



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:37 AM UTC

PDB ID : 4BP1 / pdb_00004bp1
Title : Crystal Structure of Plasmodium Falciparum Spermidine Synthase in Complex with 5'-Methylthioadenosine and Putrescine
Authors : Sprenger, J.; Halander, J.C.; Svensson, B.; Al-Karadaghi, S.; Persson, L.
Deposited on : 2013-05-23
Resolution : 2.17 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
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

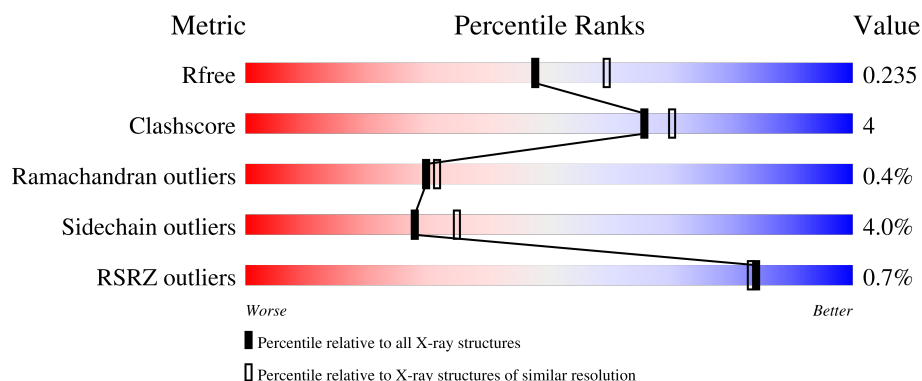
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	283	2% 88% 11% ..
1	B	283	81% 13% ..
1	C	283	90% 9% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7276 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.

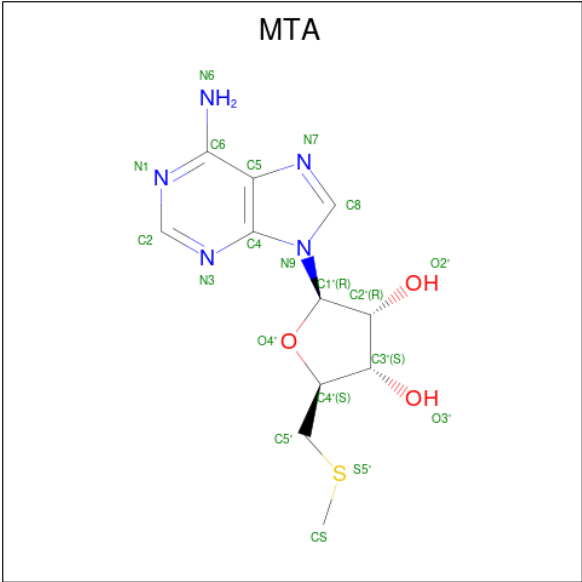
- Molecule 1 is a protein called SPERMIDINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2254	1463	352	425	14			
1	B	280	Total	C	N	O	S	0	1	0
			2251	1460	352	425	14			
1	C	281	Total	C	N	O	S	0	1	0
			2260	1466	353	427	14			

There are 6 discrepancies between the modelled and reference sequences:

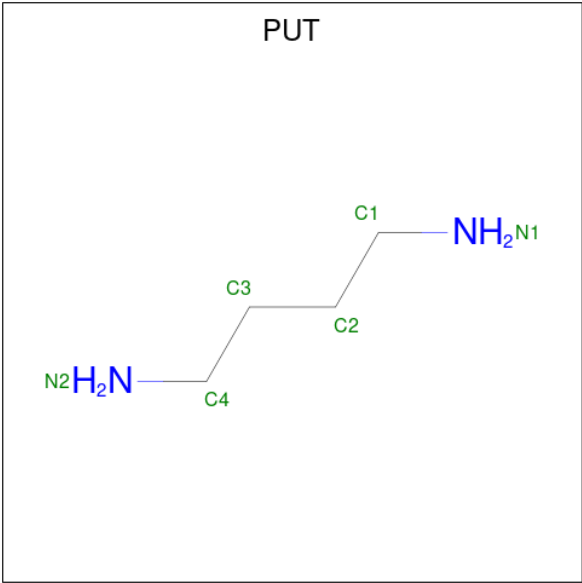
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	expression tag	UNP Q8II73
A	40	SER	-	expression tag	UNP Q8II73
B	39	GLY	-	expression tag	UNP Q8II73
B	40	SER	-	expression tag	UNP Q8II73
C	39	GLY	-	expression tag	UNP Q8II73
C	40	SER	-	expression tag	UNP Q8II73

- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 3 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



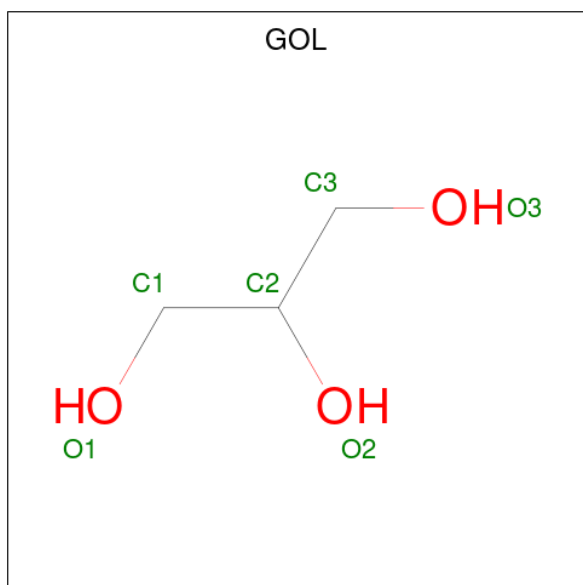
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			6	4	2		

