



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:04 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 Full wwPDB X-ray Structure Validation 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:

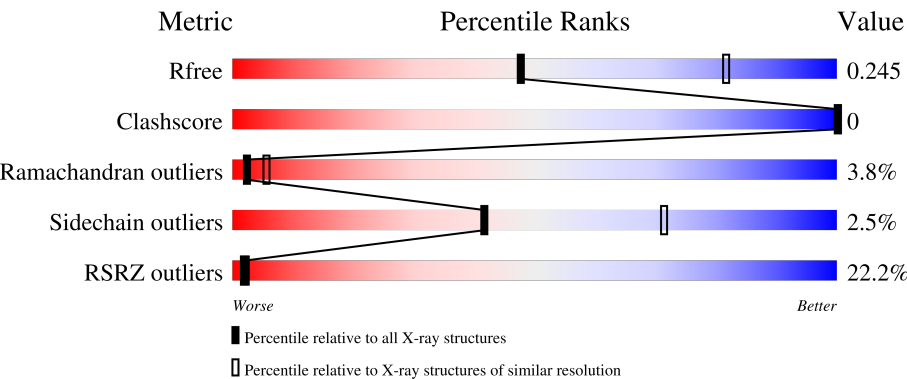
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance 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.



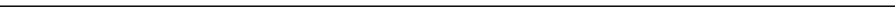
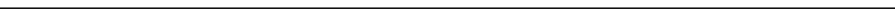
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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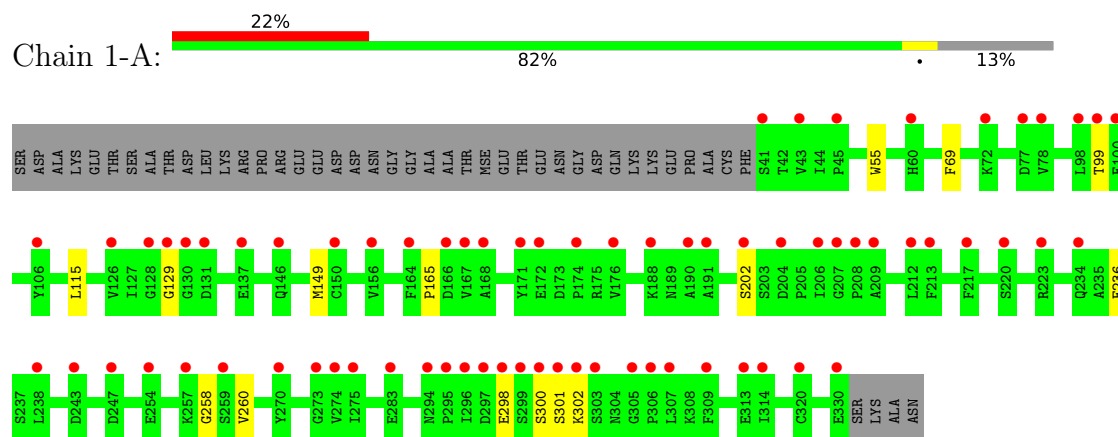
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-D	134	Total 134	O 134	0	0
2	4-D	134	Total 134	O 134	0	0
2	5-D	133	Total 133	O 133	0	0
2	6-D	133	Total 133	O 133	0	0
2	7-D	138	Total 138	O 138	0	0
2	8-D	135	Total 135	O 135	0	0

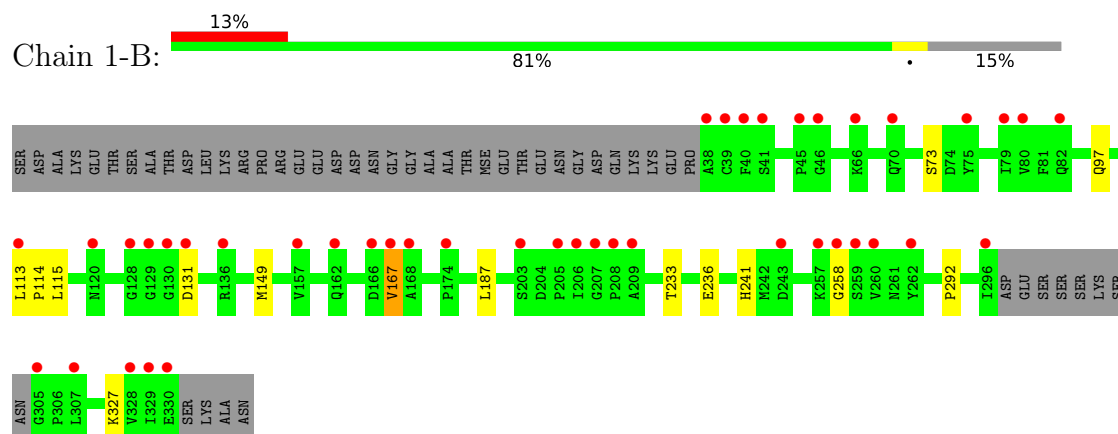
3 Residue-property plots [i](#)

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.

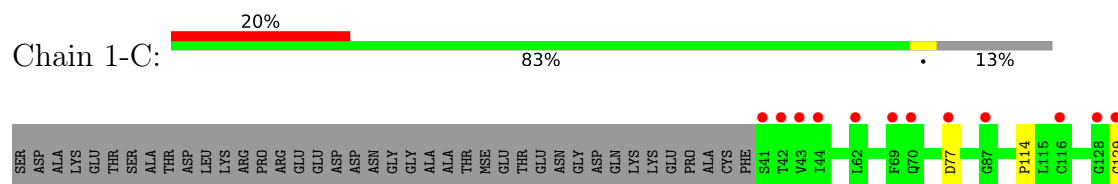
• Molecule 1: Spermidine synthase 1

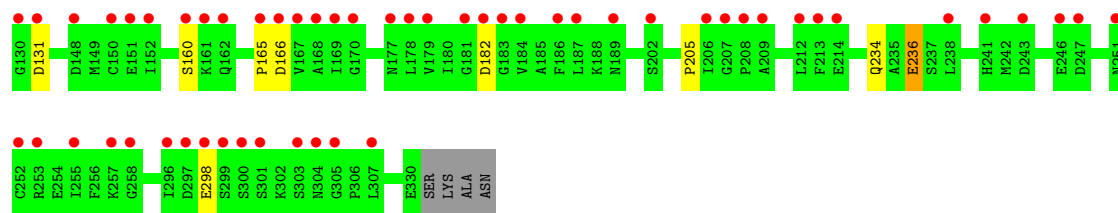


• Molecule 1: Spermidine synthase 1

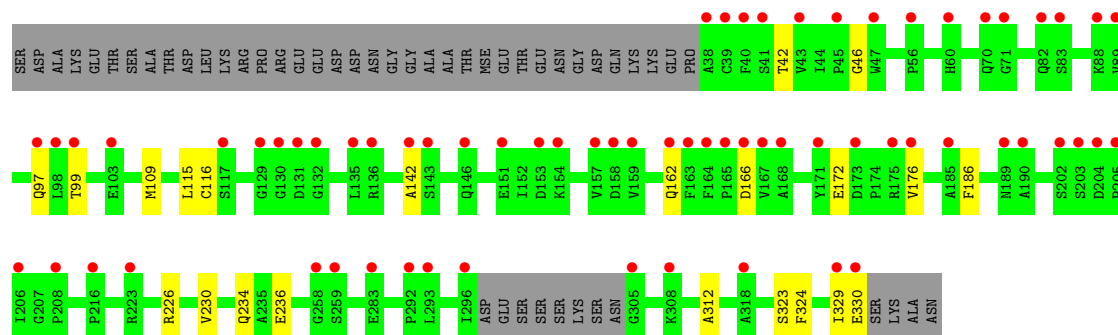
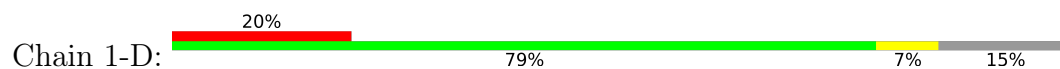


