



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:27 PM EDT

PDB ID : 6HY1 / pdb_00006hy1
Title : Plasmodium falciparum spermidine synthase in complex with 5'-methylthioadenosine and N,N'-Bis(3-aminopropyl)-1,4-cyclohexanediamine after catalysis in crystal
Authors : Sprenger, J.; Coertzen, D.; Persson, L.; Carey, J.; Birkholtz, L.M.; Louw, B.I.
Deposited on : 2018-10-19
Resolution : 1.60 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

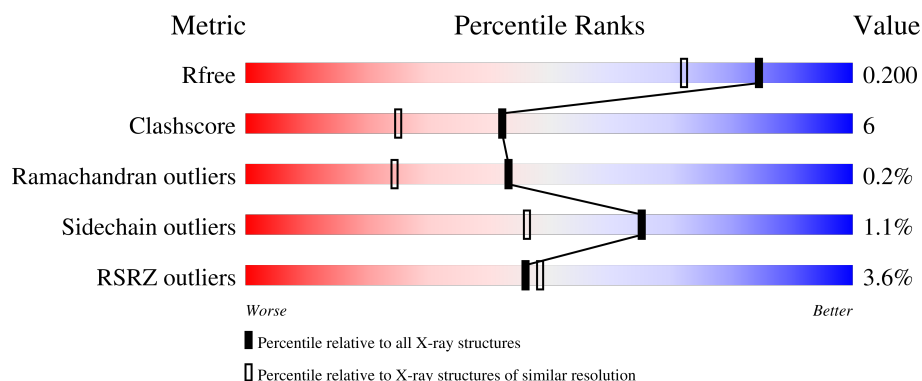
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	281	4% 89% 10%
1	B	281	6% 85% 14%
1	C	281	% 91% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	406	-	-	X	-

2 Entry composition [i](#)

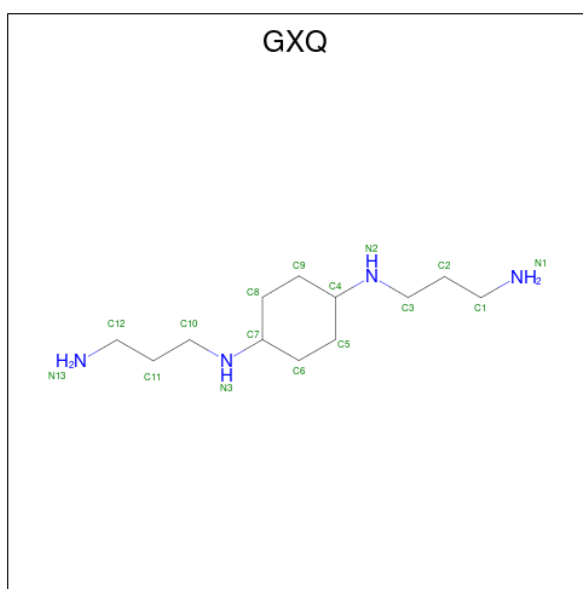
There are 7 unique types of molecules in this entry. The entry contains 7721 atoms, of which 8 are hydrogens and 0 are deuteriums.

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	0	0
			2242	1455	350	423	14			
1	C	281	Total	C	N	O	S	0	0	0
			2253	1462	352	425	14			

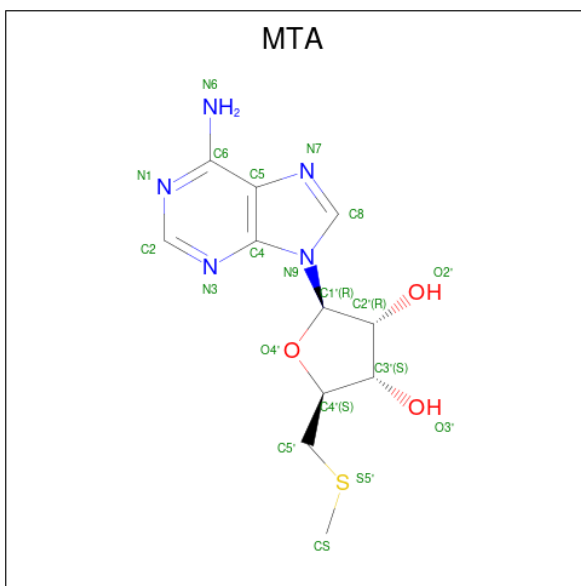
- Molecule 2 is N,N'-Bis(3-aminopropyl)-1,4-cyclohexanediamine (CCD ID: GXQ) (formula: $C_{12}H_{28}N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			16	12	4		
2	B	1	Total	C	N	0	0
			16	12	4		

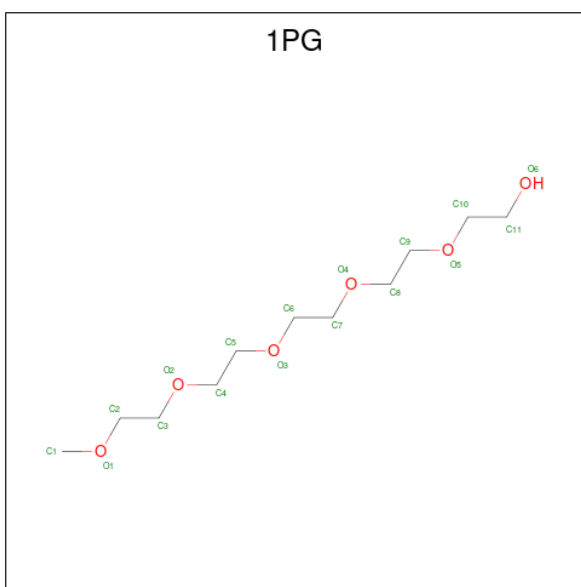
- Molecule 3 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula:

C₁₁H₁₅N₅O₃S).



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

- Molecule 4 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (CCD ID: 1PG) (formula: C₁₁H₂₄O₆).