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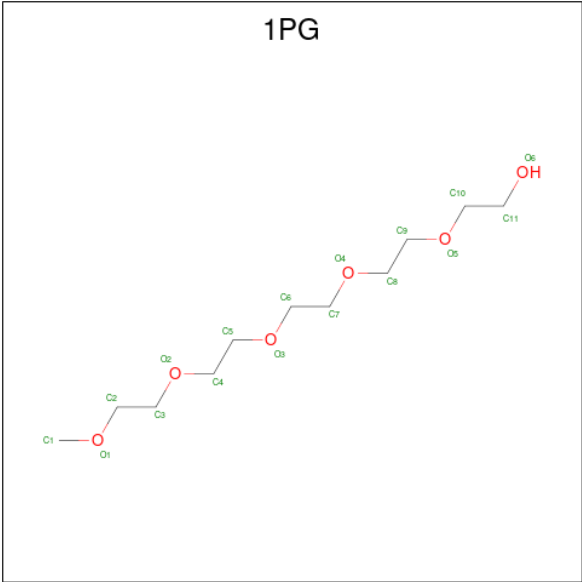
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			6	4	2		
3	C	1	Total	C	N	0	0
			6	4	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (CCD ID: 1PG) (formula: $C_{11}H_{24}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			17	11	6		

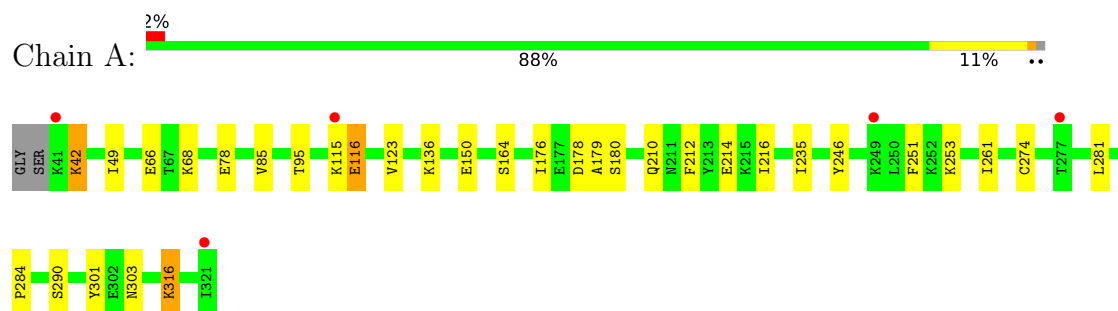
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	81	Total	O	0	0
			81	81		
6	B	153	Total	O	0	0
			153	153		
6	C	176	Total	O	0	0
			176	176		

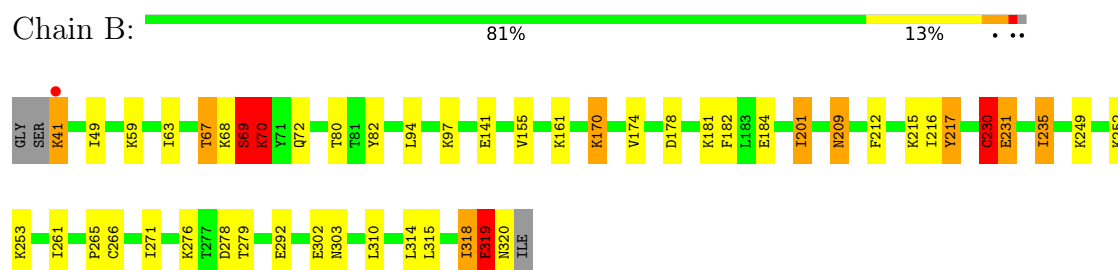
3 Residue-property plots [i](#)

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.

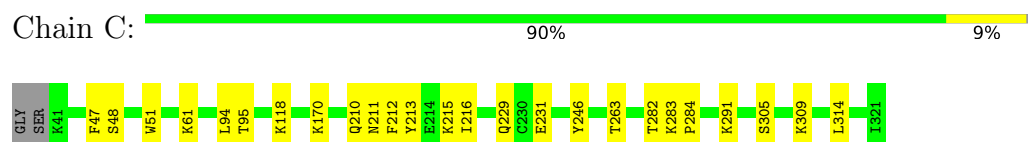
• Molecule 1: SPERMIDINE SYNTHASE



• Molecule 1: SPERMIDINE SYNTHASE



• Molecule 1: SPERMIDINE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.76Å 134.97Å 48.60Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	28.65 – 2.17 28.65 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.7 (28.65-2.17) 98.7 (28.65-2.17)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.180 , 0.231 0.187 , 0.235	Depositor DCC
R_{free} test set	3441 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7276	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: 1PG, PUT, MTA, GOL