• Molecule 1: Spermidine synthase 1

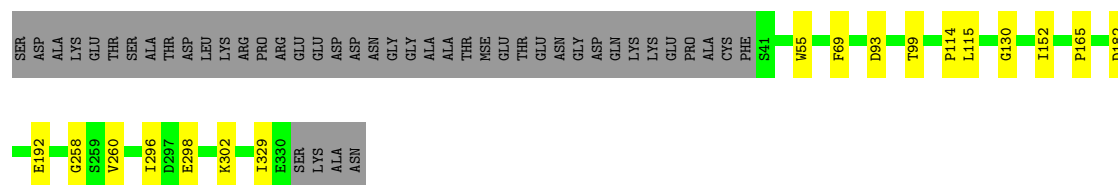
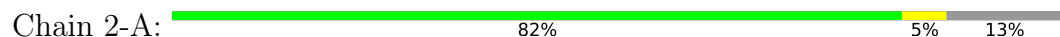




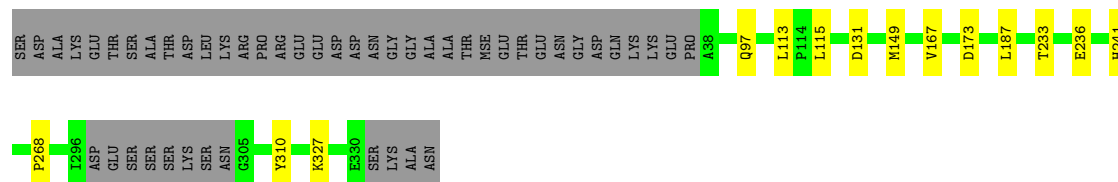
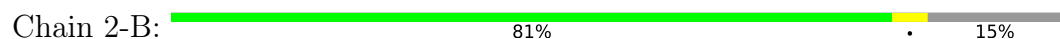
• Molecule 1: Spermidine synthase 1



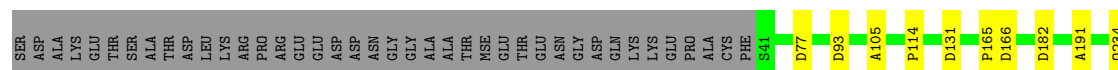
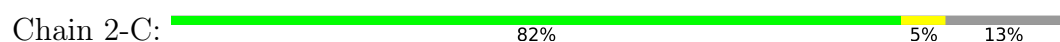
• Molecule 1: Spermidine synthase 1

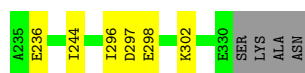


• Molecule 1: Spermidine synthase 1



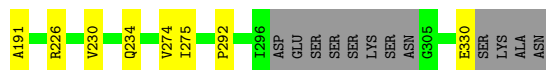
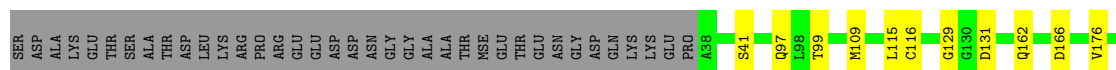
• Molecule 1: Spermidine synthase 1





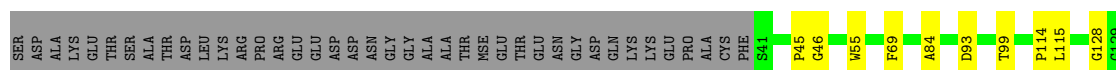
- Molecule 1: Spermidine synthase 1

Chain 2-D: 80% 6% 15%



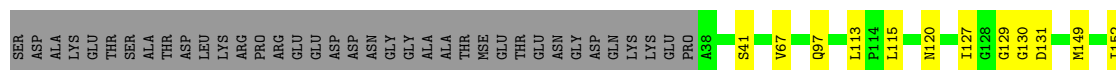
- Molecule 1: Spermidine synthase 1

Chain 3-A: 81% 5% 13%



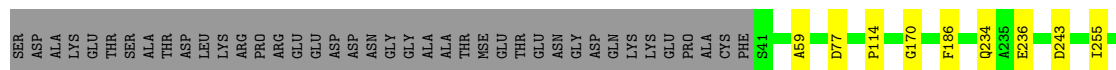
- Molecule 1: Spermidine synthase 1

Chain 3-B: 78% 8% 15%



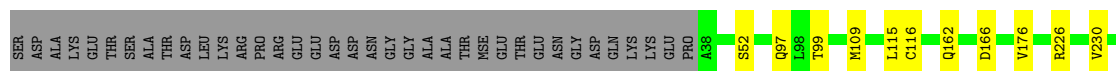
- Molecule 1: Spermidine synthase 1

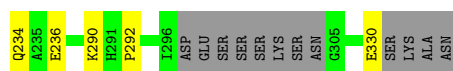
Chain 3-C: 82% 5% 13%



- Molecule 1: Spermidine synthase 1

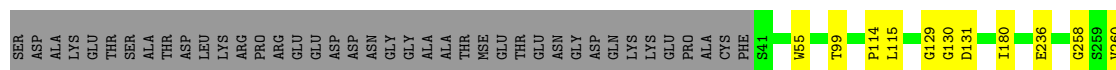
Chain 3-D: 81% 5% 15%





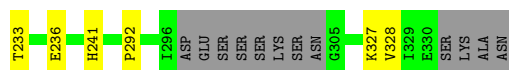
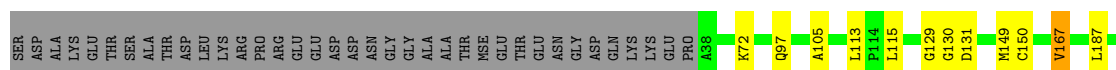
- Molecule 1: Spermidine synthase 1

Chain 4-A: 81% 6% 13%



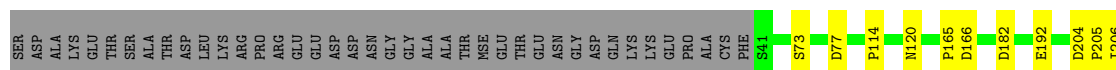
- Molecule 1: Spermidine synthase 1

Chain 4-B: 80% 5% 15%



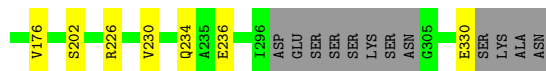
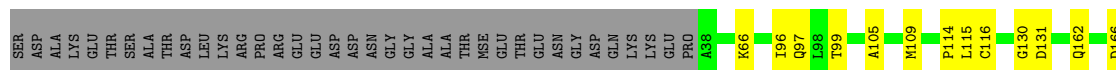
- Molecule 1: Spermidine synthase 1

