Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2016 – 07:44 PM EST

PDB ID	:	5B1S
Title	:	Crystal structure of Trypanosoma cruzi spermidine synthase in complex with 2-(2-fluorophenyl)ethanamine
Authors	:	Amano, Y.; Tateishi, Y.
Deposited on	:	2015-12-17
Resolution	:	1.58 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442
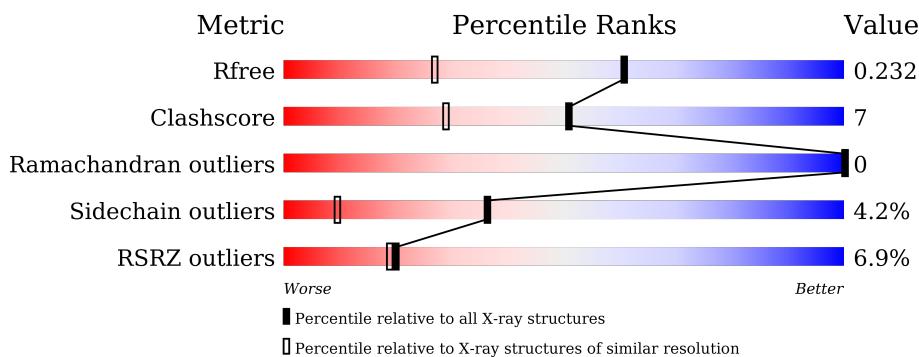
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
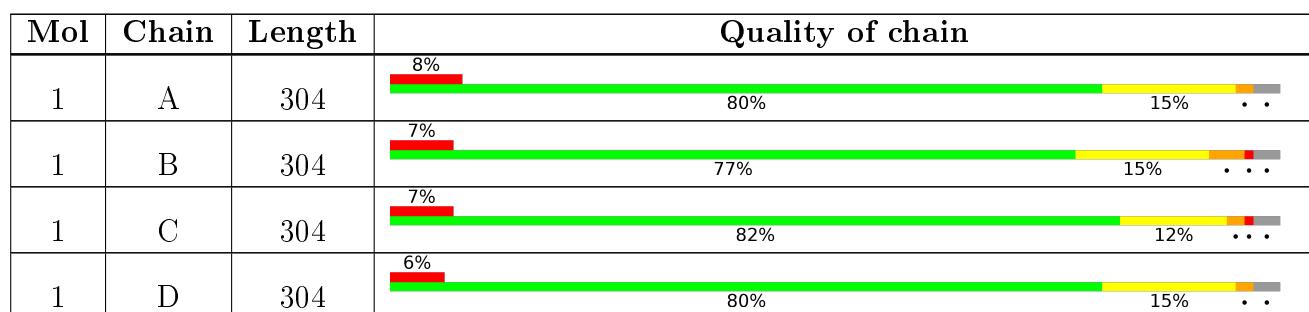
The reported resolution of this entry is 1.58 Å.

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	Percentile Ranks	Value
Rfree		0.232
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		4.2%
RSRZ outliers		6.9%

Worse ... *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	8% / 80% / 15% ··
1	B	304	7% / 77% / 15% ···
1	C	304	7% / 82% / 12% ···
1	D	304	6% / 80% / 15% ··

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9943 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, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2306	1464	393	434	15			
1	B	294	Total	C	N	O	S	0	0	0
			2306	1464	393	434	15			
1	C	294	Total	C	N	O	S	0	0	0
			2306	1464	393	434	15			
1	D	294	Total	C	N	O	S	0	0	0
			2306	1464	393	434	15			

There are 32 discrepancies between the modelled and reference sequences:
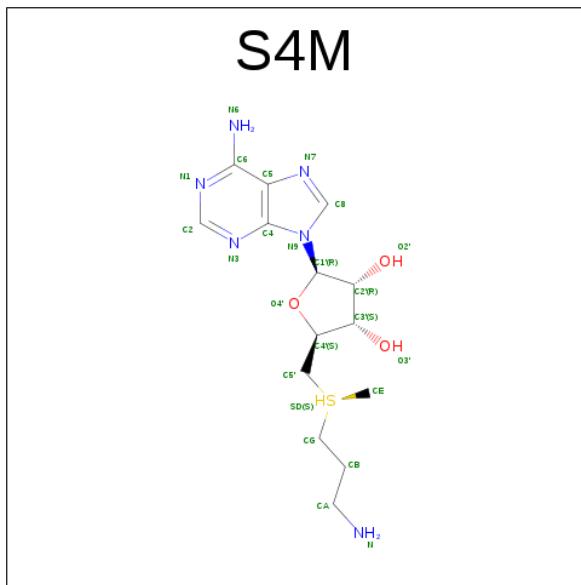
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q4DA73
A	-6	ALA	-	expression tag	UNP Q4DA73
A	-5	HIS	-	expression tag	UNP Q4DA73
A	-4	HIS	-	expression tag	UNP Q4DA73
A	-3	HIS	-	expression tag	UNP Q4DA73
A	-2	HIS	-	expression tag	UNP Q4DA73
A	-1	HIS	-	expression tag	UNP Q4DA73
A	0	HIS	-	expression tag	UNP Q4DA73
B	-7	MET	-	expression tag	UNP Q4DA73
B	-6	ALA	-	expression tag	UNP Q4DA73
B	-5	HIS	-	expression tag	UNP Q4DA73
B	-4	HIS	-	expression tag	UNP Q4DA73
B	-3	HIS	-	expression tag	UNP Q4DA73
B	-2	HIS	-	expression tag	UNP Q4DA73
B	-1	HIS	-	expression tag	UNP Q4DA73
B	0	HIS	-	expression tag	UNP Q4DA73
C	-7	MET	-	expression tag	UNP Q4DA73
C	-6	ALA	-	expression tag	UNP Q4DA73
C	-5	HIS	-	expression tag	UNP Q4DA73
C	-4	HIS	-	expression tag	UNP Q4DA73
C	-3	HIS	-	expression tag	UNP Q4DA73