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	1.19	1/2304 (0.0%)	1.19	8/3111 (0.3%)
1	B	1.34	7/2301 (0.3%)	1.21	5/3108 (0.2%)
1	C	1.29	1/2310 (0.0%)	1.20	5/3119 (0.2%)
All	All	1.28	9/6915 (0.1%)	1.20	18/9338 (0.2%)

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	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	284	PRO	C-O	-6.62	1.16	1.23
1	B	174	VAL	C-O	-6.36	1.17	1.24
1	B	141	GLU	CA-C	-6.33	1.45	1.52
1	B	292	GLU	C-O	-5.91	1.16	1.24
1	B	182	PHE	N-CA	5.88	1.53	1.46
1	B	217	TYR	C-O	-5.64	1.17	1.24
1	B	70	LYS	N-CA	5.29	1.53	1.46
1	A	176	ILE	CA-C	-5.26	1.47	1.52
1	B	230	CYS	C-O	-5.05	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	283	LYS	CA-C-N	-6.07	113.69	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	283	LYS	C-N-CA	-6.07	113.69	119.76
1	C	314	LEU	N-CA-C	-6.02	104.28	111.69
1	A	303	ASN	CB-CA-C	5.93	121.74	109.95
1	A	115	LYS	CA-C-N	-5.74	115.80	122.00
1	A	115	LYS	C-N-CA	-5.74	115.80	122.00
1	B	303	ASN	CB-CA-C	5.62	121.13	109.95
1	A	253	LYS	N-CA-C	5.47	117.12	107.61
1	B	235	ILE	N-CA-C	5.46	120.69	109.34
1	B	252	LYS	N-CA-C	5.39	117.24	111.36
1	C	118	LYS	CB-CA-C	-5.39	100.30	109.03
1	B	178	ASP	N-CA-C	-5.39	101.88	109.96
1	A	281	LEU	N-CA-C	5.19	119.57	112.88
1	A	214	GLU	CB-CA-C	-5.17	102.76	110.88
1	C	213	TYR	CA-CB-CG	-5.15	104.63	113.90
1	B	201	ILE	CB-CA-C	5.10	117.13	110.96
1	A	164	SER	CA-C-N	5.05	127.76	120.38
1	A	164	SER	C-N-CA	5.05	127.76	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	CYS	Peptide
1	B	69	SER	Peptide

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	2254	0	2265	14	0
1	B	2251	0	2258	30	0
1	C	2260	0	2269	10	0
2	A	20	0	15	0	0
2	B	20	0	15	0	0
2	C	20	0	15	0	0
3	A	6	0	12	0	0
3	B	6	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	12	0	0
4	B	6	0	8	0	0
5	C	17	0	24	1	0
6	A	81	0	0	3	0
6	B	153	0	0	4	0
6	C	176	0	0	0	0
All	All	7276	0	6905	52	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 4.

All (52) 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:B:69:SER:OG	1:B:70:LYS:HA	1.23	1.25
1:B:69:SER:OG	1:B:70:LYS:CA	1.88	1.20
1:B:68:LYS:HG3	1:B:69:SER:HB3	1.51	0.91
1:B:69:SER:HG	1:B:70:LYS:HA	1.34	0.89
1:A:68:LYS:O	1:B:161:LYS:NZ	2.22	0.73
1:A:212:PHE:CE2	1:A:216:ILE:HD11	2.26	0.70
1:B:69:SER:OG	1:B:70:LYS:C	2.36	0.69
1:B:310:LEU:HD13	1:B:314:LEU:HD23	1.76	0.68
1:A:284:PRO:HG2	1:A:301:TYR:CE1	2.32	0.64
1:B:212:PHE:CE2	1:B:216:ILE:HD11	2.33	0.63
1:B:209:ASN:ND2	1:B:212:PHE:H	2.03	0.57
1:A:136:LYS:NZ	6:A:2042:HOH:O	2.41	0.53
1:B:59:LYS:HE3	1:B:80:THR:HG21	1.90	0.53
1:B:170:LYS:HG2	6:B:2073:HOH:O	2.08	0.53
1:B:69:SER:HB2	1:B:72:GLN:H	1.74	0.53
1:B:181:LYS:O	1:B:184:GLU:HG2	2.09	0.53
1:B:315:LEU:HD21	6:B:2146:HOH:O	2.09	0.52
1:C:94:LEU:C	1:C:94:LEU:HD12	2.35	0.52
1:B:82:TYR:CD2	1:B:97:LYS:HD3	2.45	0.51
1:B:94:LEU:HD12	1:B:94:LEU:C	2.35	0.51
1:B:217:TYR:CE2	1:B:276:LYS:HE2	2.46	0.51
1:B:302:GLU:HB3	1:C:309:LYS:HD2	1.92	0.51
1:C:229:GLN:HE21	1:C:231:GLU:H	1.59	0.51
1:A:210:GLN:HE22	1:A:246:TYR:HA	1.75	0.50
1:B:265:PRO:O	1:B:266:CYS:HB2	2.11	0.50
1:C:211:ASN:HD21	1:C:215:LYS:NZ	2.10	0.49
1:A:210:GLN:NE2	1:A:246:TYR:HA	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:SER:HB2	1:B:72:GLN:N	2.28	0.48
1:C:47:PHE:CD1	5:C:702:1PG:H13	2.49	0.48
1:C:282:THR:O	1:C:305[B]:SER:HB3	2.14	0.47
1:B:318:ILE:O	1:B:319:GLU:C	2.59	0.45
1:A:116:GLU:HG2	1:A:116:GLU:O	2.16	0.45
1:A:178:ASP:OD1	1:A:180:SER:HB3	2.16	0.45
1:B:41:LYS:HE3	1:B:41:LYS:HA	1.97	0.45
1:A:42:LYS:HG2	6:A:2003:HOH:O	2.16	0.44
1:C:212:PHE:CE2	1:C:216:ILE:HD11	2.53	0.44
1:C:210:GLN:HE22	1:C:246:TYR:HA	1.83	0.44
1:B:184:GLU:HB3	1:B:215:LYS:HE2	2.00	0.43
1:B:41:LYS:HA	1:B:41:LYS:CE	2.49	0.43
1:C:48:SER:HB3	1:C:51:TRP:CE2	2.53	0.43
1:A:316:LYS:HE2	1:A:316:LYS:C	2.44	0.43
1:B:94:LEU:HA	6:B:2038:HOH:O	2.19	0.43
1:B:67:THR:HG23	1:B:68:LYS:N	2.35	0.42
1:A:150:GLU:OE2	6:A:2044:HOH:O	2.21	0.41
1:B:209:ASN:C	1:B:209:ASN:HD22	2.28	0.41
1:B:271:ILE:HD13	1:B:271:ILE:HG21	1.89	0.41
1:A:123:VAL:HG13	1:A:179:ALA:HB2	2.02	0.41
1:B:41:LYS:HD2	6:B:2021:HOH:O	2.20	0.41
1:A:251:PHE:CD2	1:A:274:CYS:HB3	2.56	0.41
1:C:95:THR:HG21	1:C:263:THR:HG21	2.02	0.41
1:A:85:VAL:HG13	1:A:95:THR:HG22	2.04	0.40
1:B:230:CYS:O	1:B:231:GLU:O	2.39	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	279/283 (99%)	262 (94%)	16 (6%)	1 (0%)	30	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	279/283 (99%)	264 (95%)	13 (5%)	2 (1%)	18	17
1	C	280/283 (99%)	270 (96%)	10 (4%)	0	100	100
All	All	838/849 (99%)	796 (95%)	39 (5%)	3 (0%)	30	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	SER
1	B	319	GLU
1	A	235	ILE

