wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 10:19 am BST

PDB ID	:	6O64
Title	:	Crystal Structure of Arabidopsis thaliana Spermidine Synthase isoform 2 (At-SPDS2)
Authors	:	Sekula, B.; Dauter, Z.
Deposited on	:	2019-03-05
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

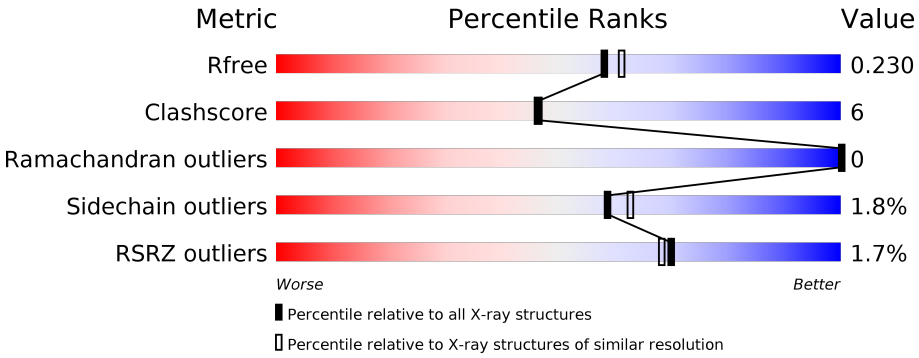
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	A	305	82% 11% • 7%
1	B	305	2% 83% 12% 5%
1	C	305	2% 80% 10% 9%
1	D	305	4% 71% 18% • 10%
1	E	305	75% 17% 8%
1	F	305	82% 12% 6%

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Mol	Chain	Length	Quality of chain
1	G	305	2% 83% 11% 6%
1	H	305	% 80% 12% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	E	402	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18590 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	1	0
			2202	1415	354	418	15			
1	B	290	Total	C	N	O	S	0	0	0
			2238	1436	362	425	15			
1	C	277	Total	C	N	O	S	0	0	0
			2145	1378	346	408	13			
1	D	275	Total	C	N	O	S	0	0	0
			2131	1371	344	403	13			
1	E	281	Total	C	N	O	S	0	3	0
			2183	1407	350	411	15			
1	F	287	Total	C	N	O	S	0	2	0
			2223	1430	358	419	16			
1	G	288	Total	C	N	O	S	0	0	0
			2220	1426	357	422	15			
1	H	281	Total	C	N	O	S	0	1	0
			2178	1401	352	411	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	SER	-	expression tag	UNP O48661
A	37	ASN	-	expression tag	UNP O48661
A	38	ALA	-	expression tag	UNP O48661
B	36	SER	-	expression tag	UNP O48661
B	37	ASN	-	expression tag	UNP O48661
B	38	ALA	-	expression tag	UNP O48661
C	36	SER	-	expression tag	UNP O48661
C	37	ASN	-	expression tag	UNP O48661
C	38	ALA	-	expression tag	UNP O48661
D	36	SER	-	expression tag	UNP O48661
D	37	ASN	-	expression tag	UNP O48661
D	38	ALA	-	expression tag	UNP O48661
E	36	SER	-	expression tag	UNP O48661

