wwPDB X-ray Structure Validation Summary Report (i)

Jul 7, 2017 – 12:58 AM EDT

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	:	unknown
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*
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:

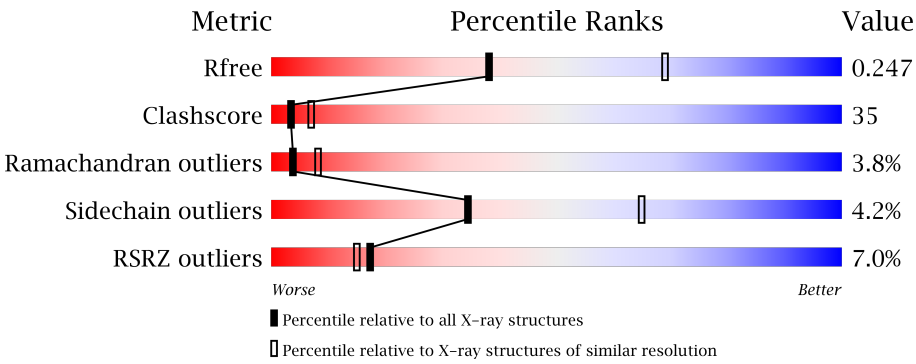
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 >=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	1-A	334	7%, 40%, 43%, •, 13%
1	1-B	334	3%, 47%, 36%, •, 15%
1	1-C	334	10%, 40%, 43%, •, 13%
1	1-D	334	4%, 43%, 38%, •, 15%
1	2-A	334	7%, 35%, 48%, •, 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	2-B	334	3% 39% 43% • 15%
1	2-C	334	10% 39% 44% • 13%
1	2-D	334	4% 47% 35% • 15%
1	3-A	334	7% 38% 44% • 13%
1	3-B	334	3% 36% 44% 5% 15%
1	3-C	334	10% 33% 47% 6% 13%
1	3-D	334	4% 45% 39% • 15%
1	4-A	334	7% 36% 46% 5% 13%
1	4-B	334	3% 41% 40% 5% 15%
1	4-C	334	10% 38% 43% 5% • 13%
1	4-D	334	4% 40% 42% • 15%
1	5-A	334	7% 34% 47% 6% 13%
1	5-B	334	3% 48% 33% • • 15%
1	5-C	334	10% 42% 41% • 13%
1	5-D	334	4% 42% 38% 5% 15%
1	6-A	334	7% 33% 48% 6% • 13%
1	6-B	334	3% 38% 43% • 15%
1	6-C	334	10% 36% 46% 5% 13%
1	6-D	334	4% 41% 41% • 15%
1	7-A	334	7% 28% 51% 7% 13%
1	7-B	334	3% 42% 39% • 15%
1	7-C	334	10% 37% 46% • 13%
1	7-D	334	4% 38% 44% • 15%
1	8-A	334	7% 38% 44% 5% 13%
1	8-B	334	3% 38% 41% 5% • 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	8-C	334	10% 42% 42% • 13%
1	8-D	334	4% 40% 41% • 15%

2 Entry composition (i)

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

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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
			Total	O		
2	1-A	130	130	130	0	0
			Total	O		
2	2-A	137	137	137	0	0
			Total	O		
2	3-A	135	135	135	0	0
			Total	O		
2	4-A	134	134	134	0	0
			Total	O		
2	5-A	134	134	134	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

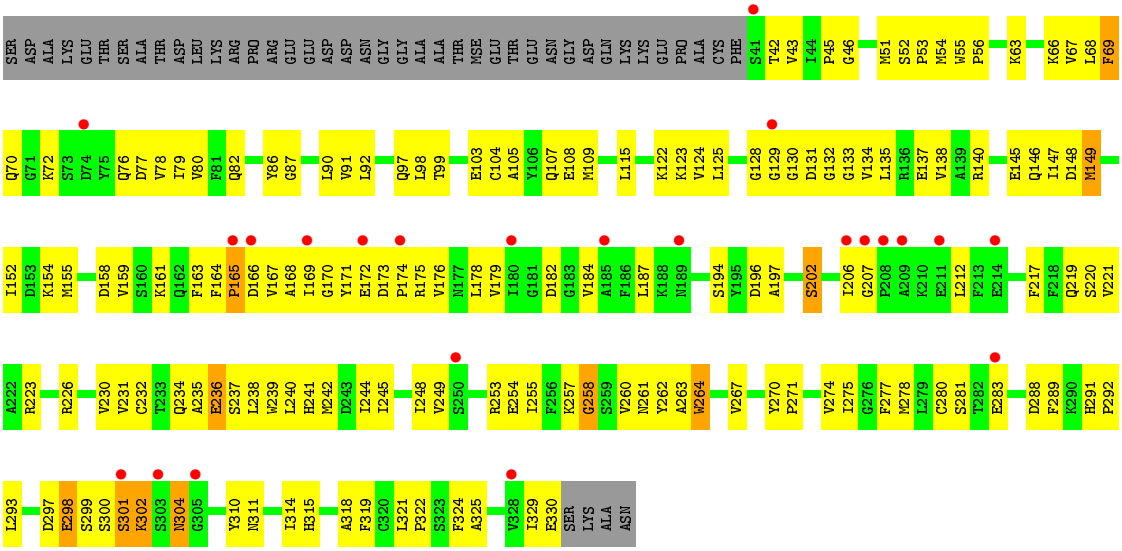
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	3-D	134	134	134	0	0
			Total	O		
2	4-D	134	134	134	0	0
			Total	O		
2	5-D	133	133	133	0	0
			Total	O		
2	6-D	133	133	133	0	0
			Total	O		
2	7-D	138	138	138	0	0
			Total	O		
2	8-D	135	135	135	0	0

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 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.

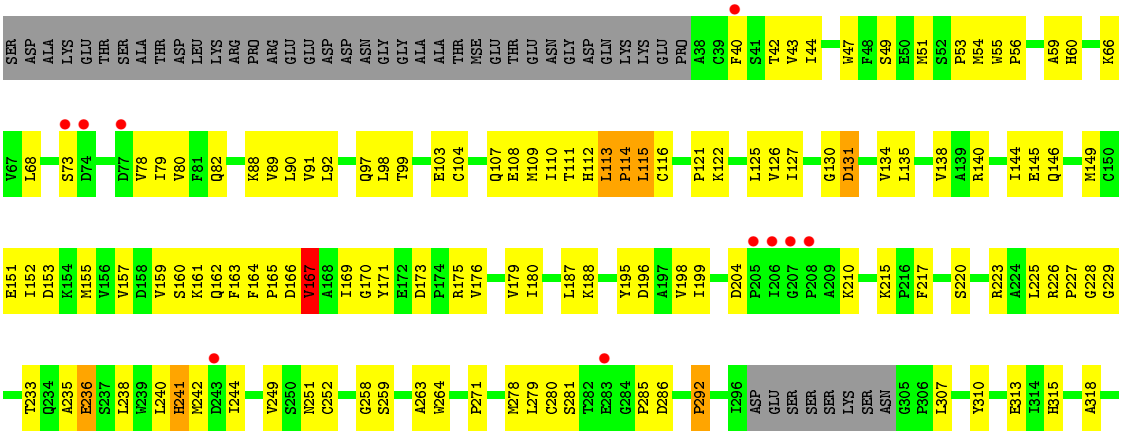
- Molecule 1: Spermidine synthase 1

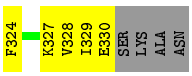
Chain 1-A:



- Molecule 1: Spermidine synthase 1

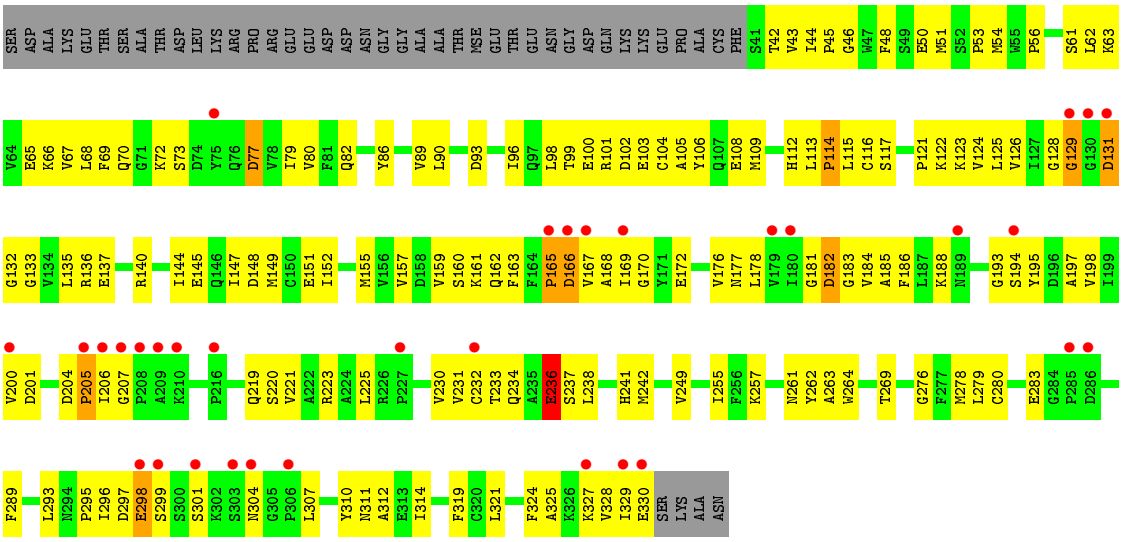
Chain 1-B:





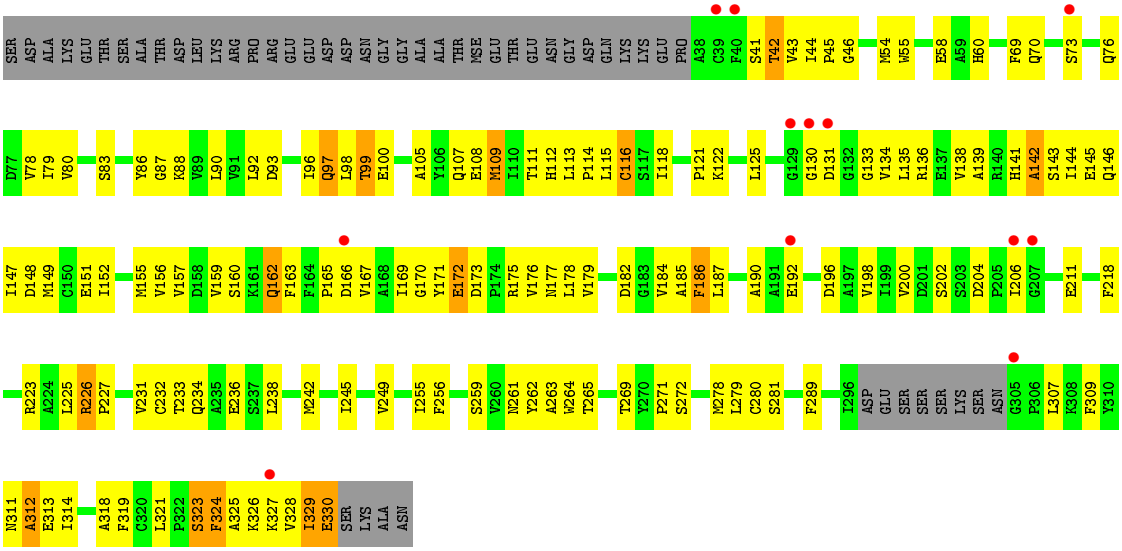
- Molecule 1: Spermidine synthase 1

Chain 1-C:



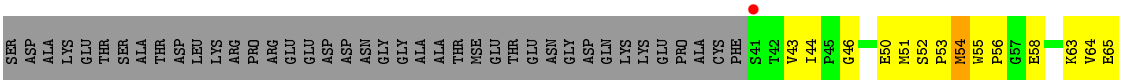
- Molecule 1: Spermidine synthase 1

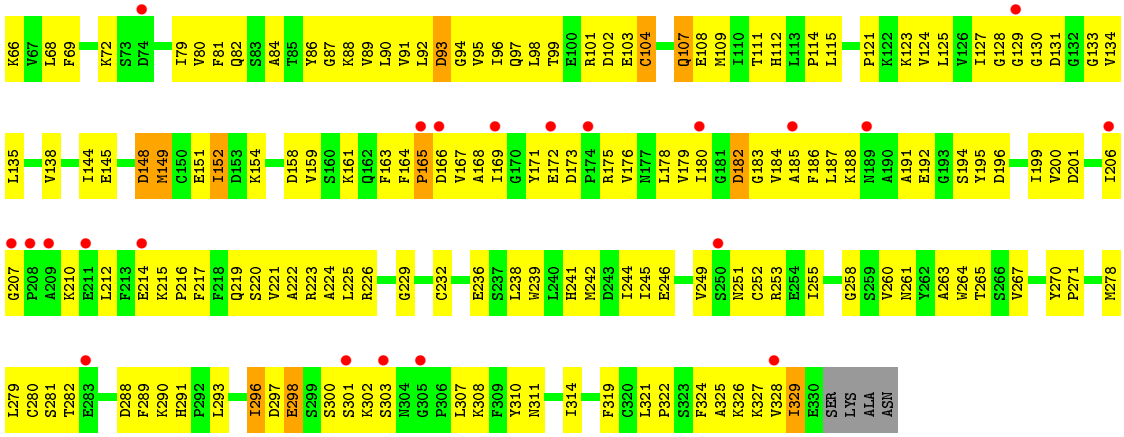
Chain 1-D:



- Molecule 1: Spermidine synthase 1

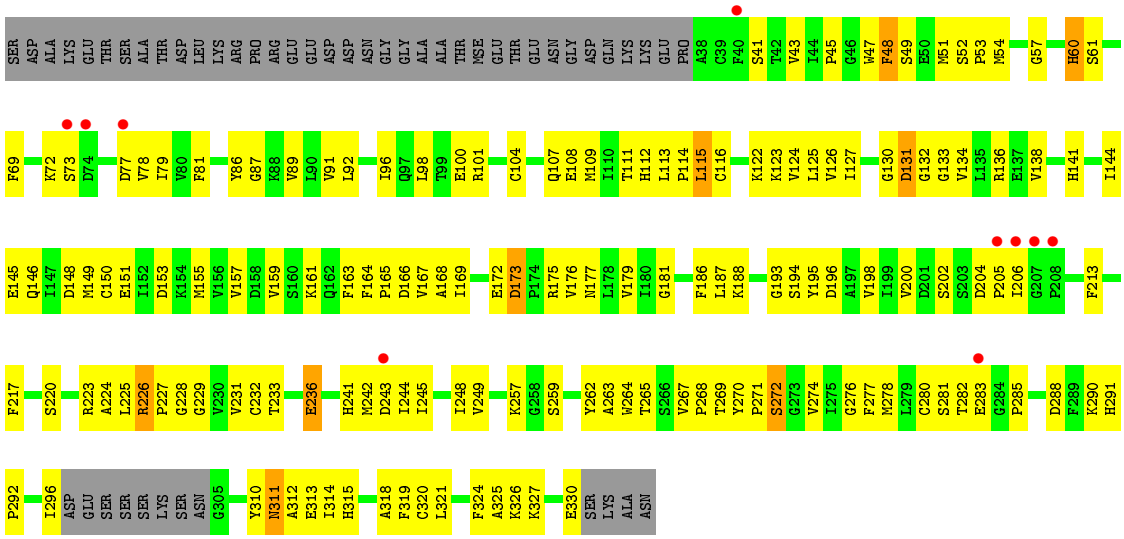
Chain 2-A:





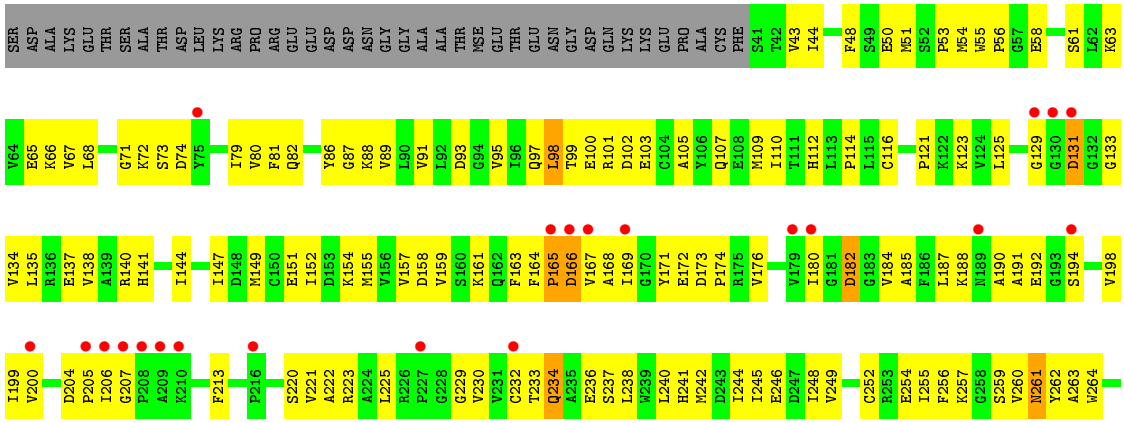
- Molecule 1: Spermidine synthase 1

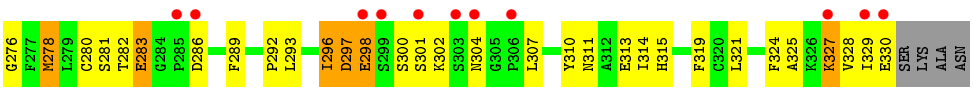
Chain 2-B:



- Molecule 1: Spermidine synthase 1

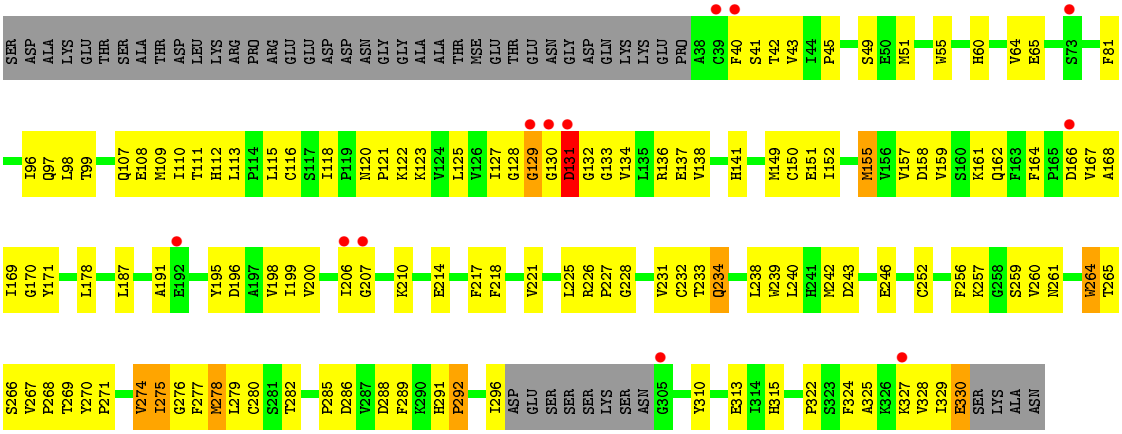
Chain 2-C:





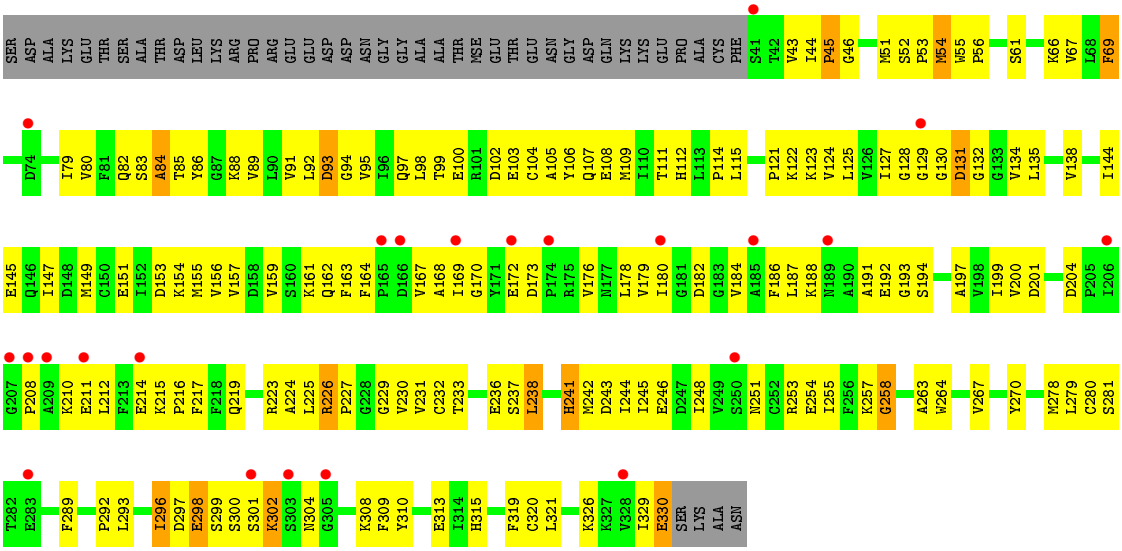
• Molecule 1: Spermidine synthase 1

Chain 2-D:



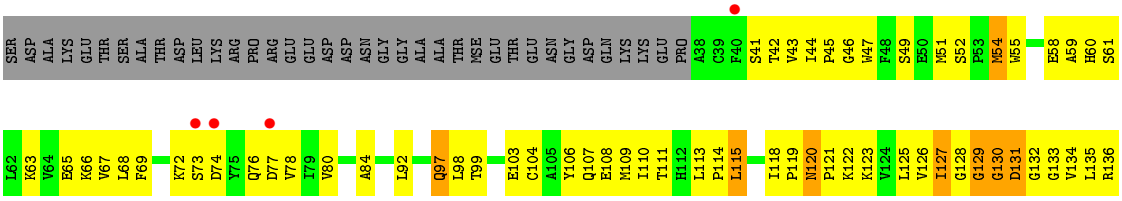
• Molecule 1: Spermidine synthase 1

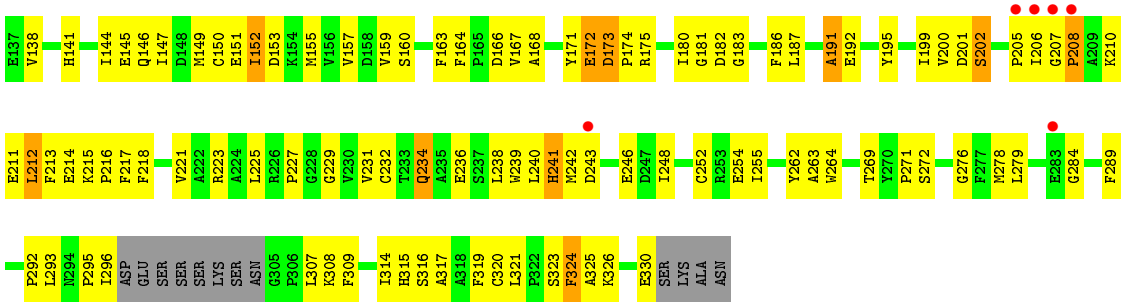
Chain 3-A:



• Molecule 1: Spermidine synthase 1

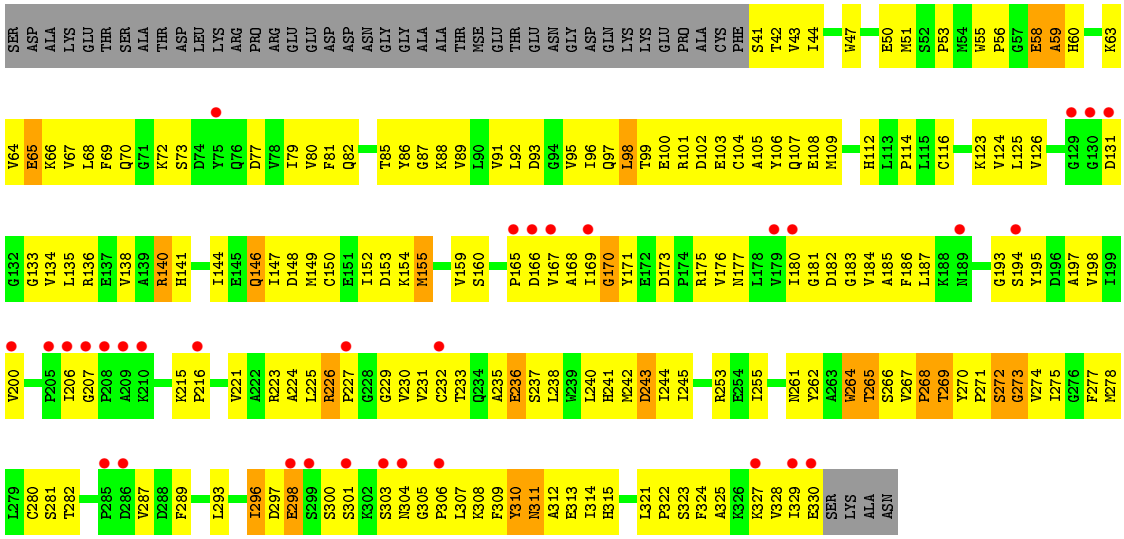
Chain 3-B:





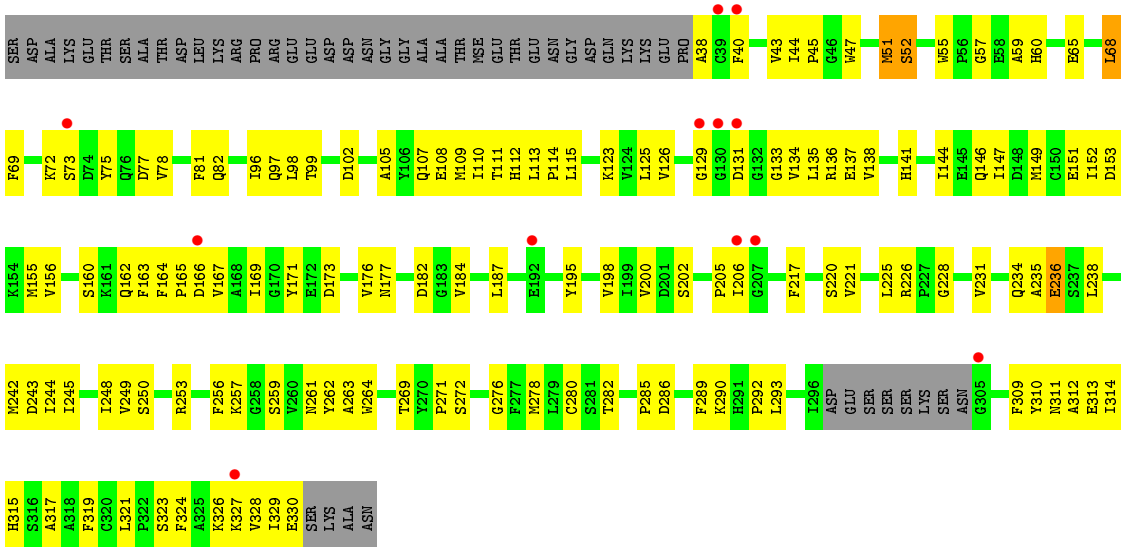
- Molecule 1: Spermidine synthase 1

Chain 3-C:



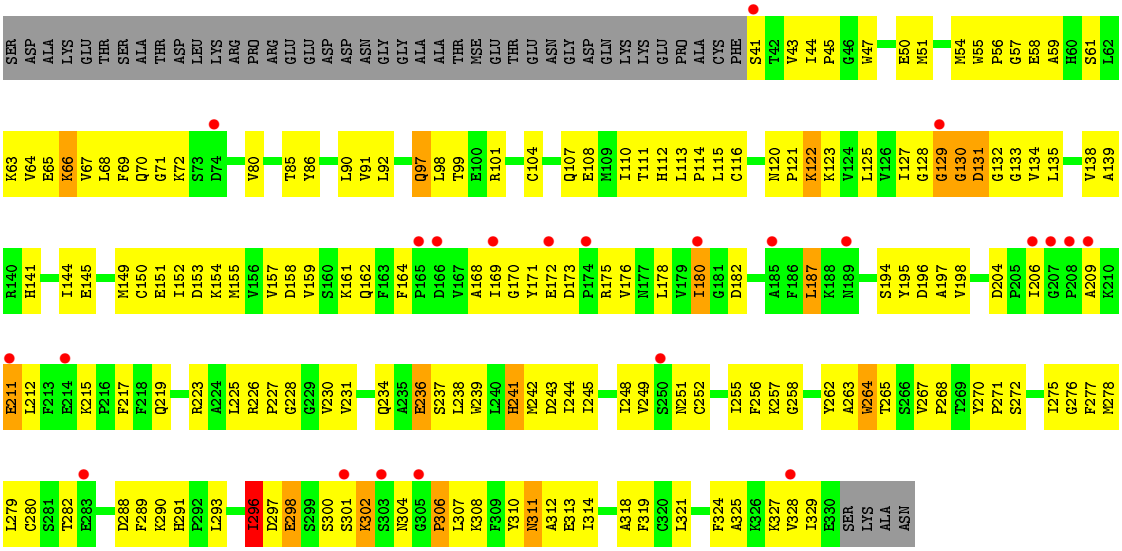
- Molecule 1: Spermidine synthase 1

Chain 3-D:



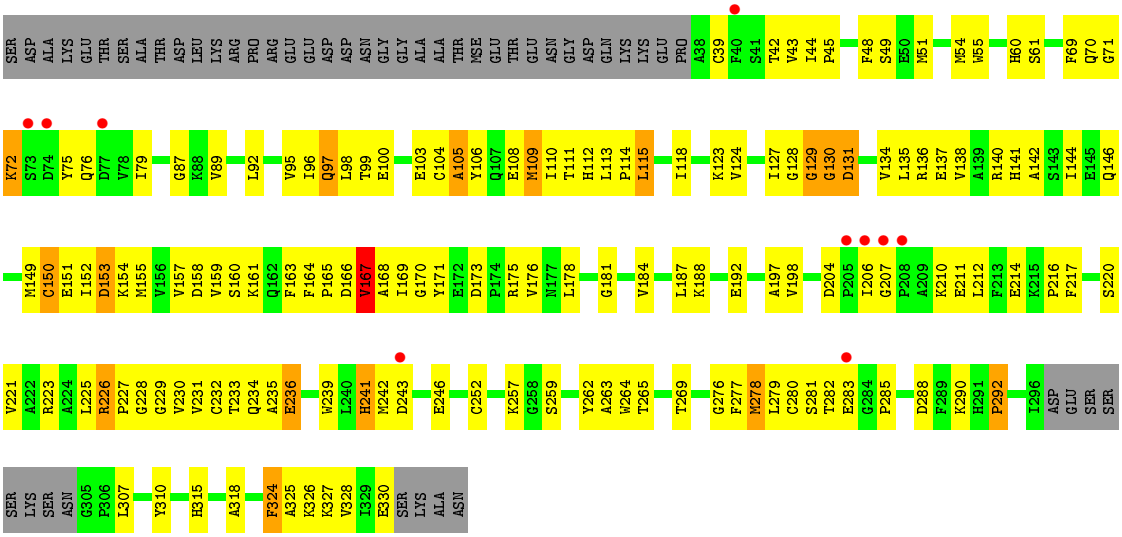
- Molecule 1: Spermidine synthase 1

Chain 4-A:



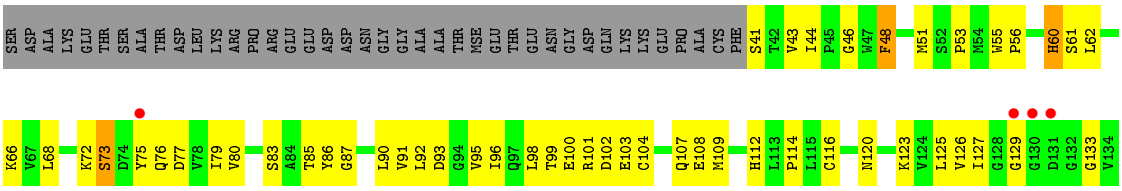
- Molecule 1: Spermidine synthase 1

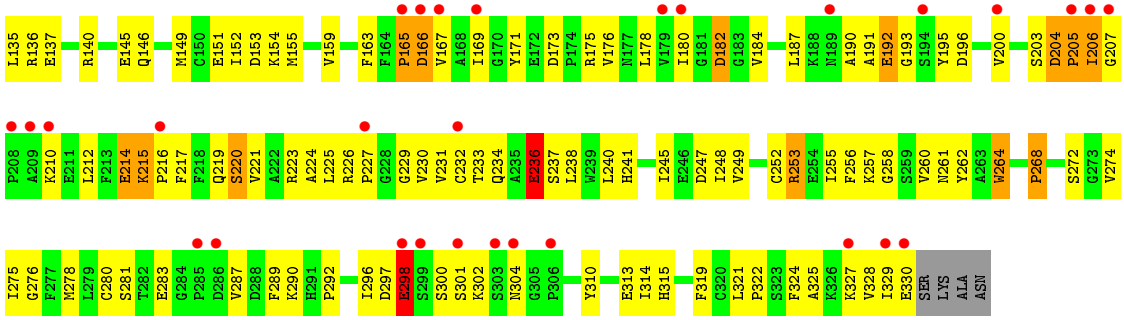
Chain 4-B:



- Molecule 1: Spermidine synthase 1

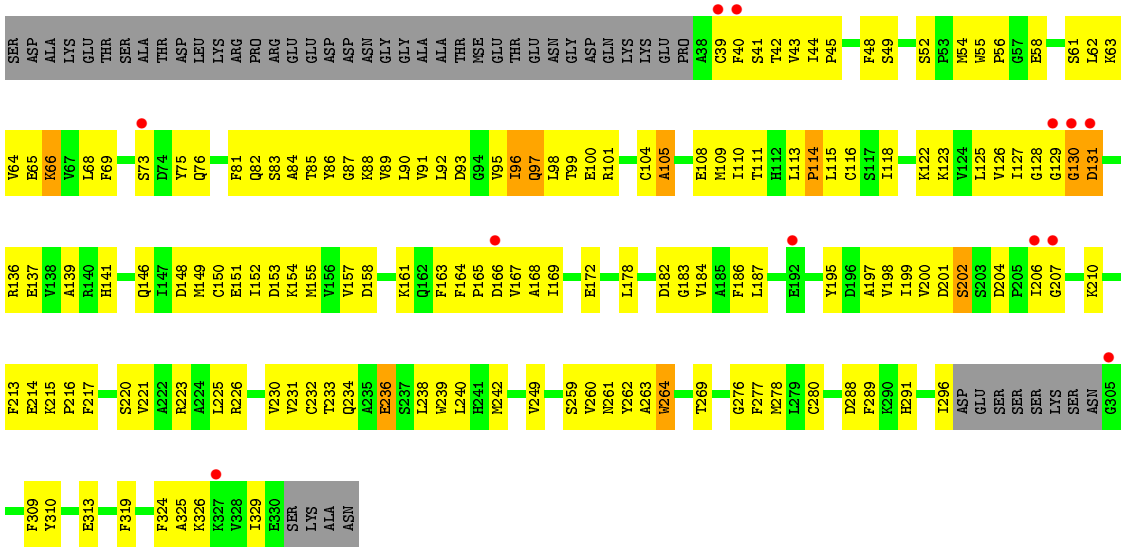
Chain 4-C:





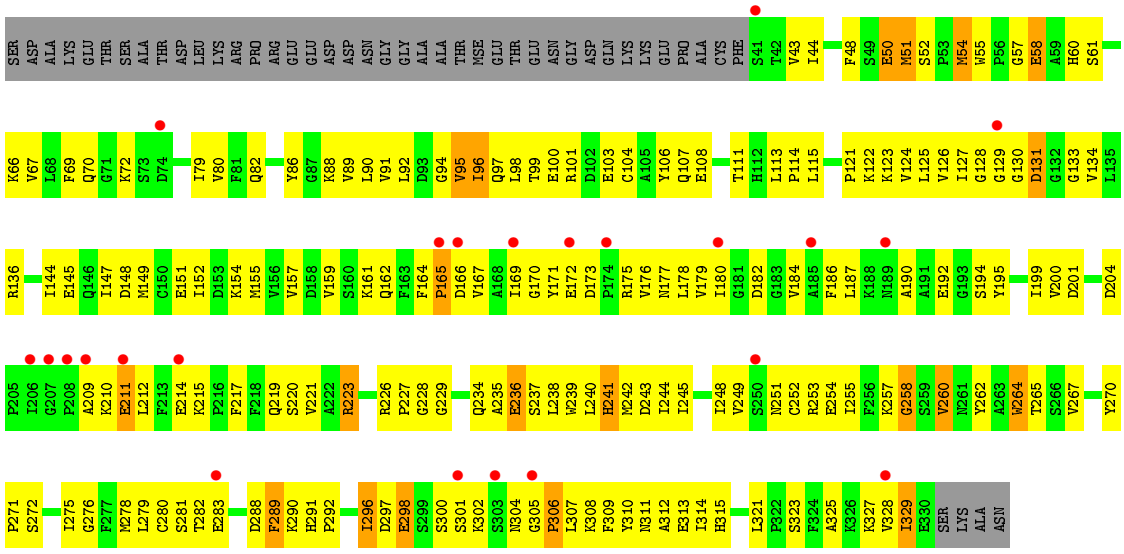
- Molecule 1: Spermidine synthase 1

Chain 4-D:



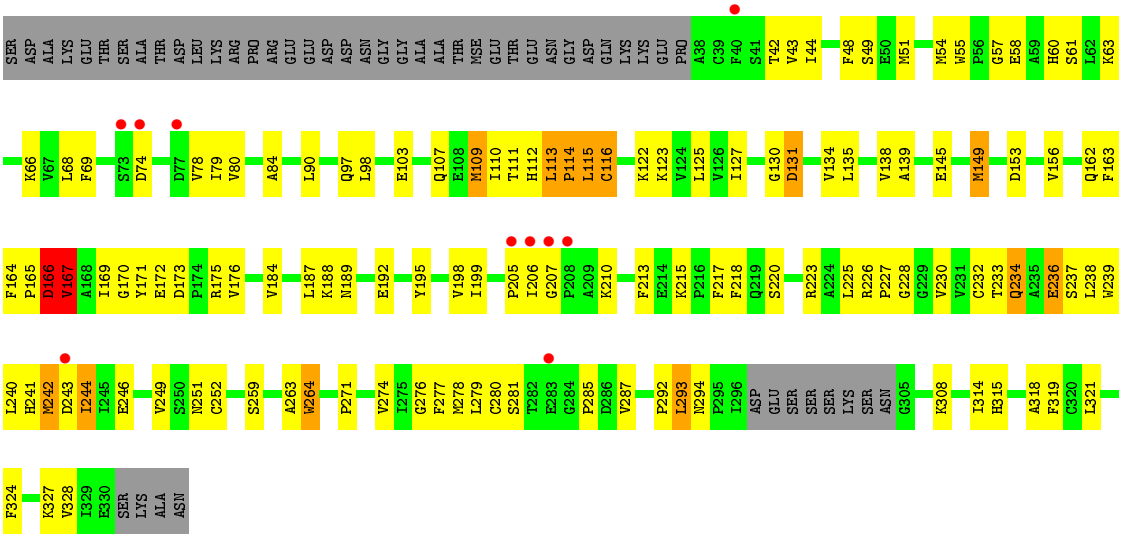
- Molecule 1: Spermidine synthase 1

Chain 5-A:



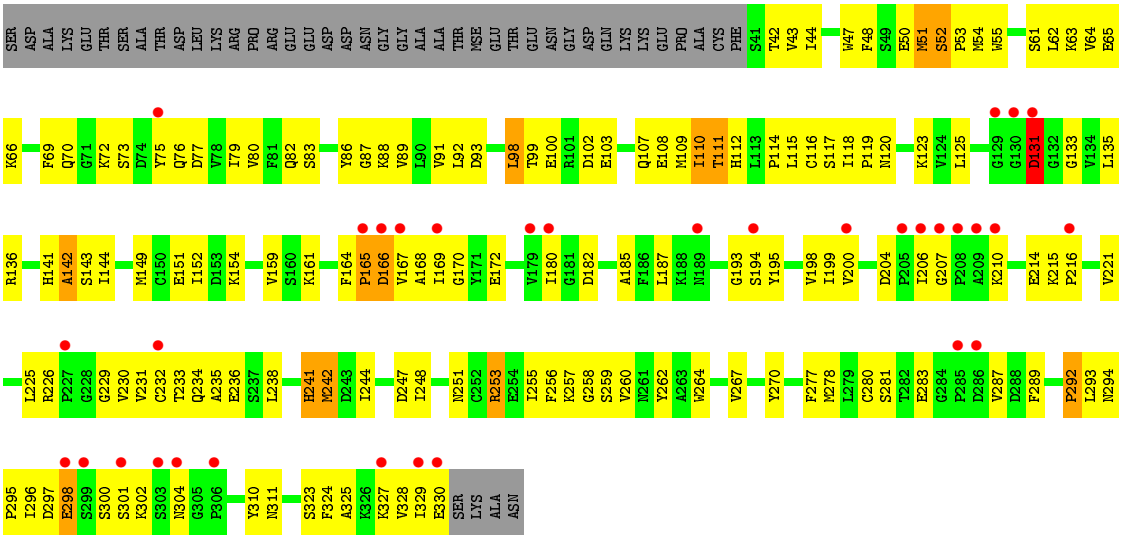
- Molecule 1: Spermidine synthase 1

Chain 5-B:



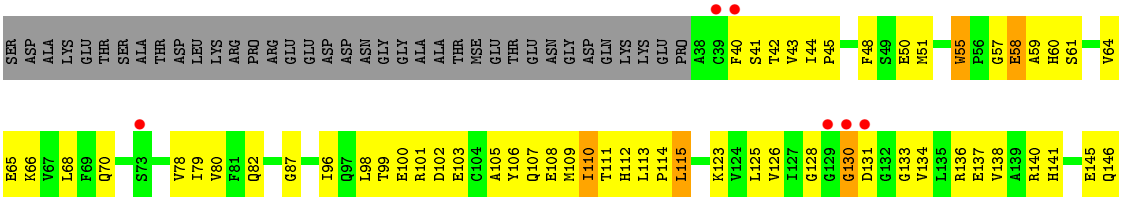
- Molecule 1: Spermidine synthase 1

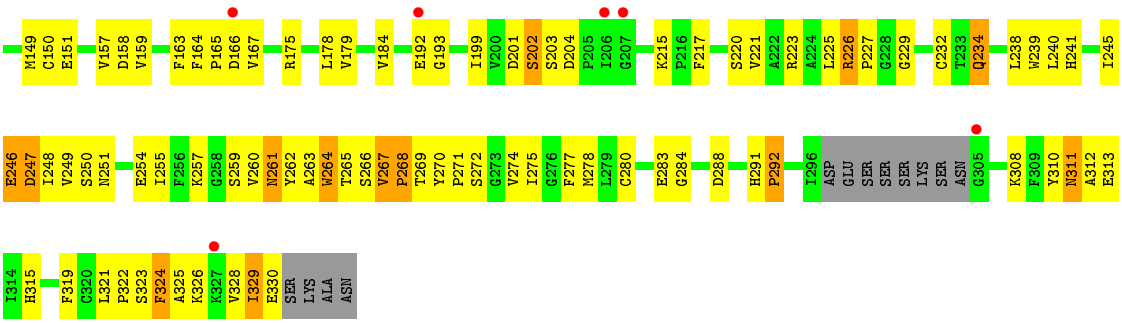
Chain 5-C:



- Molecule 1: Spermidine synthase 1

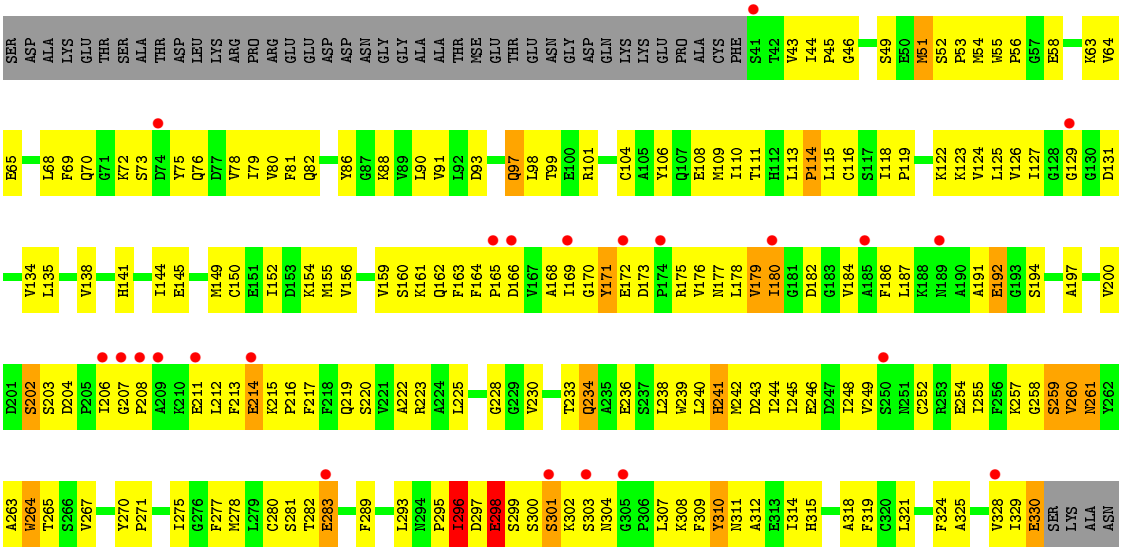
Chain 5-D:





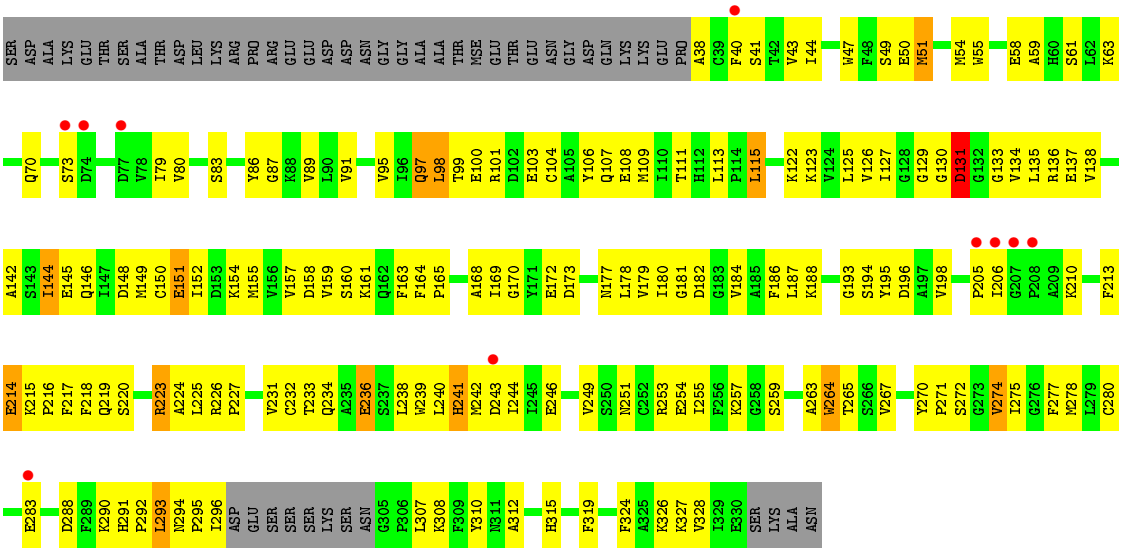
- Molecule 1: Spermidine synthase 1

Chain 6-A:



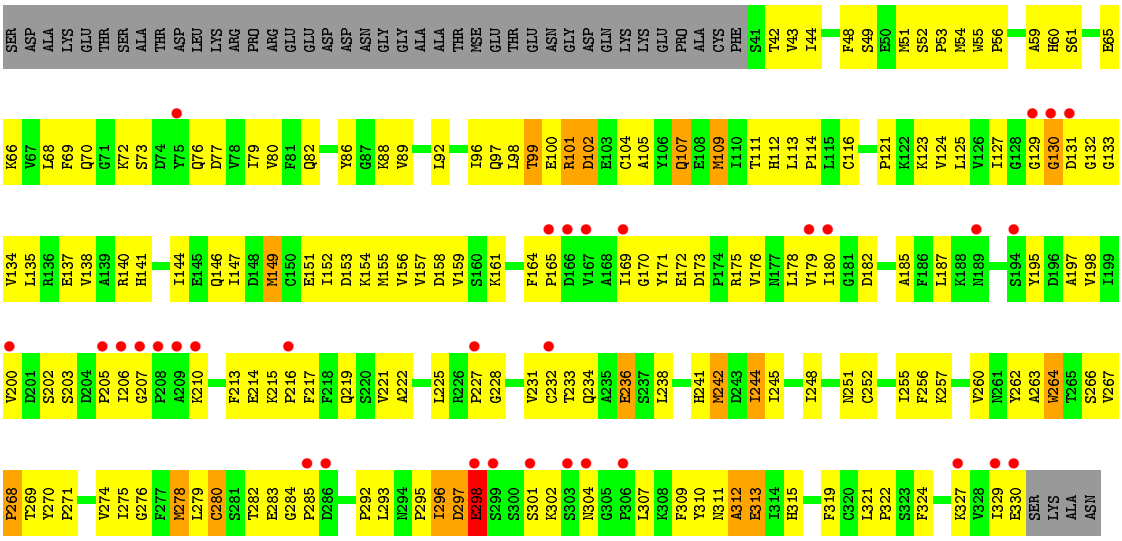
- Molecule 1: Spermidine synthase 1

Chain 6-B:



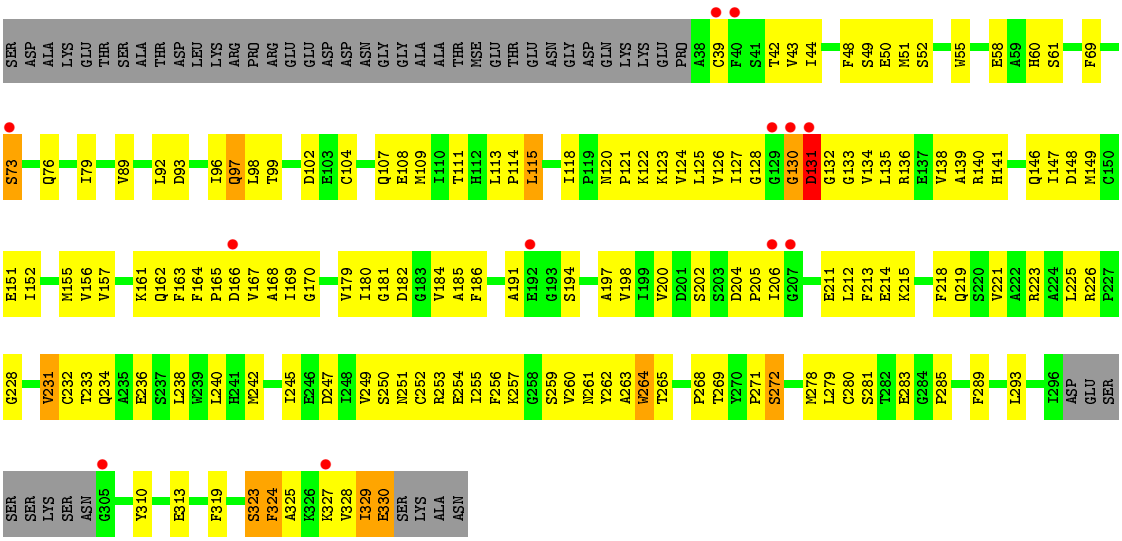
- Molecule 1: Spermidine synthase 1

Chain 6-C:



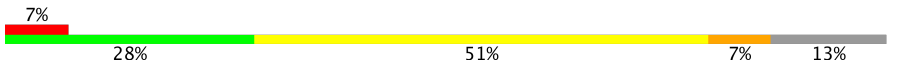
- Molecule 1: Spermidine synthase 1

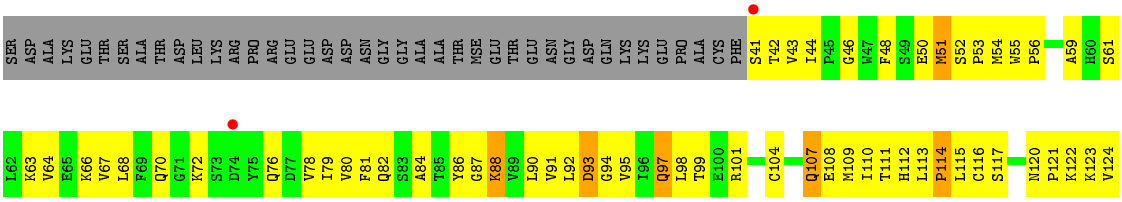
Chain 6-D:

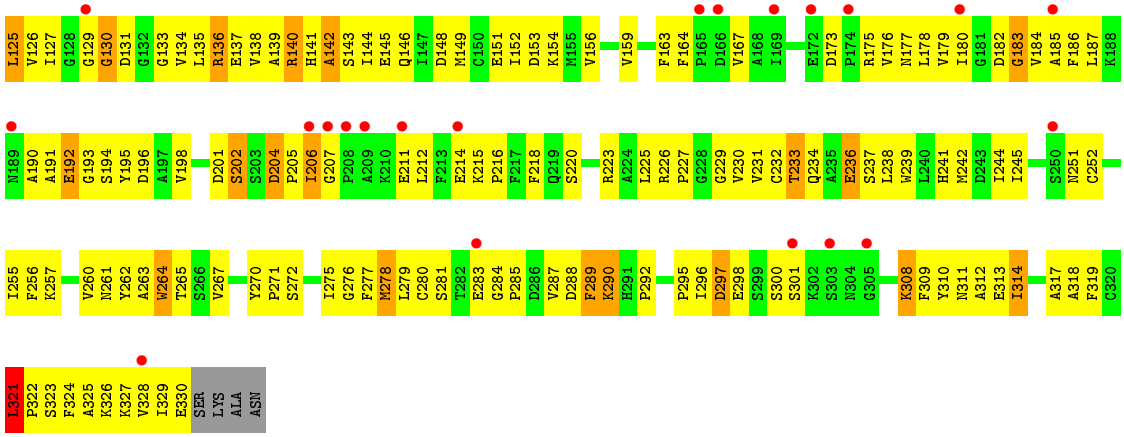


- Molecule 1: Spermidine synthase 1

Chain 7-A:

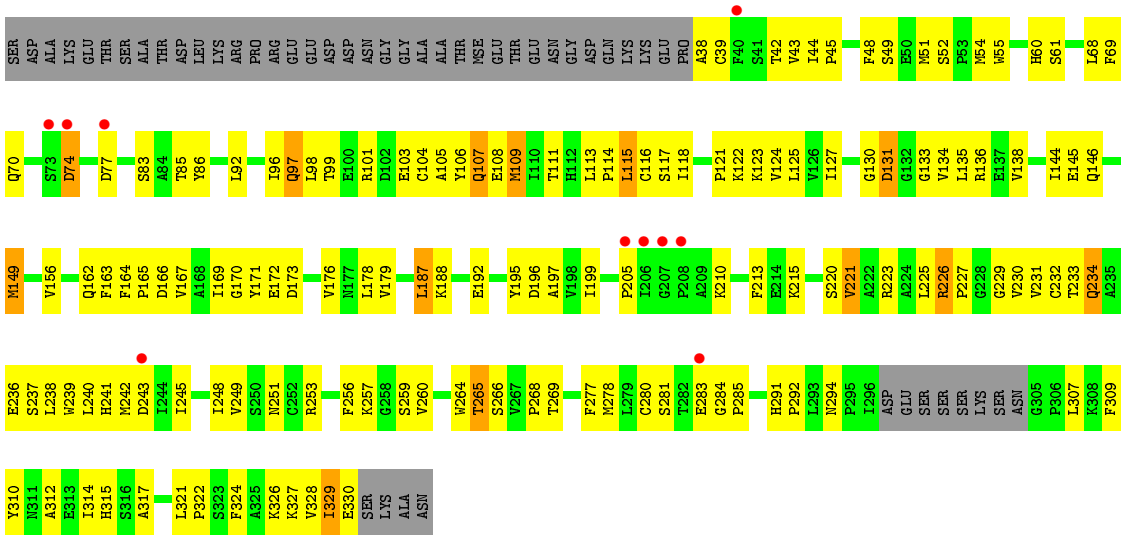






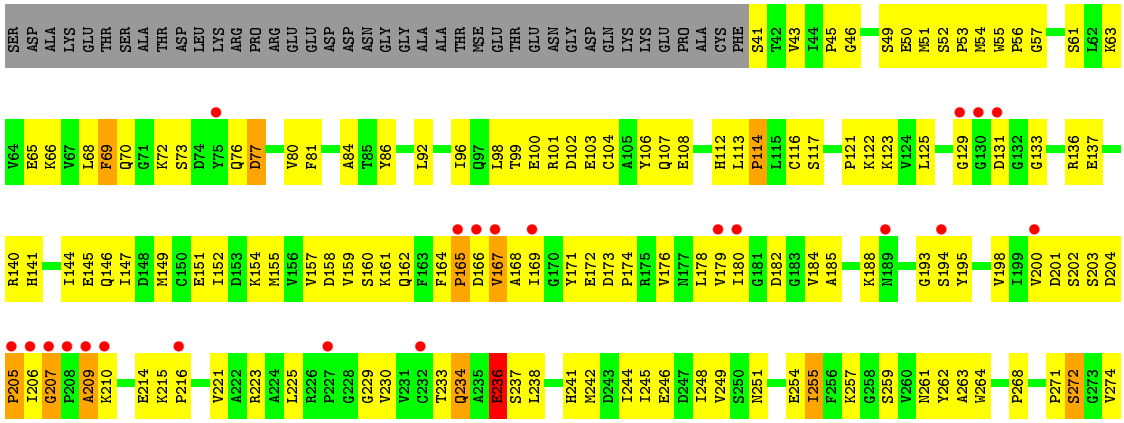
- Molecule 1: Spermidine synthase 1

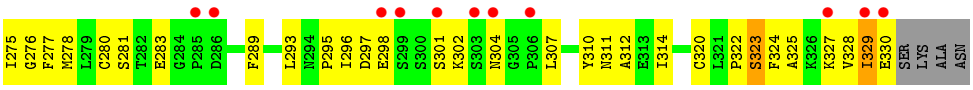
Chain 7-B:



- Molecule 1: Spermidine synthase 1

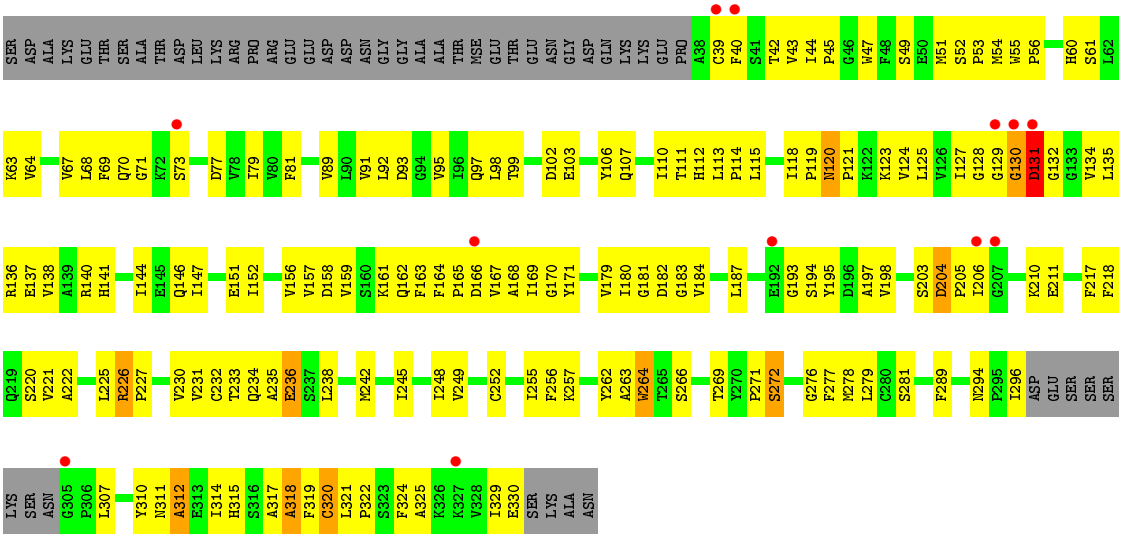
Chain 7-C:





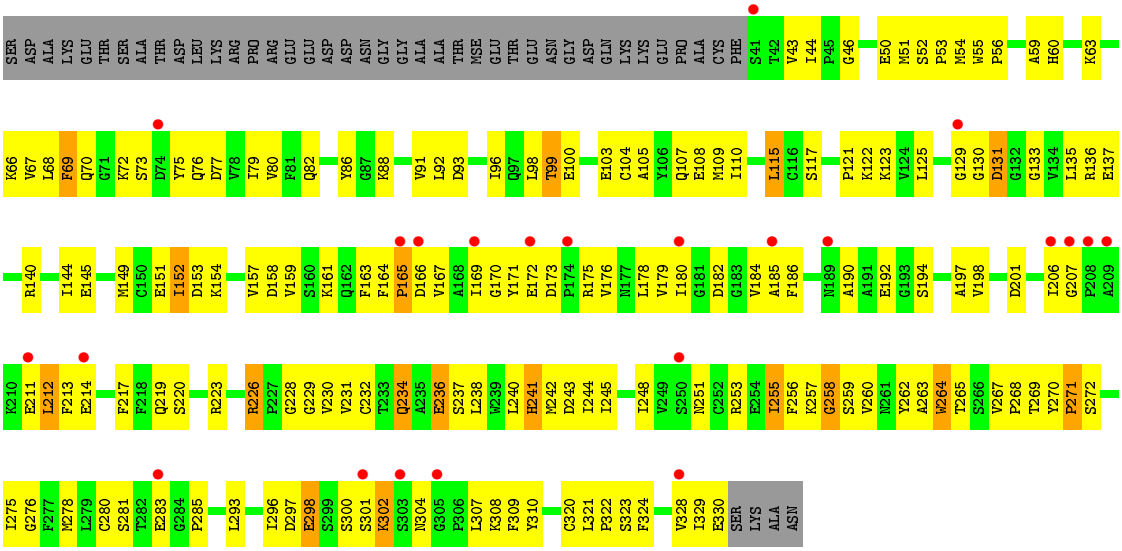
• Molecule 1: Spermidine synthase 1

Chain 7-D:



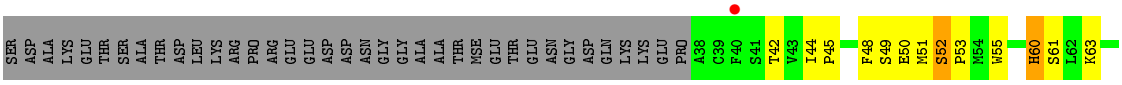
• Molecule 1: Spermidine synthase 1

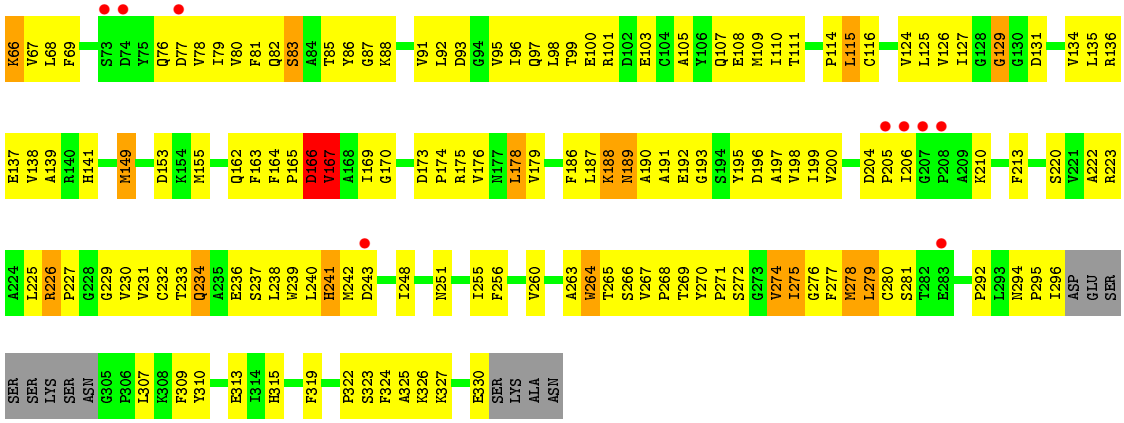
Chain 8-A:



• Molecule 1: Spermidine synthase 1

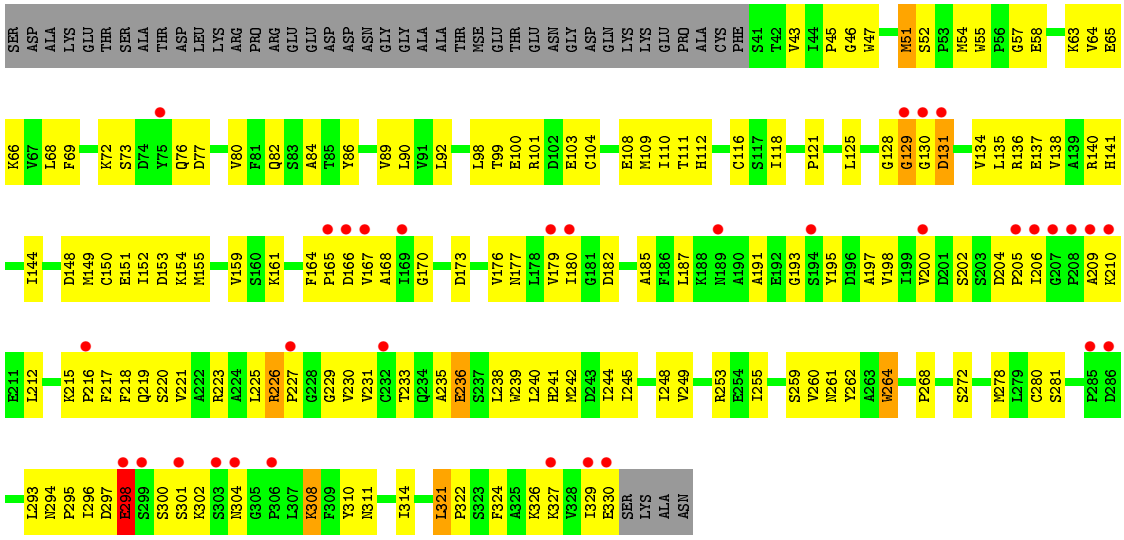
Chain 8-B:





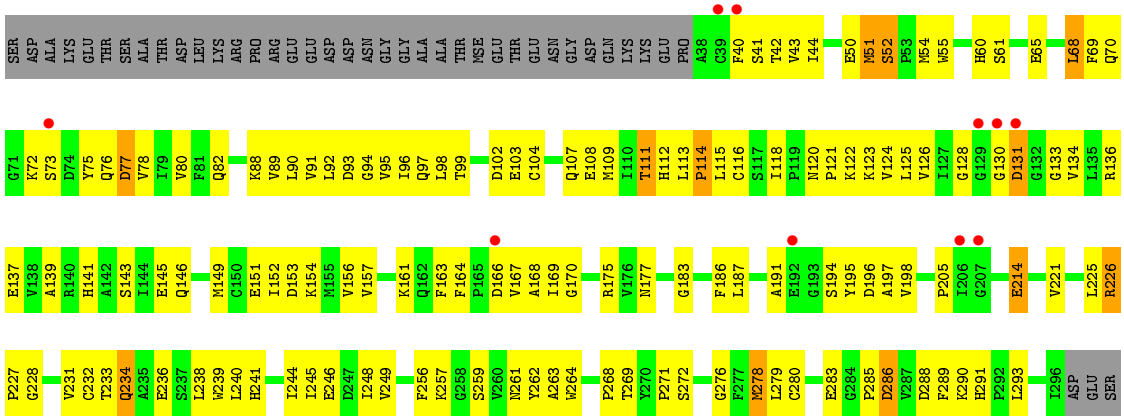
- Molecule 1: Spermidine synthase 1

Chain 8-C:



- Molecule 1: Spermidine synthase 1

Chain 8-D:



SER
SER
LYS
SER
ASN
G305
Y310
N311
A312
E313
A317
A318
F319
G320
L321
F324
A325
K326
K327
V328
I329
E330
SER
LYS
ALA
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.37 (at 2.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.164 , 0.249 0.170 , 0.247	Depositor DCC
R_{free} test set	3788 reflections (11.14%)	DCC
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 77.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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^2)	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.*

[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 (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	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(^{o})	Ideal(^{o})
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 (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	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

Continued on next page...

