



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:06 AM EDT

PDB ID : 5B1S / pdb_00005b1s
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

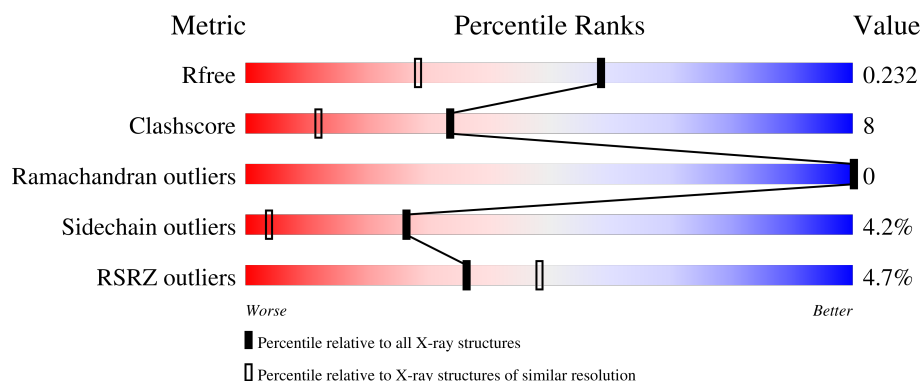
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	A	304	
1	B	304	
1	C	304	
1	D	304	

2 Entry composition

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:

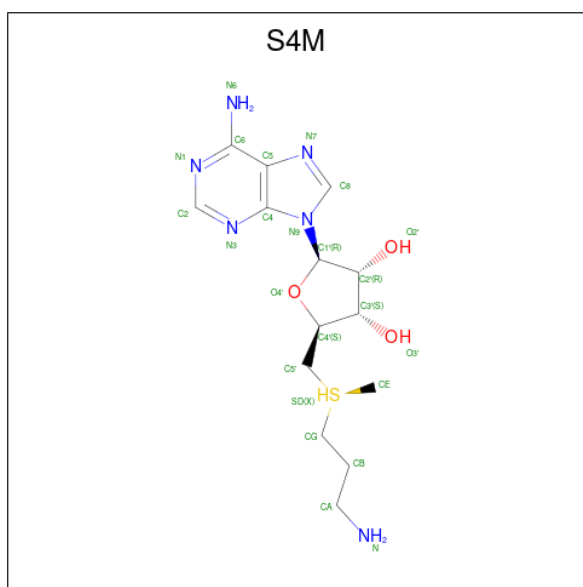
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q4DA73
A	-6	ALA	-	expression tag	UNP Q4DA73
A	-5	HIS	-	expression tag	UNP Q4DA73
A	-4	HIS	-	expression tag	UNP Q4DA73
A	-3	HIS	-	expression tag	UNP Q4DA73
A	-2	HIS	-	expression tag	UNP Q4DA73
A	-1	HIS	-	expression tag	UNP Q4DA73
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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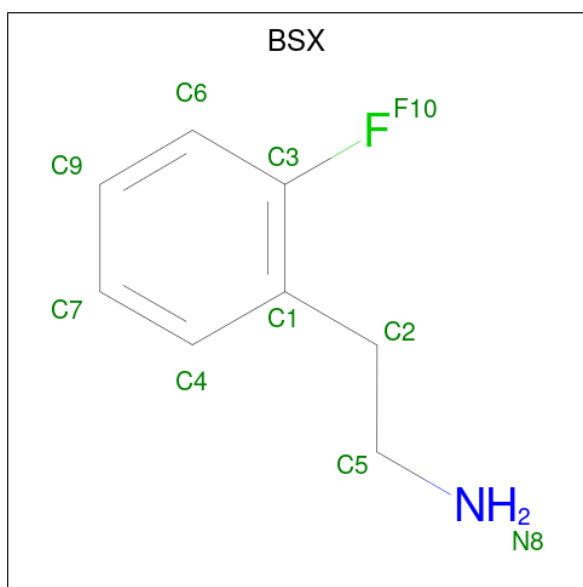
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q4DA73
C	-1	HIS	-	expression tag	UNP Q4DA73
C	0	HIS	-	expression tag	UNP Q4DA73
D	-7	MET	-	expression tag	UNP Q4DA73
D	-6	ALA	-	expression tag	UNP Q4DA73
D	-5	HIS	-	expression tag	UNP Q4DA73
D	-4	HIS	-	expression tag	UNP Q4DA73
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'-DEOXYADENOSINE (CCD ID: S4M) (formula: C₁₄H₂₄N₆O₃S).



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 (CCD ID: BSX) (formula: C₈H₁₀FN).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			10	8	1	1		
3	B	1	Total	C	F	N	0	0
			10	8	1	1		
3	C	1	Total	C	F	N	0	0
			10	8	1	1		
3	D	1	Total	C	F	N	0	0
			10	8	1	1		

