



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 12:24 AM EDT

PDB ID : 2PT9
Title : The structure of Plasmodium falciparum spermidine synthase in complex with decarboxylated S-adenosylmethionine and the inhibitor cis-4-methylcyclohexylamine (4MCHA)
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 : 2.20 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

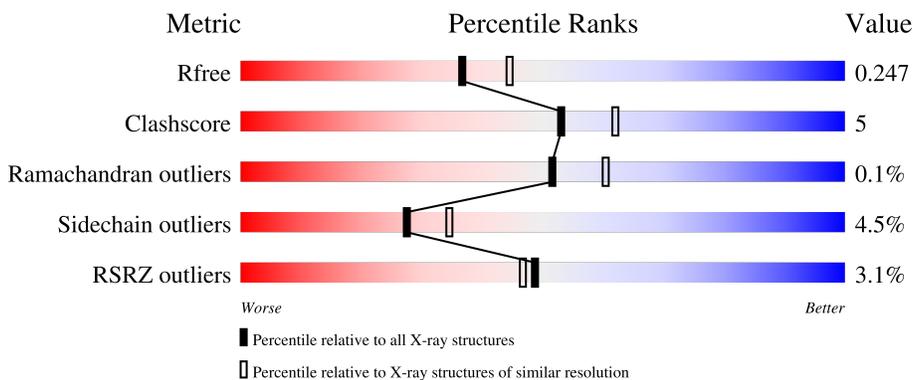
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	321	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">4% 76% 11% • 12%</p>
1	B	321	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">3% 71% 14% • 13%</p>
1	C	321	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">2% 75% 11% • 13%</p>

2 Entry composition [i](#)

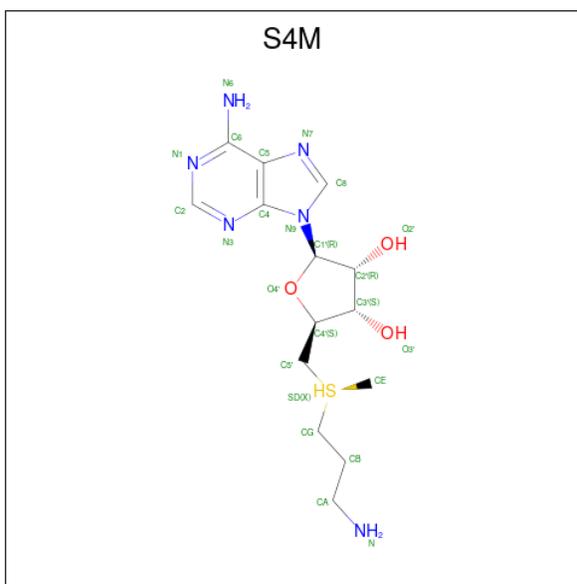
There are 7 unique types of molecules in this entry. The entry contains 7079 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

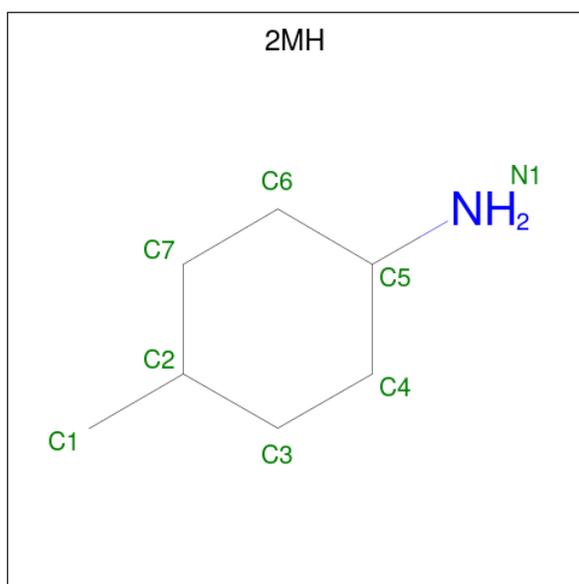
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	281	Total 2254	C 1463	N 352	O 425	S 14	0	0	0
1	B	280	Total 2245	C 1457	N 351	O 423	S 14	3	0	0
1	C	280	Total 2254	C 1463	N 350	O 427	S 14	0	2	0

- Molecule 2 is 5'-[(S)-(3-AMINOPROPYL)(METHYL)-LAMBDA 4 -SULFANYL]-5'-DEOXYADENOSINE (three-letter code: S4M) (formula: C₁₄H₂₄N₆O₃S).



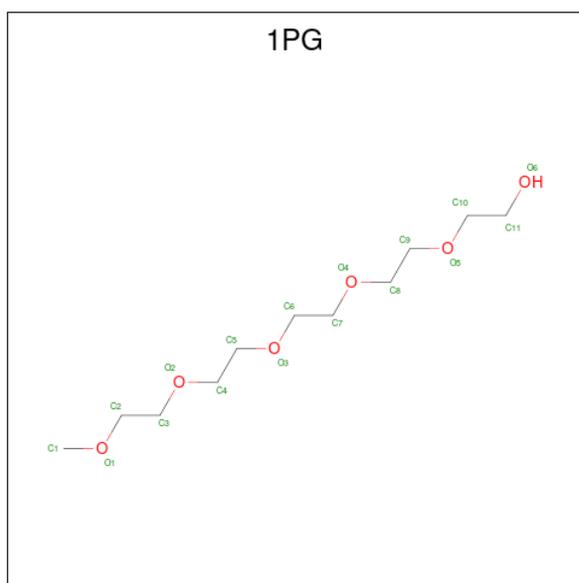
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 24	C 14	N 6	O 3	S 1	0	0
2	B	1	Total 24	C 14	N 6	O 3	S 1	0	0
2	C	1	Total 24	C 14	N 6	O 3	S 1	0	0

- Molecule 3 is cis-4-methylcyclohexanamine (three-letter code: 2MH) (formula: $C_7H_{15}N$).



