



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:39 pm BST

PDB ID : 2PT6  
Title : The structure of Plasmodium falciparum spermidine synthase in complex with decarboxylated S-adenosylmethionine  
Authors : Dufe, V.T.; Qiu, W.; Muller, I.B.; Hui, R.; Walter, R.D.; Al-Karadaghi, S.; Structural Genomics Consortium (SGC)  
Deposited on : 2007-05-08  
Resolution : 2.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

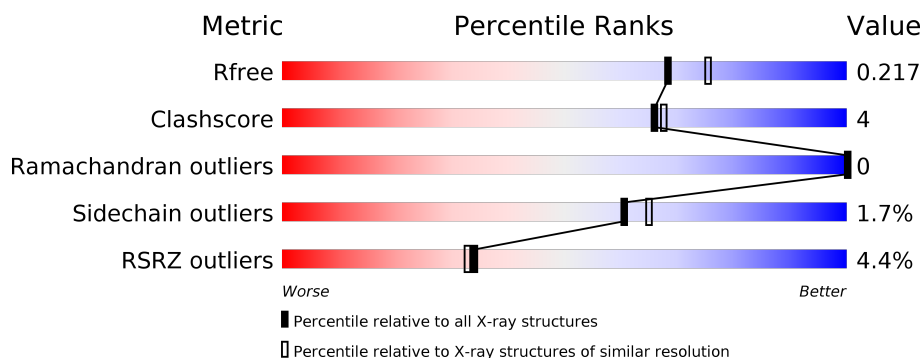
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	321	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>12%</div> </div> </div>
1	B	321	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>13%</div> </div> </div>
1	C	321	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>12%</div> </div> </div>

## 2 Entry composition [i](#)

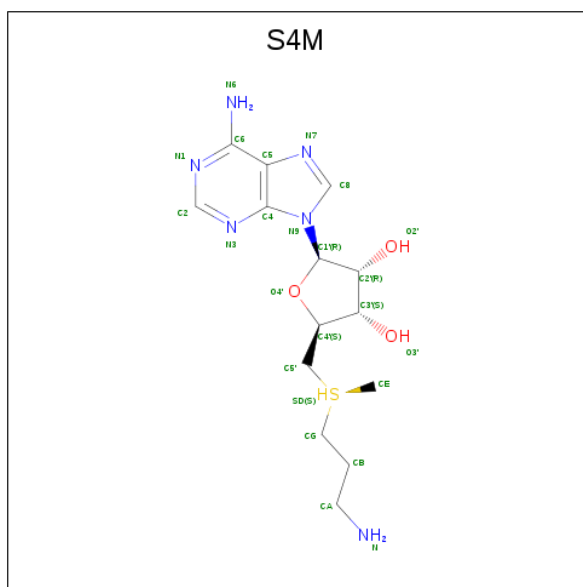
There are 5 unique types of molecules in this entry. The entry contains 7300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

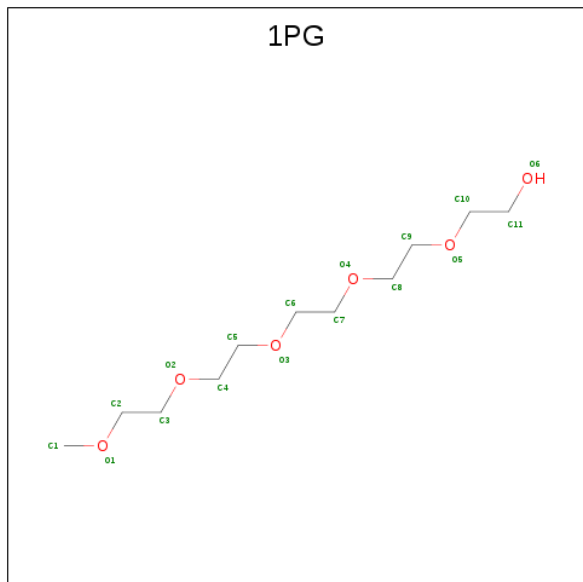
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	3	1	0
			2257	1465	352	426	14			
1	B	280	Total	C	N	O	S	6	4	0
			2259	1466	352	427	14			
1	C	281	Total	C	N	O	S	0	1	0
			2257	1465	352	426	14			

- Molecule 2 is 5'-[(S)-(3-AMINOPROPYL)(METHYL)-LAMBDA 4 -SULFANYL]-5'-DEOXYADENOSINE (three-letter code: S4M) (formula: C<sub>14</sub>H<sub>24</sub>N<sub>6</sub>O<sub>3</sub>S).



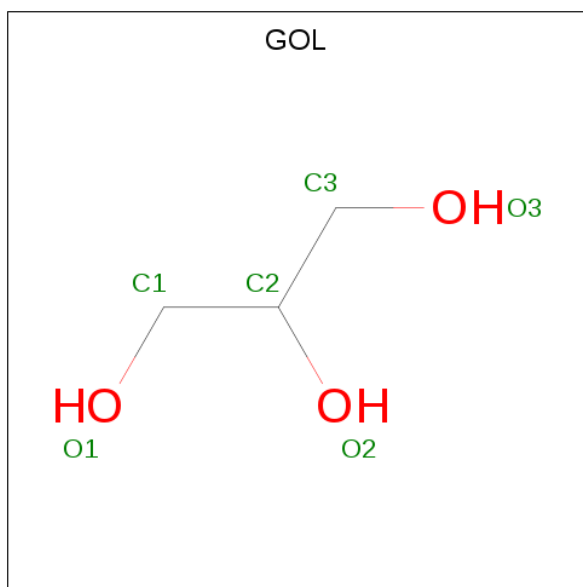
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	B	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	C	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