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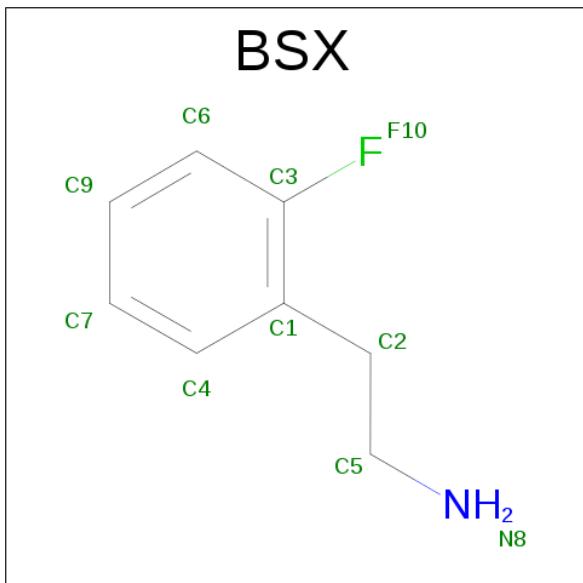
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q4DA73
C	-1	HIS	-	expression tag	UNP Q4DA73
C	0	HIS	-	expression tag	UNP Q4DA73
D	-7	MET	-	expression tag	UNP Q4DA73
D	-6	ALA	-	expression tag	UNP Q4DA73
D	-5	HIS	-	expression tag	UNP Q4DA73
D	-4	HIS	-	expression tag	UNP Q4DA73
D	-3	HIS	-	expression tag	UNP Q4DA73
D	-2	HIS	-	expression tag	UNP Q4DA73
D	-1	HIS	-	expression tag	UNP Q4DA73
D	0	HIS	-	expression tag	UNP Q4DA73

- Molecule 2 is 5'-[(S)-(3-AMINOPROPYL)(METHYL)-LAMBDA 4 -SULFANYL]-5'-DEO XYADENOSINE (three-letter code: S4M) (formula: $C_{14}H_{24}N_6O_3S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	B	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	C	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	D	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

- Molecule 3 is 2-(2-fluorophenyl)ethanamine (three-letter code: BSX) (formula: $C_8H_{10}FN$).

