



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 01:53 am BST

PDB ID : 2Q41  
Title : Ensemble refinement of the protein crystal structure of spermidine synthase from Arabidopsis thaliana gene At1g23820  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 2.70 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

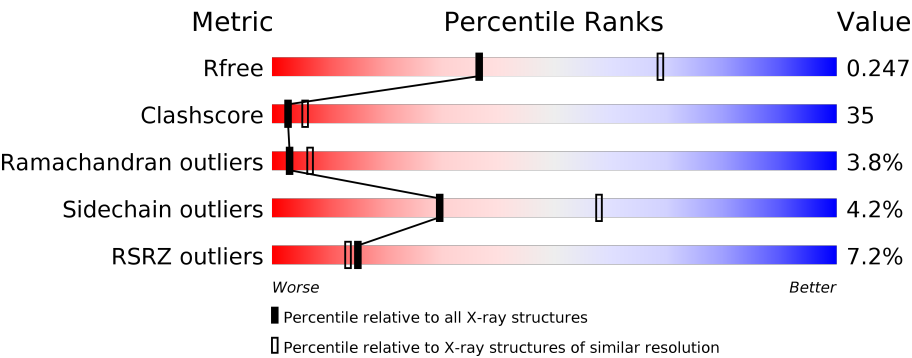
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	1-A	334	<div><div>7%</div><div><div></div><div>40%</div><div>43%</div><div>•</div><div>13%</div></div></div>
1	1-B	334	<div><div>3%</div><div><div></div><div>47%</div><div>36%</div><div>•</div><div>15%</div></div></div>
1	1-C	334	<div><div>11%</div><div><div></div><div>40%</div><div>43%</div><div>•</div><div>13%</div></div></div>
1	1-D	334	<div><div>4%</div><div><div></div><div>43%</div><div>38%</div><div>•</div><div>15%</div></div></div>
1	2-A	334	<div><div>7%</div><div><div></div><div>35%</div><div>48%</div><div>•</div><div>13%</div></div></div>
1	2-B	334	<div><div>3%</div><div><div></div><div>39%</div><div>43%</div><div>•</div><div>15%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	2-C	334	
1	2-D	334	
1	3-A	334	
1	3-B	334	
1	3-C	334	
1	3-D	334	
1	4-A	334	
1	4-B	334	
1	4-C	334	
1	4-D	334	
1	5-A	334	
1	5-B	334	
1	5-C	334	
1	5-D	334	
1	6-A	334	
1	6-B	334	
1	6-C	334	
1	6-D	334	
1	7-A	334	
1	7-B	334	
1	7-C	334	
1	7-D	334	
1	8-A	334	
1	8-B	334	
1	8-C	334	

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Mol	Chain	Length	Quality of chain
1	8-D	334	<div><div></div><div>4%</div><div>40%</div><div>41%</div><div>•</div><div>15%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 75520 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 Spermidine synthase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	2-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	3-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	4-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	5-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	6-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	7-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	8-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	1-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	2-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	3-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	4-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	5-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	6-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	7-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	8-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	2-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	3-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	4-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	5-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	6-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	7-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	8-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	1-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	2-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	3-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	4-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	5-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	6-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	7-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	8-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9ZUB3
A	26	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	51	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	54	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	149	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	155	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	242	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	278	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	1	SER	-	EXPRESSION TAG	UNP Q9ZUB3
B	26	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	51	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	54	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	109	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	149	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	155	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	242	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	278	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	1	SER	-	EXPRESSION TAG	UNP Q9ZUB3
C	26	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	51	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	54	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	109	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	149	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	155	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	242	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	278	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	1	SER	-	EXPRESSION TAG	UNP Q9ZUB3
D	26	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	51	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	54	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	109	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	149	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	155	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	242	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	278	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	130	Total O 130 130	0	0
2	2-A	137	Total O 137 137	0	0
2	3-A	135	Total O 135 135	0	0
2	4-A	134	Total O 134 134	0	0
2	5-A	134	Total O 134 134	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6-A	135	Total 135	O 135	0	0
2	7-A	128	Total 128	O 128	0	0
2	8-A	135	Total 135	O 135	0	0
2	1-B	177	Total 177	O 177	0	0
2	2-B	179	Total 179	O 179	0	0
2	3-B	175	Total 175	O 175	0	0
2	4-B	173	Total 173	O 173	0	0
2	5-B	171	Total 171	O 171	0	0
2	6-B	176	Total 176	O 176	0	0
2	7-B	177	Total 177	O 177	0	0
2	8-B	173	Total 173	O 173	0	0
2	1-C	135	Total 135	O 135	0	0
2	2-C	129	Total 129	O 129	0	0
2	3-C	132	Total 132	O 132	0	0
2	4-C	135	Total 135	O 135	0	0
2	5-C	138	Total 138	O 138	0	0
2	6-C	132	Total 132	O 132	0	0
2	7-C	133	Total 133	O 133	0	0
2	8-C	133	Total 133	O 133	0	0
2	1-D	134	Total 134	O 134	0	0
2	2-D	131	Total 131	O 131	0	0

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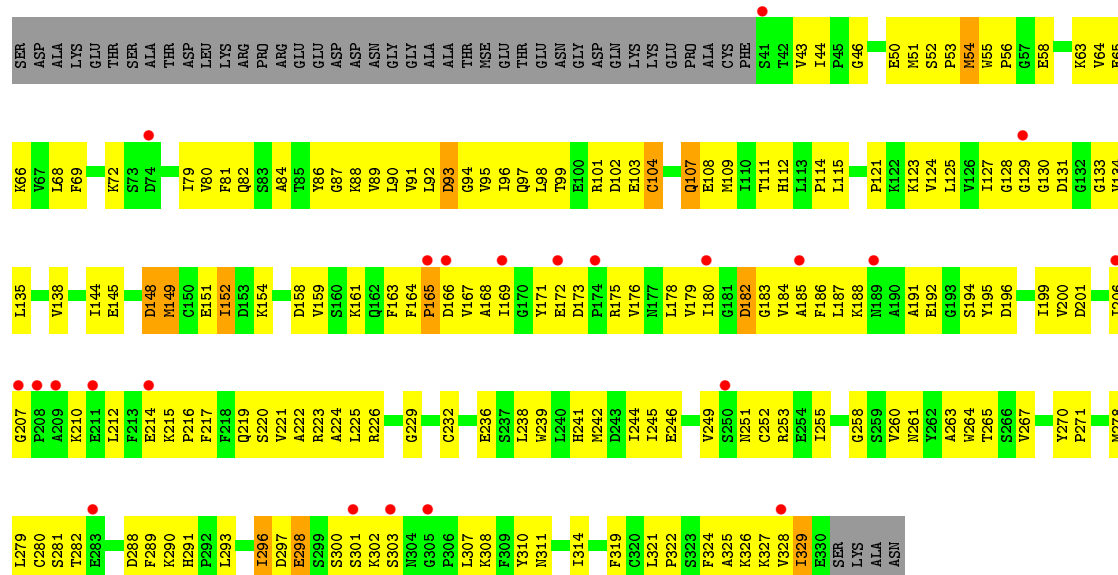