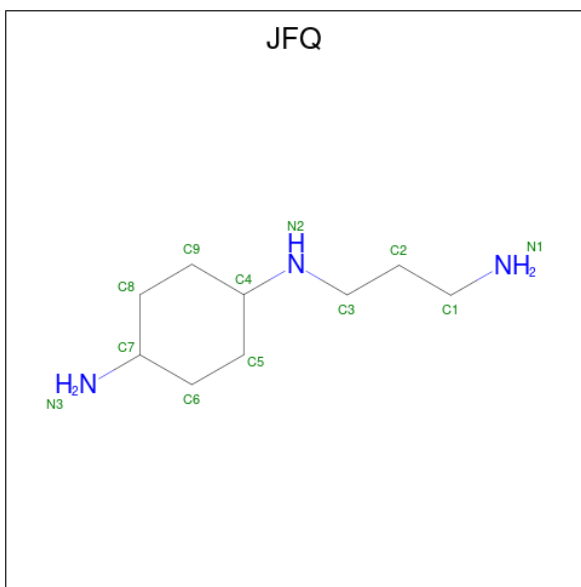
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	11	6		
4	B	1	Total	C	O	0	0
			17	11	6		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	O		0	0
			6	3	3			
5	C	1	Total	C	O		0	0
			6	3	3			
5	C	1	Total	C	O		0	0
			6	3	3			

- Molecule 6 is trans-N-(3-aminopropyl)cyclohexane-1,4-diamine (CCD ID: JFQ) (formula: $C_9H_{21}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			12	9	3		

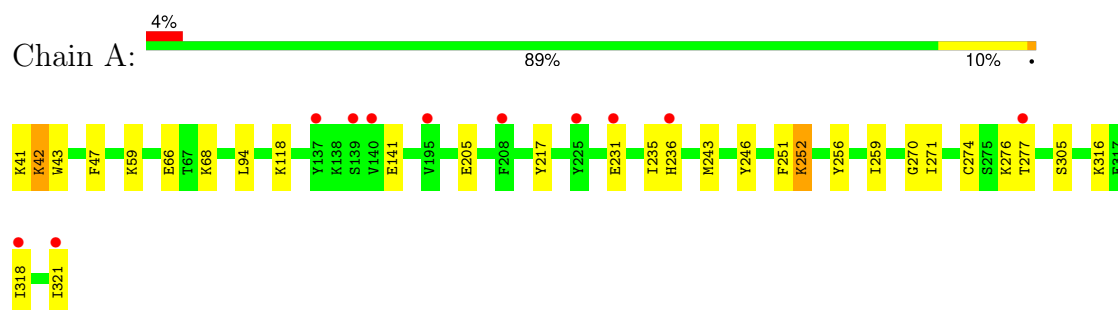
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	201	Total	O	0	0
			201	201		
7	B	239	Total	O	0	0
			239	239		
7	C	344	Total	O	0	0
			344	344		

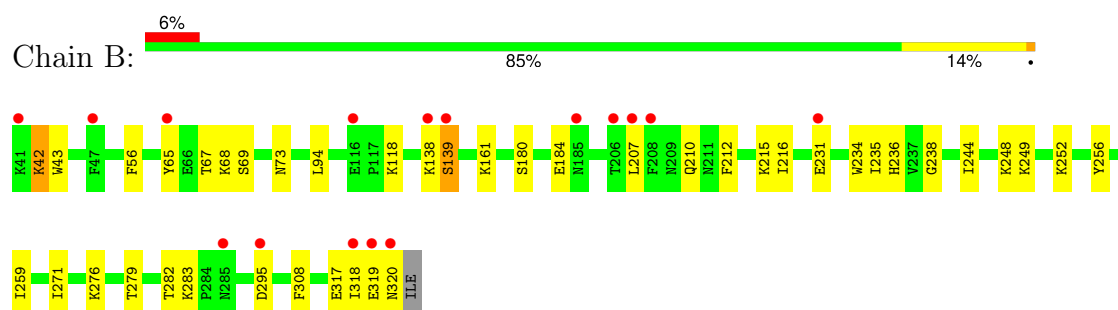
3 Residue-property plots [i](#)

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.

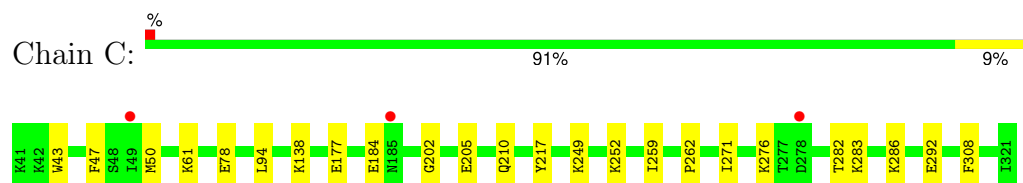
• Molecule 1: Spermidine synthase



• 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	199.87Å 135.00Å 48.57Å 90.00° 95.95° 90.00°	Depositor
Resolution (Å)	32.17 – 1.60 32.17 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (32.17-1.60) 98.0 (32.17-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.55Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.176 , 0.200 0.177 , 0.200	Depositor DCC
R_{free} test set	8829 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7721	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 1PG, MTA, JFQ, GXQ

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	0.53	0/2304	0.63	0/3111
1	B	0.62	0/2292	0.73	0/3097
1	C	0.69	0/2302	0.74	2/3109 (0.1%)
All	All	0.61	0/6898	0.70	2/9317 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	GLU	CA-C-N	-5.46	111.12	121.54
1	C	184	GLU	C-N-CA	-5.46	111.12	121.54

There are no chirality outliers.

There are no planarity outliers.

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	2254	0	2265	27	0
1	B	2242	0	2245	42	0
1	C	2253	0	2258	19	0
2	A	16	0	0	0	0
2	B	16	0	0	1	0
3	A	20	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	15	0	0
3	C	20	0	15	0	0
4	A	17	0	24	2	0
4	B	17	0	24	2	0
5	A	6	0	8	0	0
5	B	18	8	24	5	0
5	C	18	0	22	2	0
6	C	12	0	21	0	0
7	A	201	0	0	4	1
7	B	239	0	0	12	0
7	C	344	0	0	5	2
All	All	7713	8	6936	87	3

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 6.