Chain 4-C: 82% 5% 13%



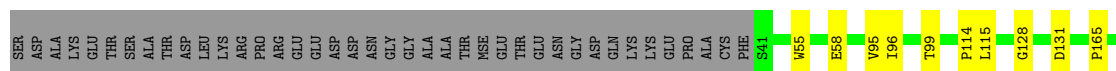
- Molecule 1: Spermidine synthase 1

Chain 4-D: 79% 6% 15%



- Molecule 1: Spermidine synthase 1

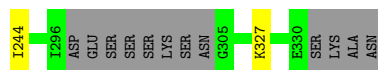
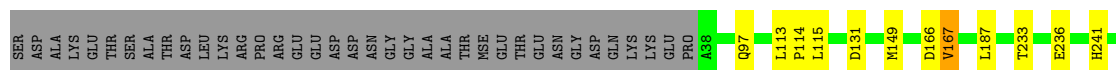
Chain 5-A: 82% 5% 13%





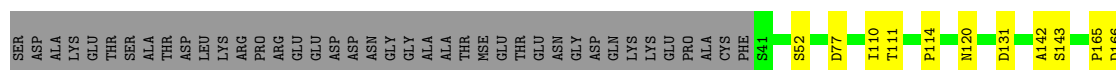
- Molecule 1: Spermidine synthase 1

Chain 5-B: 81% 15%



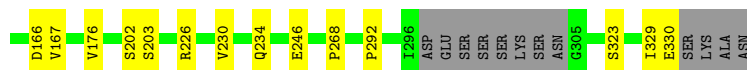
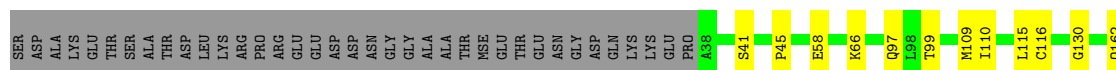
- Molecule 1: Spermidine synthase 1

Chain 5-C: 82% 5% 13%



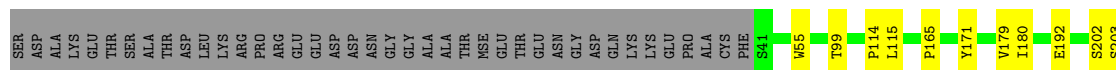
- Molecule 1: Spermidine synthase 1

Chain 5-D: 78% 8% 15%



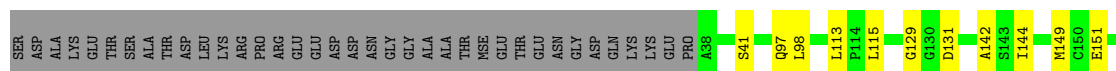
- Molecule 1: Spermidine synthase 1

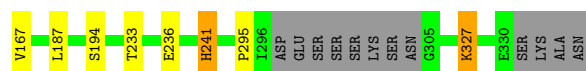
Chain 6-A: 81% 6% 13%



- Molecule 1: Spermidine synthase 1

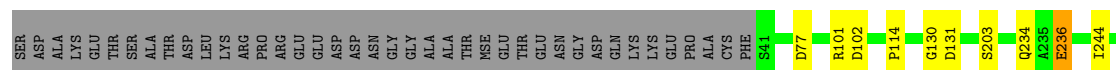
Chain 6-B: 80% 5% 15%





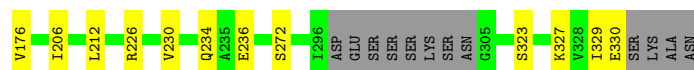
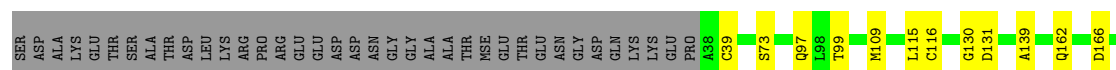
- Molecule 1: Spermidine synthase 1

Chain 6-C: 82% 13%



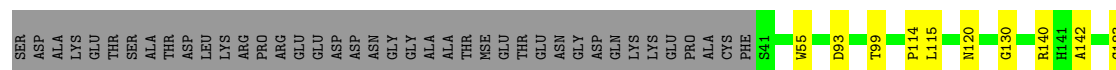
- Molecule 1: Spermidine synthase 1

Chain 6-D: 78% 7% 15%



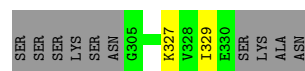
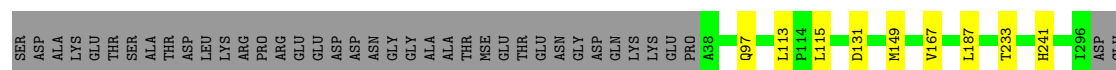
- Molecule 1: Spermidine synthase 1

Chain 7-A: 81% 6% 13%



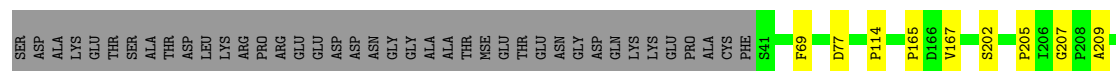
- Molecule 1: Spermidine synthase 1

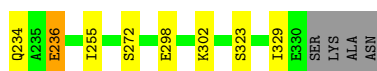
Chain 7-B: 82% 15%



- Molecule 1: Spermidine synthase 1

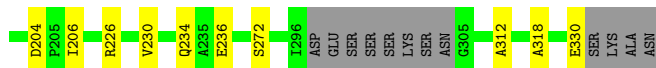
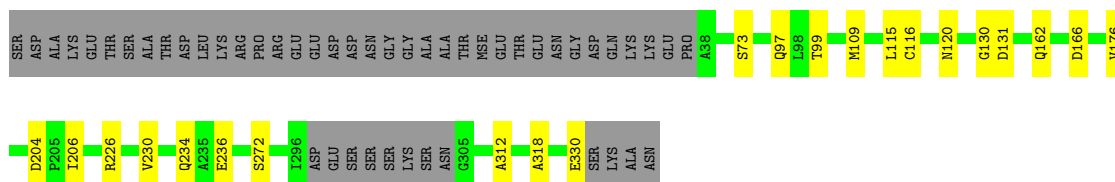
Chain 7-C: 82% 5% 13%