- Molecule 3 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula:  $C_{11}H_{24}O_6$ ).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

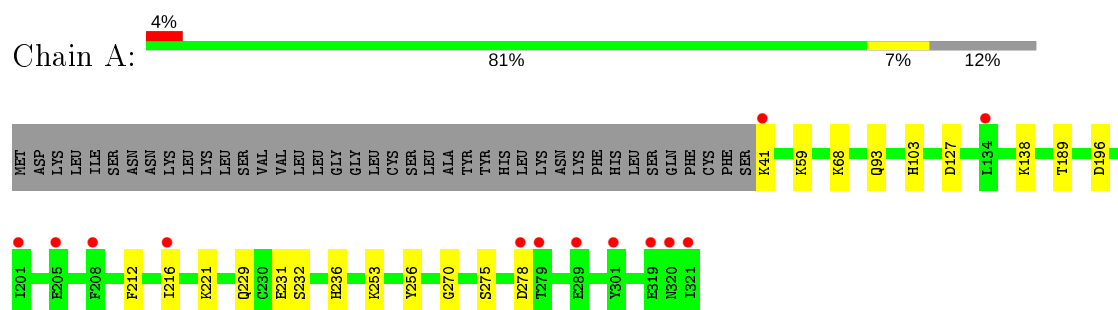
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	122	Total	O	0	0
			122	122		
5	C	173	Total	O	0	0
			173	173		

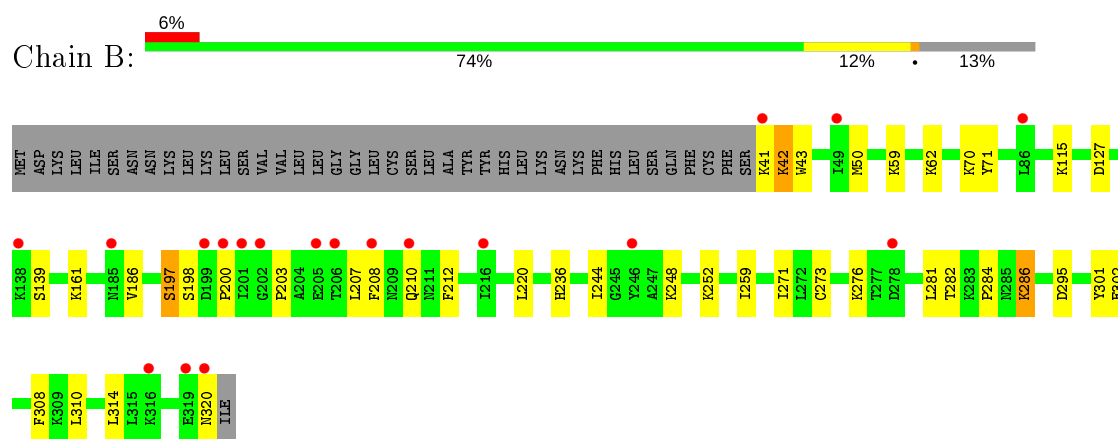
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

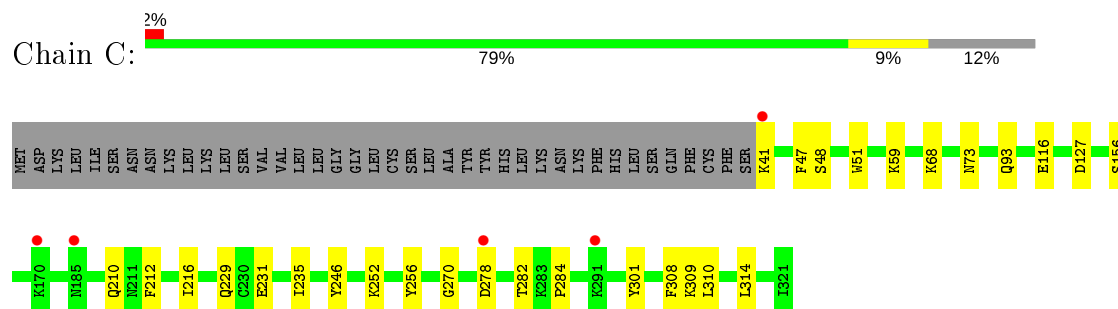
#### • Molecule 1: Spermidine synthase



#### • Molecule 1: Spermidine synthase



#### • Molecule 1: Spermidine synthase



## 4 Data and refinement statistics

Property	Value
Space group	C 1 2 1
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.30 Å   134.18 Å   48.32 Å 90.00°   94.38°   90.00°
Resolution (Å)	19.99 – 2.00 19.99 – 2.00
% Data completeness (in resolution range)	100.0 (19.99-2.00) 99.6 (19.99-2.00)
$R_{merge}$	0.72
$R_{sym}$	0.12
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.01 Å)
Refinement program	REFMAC 5.2.0019, REFMAC 5.2.0019, REFMAC 5.2.0019, REFMAC
R, $R_{free}$	0.180   ,   0.214 0.188   ,   0.217
$R_{free}$ test set	4178 reflections (5.00%)
Wilson B-factor (Å <sup>2</sup> )	28.3
Anisotropy	0.061
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 58.3
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$
Estimated twinning fraction	No twinning to report.
$F_o, F_c$ correlation	0.95
Total number of atoms	7300
Average B, all atoms (Å <sup>2</sup> )	30.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, 1PG, 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	0.55	0/2310	0.58	0/3119
1	B	0.69	3/2321 (0.1%)	0.73	8/3135 (0.3%)
1	C	0.62	0/2310	0.64	0/3119
All	All	0.63	3/6941 (0.0%)	0.65	8/9373 (0.1%)