All (87) 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)
2:B:401:GXQ:N13	7:B:503:HOH:O	1.91	1.03
1:B:231:GLU:HG2	1:B:236:HIS:HB2	1.39	1.01
1:B:317:GLU:OE2	7:B:501:HOH:O	1.81	0.98
1:B:184:GLU:OE2	7:B:502:HOH:O	1.89	0.91
1:B:295:ASP:OD2	7:B:504:HOH:O	1.93	0.85
1:C:177:GLU:OE1	7:C:501:HOH:O	1.96	0.84
1:B:231:GLU:HG3	7:B:503:HOH:O	1.78	0.84
1:C:286:LYS:NZ	7:C:502:HOH:O	2.03	0.82
1:B:283:LYS:NZ	7:B:505:HOH:O	2.11	0.81
1:C:50:MET:SD	7:C:818:HOH:O	2.39	0.80
1:A:305:SER:OG	7:A:501:HOH:O	2.03	0.75
1:A:42:LYS:HE2	1:A:43:TRP:H	1.50	0.74
1:A:205:GLU:OE2	7:A:502:HOH:O	2.06	0.73
1:B:65:TYR:OH	1:B:67:THR:HG21	1.88	0.71
1:C:61:LYS:HE2	1:C:78:GLU:CD	2.16	0.70
1:A:66:GLU:OE2	7:A:503:HOH:O	2.08	0.70
1:B:184:GLU:HG2	1:B:215:LYS:HE2	1.78	0.66
1:B:252:LYS:HE2	1:B:276:LYS:O	1.96	0.65
1:C:61:LYS:HE2	1:C:78:GLU:OE2	1.96	0.65
1:B:236:HIS:ND1	5:B:406:GOL:O2	2.18	0.62
1:B:238:GLY:H	5:B:406:GOL:C3	2.12	0.62
1:C:259:ILE:HD11	1:C:271:ILE:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LYS:HG2	1:B:73:ASN:OD1	2.00	0.61
1:B:317:GLU:CG	7:B:501:HOH:O	2.48	0.61
1:B:68:LYS:HD3	1:B:69:SER:O	2.02	0.60
1:C:249:LYS:HE2	7:C:746:HOH:O	2.01	0.59
1:B:231:GLU:O	1:B:256:TYR:OH	2.21	0.58
1:A:259:ILE:HD11	1:A:271:ILE:HD11	1.85	0.58
1:B:238:GLY:H	5:B:406:GOL:H31	1.69	0.56
1:B:65:TYR:CE1	1:B:67:THR:HG22	2.41	0.55
1:A:41:LYS:HB2	1:A:59:LYS:HE2	1.89	0.55
1:C:202:GLY:O	1:C:205:GLU:HG2	2.07	0.54
1:B:235:ILE:HG22	1:B:236:HIS:CD2	2.42	0.54
1:B:56:PHE:CD1	5:C:405:GOL:H32	2.43	0.54
1:A:68:LYS:O	1:B:161:LYS:NZ	2.41	0.54
1:C:283:LYS:HE2	7:C:577:HOH:O	2.07	0.53
1:A:41:LYS:CB	1:A:59:LYS:HE2	2.39	0.53
1:A:217:TYR:CE1	1:A:276:LYS:HE2	2.44	0.53
1:B:236:HIS:CE1	5:B:406:GOL:HO2	2.20	0.53
1:A:42:LYS:CE	1:A:43:TRP:H	2.22	0.52
1:A:243:MET:HE1	1:A:246:TYR:CE2	2.45	0.52
1:A:94:LEU:C	1:A:94:LEU:HD12	2.34	0.51
1:A:118:LYS:HE3	7:A:548:HOH:O	2.11	0.50
1:B:180:SER:O	1:B:184:GLU:HG3	2.13	0.49
1:B:238:GLY:H	5:B:406:GOL:H32	1.78	0.48
1:B:249:LYS:HE3	7:B:713:HOH:O	2.14	0.47
1:C:94:LEU:C	1:C:94:LEU:HD12	2.39	0.47
1:A:231:GLU:HG2	1:A:236:HIS:O	2.15	0.47
4:B:404:1PG:H112	1:C:43:TRP:CD1	2.50	0.47
1:A:243:MET:HE1	1:A:246:TYR:HE2	1.79	0.46
1:B:118:LYS:HA	1:B:118:LYS:HD3	1.81	0.45
1:A:217:TYR:CD1	1:A:276:LYS:HE2	2.52	0.45
1:B:210:GLN:OE1	1:B:249:LYS:HD2	2.17	0.45
1:A:252:LYS:HD3	1:A:252:LYS:HA	1.63	0.44
1:B:234:TRP:CE2	1:C:262:PRO:HD3	2.52	0.44
1:A:318:ILE:HB	1:A:321:ILE:HD12	1.99	0.44
4:B:404:1PG:H62	1:C:47:PHE:HZ	1.82	0.44
1:C:282:THR:HG22	1:C:308:PHE:CG	2.52	0.44
1:C:138:LYS:HE3	1:C:292:GLU:CD	2.43	0.44
1:C:210:GLN:OE1	1:C:249:LYS:HD2	2.17	0.44
1:B:317:GLU:CB	7:B:501:HOH:O	2.65	0.44
1:A:43:TRP:CD1	4:A:403:1PG:H32	2.53	0.44
1:B:138:LYS:HG2	7:B:650:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HD2	1:A:59:LYS:HE2	2.00	0.43
1:B:231:GLU:CG	1:B:236:HIS:HB2	2.28	0.43
1:B:94:LEU:HD12	1:B:94:LEU:C	2.43	0.43
1:B:259:ILE:HD11	1:B:271:ILE:HD11	2.00	0.43
1:B:212:PHE:CE2	1:B:216:ILE:HD11	2.54	0.42
1:B:318:ILE:O	1:B:320:ASN:N	2.52	0.42
1:B:42:LYS:NZ	1:B:43:TRP:H	2.16	0.42
1:A:243:MET:HA	1:A:243:MET:HE2	2.00	0.42
1:B:65:TYR:OH	1:B:67:THR:CG2	2.63	0.42
1:B:317:GLU:HB3	7:B:501:HOH:O	2.19	0.42
1:A:256:TYR:CZ	1:A:270:GLY:HA3	2.55	0.42
1:B:139:SER:HB3	7:B:687:HOH:O	2.19	0.41
1:B:244:ILE:HG22	1:B:248:LYS:HD2	2.03	0.41
1:A:243:MET:CE	1:A:246:TYR:CE2	3.03	0.41
1:B:282:THR:HG22	1:B:308:PHE:CD2	2.55	0.41
1:C:217:TYR:CE2	1:C:276:LYS:HE2	2.55	0.41
1:B:235:ILE:HG22	1:B:236:HIS:CG	2.56	0.41
1:C:138:LYS:HE3	1:C:292:GLU:OE2	2.21	0.40
1:A:118:LYS:HE2	1:A:141:GLU:OE2	2.21	0.40
1:C:252:LYS:HA	1:C:252:LYS:HD2	1.85	0.40
1:A:42:LYS:HA	1:A:42:LYS:HD2	1.38	0.40
1:A:47:PHE:CZ	4:A:403:1PG:H92	2.56	0.40
1:A:251:PHE:CG	1:A:274:CYS:HB3	2.56	0.40
1:B:56:PHE:CE1	5:C:405:GOL:H32	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:694:HOH:O	7:C:799:HOH:O[1_554]	1.88	0.32
7:C:725:HOH:O	7:C:774:HOH:O[1_554]	1.94	0.26
7:A:566:HOH:O	7:A:680:HOH:O[2_656]	2.10	0.10

