



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:50 PM UTC

PDB ID : 5Y4P / pdb_00005y4p
Title : Crystal structure of Trypanosoma cruzi spermidine synthase in complex with
5-methoxy-2-(5-methyl-4,5-dihydro-1H-imidazol-2-yl)phenol
Authors : Amano, Y.; Tateishi, Y.
Deposited on : 2017-08-04
Resolution : 2.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

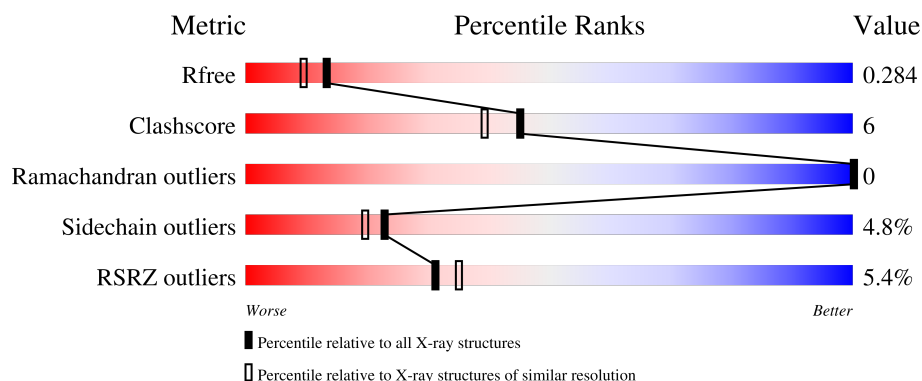
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	4% 72% 14% • 12%
1	B	304	5% 79% 12% • 9%
1	C	304	5% 76% 12% • 10%
1	D	304	5% 79% 10% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8896 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, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2111	1342	362	394	13			
1	B	278	Total	C	N	O	S	0	0	0
			2198	1396	376	412	14			
1	C	273	Total	C	N	O	S	0	0	0
			2163	1374	371	404	14			
1	D	274	Total	C	N	O	S	0	0	0
			2177	1384	372	408	13			

There are 32 discrepancies between the modelled and reference sequences:

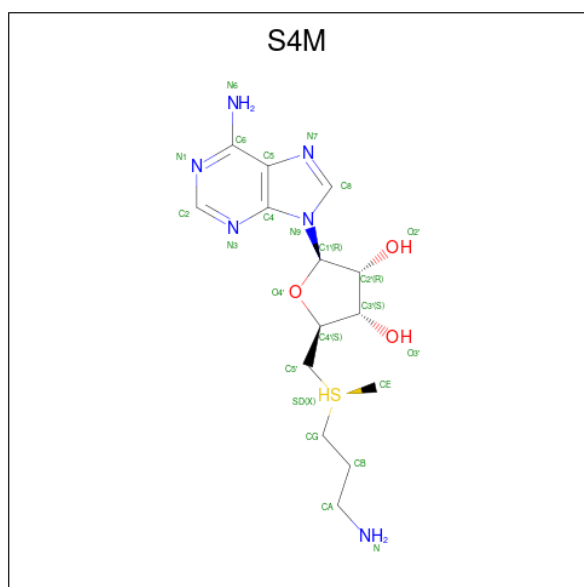
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q4DA73
A	-6	ALA	-	expression tag	UNP Q4DA73
A	-5	HIS	-	expression tag	UNP Q4DA73
A	-4	HIS	-	expression tag	UNP Q4DA73
A	-3	HIS	-	expression tag	UNP Q4DA73
A	-2	HIS	-	expression tag	UNP Q4DA73
A	-1	HIS	-	expression tag	UNP Q4DA73
A	0	HIS	-	expression tag	UNP Q4DA73
B	-7	MET	-	expression tag	UNP Q4DA73
B	-6	ALA	-	expression tag	UNP Q4DA73
B	-5	HIS	-	expression tag	UNP Q4DA73
B	-4	HIS	-	expression tag	UNP Q4DA73
B	-3	HIS	-	expression tag	UNP Q4DA73
B	-2	HIS	-	expression tag	UNP Q4DA73
B	-1	HIS	-	expression tag	UNP Q4DA73
B	0	HIS	-	expression tag	UNP Q4DA73
C	-7	MET	-	expression tag	UNP Q4DA73
C	-6	ALA	-	expression tag	UNP Q4DA73
C	-5	HIS	-	expression tag	UNP Q4DA73
C	-4	HIS	-	expression tag	UNP Q4DA73
C	-3	HIS	-	expression tag	UNP Q4DA73