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 10	C 8	F 1	N 1	0	0
3	B	1	Total 10	C 8	F 1	N 1	0	0
3	C	1	Total 10	C 8	F 1	N 1	0	0
3	D	1	Total 10	C 8	F 1	N 1	0	0
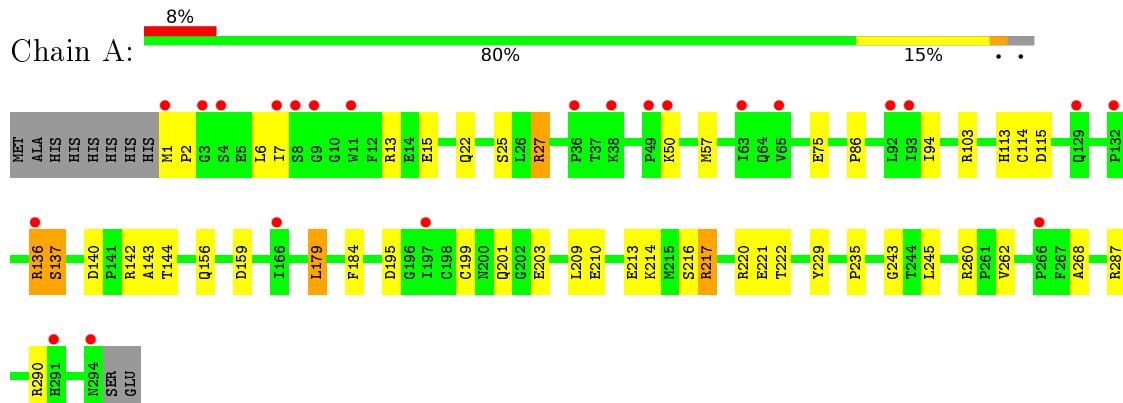
- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	149	Total 149	O 149	0	0
4	C	160	Total 160	O 160	0	0
4	D	139	Total 139	O 139	0	0
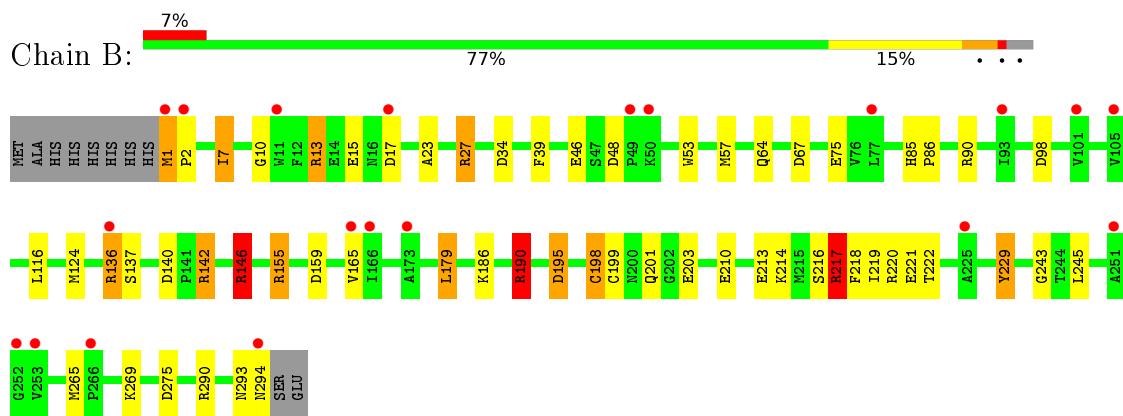
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
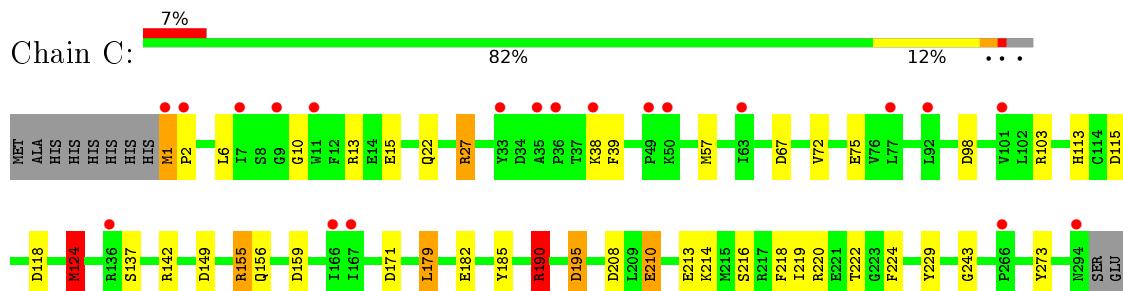
- Molecule 1: Spermidine synthase, putative
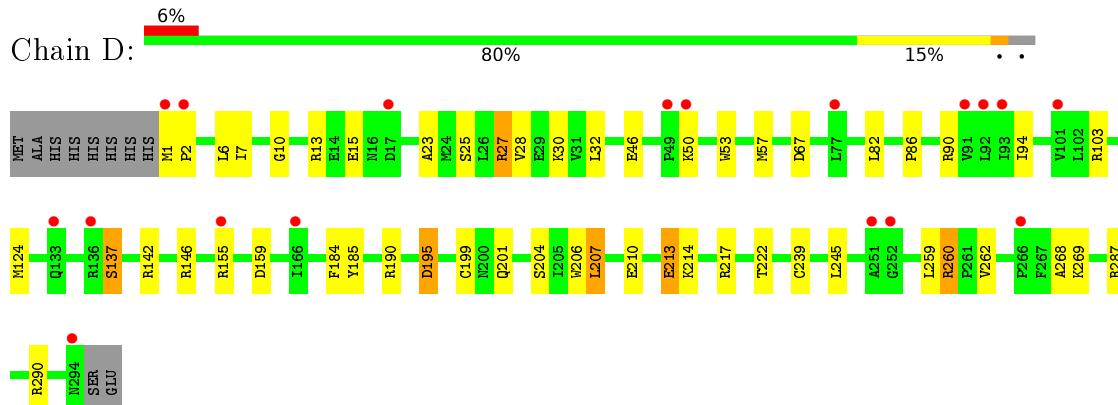
- Molecule 1: Spermidine synthase, putative

- Molecule 1: Spermidine synthase, putative

• Molecule 1: Spermidine synthase, putative

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	44.48Å 68.16Å 94.46Å 87.91° 87.18° 80.27°	Depositor
Resolution (Å)	25.02 − 1.58 25.03 − 1.58	Depositor EDS
% Data completeness (in resolution range)	81.5 (25.02-1.58) 80.8 (25.03-1.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	14.02 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.185 , 0.232 0.185 , 0.232	Depositor DCC
R_{free} test set	6148 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	10.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.47 , 71.1	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9943	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: S4M, BSX

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	1.20	4/2364 (0.2%)	1.39	20/3207 (0.6%)
1	B	1.21	7/2364 (0.3%)	1.42	27/3207 (0.8%)
1	C	1.14	7/2364 (0.3%)	1.50	23/3207 (0.7%)
1	D	1.18	5/2364 (0.2%)	1.69	25/3207 (0.8%)
All	All	1.18	23/9456 (0.2%)	1.51	95/12828 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	ARG	CZ-NH2	-14.09	1.14	1.33
1	A	137	SER	CB-OG	12.81	1.58	1.42
1	D	190	ARG	CZ-NH1	9.38	1.45	1.33
1	A	137	SER	CA-CB	8.43	1.65	1.52
1	D	190	ARG	CZ-NH2	-8.42	1.22	1.33
1	C	124	MET	CA-CB	8.29	1.72	1.53
1	C	124	MET	CB-CG	8.23	1.77	1.51
1	A	142	ARG	CZ-NH1	8.16	1.43	1.33
1	B	46	GLU	CD-OE2	7.51	1.33	1.25
1	B	203	GLU	CD-OE2	5.92	1.32	1.25
1	D	46	GLU	CD-OE2	5.92	1.32	1.25
1	B	46	GLU	CG-CD	5.77	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	GLU	CD-OE2	5.75	1.31	1.25
1	B	136	ARG	C-O	5.75	1.34	1.23
1	B	137	SER	CB-OG	5.59	1.49	1.42
1	C	190	ARG	CD-NE	-5.34	1.37	1.46
1	C	210	GLU	CD-OE2	5.32	1.31	1.25
1	C	190	ARG	CZ-NH2	-5.29	1.26	1.33
1	C	75	GLU	CD-OE2	5.27	1.31	1.25
1	B	75	GLU	CD-OE2	5.20	1.31	1.25
1	D	137	SER	CB-OG	5.15	1.49	1.42
1	C	137	SER	CB-OG	5.13	1.49	1.42
1	D	25	SER	CB-OG	5.05	1.48	1.42