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	279/281 (99%)	272 (98%)	6 (2%)	1 (0%)	30	14
1	B	278/281 (99%)	273 (98%)	4 (1%)	1 (0%)	30	14
1	C	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
All	All	836/843 (99%)	816 (98%)	18 (2%)	2 (0%)	43	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	253/253 (100%)	249 (98%)	4 (2%)	55	33
1	B	251/253 (99%)	247 (98%)	4 (2%)	55	33
1	C	252/253 (100%)	252 (100%)	0	100	100
All	All	756/759 (100%)	748 (99%)	8 (1%)	65	46

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	252	LYS
1	A	277	THR
1	A	316	LYS
1	B	42	LYS
1	B	139	SER
1	B	207	LEU
1	B	279	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	188	ASN
1	B	142	ASN
1	B	173	ASN
1	C	142	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
5	GOL	C	404	-	5,5,5	0.82	0	5,5,5	1.14	0
6	JFQ	C	401	-	12,12,12	0.90	0	14,14,14	2.16	6 (42%)
3	MTA	B	402	-	22,22,22	2.75	7 (31%)	32,32,32	2.54	11 (34%)
3	MTA	A	402	-	22,22,22	2.61	6 (27%)	32,32,32	2.27	11 (34%)
4	1PG	B	404	-	16,16,16	0.54	0	15,15,15	0.59	0
2	GXQ	A	401	-	16,16,16	0.66	0	18,18,18	1.38	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	403	-	5,5,5	1.02	0	5,5,5	1.00	0
5	GOL	A	404	-	5,5,5	0.70	0	5,5,5	1.27	1 (20%)
5	GOL	C	403	-	5,5,5	0.77	0	5,5,5	1.05	0
5	GOL	C	405	-	5,5,5	2.45	3 (60%)	5,5,5	0.49	0
2	GXQ	B	401	-	16,16,16	0.76	0	18,18,18	1.65	3 (16%)
4	1PG	A	403	-	16,16,16	0.56	0	15,15,15	0.37	0
5	GOL	B	406	-	5,5,5	0.55	0	5,5,5	0.85	0
5	GOL	B	405	-	5,5,5	0.96	0	5,5,5	1.06	0
3	MTA	C	402	-	22,22,22	2.73	9 (40%)	32,32,32	2.32	10 (31%)

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
5	GOL	C	404	-	-	0/4/4/4	-
6	JFQ	C	401	-	-	2/5/15/15	0/1/1/1
3	MTA	B	402	-	-	3/7/23/23	0/3/3/3
3	MTA	A	402	-	-	3/7/23/23	0/3/3/3
4	1PG	B	404	-	-	5/14/14/14	-
2	GXQ	A	401	-	-	3/10/20/20	0/1/1/1
5	GOL	B	403	-	-	0/4/4/4	-
5	GOL	A	404	-	-	0/4/4/4	-
5	GOL	C	403	-	-	0/4/4/4	-
5	GOL	C	405	-	-	2/4/4/4	-
2	GXQ	B	401	-	-	4/10/20/20	0/1/1/1
4	1PG	A	403	-	-	6/14/14/14	-
5	GOL	B	406	-	-	2/4/4/4	-
5	GOL	B	405	-	-	3/4/4/4	-
3	MTA	C	402	-	-	2/7/23/23	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	MTA	O4'-C1'	7.11	1.58	1.42
3	C	402	MTA	O4'-C1'	6.85	1.57	1.42
3	A	402	MTA	O4'-C1'	6.34	1.56	1.42
3	B	402	MTA	C2'-C1'	-6.26	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	MTA	C2'-C1'	-6.21	1.34	1.53
3	A	402	MTA	C2'-C1'	-5.93	1.34	1.53
3	A	402	MTA	O4'-C4'	-5.85	1.32	1.45
3	B	402	MTA	O4'-C4'	-5.14	1.33	1.45
3	C	402	MTA	O4'-C4'	-3.86	1.36	1.45
5	C	405	GOL	O2-C2	-3.84	1.32	1.43
3	C	402	MTA	O2'-C2'	3.37	1.51	1.43
3	A	402	MTA	C5-C4	-3.36	1.33	1.39
3	C	402	MTA	C5-C4	-2.98	1.33	1.39
3	B	402	MTA	C6-N6	2.96	1.41	1.34
3	C	402	MTA	C2-N3	2.87	1.39	1.33
5	C	405	GOL	C3-C2	2.86	1.62	1.51
3	B	402	MTA	O2'-C2'	2.71	1.49	1.43
3	C	402	MTA	C5-N7	-2.67	1.34	1.39
3	B	402	MTA	C5'-S5'	2.60	1.87	1.81
3	B	402	MTA	C5-C4	-2.59	1.34	1.39
3	C	402	MTA	C8-N7	2.52	1.36	1.31
5	C	405	GOL	O1-C1	-2.41	1.32	1.42
3	C	402	MTA	C3'-C2'	2.25	1.59	1.53
3	A	402	MTA	C2-N3	2.23	1.37	1.33
3	A	402	MTA	C6-N6	2.16	1.39	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	MTA	N3-C2-N1	-7.83	116.73	128.58
3	B	402	MTA	N3-C2-N1	-6.12	119.31	128.58
3	B	402	MTA	C5-C4-N3	-5.80	118.73	126.72
3	A	402	MTA	N6-C6-N1	-5.43	106.28	118.38
3	B	402	MTA	N9-C8-N7	-4.60	107.41	113.94
3	B	402	MTA	N3-C4-N9	4.23	134.36	127.17
3	A	402	MTA	N3-C2-N1	-4.22	122.20	128.58
3	A	402	MTA	C5-C6-N6	4.18	133.64	123.29
3	B	402	MTA	C2-N3-C4	3.99	121.58	111.83
3	B	402	MTA	N6-C6-N1	-3.92	109.65	118.38
3	A	402	MTA	C5-C4-N3	-3.92	121.32	126.72
3	A	402	MTA	N9-C8-N7	-3.83	108.51	113.94
3	C	402	MTA	N9-C8-N7	-3.81	108.53	113.94
3	A	402	MTA	C4'-O4'-C1'	-3.60	101.53	109.47
6	C	401	JFQ	C5-C6-C7	3.58	115.64	111.53
6	C	401	JFQ	C3-N2-C4	3.57	121.06	114.18
3	C	402	MTA	C5-C4-N3	-3.47	121.93	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GXQ	C5-C6-C7	3.45	115.28	111.49
3	C	402	MTA	C2-N3-C4	3.29	119.88	111.83
2	B	401	GXQ	C5-C6-C7	3.27	115.09	111.49
3	B	402	MTA	C4'-O4'-C1'	-3.16	102.48	109.47
2	B	401	GXQ	C10-N3-C7	-3.16	108.11	114.18
2	A	401	GXQ	C6-C5-C4	3.07	114.86	111.49
3	C	402	MTA	C2-N1-C6	3.05	123.75	118.73
3	C	402	MTA	N3-C4-N9	3.01	132.28	127.17
6	C	401	JFQ	C9-C8-C7	2.96	114.93	111.53
3	B	402	MTA	C4-N9-C8	2.95	108.84	105.74
3	C	402	MTA	C4'-O4'-C1'	-2.93	103.00	109.47
3	C	402	MTA	O4'-C1'-C2'	-2.88	100.45	106.62
3	A	402	MTA	O4'-C1'-C2'	-2.83	100.56	106.62
6	C	401	JFQ	C8-C7-C6	2.81	113.14	110.29
3	A	402	MTA	C4-N9-C8	2.81	108.68	105.74
3	C	402	MTA	C4-N9-C8	2.80	108.67	105.74
3	B	402	MTA	C5-C6-N6	2.74	130.06	123.29
6	C	401	JFQ	C8-C9-C4	2.70	114.46	111.49
3	B	402	MTA	C6-C5-C4	2.65	120.80	117.18
5	A	404	GOL	C3-C2-C1	-2.57	102.36	111.80
3	C	402	MTA	N6-C6-N1	-2.52	112.77	118.38
3	A	402	MTA	N3-C4-N9	2.51	131.43	127.17
3	B	402	MTA	C5-N7-C8	2.42	107.25	103.45
3	A	402	MTA	C2-N3-C4	2.42	117.73	111.83
6	C	401	JFQ	C6-C5-C4	2.41	114.13	111.49
2	A	401	GXQ	C11-C10-N3	-2.26	103.45	111.78
3	A	402	MTA	C5-N7-C8	2.12	106.78	103.45
2	B	401	GXQ	C11-C10-N3	2.06	119.39	111.78