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	1	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	LYS	CG-CD	12.02	1.93	1.52
1	B	197[A]	SER	CA-C	-6.71	1.35	1.52
1	B	197[B]	SER	CA-C	-6.71	1.35	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	LYS	CB-CG-CD	-9.45	87.03	111.60
1	B	295	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	197[A]	SER	CB-CA-C	-5.83	99.03	110.10
1	B	197[B]	SER	CB-CA-C	-5.83	99.03	110.10
1	B	197[A]	SER	CA-C-N	5.22	128.68	117.20
1	B	197[B]	SER	CA-C-N	5.22	128.68	117.20
1	B	197[A]	SER	CA-C-O	-5.15	109.28	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197[B]	SER	CA-C-O	-5.15	109.28	120.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	197[B]	SER	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	197[B]	SER	Mainchain

## 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	2257	0	2270	18	0
1	B	2259	0	2275	20	0
1	C	2257	0	2270	18	0
2	A	24	0	24	5	0
2	B	24	0	24	1	0
2	C	24	0	24	1	0
3	A	17	0	24	0	0
3	C	17	0	24	1	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
4	C	6	0	8	0	0
5	A	108	0	0	1	0
5	B	122	0	0	3	0
5	C	173	0	0	1	0
All	All	7300	0	6959	55	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 (55) 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:A:231:GLU:HB3	1:A:236:HIS:CD2	1.83	1.13
1:B:42:LYS:HE3	1:B:43:TRP:H	1.37	0.88
1:B:286:LYS:HE3	5:B:689:HOH:O	1.83	0.78
1:B:286:LYS:CE	5:B:689:HOH:O	2.32	0.75
1:A:232:SER:H	1:A:236:HIS:HD2	1.35	0.72
1:A:127:ASP:OD2	2:A:501:S4M:HA1	1.93	0.69
1:B:41:LYS:HD2	1:B:59:LYS:HE2	1.76	0.68
1:A:68:LYS:O	1:B:161:LYS:NZ	2.29	0.64
1:C:93:GLN:HB3	2:C:503:S4M:HG2	1.84	0.59
1:C:41:LYS:HB2	1:C:59:LYS:HE2	1.84	0.58
1:A:232:SER:N	1:A:236:HIS:HD2	2.01	0.58
1:B:259:ILE:HD11	1:B:271:ILE:HD11	1.84	0.58
1:A:41:LYS:HB2	1:A:59:LYS:HE2	1.86	0.57
1:C:229:GLN:HE21	1:C:231:GLU:H	1.51	0.56
1:A:231:GLU:HB3	1:A:236:HIS:CG	2.38	0.54
1:A:231:GLU:HB3	1:A:236:HIS:HD2	1.61	0.53
1:A:103:HIS:NE2	2:A:501:S4M:N	2.57	0.53
1:C:310:LEU:HD13	1:C:314:LEU:HD23	1.91	0.53
1:B:310:LEU:HD13	1:B:314:LEU:HD23	1.92	0.52
1:A:232:SER:H	1:A:236:HIS:CD2	2.23	0.52
1:A:138:LYS:NZ	5:A:766:HOH:O	2.23	0.51
1:A:93:GLN:HE21	2:A:501:S4M:HG1	1.77	0.49
1:B:273:CYS:HB3	1:B:281:LEU:HD12	1.93	0.49
1:C:47:PHE:CZ	3:C:702:1PG:H41	2.48	0.49
1:A:212:PHE:CE2	1:A:216:ILE:HD11	2.47	0.49
1:C:212:PHE:CE2	1:C:216:ILE:HD11	2.48	0.49
1:B:50:MET:O	1:B:236:HIS:CE1	2.65	0.48
1:B:50:MET:O	1:B:236:HIS:HE1	1.96	0.48
1:C:309:LYS:HE3	5:C:804:HOH:O	2.13	0.48
1:B:284:PRO:HG2	1:B:301:TYR:CE1	2.49	0.48
1:C:229:GLN:NE2	1:C:231:GLU:H	2.12	0.47
1:B:282:THR:HG22	1:B:308:PHE:CD1	2.50	0.47
1:C:252:LYS:HD2	1:C:278:ASP:OD1	2.14	0.46
1:B:302:GLU:HB3	1:C:309:LYS:HD2	1.97	0.46
1:B:200:PRO:HB3	1:B:208:PHE:CD1	2.51	0.46
1:C:68:LYS:HG3	1:C:73:ASN:ND2	2.31	0.45
1:B:207:LEU:HD22	1:B:212:PHE:CE1	2.51	0.45
1:A:256:TYR:CZ	1:A:270:GLY:HA3	2.51	0.45
1:B:244:ILE:HG22	1:B:248:LYS:HD2	1.98	0.45
1:C:256:TYR:CZ	1:C:270:GLY:HA3	2.52	0.45
1:A:196:ASP:OD2	2:A:501:S4M:N	2.50	0.45
1:A:189:THR:OG1	1:A:221:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLN:HE22	1:C:246:TYR:HA	1.82	0.44
1:A:253:LYS:HB3	1:A:275:SER:HB2	1.99	0.43
1:B:220:LEU:HB2	1:B:276:LYS:HE3	1.99	0.43
1:B:71:TYR:HB3	1:B:203:PRO:HG3	2.00	0.43
1:B:127:ASP:OD2	2:B:502:S4M:N	2.50	0.43
1:C:282:THR:HG22	1:C:308:PHE:CG	2.54	0.42
1:C:48:SER:HB3	1:C:51:TRP:CE2	2.54	0.42
1:C:127:ASP:HA	1:C:156[A]:SER:OG	2.21	0.41
1:B:282:THR:HG22	1:B:308:PHE:CG	2.56	0.40
1:A:127:ASP:OD2	2:A:501:S4M:CA	2.67	0.40
4:B:601:GOL:H31	5:B:677:HOH:O	2.22	0.40
1:C:284:PRO:HG2	1:C:301:TYR:CE1	2.56	0.40
1:C:51:TRP:HB3	1:C:235:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/321 (87%)	272 (97%)	8 (3%)	0	100	100
1	B	282/321 (88%)	272 (96%)	10 (4%)	0	100	100
1	C	280/321 (87%)	273 (98%)	7 (2%)	0	100	100
All	All	842/963 (87%)	817 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	254/290 (88%)	252 (99%)	2 (1%)	81	86
1	B	256/290 (88%)	246 (96%)	10 (4%)	32	30
1	C	254/290 (88%)	253 (100%)	1 (0%)	91	93
All	All	764/870 (88%)	751 (98%)	13 (2%)	60	65