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	190	ARG	NE-CZ-NH2	-45.55	97.53	120.30
1	D	190	ARG	NE-CZ-NH1	35.38	137.99	120.30
1	C	190	ARG	NE-CZ-NH2	-31.42	104.59	120.30
1	C	190	ARG	NE-CZ-NH1	24.32	132.46	120.30
1	B	190	ARG	NE-CZ-NH2	-24.23	108.19	120.30
1	A	142	ARG	NE-CZ-NH2	-18.22	111.19	120.30
1	B	142	ARG	NE-CZ-NH2	16.59	128.59	120.30
1	A	287	ARG	NE-CZ-NH1	15.44	128.02	120.30
1	A	287	ARG	NE-CZ-NH2	-15.04	112.78	120.30
1	C	57	MET	CG-SD-CE	-14.83	76.47	100.20
1	A	142	ARG	NE-CZ-NH1	14.73	127.66	120.30
1	B	142	ARG	CD-NE-CZ	-13.96	104.06	123.60
1	A	57	MET	CG-SD-CE	-13.59	78.46	100.20
1	C	142	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	D	142	ARG	NE-CZ-NH1	12.71	126.65	120.30
1	D	287	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	B	190	ARG	CD-NE-CZ	12.44	141.02	123.60
1	D	90	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	D	142	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	C	190	ARG	CD-NE-CZ	11.44	139.61	123.60
1	C	142	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	C	195	ASP	CB-CG-OD1	10.96	128.17	118.30
1	D	287	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	A	137	SER	N-CA-CB	-10.63	94.56	110.50
1	D	190	ARG	CD-NE-CZ	10.53	138.34	123.60
1	C	159	ASP	CB-CG-OD1	10.38	127.64	118.30
1	D	195	ASP	CB-CG-OD1	10.25	127.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	ASP	CB-CG-OD1	9.76	127.08	118.30
1	B	195	ASP	CB-CG-OD1	9.54	126.88	118.30
1	D	195	ASP	CB-CG-OD2	-9.52	109.74	118.30
1	B	195	ASP	CB-CG-OD2	-9.49	109.75	118.30
1	C	124	MET	CB-CA-C	9.22	128.83	110.40
1	A	179	LEU	CB-CG-CD1	9.21	126.66	111.00
1	C	179	LEU	CB-CG-CD1	8.55	125.54	111.00
1	A	103	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	A	290	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	D	57	MET	CG-SD-CE	-8.28	86.95	100.20
1	C	103	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	C	195	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	B	140	ASP	CB-CG-OD1	7.57	125.11	118.30
1	C	208	ASP	CB-CG-OD2	7.54	125.09	118.30
1	B	142	ARG	NH1-CZ-NH2	-7.47	111.19	119.40
1	C	124	MET	CA-CB-CG	7.38	125.85	113.30
1	B	90	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	90	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	290	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	217	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	D	137	SER	N-CA-CB	-6.94	100.10	110.50
1	B	159	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	142	ARG	CG-CD-NE	6.78	126.03	111.80
1	B	140	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	D	159	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	275	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	90	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	D	290	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	140	ASP	CB-CG-OD1	6.53	124.18	118.30
1	C	6	LEU	CB-CG-CD1	-6.51	99.93	111.00
1	C	103	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	217	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	142	ARG	CD-NE-CZ	6.17	132.24	123.60
1	D	103	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	185	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	B	34	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	195	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	209	LEU	CB-CG-CD2	-5.93	100.91	111.00
1	B	179	LEU	CB-CG-CD2	5.93	121.08	111.00
1	C	124	MET	CG-SD-CE	-5.90	90.76	100.20
1	A	6	LEU	CB-CG-CD2	5.88	121.00	111.00
1	C	118	ASP	CB-CG-OD1	5.86	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	195	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	D	259	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	A	159	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	13	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	B	17	ASP	CB-CG-OD1	-5.77	113.10	118.30