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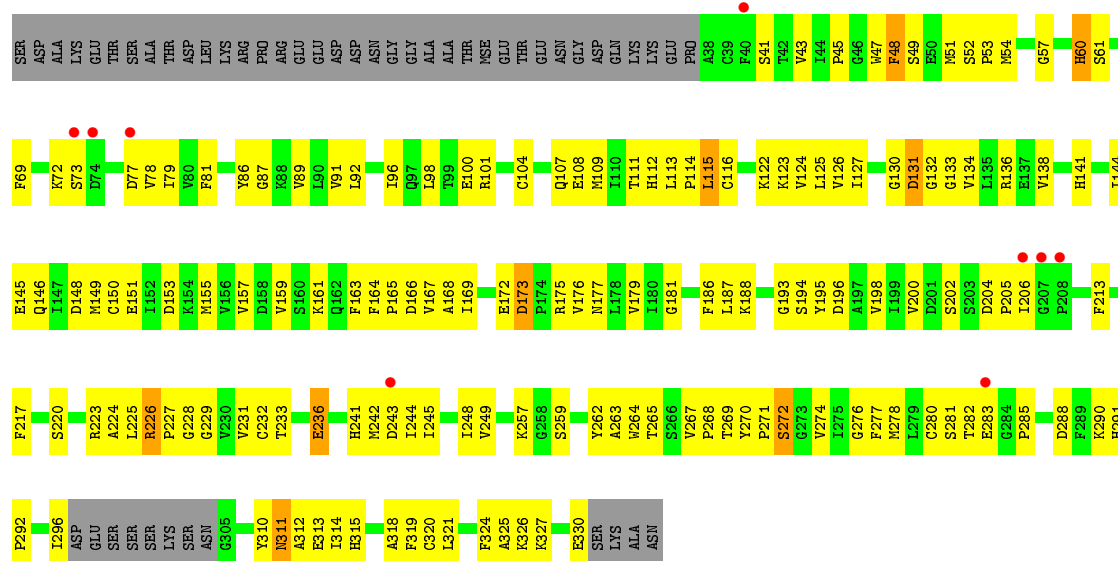
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-D	134	Total 134	O 134	0	0
2	4-D	134	Total 134	O 134	0	0
2	5-D	133	Total 133	O 133	0	0
2	6-D	133	Total 133	O 133	0	0
2	7-D	138	Total 138	O 138	0	0
2	8-D	135	Total 135	O 135	0	0



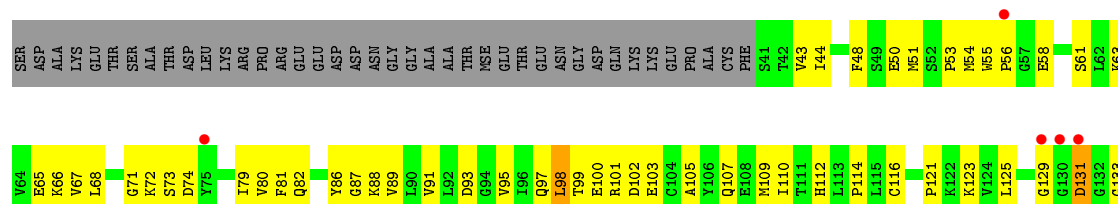
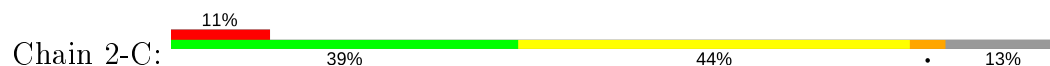




• Molecule 1: Spermidine synthase 1



• Molecule 1: Spermidine synthase 1





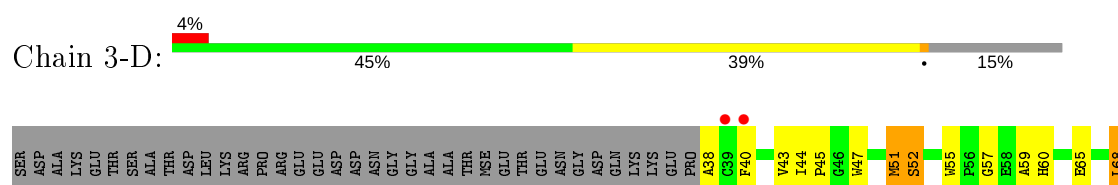
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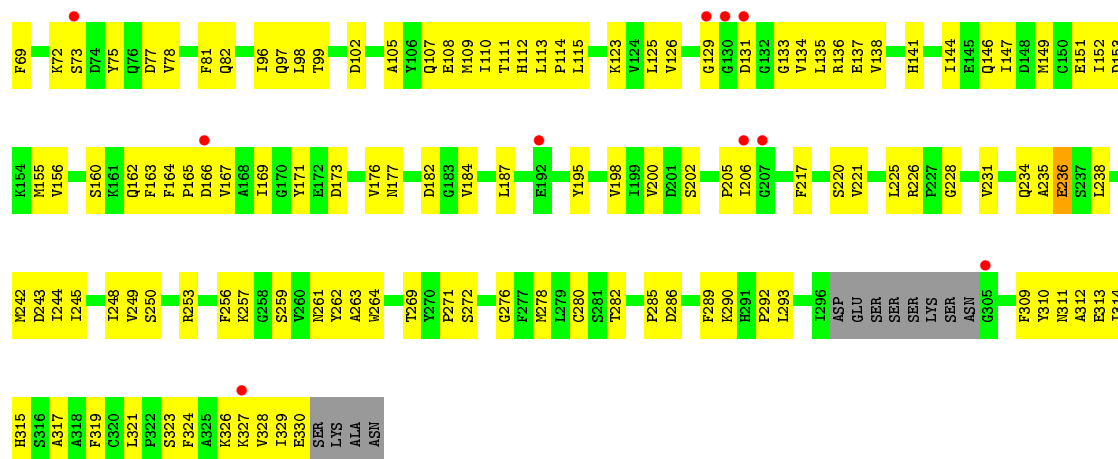


