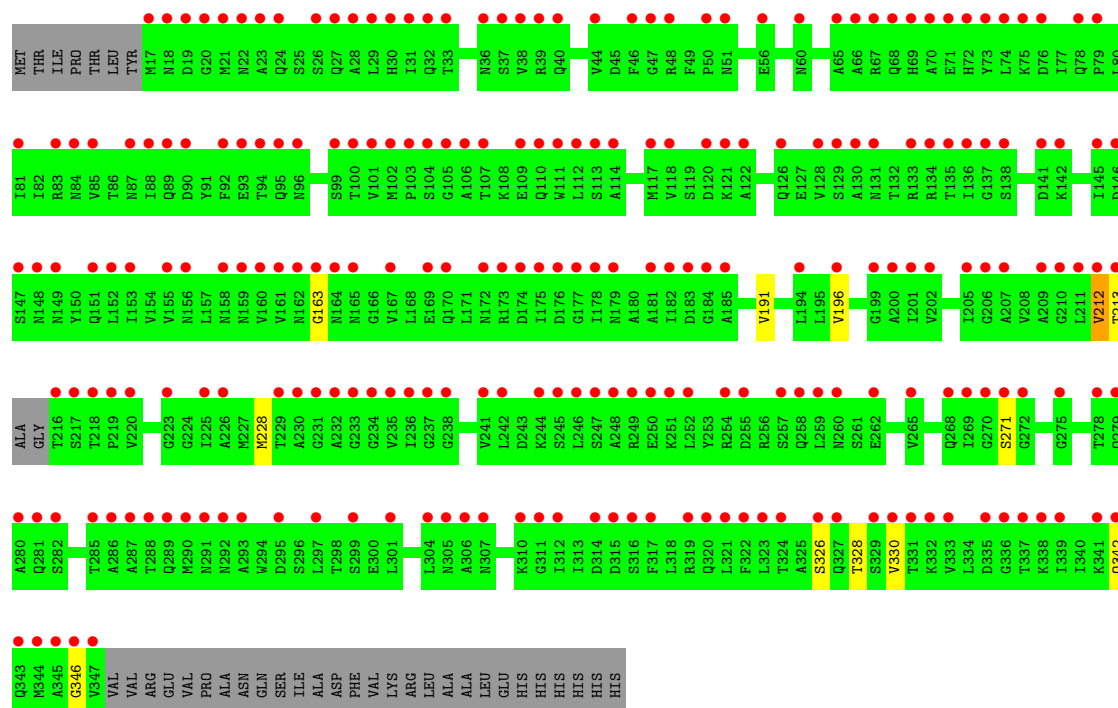
Chain	Residue	Modelled	Actual	Comment	Reference
GGG	371	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	372	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	373	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	374	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	375	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	368	LEU	-	expression tag	UNP A0A1Q4NVM7
HHH	369	GLU	-	expression tag	UNP A0A1Q4NVM7
HHH	370	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	371	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	372	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	373	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	374	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	375	HIS	-	expression tag	UNP A0A1Q4NVM7
III	368	LEU	-	expression tag	UNP A0A1Q4NVM7
III	369	GLU	-	expression tag	UNP A0A1Q4NVM7
III	370	HIS	-	expression tag	UNP A0A1Q4NVM7
III	371	HIS	-	expression tag	UNP A0A1Q4NVM7
III	372	HIS	-	expression tag	UNP A0A1Q4NVM7
III	373	HIS	-	expression tag	UNP A0A1Q4NVM7
III	374	HIS	-	expression tag	UNP A0A1Q4NVM7
III	375	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	368	LEU	-	expression tag	UNP A0A1Q4NVM7
JJJ	369	GLU	-	expression tag	UNP A0A1Q4NVM7
JJJ	370	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	371	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	372	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	373	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	374	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	375	HIS	-	expression tag	UNP A0A1Q4NVM7