Continued on next page...

Continued from previous page...

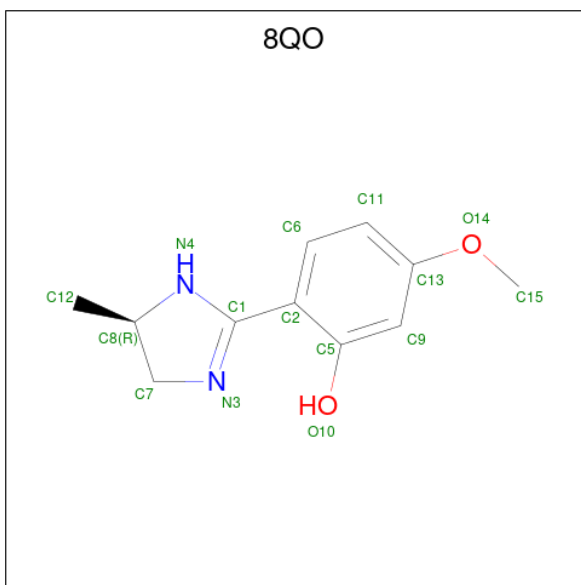
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q4DA73
C	-1	HIS	-	expression tag	UNP Q4DA73
C	0	HIS	-	expression tag	UNP Q4DA73
D	-7	MET	-	expression tag	UNP Q4DA73
D	-6	ALA	-	expression tag	UNP Q4DA73
D	-5	HIS	-	expression tag	UNP Q4DA73
D	-4	HIS	-	expression tag	UNP Q4DA73
D	-3	HIS	-	expression tag	UNP Q4DA73
D	-2	HIS	-	expression tag	UNP Q4DA73
D	-1	HIS	-	expression tag	UNP Q4DA73
D	0	HIS	-	expression tag	UNP Q4DA73

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



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		
2	D	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

- Molecule 3 is 5-methoxy-2-[(5R)-5-methyl-4,5-dihydro-1H-imidazol-2-yl]phenol (CCD ID: 8QO) (formula: C₁₁H₁₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		
3	D	1	Total	C	N	O	0	0
			15	11	2	2		

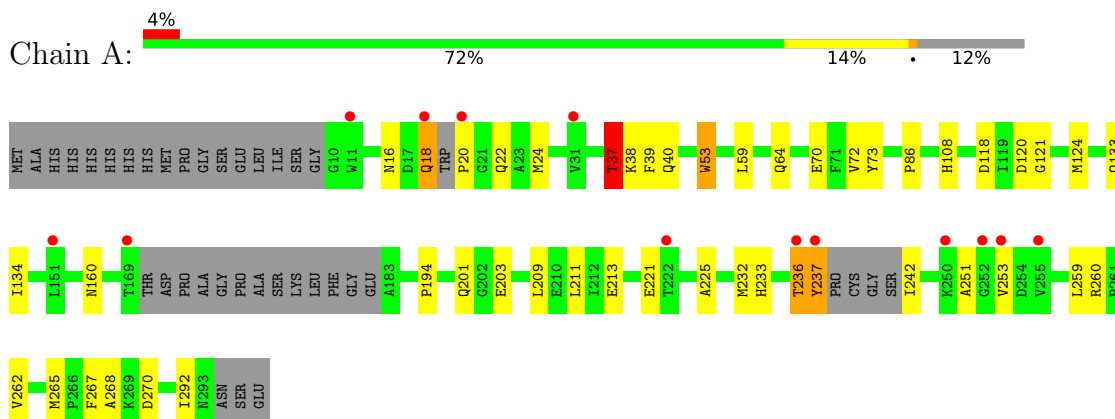
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	17	Total	O	0	0
			17	17		
4	C	27	Total	O	0	0
			27	27		
4	D	29	Total	O	0	0
			29	29		