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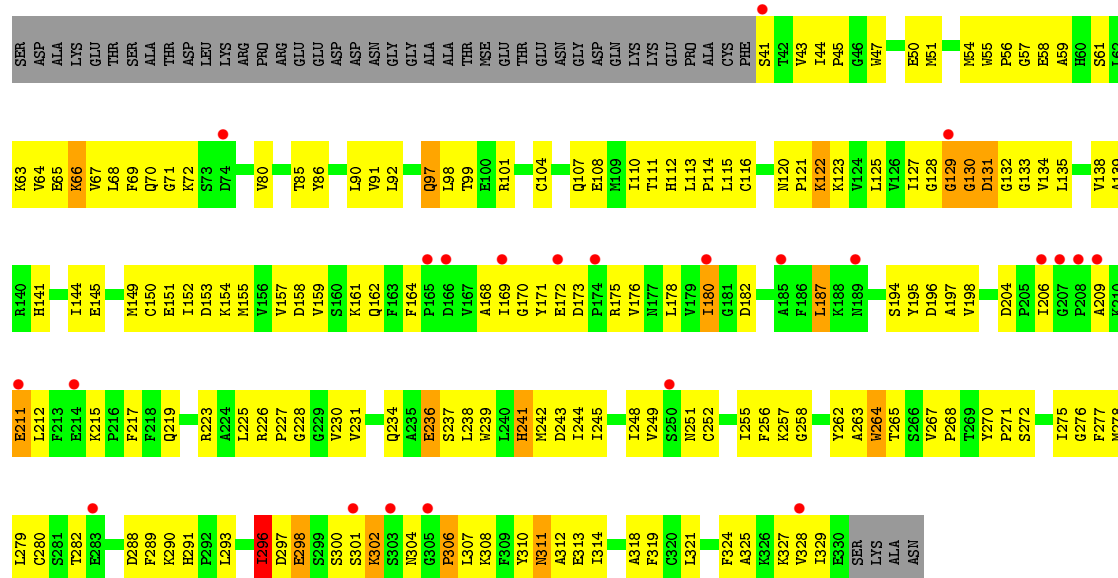


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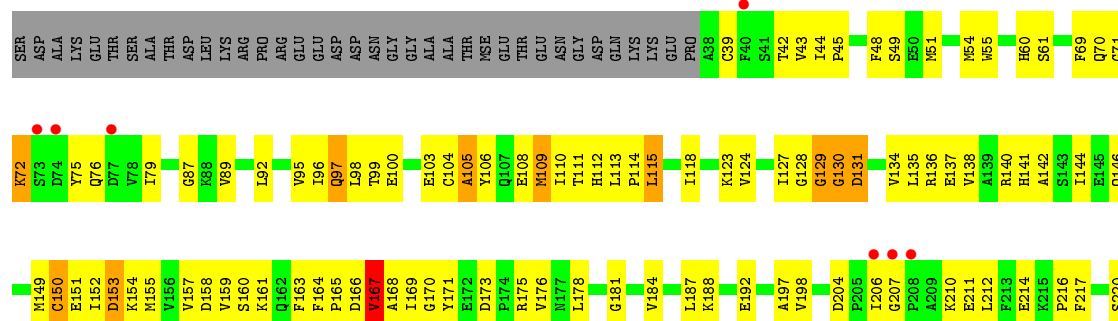


