



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:15 AM UTC

PDB ID : 2Q41 / pdb_00002q41
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

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
Mogul : 2022.3.0, CSD as543be (2022)
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

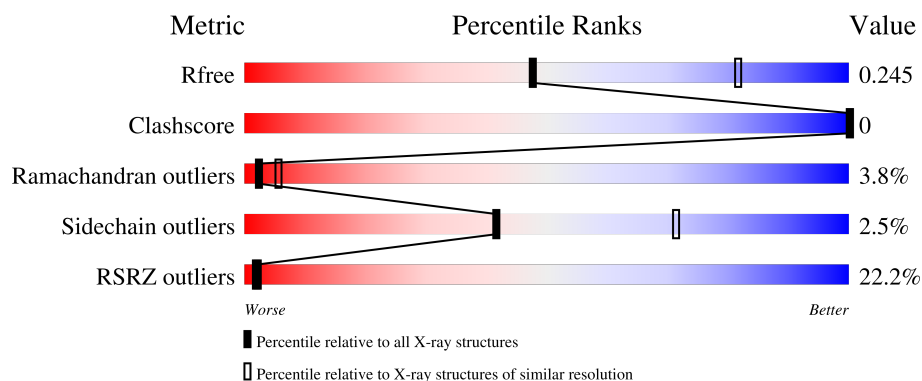
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



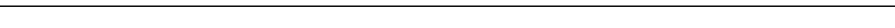
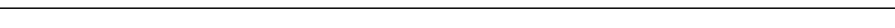
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 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	1-A	334	22% 82% 13%
1	1-B	334	13% 81% 15%
1	1-C	334	20% 83% 13%
1	1-D	334	20% 79% 7% 15%
1	2-A	334	82% 5% 13%

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Mol	Chain	Length	Quality of chain
1	2-B	334	 81% 15%
1	2-C	334	 82% 5% 13%
1	2-D	334	 80% 6% 15%
1	3-A	334	 81% 5% 13%
1	3-B	334	 78% 8% 15%
1	3-C	334	 82% 5% 13%
1	3-D	334	 81% 5% 15%
1	4-A	334	 81% 6% 13%
1	4-B	334	 80% 5% 15%
1	4-C	334	 82% 5% 13%
1	4-D	334	 79% 6% 15%
1	5-A	334	 82% 5% 13%
1	5-B	334	 81% 15%
1	5-C	334	 82% 5% 13%
1	5-D	334	 78% 8% 15%
1	6-A	334	 81% 6% 13%
1	6-B	334	 80% 5% 15%
1	6-C	334	 82% 13%
1	6-D	334	 78% 7% 15%
1	7-A	334	 81% 6% 13%
1	7-B	334	 82% 15%
1	7-C	334	 82% 5% 13%
1	7-D	334	 79% 7% 15%
1	8-A	334	 82% 5% 13%
1	8-B	334	 80% 5% 15%

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Mol	Chain	Length	Quality of chain
1	8-C	334	 83%13%
1	8-D	334	 80%5%15%

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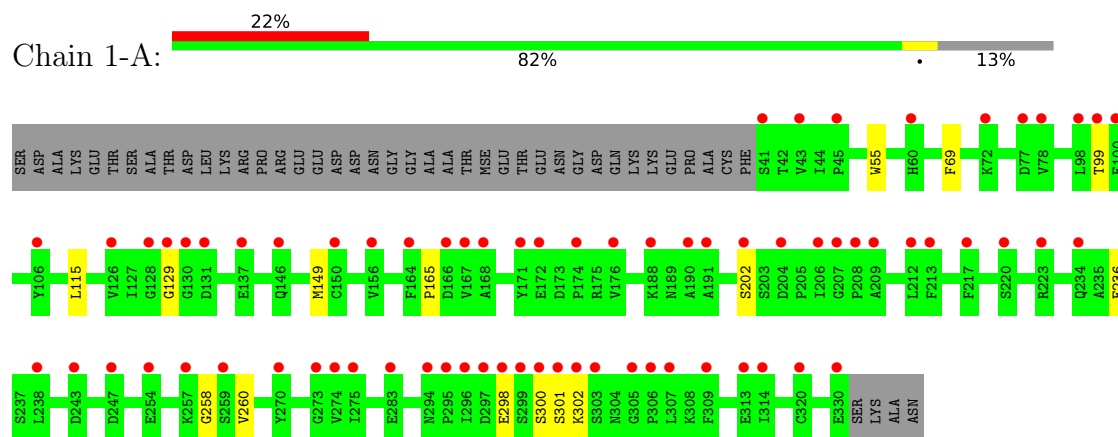
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-D	134	Total 134	O 134	0	0
2	4-D	134	Total 134	O 134	0	0
2	5-D	133	Total 133	O 133	0	0
2	6-D	133	Total 133	O 133	0	0
2	7-D	138	Total 138	O 138	0	0
2	8-D	135	Total 135	O 135	0	0