- Molecule 1: SmhB

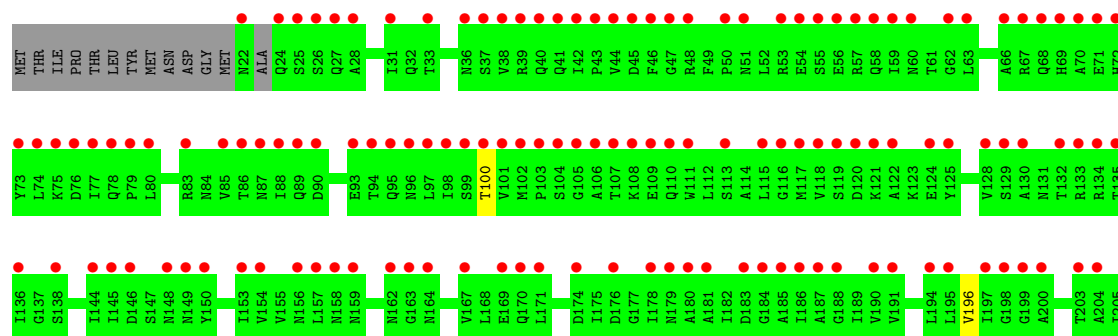




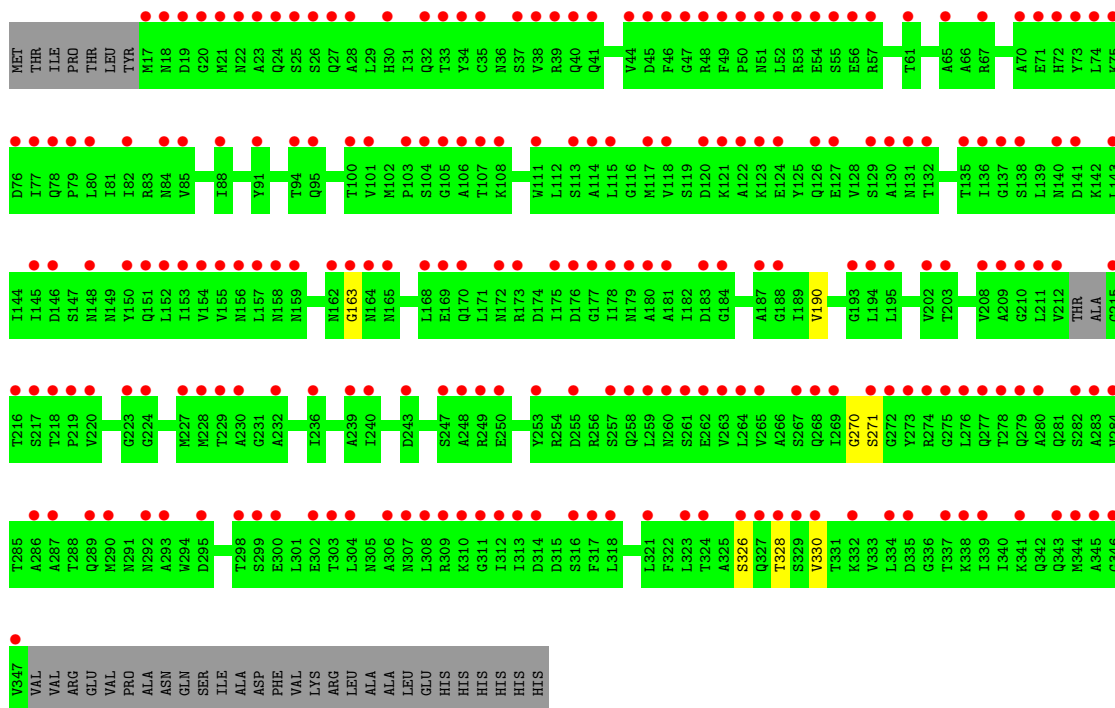
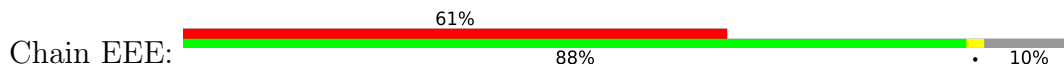
• Molecule 1: SmhB