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	278	ASP
1	B	42	LYS
1	B	62	LYS
1	B	115	LYS
1	B	139	SER
1	B	186	VAL
1	B	198	SER
1	B	210	GLN
1	B	252	LYS
1	B	286	LYS
1	B	320	ASN
1	C	116	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	142	ASN
1	A	173	ASN
1	A	210	GLN
1	A	218	ASN
1	A	229	GLN
1	A	236	HIS
1	A	303	ASN
1	B	93	GLN
1	B	142	ASN
1	B	209	ASN
1	B	211	ASN
1	B	236	HIS

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Mol	Chain	Res	Type
1	B	285	ASN
1	B	320	ASN
1	C	73	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 carbohydrates 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	$\# Z  > 2$
4	GOL	B	601	-	5,5,5	0.37	0	5,5,5	0.41	0
4	GOL	C	602	-	5,5,5	0.51	0	5,5,5	0.33	0
2	S4M	C	503	-	22,26,26	1.35	3 (13%)	21,37,37	2.36	4 (19%)
3	1PG	C	702	-	16,16,16	0.43	0	15,15,15	0.25	0
2	S4M	B	502	-	22,26,26	0.65	0	21,37,37	1.49	3 (14%)
3	1PG	A	701	-	16,16,16	0.47	0	15,15,15	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	603	-	5,5,5	0.38	0	5,5,5	0.30	0
2	S4M	A	501	-	22,26,26	0.80	1 (4%)	21,37,37	1.75	4 (19%)

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
4	GOL	B	601	-	-	0/4/4/4	-
4	GOL	C	602	-	-	0/4/4/4	-
2	S4M	C	503	-	-	3/7/28/28	0/3/3/3
3	1PG	C	702	-	-	10/14/14/14	-
2	S4M	B	502	-	-	4/7/28/28	0/3/3/3
3	1PG	A	701	-	-	10/14/14/14	-
4	GOL	A	603	-	-	2/4/4/4	-
2	S4M	A	501	-	-	5/7/28/28	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	S4M	O4'-C1'	3.73	1.46	1.41
2	C	503	S4M	C5'-C4'	3.18	1.62	1.53
2	C	503	S4M	O4'-C4'	2.76	1.51	1.45
2	A	501	S4M	O4'-C1'	2.09	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	S4M	O4'-C4'-C5'	5.99	124.03	108.88
2	C	503	S4M	O4'-C1'-C2'	-4.73	100.01	106.93
2	C	503	S4M	N3-C2-N1	-4.58	121.53	128.68
2	A	501	S4M	N3-C2-N1	-4.19	122.12	128.68
2	B	502	S4M	N3-C2-N1	-3.98	122.45	128.68
2	C	503	S4M	C5'-SD-CG	3.88	113.31	103.40
2	A	501	S4M	O4'-C1'-C2'	-3.82	101.34	106.93
2	B	502	S4M	O4'-C1'-C2'	-3.64	101.61	106.93
2	A	501	S4M	CB-CG-SD	3.27	120.58	112.39
2	A	501	S4M	O4'-C4'-C5'	2.73	115.78	108.88
2	B	502	S4M	O4'-C4'-C5'	2.50	115.20	108.88