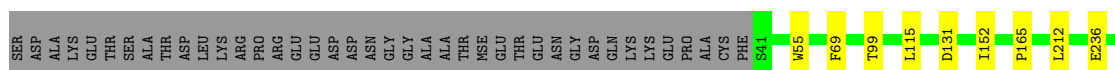
- Molecule 1: Spermidine synthase 1

Chain 7-D: 79% 7% 15%



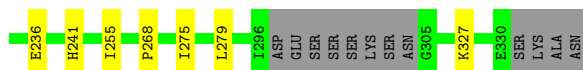
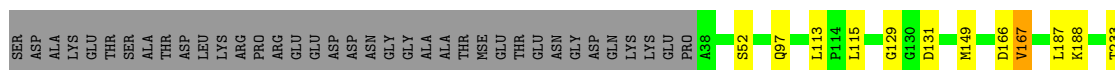
- Molecule 1: Spermidine synthase 1

Chain 8-A: 82% 5% 13%



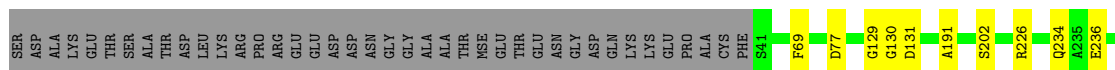
- Molecule 1: Spermidine synthase 1

Chain 8-B: 80% 5% 15%



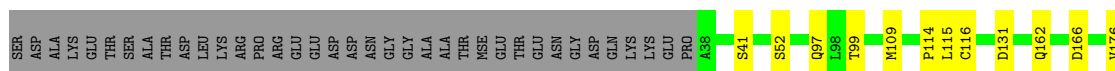
- Molecule 1: Spermidine synthase 1

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.

All (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
1	3-A	55	TRP	C-N-CA	6.21	126.42	119.90
1	4-A	55	TRP	CA-C-N	6.21	126.42	119.90
1	4-A	55	TRP	C-N-CA	6.21	126.42	119.90
1	5-A	55	TRP	CA-C-N	6.21	126.42	119.90
1	5-A	55	TRP	C-N-CA	6.21	126.42	119.90
1	6-A	55	TRP	CA-C-N	6.21	126.42	119.90
1	6-A	55	TRP	C-N-CA	6.21	126.42	119.90
1	7-A	55	TRP	CA-C-N	6.21	126.42	119.90
1	7-A	55	TRP	C-N-CA	6.21	126.42	119.90
1	8-A	55	TRP	CA-C-N	6.21	126.42	119.90
1	8-A	55	TRP	C-N-CA	6.21	126.42	119.90
1	1-D	230	VAL	N-CA-C	6.02	118.88	108.95
1	2-D	230	VAL	N-CA-C	6.02	118.88	108.95
1	3-D	230	VAL	N-CA-C	6.02	118.88	108.95
1	4-D	230	VAL	N-CA-C	6.02	118.88	108.95
1	5-D	230	VAL	N-CA-C	6.02	118.88	108.95
1	6-D	230	VAL	N-CA-C	6.02	118.88	108.95
1	7-D	230	VAL	N-CA-C	6.02	118.88	108.95
1	8-D	230	VAL	N-CA-C	6.02	118.88	108.95
1	1-D	176	VAL	N-CA-C	5.19	115.79	109.30
1	2-D	176	VAL	N-CA-C	5.19	115.79	109.30
1	3-D	176	VAL	N-CA-C	5.19	115.79	109.30
1	4-D	176	VAL	N-CA-C	5.19	115.79	109.30
1	5-D	176	VAL	N-CA-C	5.19	115.79	109.30
1	6-D	176	VAL	N-CA-C	5.19	115.79	109.30
1	7-D	176	VAL	N-CA-C	5.19	115.79	109.30
1	8-D	176	VAL	N-CA-C	5.19	115.79	109.30

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	1-C	236	GLU
1	1-D	172	GLU
1	1-D	312	ALA
1	2-A	93	ASP
1	2-B	236	GLU
1	2-C	191	ALA
1	2-C	297	ASP
1	2-D	131	ASP
1	2-D	191	ALA
1	3-A	45	PRO
1	3-A	84	ALA
1	3-A	93	ASP
1	3-B	130	GLY
1	3-B	191	ALA
1	3-C	310	TYR
1	4-A	298	GLU
1	4-A	302	LYS
1	4-A	312	ALA
1	4-B	129	GLY
1	4-B	130	GLY
1	4-B	150	CYS
1	4-B	167	VAL
1	4-B	236	GLU
1	4-C	73	SER
1	4-C	192	GLU
1	4-C	206	ILE
1	4-C	214	GLU
1	4-C	215	LYS
1	4-C	236	GLU

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Mol	Chain	Res	Type
1	4-D	202	SER
1	5-A	58	GLU
1	5-A	131	ASP
1	5-B	236	GLU
1	5-B	244	ILE
1	5-C	142	ALA
1	5-C	143	SER
1	5-D	323	SER
1	6-A	165	PRO
1	6-A	202	SER
1	6-B	151	GLU
1	6-B	194	SER
1	6-B	236	GLU
1	6-C	131	ASP
1	6-C	203	SER
1	6-C	236	GLU
1	6-D	131	ASP
1	6-D	329	ILE
1	7-A	93	ASP
1	7-A	183	GLY
1	7-A	318	ALA
1	7-B	131	ASP
1	7-C	165	PRO
1	7-C	236	GLU
1	7-C	323	SER
1	7-D	131	ASP
1	8-A	131	ASP
1	8-A	298	GLU
1	8-A	302	LYS
1	8-B	236	GLU
1	8-C	226	ARG
1	8-D	52	SER
1	8-D	131	ASP
1	1-A	129	GLY
1	1-A	149	MSE
1	1-A	165	PRO
1	1-A	236	GLU
1	1-A	302	LYS
1	1-B	73	SER
1	1-B	131	ASP
1	1-C	298	GLU
1	1-D	142	ALA

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Mol	Chain	Res	Type
1	1-D	323	SER
1	1-D	324	PHE
1	1-D	329	ILE
1	2-A	298	GLU
1	2-A	302	LYS
1	2-A	329	ILE
1	2-B	131	ASP
1	2-B	310	TYR
1	2-C	131	ASP
1	2-C	296	ILE
1	2-C	302	LYS
1	2-D	129	GLY
1	2-D	275	ILE
1	3-A	46	GLY
1	3-A	130	GLY
1	3-A	192	GLU
1	3-A	298	GLU
1	3-B	67	VAL
1	3-B	127	ILE
1	3-B	129	GLY
1	3-B	212	LEU
1	3-C	269	THR
1	3-C	273	GLY
1	3-C	298	GLU
1	4-A	129	GLY
1	4-B	72	LYS
1	4-B	131	ASP
1	4-C	165	PRO
1	4-C	182	ASP
1	4-C	298	GLU
1	4-C	302	LYS
1	4-D	130	GLY
1	5-A	95	VAL
1	5-A	128	GLY
1	5-A	165	PRO
1	5-A	312	ALA
1	5-B	131	ASP
1	5-B	167	VAL
1	5-C	110	ILE
1	5-C	131	ASP
1	5-C	298	GLU
1	5-C	302	LYS