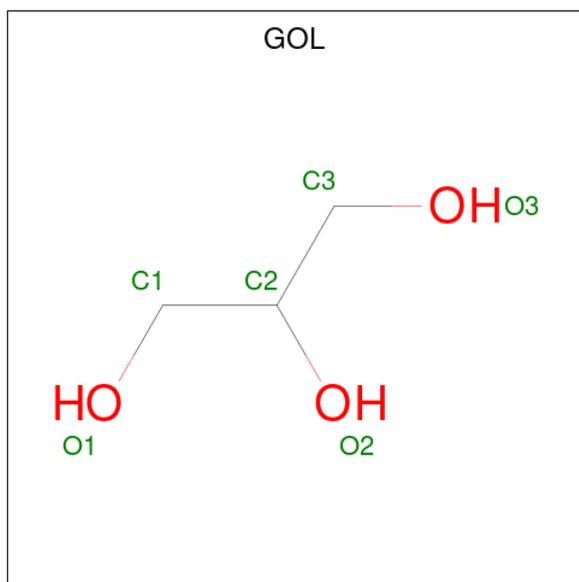
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 8 7 1	0	0
3	B	1	Total C N 8 7 1	0	0
3	C	1	Total C N 8 7 1	0	0

- Molecule 4 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula: $C_{11}H_{24}O_6$).



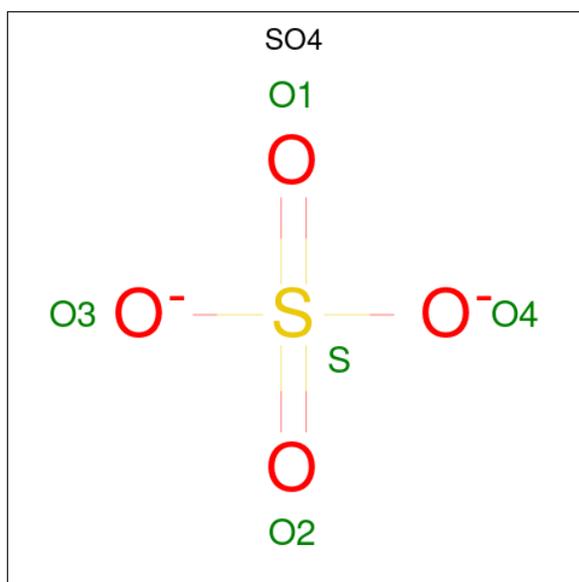
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	11	6		
4	C	1	Total	C	O	0	0
			17	11	6		

- Molecule 5 is GLYCEROL (three-letter code: 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	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

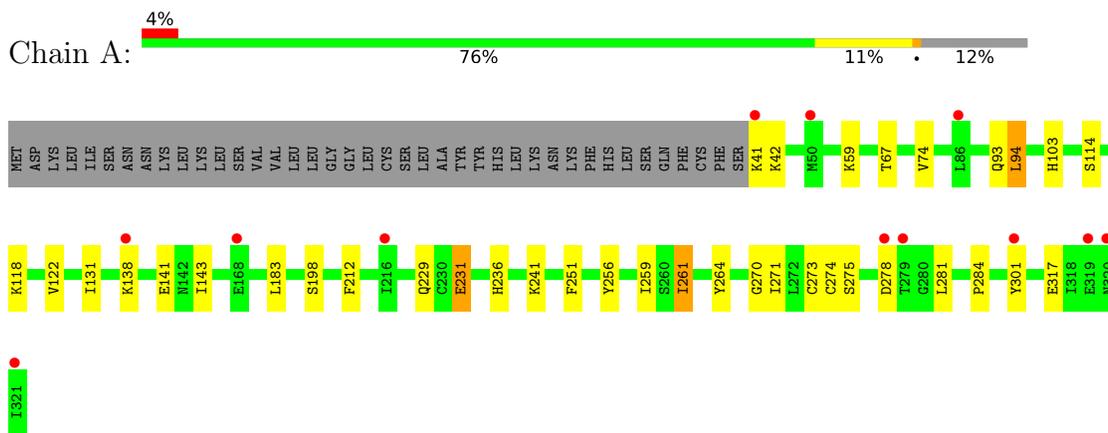
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	41	Total	O	0	0
			41	41		
7	B	59	Total	O	0	0
			59	59		
7	C	73	Total	O	0	0
			73	73		

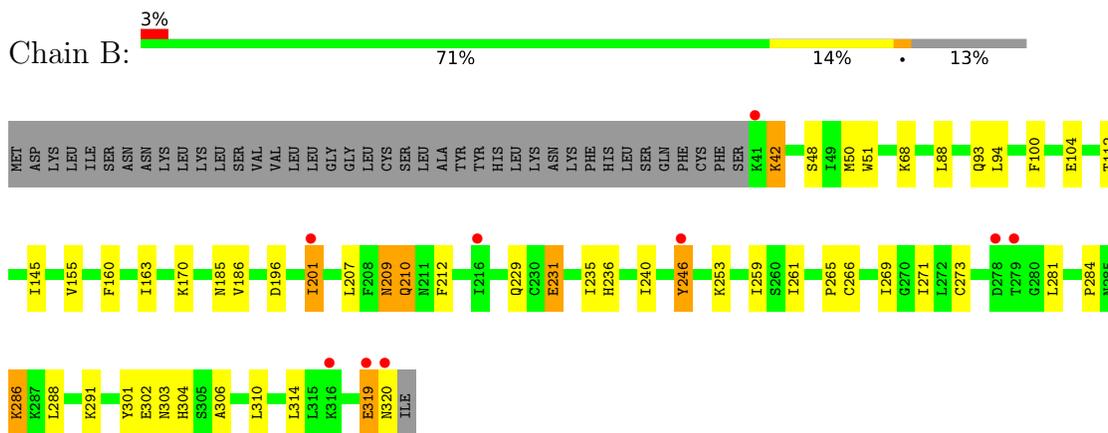
3 Residue-property plots [i](#)

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.

