



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:32 pm BST

PDB ID : 4BP3  
Title : Crystal Structure of Plasmodium Falciparum Spermidine Synthase in Complex with DECARBOXYLATED S-ADENOSYLMETHIONINE5' AND 4-METHYLANILINE  
Authors : Sprenger, J.; Halander, J.C.; Svensson, B.; Al-Karadaghi, S.; Persson, L.  
Deposited on : 2013-05-23  
Resolution : 1.75 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

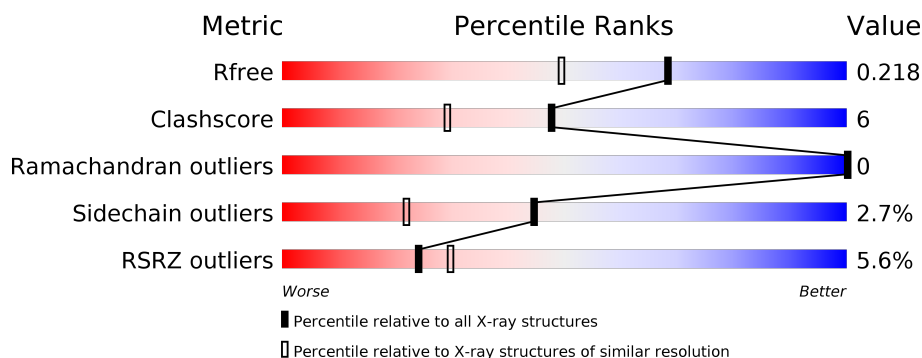
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	283	<div> <div>9%</div> <div>84%</div> <div>14%</div> <div>•</div> </div>
1	B	283	<div> <div>4%</div> <div>83%</div> <div>15%</div> <div>••</div> </div>
1	C	283	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>•</div> </div>

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	1PG	C	602	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7288 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.

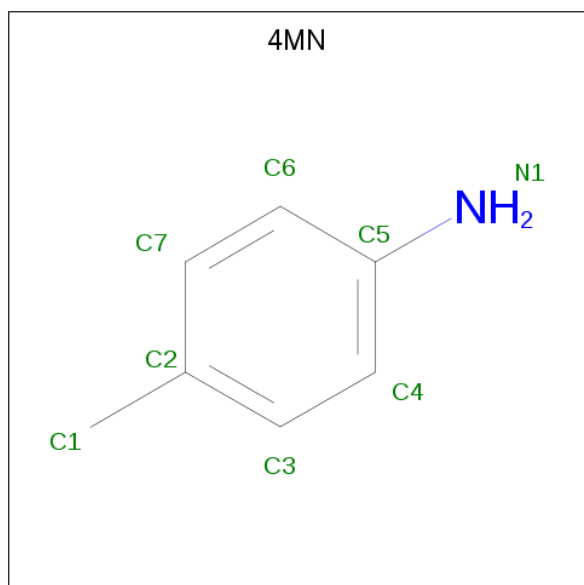
- Molecule 1 is a protein called SPERMIDINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	2	0
			2251	1462	351	423	15			
1	B	280	Total	C	N	O	S	0	3	0
			2253	1464	350	425	14			
1	C	281	Total	C	N	O	S	0	1	0
			2257	1465	352	426	14			

There are 3 discrepancies between the modelled and reference sequences:

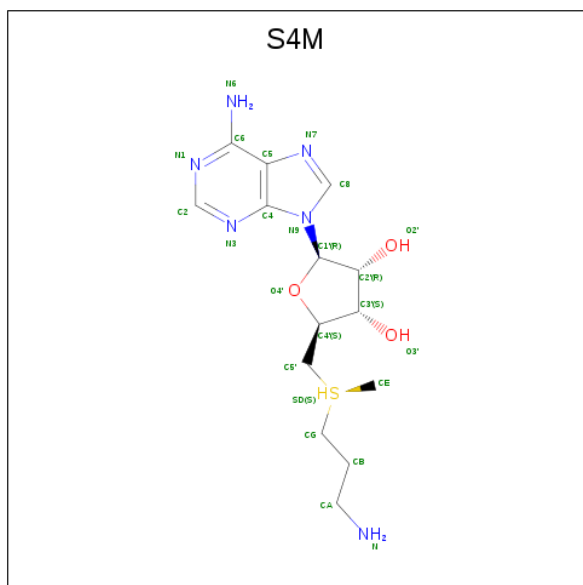
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	expression tag	UNP Q8II73
B	39	GLY	-	expression tag	UNP Q8II73
C	39	GLY	-	expression tag	UNP Q8II73

- Molecule 2 is 4-METHYLANILINE (three-letter code: 4MN) (formula: C<sub>7</sub>H<sub>9</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			8	7	1		
2	B	1	Total	C	N	0	0
			8	7	1		
2	C	1	Total	C	N	0	0
			8	7	1		

- Molecule 3 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).



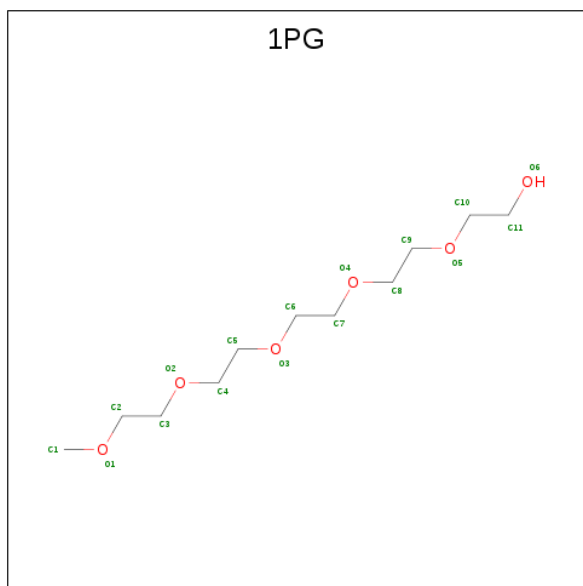
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
3	B	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
3	C	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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 (three-letter code: 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		
5	C	1	Total	C	O	0	0
			17	11	6		