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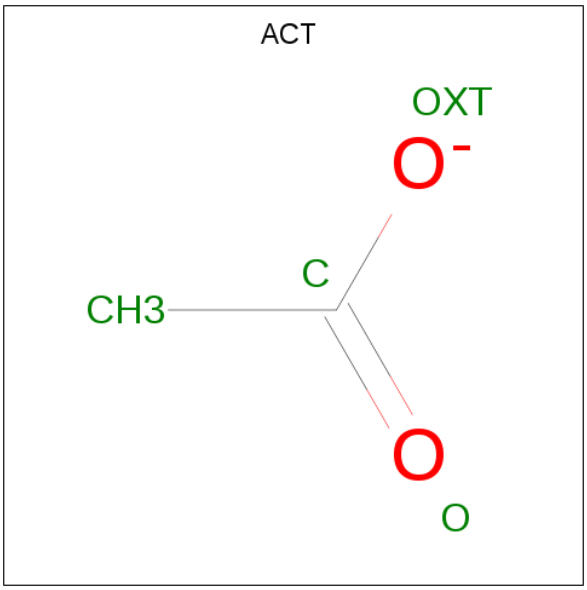
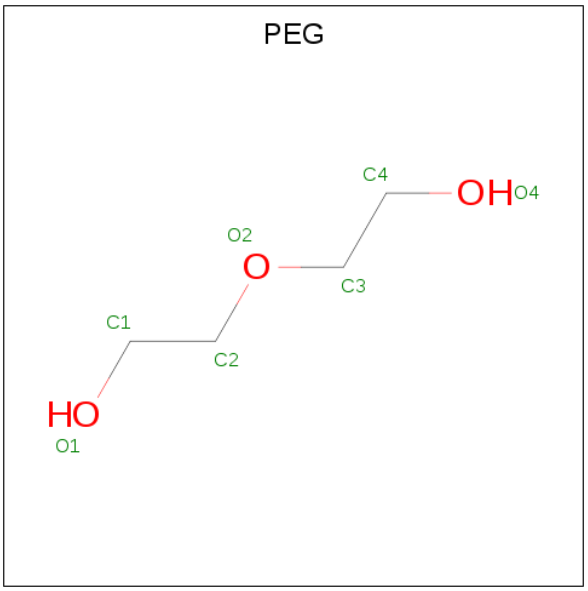
Chain	Residue	Modelled	Actual	Comment	Reference
E	37	ASN	-	expression tag	UNP O48661
E	38	ALA	-	expression tag	UNP O48661
F	36	SER	-	expression tag	UNP O48661
F	37	ASN	-	expression tag	UNP O48661
F	38	ALA	-	expression tag	UNP O48661
G	36	SER	-	expression tag	UNP O48661
G	37	ASN	-	expression tag	UNP O48661
G	38	ALA	-	expression tag	UNP O48661
H	36	SER	-	expression tag	UNP O48661
H	37	ASN	-	expression tag	UNP O48661
H	38	ALA	-	expression tag	UNP O48661

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



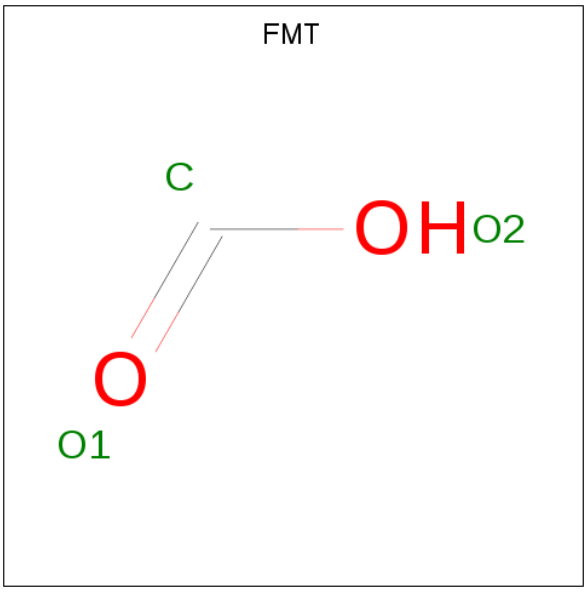
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