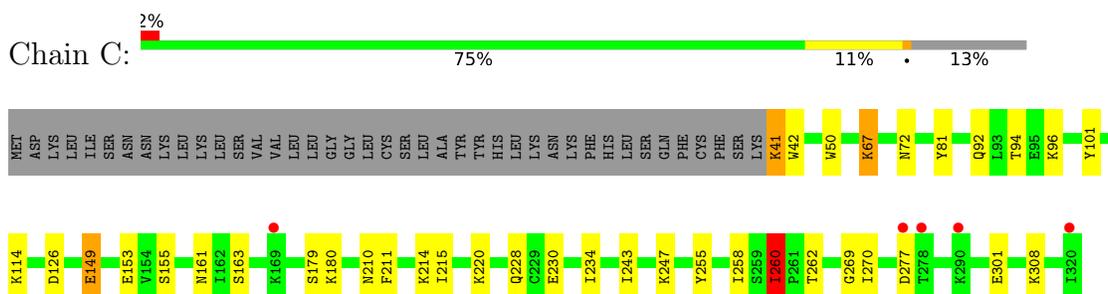
- Molecule 1: Spermidine synthase



- 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	196.24Å 134.10Å 48.35Å 90.00° 94.53° 90.00°	Depositor
Resolution (Å)	19.77 – 2.20 19.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.6 (19.77-2.20) 99.0 (19.76-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.239 0.202 , 0.247	Depositor DCC
R_{free} test set	3119 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtrriage
Anisotropy	0.131	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7079	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: SO4, S4M, 2MH, 1PG, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.57	0/2304	0.64	1/3111 (0.0%)
1	B	0.66	0/2295	0.68	1/3100 (0.0%)
1	C	0.65	0/2310	0.70	1/3120 (0.0%)
All	All	0.63	0/6909	0.67	3/9331 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	ILE	CB-CA-C	-5.19	101.21	111.60
1	B	246	TYR	CA-CB-CG	5.19	123.26	113.40
1	A	94	LEU	CA-CB-CG	5.11	127.05	115.30

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	19	0
1	B	2245	0	2254	31	0
1	C	2254	0	2263	25	0
2	A	24	0	24	2	0
2	B	24	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	24	2	0
3	A	8	0	15	0	0
3	B	8	0	15	0	0
3	C	8	0	15	1	0
4	A	17	0	24	0	0
4	C	17	0	24	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
6	B	5	0	0	0	0
7	A	41	0	0	1	0
7	B	59	0	0	1	0
7	C	73	0	0	2	0
All	All	7079	0	6971	75	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 5.

All (75) 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:ILE:HD11	1:C:270:ILE:HD11	1.17	1.06
1:C:258:ILE:HD11	1:C:270:ILE:CD1	2.00	0.92
1:B:259:ILE:HD11	1:B:271:ILE:HD11	1.56	0.86
1:C:41:LYS:HD3	1:C:42:TRP:H	1.57	0.69
1:C:155[B]:SER:OG	1:C:163:SER:HB3	1.93	0.69
1:A:259:ILE:HD11	1:A:271:ILE:HD11	1.76	0.68
1:C:211:PHE:CE2	1:C:215:ILE:HD11	2.31	0.66
1:C:228:GLN:HE21	1:C:230:GLU:H	1.43	0.66
1:A:41:LYS:HB2	1:A:59:LYS:HE2	1.82	0.61
1:B:209:ASN:ND2	1:B:212:PHE:H	2.00	0.58
1:C:228:GLN:NE2	1:C:230:GLU:H	2.02	0.58
1:C:210:ASN:HD21	1:C:214:LYS:NZ	2.02	0.58
1:B:207:LEU:HD22	1:B:212:PHE:CE1	2.40	0.57
1:B:201:ILE:HG13	1:B:201:ILE:O	2.04	0.56
1:A:122:VAL:HG21	1:A:131:ILE:HD13	1.89	0.55
1:C:126:ASP:HA	1:C:155[A]:SER:OG	2.07	0.55
1:B:209:ASN:HD22	1:B:212:PHE:H	1.55	0.55
1:B:319:GLU:OE2	1:B:319:GLU:HA	2.08	0.54
1:A:122:VAL:HG21	1:A:131:ILE:CD1	2.39	0.53
1:B:273:CYS:HB3	1:B:281:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:TYR:CD2	1:C:96:LYS:HD3	2.45	0.52
1:B:210:GLN:NE2	1:B:246:TYR:HB3	2.24	0.52
1:A:198:SER:HB2	7:A:714:HOH:O	2.10	0.51
2:C:503:S4M:HB1	3:C:403:2MH:H13	1.92	0.51
1:C:255:TYR:OH	1:C:269:GLY:HA3	2.11	0.50
1:C:92:GLN:HB3	2:C:503:S4M:HG2	1.93	0.50
1:A:241:LYS:HE3	1:A:317:GLU:O	2.11	0.50
1:A:131:ILE:HD12	1:A:143:ILE:HG21	1.94	0.50
1:B:93:GLN:HE21	2:B:502:S4M:HG1	1.76	0.49
1:A:118:LYS:HD2	1:A:141:GLU:CD	2.33	0.49
1:B:100:PHE:O	1:B:104:GLU:HG3	2.13	0.49
1:B:160:PHE:HB3	1:B:163:ILE:HD12	1.94	0.49
1:C:243:ILE:HG22	1:C:247:LYS:HD2	1.95	0.48
1:B:310:LEU:HD13	1:B:314:LEU:HD23	1.95	0.48
1:B:170:LYS:NZ	7:B:629:HOH:O	2.47	0.48
1:C:41:LYS:HD3	1:C:42:TRP:N	2.25	0.48
1:B:236:HIS:O	1:B:240:ILE:HG13	2.13	0.47
1:C:301:GLU:HG3	7:C:770:HOH:O	2.14	0.47
1:C:255:TYR:CZ	1:C:269:GLY:HA3	2.49	0.47
1:A:103:HIS:NE2	2:A:501:S4M:N	2.62	0.46
1:B:265:PRO:O	1:B:266:CYS:HB2	2.15	0.46
1:A:93:GLN:HE21	2:A:501:S4M:HG2	1.81	0.46
1:A:273:CYS:HB3	1:A:281:LEU:HD13	1.98	0.46
1:B:112:THR:HG22	1:B:288:LEU:HD21	1.97	0.45
1:C:243:ILE:O	1:C:247:LYS:HG3	2.16	0.45
1:A:284:PRO:HG2	1:A:301:TYR:CE1	2.52	0.45
1:B:302:GLU:HB3	1:C:308:LYS:HD2	1.99	0.44
1:A:231:GLU:HB3	1:A:236:HIS:ND1	2.32	0.44
1:C:210:ASN:HD21	1:C:214:LYS:HZ1	1.65	0.44
1:C:67:LYS:HG3	1:C:72:ASN:ND2	2.33	0.43
1:C:161:ASN:HB2	7:C:715:HOH:O	2.18	0.43
1:B:284:PRO:HG2	1:B:301:TYR:CE1	2.54	0.43
1:B:88:LEU:HG	1:B:93:GLN:HG3	2.01	0.43
1:B:68:LYS:HB2	1:B:68:LYS:HE2	1.81	0.43
1:B:273:CYS:HB3	1:B:281:LEU:CD1	2.49	0.43
1:A:261:ILE:HG21	1:A:264:TYR:CD2	2.54	0.42
1:C:50:TRP:HB3	1:C:234:ILE:HD12	2.01	0.42
1:C:94:THR:HG21	1:C:262:THR:HG21	2.01	0.42
1:B:48:SER:HB3	1:B:51:TRP:CE2	2.54	0.42
1:B:196:ASP:OD2	2:B:502:S4M:N	2.53	0.42
1:C:101:TYR:HB2	1:C:260:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:HIS:CD2	1:B:304:HIS:C	2.93	0.42
1:B:50:MET:O	1:B:236:HIS:CE1	2.73	0.41
1:A:256:TYR:CZ	1:A:270:GLY:HA3	2.55	0.41
1:C:149:GLU:O	1:C:153[A]:GLU:HG3	2.20	0.41
1:A:183:LEU:HD12	1:A:212:PHE:CE1	2.55	0.41
1:B:112:THR:HA	1:B:286:LYS:HD3	2.02	0.41
1:A:67:THR:HG22	1:A:74:VAL:HB	2.03	0.41
1:B:303:ASN:HA	1:B:306:ALA:HB3	2.03	0.41
1:A:251:PHE:CD1	1:A:274:CYS:HB3	2.56	0.40
1:A:256:TYR:OH	1:A:270:GLY:HA3	2.21	0.40
1:B:231:GLU:HG2	1:B:236:HIS:HB2	2.03	0.40
1:B:94:LEU:C	1:B:94:LEU:HD12	2.42	0.40
1:B:42:LYS:HD2	1:B:42:LYS:HA	1.82	0.40
1:B:51:TRP:HB3	1:B:235:ILE:HD12	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	279/321 (87%)	267 (96%)	11 (4%)	1 (0%)	34	37
1	B	278/321 (87%)	264 (95%)	14 (5%)	0	100	100
1	C	280/321 (87%)	268 (96%)	12 (4%)	0	100	100
All	All	837/963 (87%)	799 (96%)	37 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	GLU