1	B	67	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	D	67	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	229	TYR	CG-CD1-CE1	-5.63	116.80	121.30
1	B	67	ASP	CB-CG-OD1	5.62	123.35	118.30
1	D	6	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	D	260	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	39	PHE	CB-CG-CD1	-5.38	117.03	120.80
1	D	185	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	B	179	LEU	CB-CG-CD1	5.34	120.07	111.00
1	C	171	ASP	CB-CG-OD2	5.32	123.09	118.30
1	D	67	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	185	TYR	CZ-CE2-CD2	-5.28	115.05	119.80
1	D	190	ARG	CG-CD-NE	-5.23	100.81	111.80
1	A	290	ARG	CD-NE-CZ	5.20	130.88	123.60
1	B	155	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	67	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	290	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	82	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	B	146	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	185	TYR	CG-CD1-CE1	-5.01	117.29	121.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	190	ARG	Sidechain
1	C	190	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2306	0	2257	27	0
1	B	2306	0	2257	36	0
1	C	2306	0	2257	30	0
1	D	2306	0	2257	37	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0
2	C	24	0	24	0	0
2	D	24	0	24	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	135	0	0	1	0
4	B	149	0	0	4	0
4	C	160	0	0	5	0
4	D	139	0	0	3	0
All	All	9943	0	9124	128	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 7.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:MET:CG	1:C:124:MET:CB	1.77	1.60
1:C:156:GLN:HG2	4:C:604:HOH:O	1.34	1.27
1:D:207:LEU:HD11	1:D:239:CYS:SG	1.95	1.07
1:B:13:ARG:HD2	1:B:15:GLU:OE2	1.54	1.04
1:B:57:MET:HE2	1:B:64:GLN:HB2	1.34	1.03
1:D:146:ARG:HG2	1:D:146:ARG:HH11	1.26	0.99
1:C:13:ARG:CD	1:C:15:GLU:OE2	2.16	0.93
1:D:210:GLU:HA	1:D:213:GLU:OE2	1.67	0.93
1:A:214:LYS:HG2	1:A:217:ARG:NH2	1.84	0.91
1:D:13:ARG:HD2	1:D:15:GLU:OE2	1.69	0.91
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.37	0.90
1:B:13:ARG:CD	1:B:15:GLU:OE2	2.19	0.90
1:C:13:ARG:HD2	1:C:15:GLU:OE2	1.72	0.89
1:C:10:GLY:HA3	1:C:27:ARG:HH21	1.39	0.88
1:C:124:MET:SD	1:C:124:MET:CB	2.67	0.83
1:D:213:GLU:HG2	1:D:217:ARG:NH2	1.94	0.82
1:B:57:MET:HE2	1:B:64:GLN:CB	2.09	0.81
1:B:293:ASN:O	1:B:294:ASN:HB2	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ARG:HH11	1:B:146:ARG:CG	1.98	0.77
1:D:204:SER:OG	1:D:207:LEU:HD13	1.86	0.76
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.50	0.76
1:C:182:GLU:HG3	4:C:688:HOH:O	1.87	0.74
1:B:210:GLU:O	1:B:213:GLU:HG2	1.89	0.72
1:D:213:GLU:CG	1:D:217:ARG:NH2	2.53	0.72
1:B:10:GLY:HA3	1:B:27:ARG:HH21	1.54	0.70
1:A:27:ARG:NH1	1:A:27:ARG:HG3	2.06	0.70
1:D:146:ARG:CG	1:D:146:ARG:HH11	2.03	0.69
1:A:113:HIS:NE2	1:A:115:ASP:OD1	2.25	0.69
1:C:13:ARG:HD3	1:C:15:GLU:OE2	1.90	0.69
1:B:57:MET:CE	1:B:64:GLN:CB	2.72	0.68
1:A:156:GLN:NE2	4:A:601:HOH:O	2.26	0.68
1:D:1:MET:HB3	1:D:2:PRO:HD3	1.76	0.68
1:A:210:GLU:O	1:A:213:GLU:HG2	1.95	0.67
1:B:57:MET:CE	1:B:64:GLN:HB2	2.18	0.66
1:C:155:ARG:HD3	4:C:675:HOH:O	1.94	0.66
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.76	0.65
1:D:207:LEU:N	1:D:207:LEU:HD12	2.12	0.64
1:D:213:GLU:CG	1:D:217:ARG:HH22	2.10	0.64
1:B:146:ARG:HG2	1:B:146:ARG:NH1	2.11	0.64
1:D:213:GLU:HG3	1:D:217:ARG:HH22	1.63	0.64
1:C:155:ARG:NH2	4:C:602:HOH:O	2.30	0.63
1:A:27:ARG:CG	1:A:27:ARG:HH11	2.12	0.62