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Mol	Chain	Res	Type
1	5-D	41	SER
1	5-D	110	ILE
1	5-D	130	GLY
1	5-D	202	SER
1	6-A	180	ILE
1	6-A	203	SER
1	6-A	243	ASP
1	6-A	258	GLY
1	6-A	283	GLU
1	6-A	298	GLU
1	6-A	301	SER
1	6-A	302	LYS
1	6-B	41	SER
1	6-B	129	GLY
1	6-B	131	ASP
1	6-B	241	HIS
1	6-C	298	GLU
1	6-D	39	CYS
1	6-D	73	SER
1	6-D	130	GLY
1	6-D	212	LEU
1	7-A	140	ARG
1	7-A	142	ALA
1	7-A	206	ILE
1	7-A	236	GLU
1	7-A	283	GLU
1	7-A	297	ASP
1	7-C	69	PHE
1	7-C	298	GLU
1	7-D	130	GLY
1	7-D	236	GLU
1	7-D	272	SER
1	8-A	165	PRO
1	8-B	131	ASP
1	8-B	255	ILE
1	8-B	279	LEU
1	8-C	131	ASP
1	8-C	298	GLU
1	1-C	166	ASP
1	1-C	182	ASP
1	1-D	236	GLU
1	2-C	93	ASP

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Mol	Chain	Res	Type
1	2-D	41	SER
1	3-A	69	PHE
1	3-A	302	LYS
1	3-B	131	ASP
1	3-B	172	GLU
1	3-B	173	ASP
1	3-B	208	PRO
1	3-B	324	PHE
1	3-C	272	SER
1	3-D	52	SER
1	3-D	236	GLU
1	3-D	292	PRO
1	4-A	131	ASP
1	4-A	236	GLU
1	4-B	328	VAL
1	4-D	114	PRO
1	4-D	131	ASP
1	4-D	236	GLU
1	5-A	236	GLU
1	5-A	289	PHE
1	5-C	111	THR
1	5-D	268	PRO
1	5-D	329	ILE
1	6-A	114	PRO
1	6-A	171	TYR
1	6-A	214	GLU
1	6-C	101	ARG
1	6-C	302	LYS
1	6-D	139	ALA
1	7-A	114	PRO
1	7-A	202	SER
1	7-C	272	SER
1	7-C	302	LYS
1	7-D	73	SER
1	7-D	312	ALA
1	7-D	318	ALA
1	8-A	69	PHE
1	8-A	271	PRO
1	8-B	166	ASP
1	8-C	129	GLY
1	8-C	302	LYS
1	8-D	41	SER

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Mol	Chain	Res	Type
1	1-A	300	SER
1	1-C	114	PRO
1	1-D	186	PHE
1	2-A	152	ILE
1	2-A	182	ASP
1	2-B	173	ASP
1	2-C	105	ALA
1	2-C	298	GLU
1	3-A	128	GLY
1	3-B	120	ASN
1	3-B	174	PRO
1	3-C	186	PHE
1	4-A	114	PRO
1	4-A	258	GLY
1	4-C	166	ASP
1	4-C	204	ASP
1	4-D	66	LYS
1	4-D	96	ILE
1	5-C	120	ASN
1	5-C	165	PRO
1	5-C	166	ASP
1	5-D	58	GLU
1	5-D	246	GLU
1	6-B	295	PRO
1	6-C	296	ILE
1	6-D	236	GLU
1	7-A	321	LEU
1	7-C	114	PRO
1	7-C	209	ALA
1	7-C	255	ILE
1	8-A	236	GLU
1	8-B	167	VAL
1	8-B	188	LYS
1	8-C	191	ALA
1	8-D	114	PRO
1	1-A	202	SER
1	1-B	292	PRO
1	1-C	131	ASP
1	1-C	160	SER
1	1-D	42	THR
1	2-A	192	GLU
1	2-C	114	PRO

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Mol	Chain	Res	Type
1	2-C	166	ASP
1	2-D	292	PRO
1	3-B	41	SER
1	3-C	59	ALA
1	3-C	243	ASP
1	3-C	296	ILE
1	3-D	290	LYS
1	4-A	180	ILE
1	4-A	272	SER
1	4-A	306	PRO
1	4-A	311	ASN
1	4-B	105	ALA
1	4-C	120	ASN
1	4-D	105	ALA
1	5-A	114	PRO
1	5-B	166	ASP
1	5-C	52	SER
1	5-D	66	LYS
1	5-D	203	SER
1	6-A	192	GLU
1	6-B	327	LYS
1	6-C	114	PRO
1	6-C	297	ASP
1	6-D	272	SER
1	6-D	323	SER
1	7-C	202	SER
1	7-D	120	ASN
1	8-A	255	ILE
1	8-A	268	PRO
1	8-B	268	PRO
1	8-C	202	SER
1	8-D	286	ASP
1	1-A	301	SER
1	1-B	114	PRO
1	1-D	46	GLY
1	2-A	69	PHE
1	2-A	130	GLY
1	2-C	182	ASP
1	3-A	131	ASP
1	3-B	180	ILE
1	3-B	202	SER
1	3-C	255	ILE

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Mol	Chain	Res	Type
1	3-C	268	PRO
1	4-A	318	ALA
1	4-B	292	PRO
1	5-A	306	PRO
1	5-B	114	PRO
1	5-D	45	PRO
1	6-B	98	LEU
1	6-B	142	ALA
1	6-C	102	ASP
1	6-C	312	ALA
1	6-D	327	LYS
1	7-A	289	PHE
1	7-C	207	GLY
1	7-D	204	ASP
1	8-A	212	LEU
1	8-A	258	GLY
1	8-C	69	PHE
1	1-B	258	GLY
1	2-A	114	PRO
1	2-A	258	GLY
1	2-C	165	PRO
1	3-A	296	ILE
1	4-C	205	PRO
1	5-D	167	VAL
1	6-C	268	PRO
1	7-C	205	PRO
1	8-A	152	ILE
1	1-C	129	GLY
1	2-C	244	ILE
1	3-A	114	PRO
1	3-B	152	ILE
1	3-C	114	PRO
1	4-C	114	PRO
1	5-A	96	ILE
1	5-D	292	PRO
1	6-A	179	VAL
1	6-B	144	ILE
1	6-C	244	ILE
1	7-A	120	ASN
1	7-A	130	GLY
1	1-C	205	PRO
1	2-A	296	ILE

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Mol	Chain	Res	Type
1	2-B	268	PRO
1	3-C	170	GLY
1	4-A	130	GLY
1	4-A	296	ILE
1	5-A	258	GLY
1	6-D	206	ILE
1	7-C	329	ILE
1	7-D	206	ILE
1	8-B	129	GLY
1	1-A	258	GLY
1	2-D	274	VAL
1	3-A	258	GLY
1	5-C	114	PRO
1	5-C	292	PRO
1	6-A	296	ILE
1	7-B	329	ILE
1	7-C	167	VAL
1	8-B	52	SER
1	8-B	275	ILE
1	8-C	130	GLY
1	2-A	165	PRO
1	6-C	130	GLY

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

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

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	99	THR
1	1-A	115	LEU
1	1-A	260	VAL