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	503	S4M	CA-CB-CG-SD
2	B	502	S4M	CA-CB-CG-SD
2	B	502	S4M	O4'-C4'-C5'-SD
2	B	502	S4M	C3'-C4'-C5'-SD
2	A	501	S4M	CA-CB-CG-SD
2	A	501	S4M	O4'-C4'-C5'-SD
2	A	501	S4M	C3'-C4'-C5'-SD
3	A	701	1PG	O2-C4-C5-O3
3	C	702	1PG	O1-C2-C3-O2
3	C	702	1PG	O5-C10-C11-O6
3	C	702	1PG	C3-C2-O1-C1
3	C	702	1PG	C2-C3-O2-C4
3	A	701	1PG	C8-C9-O5-C10
3	A	701	1PG	C4-C5-O3-C6
3	A	701	1PG	C9-C8-O4-C7
4	A	603	GOL	O1-C1-C2-O2
3	C	702	1PG	C5-C4-O2-C3
2	C	503	S4M	O4'-C4'-C5'-SD
2	C	503	S4M	C3'-C4'-C5'-SD
3	A	701	1PG	C2-C3-O2-C4
3	A	701	1PG	C3-C2-O1-C1
3	A	701	1PG	O3-C6-C7-O4
2	A	501	S4M	N-CA-CB-CG
3	C	702	1PG	C4-C5-O3-C6
4	A	603	GOL	O1-C1-C2-C3
3	C	702	1PG	O2-C4-C5-O3
3	C	702	1PG	C8-C9-O5-C10
3	C	702	1PG	O3-C6-C7-O4
3	A	701	1PG	O1-C2-C3-O2
3	A	701	1PG	C6-C7-O4-C8
2	A	501	S4M	CB-CG-SD-CE
2	B	502	S4M	CB-CG-SD-C5'
3	C	702	1PG	O4-C8-C9-O5
3	A	701	1PG	O4-C8-C9-O5

There are no ring outliers.

5 monomers are involved in 9 short contacts:

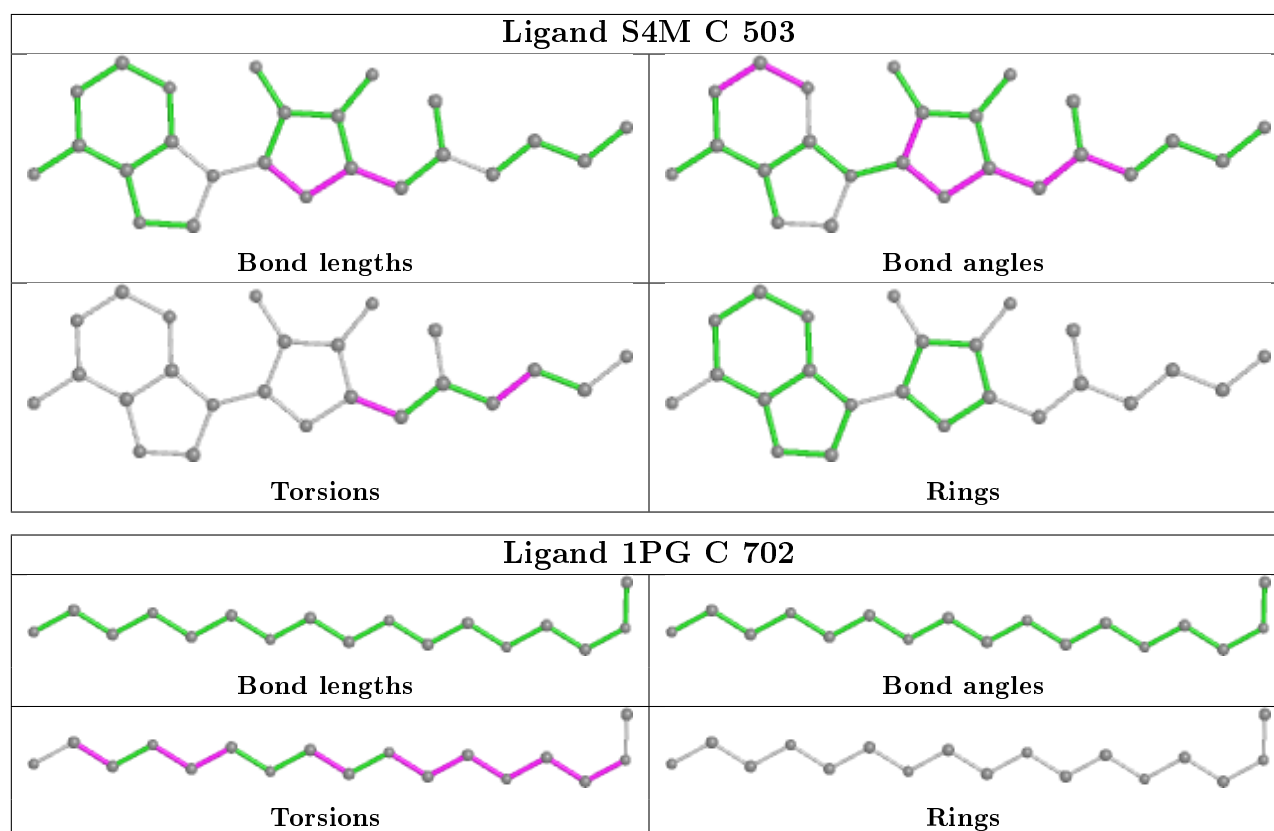
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	GOL	1	0