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	253/290 (87%)	245 (97%)	8 (3%)	39	50
1	B	252/290 (87%)	235 (93%)	17 (7%)	16	18
1	C	254/290 (88%)	245 (96%)	9 (4%)	36	46
All	All	759/870 (87%)	725 (96%)	34 (4%)	27	34

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	94	LEU
1	A	114	SER
1	A	138	LYS
1	A	229	GLN
1	A	261	ILE
1	A	275	SER
1	A	278	ASP
1	B	42	LYS
1	B	145	ILE
1	B	155	VAL
1	B	185	ASN
1	B	186	VAL
1	B	201	ILE
1	B	209	ASN
1	B	210	GLN
1	B	229	GLN
1	B	231	GLU
1	B	253	LYS
1	B	261	ILE
1	B	269	ILE
1	B	286	LYS
1	B	291	LYS
1	B	319	GLU
1	B	320	ASN
1	C	41	LYS

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Mol	Chain	Res	Type
1	C	67	LYS
1	C	114	LYS
1	C	149	GLU
1	C	179	SER
1	C	180	LYS
1	C	220	LYS
1	C	260	ILE
1	C	277	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	142	ASN
1	A	210	GLN
1	A	218	ASN
1	B	93	GLN
1	B	185	ASN
1	B	209	ASN
1	B	236	HIS
1	B	285	ASN
1	B	320	ASN
1	C	72	ASN
1	C	209	GLN
1	C	210	ASN
1	C	228	GLN
1	C	284	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 monosaccharides in this entry.