1:C:13:ARG:HD3	1:C:15:GLU:CG	2.29	0.62
1:D:13:ARG:CD	1:D:15:GLU:OE2	2.44	0.62
1:A:7:ILE:HG13	1:A:7:ILE:O	2.00	0.62
1:A:214:LYS:HG2	1:A:217:ARG:HH22	1.63	0.61
1:B:219:ILE:O	1:B:222:THR:HG22	2.02	0.59
1:D:206:TRP:C	1:D:207:LEU:HD12	2.23	0.58
1:C:13:ARG:HD3	1:C:15:GLU:HG3	1.86	0.57
1:A:94:ILE:HD13	1:A:184:PHE:HZ	1.69	0.57
1:B:265:MET:HE2	4:B:714:HOH:O	2.04	0.57
1:D:207:LEU:N	1:D:207:LEU:CD1	2.68	0.57
1:A:229:TYR:CZ	1:A:243:GLY:HA3	2.40	0.56
1:C:10:GLY:CA	1:C:27:ARG:HH21	2.15	0.56
1:C:216:SER:OG	1:C:220:ARG:NH2	2.38	0.56
1:C:156:GLN:NE2	4:C:603:HOH:O	2.39	0.56
1:D:206:TRP:HB2	1:D:207:LEU:CD1	2.35	0.55
1:B:229:TYR:CZ	1:B:243:GLY:HA3	2.41	0.55
1:D:94:ILE:HD13	1:D:184:PHE:HZ	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:GLU:H	1:D:210:GLU:CD	2.10	0.54
1:D:30:LYS:HE3	1:D:32:LEU:CD2	2.37	0.54
1:B:13:ARG:HG2	1:B:23:ALA:HB1	1.88	0.54
1:B:13:ARG:HD3	1:B:15:GLU:OE2	2.05	0.54
1:D:10:GLY:HA3	1:D:27:ARG:HH21	1.73	0.53
1:C:155:ARG:HG3	1:C:155:ARG:HH11	1.75	0.51
1:D:13:ARG:HG2	1:D:23:ALA:HB1	1.91	0.51
1:C:22:GLN:NE2	1:D:53:TRP:HE1	2.09	0.51
1:D:30:LYS:HE3	1:D:32:LEU:HD21	1.93	0.51
1:B:27:ARG:HG2	1:B:48:ASP:HB2	1.92	0.51
1:D:146:ARG:HG2	1:D:146:ARG:NH1	2.06	0.51
1:B:210:GLU:CD	1:B:210:GLU:H	2.13	0.50
1:C:182:GLU:HG2	1:C:218:PHE:CD2	2.45	0.50
1:D:137:SER:HB3	4:D:727:HOH:O	2.11	0.50
1:B:7:ILE:HG12	1:B:7:ILE:O	2.11	0.50
1:B:293:ASN:O	1:B:294:ASN:CB	2.55	0.50
1:D:210:GLU:CD	1:D:210:GLU:N	2.65	0.49
1:B:265:MET:CE	4:B:714:HOH:O	2.57	0.49
1:B:217:ARG:O	1:B:221:GLU:HG3	2.12	0.49
1:B:210:GLU:HB3	1:B:214:LYS:NZ	2.27	0.48
1:C:229:TYR:CZ	1:C:243:GLY:HA3	2.48	0.48
1:D:206:TRP:CB	1:D:207:LEU:HD12	2.44	0.48
1:A:94:ILE:HD13	1:A:184:PHE:CZ	2.49	0.47
1:B:13:ARG:HD3	1:B:15:GLU:CG	2.43	0.47
1:C:72:VAL:HG22	1:C:273:TYR:CD1	2.49	0.47
1:A:1:MET:HB3	1:A:2:PRO:HD3	1.97	0.47
1:A:214:LYS:HE3	1:A:217:ARG:NH2	2.29	0.47
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.96	0.47
1:A:201:GLN:NE2	1:A:203:GLU:H	2.13	0.47
1:A:13:ARG:HD2	1:A:15:GLU:OE2	2.14	0.47
1:B:165:VAL:O	1:B:198:CYS:HA	2.15	0.47
1:A:22:GLN:NE2	1:B:53:TRP:HE1	2.12	0.47
1:C:182:GLU:HG2	1:C:218:PHE:CG	2.50	0.47
1:C:124:MET:SD	1:C:124:MET:HB3	2.52	0.46
1:A:136:ARG:HG3	1:A:136:ARG:O	2.14	0.46
1:D:206:TRP:HB2	1:D:207:LEU:HD12	1.97	0.46
1:D:199:CYS:HA	1:D:245:LEU:O	2.17	0.45
1:C:13:ARG:CD	1:C:15:GLU:HG3	2.47	0.45
1:A:13:ARG:HG3	1:A:25:SER:OG	2.16	0.45
1:B:265:MET:CE	4:B:726:HOH:O	2.63	0.45
1:B:265:MET:HE1	4:B:726:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ARG:CG	1:D:146:ARG:NH1	2.68	0.45
1:D:50:LYS:HA	1:D:50:LYS:HD3	1.82	0.45
1:D:94:ILE:HD13	1:D:184:PHE:CZ	2.52	0.45
1:B:85:HIS:CG	1:B:86:PRO:HD2	2.52	0.45
1:A:262:VAL:O	1:A:268:ALA:HB2	2.17	0.44
1:A:50:LYS:HD3	1:A:50:LYS:HA	1.69	0.44
1:D:269:LYS:HG3	4:D:713:HOH:O	2.18	0.44
1:C:219:ILE:O	1:C:222:THR:HG22	2.18	0.44
1:B:142:ARG:HH11	1:B:142:ARG:HD2	1.38	0.43
1:B:116:LEU:HD23	1:B:116:LEU:C	2.38	0.43
1:C:210:GLU:O	1:C:214:LYS:HG3	2.18	0.43
1:B:199:CYS:HA	1:B:245:LEU:O	2.19	0.43
1:B:216:SER:OG	1:B:220:ARG:CZ	2.66	0.43
1:D:86:PRO:O	1:D:260:ARG:HD3	2.18	0.42
1:B:146:ARG:NH1	1:B:146:ARG:CG	2.67	0.42
1:A:1:MET:CB	1:A:2:PRO:HD3	2.49	0.42
1:A:113:HIS:HE1	1:A:144:THR:OG1	2.03	0.42
1:C:13:ARG:NH2	1:C:15:GLU:OE2	2.52	0.42
1:A:86:PRO:O	1:A:260:ARG:HD3	2.20	0.41
1:C:219:ILE:HG23	1:C:224:PHE:CD2	2.56	0.41
1:A:199:CYS:HA	1:A:245:LEU:O	2.20	0.41
1:D:27:ARG:HG3	1:D:28:VAL:N	2.36	0.41
1:D:262:VAL:O	1:D:268:ALA:HB2	2.21	0.41
1:A:114:CYS:O	1:A:143:ALA:HA	2.20	0.40
1:C:38:LYS:HD3	1:C:39:PHE:CE2	2.56	0.40
1:D:155:ARG:NH1	4:D:605:HOH:O	2.54	0.40
1:C:113:HIS:NE2	1:C:115:ASP:OD1	2.45	0.40
1:A:216:SER:OG	1:A:220:ARG:CZ	2.70	0.40