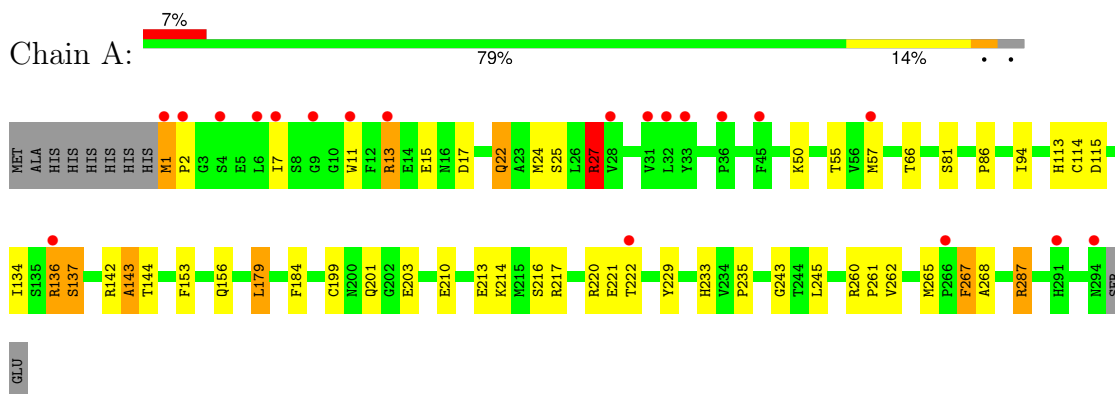
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	149	Total	O	0	0
			149	149		
4	C	160	Total	O	0	0
			160	160		
4	D	139	Total	O	0	0
			139	139		

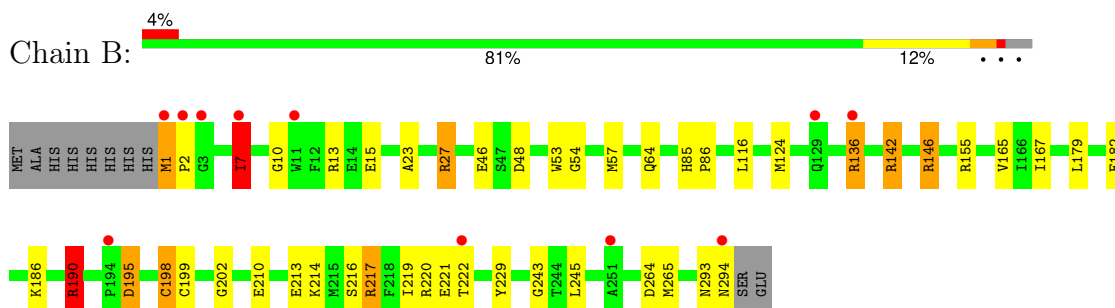
3 Residue-property plots [i](#)

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.

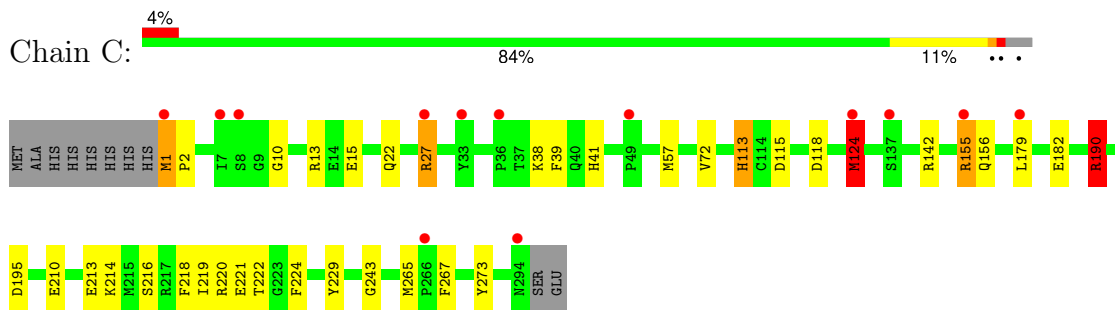
- Molecule 1: Spermidine synthase, putative



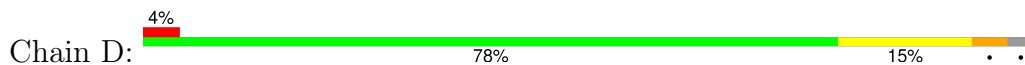
- Molecule 1: Spermidine synthase, putative

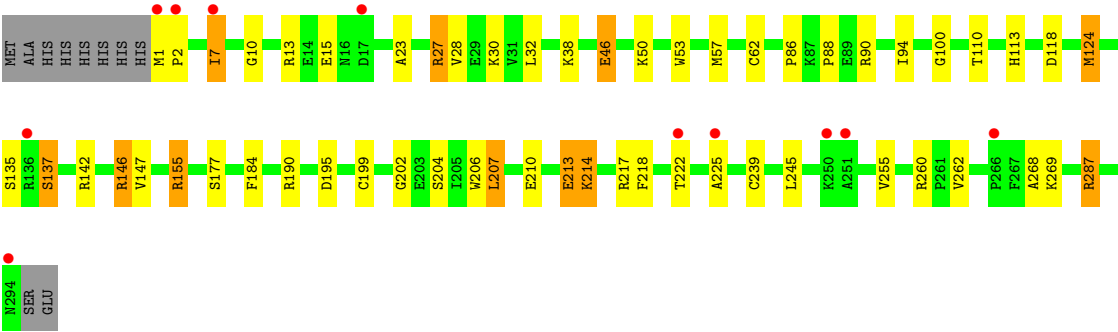


- Molecule 1: Spermidine synthase, putative



- Molecule 1: Spermidine synthase, putative





4 Data and refinement statistics

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 25.02 – 1.58	Depositor EDS
% Data completeness (in resolution range)	81.5 (25.02-1.58) 81.5 (25.02-1.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.11%)	wwPDB-VP
Wilson B-factor (Å ²)	10.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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

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

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	1.48	17/2364 (0.7%)	1.45	15/3207 (0.5%)
1	B	1.50	4/2364 (0.2%)	1.42	11/3207 (0.3%)
1	C	1.43	8/2364 (0.3%)	1.41	8/3207 (0.2%)
1	D	1.46	14/2364 (0.6%)	1.50	16/3207 (0.5%)
All	All	1.47	43/9456 (0.5%)	1.45	50/12828 (0.4%)