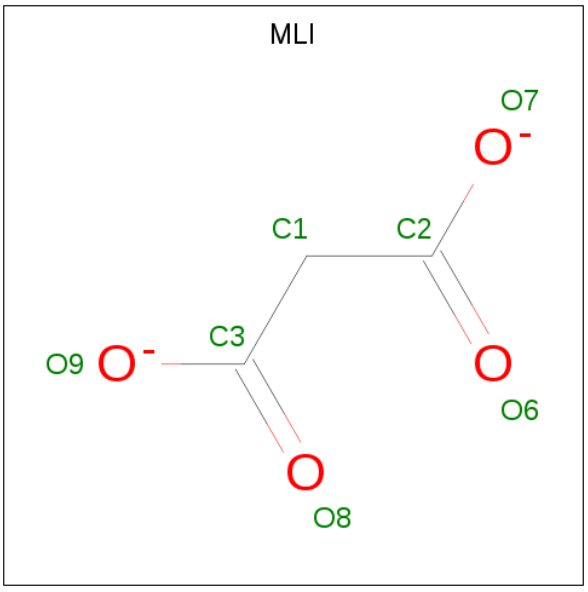
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 6 2 4	0	1

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 7 3 4	0	0

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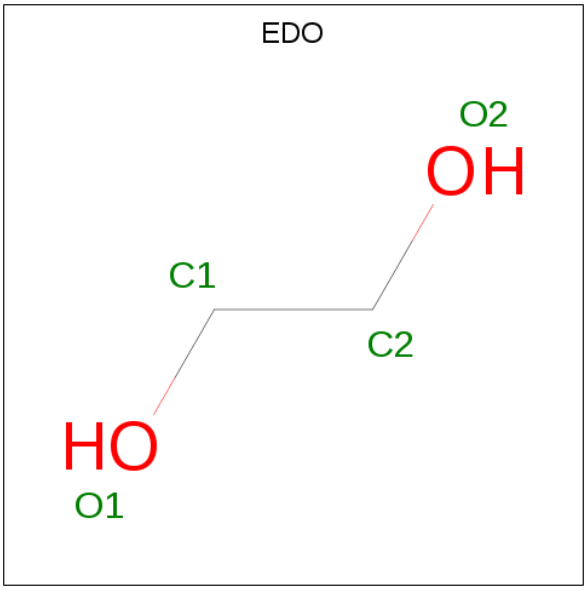
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 7 3 4	0	0
5	E	1	Total C O 7 3 4	0	0
5	H	1	Total C O 7 3 4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	79	Total O 79 79	0	0
7	B	99	Total O 99 99	0	0
7	C	84	Total O 84 84	0	0
7	D	67	Total O 67 67	0	0
7	E	186	Total O 186 186	0	0

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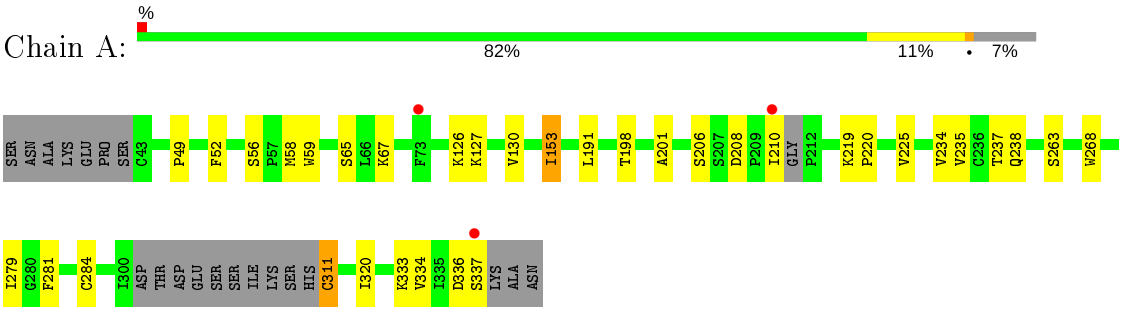
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	162	Total O 162 162	0	0
7	G	143	Total O 143 143	0	0
7	H	116	Total O 116 116	0	0