5.6 Ligand geometry

12 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	2MH	C	403	-	8,8,8	0.37	0	10,10,10	1.18	1 (10%)
2	S4M	C	503	-	22,26,26	0.84	1 (4%)	21,37,37	2.33	5 (23%)
5	GOL	A	603	-	5,5,5	0.39	0	5,5,5	0.26	0
2	S4M	B	502	-	22,26,26	0.78	0	21,37,37	1.72	3 (14%)
5	GOL	B	601	-	5,5,5	0.36	0	5,5,5	0.28	0
6	SO4	B	604	-	4,4,4	0.16	0	6,6,6	0.34	0
3	2MH	A	401	-	8,8,8	0.43	0	10,10,10	0.97	1 (10%)
4	1PG	A	701	-	16,16,16	0.55	0	15,15,15	0.27	0
4	1PG	C	702	-	16,16,16	0.52	0	15,15,15	0.27	0
3	2MH	B	402	-	8,8,8	0.44	0	10,10,10	2.37	4 (40%)
5	GOL	C	602	-	5,5,5	0.44	0	5,5,5	0.34	0
2	S4M	A	501	-	22,26,26	0.79	0	21,37,37	2.12	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
3	2MH	C	403	-	-	-	0/1/1/1
2	S4M	C	503	-	-	3/7/28/28	0/3/3/3
5	GOL	A	603	-	-	2/4/4/4	-
2	S4M	B	502	-	-	4/7/28/28	0/3/3/3
5	GOL	B	601	-	-	2/4/4/4	-
3	2MH	A	401	-	-	-	0/1/1/1
4	1PG	A	701	-	-	10/14/14/14	-
4	1PG	C	702	-	-	7/14/14/14	-
3	2MH	B	402	-	-	-	0/1/1/1
5	GOL	C	602	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S4M	A	501	-	-	6/7/28/28	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	S4M	C5-N7	-2.06	1.32	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	S4M	O4'-C1'-C2'	-6.01	98.15	106.93
2	C	503	S4M	O4'-C1'-C2'	-5.94	98.24	106.93
2	C	503	S4M	O4'-C4'-C5'	5.37	122.44	108.88
2	C	503	S4M	N3-C2-N1	-4.86	121.09	128.68
3	B	402	2MH	C3-C4-C5	4.62	116.83	111.53
3	B	402	2MH	C7-C6-C5	4.35	116.52	111.53
2	A	501	S4M	N3-C2-N1	-4.28	121.98	128.68
2	B	502	S4M	O4'-C4'-C5'	4.28	119.70	108.88
2	A	501	S4M	O4'-C4'-C5'	4.15	119.37	108.88
2	B	502	S4M	O4'-C1'-C2'	-3.93	101.19	106.93
2	B	502	S4M	N3-C2-N1	-3.69	122.92	128.68
2	A	501	S4M	C4-C5-N7	-2.96	106.32	109.40
3	C	403	2MH	C6-C7-C2	2.66	116.07	111.98
3	B	402	2MH	C4-C3-C2	2.47	115.78	111.98
3	A	401	2MH	C3-C4-C5	2.42	114.31	111.53
2	C	503	S4M	C2-N1-C6	2.18	122.48	118.75
2	C	503	S4M	CG-SD-C5'	2.07	108.67	103.40
3	B	402	2MH	C6-C7-C2	2.05	115.13	111.98

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	S4M	O4'-C4'-C5'-SD
2	A	501	S4M	C3'-C4'-C5'-SD
2	B	502	S4M	O4'-C4'-C5'-SD
2	B	502	S4M	C3'-C4'-C5'-SD
2	C	503	S4M	CA-CB-CG-SD
2	C	503	S4M	C3'-C4'-C5'-SD
5	B	601	GOL	O1-C1-C2-C3
4	A	701	1PG	O4-C8-C9-O5

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Mol	Chain	Res	Type	Atoms
4	C	702	1PG	O1-C2-C3-O2
4	A	701	1PG	O3-C6-C7-O4
4	A	701	1PG	O1-C2-C3-O2
4	C	702	1PG	O5-C10-C11-O6
4	C	702	1PG	O4-C8-C9-O5
4	C	702	1PG	O3-C6-C7-O4
2	B	502	S4M	N-CA-CB-CG
4	C	702	1PG	O2-C4-C5-O3
5	B	601	GOL	O1-C1-C2-O2
4	A	701	1PG	C8-C9-O5-C10
2	A	501	S4M	CB-CG-SD-CE
5	A	603	GOL	O1-C1-C2-O2
2	A	501	S4M	N-CA-CB-CG
4	A	701	1PG	C11-C10-O5-C9
4	A	701	1PG	C9-C8-O4-C7
4	A	701	1PG	C5-C4-O2-C3
2	A	501	S4M	CB-CG-SD-C5'
2	C	503	S4M	O4'-C4'-C5'-SD
4	A	701	1PG	C2-C3-O2-C4
4	A	701	1PG	C4-C5-O3-C6
4	C	702	1PG	C8-C9-O5-C10
4	C	702	1PG	C6-C7-O4-C8
4	A	701	1PG	O5-C10-C11-O6
5	A	603	GOL	O1-C1-C2-C3
2	A	501	S4M	CA-CB-CG-SD
2	B	502	S4M	CA-CB-CG-SD

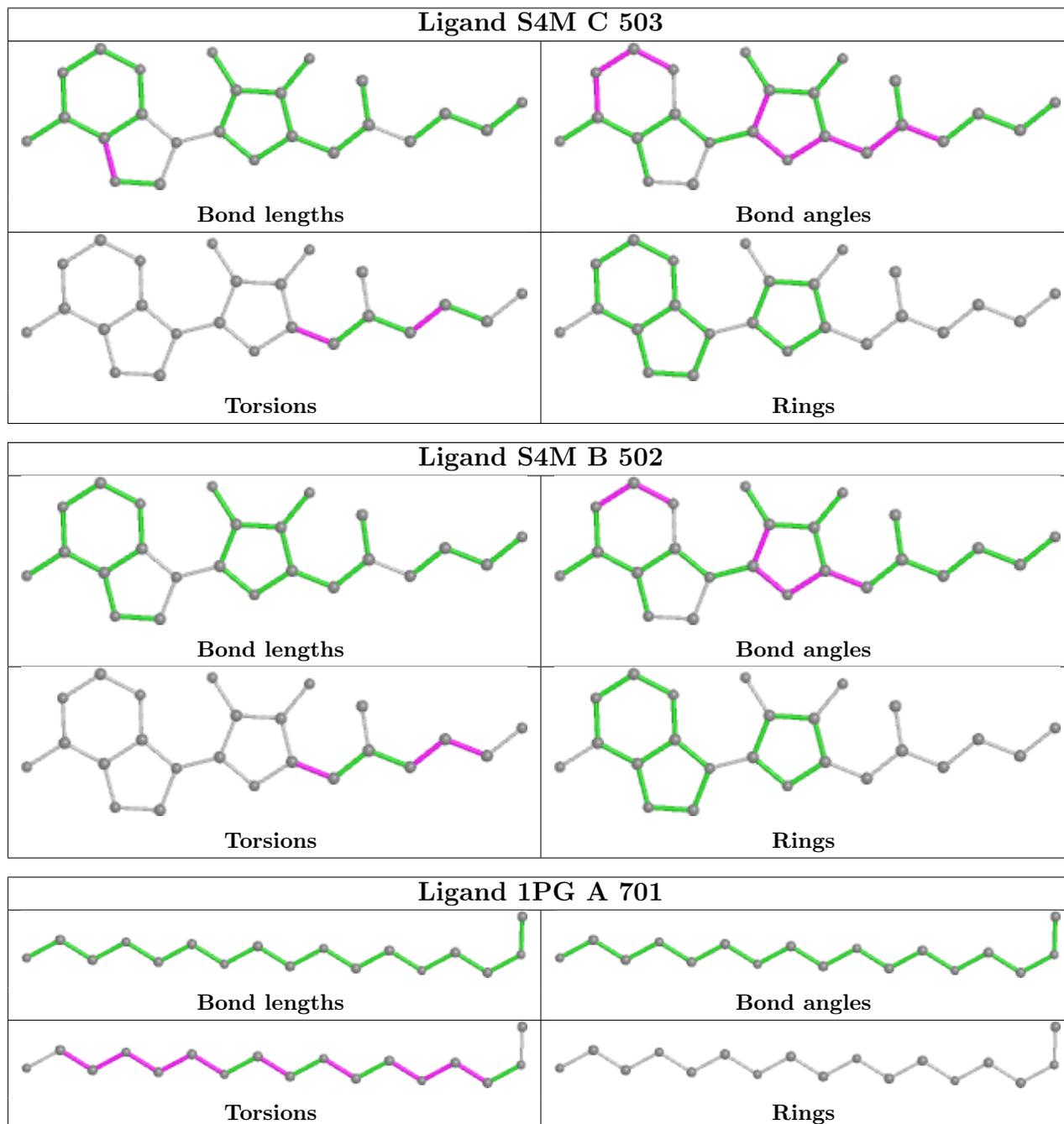
There are no ring outliers.