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 (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	ARG	CZ-NH2	-14.40	1.14	1.33
1	C	124	MET	CA-CB	11.64	1.72	1.53
1	D	190	ARG	CZ-NH1	8.93	1.45	1.32
1	D	190	ARG	CZ-NH2	-8.73	1.22	1.33
1	B	136	ARG	C-O	8.68	1.34	1.24
1	C	124	MET	CB-CG	8.42	1.77	1.52
1	A	137	SER	CB-OG	8.38	1.58	1.42
1	A	142	ARG	CZ-NH1	7.79	1.43	1.32
1	A	137	SER	CA-CB	7.46	1.65	1.53
1	A	66	THR	N-CA	7.17	1.55	1.45
1	D	214	LYS	N-CA	7.15	1.54	1.46
1	C	124	MET	CA-C	7.00	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	THR	N-CA	-6.93	1.36	1.45
1	A	137	SER	N-CA	-6.86	1.36	1.46
1	C	190	ARG	CD-NE	-6.34	1.37	1.46
1	A	11	TRP	N-CA	6.29	1.53	1.45
1	D	88	PRO	CA-C	-6.04	1.46	1.52
1	B	54	GLY	C-O	5.88	1.31	1.24
1	A	27	ARG	N-CA	5.81	1.53	1.46
1	A	233	HIS	C-O	5.70	1.30	1.24
1	A	267	PHE	CA-C	5.65	1.60	1.52
1	A	143	ALA	N-CA	5.62	1.52	1.45
1	C	190	ARG	CZ-NH2	-5.59	1.26	1.33
1	A	24	MET	N-CA	-5.58	1.38	1.46
1	B	202	GLY	N-CA	5.58	1.52	1.45
1	D	100	GLY	CA-C	5.54	1.58	1.52
1	D	62	CYS	C-O	5.46	1.30	1.24
1	D	255	VAL	N-CA	5.38	1.53	1.46
1	D	225	ALA	N-CA	5.31	1.52	1.46
1	D	90	ARG	CZ-NH2	-5.30	1.26	1.33
1	A	261	PRO	C-O	5.27	1.29	1.23
1	C	113	HIS	N-CA	-5.25	1.39	1.46
1	A	17	ASP	N-CA	-5.19	1.39	1.46
1	D	113	HIS	CA-C	5.18	1.59	1.52
1	D	110	THR	C-O	5.17	1.30	1.24
1	D	177	SER	C-O	5.15	1.29	1.24
1	A	134	ILE	C-O	5.14	1.28	1.23
1	D	7	ILE	CA-CB	5.14	1.60	1.54
1	C	41	HIS	N-CA	-5.14	1.39	1.46
1	A	13	ARG	N-CA	5.12	1.52	1.46
1	D	202	GLY	N-CA	5.11	1.51	1.45
1	C	221	GLU	C-O	5.09	1.30	1.24
1	A	22	GLN	N-CA	-5.01	1.39	1.45

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	190	ARG	NE-CZ-NH2	-24.08	97.53	119.20
1	D	190	ARG	NE-CZ-NH1	16.49	137.99	121.50
1	C	190	ARG	NE-CZ-NH2	-16.23	104.59	119.20
1	B	142	ARG	CD-NE-CZ	-14.53	104.06	124.40
1	B	190	ARG	NE-CZ-NH2	-12.24	108.19	119.20
1	B	190	ARG	CD-NE-CZ	11.87	141.02	124.40
1	C	57	MET	CG-SD-CE	-11.11	76.47	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	ARG	NE-CZ-NH1	10.96	132.46	121.50
1	A	137	SER	N-CA-CB	-10.86	94.56	110.53
1	C	190	ARG	CD-NE-CZ	10.86	139.61	124.40
1	B	142	ARG	NE-CZ-NH2	10.44	128.59	119.20
1	A	57	MET	CG-SD-CE	-10.20	78.46	100.90
1	D	190	ARG	CD-NE-CZ	9.96	138.34	124.40
1	C	124	MET	CB-CA-C	9.91	128.83	110.70
1	D	7	ILE	N-CA-CB	9.01	121.28	111.00
1	A	142	ARG	NE-CZ-NH2	-8.90	111.19	119.20
1	C	124	MET	N-CA-C	-7.57	102.37	111.69
1	D	46	GLU	CB-CG-CD	7.54	125.42	112.60
1	B	7	ILE	N-CA-CB	7.42	118.81	110.72
1	A	134	ILE	N-CA-C	-7.21	105.61	111.81
1	A	287	ARG	NE-CZ-NH2	-7.13	112.78	119.20
1	B	46	GLU	CB-CG-CD	6.92	124.36	112.60
1	A	287	ARG	NE-CZ-NH1	6.52	128.02	121.50
1	B	142	ARG	CG-CD-NE	6.38	126.03	112.00
1	D	57	MET	CG-SD-CE	-6.34	86.95	100.90
1	B	195	ASP	N-CA-C	-6.27	105.57	112.72
1	B	142	ARG	NH1-CZ-NH2	-6.24	111.19	119.30
1	A	142	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	B	264	ASP	N-CA-C	-6.06	105.65	113.16
1	D	137	SER	N-CA-CB	-6.01	100.10	110.32
1	D	7	ILE	CB-CA-C	6.01	118.23	110.96
1	D	137	SER	N-CA-C	5.90	119.58	112.38
1	C	124	MET	CA-CB-CG	5.88	125.85	114.10
1	D	287	ARG	NE-CZ-NH2	-5.75	114.02	119.20
1	A	1	MET	CA-C-N	-5.62	114.53	120.66
1	A	1	MET	C-N-CA	-5.62	114.53	120.66
1	A	142	ARG	CD-NE-CZ	5.60	132.24	124.40
1	C	142	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	A	136	ARG	CA-C-N	5.45	131.34	121.92
1	A	136	ARG	C-N-CA	5.45	131.34	121.92
1	A	81	SER	N-CA-C	5.41	116.98	111.14
1	D	90	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	B	167	ILE	N-CA-CB	-5.35	106.33	111.89
1	D	142	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	A	179	LEU	CB-CG-CD1	5.32	126.66	110.70
1	A	153	PHE	N-CA-C	5.23	116.98	111.28
1	D	218	PHE	N-CA-CB	5.18	118.31	110.28
1	D	142	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	D	135	SER	N-CA-C	5.11	119.60	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	190	ARG	CG-CD-NE	-5.09	100.81	112.00