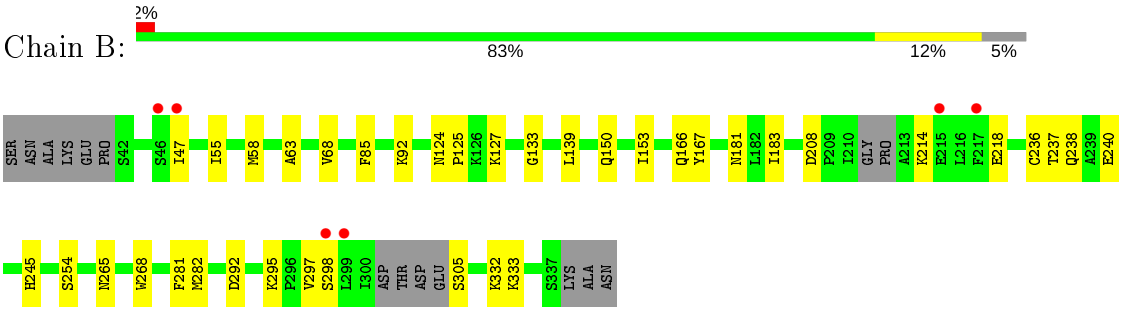
3 Residue-property plots

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.

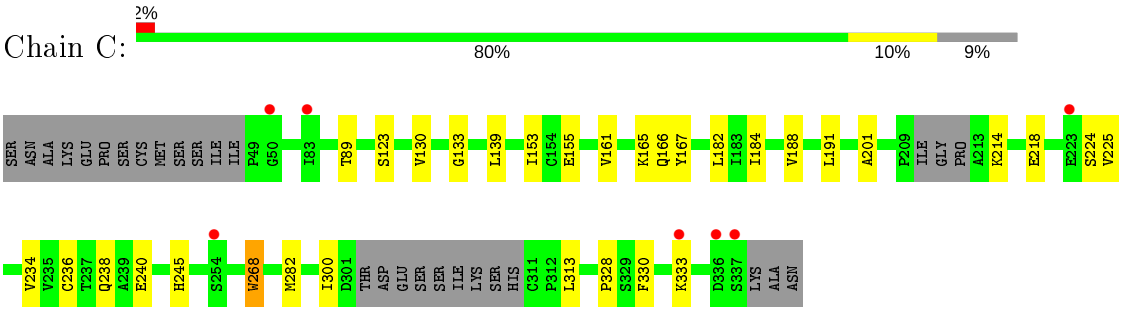
- Molecule 1: Spermidine synthase 2



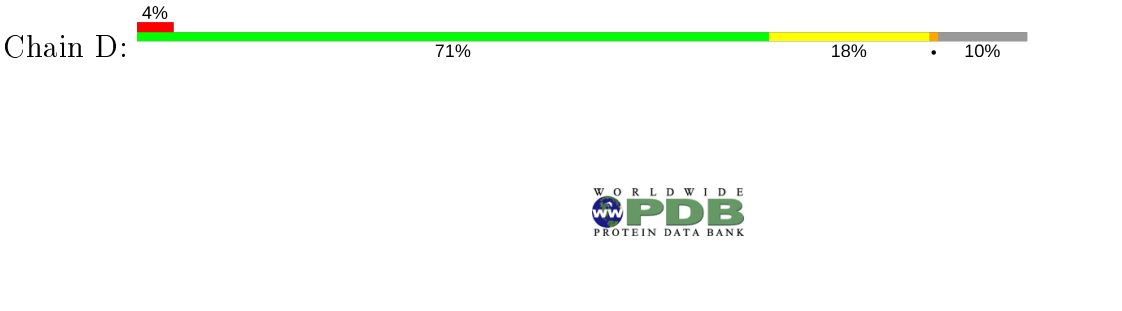
- Molecule 1: Spermidine synthase 2

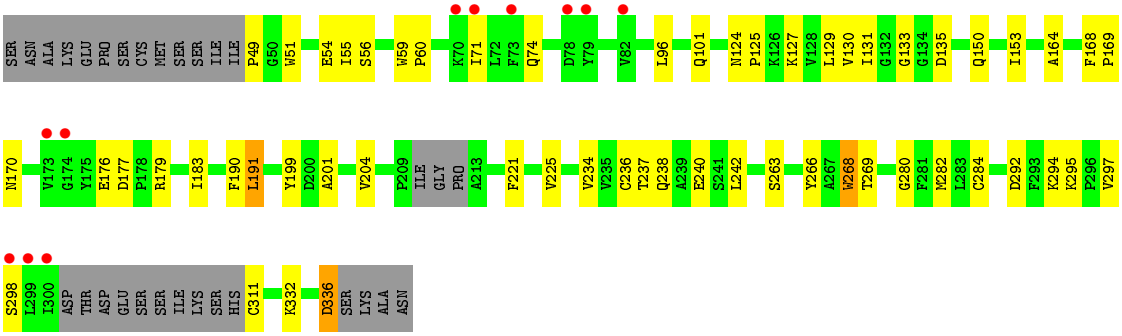