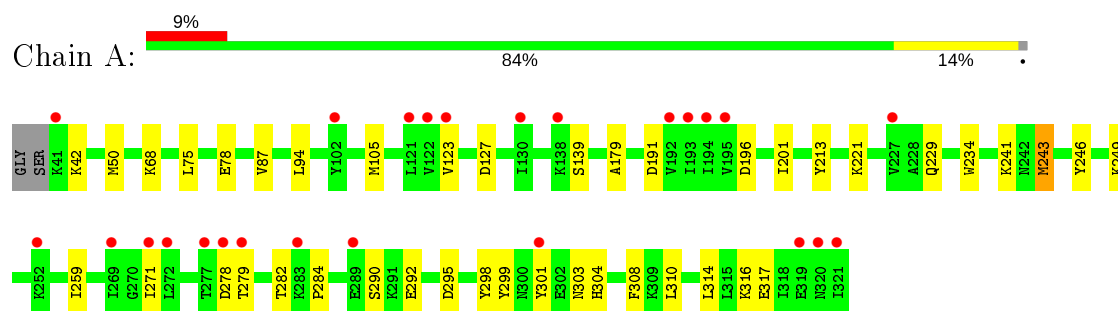
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total 84	O 84	0	0
6	B	147	Total 147	O 147	0	0
6	C	160	Total 160	O 160	0	0

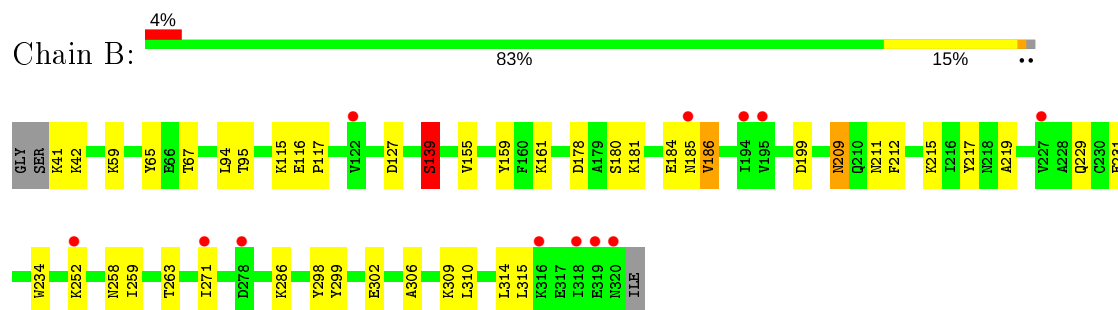
### 3 Residue-property plots [i](#)

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.

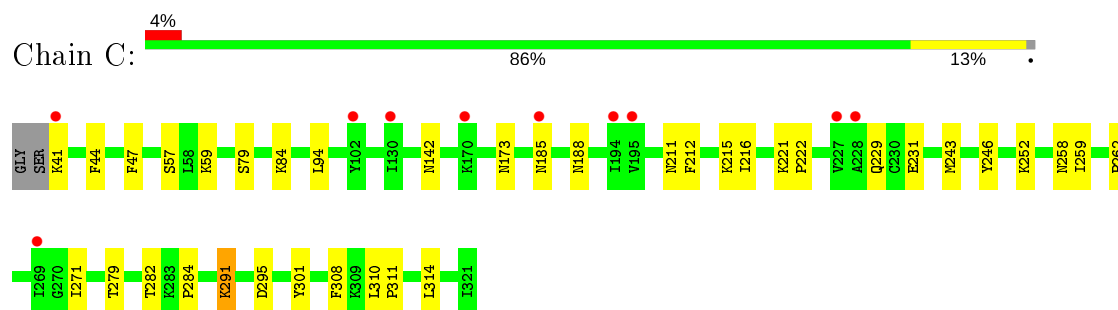
#### • Molecule 1: SPERMIDINE SYNTHASE



#### • Molecule 1: SPERMIDINE SYNTHASE



#### • Molecule 1: SPERMIDINE SYNTHASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.46 Å   132.79 Å   49.16 Å 90.00°   94.86°   90.00°	Depositor
Resolution (Å)	28.66 – 1.75 28.66 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.1 (28.66-1.75) 94.1 (28.66-1.75)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.76 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.180   ,   0.212 0.187   ,   0.218	Depositor DCC
$R_{free}$ test set	5852 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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, 4MN, 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	1.12	1/2306 (0.0%)	1.08	4/3115 (0.1%)
1	B	1.21	7/2312 (0.3%)	1.10	4/3124 (0.1%)
1	C	1.26	2/2310 (0.1%)	1.13	5/3119 (0.2%)
All	All	1.20	10/6928 (0.1%)	1.10	13/9358 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	SER	CB-OG	10.73	1.56	1.42
1	B	139	SER	CA-CB	7.97	1.65	1.52
1	A	234	TRP	CB-CG	-7.61	1.36	1.50
1	B	302	GLU	CG-CD	-6.72	1.41	1.51
1	B	217	TYR	CB-CG	-5.79	1.43	1.51
1	B	159	TYR	CE1-CZ	-5.71	1.31	1.38
1	B	299	TYR	N-CA	-5.63	1.35	1.46
1	C	246	TYR	CB-CG	-5.29	1.43	1.51
1	C	79	SER	CB-OG	-5.14	1.35	1.42
1	B	180	SER	CA-CB	5.11	1.60	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	ASP	CB-CG-OD1	7.40	124.96	118.30
1	A	295	ASP	CB-CG-OD1	7.16	124.74	118.30
1	C	295	ASP	CB-CG-OD1	6.93	124.54	118.30
1	B	302	GLU	OE1-CD-OE2	6.62	131.25	123.30
1	B	309	LYS	CD-CE-NZ	-6.08	97.72	111.70
1	C	279	THR	N-CA-C	5.88	126.87	111.00
1	A	303	ASN	CB-CA-C	5.78	121.97	110.40
1	A	243	MET	CG-SD-CE	-5.71	91.07	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	TYR	CZ-CE2-CD2	5.65	124.88	119.80
1	C	295	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	C	243	MET	CG-SD-CE	-5.50	91.39	100.20
1	A	213	TYR	CA-CB-CG	-5.34	103.25	113.40
1	C	84	LYS	CD-CE-NZ	5.10	123.43	111.70

There are no chirality outliers.