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 ⓘ

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	28	0
1	B	2306	0	2257	43	0
1	C	2306	0	2257	33	0
1	D	2306	0	2257	39	0
2	A	24	0	24	0	0
2	B	24	0	24	1	0
2	C	24	0	24	0	0
2	D	24	0	24	1	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	142	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 8.

All (142) 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:CB	1:C:124:MET:CG	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: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:HH11	1:B:146:ARG:HG2	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:CB	1:C:124:MET:SD	2.67	0.83
1:D:213:GLU:HG2	1:D:217:ARG:NH2	1.94	0.82
1:B:293:ASN:O	1:B:294:ASN:HB2	1.79	0.80
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:HH11	1:A:27:ARG:HG3	1.50	0.76
1:C:182:GLU:HG3	4:C:688:HOH:O	1.87	0.74
1:B:57:MET:HE3	1:B:64:GLN:CB	2.18	0.73
1:B:57:MET:CE	1:B:64:GLN:HB2	2.18	0.73
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:HG3	1:A:27:ARG:NH1	2.06	0.70
1:D:146:ARG:HH11	1:D:146:ARG:CG	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:C:155:ARG:HD3	4:C:675:HOH:O	1.94	0.66
1:B:57:MET:HE2	1:B:64:GLN:HB2	1.77	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:D:206:TRP:C	1:D:207:LEU:HD12	2.23	0.63
1:C:155:ARG:NH2	4:C:602:HOH:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:HH11	1:A:27:ARG:CG	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:B:265:MET:HE2	4:B:714:HOH:O	2.01	0.61
1:A:214:LYS:HG2	1:A:217:ARG:HH22	1.63	0.61
1:B:1:MET:HE3	1:B:1:MET:HA	1.84	0.60
1:D:210:GLU:CD	1:D:210:GLU:H	2.10	0.59
1:B:219:ILE:O	1:B:222:THR:HG22	2.02	0.59
1:B:57:MET:HE3	1:B:64:GLN:HB2	1.83	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:D:207:LEU:N	1:D:207:LEU:CD1	2.68	0.57
1:B:57:MET:HE3	1:B:64:GLN:HG3	1.87	0.57
1:A:229:TYR:CZ	1:A:243:GLY:HA3	2.40	0.56
1:B:210:GLU:H	1:B:210:GLU:CD	2.13	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
1:D:30:LYS:HE3	1:D:32:LEU:CD2	2.37	0.54
1:D:210:GLU:CD	1:D:210:GLU:N	2.65	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:B:57:MET:HE3	1:B:64:GLN:CG	2.39	0.53
1:D:10:GLY:HA3	1:D:27:ARG:HH21	1.73	0.53
1:C:118:ASP:HB3	1:C:124:MET:HE2	1.92	0.52
1:C:22:GLN:NE2	1:D:53:TRP:HE1	2.09	0.51
1:C:155:ARG:HH11	1:C:155:ARG:HG3	1.75	0.51
1:D:13:ARG:HG2	1:D:23:ALA:HB1	1.91	0.51
1:D:118:ASP:HB3	1:D:124:MET:HE1	1.91	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: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:O	1:B:7:ILE:HG12	2.11	0.50
1:B:293:ASN:O	1:B:294:ASN:CB	2.55	0.50
1:B:57:MET:HE1	2:B:501:S4M:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:265:MET:HE2	1:A:267:PHE:HE2	1.78	0.49
1:D:124:MET:HE2	1:D:147:VAL:HG22	1.95	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:B:116:LEU:C	1:B:116:LEU:HD23	2.38	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:D:206:TRP:HB2	1:D:207:LEU:HD12	1.97	0.46
1:A:136:ARG:O	1:A:136:ARG:HG3	2.14	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:D:50:LYS:HA	1:D:50:LYS:HD3	1.82	0.45
1:D:146:ARG:CG	1:D:146:ARG:NH1	2.68	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: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:210:GLU:CD	1:B:210:GLU:N	2.77	0.43
1:B:216:SER:OG	1:B:220:ARG:CZ	2.66	0.43
1:C:265:MET:HE2	1:C:267:PHE:HE2	1.83	0.43
1:D:86:PRO:O	1:D:260:ARG:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ARG:CG	1:B:146:ARG:NH1	2.67	0.42
1:A:1:MET:CB	1:A:2:PRO:HD3	2.49	0.42
1:B:210:GLU:HB3	1:B:214:LYS:HZ1	1.84	0.42
1:C:13:ARG:HD3	1:C:15:GLU:CD	2.44	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:B:265:MET:HE3	4:B:726:HOH:O	2.20	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
2:D:501:S4M:HE2	2:D:501:S4M:HB1	1.96	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