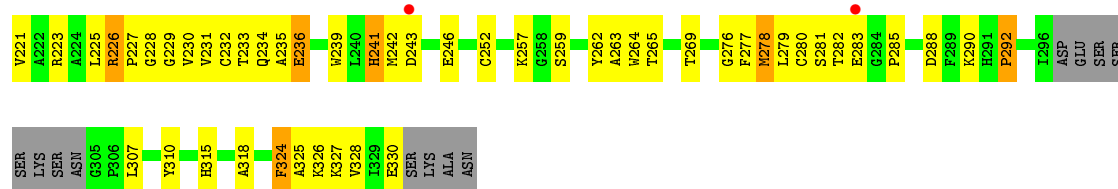


• Molecule 1: Spermidine synthase 1

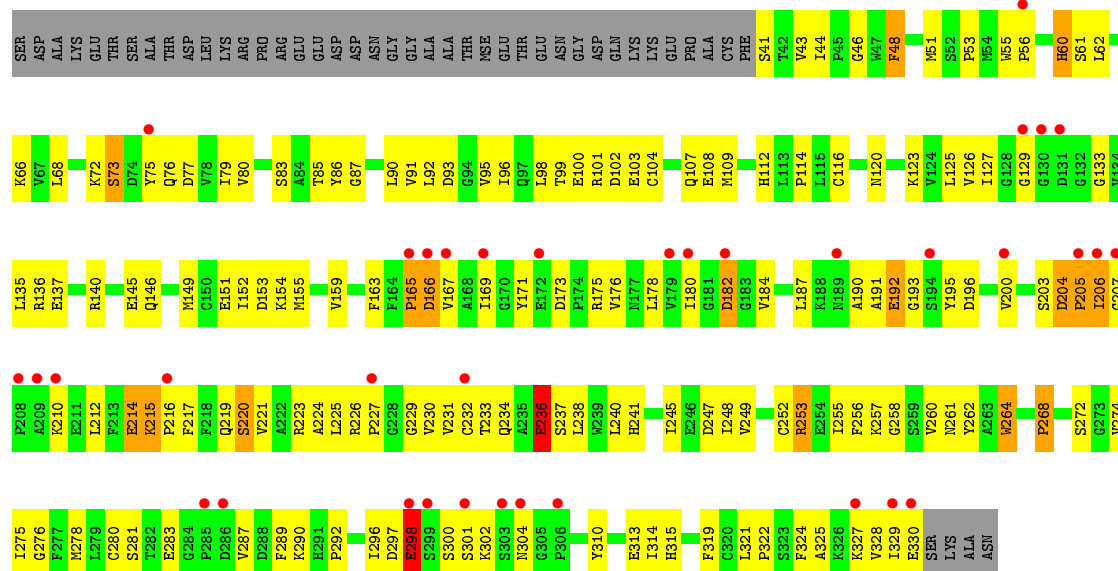


• Molecule 1: Spermidine synthase 1

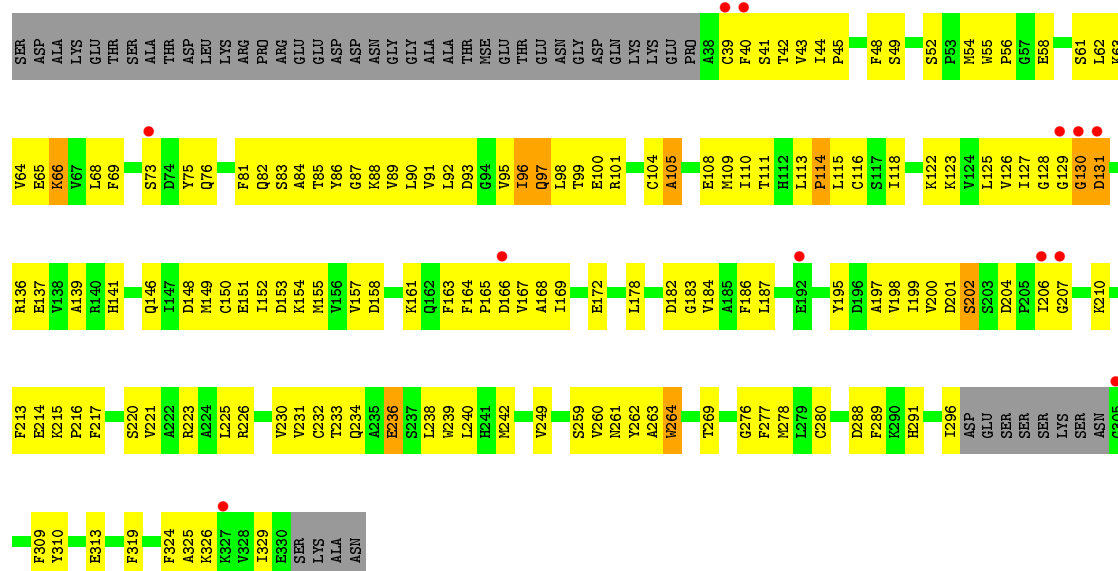
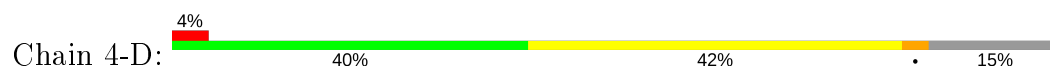




• Molecule 1: Spermidine synthase 1

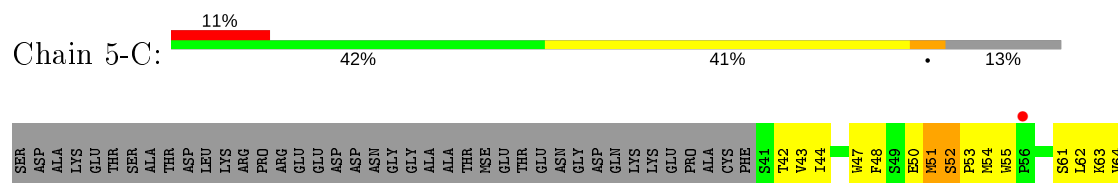


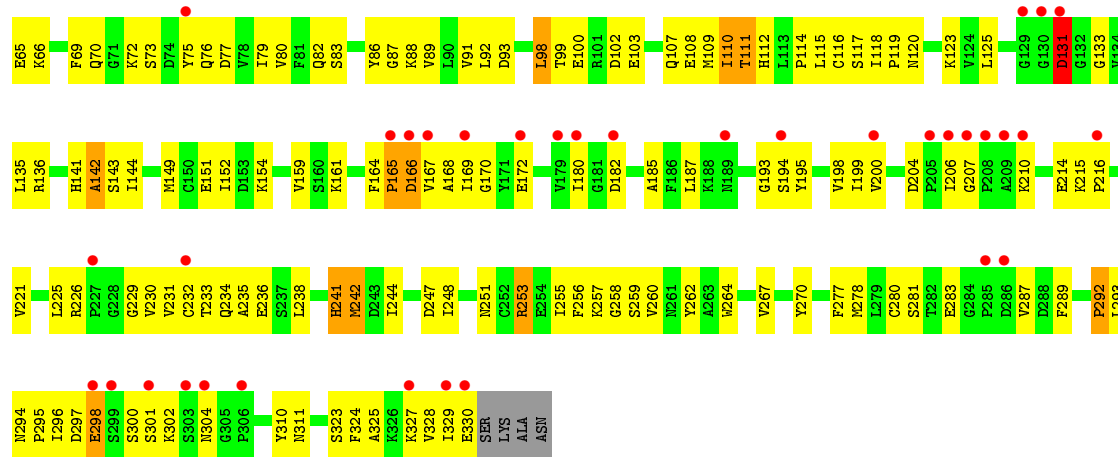
• Molecule 1: Spermidine synthase 1



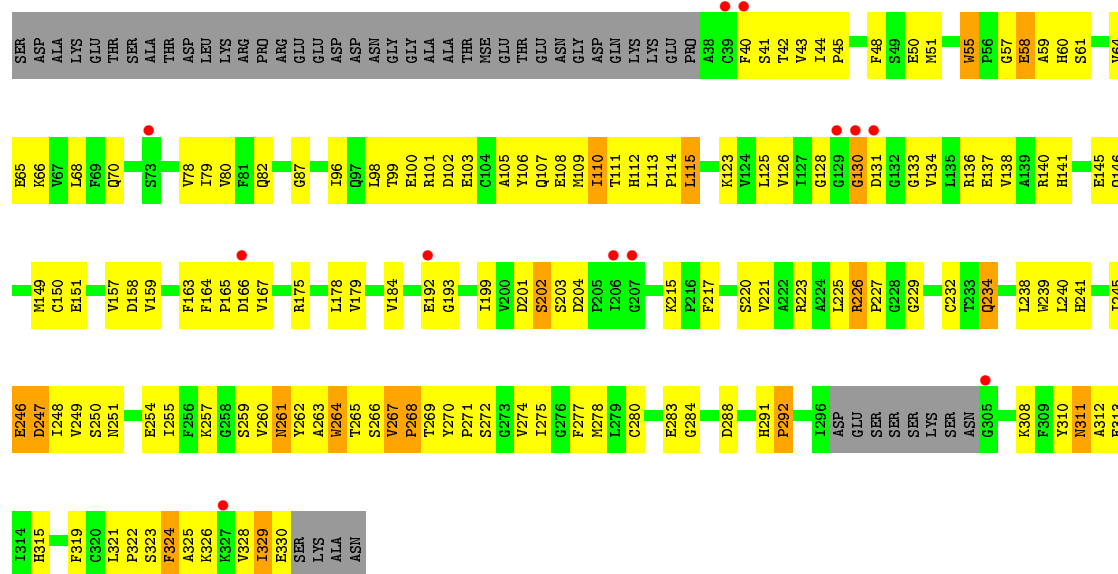
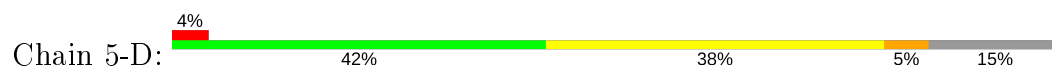
• Molecule 1: Spermidine synthase 1