There are no planarity outliers.

## 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	2251	0	2260	24	0
1	B	2253	0	2266	26	0
1	C	2257	0	2270	25	0
2	A	8	0	9	0	0
2	B	8	0	9	0	0
2	C	8	0	9	0	0
3	A	24	0	24	2	0
3	B	24	0	24	1	0
3	C	24	0	24	0	0
4	B	6	0	7	0	0
5	C	34	0	48	23	0
6	A	84	0	0	0	0
6	B	147	0	0	5	0
6	C	160	0	0	5	0
All	All	7288	0	6950	84	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 6.

All (84) 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:258:ASN:HD22	5:C:602:1PG:H12	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:602:1PG:H92	6:C:2140:HOH:O	1.73	0.86
1:B:258:ASN:HD22	5:C:602:1PG:H81	1.41	0.86
5:C:602:1PG:O3	5:C:602:1PG:H101	1.79	0.82
1:C:258:ASN:HD22	5:C:602:1PG:C1	1.95	0.80
1:C:311:PRO:HD3	5:C:602:1PG:H21	1.63	0.80
1:B:258:ASN:HD22	5:C:602:1PG:C8	1.97	0.78
6:B:2137:HOH:O	5:C:602:1PG:H52	1.84	0.76
1:B:306:ALA:O	5:C:602:1PG:H102	1.88	0.73
1:A:241:LYS:HE3	1:A:317:GLU:O	1.94	0.67
1:C:188:ASN:HD21	1:C:222:PRO:HD3	1.60	0.65
5:C:602:1PG:H13	5:C:602:1PG:H62	1.81	0.63
1:B:181:LYS:O	1:B:184:GLU:HG2	2.00	0.61
1:C:188:ASN:ND2	1:C:222:PRO:HD3	2.14	0.60
1:C:258:ASN:ND2	5:C:602:1PG:H12	2.08	0.58
1:A:243:MET:HE1	1:A:246:TYR:HE2	1.68	0.57
1:A:243:MET:HE1	1:A:246:TYR:CE2	2.39	0.57
1:C:212:PHE:CE2	1:C:216:ILE:HD11	2.40	0.57
1:A:105[B]:MET:CE	1:A:299:TYR:HA	2.35	0.57
1:C:229:GLN:HE21	1:C:231:GLU:H	1.52	0.56
1:B:310:LEU:HD13	1:B:314:LEU:HD23	1.87	0.56
1:A:243:MET:CE	1:A:246:TYR:CE2	2.88	0.56
1:A:259:ILE:HD11	1:A:271:ILE:HD11	1.88	0.55
1:A:105[B]:MET:HE1	1:A:299:TYR:HA	1.89	0.54
5:C:602:1PG:C9	6:C:2140:HOH:O	2.44	0.54
1:B:209:ASN:ND2	1:B:212:PHE:H	2.06	0.53
1:A:290:SER:HB2	1:A:292:GLU:OE1	2.09	0.53
1:B:258:ASN:ND2	5:C:602:1PG:H81	2.17	0.53
5:C:602:1PG:H41	5:C:602:1PG:O6	2.08	0.52
1:B:315:LEU:HD21	6:B:2139:HOH:O	2.10	0.52
5:C:602:1PG:C6	5:C:602:1PG:H13	2.39	0.52
1:B:65:TYR:OH	1:B:67:THR:HG21	2.10	0.52
1:B:41:LYS:CD	1:B:59:LYS:HE2	2.40	0.51
1:C:142:ASN:HD21	1:C:173:ASN:HD22	1.58	0.51
1:C:94:LEU:HD12	1:C:94:LEU:C	2.31	0.51
1:B:94:LEU:C	1:B:94:LEU:HD12	2.31	0.51
1:C:291:LYS:HD3	6:C:2137:HOH:O	2.11	0.51
1:A:191:ASP:OD1	1:A:221:LYS:HD2	2.11	0.50
1:C:284:PRO:HG2	1:C:301:TYR:CE1	2.47	0.50
1:A:105[B]:MET:HE3	1:A:298:TYR:CD1	2.47	0.49
1:B:258:ASN:HB3	5:C:602:1PG:H81	1.94	0.49
1:C:291:LYS:CD	6:C:2137:HOH:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:602:1PG:O2	5:C:602:1PG:H62	2.13	0.49
1:B:116:GLU:N	1:B:117:PRO:CD	2.77	0.48
1:C:211:ASN:HD21	1:C:215:LYS:NZ	2.12	0.48
6:B:2137:HOH:O	5:C:602:1PG:C5	2.53	0.47
5:C:602:1PG:C8	6:C:2140:HOH:O	2.62	0.47
1:C:47:PHE:HZ	5:C:702:1PG:H72	1.78	0.47
1:B:41:LYS:HD2	1:B:59:LYS:HE2	1.97	0.47
1:B:139:SER:HB3	6:B:2058:HOH:O	2.15	0.47
1:A:105[B]:MET:CE	1:A:298:TYR:HD1	2.28	0.46
1:C:229:GLN:NE2	1:C:231:GLU:H	2.13	0.46
1:A:310:LEU:HD13	1:A:314:LEU:HD23	1.96	0.46
1:C:188:ASN:HD22	1:C:221:LYS:HA	1.80	0.46
1:A:282:THR:HG22	1:A:308:PHE:CG	2.51	0.46
1:A:68:LYS:O	1:B:161:LYS:NZ	2.49	0.45
1:A:243:MET:HE2	1:A:246:TYR:CE2	2.52	0.45
1:A:123:VAL:HG13	1:A:179:ALA:CB	2.47	0.44
1:C:310:LEU:HD13	1:C:314:LEU:HD23	2.00	0.44
1:C:258:ASN:HB3	5:C:602:1PG:H31	1.98	0.44
1:B:258:ASN:HD22	5:C:602:1PG:H82	1.79	0.44
1:C:259:ILE:HD11	1:C:271:ILE:HD11	2.00	0.44
1:A:50:MET:HG3	1:A:201:ILE:HD12	1.99	0.44
1:C:284:PRO:HG2	1:C:301:TYR:CD1	2.53	0.43
1:B:186:VAL:HG22	1:B:219:ALA:CB	2.49	0.43
1:B:199:ASP:OD1	1:B:231:GLU:OE2	2.37	0.43
1:B:234:TRP:CE2	1:C:262:PRO:HD3	2.53	0.43
1:A:284:PRO:HG2	1:A:301:TYR:CE2	2.54	0.42
1:A:127:ASP:OD2	3:A:501:S4M:HE1	2.20	0.42
1:B:211:ASN:HD21	1:B:215:LYS:NZ	2.17	0.42
1:A:196:ASP:OD1	3:A:501:S4M:HG2	2.19	0.42
1:C:282:THR:HG22	1:C:308:PHE:CG	2.56	0.41
1:C:44:PHE:O	1:C:57:SER:HA	2.21	0.41
5:C:602:1PG:C1	5:C:602:1PG:H61	2.51	0.41
1:A:304:HIS:CD2	1:A:304:HIS:C	2.94	0.41
1:B:127:ASP:OD2	3:B:501:S4M:HE1	2.20	0.41
1:C:41:LYS:HB2	1:C:59:LYS:HE2	2.01	0.41
1:A:75:LEU:HB3	1:A:87:VAL:HB	2.02	0.41
1:A:94:LEU:C	1:A:94:LEU:HD12	2.40	0.41
1:B:209:ASN:HD22	1:B:212:PHE:H	1.69	0.41
1:B:286:LYS:NZ	6:B:2126:HOH:O	2.53	0.41
1:A:105[B]:MET:CE	1:A:298:TYR:CD1	3.04	0.40
1:B:95:THR:HG21	1:B:263:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HD11	1:B:271:ILE:HD11	2.03	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	281/283 (99%)	272 (97%)	9 (3%)	0	100	100
1	B	281/283 (99%)	272 (97%)	9 (3%)	0	100	100
1	C	280/283 (99%)	271 (97%)	9 (3%)	0	100	100
All	All	842/849 (99%)	815 (97%)	27 (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	252/254 (99%)	244 (97%)	8 (3%)	39	16
1	B	254/254 (100%)	245 (96%)	9 (4%)	36	13
1	C	254/254 (100%)	251 (99%)	3 (1%)	71	56
All	All	760/762 (100%)	740 (97%)	20 (3%)	44	23