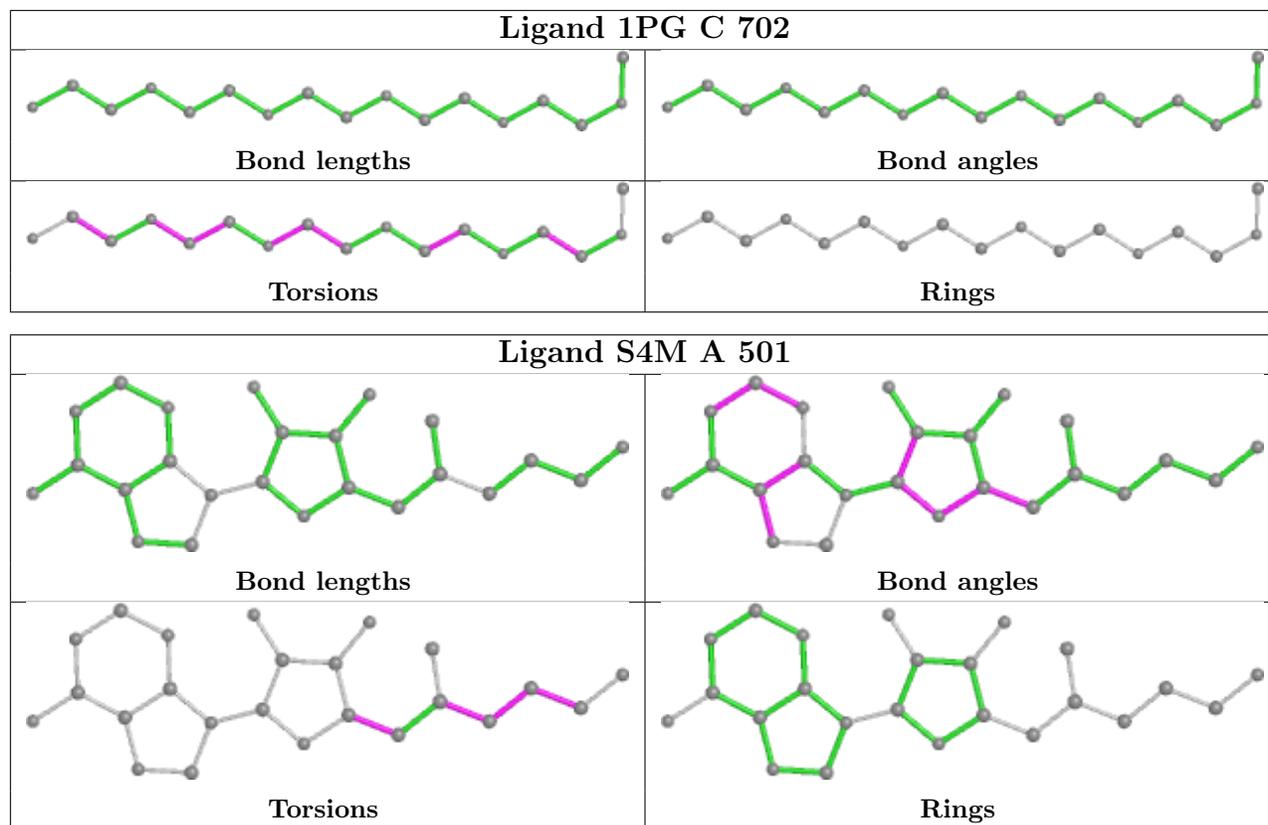
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	2MH	1	0
2	C	503	S4M	2	0
2	B	502	S4M	2	0
2	A	501	S4M	2	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	281/321 (87%)	-0.03	12 (4%) 35 33	26, 38, 52, 66	20 (7%)
1	B	280/321 (87%)	-0.09	9 (3%) 47 45	21, 32, 48, 64	16 (5%)
1	C	280/321 (87%)	-0.31	5 (1%) 68 66	19, 31, 42, 48	5 (1%)
All	All	841/963 (87%)	-0.14	26 (3%) 49 47	19, 34, 48, 66	41 (4%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	TYR	4.7
1	B	320	ASN	4.6
1	A	216	ILE	4.0
1	B	216	ILE	3.9
1	A	278	ASP	3.7
1	B	278	ASP	3.3
1	C	277	ASP	3.2
1	A	320	ASN	2.9
1	B	246	TYR	2.8
1	A	279	THR	2.7
1	C	169	LYS	2.7
1	C	278	THR	2.7
1	A	319	GLU	2.6
1	B	319	GLU	2.5
1	A	138	LYS	2.3
1	C	320	ILE	2.3
1	B	41	LYS	2.3
1	A	41	LYS	2.3
1	A	50	MET	2.2
1	B	201	ILE	2.2
1	B	316	LYS	2.2
1	C	290	LYS	2.2
1	A	168	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	ILE	2.1
1	B	279	THR	2.1
1	A	86	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 monosaccharides in this entry.