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Mol	Chain	Res	Type
1	1-B	97	GLN
1	1-B	113	LEU
1	1-B	115	LEU
1	1-B	149	MSE
1	1-B	167	VAL
1	1-B	187	LEU
1	1-B	233	THR
1	1-B	241	HIS
1	1-B	327	LYS
1	1-C	77	ASP
1	1-C	234	GLN
1	1-C	236	GLU
1	1-D	97	GLN
1	1-D	99	THR
1	1-D	109	MSE
1	1-D	115	LEU
1	1-D	116	CYS
1	1-D	162	GLN
1	1-D	166	ASP
1	1-D	226	ARG
1	1-D	234	GLN
1	1-D	330	GLU
1	2-A	99	THR
1	2-A	115	LEU
1	2-A	260	VAL
1	2-B	97	GLN
1	2-B	113	LEU
1	2-B	115	LEU
1	2-B	149	MSE
1	2-B	167	VAL
1	2-B	187	LEU
1	2-B	233	THR
1	2-B	241	HIS
1	2-B	327	LYS
1	2-C	77	ASP
1	2-C	234	GLN
1	2-C	236	GLU
1	2-D	97	GLN
1	2-D	99	THR
1	2-D	109	MSE
1	2-D	115	LEU
1	2-D	116	CYS

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Mol	Chain	Res	Type
1	2-D	162	GLN
1	2-D	166	ASP
1	2-D	226	ARG
1	2-D	234	GLN
1	2-D	330	GLU
1	3-A	99	THR
1	3-A	115	LEU
1	3-A	260	VAL
1	3-B	97	GLN
1	3-B	113	LEU
1	3-B	115	LEU
1	3-B	149	MSE
1	3-B	167	VAL
1	3-B	187	LEU
1	3-B	233	THR
1	3-B	241	HIS
1	3-B	327	LYS
1	3-C	77	ASP
1	3-C	234	GLN
1	3-C	236	GLU
1	3-D	97	GLN
1	3-D	99	THR
1	3-D	109	MSE
1	3-D	115	LEU
1	3-D	116	CYS
1	3-D	162	GLN
1	3-D	166	ASP
1	3-D	226	ARG
1	3-D	234	GLN
1	3-D	330	GLU
1	4-A	99	THR
1	4-A	115	LEU
1	4-A	260	VAL
1	4-B	97	GLN
1	4-B	113	LEU
1	4-B	115	LEU
1	4-B	149	MSE
1	4-B	167	VAL
1	4-B	187	LEU
1	4-B	233	THR
1	4-B	241	HIS
1	4-B	327	LYS

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Mol	Chain	Res	Type
1	4-C	77	ASP
1	4-C	234	GLN
1	4-C	236	GLU
1	4-D	97	GLN
1	4-D	99	THR
1	4-D	109	MSE
1	4-D	115	LEU
1	4-D	116	CYS
1	4-D	162	GLN
1	4-D	166	ASP
1	4-D	226	ARG
1	4-D	234	GLN
1	4-D	330	GLU
1	5-A	99	THR
1	5-A	115	LEU
1	5-A	260	VAL
1	5-B	97	GLN
1	5-B	113	LEU
1	5-B	115	LEU
1	5-B	149	MSE
1	5-B	167	VAL
1	5-B	187	LEU
1	5-B	233	THR
1	5-B	241	HIS
1	5-B	327	LYS
1	5-C	77	ASP
1	5-C	234	GLN
1	5-C	236	GLU
1	5-D	97	GLN
1	5-D	99	THR
1	5-D	109	MSE
1	5-D	115	LEU
1	5-D	116	CYS
1	5-D	162	GLN
1	5-D	166	ASP
1	5-D	226	ARG
1	5-D	234	GLN
1	5-D	330	GLU
1	6-A	99	THR
1	6-A	115	LEU
1	6-A	260	VAL
1	6-B	97	GLN

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Mol	Chain	Res	Type
1	6-B	113	LEU
1	6-B	115	LEU
1	6-B	149	MSE
1	6-B	167	VAL
1	6-B	187	LEU
1	6-B	233	THR
1	6-B	241	HIS
1	6-B	327	LYS
1	6-C	77	ASP
1	6-C	234	GLN
1	6-C	236	GLU
1	6-D	97	GLN
1	6-D	99	THR
1	6-D	109	MSE
1	6-D	115	LEU
1	6-D	116	CYS
1	6-D	162	GLN
1	6-D	166	ASP
1	6-D	226	ARG
1	6-D	234	GLN
1	6-D	330	GLU
1	7-A	99	THR
1	7-A	115	LEU
1	7-A	260	VAL
1	7-B	97	GLN
1	7-B	113	LEU
1	7-B	115	LEU
1	7-B	149	MSE
1	7-B	167	VAL
1	7-B	187	LEU
1	7-B	233	THR
1	7-B	241	HIS
1	7-B	327	LYS
1	7-C	77	ASP
1	7-C	234	GLN
1	7-C	236	GLU
1	7-D	97	GLN
1	7-D	99	THR
1	7-D	109	MSE
1	7-D	115	LEU
1	7-D	116	CYS
1	7-D	162	GLN

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Mol	Chain	Res	Type
1	7-D	166	ASP
1	7-D	226	ARG
1	7-D	234	GLN
1	7-D	330	GLU
1	8-A	99	THR
1	8-A	115	LEU
1	8-A	260	VAL
1	8-B	97	GLN
1	8-B	113	LEU
1	8-B	115	LEU
1	8-B	149	MSE
1	8-B	167	VAL
1	8-B	187	LEU
1	8-B	233	THR
1	8-B	241	HIS
1	8-B	327	LYS
1	8-C	77	ASP
1	8-C	234	GLN
1	8-C	236	GLU
1	8-D	97	GLN
1	8-D	99	THR
1	8-D	109	MSE
1	8-D	115	LEU
1	8-D	116	CYS
1	8-D	162	GLN
1	8-D	166	ASP
1	8-D	226	ARG
1	8-D	234	GLN
1	8-D	330	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (189) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	60	HIS
1	1-A	70	GLN
1	1-A	82	GLN
1	1-A	97	GLN
1	1-A	146	GLN
1	1-A	241	HIS
1	1-A	304	ASN
1	1-B	76	GLN
1	1-B	82	GLN

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Mol	Chain	Res	Type
1	1-B	120	ASN
1	1-B	146	GLN
1	1-C	70	GLN
1	1-C	82	GLN
1	1-C	107	GLN
1	1-C	162	GLN
1	1-C	219	GLN
1	1-C	241	HIS
1	1-C	261	ASN
1	1-C	304	ASN
1	1-D	60	HIS
1	1-D	70	GLN
1	1-D	120	ASN
1	1-D	146	GLN
1	1-D	162	GLN
1	1-D	261	ASN
1	2-A	70	GLN
1	2-A	82	GLN
1	2-A	97	GLN
1	2-A	107	GLN
1	2-A	120	ASN
1	2-A	241	HIS
1	2-A	251	ASN
1	2-A	261	ASN
1	2-B	120	ASN
1	2-B	146	GLN
1	2-B	162	GLN
1	2-B	311	ASN
1	2-C	70	GLN
1	2-C	82	GLN
1	2-C	97	GLN
1	2-C	146	GLN
1	2-C	241	HIS
1	2-C	261	ASN
1	2-C	304	ASN
1	2-D	97	GLN
1	2-D	120	ASN
1	2-D	146	GLN
1	2-D	162	GLN
1	2-D	177	ASN
1	2-D	261	ASN
1	3-A	97	GLN