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	78	GLU
1	A	139	SER
1	A	229	GLN
1	A	249	LYS
1	A	278	ASP
1	A	279	THR
1	A	316	LYS
1	B	42	LYS
1	B	115	LYS
1	B	139	SER
1	B	155	VAL
1	B	185	ASN
1	B	186	VAL
1	B	209	ASN
1	B	229	GLN
1	B	252	LYS
1	C	185	ASN
1	C	252	LYS
1	C	291	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	218	ASN
1	A	320	ASN
1	B	54	GLN
1	B	73	ASN
1	B	162	ASN
1	B	173	ASN
1	B	188	ASN
1	B	209	ASN
1	B	210	GLN
1	B	211	ASN
1	B	258	ASN
1	B	285	ASN
1	C	54	GLN
1	C	142	ASN
1	C	188	ASN
1	C	211	ASN

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Mol	Chain	Res	Type
1	C	229	GLN
1	C	258	ASN
1	C	285	ASN
1	C	320	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 ⓘ

9 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	S4M	C	503	-	22,26,26	0.89	0	21,37,37	1.95	4 (19%)
2	4MN	B	401	-	8,8,8	0.86	1 (12%)	10,10,10	1.05	0
2	4MN	A	401	-	8,8,8	1.00	0	10,10,10	0.78	0
2	4MN	C	401	-	8,8,8	0.89	0	10,10,10	1.98	3 (30%)
3	S4M	A	501	-	22,26,26	1.34	2 (9%)	21,37,37	2.27	8 (38%)
5	1PG	C	702	-	16,16,16	0.50	0	15,15,15	0.87	0
5	1PG	C	602	-	16,16,16	1.11	0	15,15,15	1.65	4 (26%)
3	S4M	B	501	-	22,26,26	0.92	0	21,37,37	2.48	9 (42%)
4	GOL	B	601	-	5,5,5	1.31	1 (20%)	5,5,5	0.90	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	S4M	C	503	-	-	4/7/28/28	0/3/3/3
2	4MN	B	401	-	-	-	0/1/1/1
4	GOL	B	601	-	-	3/4/4/4	-
2	4MN	C	401	-	-	-	0/1/1/1
3	S4M	A	501	-	-	5/7/28/28	0/3/3/3
2	4MN	A	401	-	-	-	0/1/1/1
5	1PG	C	702	-	-	10/14/14/14	-
5	1PG	C	602	-	-	7/14/14/14	-
3	S4M	B	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)
3	A	501	S4M	O4'-C1'	3.81	1.46	1.41
4	B	601	GOL	O2-C2	-2.91	1.34	1.43
3	A	501	S4M	C5-C4	-2.61	1.34	1.40
2	B	401	4MN	C6-C5	-2.14	1.35	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	S4M	N3-C2-N1	-6.47	118.56	128.68
3	B	501	S4M	N3-C2-N1	-5.33	120.35	128.68
3	B	501	S4M	O4'-C1'-C2'	-5.14	99.42	106.93
3	C	503	S4M	N3-C2-N1	-4.59	121.51	128.68
3	C	503	S4M	O4'-C1'-C2'	-4.37	100.54	106.93
3	A	501	S4M	O4'-C1'-C2'	-4.31	100.63	106.93
3	B	501	S4M	C3'-C2'-C1'	4.22	107.34	100.98
3	C	503	S4M	CB-CG-SD	3.52	121.22	112.39
2	C	401	4MN	C6-C5-N1	3.32	127.09	120.91
3	B	501	S4M	O2'-C2'-C1'	3.08	122.21	110.85
5	C	602	1PG	O5-C10-C11	3.03	123.37	110.07
3	A	501	S4M	CB-CG-SD	2.99	119.90	112.39
2	C	401	4MN	C4-C5-C6	-2.99	113.51	118.15
3	C	503	S4M	CE-SD-C5'	2.85	122.94	100.54
3	B	501	S4M	O4'-C4'-C5'	2.78	115.91	108.88
5	C	602	1PG	O4-C8-C9	2.52	121.77	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	S4M	C1'-N9-C4	-2.43	122.36	126.64
3	B	501	S4M	C1'-N9-C4	-2.43	122.38	126.64
3	A	501	S4M	CE-SD-C5'	2.41	119.51	100.54
3	A	501	S4M	N6-C6-N1	2.29	123.33	118.57
2	C	401	4MN	C1-C2-C3	2.26	128.01	120.94
3	B	501	S4M	CE-SD-C5'	2.24	118.18	100.54
3	B	501	S4M	C2-N1-C6	2.19	122.49	118.75
5	C	602	1PG	O3-C6-C7	2.18	120.25	110.39
3	A	501	S4M	O4'-C4'-C5'	2.10	114.19	108.88
3	A	501	S4M	C2-N1-C6	2.06	122.27	118.75
5	C	602	1PG	O3-C5-C4	2.05	119.64	110.39
3	B	501	S4M	N6-C6-N1	2.03	122.80	118.57