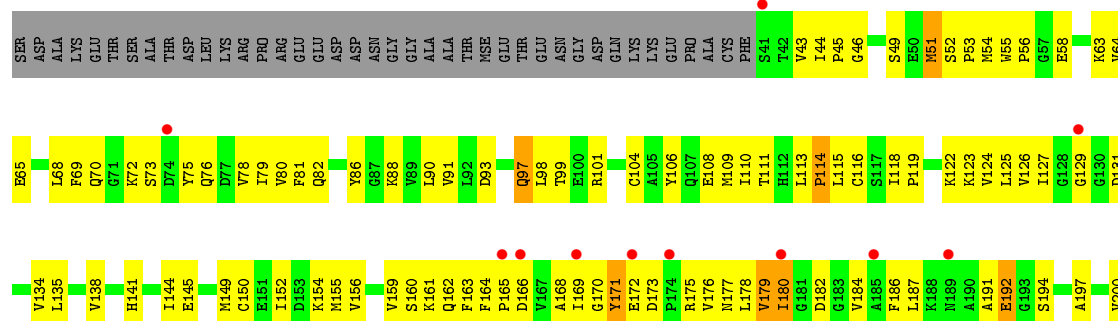


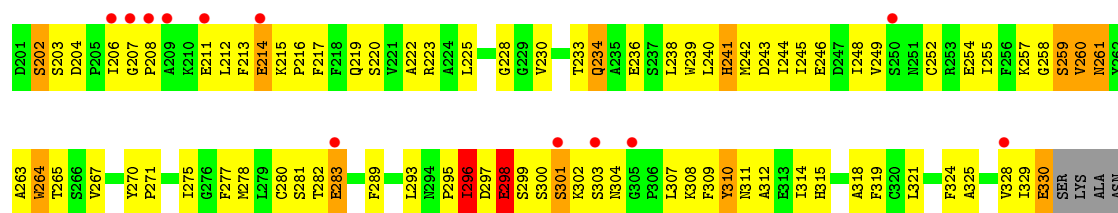


• Molecule 1: Spermidine synthase 1

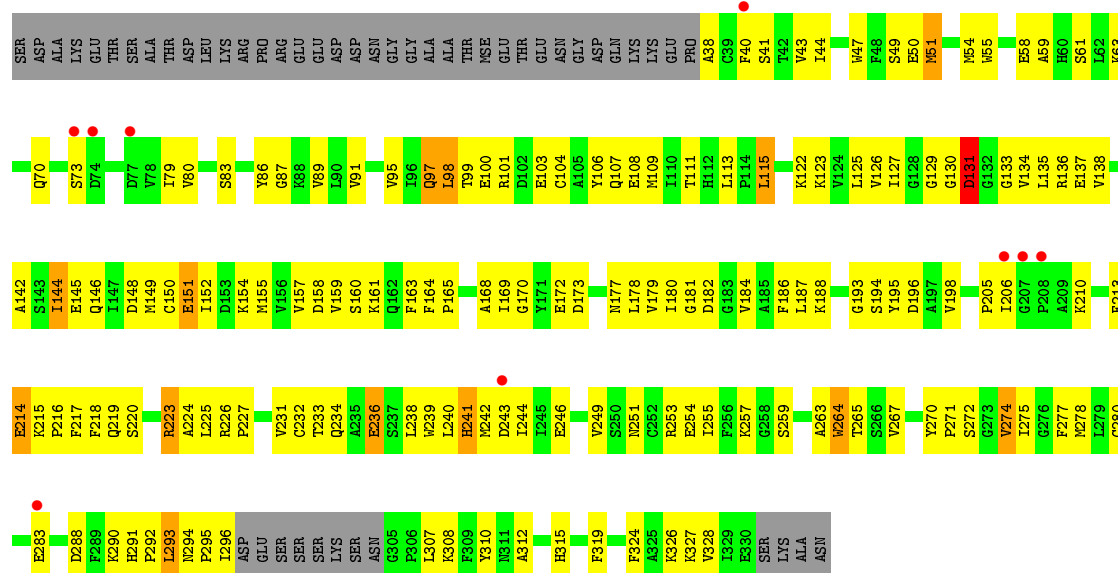


• Molecule 1: Spermidine synthase 1

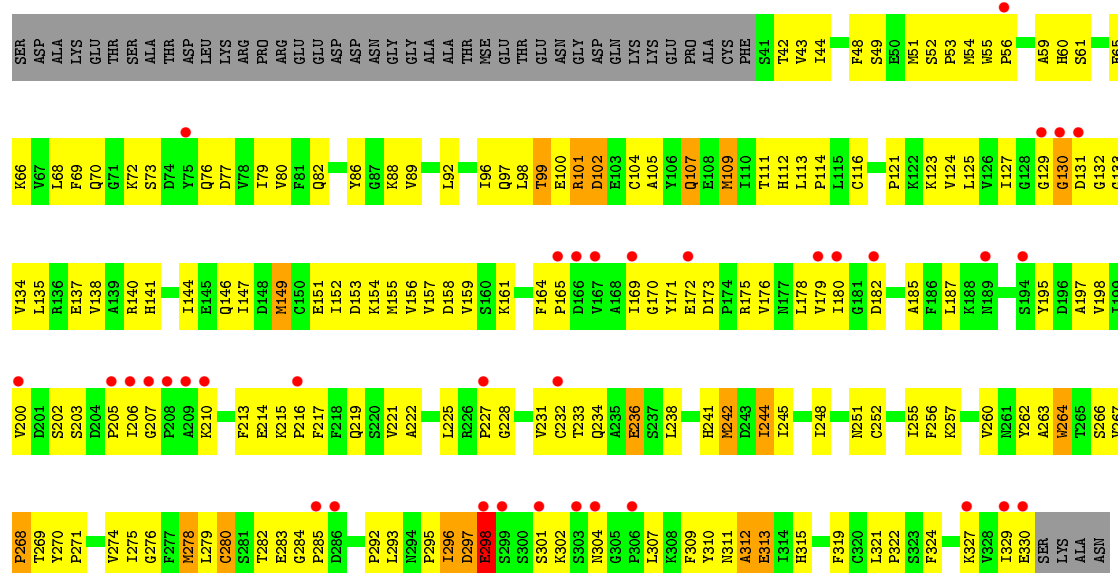




• Molecule 1: Spermidine synthase 1



• Molecule 1: Spermidine synthase 1



## Chain 6-D:

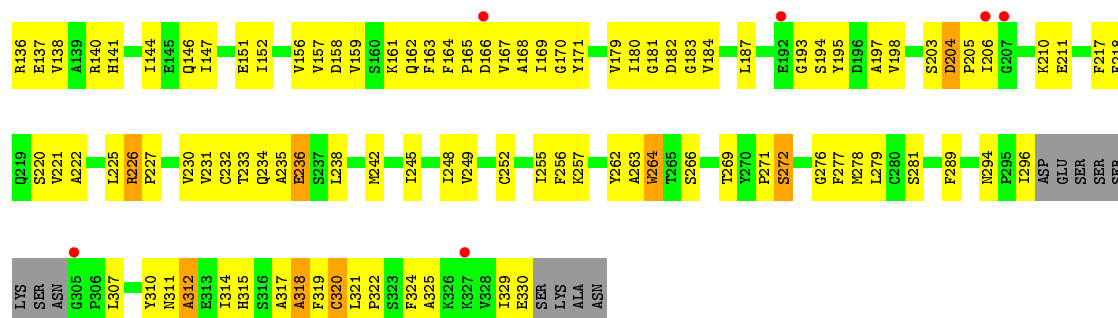


Chain 7-A:

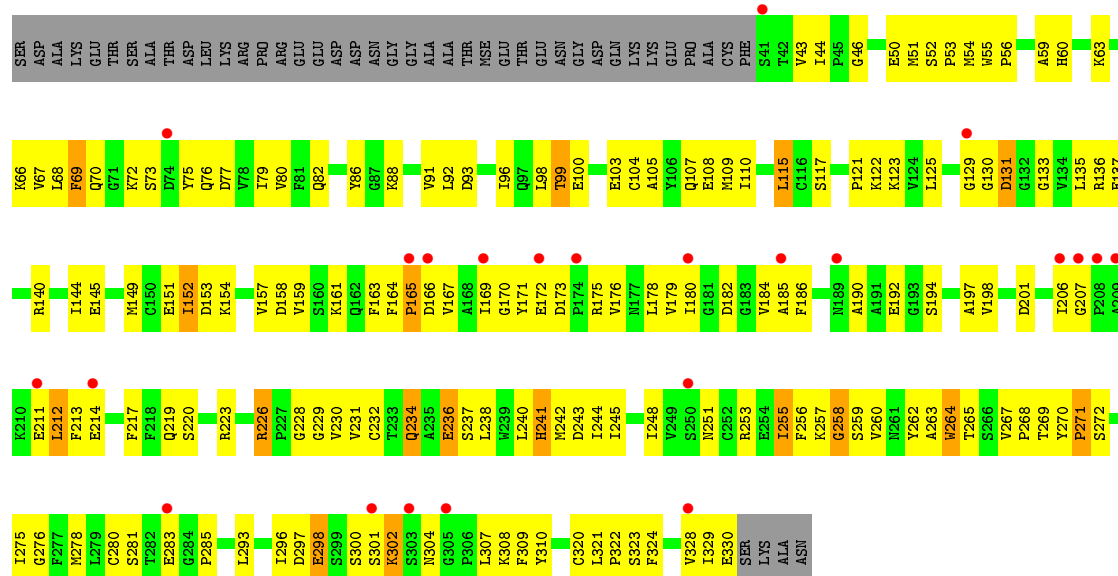


## Chain 7-B:

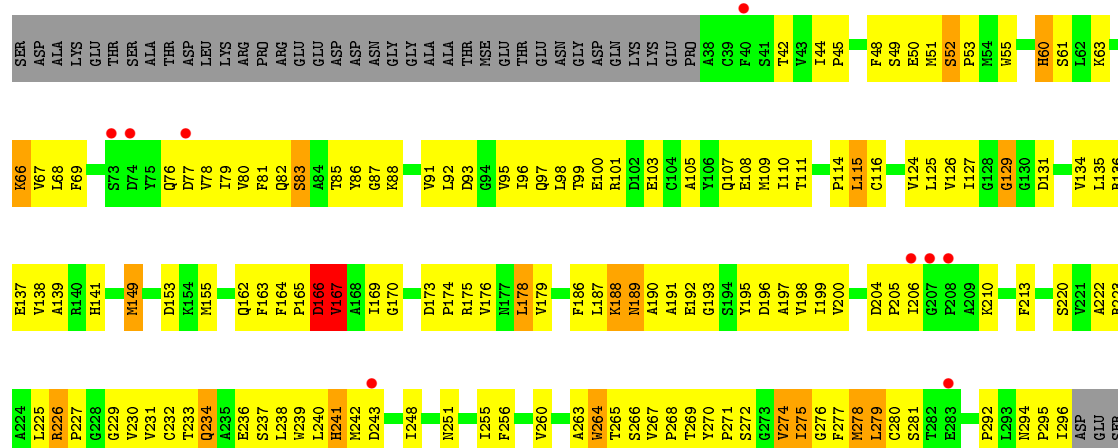


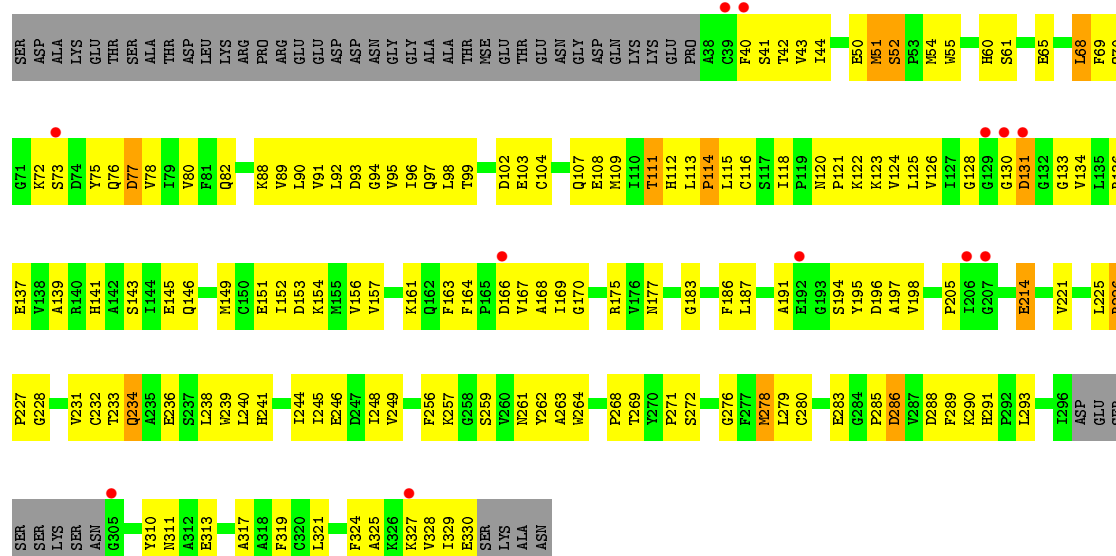


### • Molecule 1: Spermidine synthase 1



### • Molecule 1: Spermidine synthase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.81Å 95.21Å 89.16Å 90.00° 104.96° 90.00°	Depositor
Resolution (Å)	26.29 – 2.70 26.28 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.5 (26.29-2.70) 94.0 (26.28-2.66)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.164 , 0.249 0.167 , 0.247	Depositor DCC
$R_{free}$ test set	3788 reflections (9.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	75520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	1-A	0.37	0/2282	0.61	0/3089
1	1-B	0.39	0/2246	0.61	0/3040
1	1-C	0.37	0/2282	0.62	0/3089
1	1-D	0.39	0/2246	0.61	0/3040
1	2-A	0.36	0/2282	0.60	0/3089
1	2-B	0.39	0/2246	0.62	0/3040
1	2-C	0.37	0/2282	0.62	0/3089
1	2-D	0.39	0/2246	0.62	0/3040
1	3-A	0.37	0/2282	0.61	0/3089
1	3-B	0.40	0/2246	0.62	0/3040
1	3-C	0.38	0/2282	0.61	0/3089
1	3-D	0.39	0/2246	0.62	0/3040
1	4-A	0.38	0/2282	0.59	0/3089
1	4-B	0.41	0/2246	0.63	1/3040 (0.0%)
1	4-C	0.38	0/2282	0.62	0/3089
1	4-D	0.38	0/2246	0.61	0/3040
1	5-A	0.39	0/2282	0.63	0/3089
1	5-B	0.43	0/2246	0.65	1/3040 (0.0%)
1	5-C	0.40	0/2282	0.64	0/3089
1	5-D	0.41	0/2246	0.65	0/3040
1	6-A	0.40	0/2282	0.63	0/3089
1	6-B	0.41	0/2246	0.63	0/3040
1	6-C	0.39	0/2282	0.64	0/3089
1	6-D	0.40	0/2246	0.65	0/3040
1	7-A	0.38	0/2282	0.63	0/3089
1	7-B	0.40	0/2246	0.62	0/3040
1	7-C	0.41	0/2282	0.64	0/3089
1	7-D	0.41	0/2246	0.64	0/3040
1	8-A	0.39	0/2282	0.63	0/3089
1	8-B	0.41	0/2246	0.63	0/3040
1	8-C	0.41	0/2282	0.66	0/3089
1	8-D	0.41	0/2246	0.64	0/3040