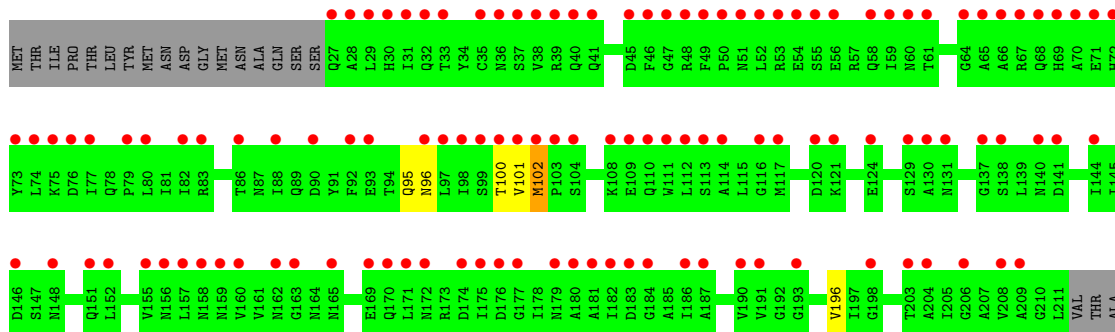
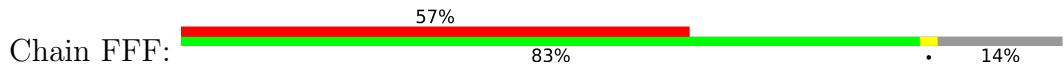
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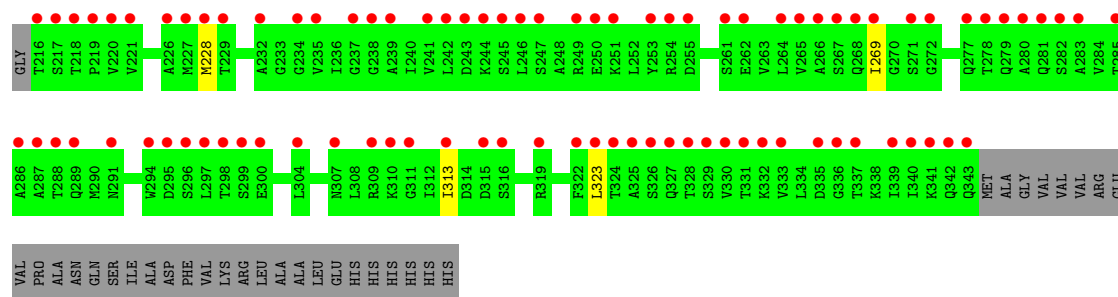