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	S4M	CA-CB-CG-SD
3	A	501	S4M	CA-CB-CG-SD
3	A	501	S4M	CB-CG-SD-CE
3	A	501	S4M	O4'-C4'-C5'-SD
3	A	501	S4M	C3'-C4'-C5'-SD
3	B	501	S4M	CA-CB-CG-SD
3	B	501	S4M	O4'-C4'-C5'-SD
4	B	601	GOL	C1-C2-C3-O3
5	C	602	1PG	C11-C10-O5-C9
5	C	602	1PG	C3-C2-O1-C1
5	C	702	1PG	O4-C8-C9-O5
5	C	602	1PG	O5-C10-C11-O6
4	B	601	GOL	O1-C1-C2-C3
4	B	601	GOL	O2-C2-C3-O3
5	C	702	1PG	O5-C10-C11-O6
5	C	702	1PG	O2-C4-C5-O3
5	C	602	1PG	C4-C5-O3-C6
5	C	702	1PG	O1-C2-C3-O2
5	C	702	1PG	C9-C8-O4-C7
5	C	602	1PG	C9-C8-O4-C7
5	C	702	1PG	C5-C4-O2-C3
5	C	602	1PG	C6-C7-O4-C8
3	C	503	S4M	O4'-C4'-C5'-SD
3	A	501	S4M	CB-CG-SD-C5'
5	C	702	1PG	C8-C9-O5-C10