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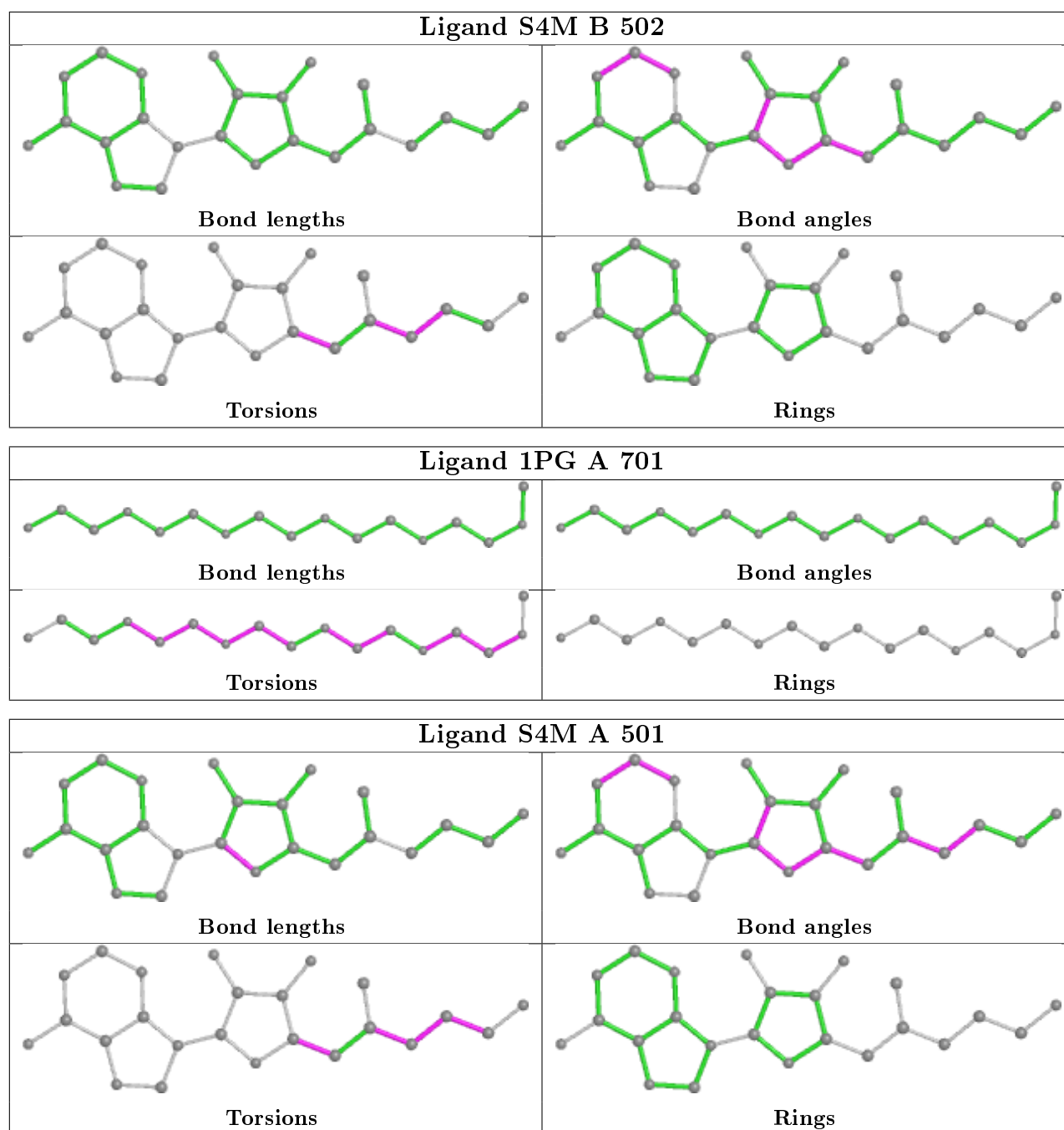
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	503	S4M	1	0
3	C	702	1PG	1	0
2	B	502	S4M	1	0
2	A	501	S4M	5	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	281/321 (87%)	0.08	13 (4%) 32 31	23, 31, 51, 61	17 (6%)
1	B	280/321 (87%)	0.09	19 (6%) 17 16	18, 27, 52, 69	14 (5%)
1	C	281/321 (87%)	-0.30	5 (1%) 68 66	17, 25, 35, 47	5 (1%)
All	All	842/963 (87%)	-0.04	37 (4%) 34 33	17, 28, 45, 69	36 (4%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	PHE	8.5
1	B	201	ILE	6.9
1	B	320	ASN	5.6
1	B	200	PRO	4.9
1	A	216	ILE	4.6
1	B	216	ILE	4.6
1	A	41	LYS	4.5
1	C	41	LYS	4.4
1	B	49	ILE	3.7
1	A	319	GLU	3.7
1	B	246	TYR	3.6
1	A	278	ASP	3.6
1	A	321	ILE	3.5
1	B	205	GLU	3.5
1	C	185	ASN	3.2
1	A	301	TYR	3.2
1	A	201	ILE	3.0
1	A	279	THR	3.0
1	A	208	PHE	3.0
1	B	210	GLN	2.9
1	B	199	ASP	2.9
1	B	138	LYS	2.9
1	B	319	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	291	LYS	2.7
1	B	41	LYS	2.7
1	B	202	GLY	2.7
1	A	320	ASN	2.5
1	A	289	GLU	2.5
1	A	205	GLU	2.5
1	B	278	ASP	2.4
1	B	316	LYS	2.4
1	C	170	LYS	2.3
1	B	86	LEU	2.3
1	B	206	THR	2.2
1	B	185	ASN	2.2
1	C	278	ASP	2.1
1	A	134	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