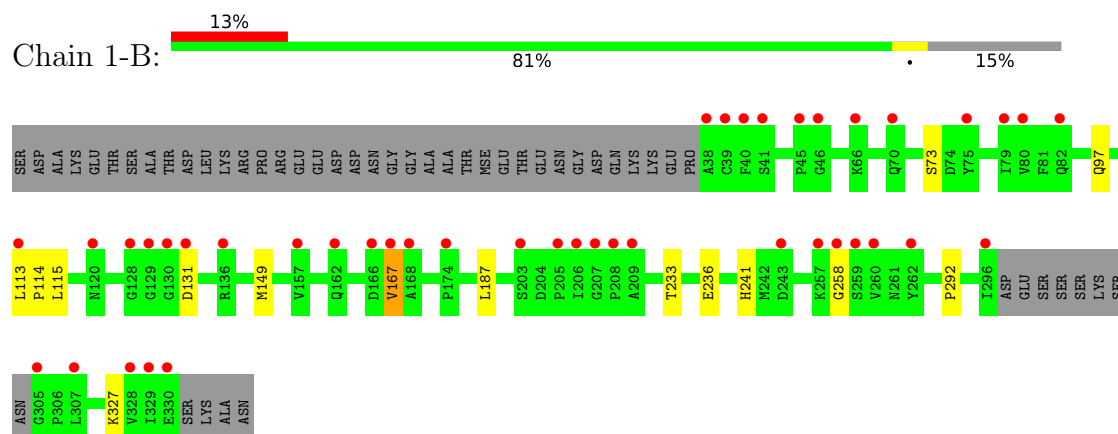
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