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	292/304 (96%)	282 (97%)	10 (3%)	0	100	100
1	B	292/304 (96%)	284 (97%)	8 (3%)	0	100	100
1	C	292/304 (96%)	282 (97%)	10 (3%)	0	100	100
1	D	292/304 (96%)	284 (97%)	8 (3%)	0	100	100
All	All	1168/1216 (96%)	1132 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	253/262 (97%)	246 (97%)	7 (3%)	51	20
1	B	253/262 (97%)	236 (93%)	17 (7%)	20	3
1	C	253/262 (97%)	244 (96%)	9 (4%)	42	13
1	D	253/262 (97%)	244 (96%)	9 (4%)	42	13
All	All	1012/1048 (97%)	970 (96%)	42 (4%)	36	9

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	136	ARG
1	A	137	SER
1	A	179	LEU
1	A	221	GLU
1	A	222	THR
1	A	235	PRO
1	B	1	MET
1	B	7	ILE
1	B	27	ARG
1	B	98	ASP
1	B	124	MET
1	B	136	ARG

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Mol	Chain	Res	Type
1	B	146	ARG
1	B	155	ARG
1	B	179	LEU
1	B	186	LYS
1	B	190	ARG
1	B	195	ASP
1	B	198	CYS
1	B	201	GLN
1	B	217	ARG
1	B	218	PHE
1	B	269	LYS
1	C	1	MET
1	C	27	ARG
1	C	98	ASP
1	C	124	MET
1	C	155	ARG
1	C	179	LEU
1	C	190	ARG
1	C	195	ASP
1	C	213	GLU
1	D	7	ILE
1	D	27	ARG
1	D	124	MET
1	D	195	ASP
1	D	201	GLN
1	D	207	LEU
1	D	213	GLU
1	D	214	LYS
1	D	222	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	201	GLN
1	A	233	HIS
1	B	233	HIS
1	C	22	GLN
1	C	156	GLN
1	C	201	GLN
1	C	233	HIS
1	D	233	HIS

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)

8 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	$\#|Z| > 2$
2	S4M	A	501	-	23,26,26	1.10	2 (8%)	17,37,37	2.59	6 (35%)
3	BSX	A	502	-	10,10,10	0.77	0	10,12,12	1.51	2 (20%)
2	S4M	B	501	-	23,26,26	1.12	3 (13%)	17,37,37	2.65	1 (5%)
3	BSX	B	502	-	10,10,10	1.20	1 (10%)	10,12,12	2.52	5 (50%)
2	S4M	C	501	-	23,26,26	1.40	4 (17%)	17,37,37	2.60	3 (17%)
3	BSX	C	502	-	10,10,10	0.98	1 (10%)	10,12,12	1.18	0
2	S4M	D	501	-	23,26,26	0.94	1 (4%)	17,37,37	2.07	4 (23%)
3	BSX	D	502	-	10,10,10	0.67	0	10,12,12	1.04	1 (10%)