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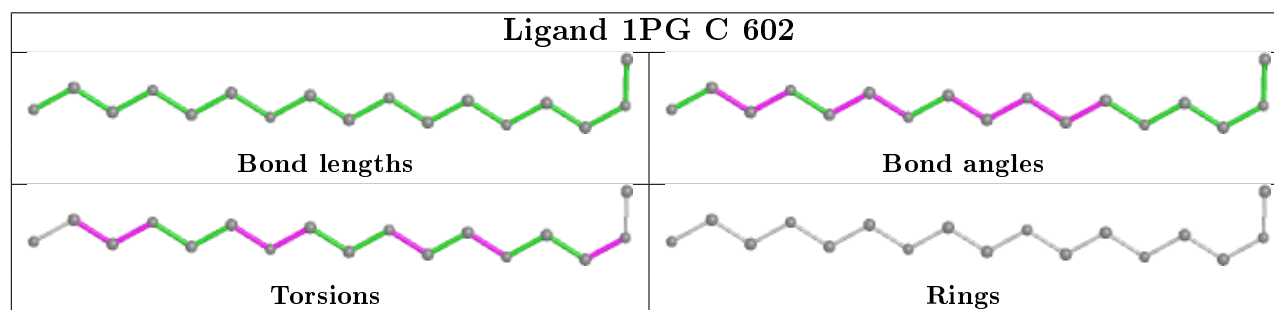
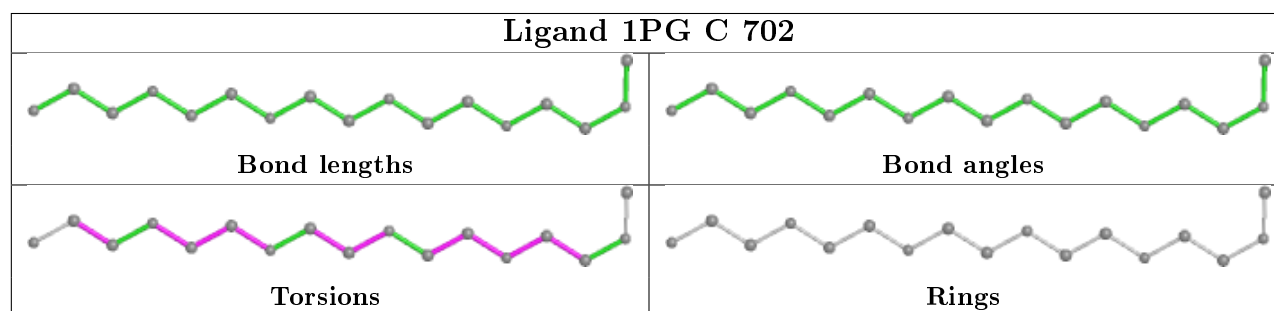
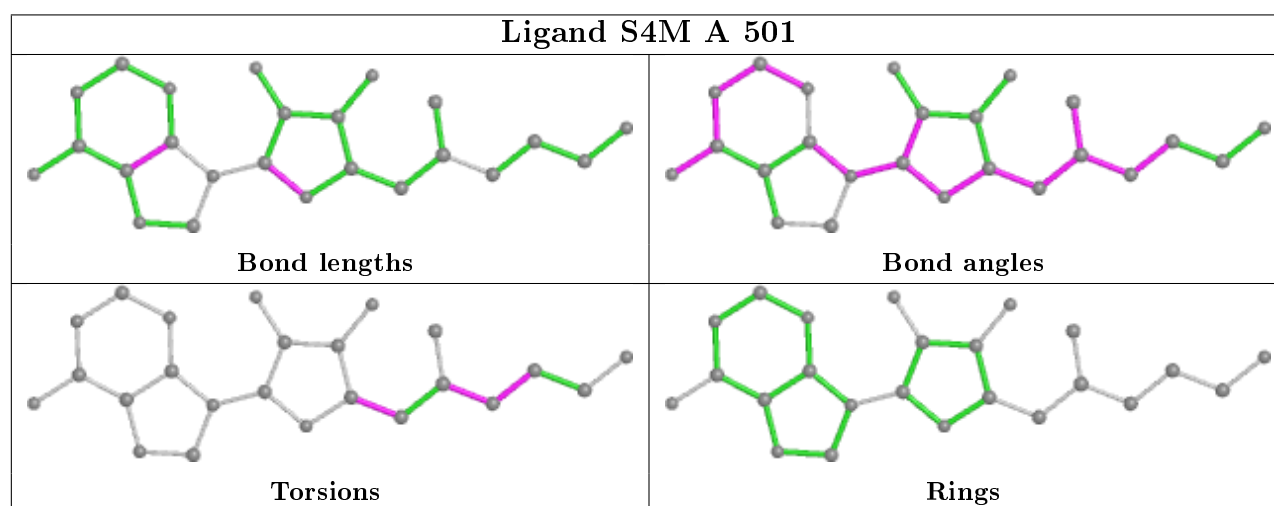
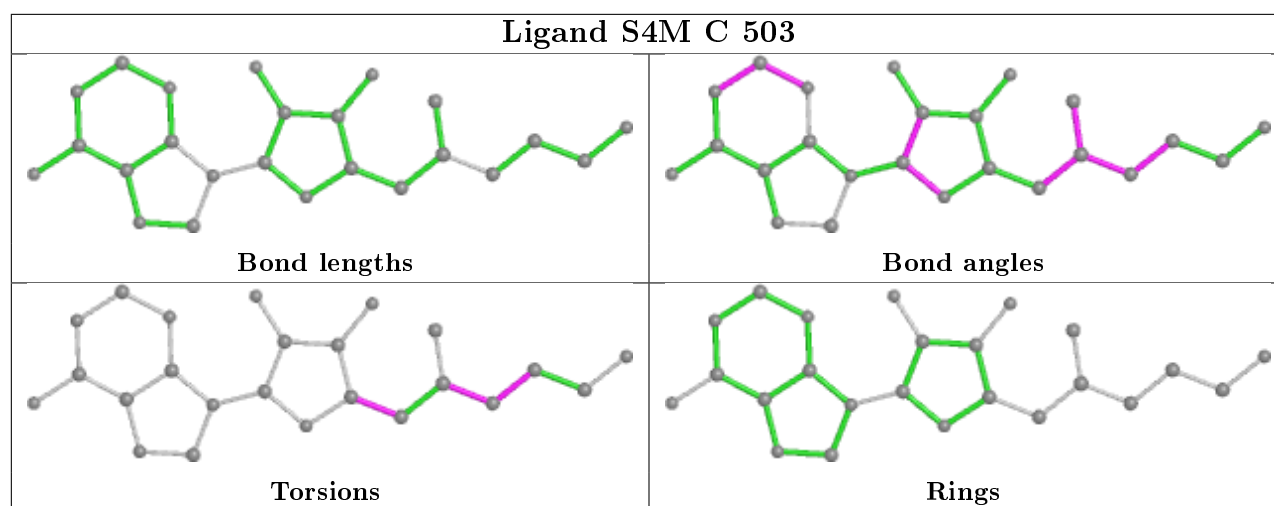
Mol	Chain	Res	Type	Atoms
3	C	503	S4M	C3'-C4'-C5'-SD
3	B	501	S4M	C3'-C4'-C5'-SD
5	C	702	1PG	O3-C6-C7-O4
5	C	702	1PG	C2-C3-O2-C4
5	C	702	1PG	C7-C6-O3-C5
3	C	503	S4M	CB-CG-SD-CE
3	B	501	S4M	CB-CG-SD-CE
5	C	602	1PG	C5-C4-O2-C3
3	B	501	S4M	N-CA-CB-CG

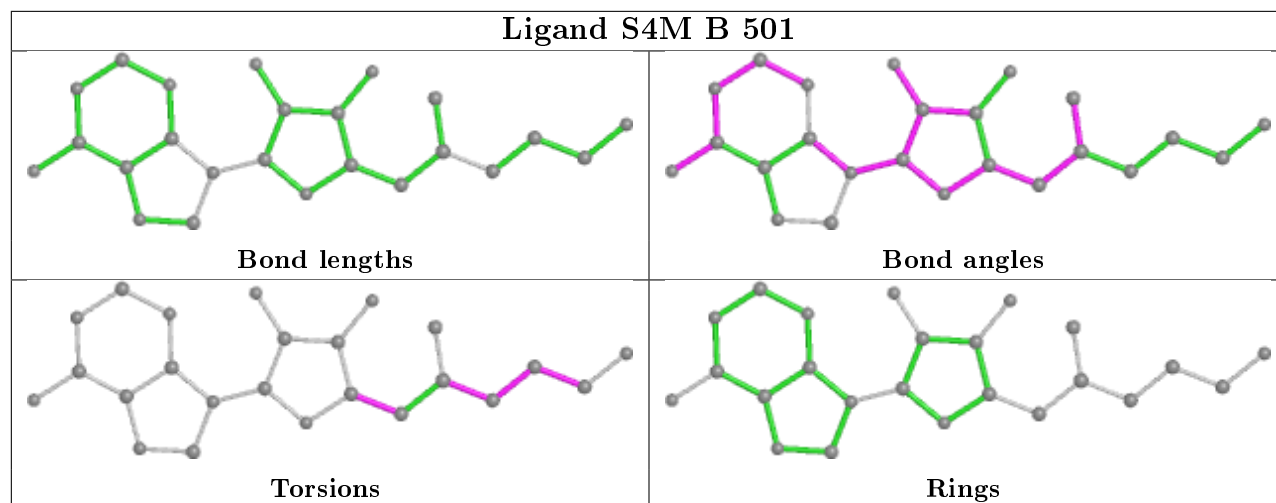
There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	S4M	2	0
5	C	702	1PG	1	0
5	C	602	1PG	22	0
3	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, 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	281/283 (99%)	0.28	25 (8%) 9 12	19, 25, 42, 60	0
1	B	280/283 (98%)	0.02	12 (4%) 35 41	12, 19, 39, 78	0
1	C	281/283 (99%)	-0.10	10 (3%) 42 49	12, 17, 33, 52	0
All	All	842/849 (99%)	0.07	47 (5%) 24 30	12, 21, 40, 78	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	ASN	5.6
1	B	319	GLU	5.0
1	A	194	ILE	4.2
1	B	195	VAL	4.1
1	A	278	ASP	4.1
1	A	195	VAL	4.0
1	A	41	LYS	3.5
1	C	195	VAL	3.5
1	B	194	ILE	3.4
1	C	227	VAL	3.2
1	A	252	LYS	3.1
1	B	227	VAL	3.0
1	C	194	ILE	3.0
1	A	122	VAL	3.0
1	A	227	VAL	3.0
1	A	320	ASN	2.8
1	C	185	ASN	2.8
1	A	289	GLU	2.8
1	B	185	ASN	2.8
1	A	301	TYR	2.7
1	B	318	ILE	2.7
1	A	321	ILE	2.6
1	A	123	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	271	ILE	2.5
1	A	130	ILE	2.5
1	A	102	TYR	2.5
1	C	41	LYS	2.5
1	A	279	THR	2.4
1	B	278	ASP	2.4
1	A	283	LYS	2.3
1	C	102	TYR	2.3
1	A	271	ILE	2.3
1	C	130	ILE	2.3
1	A	121	LEU	2.2
1	C	228	ALA	2.2
1	C	269	ILE	2.2
1	B	122	VAL	2.1
1	A	138	LYS	2.1
1	B	316	LYS	2.1
1	A	269	ILE	2.1
1	C	170	LYS	2.1
1	A	272	LEU	2.1
1	A	277	THR	2.0
1	B	252	LYS	2.0
1	A	192	VAL	2.0
1	A	319	GLU	2.0
1	A	193	ILE	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](#)