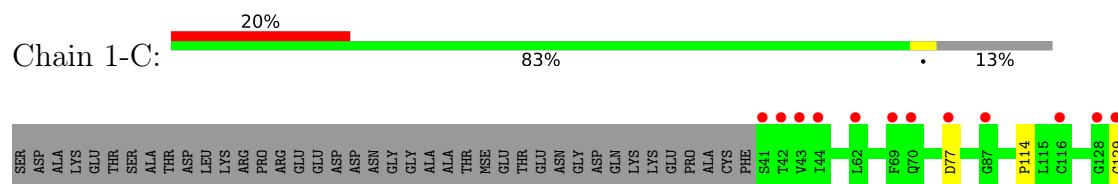
• Molecule 1: Spermidine synthase 1

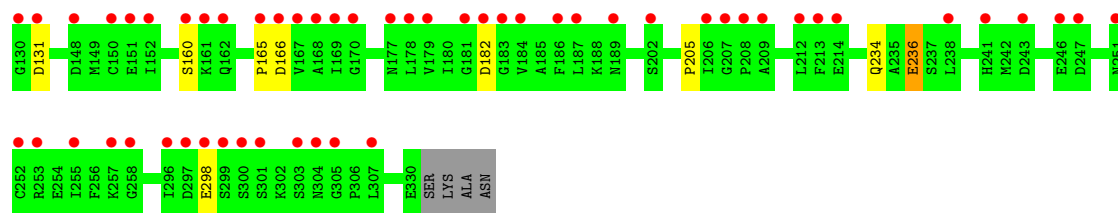


• Molecule 1: Spermidine synthase 1

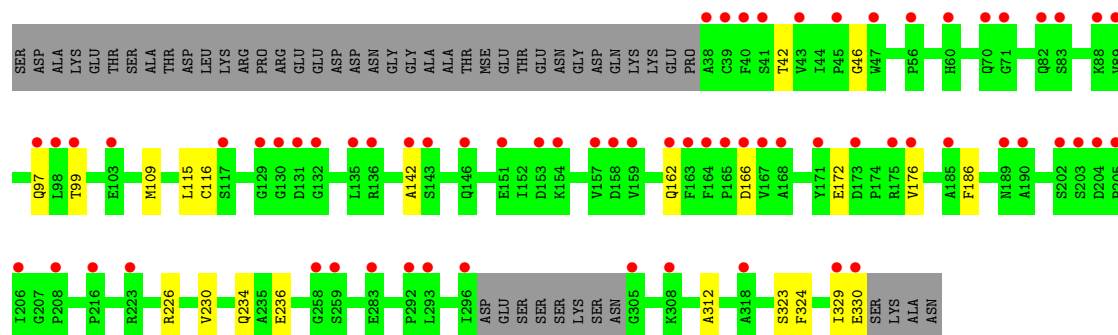
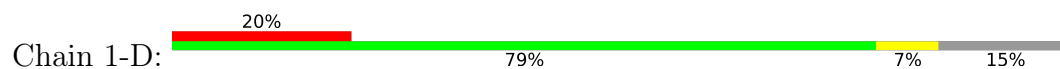


• Molecule 1: Spermidine synthase 1

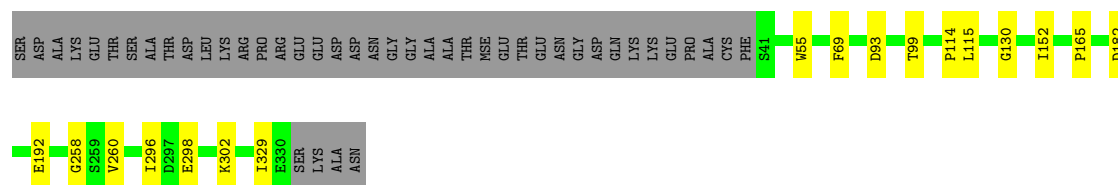
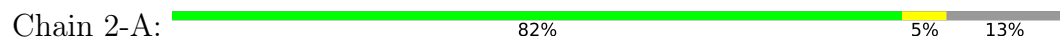




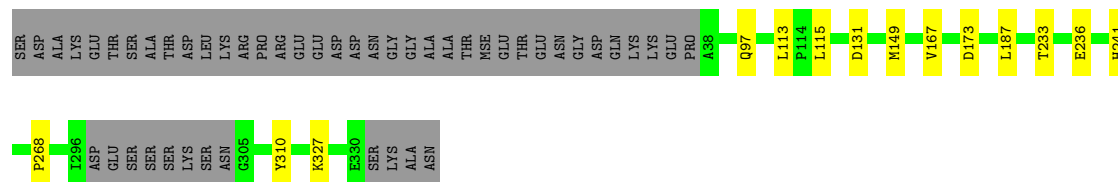
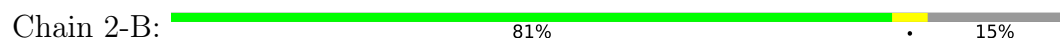
• Molecule 1: Spermidine synthase 1



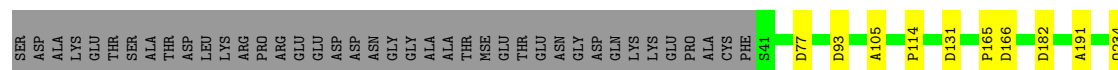
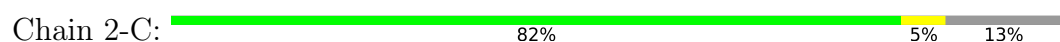
• Molecule 1: Spermidine synthase 1

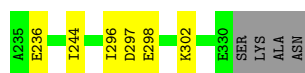


• Molecule 1: Spermidine synthase 1



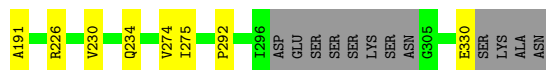
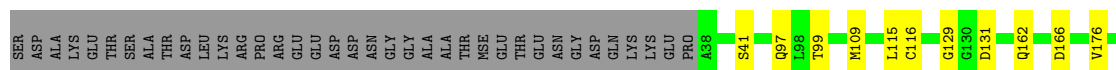
• Molecule 1: Spermidine synthase 1