6.4 Ligands [i](#)

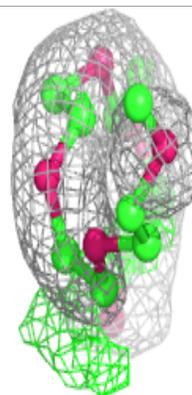
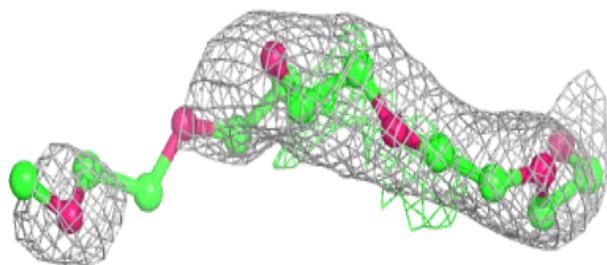
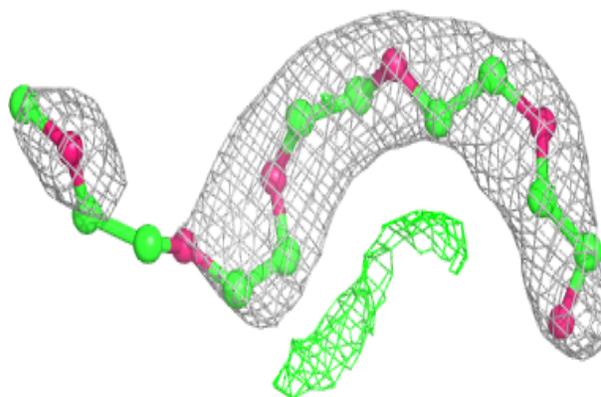
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	603	6/6	0.67	0.20	64,67,68,69	0
4	1PG	C	702	17/17	0.75	0.26	55,60,74,74	0
4	1PG	A	701	17/17	0.76	0.26	46,50,58,58	17
5	GOL	C	602	6/6	0.84	0.23	51,55,57,59	0
5	GOL	B	601	6/6	0.86	0.14	63,65,65,65	0
3	2MH	A	401	8/8	0.89	0.18	60,62,63,64	0
3	2MH	B	402	8/8	0.93	0.13	38,41,42,43	0
2	S4M	B	502	24/24	0.94	0.14	33,39,42,44	1
2	S4M	C	503	24/24	0.95	0.12	29,34,48,49	1
2	S4M	A	501	24/24	0.95	0.14	32,37,51,51	1
3	2MH	C	403	8/8	0.96	0.12	39,43,44,45	0
6	SO4	B	604	5/5	0.97	0.14	54,55,56,57	0

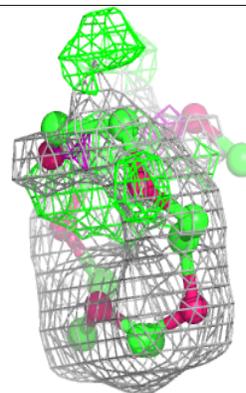
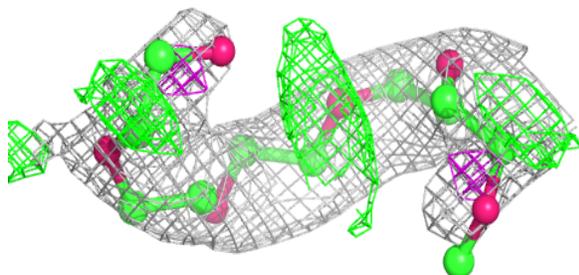
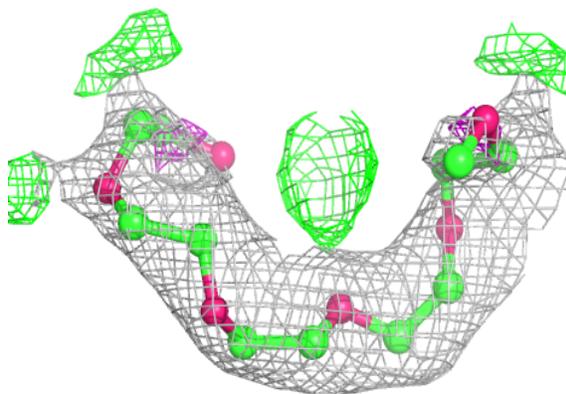
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1PG C 702:

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

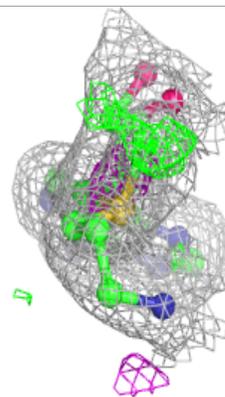
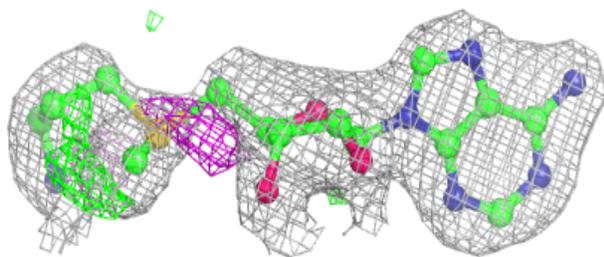
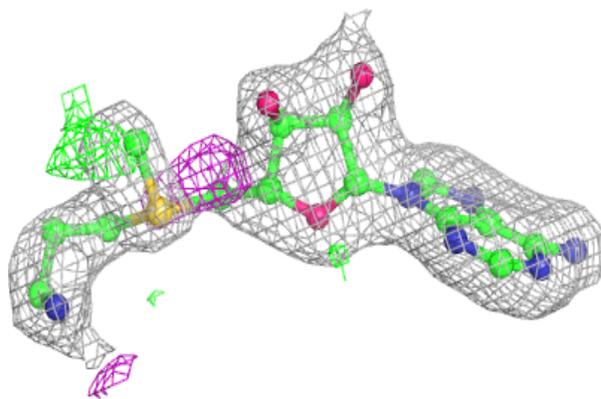
**Electron density around 1PG A 701:**