- Molecule 1: SmhB

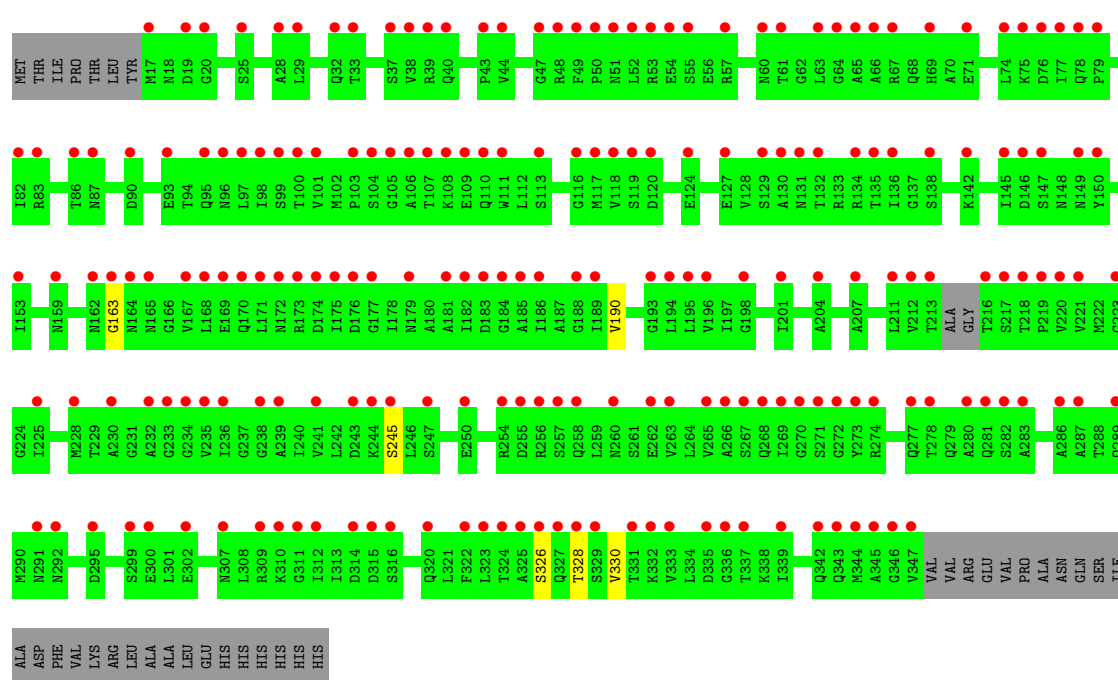


- Molecule 1: SmhB

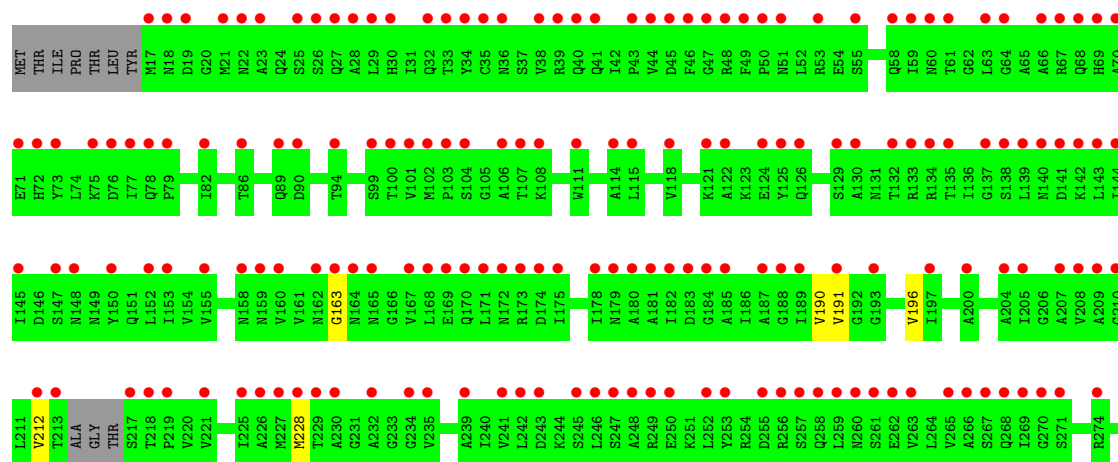


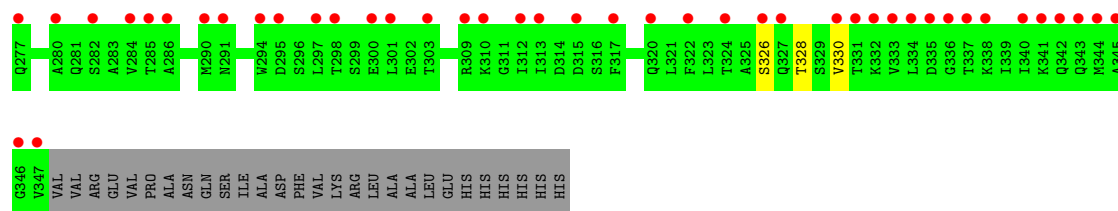


• Molecule 1: SmhB

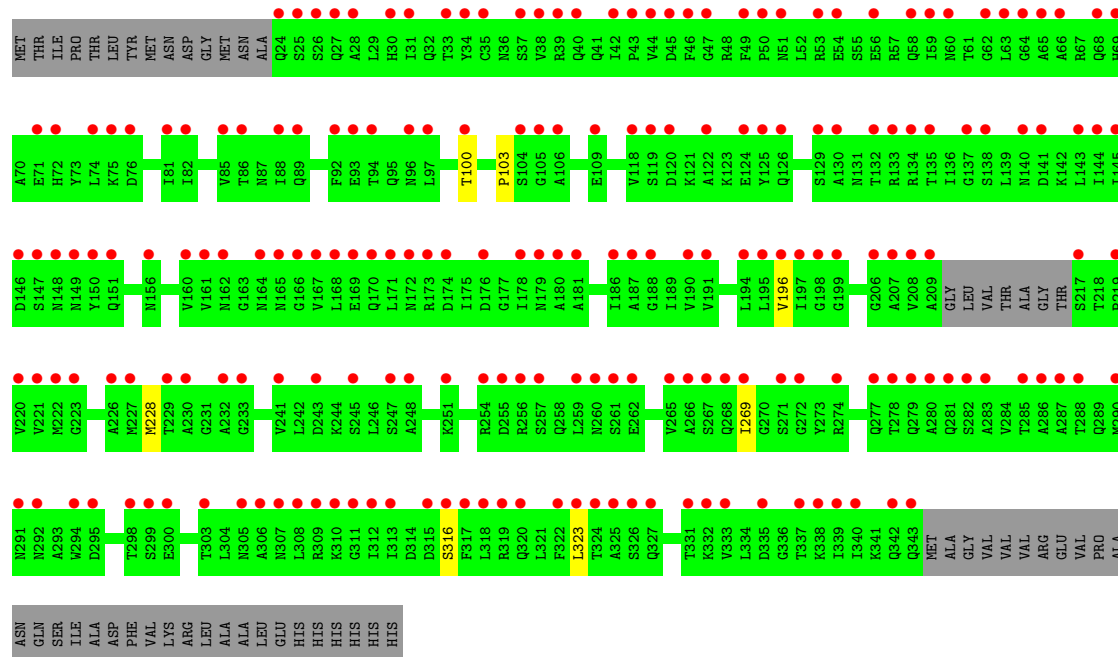
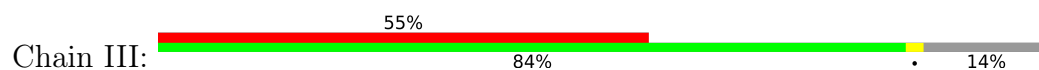