All	All	0.39	0/72448	0.63	2/98064 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	4-B	109	MSE	CA-CB-CG	-6.46	102.32	113.30
1	5-B	109	MSE	CB-CA-C	5.31	121.01	110.40

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	1-A	2234	0	2199	160	0
1	1-B	2198	0	2168	122	0
1	1-C	2234	0	2199	148	0
1	1-D	2198	0	2168	142	0
1	2-A	2234	0	2199	181	0
1	2-B	2198	0	2168	140	0
1	2-C	2234	0	2199	167	0
1	2-D	2198	0	2168	128	0
1	3-A	2234	0	2199	152	0
1	3-B	2198	0	2168	180	0
1	3-C	2234	0	2199	213	0
1	3-D	2198	0	2168	126	0
1	4-A	2234	0	2199	204	0
1	4-B	2198	0	2168	154	0
1	4-C	2234	0	2199	172	0
1	4-D	2198	0	2168	155	0
1	5-A	2234	0	2199	188	0
1	5-B	2198	0	2168	115	0
1	5-C	2234	0	2199	150	0
1	5-D	2198	0	2168	149	0
1	6-A	2234	0	2199	209	0
1	6-B	2198	0	2168	148	0
1	6-C	2234	0	2199	200	0
1	6-D	2198	0	2168	140	0
1	7-A	2234	0	2199	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7-B	2198	0	2168	136	0
1	7-C	2234	0	2199	161	0
1	7-D	2198	0	2168	156	0
1	8-A	2234	0	2199	162	0
1	8-B	2198	0	2168	169	0
1	8-C	2234	0	2199	146	0
1	8-D	2198	0	2168	167	0
2	1-A	130	0	0	4	0
2	1-B	177	0	0	10	0
2	1-C	135	0	0	9	0
2	1-D	134	0	0	6	0
2	2-A	137	0	0	5	0
2	2-B	179	0	0	13	0
2	2-C	129	0	0	9	0
2	2-D	131	0	0	8	0
2	3-A	135	0	0	6	0
2	3-B	175	0	0	10	0
2	3-C	132	0	0	16	0
2	3-D	134	0	0	4	0
2	4-A	134	0	0	10	0
2	4-B	173	0	0	11	0
2	4-C	135	0	0	15	0
2	4-D	134	0	0	6	0
2	5-A	134	0	0	7	0
2	5-B	171	0	0	14	0
2	5-C	138	0	0	7	0
2	5-D	133	0	0	16	0
2	6-A	135	0	0	7	0
2	6-B	176	0	0	12	0
2	6-C	132	0	0	7	0
2	6-D	133	0	0	9	0
2	7-A	128	0	0	13	0
2	7-B	177	0	0	12	0
2	7-C	133	0	0	9	0
2	7-D	138	0	0	13	0
2	8-A	135	0	0	7	0
2	8-B	173	0	0	16	0
2	8-C	133	0	0	7	0
2	8-D	135	0	0	14	0
All	All	75520	0	69872	4966	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 35.