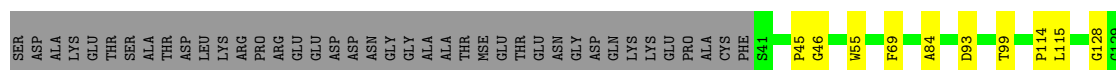
- Molecule 1: Spermidine synthase 1

Chain 2-D: 80% 6% 15%



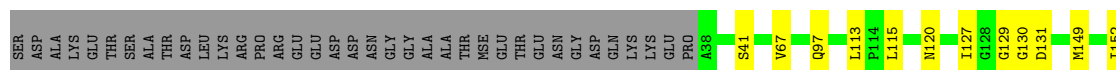
- Molecule 1: Spermidine synthase 1

Chain 3-A: 81% 5% 13%



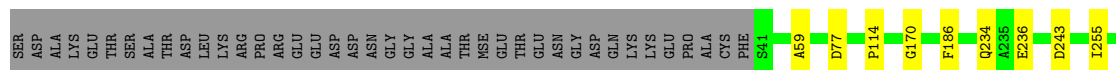
- Molecule 1: Spermidine synthase 1

Chain 3-B: 78% 8% 15%



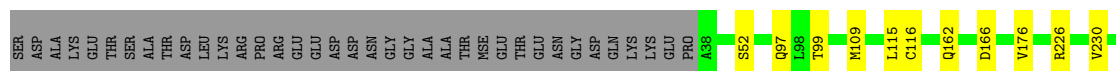
- Molecule 1: Spermidine synthase 1

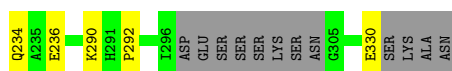
Chain 3-C: 82% 5% 13%



- Molecule 1: Spermidine synthase 1

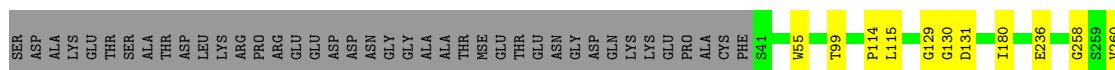
Chain 3-D: 81% 5% 15%





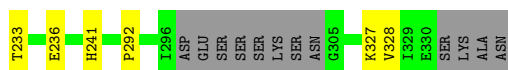
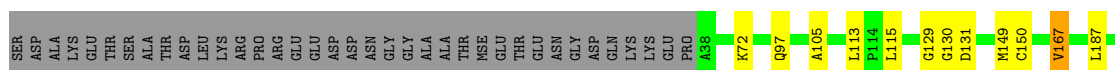
- Molecule 1: Spermidine synthase 1

Chain 4-A: 81% 6% 13%



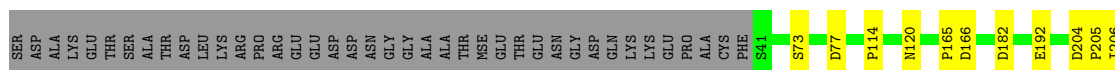
- Molecule 1: Spermidine synthase 1

Chain 4-B: 80% 5% 15%



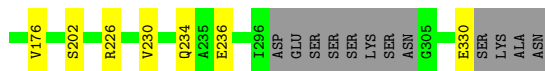
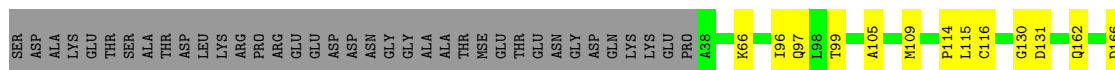
- Molecule 1: Spermidine synthase 1

Chain 4-C: 82% 5% 13%



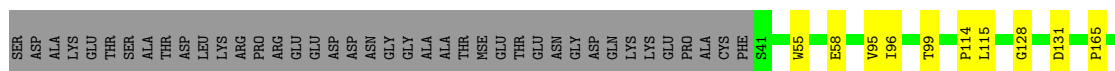
- Molecule 1: Spermidine synthase 1

Chain 4-D: 79% 6% 15%



- Molecule 1: Spermidine synthase 1

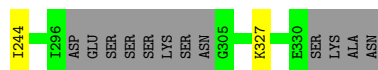
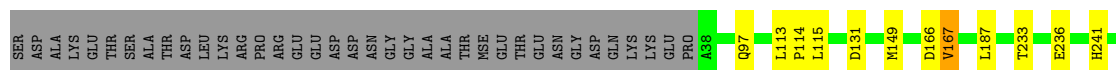
Chain 5-A: 82% 5% 13%