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GXQ	C9-C4-N2-C3
3	A	402	MTA	C3'-C4'-C5'-S5'
6	C	401	JFQ	C9-C4-N2-C3
4	A	403	1PG	O1-C2-C3-O2
5	B	405	GOL	O1-C1-C2-C3
5	B	406	GOL	C1-C2-C3-O3
5	C	405	GOL	O1-C1-C2-C3
5	B	405	GOL	O1-C1-C2-O2
4	A	403	1PG	O3-C6-C7-O4

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Mol	Chain	Res	Type	Atoms
4	B	404	1PG	C4-C5-O3-C6
4	B	404	1PG	C8-C9-O5-C10
2	A	401	GXQ	C11-C10-N3-C7
5	B	406	GOL	O2-C2-C3-O3
4	A	403	1PG	C6-C7-O4-C8
2	A	401	GXQ	C10-C11-C12-N13
4	A	403	1PG	O4-C8-C9-O5
2	A	401	GXQ	C2-C3-N2-C4
4	A	403	1PG	C3-C2-O1-C1
4	B	404	1PG	O2-C4-C5-O3
3	A	402	MTA	O4'-C4'-C5'-S5'
3	B	402	MTA	O4'-C4'-C5'-S5'
2	B	401	GXQ	C10-C11-C12-N13
2	B	401	GXQ	C2-C3-N2-C4
2	B	401	GXQ	C11-C10-N3-C7
6	C	401	JFQ	C2-C3-N2-C4
4	B	404	1PG	O1-C2-C3-O2
4	A	403	1PG	O5-C10-C11-O6
5	C	405	GOL	O1-C1-C2-O2
3	C	402	MTA	C2'-C1'-N9-C8
3	B	402	MTA	C3'-C4'-C5'-S5'
3	C	402	MTA	C3'-C4'-C5'-S5'
5	B	405	GOL	O2-C2-C3-O3
3	A	402	MTA	C2'-C1'-N9-C8
3	B	402	MTA	C2'-C1'-N9-C8
4	B	404	1PG	O4-C8-C9-O5