• Molecule 1: SmhB

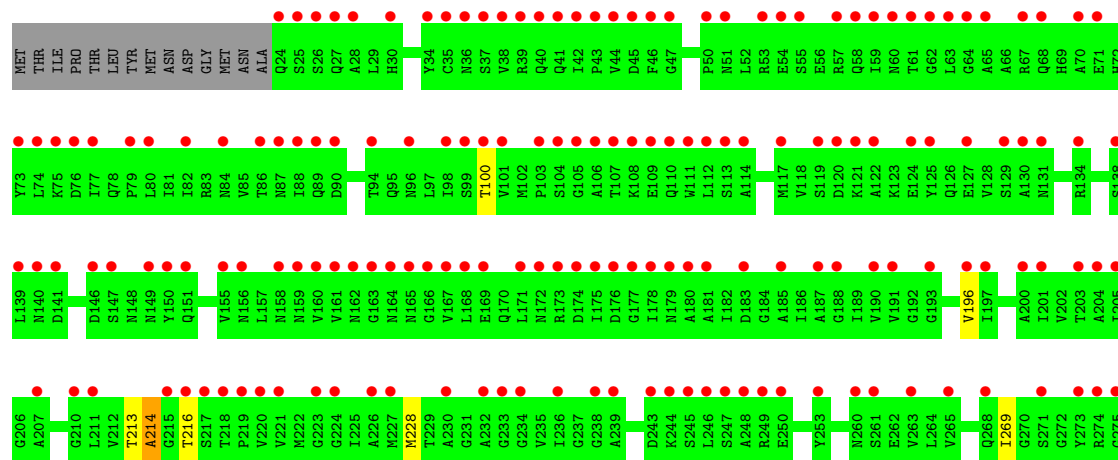
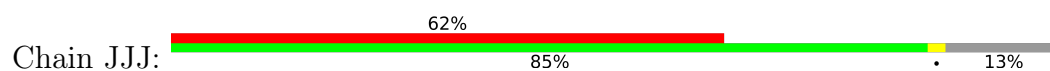




● Molecule 1: SmhB



● Molecule 1: SmhB





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.48Å 118.06Å 209.53Å 90.00° 109.44° 90.00°	Depositor
Resolution (Å)	66.77 – 6.98 66.77 – 6.98	Depositor EDS
% Data completeness (in resolution range)	98.7 (66.77-6.98) 80.4 (66.77-6.98)	Depositor EDS
R_{merge}	2.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.33 (at 6.71Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.334 , 0.335 0.350 , 0.391	Depositor DCC
R_{free} test set	380 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	-102.2	Xtriage
Anisotropy	-2.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.66	EDS
Total number of atoms	27767	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% 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	1.34	0/1606	2.39	10/2223 (0.4%)
1	BBB	1.36	0/1563	2.34	2/2165 (0.1%)
1	CCC	1.34	0/1606	2.39	7/2223 (0.3%)
1	DDD	1.34	0/1552	2.35	2/2147 (0.1%)
1	EEE	1.36	2/1610 (0.1%)	2.37	5/2228 (0.2%)
1	FFF	1.35	0/1528	2.35	2/2115 (0.1%)
1	GGG	1.35	1/1606 (0.1%)	2.38	4/2223 (0.2%)
1	HHH	1.35	1/1601 (0.1%)	2.38	5/2216 (0.2%)
1	III	1.36	0/1529	2.35	4/2117 (0.2%)
1	JJJ	1.35	0/1563	2.35	2/2165 (0.1%)
All	All	1.35	4/15764 (0.0%)	2.37	43/21822 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	HHH	190	VAL	C-O	5.87	1.30	1.24
1	EEE	190	VAL	C-O	5.38	1.29	1.24
1	EEE	270	GLY	C-O	5.25	1.30	1.23
1	GGG	190	VAL	C-O	5.03	1.29	1.24