The worst 5 of 4966 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:124:VAL:HG22	1:C:197:ALA:HB3	1.25	1.18
1:A:135:LEU:HD22	1:A:149:MSE:HE2	1.28	1.14
1:A:241:HIS:HB3	2:A:427:HOH:O	1.45	1.13
1:A:238:LEU:HA	1:A:242:MSE:HE3	1.37	1.06
1:C:198:VAL:HB	1:C:231:VAL:HG22	1.34	1.04

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	1-A	288/334 (86%)	244 (85%)	33 (12%)	11 (4%)	3	7
1	1-B	281/334 (84%)	241 (86%)	33 (12%)	7 (2%)	5	14
1	1-C	288/334 (86%)	249 (86%)	29 (10%)	10 (4%)	3	8
1	1-D	281/334 (84%)	227 (81%)	44 (16%)	10 (4%)	3	7
1	2-A	288/334 (86%)	243 (84%)	32 (11%)	13 (4%)	2	5
1	2-B	281/334 (84%)	245 (87%)	31 (11%)	5 (2%)	8	21
1	2-C	288/334 (86%)	242 (84%)	33 (12%)	13 (4%)	2	5
1	2-D	281/334 (84%)	246 (88%)	28 (10%)	7 (2%)	5	14
1	3-A	288/334 (86%)	243 (84%)	31 (11%)	14 (5%)	2	4
1	3-B	281/334 (84%)	217 (77%)	47 (17%)	17 (6%)	1	2
1	3-C	288/334 (86%)	229 (80%)	46 (16%)	13 (4%)	2	5
1	3-D	281/334 (84%)	244 (87%)	33 (12%)	4 (1%)	11	28
1	4-A	288/334 (86%)	242 (84%)	31 (11%)	15 (5%)	2	3
1	4-B	281/334 (84%)	243 (86%)	28 (10%)	10 (4%)	3	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-C	288/334 (86%)	243 (84%)	30 (10%)	15 (5%)	2	3
1	4-D	281/334 (84%)	233 (83%)	40 (14%)	8 (3%)	5	11
1	5-A	288/334 (86%)	232 (81%)	44 (15%)	12 (4%)	3	5
1	5-B	281/334 (84%)	242 (86%)	33 (12%)	6 (2%)	7	18
1	5-C	288/334 (86%)	233 (81%)	42 (15%)	13 (4%)	2	5
1	5-D	281/334 (84%)	225 (80%)	42 (15%)	14 (5%)	2	4
1	6-A	288/334 (86%)	241 (84%)	31 (11%)	16 (6%)	2	3
1	6-B	281/334 (84%)	234 (83%)	35 (12%)	12 (4%)	2	5
1	6-C	288/334 (86%)	238 (83%)	36 (12%)	14 (5%)	2	4
1	6-D	281/334 (84%)	234 (83%)	35 (12%)	12 (4%)	2	5
1	7-A	288/334 (86%)	234 (81%)	39 (14%)	15 (5%)	2	3
1	7-B	281/334 (84%)	247 (88%)	32 (11%)	2 (1%)	22	46
1	7-C	288/334 (86%)	248 (86%)	25 (9%)	15 (5%)	2	3
1	7-D	281/334 (84%)	235 (84%)	36 (13%)	10 (4%)	3	7
1	8-A	288/334 (86%)	249 (86%)	27 (9%)	12 (4%)	3	5
1	8-B	281/334 (84%)	229 (82%)	41 (15%)	11 (4%)	3	6
1	8-C	288/334 (86%)	242 (84%)	37 (13%)	9 (3%)	4	9
1	8-D	281/334 (84%)	240 (85%)	36 (13%)	5 (2%)	8	21
All	All	9104/10688 (85%)	7634 (84%)	1120 (12%)	350 (4%)	3	7

5 of 350 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	69	PHE
1	1-A	298	GLU
1	1-B	167	VAL
1	1-B	236	GLU
1	1-C	165	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	1-A	249/276 (90%)	245 (98%)	4 (2%)	62	85
1	1-B	243/276 (88%)	234 (96%)	9 (4%)	34	63
1	1-C	249/276 (90%)	244 (98%)	5 (2%)	55	81
1	1-D	243/276 (88%)	233 (96%)	10 (4%)	30	59
1	2-A	249/276 (90%)	242 (97%)	7 (3%)	43	73
1	2-B	243/276 (88%)	235 (97%)	8 (3%)	38	67
1	2-C	249/276 (90%)	240 (96%)	9 (4%)	35	64
1	2-D	243/276 (88%)	234 (96%)	9 (4%)	34	63
1	3-A	249/276 (90%)	240 (96%)	9 (4%)	35	64
1	3-B	243/276 (88%)	232 (96%)	11 (4%)	27	55
1	3-C	249/276 (90%)	237 (95%)	12 (5%)	25	53
1	3-D	243/276 (88%)	235 (97%)	8 (3%)	38	67
1	4-A	249/276 (90%)	237 (95%)	12 (5%)	25	53
1	4-B	243/276 (88%)	231 (95%)	12 (5%)	25	52
1	4-C	249/276 (90%)	239 (96%)	10 (4%)	31	60
1	4-D	243/276 (88%)	238 (98%)	5 (2%)	53	80
1	5-A	249/276 (90%)	234 (94%)	15 (6%)	19	42
1	5-B	243/276 (88%)	228 (94%)	15 (6%)	18	40
1	5-C	249/276 (90%)	240 (96%)	9 (4%)	35	64
1	5-D	243/276 (88%)	228 (94%)	15 (6%)	18	40
1	6-A	249/276 (90%)	236 (95%)	13 (5%)	23	49
1	6-B	243/276 (88%)	231 (95%)	12 (5%)	25	52
1	6-C	249/276 (90%)	238 (96%)	11 (4%)	28	56
1	6-D	243/276 (88%)	233 (96%)	10 (4%)	30	59
1	7-A	249/276 (90%)	231 (93%)	18 (7%)	14	34
1	7-B	243/276 (88%)	227 (93%)	16 (7%)	16	38
1	7-C	249/276 (90%)	244 (98%)	5 (2%)	55	81
1	7-D	243/276 (88%)	236 (97%)	7 (3%)	42	71
1	8-A	249/276 (90%)	241 (97%)	8 (3%)	39	68
1	8-B	243/276 (88%)	227 (93%)	16 (7%)	16	38
1	8-C	249/276 (90%)	241 (97%)	8 (3%)	39	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-D	243/276 (88%)	231 (95%)	12 (5%)	25	52
All	All	7872/8832 (89%)	7542 (96%)	330 (4%)	30	58

5 of 330 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5-A	260	VAL
1	5-D	226	ARG
1	8-B	226	ARG
1	5-A	306	PRO
1	5-B	264	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
1	4-C	107	GLN
1	5-B	120	ASN
1	8-B	146	GLN
1	4-C	241	HIS
1	4-D	261	ASN

### 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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	1-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	1-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	1-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	2-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	2-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	2-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	2-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	3-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	3-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	3-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	3-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	4-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	4-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	4-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	4-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	5-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	5-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	5-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	5-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	6-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	6-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	6-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	6-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	7-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	7-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	7-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	7-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	8-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	8-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	8-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	8-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
All	All	8976/10688 (83%)	0.13	640 (7%) 15 14	10, 33, 75, 112	8976 (100%)

The worst 5 of 640 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-C	207	GLY	10.5
1	2-C	207	GLY	10.5
1	3-C	207	GLY	10.5
1	4-C	207	GLY	10.5
1	5-C	207	GLY	10.5

## 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.