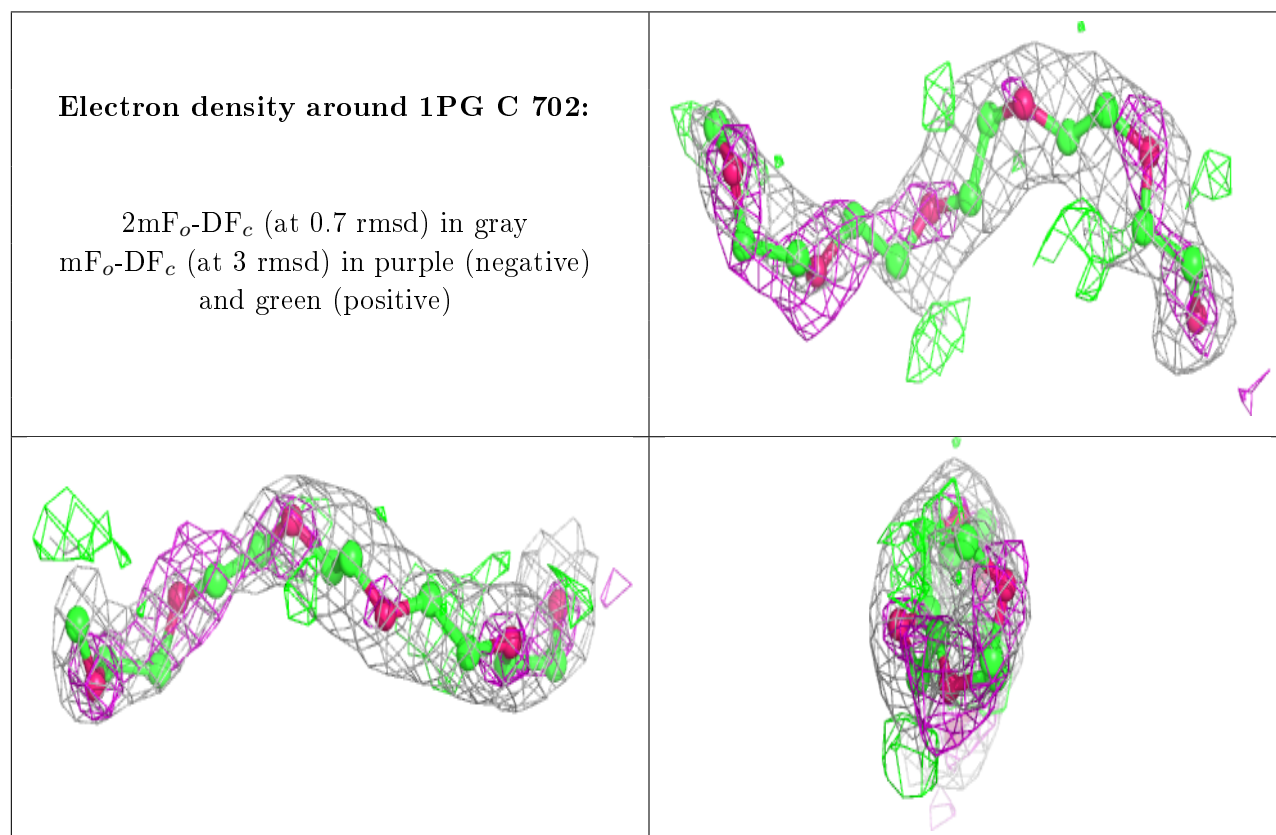
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

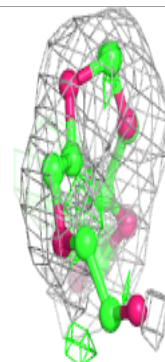
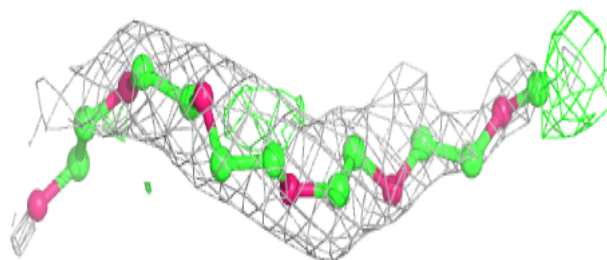
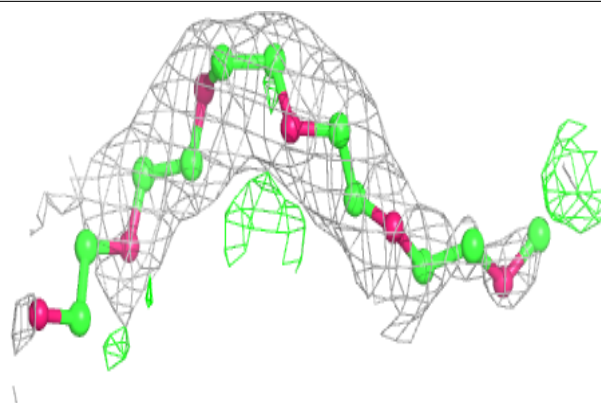
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1PG	C	702	17/17	0.76	0.34	25,28,39,40	0
4	GOL	A	603	6/6	0.77	0.17	57,60,61,61	0
3	1PG	A	701	17/17	0.83	0.19	47,48,54,54	17
4	GOL	B	601	6/6	0.90	0.13	47,51,52,53	0
4	GOL	C	602	6/6	0.94	0.16	46,47,48,49	0
2	S4M	B	502	24/24	0.94	0.11	32,34,46,51	1
2	S4M	A	501	24/24	0.94	0.12	29,33,49,52	1
2	S4M	C	503	24/24	0.95	0.11	21,26,44,47	1

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.