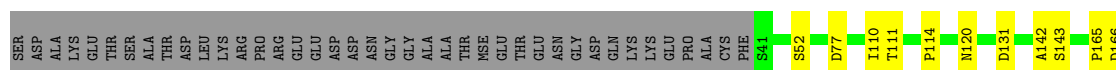
- Molecule 1: Spermidine synthase 1

Chain 5-B: 81% 15%



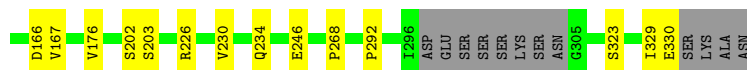
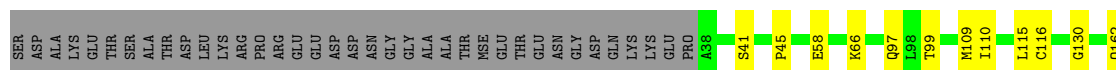
- Molecule 1: Spermidine synthase 1

Chain 5-C: 82% 5% 13%



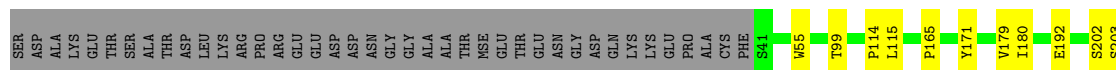
- Molecule 1: Spermidine synthase 1

Chain 5-D: 78% 8% 15%



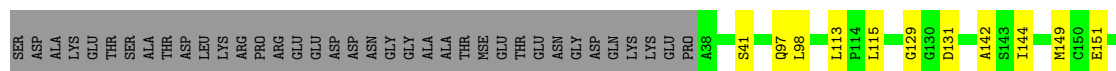
- Molecule 1: Spermidine synthase 1

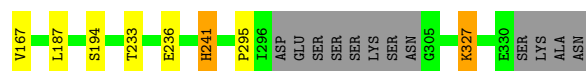
Chain 6-A: 81% 6% 13%



- Molecule 1: Spermidine synthase 1

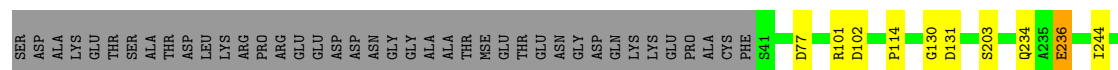
Chain 6-B: 80% 5% 15%





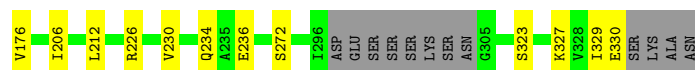
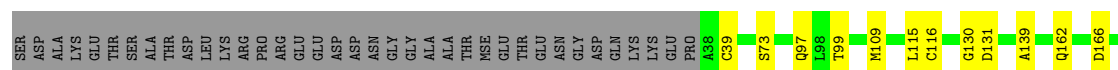
- Molecule 1: Spermidine synthase 1

Chain 6-C: 82% 13%



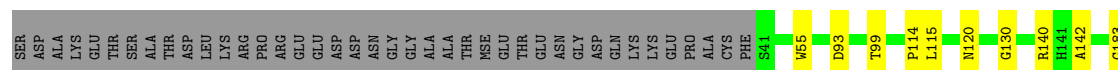
- Molecule 1: Spermidine synthase 1

Chain 6-D: 78% 7% 15%



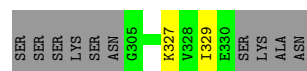
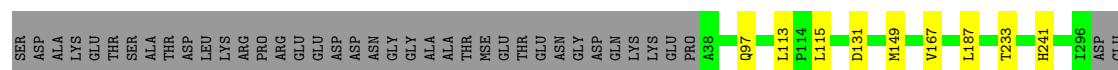
- Molecule 1: Spermidine synthase 1

Chain 7-A: 81% 6% 13%



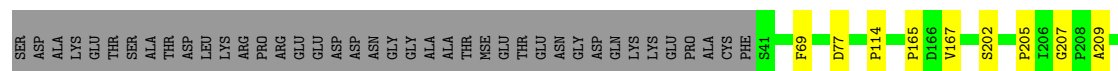
- Molecule 1: Spermidine synthase 1

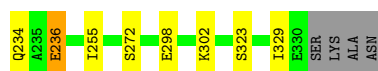
Chain 7-B: 82% 15%



- Molecule 1: Spermidine synthase 1

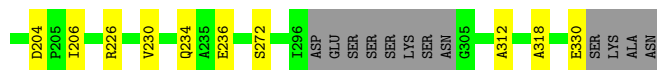
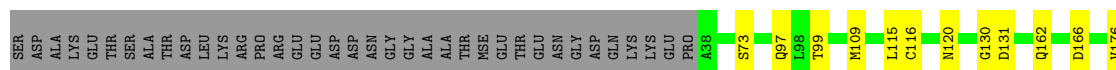
Chain 7-C: 82% 5% 13%