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	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%)	38	9
1	B	253/262 (97%)	239 (94%)	14 (6%)	19	2
1	C	253/262 (97%)	245 (97%)	8 (3%)	34	7
1	D	253/262 (97%)	240 (95%)	13 (5%)	21	2
All	All	1012/1048 (97%)	970 (96%)	42 (4%)	26	4

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

Mol	Chain	Res	Type
1	A	27	ARG
1	A	137	SER
1	A	179	LEU
1	A	221	GLU
1	A	222	THR
1	A	235	PRO
1	A	287	ARG
1	B	1	MET
1	B	7	ILE
1	B	27	ARG
1	B	124	MET
1	B	136	ARG
1	B	146	ARG
1	B	155	ARG
1	B	179	LEU
1	B	182	GLU
1	B	186	LYS
1	B	190	ARG
1	B	195	ASP
1	B	198	CYS
1	B	217	ARG
1	C	1	MET
1	C	27	ARG
1	C	124	MET

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Mol	Chain	Res	Type
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	38	LYS
1	D	46	GLU
1	D	124	MET
1	D	146	ARG
1	D	155	ARG
1	D	195	ASP
1	D	207	LEU
1	D	213	GLU
1	D	214	LYS
1	D	222	THR
1	D	287	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	201	GLN
1	A	233	HIS
1	B	156	GLN
1	B	228	GLN
1	C	22	GLN
1	C	156	GLN
1	C	160	ASN
1	C	201	GLN
1	C	233	HIS
1	D	233	HIS

5.3.3 RNA ⓘ

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](#)

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	-	25,26,26	0.82	1 (4%)	33,37,37	1.76	8 (24%)
2	S4M	D	501	-	25,26,26	0.87	1 (4%)	33,37,37	1.70	5 (15%)
3	BSX	D	502	-	10,10,10	0.65	0	12,12,12	1.22	1 (8%)
2	S4M	B	501	-	25,26,26	1.17	1 (4%)	33,37,37	1.70	7 (21%)
3	BSX	C	502	-	10,10,10	0.98	0	12,12,12	1.53	1 (8%)
3	BSX	A	502	-	10,10,10	0.75	0	12,12,12	1.74	3 (25%)
2	S4M	C	501	-	25,26,26	0.96	1 (4%)	33,37,37	1.66	5 (15%)
3	BSX	B	502	-	10,10,10	1.23	1 (10%)	12,12,12	2.84	7 (58%)

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	-	-	3/12/28/28	0/3/3/3
2	S4M	D	501	-	-	3/12/28/28	0/3/3/3
3	BSX	D	502	-	-	0/3/3/3	0/1/1/1
2	S4M	B	501	-	-	1/12/28/28	0/3/3/3
3	BSX	C	502	-	-	0/3/3/3	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BSX	A	502	-	-	0/3/3/3	0/1/1/1
2	S4M	C	501	-	-	3/12/28/28	0/3/3/3
3	BSX	B	502	-	-	0/3/3/3	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	S4M	C6-N6	4.39	1.45	1.34
3	B	502	BSX	C2-C1	2.76	1.56	1.51
2	C	501	S4M	O4'-C4'	2.42	1.50	1.45
2	D	501	S4M	C2-N1	2.19	1.37	1.33
2	A	501	S4M	C6-N6	2.14	1.39	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	BSX	C9-C7-C4	5.94	127.56	120.24
2	B	501	S4M	C4'-O4'-C1'	-4.89	98.67	109.47
2	D	501	S4M	O4'-C1'-C2'	-4.84	96.26	106.62
2	A	501	S4M	CG-SD-C5'	-4.37	92.76	103.43
2	C	501	S4M	C4'-O4'-C1'	-4.21	100.17	109.47
2	B	501	S4M	C5-C4-N9	4.19	110.38	105.81
3	B	502	BSX	C5-C2-C1	-4.16	104.08	112.85
2	A	501	S4M	C4'-O4'-C1'	-3.93	100.79	109.47
2	D	501	S4M	CG-SD-C5'	-3.80	94.15	103.43
2	B	501	S4M	CG-SD-C5'	-3.72	94.33	103.43
2	C	501	S4M	C4-N9-C8	3.68	109.61	105.74
3	A	502	BSX	C9-C7-C4	3.65	124.74	120.24
2	A	501	S4M	O4'-C1'-C2'	-3.62	98.87	106.62
3	A	502	BSX	C7-C9-C6	-3.33	116.12	120.24
2	A	501	S4M	C3'-C2'-C1'	3.32	107.75	101.46
2	C	501	S4M	O4'-C1'-C2'	-3.31	99.53	106.62
2	C	501	S4M	CG-SD-C5'	-3.24	95.50	103.43
3	B	502	BSX	C7-C9-C6	-3.23	116.26	120.24
3	B	502	BSX	F10-C3-C6	-3.10	111.45	118.65
3	C	502	BSX	C5-C2-C1	-3.07	106.38	112.85
2	D	501	S4M	C4'-O4'-C1'	-3.02	102.79	109.47
2	C	501	S4M	N9-C8-N7	-2.94	109.76	113.94
2	B	501	S4M	C4-N9-C8	-2.88	102.72	105.74
2	A	501	S4M	O4'-C1'-N9	2.59	113.06	108.09
2	A	501	S4M	O4'-C4'-C3'	2.58	110.28	105.15
3	A	502	BSX	C5-C2-C1	-2.54	107.50	112.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	S4M	C2'-C3'-C4'	-2.45	97.87	102.61
2	D	501	S4M	N9-C8-N7	-2.43	110.48	113.94
2	D	501	S4M	O4'-C1'-N9	2.43	112.75	108.09
3	B	502	BSX	C7-C4-C1	-2.34	117.45	120.88
3	D	502	BSX	C9-C7-C4	2.30	123.08	120.24
3	B	502	BSX	C6-C3-C1	2.30	127.68	123.60
2	B	501	S4M	C5-C4-N3	-2.26	123.60	126.72
2	A	501	S4M	C2-N1-C6	-2.23	115.06	118.73
3	B	502	BSX	C2-C1-C3	2.17	127.40	121.06
2	B	501	S4M	C4-C5-N7	-2.12	108.16	110.58
2	B	501	S4M	C1'-N9-C8	2.06	131.66	127.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	S4M	CA-CB-CG-SD
2	B	501	S4M	CA-CB-CG-SD
2	C	501	S4M	CA-CB-CG-SD
2	C	501	S4M	C3'-C4'-C5'-SD
2	D	501	S4M	CA-CB-CG-SD
2	D	501	S4M	C3'-C4'-C5'-SD
2	A	501	S4M	O4'-C4'-C5'-SD
2	D	501	S4M	O4'-C4'-C5'-SD
2	A	501	S4M	CB-CG-SD-C5'
2	C	501	S4M	CB-CG-SD-C5'