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
2	S4M	A	501	-	-	0/7/28/28	0/3/3/3
3	BSX	A	502	-	-	0/3/3/3	0/1/1/1
2	S4M	B	501	-	-	0/7/28/28	0/3/3/3
3	BSX	B	502	-	-	0/3/3/3	0/1/1/1
2	S4M	C	501	-	-	0/7/28/28	0/3/3/3
3	BSX	C	502	-	-	0/3/3/3	0/1/1/1
2	S4M	D	501	-	-	0/7/28/28	0/3/3/3
3	BSX	D	502	-	-	0/3/3/3	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	S4M	C8-N7	-2.93	1.29	1.34
2	C	501	S4M	C4-N3	-2.28	1.32	1.35
2	D	501	S4M	C2-N1	2.04	1.37	1.33
3	C	502	BSX	C2-C1	2.04	1.55	1.51
2	B	501	S4M	CG-SD	2.04	1.85	1.80
2	C	501	S4M	CG-SD	2.24	1.85	1.80
2	C	501	S4M	O4'-C4'	2.34	1.50	1.45
2	B	501	S4M	O4'-C1'	2.41	1.44	1.41
2	A	501	S4M	O4'-C1'	2.56	1.44	1.41
2	B	501	S4M	C6-N6	2.76	1.45	1.34
3	B	502	BSX	C2-C1	2.92	1.56	1.51
2	C	501	S4M	O4'-C1'	3.22	1.45	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	S4M	C4'-O4'-C1'	-10.35	98.67	109.64
2	C	501	S4M	C4'-O4'-C1'	-8.94	100.17	109.64
2	A	501	S4M	C4'-O4'-C1'	-8.35	100.79	109.64
2	D	501	S4M	C4'-O4'-C1'	-6.47	102.79	109.64
2	C	501	S4M	C1'-N9-C4	-3.62	122.77	126.81
3	B	502	BSX	F10-C3-C6	-3.08	111.45	118.46
2	D	501	S4M	C1'-N9-C4	-2.94	123.52	126.81
3	A	502	BSX	C7-C9-C6	-2.94	116.12	120.20
3	B	502	BSX	C7-C9-C6	-2.84	116.26	120.20
2	A	501	S4M	C2'-C3'-C4'	-2.33	97.87	102.64
3	B	502	BSX	C7-C4-C1	-2.24	117.45	120.90
2	A	501	S4M	C2-N1-C6	-2.08	115.06	118.77
3	D	502	BSX	C9-C7-C4	2.07	123.08	120.20
3	B	502	BSX	C6-C3-C1	2.26	127.68	123.50
2	A	501	S4M	N3-C2-N1	2.44	130.79	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	S4M	CG-CB-CA	2.44	117.65	112.53
2	D	501	S4M	O4'-C1'-N9	2.46	112.75	108.11
2	A	501	S4M	O4'-C4'-C3'	2.52	110.28	105.16
2	A	501	S4M	O4'-C1'-N9	2.62	113.06	108.11
3	A	502	BSX	C9-C7-C4	3.27	124.74	120.20
2	C	501	S4M	N3-C2-N1	3.38	131.52	128.87
3	B	502	BSX	C9-C7-C4	5.30	127.56	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	294/304 (96%)	0.82	23 (7%)	16	14	8, 14, 28, 39	0
1	B	294/304 (96%)	0.79	20 (6%)	20	19	8, 13, 25, 54	0
1	C	294/304 (96%)	0.82	20 (6%)	20	19	8, 14, 27, 56	0
1	D	294/304 (96%)	0.76	18 (6%)	25	23	8, 14, 25, 46	0
All	All	1176/1216 (96%)	0.80	81 (6%)	20	19	8, 14, 26, 56	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	9.2
1	C	1	MET	7.7
1	D	1	MET	7.4
1	B	294	ASN	6.4
1	A	294	ASN	4.6
1	C	266	PRO	4.4
1	A	7	ILE	4.1
1	C	294	ASN	4.0
1	B	251	ALA	3.9
1	D	294	ASN	3.9
1	A	1	MET	3.8
1	B	252	GLY	3.8
1	A	36	PRO	3.6
1	D	136	ARG	3.4
1	A	266	PRO	3.3
1	C	36	PRO	3.2
1	D	2	PRO	3.1
1	B	136	ARG	3.1
1	C	7	ILE	3.0
1	B	11	TRP	3.0
1	A	136	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	251	ALA	2.8
1	D	17	ASP	2.8
1	B	2	PRO	2.8
1	D	50	LYS	2.8
1	A	8	SER	2.8
1	C	136	ARG	2.7
1	D	252	GLY	2.7
1	D	266	PRO	2.7
1	D	166	ILE	2.7
1	B	50	LYS	2.7
1	C	50	LYS	2.7
1	C	9	GLY	2.7
1	A	63	ILE	2.6
1	B	166	ILE	2.6
1	A	49	PRO	2.6
1	C	2	PRO	2.6
1	C	35	ALA	2.6
1	B	93	ILE	2.6
1	C	49	PRO	2.5
1	C	63	ILE	2.5
1	D	155	ARG	2.5
1	A	93	ILE	2.5
1	C	166	ILE	2.5
1	D	49	PRO	2.4
1	D	92	LEU	2.4
1	D	93	ILE	2.4
1	A	132	PRO	2.4
1	D	133	GLN	2.3
1	B	173	ALA	2.3
1	A	38	LYS	2.3
1	A	4	SER	2.3
1	B	49	PRO	2.3
1	A	11	TRP	2.3
1	C	11	TRP	2.3
1	A	50	LYS	2.3
1	B	225	ALA	2.2
1	C	33	TYR	2.2
1	C	38	LYS	2.2
1	D	101	VAL	2.2
1	A	3	GLY	2.1
1	A	197	ILE	2.1
1	A	92	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	92	LEU	2.1
1	A	166	ILE	2.1
1	B	165	VAL	2.1
1	C	77	LEU	2.1
1	C	101	VAL	2.1
1	A	9	GLY	2.1
1	B	17	ASP	2.1
1	B	77	LEU	2.1
1	D	77	LEU	2.1
1	C	167	ILE	2.0
1	B	101	VAL	2.0
1	A	291	HIS	2.0
1	A	129	GLN	2.0
1	A	65	VAL	2.0
1	B	105	VAL	2.0
1	B	253	VAL	2.0
1	D	91	VAL	2.0
1	B	266	PRO	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 carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å^2)	Q<0.9
3	BSX	D	502	10/10	0.92	0.14	1.48	11,14,16,17	0
3	BSX	C	502	10/10	0.92	0.13	0.67	11,16,16,20	0
3	BSX	B	502	10/10	0.93	0.13	0.51	12,14,15,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BSX	A	502	10/10	0.93	0.13	0.42	10,12,15,15	0
2	S4M	C	501	24/24	0.93	0.12	0.37	9,13,20,22	0
2	S4M	A	501	24/24	0.93	0.12	0.22	9,12,19,22	0
2	S4M	D	501	24/24	0.94	0.11	-0.19	9,10,19,19	0
2	S4M	B	501	24/24	0.93	0.11	-0.42	9,11,18,22	0

6.5 Other polymers (i)

There are no such residues in this entry.