- Molecule 1: Spermidine synthase 2



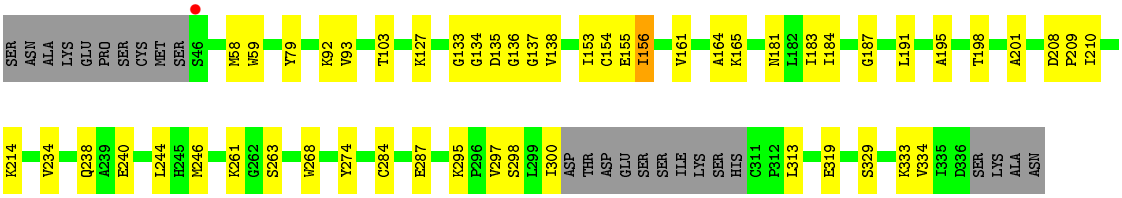
- Molecule 1: Spermidine synthase 2





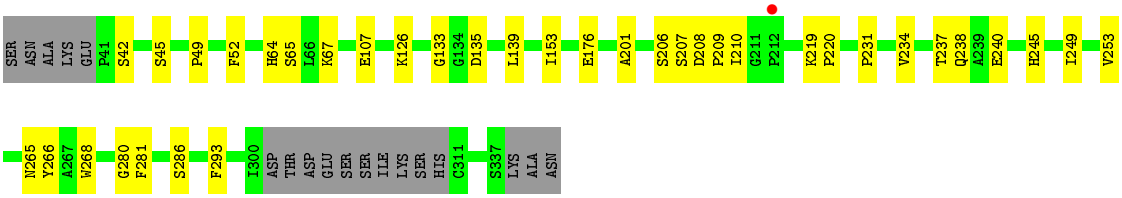
• Molecule 1: Spermidine synthase 2

Chain E:



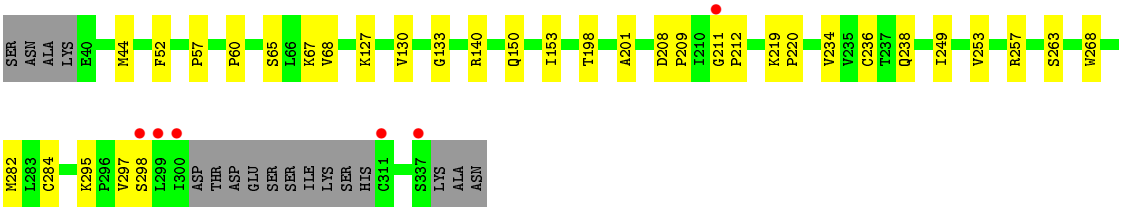
• Molecule 1: Spermidine synthase 2

Chain F:



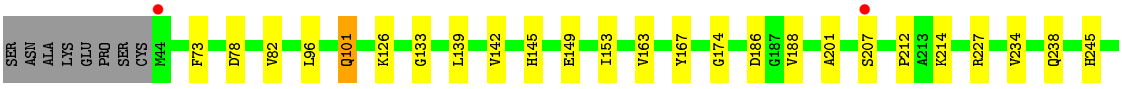
• Molecule 1: Spermidine synthase 2

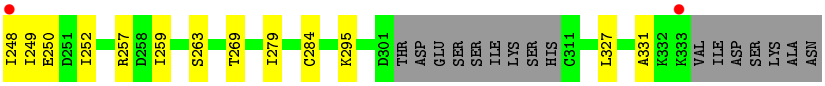
Chain G:



• Molecule 1: Spermidine synthase 2

Chain H:




I248
I249
E250
D251
I252
R257
D258
I259
S263
T269
I279
C284
K295
D301
THR
ASP
GLU
SER
SER
ILE
LYS
SER
HIS
C311
L327
A331
K332
K333
VAL
ILE
ASP
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	75.65Å 162.70Å 97.49Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	42.54 – 2.00 42.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	80.2 (42.54-2.00) 80.2 (42.51-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.231 0.185 , 0.230	Depositor DCC
R_{free} test set	1234 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18590	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 5.38% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, FMT, MLI, EDO, ACT

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	A	0.78	0/2252	0.90	0/3056
1	B	0.83	0/2288	0.94	0/3103
1	C	0.80	0/2194	0.92	0/2977
1	D	0.80	0/2180	0.90	0/2958
1	E	0.92	0/2243	1.02	0/3046
1	F	0.95	0/2282	1.00	0/3098
1	G	0.89	0/2272	0.98	0/3086
1	H	0.92	0/2233	1.01	0/3032
All	All	0.86	0/17944	0.96	0/24356

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A	2202	0	2180	21	0
1	B	2238	0	2220	22	0
1	C	2145	0	2117	19	0
1	D	2131	0	2108	36	0
1	E	2183	0	2175	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2223	0	2209	24	0
1	G	2220	0	2198	22	0
1	H	2178	0	2157	33	0
2	A	4	0	3	0	0
2	F	4	0	3	0	0
2	H	12	0	9	0	0
3	A	7	0	10	1	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	D	21	0	30	0	0
3	E	7	0	10	1	0
3	F	14	0	20	2	0
3	G	7	0	10	1	0
4	B	3	0	1	0	0
4	E	9	0	3	0	0
5	D	7	0	2	0	0
5	E	14	0	4	0	0
5	H	7	0	2	0	0
6	E	4	0	6	17	0
7	A	79	0	0	2	0
7	B	99	0	0	2	0
7	C	84	0	0	1	0
7	D	67	0	0	1	0
7	E	186	0	0	2	0
7	F	162	0	0	7	0
7	G	143	0	0	0	0
7	H	116	0	0	5	0
All	All	18590	0	17497	220	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 6.

The worst 5 of 220 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:E:58[A]:MET:SD	1:E:210:ILE:HG12	2.10	0.91
1:E:138:VAL:H	6:E:402:EDO:C2	1.86	0.87
1:E:138:VAL:H	6:E:402:EDO:H22	1.40	0.87
1:G:127:LYS:HE3	1:G:150:GLN:NE2	1.93	0.82
1:F:126:LYS:HG3	3:F:403:PEG:H12	1.63	0.80