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Mol	Chain	Res	Type
1	3-A	107	GLN
1	3-A	146	GLN
1	3-A	241	HIS
1	3-B	76	GLN
1	3-B	146	GLN
1	3-C	82	GLN
1	3-C	234	GLN
1	3-C	241	HIS
1	3-C	261	ASN
1	3-C	304	ASN
1	3-C	315	HIS
1	3-D	97	GLN
1	3-D	146	GLN
1	3-D	162	GLN
1	3-D	219	GLN
1	3-D	234	GLN
1	3-D	261	ASN
1	3-D	291	HIS
1	4-A	70	GLN
1	4-A	97	GLN
1	4-A	162	GLN
1	4-A	251	ASN
1	4-A	304	ASN
1	4-B	70	GLN
1	4-B	97	GLN
1	4-B	107	GLN
1	4-B	120	ASN
1	4-B	141	HIS
1	4-B	146	GLN
1	4-B	162	GLN
1	4-B	234	GLN
1	4-B	241	HIS
1	4-C	107	GLN
1	4-C	219	GLN
1	4-C	241	HIS
1	4-C	261	ASN
1	4-C	304	ASN
1	4-D	76	GLN
1	4-D	82	GLN
1	4-D	162	GLN
1	4-D	234	GLN
1	4-D	261	ASN

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Mol	Chain	Res	Type
1	5-A	70	GLN
1	5-A	76	GLN
1	5-A	97	GLN
1	5-A	120	ASN
1	5-B	97	GLN
1	5-B	107	GLN
1	5-B	120	ASN
1	5-B	162	GLN
1	5-B	177	ASN
1	5-B	189	ASN
1	5-B	291	HIS
1	5-C	70	GLN
1	5-C	82	GLN
1	5-C	251	ASN
1	5-C	261	ASN
1	5-C	304	ASN
1	5-D	60	HIS
1	5-D	70	GLN
1	5-D	82	GLN
1	5-D	97	GLN
1	5-D	219	GLN
1	5-D	251	ASN
1	5-D	311	ASN
1	6-A	70	GLN
1	6-A	97	GLN
1	6-A	162	GLN
1	6-A	261	ASN
1	6-B	70	GLN
1	6-B	82	GLN
1	6-B	97	GLN
1	6-B	107	GLN
1	6-B	146	GLN
1	6-B	177	ASN
1	6-B	234	GLN
1	6-C	76	GLN
1	6-C	97	GLN
1	6-C	189	ASN
1	6-C	241	HIS
1	6-C	261	ASN
1	6-C	304	ASN
1	6-D	70	GLN
1	6-D	76	GLN

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Mol	Chain	Res	Type
1	6-D	82	GLN
1	6-D	120	ASN
1	6-D	146	GLN
1	6-D	162	GLN
1	6-D	241	HIS
1	6-D	251	ASN
1	6-D	261	ASN
1	7-A	70	GLN
1	7-A	82	GLN
1	7-A	97	GLN
1	7-A	234	GLN
1	7-A	241	HIS
1	7-A	261	ASN
1	7-B	60	HIS
1	7-B	97	GLN
1	7-B	120	ASN
1	7-B	146	GLN
1	7-B	234	GLN
1	7-B	261	ASN
1	7-C	70	GLN
1	7-C	82	GLN
1	7-C	107	GLN
1	7-C	146	GLN
1	7-C	162	GLN
1	7-C	241	HIS
1	7-C	261	ASN
1	7-C	304	ASN
1	7-D	60	HIS
1	7-D	76	GLN
1	7-D	97	GLN
1	7-D	141	HIS
1	7-D	162	GLN
1	8-A	97	GLN
1	8-A	146	GLN
1	8-A	251	ASN
1	8-A	261	ASN
1	8-B	120	ASN
1	8-B	146	GLN
1	8-B	219	GLN
1	8-B	234	GLN
1	8-C	70	GLN
1	8-C	82	GLN

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Mol	Chain	Res	Type
1	8-C	146	GLN
1	8-C	234	GLN
1	8-C	241	HIS
1	8-C	304	ASN
1	8-D	60	HIS
1	8-D	97	GLN
1	8-D	120	ASN
1	8-D	146	GLN
1	8-D	162	GLN
1	8-D	189	ASN
1	8-D	219	GLN
1	8-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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)  	2, 4, 10, 12	283 (100%)
1	1-B	278/334 (83%)	1.08	43 (15%)  	1, 4, 7, 12	278 (100%)
1	1-C	283/334 (84%)	1.36	66 (23%)  	2, 4, 10, 13	283 (100%)
1	1-D	278/334 (83%)	1.36	68 (24%)  	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%)