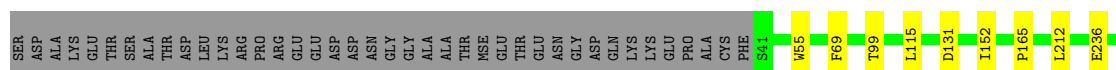
- Molecule 1: Spermidine synthase 1

Chain 7-D: 79% 7% 15%



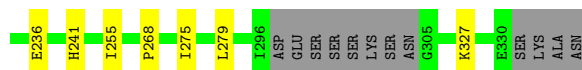
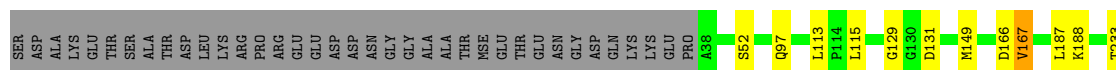
- Molecule 1: Spermidine synthase 1

Chain 8-A: 82% 5% 13%



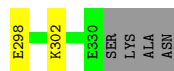
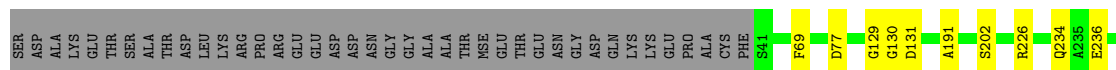
- Molecule 1: Spermidine synthase 1

Chain 8-B: 80% 5% 15%



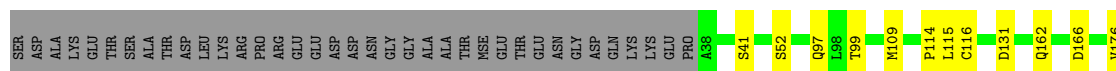
- Molecule 1: Spermidine synthase 1

Chain 8-C: 83% 13%



- Molecule 1: Spermidine synthase 1

Chain 8-D: 80% 5% 15%



R226	V230	Q234	D286	I296	ASP	GLU	SER	SER	SER	LYS	SER	ASN	G305	E330	SER	LYS	ALA	ASN
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4 Data and refinement statistics

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 26.29 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.5 (26.29-2.70) 95.5 (26.29-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.164 , 0.249 0.166 , 0.245	Depositor DCC
R_{free} test set	3788 reflections (9.55%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.87	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.*

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

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	0.25	0/2282	0.53	2/3089 (0.1%)
1	1-B	0.27	0/2246	0.52	0/3040
1	1-C	0.26	0/2282	0.52	0/3089
1	1-D	0.26	0/2246	0.53	2/3040 (0.1%)
1	2-A	0.25	0/2282	0.53	2/3089 (0.1%)
1	2-B	0.27	0/2246	0.52	0/3040
1	2-C	0.26	0/2282	0.52	0/3089
1	2-D	0.26	0/2246	0.53	2/3040 (0.1%)
1	3-A	0.25	0/2282	0.53	2/3089 (0.1%)
1	3-B	0.27	0/2246	0.52	0/3040
1	3-C	0.26	0/2282	0.52	0/3089
1	3-D	0.26	0/2246	0.53	2/3040 (0.1%)
1	4-A	0.25	0/2282	0.53	2/3089 (0.1%)
1	4-B	0.27	0/2246	0.52	0/3040
1	4-C	0.26	0/2282	0.52	0/3089
1	4-D	0.26	0/2246	0.53	2/3040 (0.1%)
1	5-A	0.25	0/2282	0.53	2/3089 (0.1%)
1	5-B	0.27	0/2246	0.52	0/3040
1	5-C	0.26	0/2282	0.52	0/3089
1	5-D	0.26	0/2246	0.53	2/3040 (0.1%)
1	6-A	0.25	0/2282	0.53	2/3089 (0.1%)
1	6-B	0.27	0/2246	0.52	0/3040
1	6-C	0.26	0/2282	0.52	0/3089
1	6-D	0.26	0/2246	0.53	2/3040 (0.1%)
1	7-A	0.25	0/2282	0.53	2/3089 (0.1%)
1	7-B	0.27	0/2246	0.52	0/3040
1	7-C	0.26	0/2282	0.52	0/3089
1	7-D	0.26	0/2246	0.53	2/3040 (0.1%)
1	8-A	0.25	0/2282	0.53	2/3089 (0.1%)
1	8-B	0.27	0/2246	0.52	0/3040
1	8-C	0.26	0/2282	0.52	0/3089
1	8-D	0.26	0/2246	0.53	2/3040 (0.1%)
All	All	0.26	0/72448	0.52	32/98064 (0.0%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	55	TRP	CA-C-N	6.21	126.42	119.90
1	1-A	55	TRP	C-N-CA	6.21	126.42	119.90
1	2-A	55	TRP	CA-C-N	6.21	126.42	119.90
1	2-A	55	TRP	C-N-CA	6.21	126.42	119.90
1	3-A	55	TRP	CA-C-N	6.21	126.42	119.90