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	A	279/305 (92%)	254 (91%)	25 (9%)	0	100	100
1	B	284/305 (93%)	270 (95%)	14 (5%)	0	100	100
1	C	271/305 (89%)	259 (96%)	12 (4%)	0	100	100
1	D	269/305 (88%)	257 (96%)	12 (4%)	0	100	100
1	E	280/305 (92%)	273 (98%)	7 (2%)	0	100	100
1	F	285/305 (93%)	270 (95%)	15 (5%)	0	100	100
1	G	284/305 (93%)	270 (95%)	14 (5%)	0	100	100
1	H	278/305 (91%)	266 (96%)	12 (4%)	0	100	100
All	All	2230/2440 (91%)	2119 (95%)	111 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	A	247/264 (94%)	241 (98%)	6 (2%)	49	51
1	B	252/264 (96%)	247 (98%)	5 (2%)	55	58
1	C	239/264 (90%)	235 (98%)	4 (2%)	60	65
1	D	237/264 (90%)	231 (98%)	6 (2%)	47	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	245/264 (93%)	241 (98%)	4 (2%)	62	67
1	F	250/264 (95%)	247 (99%)	3 (1%)	71	76
1	G	249/264 (94%)	246 (99%)	3 (1%)	71	76
1	H	243/264 (92%)	239 (98%)	4 (2%)	62	67
All	All	1962/2112 (93%)	1927 (98%)	35 (2%)	59	63