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

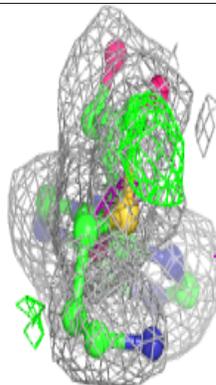
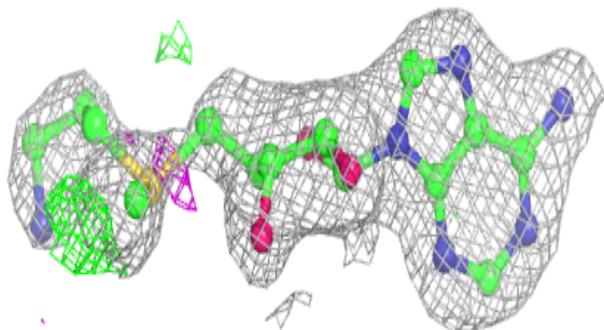
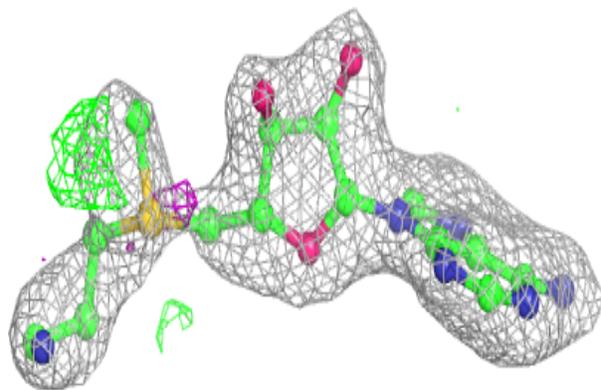


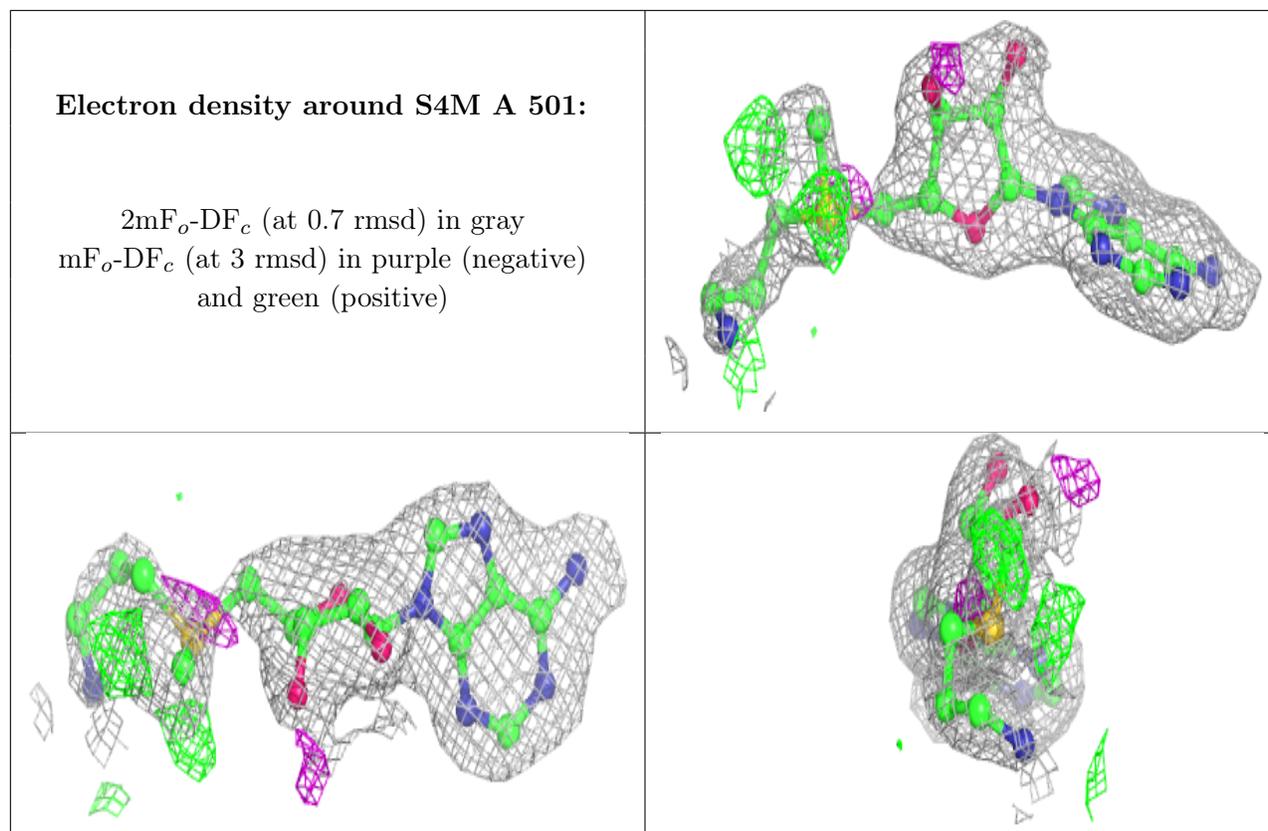
Electron density around S4M B 502:

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

**Electron density around S4M 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.