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	0	0
1	1-B	2198	0	2168	0	0
1	1-C	2234	0	2199	0	0
1	1-D	2198	0	2168	0	0
1	2-A	2234	0	2199	0	0
1	2-B	2198	0	2168	0	0
1	2-C	2234	0	2199	0	0
1	2-D	2198	0	2168	0	0
1	3-A	2234	0	2199	0	0
1	3-B	2198	0	2168	0	0
1	3-C	2234	0	2199	0	0
1	3-D	2198	0	2168	0	0
1	4-A	2234	0	2199	0	0
1	4-B	2198	0	2168	0	0
1	4-C	2234	0	2199	0	0
1	4-D	2198	0	2168	0	0
1	5-A	2234	0	2199	0	0
1	5-B	2198	0	2168	0	0
1	5-C	2234	0	2199	0	0
1	5-D	2198	0	2168	0	0
1	6-A	2234	0	2199	0	0
1	6-B	2198	0	2168	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6-C	2234	0	2199	0	0
1	6-D	2198	0	2168	0	0
1	7-A	2234	0	2199	0	0
1	7-B	2198	0	2168	0	0
1	7-C	2234	0	2199	0	0
1	7-D	2198	0	2168	0	0
1	8-A	2234	0	2199	0	0
1	8-B	2198	0	2168	0	0
1	8-C	2234	0	2199	0	0
1	8-D	2198	0	2168	0	0
2	1-A	130	0	0	0	0
2	1-B	177	0	0	0	0
2	1-C	135	0	0	0	0
2	1-D	134	0	0	0	0
2	2-A	137	0	0	0	0
2	2-B	179	0	0	0	0
2	2-C	129	0	0	0	0
2	2-D	131	0	0	0	0
2	3-A	135	0	0	0	0
2	3-B	175	0	0	0	0
2	3-C	132	0	0	0	0
2	3-D	134	0	0	0	0
2	4-A	134	0	0	0	0
2	4-B	173	0	0	0	0
2	4-C	135	0	0	0	0
2	4-D	134	0	0	0	0
2	5-A	134	0	0	0	0
2	5-B	171	0	0	0	0
2	5-C	138	0	0	0	0
2	5-D	133	0	0	0	0
2	6-A	135	0	0	0	0
2	6-B	176	0	0	0	0
2	6-C	132	0	0	0	0
2	6-D	133	0	0	0	0
2	7-A	128	0	0	0	0
2	7-B	177	0	0	0	0
2	7-C	133	0	0	0	0
2	7-D	138	0	0	0	0
2	8-A	135	0	0	0	0
2	8-B	173	0	0	0	0
2	8-C	133	0	0	0	0
2	8-D	135	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	75520	0	69872	0	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 0.

There are no clashes within the asymmetric unit.

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%)	2	5
1	1-B	281/334 (84%)	241 (86%)	33 (12%)	7 (2%)	4	11
1	1-C	288/334 (86%)	249 (86%)	29 (10%)	10 (4%)	3	6
1	1-D	281/334 (84%)	227 (81%)	44 (16%)	10 (4%)	2	6
1	2-A	288/334 (86%)	243 (84%)	32 (11%)	13 (4%)	2	4
1	2-B	281/334 (84%)	245 (87%)	31 (11%)	5 (2%)	6	18
1	2-C	288/334 (86%)	242 (84%)	33 (12%)	13 (4%)	2	4
1	2-D	281/334 (84%)	246 (88%)	28 (10%)	7 (2%)	4	11
1	3-A	288/334 (86%)	243 (84%)	31 (11%)	14 (5%)	1	3
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	4
1	3-D	281/334 (84%)	244 (87%)	33 (12%)	4 (1%)	9	23
1	4-A	288/334 (86%)	242 (84%)	31 (11%)	15 (5%)	1	3
1	4-B	281/334 (84%)	243 (86%)	28 (10%)	10 (4%)	2	6
1	4-C	288/334 (86%)	243 (84%)	30 (10%)	15 (5%)	1	3
1	4-D	281/334 (84%)	233 (83%)	40 (14%)	8 (3%)	4	9