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	191	LEU
1	D	311	CYS
1	H	101	GLN
1	D	238	GLN
1	D	268	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	265	ASN
1	E	265	ASN
1	G	170	ASN
1	D	74	GLN
1	G	265	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)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEG	B	401	-	6,6,6	0.23	0	5,5,5	0.12	0
3	PEG	A	402	-	6,6,6	0.14	0	5,5,5	0.13	0
3	PEG	C	401	-	6,6,6	0.30	0	5,5,5	0.21	0
5	MLI	E	403	-	0,6,6	0.00	-	0,7,7	0.00	-
3	PEG	F	403	-	6,6,6	0.21	0	5,5,5	0.31	0
3	PEG	D	404	-	6,6,6	0.23	0	5,5,5	0.14	0
2	ACT	F	401	-	1,3,3	3.58	1 (100%)	0,3,3	0.00	-
3	PEG	F	402	-	6,6,6	0.24	0	5,5,5	0.18	0
5	MLI	D	401	-	0,6,6	0.00	-	0,7,7	0.00	-
4	FMT	E	406[A]	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	406[B]	-	0,2,2	0.00	-	0,1,1	0.00	-
2	ACT	A	401	-	1,3,3	3.44	1 (100%)	0,3,3	0.00	-
4	FMT	B	402	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	E	402	-	3,3,3	0.08	0	2,2,2	0.28	0
5	MLI	E	401	-	0,6,6	0.00	-	0,7,7	0.00	-
2	ACT	H	404	-	1,3,3	3.43	1 (100%)	0,3,3	0.00	-
3	PEG	D	402	-	6,6,6	0.21	0	5,5,5	0.18	0
2	ACT	H	403	-	1,3,3	3.63	1 (100%)	0,3,3	0.00	-
3	PEG	G	401	-	6,6,6	0.45	0	5,5,5	0.30	0
3	PEG	E	404	-	6,6,6	0.48	0	5,5,5	0.41	0
5	MLI	H	401	-	0,6,6	0.00	-	0,7,7	0.00	-
3	PEG	D	403	-	6,6,6	0.26	0	5,5,5	0.19	0
2	ACT	H	402	-	1,3,3	3.59	1 (100%)	0,3,3	0.00	-
4	FMT	E	405	-	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLI	E	403	-	-	0/0/4/4	-
6	EDO	E	402	-	-	0/1/1/1	-
5	MLI	E	401	-	-	0/0/4/4	-
3	PEG	B	401	-	-	2/4/4/4	-
5	MLI	H	401	-	-	0/0/4/4	-
3	PEG	F	403	-	-	1/4/4/4	-
3	PEG	D	403	-	-	3/4/4/4	-
3	PEG	D	402	-	-	3/4/4/4	-
3	PEG	F	402	-	-	1/4/4/4	-
3	PEG	A	402	-	-	2/4/4/4	-
3	PEG	C	401	-	-	2/4/4/4	-
3	PEG	G	401	-	-	0/4/4/4	-
5	MLI	D	401	-	-	0/0/4/4	-
3	PEG	E	404	-	-	0/4/4/4	-
3	PEG	D	404	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	403	ACT	CH3-C	3.63	1.53	1.48
2	H	402	ACT	CH3-C	3.59	1.53	1.48
2	F	401	ACT	CH3-C	3.58	1.53	1.48
2	A	401	ACT	CH3-C	3.44	1.53	1.48
2	H	404	ACT	CH3-C	3.43	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402	PEG	O1-C1-C2-O2
3	C	401	PEG	O2-C3-C4-O4
3	F	403	PEG	O1-C1-C2-O2
3	B	401	PEG	O2-C3-C4-O4
3	D	403	PEG	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	PEG	1	0
3	F	403	PEG	1	0
3	F	402	PEG	1	0
6	E	402	EDO	17	0
3	G	401	PEG	1	0
3	E	404	PEG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	284/305 (93%)	-0.03	3 (1%)	80	79	24, 42, 64, 90	0
1	B	290/305 (95%)	-0.18	6 (2%)	63	62	21, 38, 64, 82	0
1	C	277/305 (90%)	-0.03	7 (2%)	57	56	21, 42, 71, 87	0
1	D	275/305 (90%)	0.19	11 (4%)	38	37	25, 47, 83, 109	0
1	E	281/305 (92%)	-0.38	1 (0%)	92	92	11, 20, 43, 69	0
1	F	287/305 (94%)	-0.37	1 (0%)	94	93	11, 27, 57, 89	0
1	G	288/305 (94%)	-0.29	6 (2%)	63	62	13, 32, 56, 103	0
1	H	281/305 (92%)	-0.23	4 (1%)	75	74	15, 35, 59, 80	0
All	All	2263/2440 (92%)	-0.17	39 (1%)	70	68	11, 36, 69, 109	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	299	LEU	10.0
1	G	337	SER	5.9
1	A	337	SER	5.8
1	C	337	SER	4.3
1	G	211	GLY	3.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	H	402	4/4	0.71	0.21	48,49,52,54	0
5	MLI	D	401	7/7	0.81	0.25	41,42,43,44	7
3	PEG	C	401	7/7	0.82	0.18	50,53,56,57	0
3	PEG	D	403	7/7	0.85	0.12	46,53,56,57	0
4	FMT	B	402	3/3	0.86	0.12	67,67,68,69	0
3	PEG	D	402	7/7	0.87	0.16	55,57,61,63	0
4	FMT	E	405	3/3	0.87	0.15	49,49,51,54	0
3	PEG	A	402	7/7	0.88	0.17	48,56,57,59	0
5	MLI	E	401	7/7	0.89	0.23	26,28,30,32	7
6	EDO	E	402	4/4	0.91	0.25	21,21,21,23	4
2	ACT	H	404	4/4	0.91	0.12	25,32,33,38	4
3	PEG	D	404	7/7	0.92	0.10	25,27,37,39	7
3	PEG	F	403	7/7	0.92	0.21	36,38,43,46	7
5	MLI	H	401	7/7	0.93	0.20	32,37,40,43	7
5	MLI	E	403	7/7	0.93	0.09	27,35,38,39	7
2	ACT	F	401	4/4	0.93	0.21	21,24,25,30	4
3	PEG	F	402	7/7	0.93	0.11	28,30,37,39	0
3	PEG	B	401	7/7	0.94	0.13	44,47,51,51	0
2	ACT	H	403	4/4	0.94	0.21	26,26,28,32	4
2	ACT	A	401	4/4	0.94	0.34	30,30,33,36	4
4	FMT	E	406[B]	3/3	0.95	0.26	13,13,14,15	3
4	FMT	E	406[A]	3/3	0.95	0.26	7,7,7,7	3
3	PEG	G	401	7/7	0.96	0.09	17,23,25,26	0
3	PEG	E	404	7/7	0.98	0.08	12,13,16,17	0

6.5 Other polymers

There are no such residues in this entry.