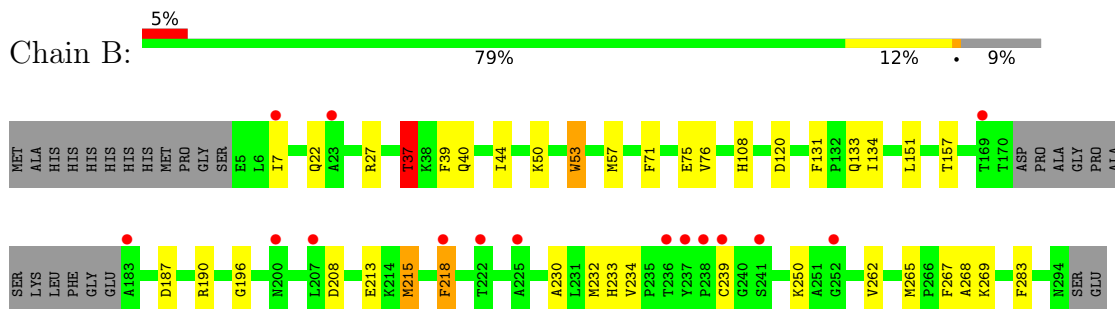
3 Residue-property plots [i](#)

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.

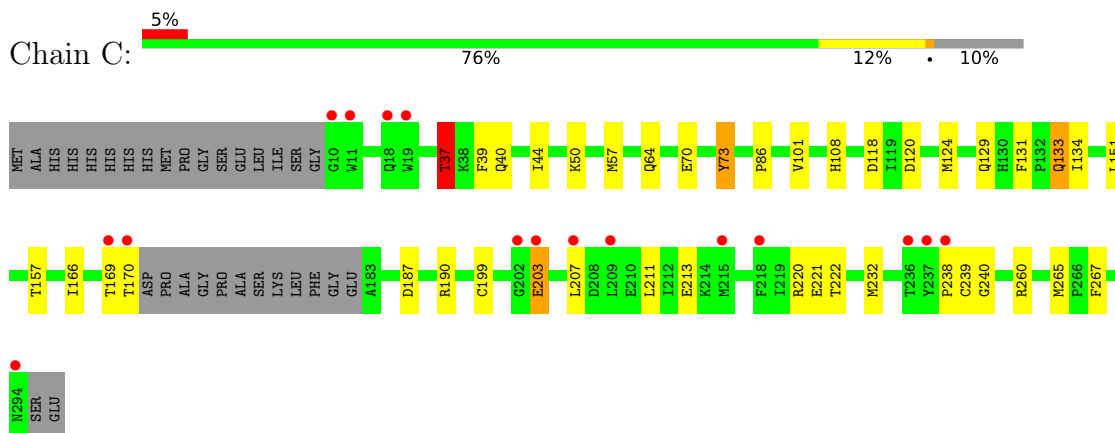
- Molecule 1: Spermidine synthase, putative



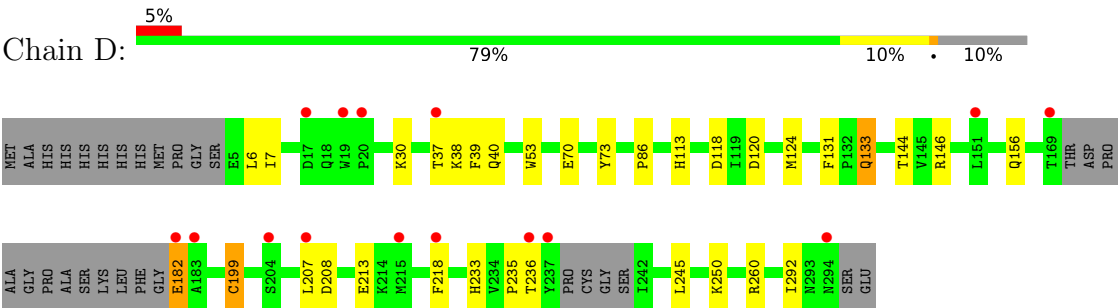
- Molecule 1: Spermidine synthase, putative