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

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%)	246 (99%)	3 (1%)	63	84
1	1-B	243/276 (88%)	234 (96%)	9 (4%)	30	59
1	1-C	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	1-D	243/276 (88%)	233 (96%)	10 (4%)	27	56
1	2-A	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	2-B	243/276 (88%)	234 (96%)	9 (4%)	30	59
1	2-C	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	2-D	243/276 (88%)	233 (96%)	10 (4%)	27	56
1	3-A	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	3-B	243/276 (88%)	234 (96%)	9 (4%)	30	59
1	3-C	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	3-D	243/276 (88%)	233 (96%)	10 (4%)	27	56
1	4-A	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	4-B	243/276 (88%)	234 (96%)	9 (4%)	30	59
1	4-C	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	4-D	243/276 (88%)	233 (96%)	10 (4%)	27	56
1	5-A	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	5-B	243/276 (88%)	234 (96%)	9 (4%)	30	59
1	5-C	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	5-D	243/276 (88%)	233 (96%)	10 (4%)	27	56
1	6-A	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	6-B	243/276 (88%)	234 (96%)	9 (4%)	30	59
1	6-C	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	6-D	243/276 (88%)	233 (96%)	10 (4%)	27	56
1	7-A	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	7-B	243/276 (88%)	234 (96%)	9 (4%)	30	59
1	7-C	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	7-D	243/276 (88%)	233 (96%)	10 (4%)	27	56
1	8-A	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	8-B	243/276 (88%)	234 (96%)	9 (4%)	30	59
1	8-C	249/276 (90%)	246 (99%)	3 (1%)	63	84
1	8-D	243/276 (88%)	233 (96%)	10 (4%)	27	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7872/8832 (89%)	7672 (98%)	200 (2%)	42 71

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5-D	97	GLN
1	6-D	115	LEU
1	8-D	330	GLU
1	5-D	116	CYS
1	6-B	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 189 such sidechains are listed below:

Mol	Chain	Res	Type
1	5-D	311	ASN
1	7-A	82	GLN
1	6-A	261	ASN
1	6-C	241	HIS
1	7-B	120	ASN

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 ⓘ

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, 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%)	1.41	72 (25%) 1 1	2, 4, 10, 12	283 (100%)
1	1-B	278/334 (83%)	1.08	43 (15%) 5 4	1, 4, 7, 12	278 (100%)
1	1-C	283/334 (84%)	1.36	66 (23%) 2 2	2, 4, 10, 13	283 (100%)
1	1-D	278/334 (83%)	1.36	68 (24%) 2 1	2, 4, 8, 12	278 (100%)
1	2-A	0/334	-	-	-	-
1	2-B	0/334	-	-	-	-
1	2-C	0/334	-	-	-	-
1	2-D	0/334	-	-	-	-
1	3-A	0/334	-	-	-	-
1	3-B	0/334	-	-	-	-
1	3-C	0/334	-	-	-	-
1	3-D	0/334	-	-	-	-
1	4-A	0/334	-	-	-	-
1	4-B	0/334	-	-	-	-
1	4-C	0/334	-	-	-	-
1	4-D	0/334	-	-	-	-
1	5-A	0/334	-	-	-	-
1	5-B	0/334	-	-	-	-
1	5-C	0/334	-	-	-	-
1	5-D	0/334	-	-	-	-
1	6-A	0/334	-	-	-	-
1	6-B	0/334	-	-	-	-
1	6-C	0/334	-	-	-	-
1	6-D	0/334	-	-	-	-
1	7-A	0/334	-	-	-	-
1	7-B	0/334	-	-	-	-
1	7-C	0/334	-	-	-	-
1	7-D	0/334	-	-	-	-
1	8-A	0/334	-	-	-	-
1	8-B	0/334	-	-	-	-
1	8-C	0/334	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	8-D	0/334	-	-	-	-
All	All	1122/10688 (10%)	1.31	249 (22%) 2 2	1, 4, 9, 13	1122 (100%)

The worst 5 of 249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-D	131	ASP	12.7
1	1-A	274	VAL	7.2
1	1-A	301	SER	6.6
1	1-D	40	PHE	6.1
1	1-B	41	SER	6.0

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.