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	253/254 (100%)	245 (97%)	8 (3%)	34	43
1	B	253/254 (100%)	234 (92%)	19 (8%)	12	12
1	C	254/254 (100%)	251 (99%)	3 (1%)	63	75
All	All	760/762 (100%)	730 (96%)	30 (4%)	28	36

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	49	ILE
1	A	66	GLU
1	A	78	GLU
1	A	116	GLU
1	A	261	ILE
1	A	290	SER
1	A	316	LYS
1	B	41	LYS
1	B	49	ILE
1	B	63	ILE

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Mol	Chain	Res	Type
1	B	67	THR
1	B	70	LYS
1	B	155	VAL
1	B	170	LYS
1	B	201	ILE
1	B	209	ASN
1	B	231	GLU
1	B	235	ILE
1	B	249	LYS
1	B	253	LYS
1	B	261	ILE
1	B	278	ASP
1	B	279	THR
1	B	318	ILE
1	B	319	GLU
1	B	320	ASN
1	C	61	LYS
1	C	170	LYS
1	C	291	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	185	ASN
1	A	188	ASN
1	A	210	GLN
1	A	218	ASN
1	B	173	ASN
1	B	209	ASN
1	B	211	ASN
1	B	285	ASN
1	C	72	GLN
1	C	73	ASN
1	C	142	ASN
1	C	210	GLN
1	C	211	ASN
1	C	229	GLN
1	C	285	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
3	PUT	A	601	-	5,5,5	0.56	0	4,4,4	0.61	0
3	PUT	B	601	-	5,5,5	0.70	0	4,4,4	0.77	0
3	PUT	C	601	-	5,5,5	0.19	0	4,4,4	0.40	0
5	1PG	C	702	-	16,16,16	0.63	0	15,15,15	0.67	0
2	MTA	C	501	-	22,22,22	1.41	3 (13%)	32,32,32	2.05	10 (31%)
2	MTA	A	501	-	22,22,22	1.69	3 (13%)	32,32,32	2.04	9 (28%)
2	MTA	B	501	-	22,22,22	1.62	4 (18%)	32,32,32	2.07	11 (34%)
4	GOL	B	701	-	5,5,5	0.97	0	5,5,5	0.75	0