- Molecule 1: Spermidine synthase, putative



● Molecule 1: Spermidine synthase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.82Å 99.73Å 134.25Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	49.86 – 2.16 49.86 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.86-2.16) 98.3 (49.86-2.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.233 , 0.283 0.233 , 0.284	Depositor DCC
R_{free} test set	2985 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8896	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7533e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: S4M, 8QO

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	0.75	0/2159	1.01	2/2921 (0.1%)
1	B	0.74	0/2251	1.04	3/3052 (0.1%)
1	C	0.81	1/2216 (0.0%)	1.03	3/3005 (0.1%)
1	D	0.77	0/2228	1.01	1/3018 (0.0%)
All	All	0.77	1/8854 (0.0%)	1.02	9/11996 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	220	ARG	CA-C	5.21	1.59	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	THR	N-CA-C	-6.48	99.56	109.41
1	A	37	THR	N-CA-C	-6.40	100.09	109.18
1	B	196	GLY	N-CA-C	6.16	118.56	111.36
1	D	53	TRP	N-CA-C	5.94	118.71	111.82
1	C	213	GLU	CA-C-N	5.76	127.93	120.44
1	C	213	GLU	C-N-CA	5.76	127.93	120.44
1	B	37	THR	N-CA-C	-5.71	101.47	109.69
1	B	53	TRP	N-CA-C	5.41	118.09	111.82
1	A	53	TRP	N-CA-C	5.15	117.79	111.82