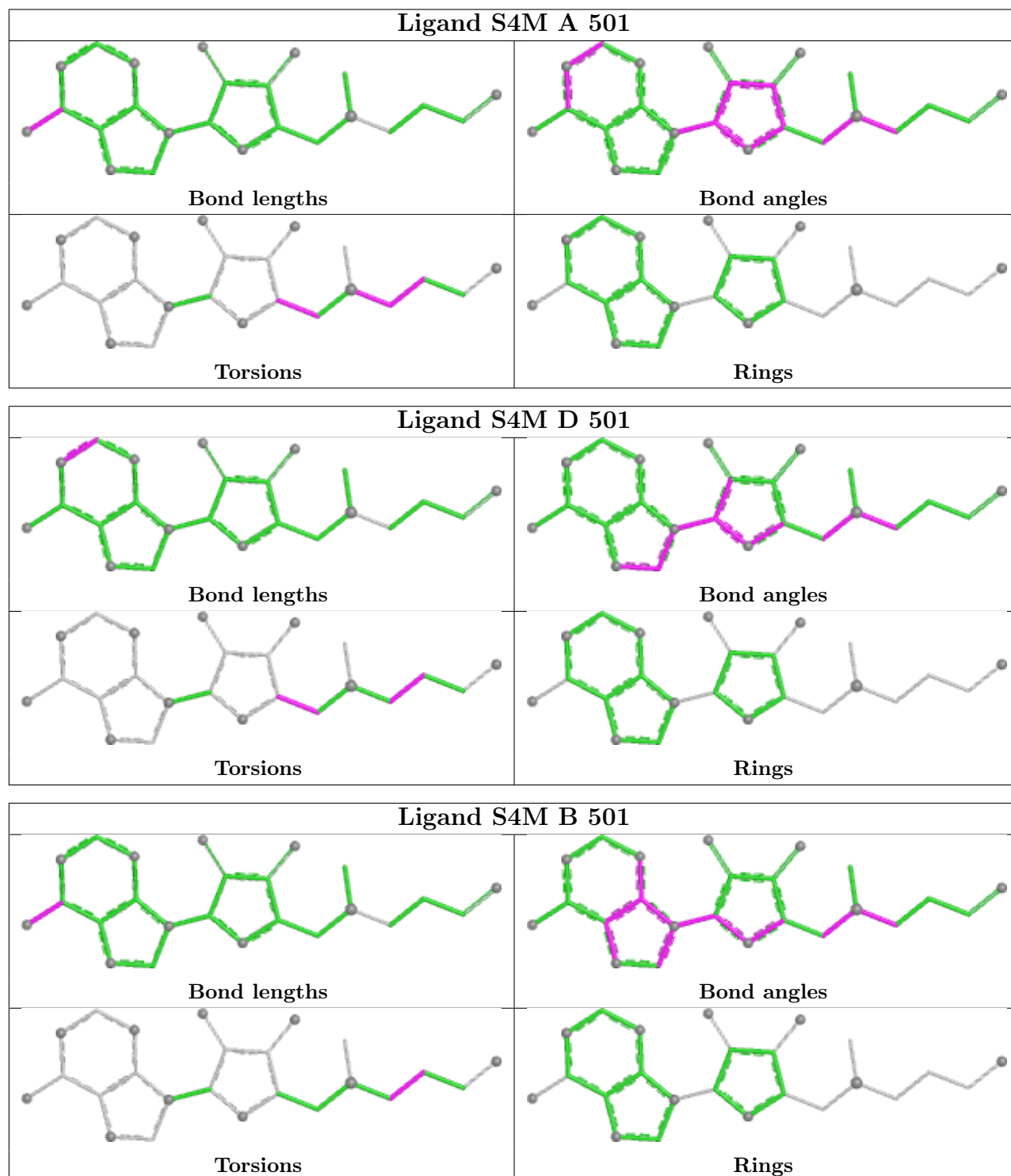
There are no ring outliers.