All (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
1	1-B	329	ILE	5.6
1	1-B	206	ILE	5.5
1	1-C	70	GLN	5.5
1	1-C	131	ASP	5.5
1	1-C	167	VAL	5.5
1	1-D	142	ALA	5.4
1	1-D	165	PRO	5.3
1	1-C	130	GLY	5.3
1	1-D	130	GLY	5.3
1	1-C	296	ILE	5.2
1	1-C	42	THR	5.2
1	1-A	129	GLY	5.2
1	1-A	300	SER	5.2
1	1-B	39	CYS	5.1
1	1-D	166	ASP	5.1
1	1-B	307	LEU	5.0
1	1-B	259	SER	4.9
1	1-B	205	PRO	4.9
1	1-A	130	GLY	4.9
1	1-C	150	CYS	4.8
1	1-D	43	VAL	4.8
1	1-B	330	GLU	4.7
1	1-C	301	SER	4.7
1	1-C	300	SER	4.5
1	1-C	161	LYS	4.5
1	1-B	79	ILE	4.5
1	1-C	41	SER	4.5
1	1-A	209	ALA	4.4
1	1-C	69	PHE	4.4
1	1-A	167	VAL	4.4
1	1-A	77	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	1-C	299	SER	4.3
1	1-D	163	PHE	4.2
1	1-A	296	ILE	4.1
1	1-C	209	ALA	4.1
1	1-D	167	VAL	4.0
1	1-A	283	GLU	3.9
1	1-D	129	GLY	3.9
1	1-D	70	GLN	3.9
1	1-D	132	GLY	3.9
1	1-C	208	PRO	3.9
1	1-D	318	ALA	3.9
1	1-B	207	GLY	3.9
1	1-A	166	ASP	3.8
1	1-A	294	ASN	3.8
1	1-C	168	ALA	3.8
1	1-C	177	ASN	3.7
1	1-C	129	GLY	3.7
1	1-C	297	ASP	3.7
1	1-B	38	ALA	3.7
1	1-B	129	GLY	3.7
1	1-D	305	GLY	3.7
1	1-D	205	PRO	3.7
1	1-C	169	ILE	3.6
1	1-C	206	ILE	3.6
1	1-A	191	ALA	3.6
1	1-D	41	SER	3.6
1	1-B	131	ASP	3.6
1	1-D	60	HIS	3.6
1	1-A	259	SER	3.6
1	1-C	307	LEU	3.6
1	1-C	179	VAL	3.5
1	1-B	203	SER	3.5
1	1-B	113	LEU	3.5
1	1-C	166	ASP	3.5
1	1-C	148	ASP	3.5
1	1-D	159	VAL	3.5
1	1-A	126	VAL	3.4
1	1-C	160	SER	3.4
1	1-B	40	PHE	3.4
1	1-A	146	GLN	3.4
1	1-A	206	ILE	3.3
1	1-D	39	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	1-D	189	ASN	3.3
1	1-D	206	ILE	3.3
1	1-A	213	PHE	3.3
1	1-D	99	THR	3.3
1	1-C	241	HIS	3.3
1	1-B	243	ASP	3.3
1	1-A	307	LEU	3.3
1	1-C	255	ILE	3.3
1	1-D	158	ASP	3.3
1	1-B	45	PRO	3.2
1	1-D	56	PRO	3.2
1	1-A	257	LYS	3.2
1	1-C	246	GLU	3.2
1	1-C	77	ASP	3.1
1	1-A	60	HIS	3.1
1	1-B	328	VAL	3.1
1	1-B	70	GLN	3.1
1	1-B	209	ALA	3.1
1	1-C	44	ILE	3.1
1	1-A	303	SER	3.1
1	1-C	251	ASN	3.1
1	1-D	157	VAL	3.1
1	1-A	106	TYR	3.0
1	1-C	165	PRO	3.0
1	1-A	297	ASP	3.0
1	1-C	184	VAL	3.0
1	1-B	157	VAL	3.0
1	1-D	330	GLU	3.0
1	1-A	208	PRO	3.0
1	1-A	298	GLU	2.9
1	1-B	296	ILE	2.9
1	1-B	258	GLY	2.9
1	1-C	128	GLY	2.9
1	1-A	72	LYS	2.9
1	1-A	190	ALA	2.9
1	1-D	190	ALA	2.9
1	1-B	257	LYS	2.9
1	1-D	283	GLU	2.9
1	1-A	45	PRO	2.9
1	1-D	175	ARG	2.9
1	1-C	87	GLY	2.9
1	1-B	208	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-C	182	ASP	2.9
1	1-B	260	VAL	2.9
1	1-B	162	GLN	2.8
1	1-D	136	ARG	2.8
1	1-D	89	VAL	2.8
1	1-C	298	GLU	2.8
1	1-C	162	GLN	2.8
1	1-D	164	PHE	2.8
1	1-D	162	GLN	2.8
1	1-D	146	GLN	2.8
1	1-D	143	SER	2.8
1	1-A	202	SER	2.7
1	1-D	258	GLY	2.7
1	1-A	309	PHE	2.7
1	1-A	98	LEU	2.7
1	1-B	174	PRO	2.7
1	1-A	150	CYS	2.7
1	1-A	220	SER	2.7
1	1-C	181	GLY	2.7
1	1-C	304	ASN	2.7
1	1-D	202	SER	2.7
1	1-D	38	ALA	2.7
1	1-B	166	ASP	2.7
1	1-D	329	ILE	2.7
1	1-A	330	GLU	2.7
1	1-C	303	SER	2.7
1	1-D	151	GLU	2.7
1	1-A	174	PRO	2.7
1	1-B	82	GLN	2.6
1	1-D	223	ARG	2.6
1	1-B	167	VAL	2.6
1	1-D	153	ASP	2.6
1	1-C	151	GLU	2.6
1	1-C	170	GLY	2.6
1	1-C	43	VAL	2.6
1	1-A	212	LEU	2.6
1	1-A	313	GLU	2.6
1	1-A	314	ILE	2.6
1	1-D	45	PRO	2.6
1	1-D	168	ALA	2.6
1	1-D	203	SER	2.5
1	1-D	296	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-D	135	LEU	2.5
1	1-A	128	GLY	2.5
1	1-B	262	TYR	2.5
1	1-B	130	GLY	2.5
1	1-A	254	GLU	2.5
1	1-A	305	GLY	2.5
1	1-D	292	PRO	2.5
1	1-A	275	ILE	2.5
1	1-A	131	ASP	2.5
1	1-A	204	ASP	2.5
1	1-D	47	TRP	2.5
1	1-B	46	GLY	2.5
1	1-D	82	GLN	2.5
1	1-A	137	GLU	2.4
1	1-A	171	TYR	2.4
1	1-A	188	LYS	2.4
1	1-A	234	GLN	2.4
1	1-A	156	VAL	2.4
1	1-A	273	GLY	2.4
1	1-A	43	VAL	2.4
1	1-C	186	PHE	2.4
1	1-A	302	LYS	2.4
1	1-D	208	PRO	2.4
1	1-C	305	GLY	2.4
1	1-C	187	LEU	2.3
1	1-D	71	GLY	2.3
1	1-A	41	SER	2.3
1	1-A	217	PHE	2.3
1	1-C	212	LEU	2.3
1	1-C	152	ILE	2.3
1	1-A	247	ASP	2.3
1	1-C	243	ASP	2.3
1	1-B	136	ARG	2.3
1	1-C	253	ARG	2.3
1	1-D	154	LYS	2.3
1	1-D	117	SER	2.3
1	1-D	204	ASP	2.3
1	1-A	78	VAL	2.3
1	1-D	176	VAL	2.3
1	1-C	213	PHE	2.3
1	1-B	66	LYS	2.2
1	1-B	75	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	295	PRO	2.2
1	1-D	216	PRO	2.2
1	1-C	62	LEU	2.2
1	1-A	164	PHE	2.2
1	1-A	100	GLU	2.2
1	1-C	214	GLU	2.2
1	1-A	223	ARG	2.2
1	1-C	258	GLY	2.2
1	1-D	173	ASP	2.2
1	1-D	98	LEU	2.2
1	1-A	320	CYS	2.2
1	1-A	306	PRO	2.2
1	1-C	183	GLY	2.2
1	1-D	308	LYS	2.2
1	1-B	168	ALA	2.2
1	1-D	293	LEU	2.2
1	1-A	299	SER	2.2
1	1-D	103	GLU	2.1
1	1-B	120	ASN	2.1
1	1-C	257	LYS	2.1
1	1-D	97	GLN	2.1
1	1-D	171	TYR	2.1
1	1-C	178	LEU	2.1
1	1-B	128	GLY	2.1
1	1-A	176	VAL	2.1
1	1-C	247	ASP	2.1
1	1-D	83	SER	2.1
1	1-A	172	GLU	2.1
1	1-A	99	THR	2.1
1	1-A	238	LEU	2.1
1	1-A	270	TYR	2.1
1	1-B	80	VAL	2.1
1	1-D	88	LYS	2.1
1	1-C	189	ASN	2.1
1	1-C	207	GLY	2.1
1	1-A	168	ALA	2.1
1	1-C	202	SER	2.1
1	1-C	116	CYS	2.1
1	1-C	252	CYS	2.1
1	1-A	243	ASP	2.0
1	1-D	185	ALA	2.0
1	1-C	238	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	1-D	259	SER	2.0
1	1-A	207	GLY	2.0
1	1-B	305	GLY	2.0

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.