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
3	PUT	A	601	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PUT	B	601	-	-	0/3/3/3	-
3	PUT	C	601	-	-	0/3/3/3	-
5	1PG	C	702	-	-	7/14/14/14	-
2	MTA	C	501	-	-	2/7/23/23	0/3/3/3
2	MTA	A	501	-	-	2/7/23/23	0/3/3/3
2	MTA	B	501	-	-	2/7/23/23	0/3/3/3
4	GOL	B	701	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MTA	C5-C4	4.39	1.46	1.39
2	A	501	MTA	C4-N9	-4.29	1.28	1.37
2	A	501	MTA	C5-C4	4.08	1.46	1.39
2	B	501	MTA	C4-N9	-3.69	1.30	1.37
2	C	501	MTA	C5-C4	3.49	1.45	1.39
2	B	501	MTA	C5-N7	-3.36	1.33	1.39
2	A	501	MTA	C5'-S5'	-3.36	1.73	1.81
2	C	501	MTA	C4-N9	-2.87	1.31	1.37
2	C	501	MTA	C5-C6	2.52	1.48	1.41
2	B	501	MTA	C5-C6	2.35	1.47	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	MTA	C5-C4-N3	-5.39	119.29	126.72
2	A	501	MTA	C4-N9-C8	5.15	111.14	105.74
2	B	501	MTA	N3-C4-N9	5.00	135.67	127.17
2	B	501	MTA	C5-C4-N3	-4.96	119.89	126.72
2	A	501	MTA	C2-N1-C6	4.26	125.73	118.73
2	C	501	MTA	N3-C4-N9	4.18	134.28	127.17
2	A	501	MTA	N3-C2-N1	-4.13	122.32	128.58
2	B	501	MTA	C4-N9-C8	3.86	109.79	105.74
2	A	501	MTA	N3-C4-N9	3.53	133.16	127.17
2	B	501	MTA	C2-N3-C4	3.35	120.01	111.83
2	C	501	MTA	C4-C5-N7	-3.27	106.84	110.58
2	C	501	MTA	C4-N9-C8	3.21	109.11	105.74
2	C	501	MTA	C2-N3-C4	2.86	118.82	111.83
2	A	501	MTA	C4'-O4'-C1'	-2.86	103.16	109.47
2	C	501	MTA	O4'-C1'-N9	2.79	113.44	108.09
2	A	501	MTA	C5-C4-N3	-2.77	122.91	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MTA	O4'-C4'-C5'	2.70	115.78	108.83
2	B	501	MTA	N3-C2-N1	-2.66	124.56	128.58
2	C	501	MTA	N9-C8-N7	-2.63	110.20	113.94
2	C	501	MTA	C5-N7-C8	2.53	107.42	103.45
2	A	501	MTA	C4-N9-C1'	-2.41	120.99	126.63
2	B	501	MTA	N9-C8-N7	-2.39	110.55	113.94
2	B	501	MTA	N6-C6-N1	2.38	123.68	118.38
2	C	501	MTA	O4'-C1'-C2'	-2.37	101.54	106.62
2	C	501	MTA	N3-C2-N1	-2.33	125.06	128.58
2	B	501	MTA	C5-N7-C8	2.22	106.94	103.45
2	A	501	MTA	C2-N3-C4	2.20	117.21	111.83
2	B	501	MTA	C5-C6-N6	-2.19	117.86	123.29
2	A	501	MTA	N9-C8-N7	-2.10	110.95	113.94
2	B	501	MTA	O2'-C2'-C3'	2.02	118.29	111.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