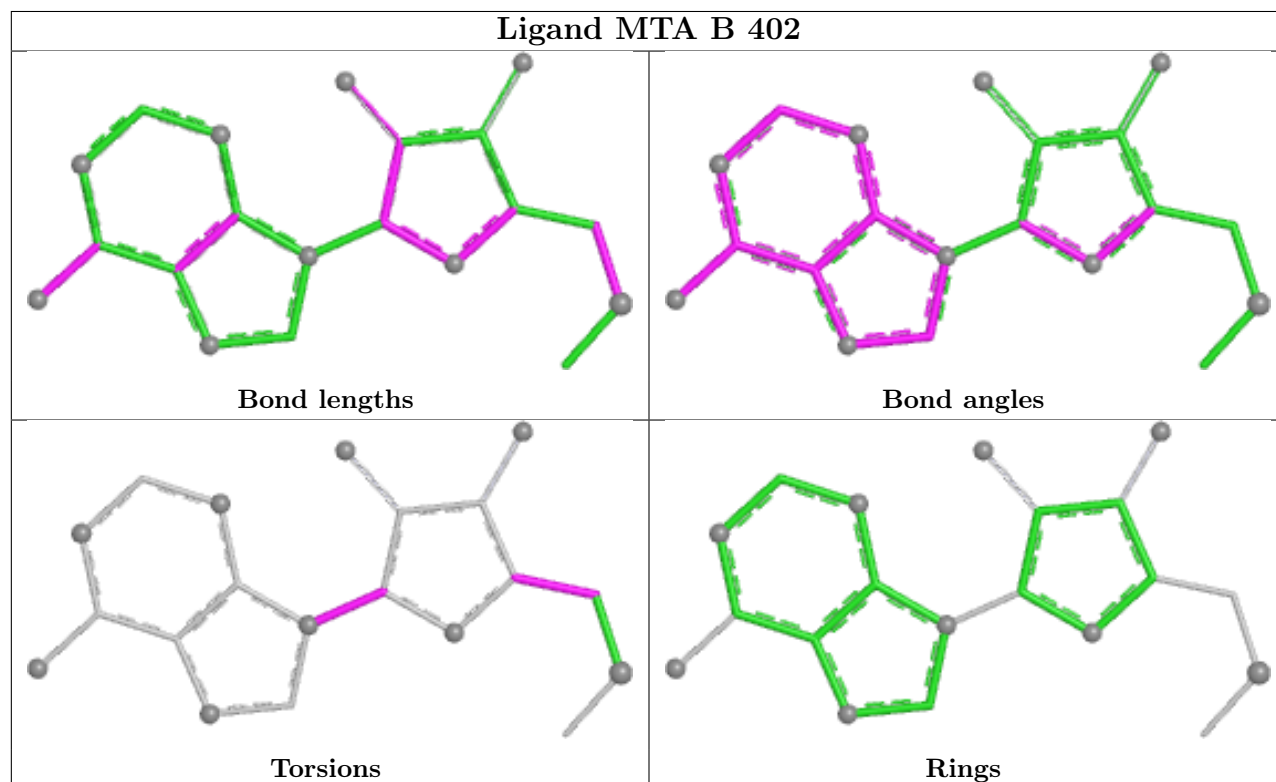
There are no ring outliers.

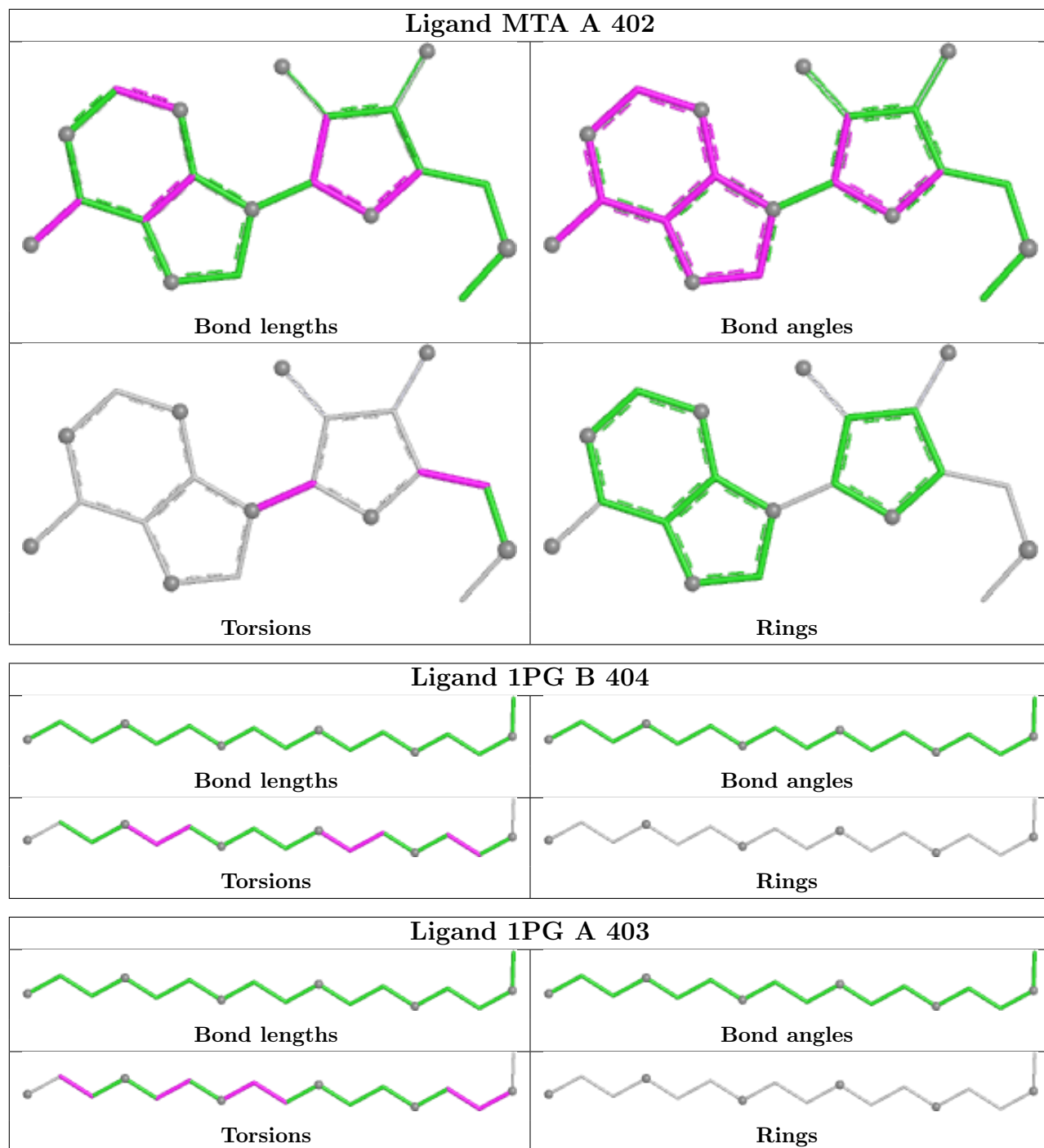
5 monomers are involved in 12 short contacts:

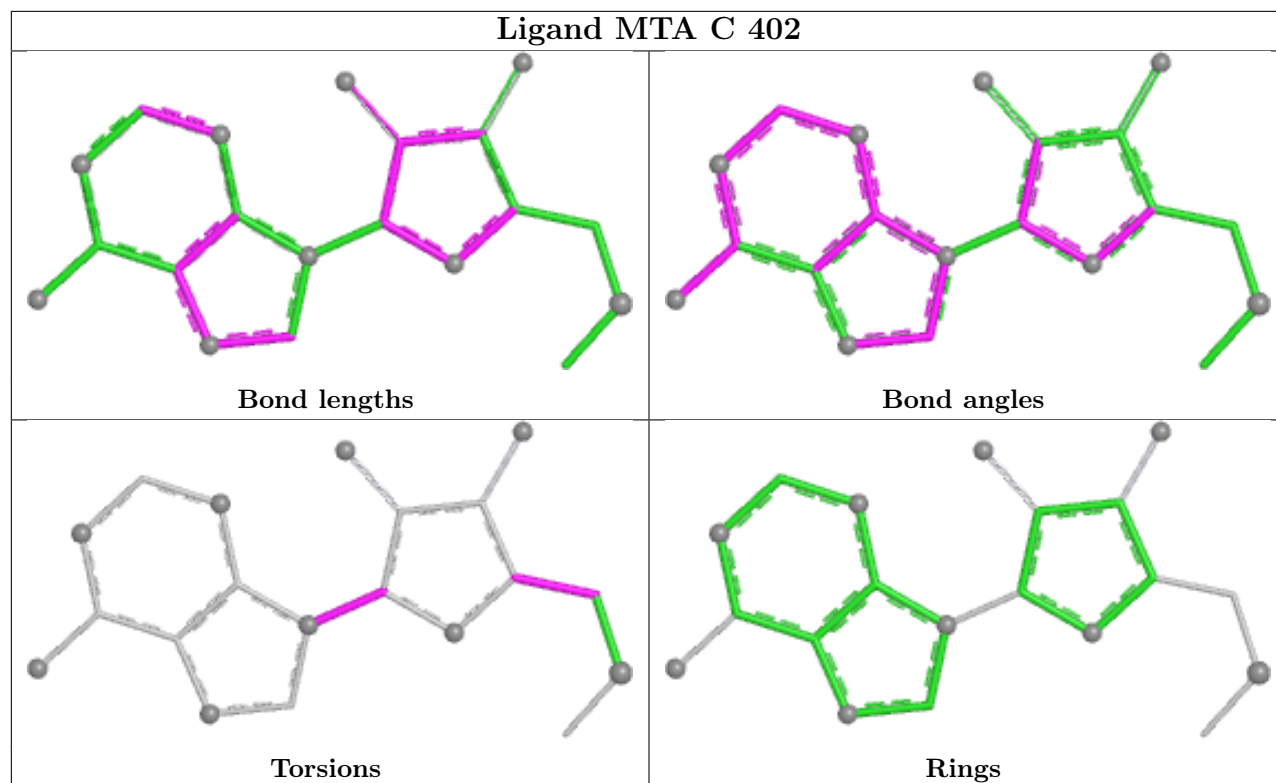
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	1PG	2	0
5	C	405	GOL	2	0
2	B	401	GXQ	1	0
4	A	403	1PG	2	0
5	B	406	GOL	5	0

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	281/281 (100%)	0.68	11 (3%) 43 45	27, 35, 53, 71	0
1	B	280/281 (99%)	0.20	16 (5%) 29 30	21, 29, 49, 79	0
1	C	281/281 (100%)	-0.05	3 (1%) 78 82	21, 27, 42, 59	0
All	All	842/843 (99%)	0.28	30 (3%) 46 48	21, 31, 50, 79	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	PHE	3.8
1	A	321	ILE	3.8
1	B	47	PHE	3.6
1	B	319	GLU	3.4
1	C	278	ASP	3.3
1	A	208	PHE	3.3
1	A	236	HIS	3.1
1	A	231	GLU	3.0
1	A	318	ILE	2.9
1	B	185	ASN	2.8
1	C	185	ASN	2.7
1	B	65	TYR	2.6
1	B	116	GLU	2.5
1	A	277	THR	2.4
1	B	41	LYS	2.4
1	B	320	ASN	2.4
1	B	231	GLU	2.4
1	B	318	ILE	2.4
1	C	49	ILE	2.3
1	B	139	SER	2.3
1	B	295	ASP	2.3
1	B	207	LEU	2.3
1	B	206	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	138	LYS	2.2
1	B	285	ASN	2.2
1	A	137	TYR	2.2
1	A	225	TYR	2.2
1	A	140	VAL	2.1
1	A	139	SER	2.1
1	A	195	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

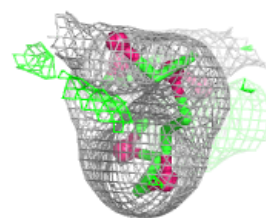
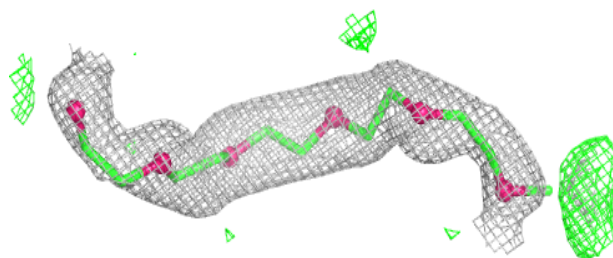
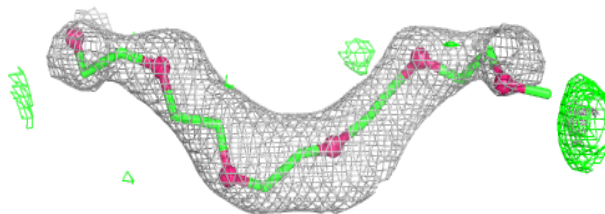
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GXQ	A	401	16/16	0.82	0.18	28,43,57,58	0
5	GOL	B	406	6/6	0.82	0.15	37,61,80,87	0
2	GXQ	B	401	16/16	0.84	0.16	27,38,50,56	0
4	1PG	A	403	17/17	0.87	0.15	34,45,55,57	17
5	GOL	B	405	6/6	0.88	0.12	37,47,56,57	0
4	1PG	B	404	17/17	0.89	0.14	38,57,64,68	0
5	GOL	C	404	6/6	0.89	0.11	41,49,52,52	0
6	JFQ	C	401	12/12	0.91	0.13	23,32,39,41	0
5	GOL	A	404	6/6	0.92	0.10	41,46,52,55	0
5	GOL	B	403	6/6	0.92	0.10	34,42,44,46	0
5	GOL	C	403	6/6	0.95	0.07	31,31,36,41	0
5	GOL	C	405	6/6	0.96	0.10	26,29,33,33	0
3	MTA	B	402	20/20	0.96	0.07	26,28,32,33	0
3	MTA	A	402	20/20	0.97	0.06	28,30,34,35	0
3	MTA	C	402	20/20	0.97	0.07	22,25,28,28	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.