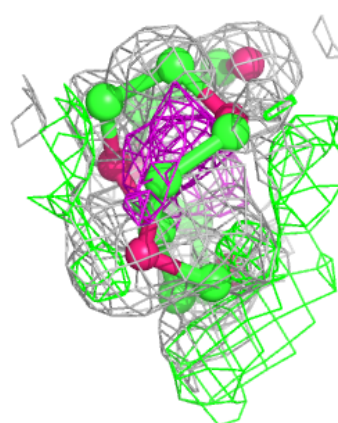
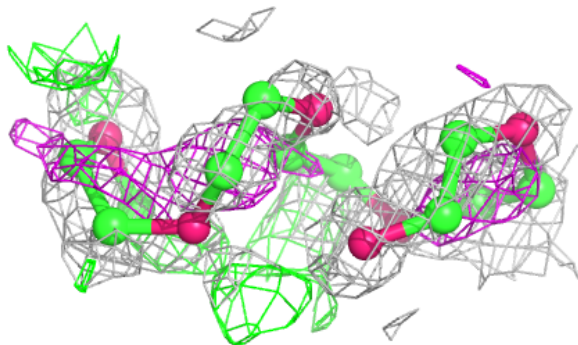
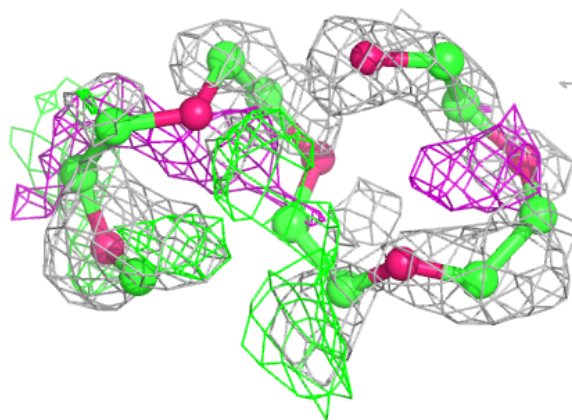
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	1PG	C	602	17/17	0.58	0.36	39,54,78,87	0
5	1PG	C	702	17/17	0.86	0.20	31,43,74,75	0
3	S4M	C	503	24/24	0.92	0.11	13,16,29,35	0
3	S4M	A	501	24/24	0.93	0.11	16,20,39,44	0
3	S4M	B	501	24/24	0.93	0.12	16,18,33,37	0
4	GOL	B	601	6/6	0.94	0.13	22,31,35,40	0
2	4MN	C	401	8/8	0.96	0.16	13,14,16,17	0
2	4MN	B	401	8/8	0.96	0.14	15,18,18,19	0
2	4MN	A	401	8/8	0.96	0.15	24,25,26,30	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 602:**

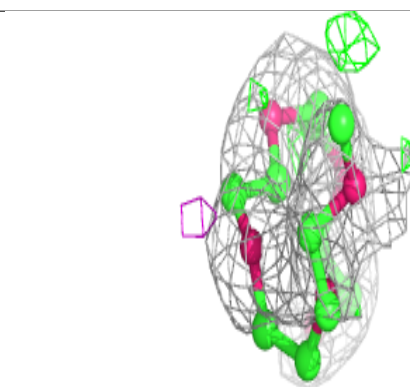
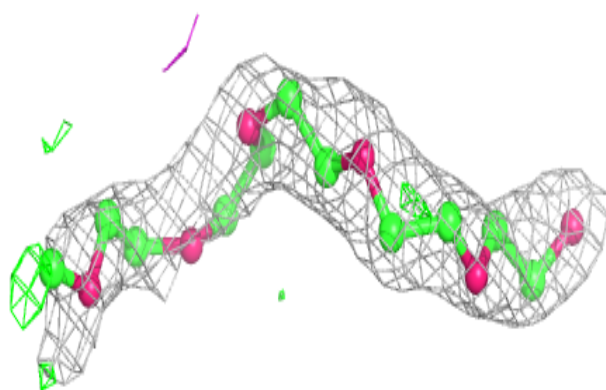
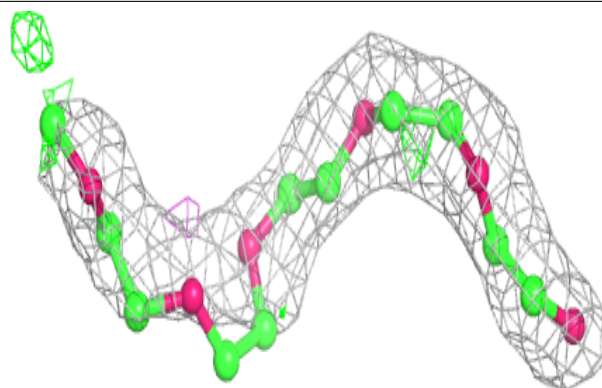
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