Continued from previous page...

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%)	4 8
1	1-B	281/334 (84%)	241 (86%)	33 (12%)	7 (2%)	6 17
1	1-C	288/334 (86%)	249 (86%)	29 (10%)	10 (4%)	4 9
1	1-D	281/334 (84%)	227 (81%)	44 (16%)	10 (4%)	4 9
1	2-A	288/334 (86%)	243 (84%)	32 (11%)	13 (4%)	3 6
1	2-B	281/334 (84%)	245 (87%)	31 (11%)	5 (2%)	10 25
1	2-C	288/334 (86%)	242 (84%)	33 (12%)	13 (4%)	3 6
1	2-D	281/334 (84%)	246 (88%)	28 (10%)	7 (2%)	6 17
1	3-A	288/334 (86%)	243 (84%)	31 (11%)	14 (5%)	2 5
1	3-B	281/334 (84%)	217 (77%)	47 (17%)	17 (6%)	2 3
1	3-C	288/334 (86%)	229 (80%)	46 (16%)	13 (4%)	3 6
1	3-D	281/334 (84%)	244 (87%)	33 (12%)	4 (1%)	13 33
1	4-A	288/334 (86%)	242 (84%)	31 (11%)	15 (5%)	2 4
1	4-B	281/334 (84%)	243 (86%)	28 (10%)	10 (4%)	4 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	4-C	288/334 (86%)	243 (84%)	30 (10%)	15 (5%)	2 4
1	4-D	281/334 (84%)	233 (83%)	40 (14%)	8 (3%)	6 14
1	5-A	288/334 (86%)	232 (81%)	44 (15%)	12 (4%)	3 7
1	5-B	281/334 (84%)	242 (86%)	33 (12%)	6 (2%)	8 21
1	5-C	288/334 (86%)	233 (81%)	42 (15%)	13 (4%)	3 6
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%)	3 6
1	6-C	288/334 (86%)	238 (83%)	36 (12%)	14 (5%)	2 5
1	6-D	281/334 (84%)	234 (83%)	35 (12%)	12 (4%)	3 6
1	7-A	288/334 (86%)	234 (81%)	39 (14%)	15 (5%)	2 4
1	7-B	281/334 (84%)	247 (88%)	32 (11%)	2 (1%)	25 53
1	7-C	288/334 (86%)	248 (86%)	25 (9%)	15 (5%)	2 4
1	7-D	281/334 (84%)	235 (84%)	36 (13%)	10 (4%)	4 9
1	8-A	288/334 (86%)	249 (86%)	27 (9%)	12 (4%)	3 7
1	8-B	281/334 (84%)	229 (82%)	41 (15%)	11 (4%)	3 8
1	8-C	288/334 (86%)	242 (84%)	37 (13%)	9 (3%)	5 11
1	8-D	281/334 (84%)	240 (85%)	36 (13%)	5 (2%)	10 25
All	All	9104/10688 (85%)	7634 (84%)	1120 (12%)	350 (4%)	4 8

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 (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	1-A	249/276 (90%)	245 (98%)	4 (2%)	68	89
1	1-B	243/276 (88%)	234 (96%)	9 (4%)	39	70
1	1-C	249/276 (90%)	244 (98%)	5 (2%)	60	86
1	1-D	243/276 (88%)	233 (96%)	10 (4%)	35	66
1	2-A	249/276 (90%)	242 (97%)	7 (3%)	49	79
1	2-B	243/276 (88%)	235 (97%)	8 (3%)	43	73
1	2-C	249/276 (90%)	240 (96%)	9 (4%)	40	70
1	2-D	243/276 (88%)	234 (96%)	9 (4%)	39	70
1	3-A	249/276 (90%)	240 (96%)	9 (4%)	40	70
1	3-B	243/276 (88%)	232 (96%)	11 (4%)	32	62
1	3-C	249/276 (90%)	237 (95%)	12 (5%)	30	59
1	3-D	243/276 (88%)	235 (97%)	8 (3%)	43	73
1	4-A	249/276 (90%)	237 (95%)	12 (5%)	30	59
1	4-B	243/276 (88%)	231 (95%)	12 (5%)	29	58
1	4-C	249/276 (90%)	239 (96%)	10 (4%)	36	67
1	4-D	243/276 (88%)	238 (98%)	5 (2%)	59	85
1	5-A	249/276 (90%)	234 (94%)	15 (6%)	22	48
1	5-B	243/276 (88%)	228 (94%)	15 (6%)	21	46
1	5-C	249/276 (90%)	240 (96%)	9 (4%)	40	70
1	5-D	243/276 (88%)	228 (94%)	15 (6%)	21	46
1	6-A	249/276 (90%)	236 (95%)	13 (5%)	27	55
1	6-B	243/276 (88%)	231 (95%)	12 (5%)	29	58
1	6-C	249/276 (90%)	238 (96%)	11 (4%)	33	63
1	6-D	243/276 (88%)	233 (96%)	10 (4%)	35	66
1	7-A	249/276 (90%)	231 (93%)	18 (7%)	17	39
1	7-B	243/276 (88%)	227 (93%)	16 (7%)	19	43
1	7-C	249/276 (90%)	244 (98%)	5 (2%)	60	86
1	7-D	243/276 (88%)	236 (97%)	7 (3%)	48	77
1	8-A	249/276 (90%)	241 (97%)	8 (3%)	44	75
1	8-B	243/276 (88%)	227 (93%)	16 (7%)	19	43
1	8-C	249/276 (90%)	241 (97%)	8 (3%)	44	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-D	243/276 (88%)	231 (95%)	12 (5%)	29	58
All	All	7872/8832 (89%)	7542 (96%)	330 (4%)	34	65

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 (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	1-A	283/334 (84%)	0.23	23 (8%)	13	10	12, 35, 82, 101	283 (100%)
1	1-B	278/334 (83%)	-0.13	10 (3%)	43	42	10, 30, 62, 100	278 (100%)
1	1-C	283/334 (84%)	0.32	33 (11%)	5	4	15, 35, 80, 112	283 (100%)
1	1-D	278/334 (83%)	0.06	12 (4%)	36	34	11, 31, 70, 104	278 (100%)
1	2-A	283/334 (84%)	0.23	23 (8%)	13	10	12, 35, 82, 101	283 (100%)
1	2-B	278/334 (83%)	-0.13	10 (3%)	43	42	10, 30, 62, 100	278 (100%)
1	2-C	283/334 (84%)	0.32	33 (11%)	5	4	15, 35, 80, 112	283 (100%)
1	2-D	278/334 (83%)	0.06	12 (4%)	36	34	11, 31, 70, 104	278 (100%)
1	3-A	283/334 (84%)	0.23	23 (8%)	13	10	12, 35, 82, 101	283 (100%)
1	3-B	278/334 (83%)	-0.13	10 (3%)	43	42	10, 30, 62, 100	278 (100%)
1	3-C	283/334 (84%)	0.32	33 (11%)	5	4	15, 35, 80, 112	283 (100%)
1	3-D	278/334 (83%)	0.06	12 (4%)	36	34	11, 31, 70, 104	278 (100%)
1	4-A	283/334 (84%)	0.23	23 (8%)	13	10	12, 35, 82, 101	283 (100%)
1	4-B	278/334 (83%)	-0.13	10 (3%)	43	42	10, 30, 62, 100	278 (100%)
1	4-C	283/334 (84%)	0.32	33 (11%)	5	4	15, 35, 80, 112	283 (100%)
1	4-D	278/334 (83%)	0.06	12 (4%)	36	34	11, 31, 70, 104	278 (100%)
1	5-A	283/334 (84%)	0.23	23 (8%)	13	10	12, 35, 82, 101	283 (100%)
1	5-B	278/334 (83%)	-0.13	10 (3%)	43	42	10, 30, 62, 100	278 (100%)
1	5-C	283/334 (84%)	0.32	33 (11%)	5	4	15, 35, 80, 112	283 (100%)
1	5-D	278/334 (83%)	0.06	12 (4%)	36	34	11, 31, 70, 104	278 (100%)
1	6-A	283/334 (84%)	0.23	23 (8%)	13	10	12, 35, 82, 101	283 (100%)
1	6-B	278/334 (83%)	-0.13	10 (3%)	43	42	10, 30, 62, 100	278 (100%)
1	6-C	283/334 (84%)	0.32	33 (11%)	5	4	15, 35, 80, 112	283 (100%)
1	6-D	278/334 (83%)	0.06	12 (4%)	36	34	11, 31, 70, 104	278 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	7-A	283/334 (84%)	0.23	23 (8%)	13	10	12, 35, 82, 101	283 (100%)
1	7-B	278/334 (83%)	-0.13	10 (3%)	43	42	10, 30, 62, 100	278 (100%)
1	7-C	283/334 (84%)	0.32	33 (11%)	5	4	15, 35, 80, 112	283 (100%)
1	7-D	278/334 (83%)	0.06	12 (4%)	36	34	11, 31, 70, 104	278 (100%)
1	8-A	283/334 (84%)	0.23	23 (8%)	13	10	12, 35, 82, 101	283 (100%)
1	8-B	278/334 (83%)	-0.13	10 (3%)	43	42	10, 30, 62, 100	278 (100%)
1	8-C	283/334 (84%)	0.32	33 (11%)	5	4	15, 35, 80, 112	283 (100%)
1	8-D	278/334 (83%)	0.06	12 (4%)	36	34	11, 31, 70, 104	278 (100%)
All	All	8976/10688 (83%)	0.12	624 (6%)	17	15	10, 33, 75, 112	8976 (100%)

The worst 5 of 624 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 (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates 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.