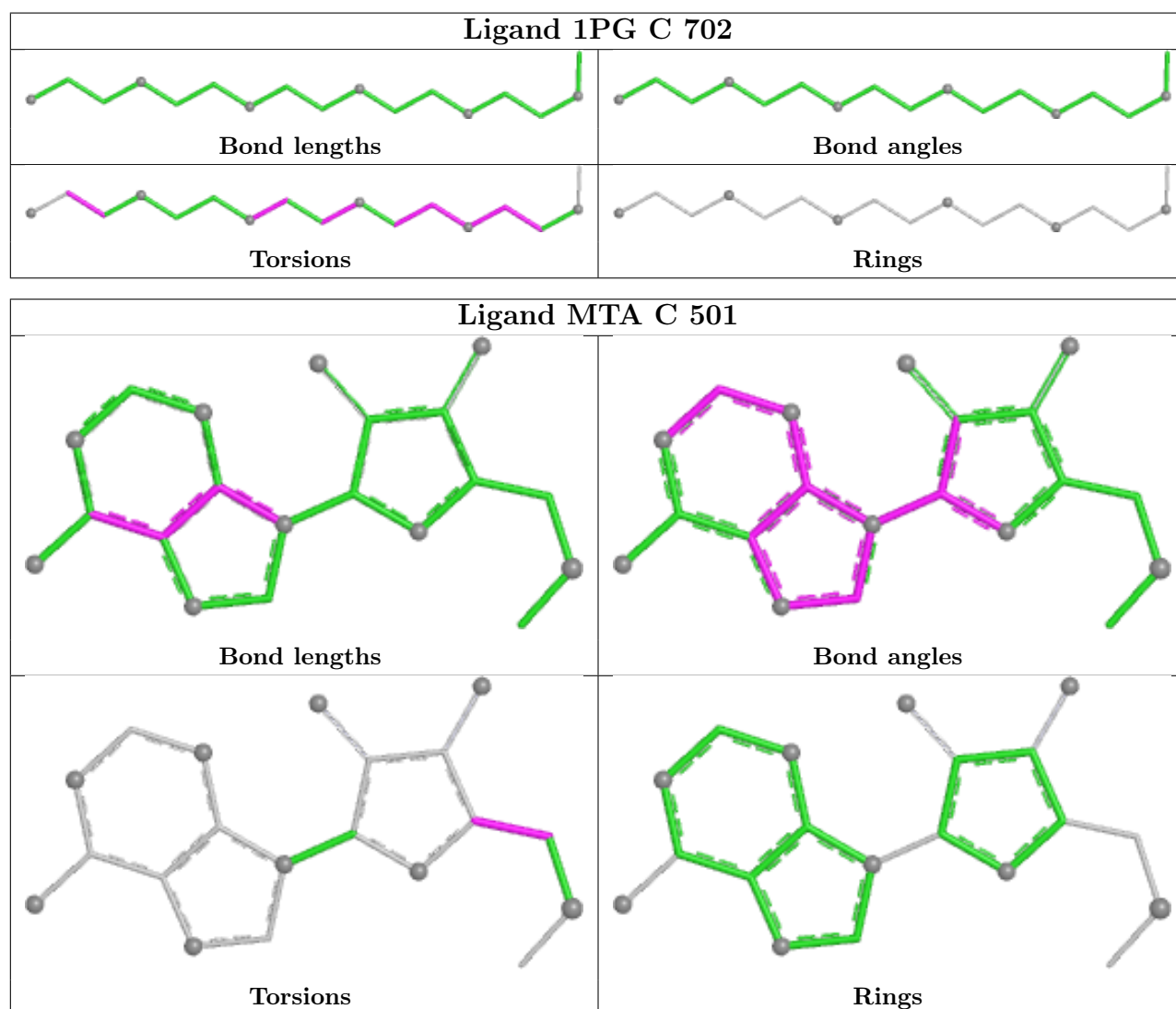
Mol	Chain	Res	Type	Atoms
2	A	501	MTA	O4'-C4'-C5'-S5'
2	A	501	MTA	C3'-C4'-C5'-S5'
2	C	501	MTA	O4'-C4'-C5'-S5'
2	C	501	MTA	C3'-C4'-C5'-S5'
4	B	701	GOL	O1-C1-C2-O2
4	B	701	GOL	O1-C1-C2-C3
5	C	702	1PG	O1-C2-C3-O2
5	C	702	1PG	O5-C10-C11-O6
5	C	702	1PG	C7-C6-O3-C5
5	C	702	1PG	C2-C3-O2-C4
2	B	501	MTA	O4'-C4'-C5'-S5'
5	C	702	1PG	C5-C4-O2-C3
5	C	702	1PG	C6-C7-O4-C8
5	C	702	1PG	O2-C4-C5-O3
2	B	501	MTA	C3'-C4'-C5'-S5'

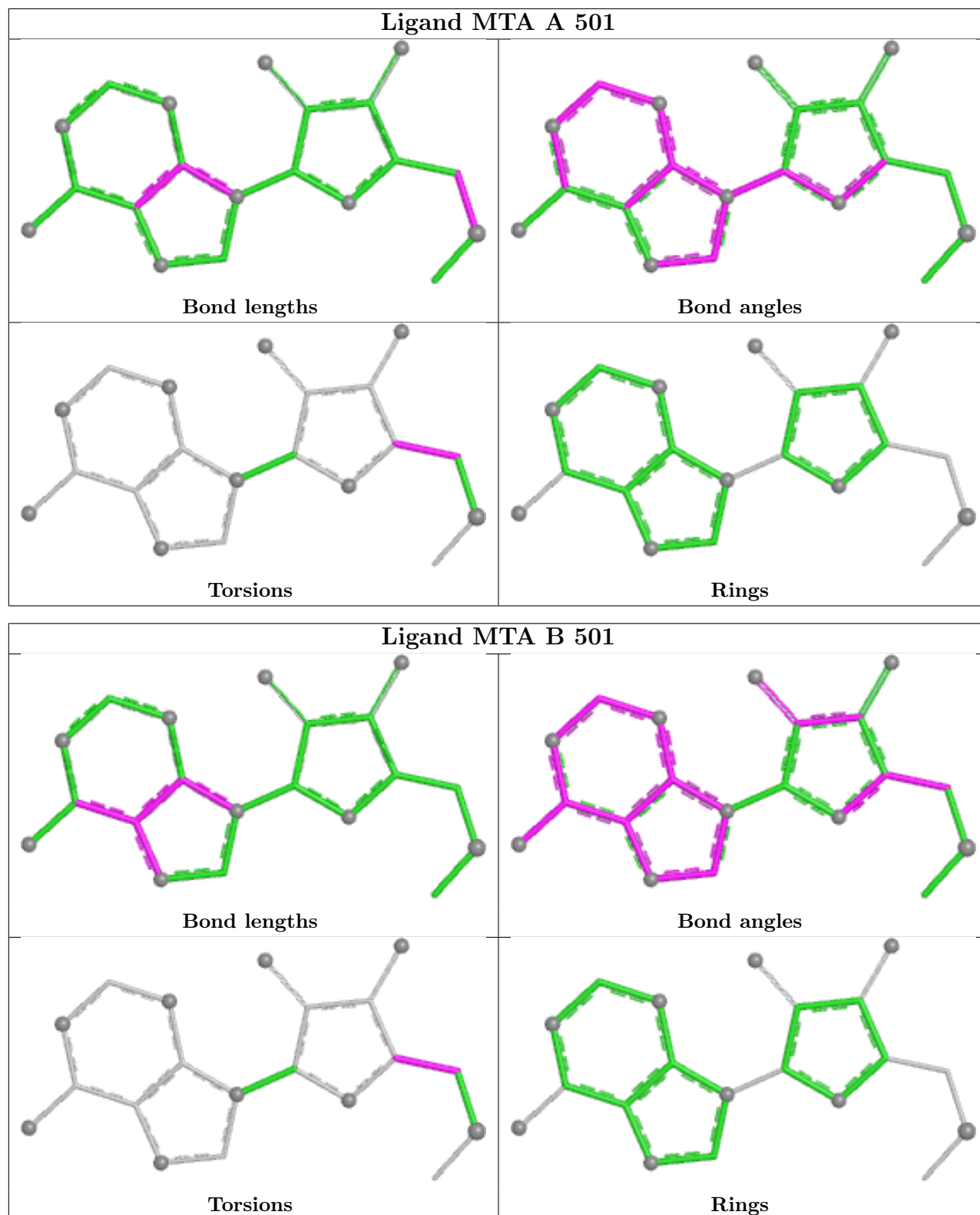
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	702	1PG	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 ⓘ