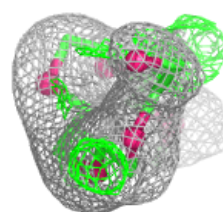
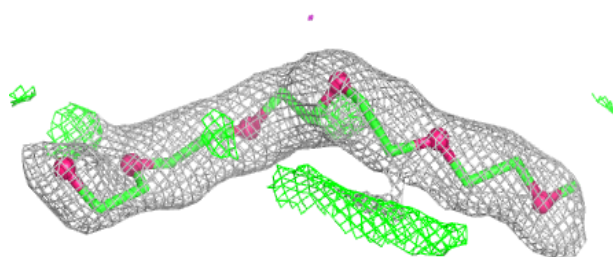
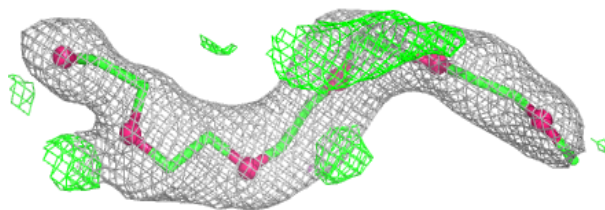
Electron density around 1PG A 403:

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

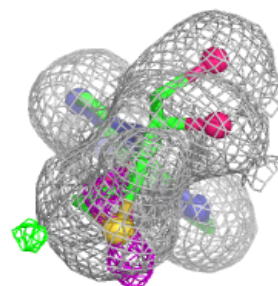
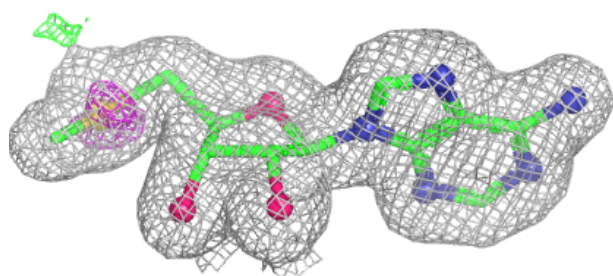
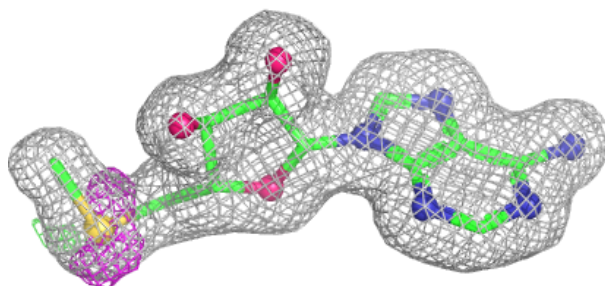


Electron density around 1PG B 404:

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

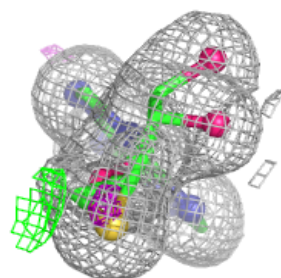
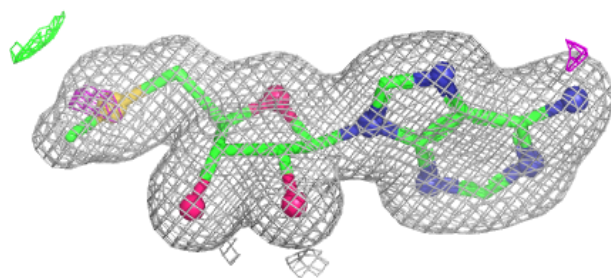
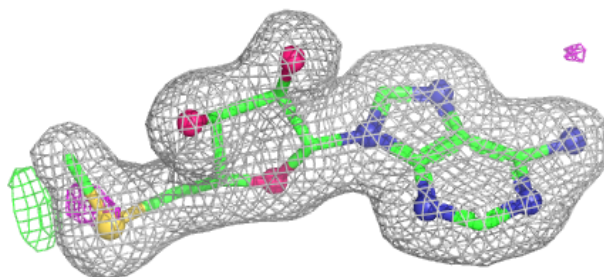
**Electron density around MTA B 402:**

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

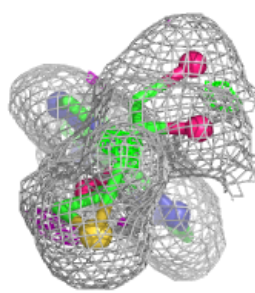
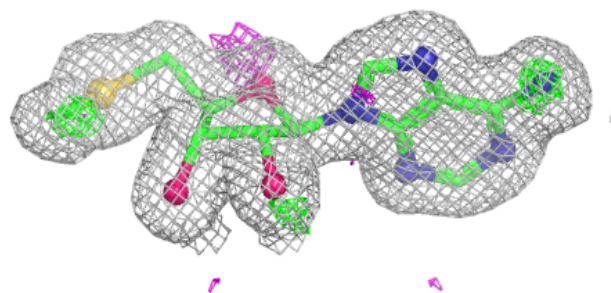
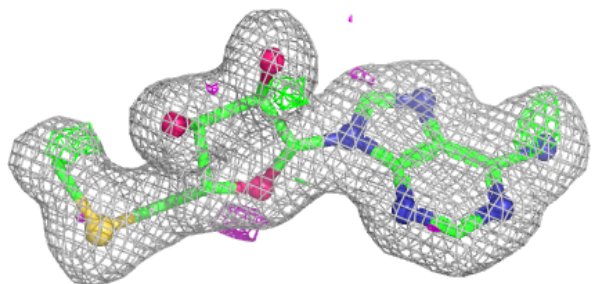


Electron density around MTA A 402:

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

**Electron density around MTA C 402:**

$2mF_o-DF_c$ (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.