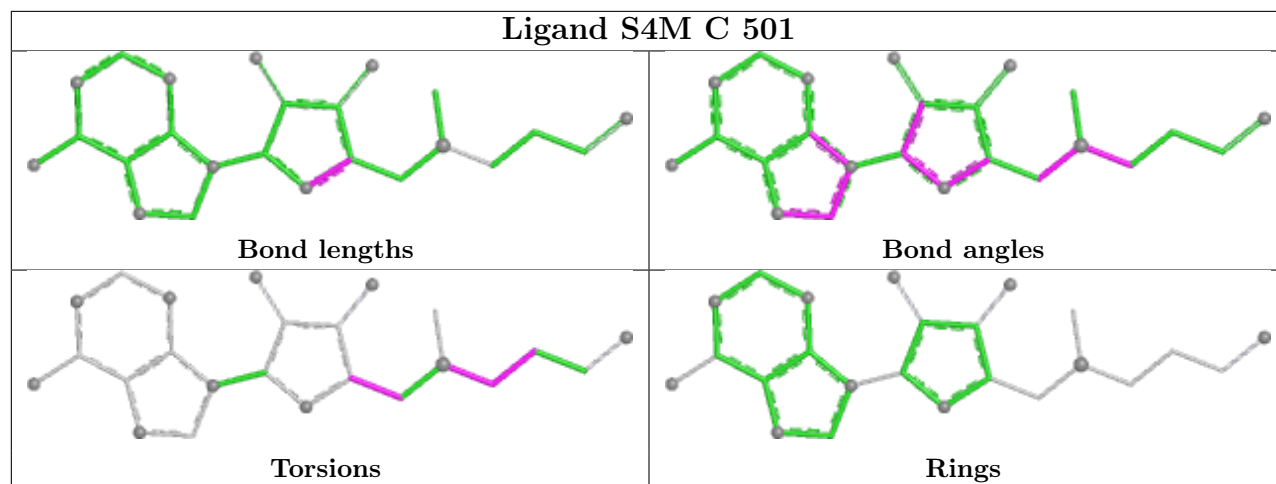
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	S4M	1	0
2	B	501	S4M	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	A	294/304 (96%)	0.60	20 (6%)	23 33	8, 14, 28, 38	0
1	B	294/304 (96%)	0.54	11 (3%)	45 56	8, 13, 25, 54	0
1	C	294/304 (96%)	0.55	13 (4%)	39 51	8, 14, 27, 56	0
1	D	294/304 (96%)	0.51	11 (3%)	45 56	8, 14, 25, 46	0
All	All	1176/1216 (96%)	0.55	55 (4%)	36 48	8, 14, 26, 56	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	ILE	4.5
1	A	7	ILE	4.2
1	A	11	TRP	4.0
1	A	9	GLY	3.9
1	C	1	MET	3.6
1	B	11	TRP	3.6
1	C	294	ASN	3.5
1	D	7	ILE	3.3
1	A	36	PRO	3.3
1	B	1	MET	3.3
1	A	294	ASN	3.2
1	D	1	MET	3.1
1	A	1	MET	3.0
1	B	251	ALA	2.9
1	C	266	PRO	2.9
1	A	266	PRO	2.9
1	B	222	THR	2.9
1	C	36	PRO	2.9
1	D	294	ASN	2.9
1	B	7	ILE	2.8
1	A	291	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	31	VAL	2.6
1	A	136	ARG	2.6
1	C	124	MET	2.6
1	A	28	VAL	2.6
1	D	222	THR	2.6
1	D	2	PRO	2.5
1	A	4	SER	2.4
1	A	13	ARG	2.4
1	B	2	PRO	2.4
1	D	266	PRO	2.4
1	C	155	ARG	2.4
1	D	17	ASP	2.3
1	A	2	PRO	2.3
1	A	32	LEU	2.3
1	B	3	GLY	2.3
1	A	45	PHE	2.3
1	A	33	TYR	2.3
1	C	8	SER	2.3
1	B	129	GLN	2.3
1	C	179	LEU	2.2
1	C	33	TYR	2.2
1	C	137	SER	2.2
1	A	222	THR	2.1
1	A	57	MET	2.1
1	D	250	LYS	2.1
1	A	6	LEU	2.1
1	B	136	ARG	2.1
1	D	136	ARG	2.1
1	B	194	PRO	2.1
1	B	294	ASN	2.1
1	D	225	ALA	2.1
1	C	49	PRO	2.1
1	D	251	ALA	2.0
1	C	27	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