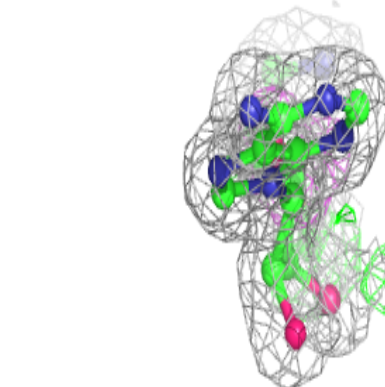
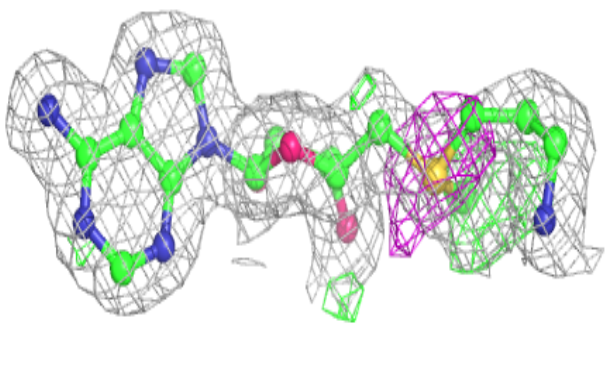
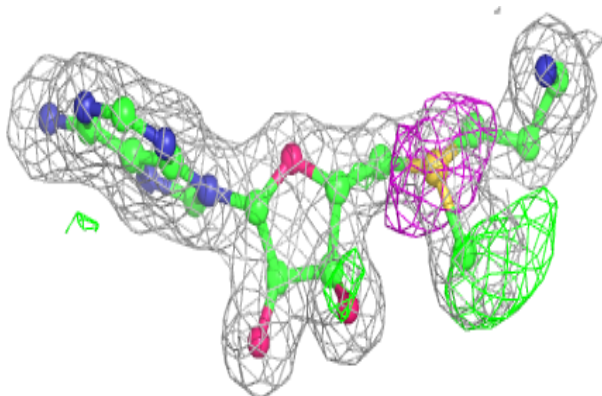


**Electron density around 1PG C 702:**

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

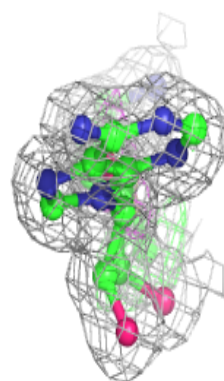
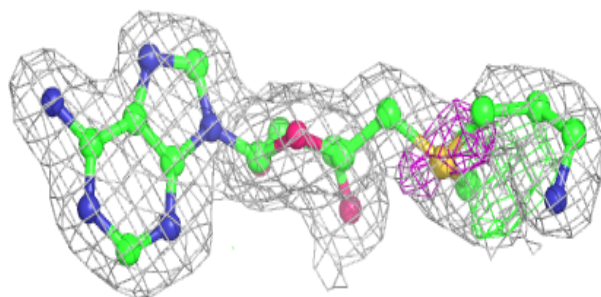
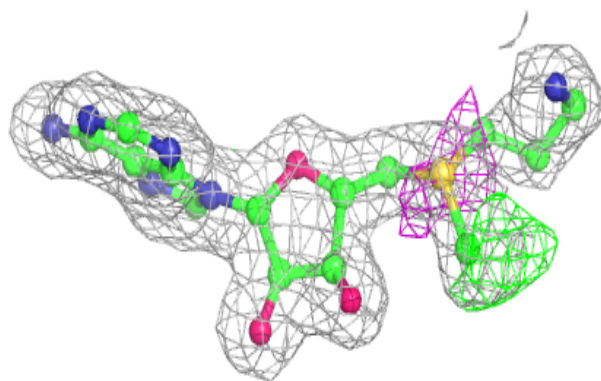
**Electron density around S4M C 503:**

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

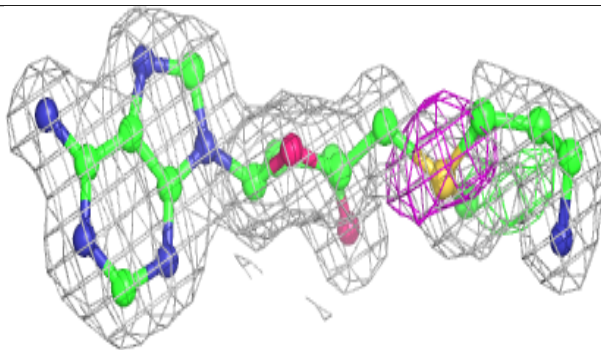
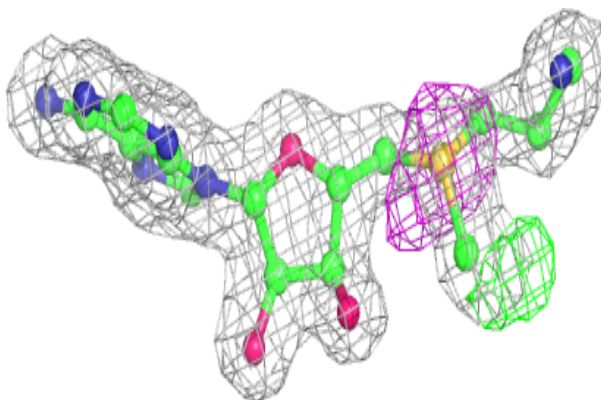


**Electron density around S4M A 501:**

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

**Electron density around S4M 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)



## 6.5 Other polymers

There are no such residues in this entry.