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GGG	163	GLY	CA-C-O	-6.08	118.03	122.23
1	HHH	163	GLY	CA-C-O	-6.01	118.08	122.23
1	III	316	SER	CA-C-O	-5.98	116.36	119.77
1	GGG	328	THR	O-C-N	5.95	125.23	120.83
1	EEE	328	THR	O-C-N	5.89	125.19	120.83

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	1608	1222	769	2	0
1	BBB	1564	1187	748	2	0
1	CCC	1608	1221	766	4	0
1	DDD	1555	1180	738	2	0
1	EEE	1609	1225	772	1	0
1	FFF	1530	1161	729	3	0
1	GGG	1608	1222	769	1	0
1	HHH	1603	1219	767	2	0
1	III	1531	1163	728	2	0
1	JJJ	1564	1187	748	3	0
All	All	15780	11987	7534	22	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 1.

The worst 5 of 22 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:III:100:THR:CB	1:III:323:LEU:CB	2.67	0.72
1:FFF:101:VAL:O	1:FFF:102:MET:CB	2.41	0.68
1:BBB:100:THR:HA	1:BBB:323:LEU:CB	2.26	0.64
1:DDD:100:THR:HA	1:DDD:323:LEU:CB	2.28	0.63
1:JJJ:100:THR:HA	1:JJJ:323:LEU:CB	2.29	0.62

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	325/366 (89%)	313 (96%)	12 (4%)	0	100	100
1	BBB	318/366 (87%)	303 (95%)	12 (4%)	3 (1%)	14	51
1	CCC	325/366 (89%)	314 (97%)	10 (3%)	1 (0%)	36	72
1	DDD	313/366 (86%)	302 (96%)	10 (3%)	1 (0%)	36	72
1	EEE	326/366 (89%)	315 (97%)	11 (3%)	0	100	100
1	FFF	309/366 (84%)	297 (96%)	8 (3%)	4 (1%)	9	42
1	GGG	325/366 (89%)	313 (96%)	12 (4%)	0	100	100
1	HHH	324/366 (88%)	313 (97%)	10 (3%)	1 (0%)	36	72
1	III	309/366 (84%)	297 (96%)	11 (4%)	1 (0%)	36	72
1	JJJ	318/366 (87%)	304 (96%)	11 (4%)	3 (1%)	14	51
All	All	3192/3660 (87%)	3071 (96%)	107 (3%)	14 (0%)	30	67

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	214	ALA
1	BBB	216	THR
1	BBB	315	ASP
1	DDD	315	ASP
1	FFF	95	GLN

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 [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	329/366 (89%)	3.22	229 (69%) 0 2	0, 0, 0, 0	0
1	BBB	320/366 (87%)	2.91	217 (67%) 0 2	0, 0, 0, 0	0
1	CCC	329/366 (89%)	3.31	234 (71%) 0 2	0, 0, 0, 0	0
1	DDD	318/366 (86%)	3.30	222 (69%) 0 2	0, 0, 0, 0	0
1	EEE	329/366 (89%)	3.25	225 (68%) 0 2	0, 0, 0, 0	1 (0%)
1	FFF	313/366 (85%)	2.93	208 (66%) 0 2	0, 0, 0, 0	0
1	GGG	329/366 (89%)	2.86	206 (62%) 0 2	0, 0, 0, 0	0
1	HHH	328/366 (89%)	2.98	219 (66%) 0 2	0, 0, 0, 0	0
1	III	313/366 (85%)	2.91	203 (64%) 0 2	0, 0, 0, 0	0
1	JJJ	320/366 (87%)	3.16	226 (70%) 0 2	0, 0, 0, 0	0
All	All	3228/3660 (88%)	3.09	2189 (67%) 0 2	0, 0, 0, 0	1 (0%)

The worst 5 of 2189 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	25	SER	23.2
1	AAA	50	PRO	13.9
1	III	105	GLY	13.8
1	AAA	312	ILE	13.4
1	GGG	165	ASN	13.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.