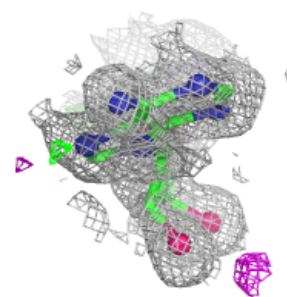
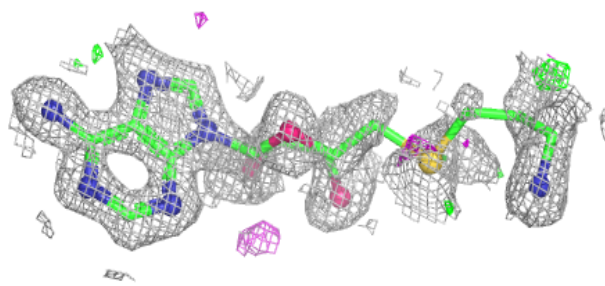
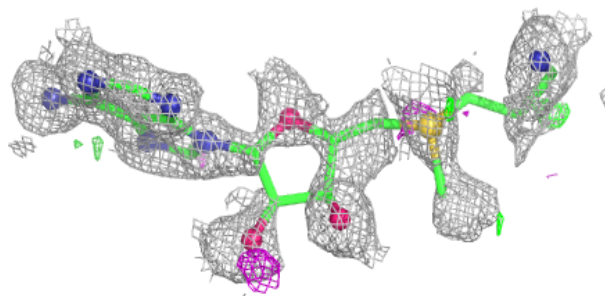
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BSX	B	502	10/10	0.95	0.09	12,14,15,17	0
2	S4M	C	501	24/24	0.96	0.09	9,13,20,22	0
2	S4M	D	501	24/24	0.96	0.07	9,10,19,19	0
3	BSX	A	502	10/10	0.96	0.07	10,12,15,15	0
2	S4M	B	501	24/24	0.96	0.08	9,11,18,22	0
3	BSX	C	502	10/10	0.96	0.09	11,16,16,20	0
3	BSX	D	502	10/10	0.96	0.08	11,14,16,17	0
2	S4M	A	501	24/24	0.97	0.07	9,12,19,22	0

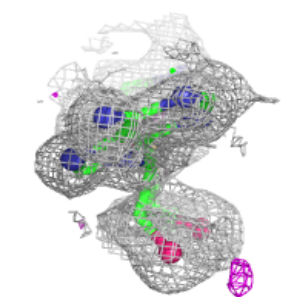
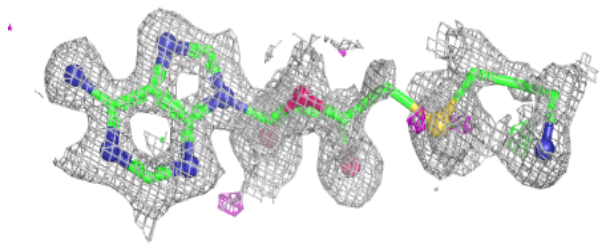
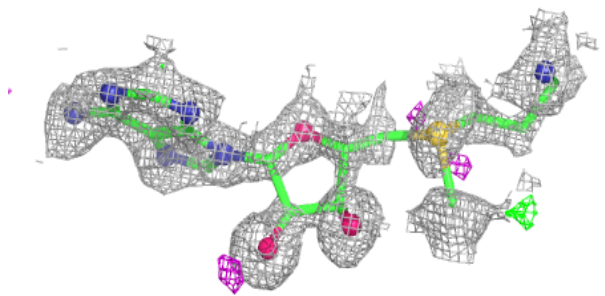
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around S4M C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

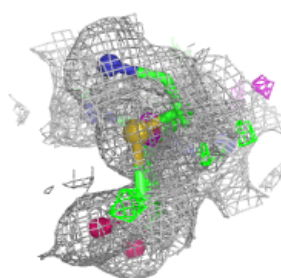
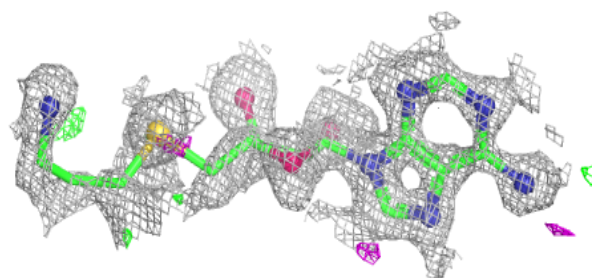
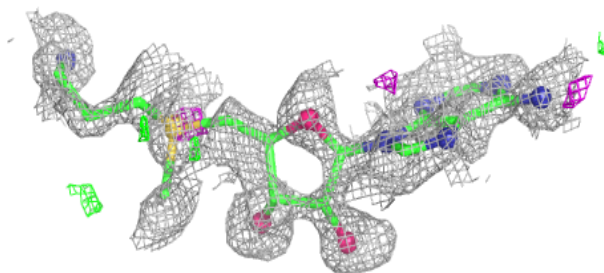
**Electron density around S4M D 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

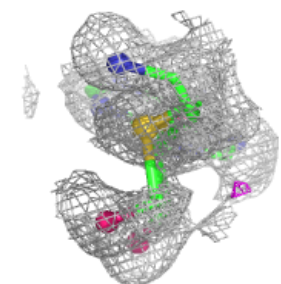
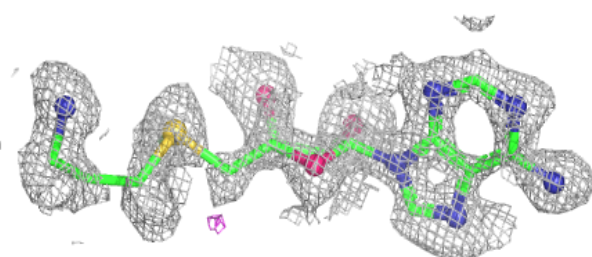
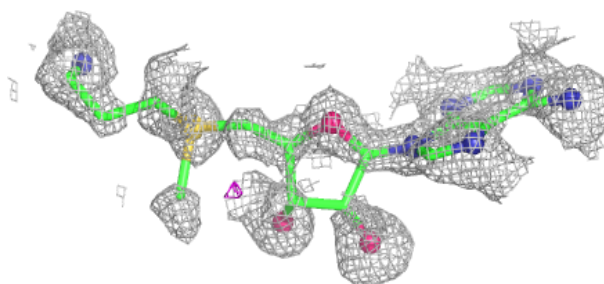


Electron density around S4M B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around S4M A 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.