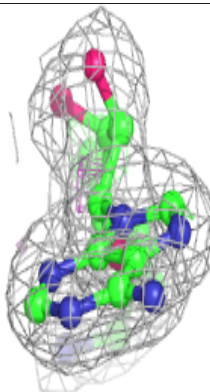
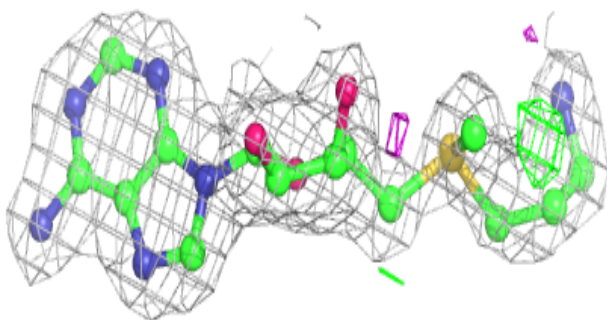
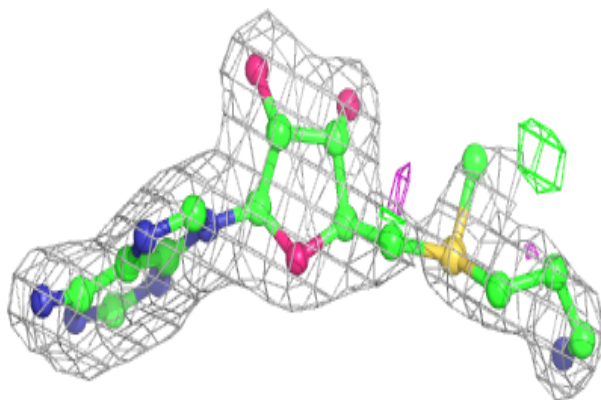


**Electron density around 1PG A 701:**

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

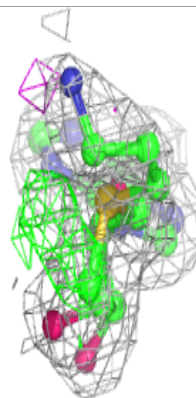
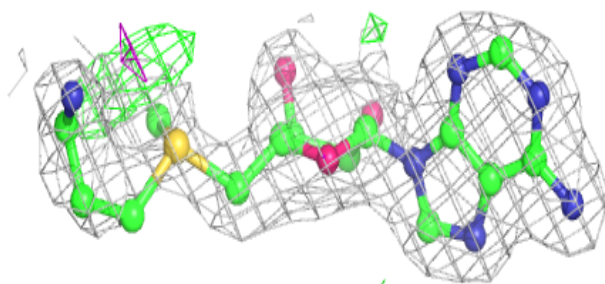
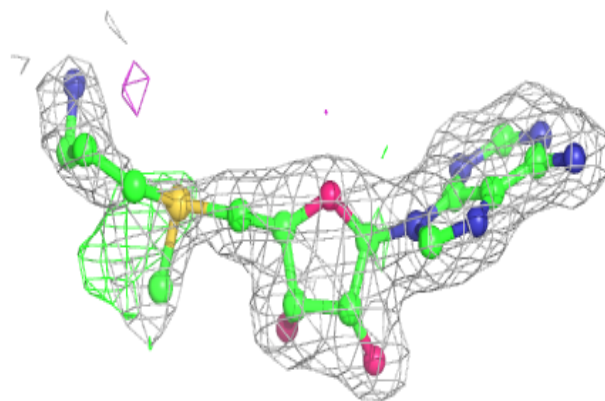
**Electron density around S4M B 502:**

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

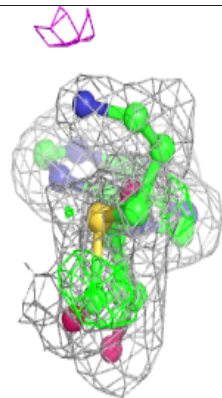
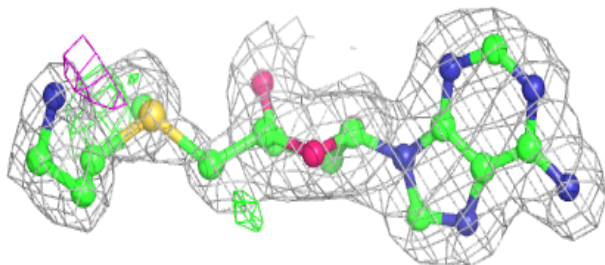
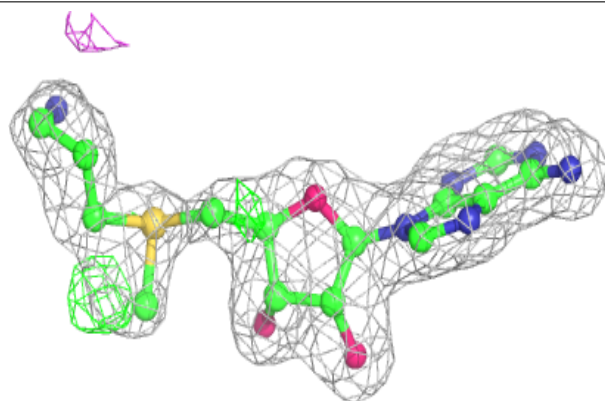


**Electron density around S4M A 501:**

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

**Electron density around S4M C 503:**

$2mF_o-DF_c$  (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.