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(Å ²)	Q<0.9
1	A	281/283 (99%)	0.14	5 (1%) 67 67	22, 32, 55, 75	0
1	B	280/283 (98%)	-0.39	1 (0%) 88 88	11, 22, 45, 87	1 (0%)
1	C	281/283 (99%)	-0.50	0 100 100	6, 20, 39, 55	1 (0%)
All	All	842/849 (99%)	-0.25	6 (0%) 84 83	6, 25, 48, 87	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	ILE	3.1
1	B	41	LYS	3.1
1	A	277	THR	3.0
1	A	41	LYS	2.4
1	A	249	LYS	2.2
1	A	115	LYS	2.1

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](#)

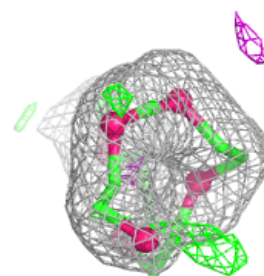
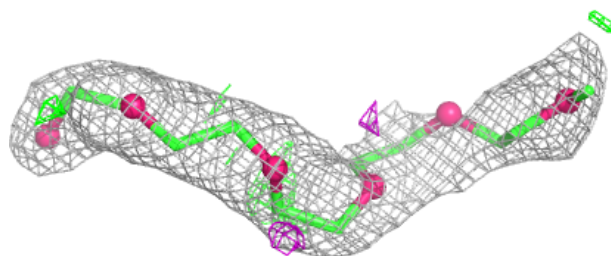
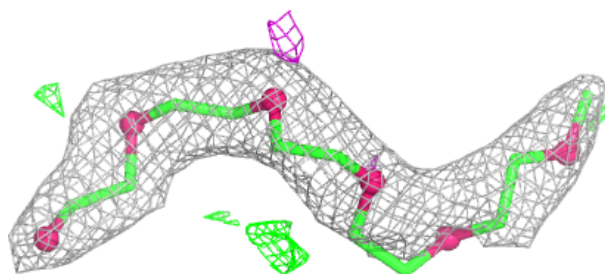
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	PUT	A	601	6/6	0.85	0.15	41,42,45,45	0
4	GOL	B	701	6/6	0.86	0.15	30,41,43,48	0
5	1PG	C	702	17/17	0.86	0.15	35,49,74,77	0
3	PUT	B	601	6/6	0.91	0.10	22,24,25,27	0
3	PUT	C	601	6/6	0.97	0.09	22,22,23,25	0
2	MTA	C	501	20/20	0.98	0.04	16,17,21,21	0
2	MTA	A	501	20/20	0.98	0.04	20,21,31,31	0
2	MTA	B	501	20/20	0.98	0.05	18,21,23,25	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.

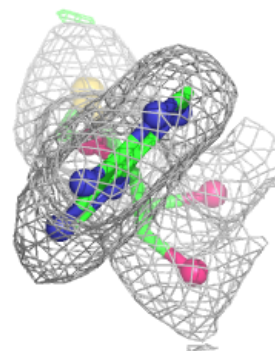
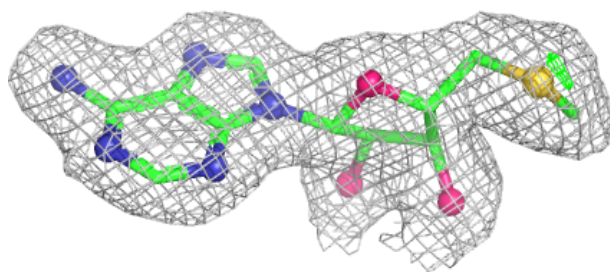
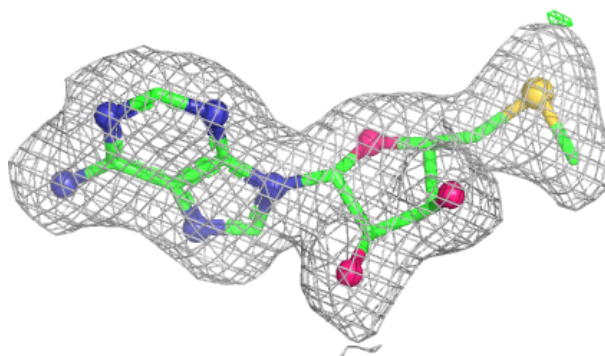
Electron density around 1PG C 702:

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

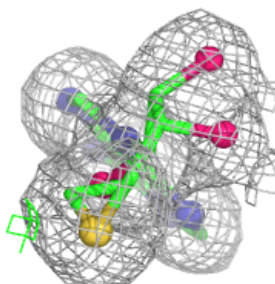
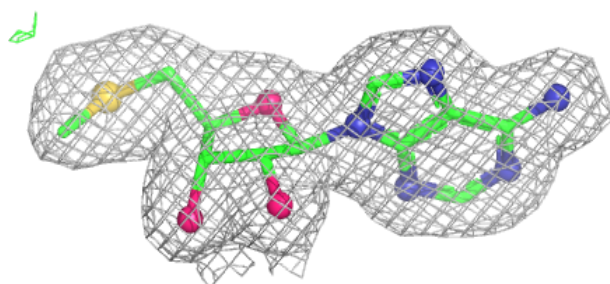
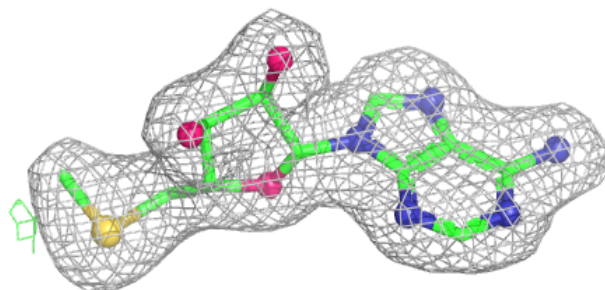


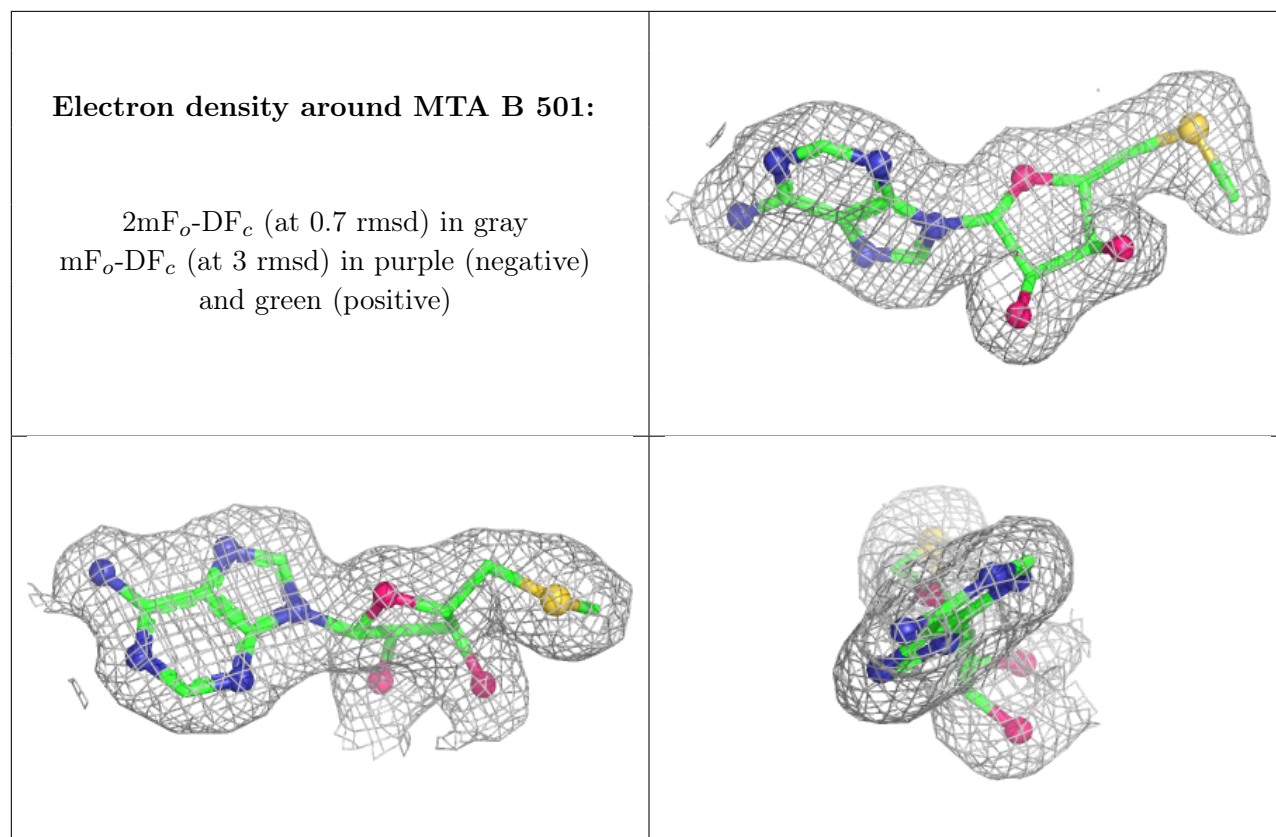
Electron density around MTA C 501:

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

**Electron density around MTA 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.