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	2111	0	2071	45	0
1	B	2198	0	2151	26	0
1	C	2163	0	2115	27	0
1	D	2177	0	2129	19	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0
2	C	24	0	24	2	0
2	D	24	0	24	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	18	0	0	3	0
4	B	17	0	0	0	0
4	C	27	0	0	4	0
4	D	29	0	0	0	0
All	All	8896	0	8562	103	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 (103) 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:157:THR:O	1:C:190:ARG:NH2	2.01	0.92
1:D:118:ASP:HB3	1:D:124:MET:HE2	1.51	0.92
1:B:37:THR:HG21	1:B:120:ASP:OD2	1.68	0.90
1:B:37:THR:HG22	1:B:40:GLN:H	1.34	0.88
1:A:118:ASP:HB3	1:A:124:MET:HE2	1.53	0.88
1:A:18:GLN:C	1:A:20:PRO:HD3	2.02	0.85
1:A:232:MET:O	1:B:233:HIS:HE1	1.62	0.82
1:C:118:ASP:HB3	1:C:124:MET:HE2	1.63	0.80
1:C:37:THR:HG21	1:C:120:ASP:OD2	1.82	0.80
1:A:37:THR:HG22	1:A:40:GLN:H	1.47	0.79
1:A:251:ALA:H	1:D:156:GLN:HE22	1.29	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:THR:HG21	1:D:120:ASP:OD2	1.84	0.78
1:B:265:MET:HE3	1:B:267:PHE:CZ	2.19	0.77
1:A:37:THR:HG21	1:A:120:ASP:OD2	1.84	0.77
1:D:37:THR:HG23	1:D:39:PHE:H	1.49	0.77
1:A:203:GLU:HG3	1:A:211:LEU:HD23	1.67	0.75
1:C:37:THR:HG22	1:C:40:GLN:H	1.53	0.73
1:A:22:GLN:NE2	1:B:53:TRP:HE1	1.85	0.73
1:A:72:VAL:HG12	1:A:232:MET:HE3	1.70	0.72
1:A:37:THR:CG2	1:A:39:PHE:H	2.04	0.70
1:A:201:GLN:HG3	4:A:409:HOH:O	1.91	0.70
1:B:108:HIS:CE1	1:B:265:MET:HE1	2.28	0.67
1:A:251:ALA:H	1:D:156:GLN:NE2	1.97	0.63
1:A:251:ALA:N	1:D:156:GLN:HE22	1.97	0.62
1:D:37:THR:HG22	1:D:40:GLN:O	1.99	0.62
1:D:70:GLU:HA	1:D:73:TYR:CZ	2.34	0.62
1:A:225:ALA:HB1	1:A:251:ALA:HB2	1.81	0.62
1:A:121:GLY:HA2	1:A:124:MET:HE3	1.82	0.62
1:A:22:GLN:HE22	1:B:53:TRP:HE1	1.46	0.61
1:B:37:THR:CG2	1:B:39:PHE:H	2.15	0.60
1:C:240:GLY:HA2	1:D:235:PRO:O	2.02	0.59
1:D:213:GLU:HG3	1:D:292:ILE:HD11	1.83	0.59
1:A:37:THR:HG23	1:A:39:PHE:H	1.67	0.58
1:C:86:PRO:O	1:C:260:ARG:HD3	2.03	0.58
1:C:133:GLN:HG2	4:C:422:HOH:O	2.03	0.58
1:C:44:ILE:HG12	1:C:57:MET:HG3	1.86	0.57
1:A:73:TYR:HB3	1:A:232:MET:HE1	1.85	0.57
1:A:37:THR:HG22	1:A:39:PHE:H	1.70	0.57
1:C:133:GLN:HG3	1:C:134:ILE:HG13	1.86	0.56
1:A:53:TRP:HE1	1:B:22:GLN:NE2	2.04	0.55
1:C:37:THR:CG2	1:C:39:PHE:H	2.20	0.54
1:A:24:MET:HE3	1:A:236:THR:HG21	1.88	0.54
1:C:169:THR:HA	2:C:301:S4M:H5'2	1.90	0.54
1:D:86:PRO:O	1:D:260:ARG:HD3	2.09	0.53
1:A:237:TYR:N	1:A:237:TYR:CD1	2.77	0.53
1:B:37:THR:HG22	1:B:39:PHE:H	1.74	0.53
1:C:232:MET:O	1:D:233:HIS:HE1	1.91	0.52
1:D:37:THR:HG22	1:D:40:GLN:H	1.74	0.52
1:A:59:LEU:HD12	1:A:64:GLN:HG3	1.91	0.51
1:A:232:MET:O	1:B:233:HIS:CE1	2.54	0.51
1:A:86:PRO:O	1:A:260:ARG:HD3	2.11	0.51
1:B:157:THR:O	1:B:190:ARG:NH2	2.36	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:HG12	1:B:57:MET:HG3	1.92	0.50
1:B:76:VAL:HG21	1:B:232:MET:HG2	1.93	0.50
1:B:37:THR:HG22	1:B:40:GLN:N	2.16	0.49
1:A:18:GLN:HE21	1:A:18:GLN:H	1.60	0.49
1:A:209:LEU:O	1:A:213:GLU:HG3	2.12	0.49
1:A:72:VAL:HG12	1:A:232:MET:CE	2.39	0.49
1:A:70:GLU:HA	1:A:73:TYR:CZ	2.47	0.49
1:C:108:HIS:ND1	1:C:265:MET:HE1	2.28	0.48
1:A:233:HIS:HD2	4:A:408:HOH:O	1.97	0.48
1:A:16:ASN:HD22	1:A:18:GLN:NE2	2.11	0.48
1:A:18:GLN:H	1:A:18:GLN:NE2	2.12	0.47
1:B:262:VAL:O	1:B:268:ALA:HB2	2.15	0.47
1:C:131:PHE:HB3	1:C:134:ILE:HD12	1.96	0.47
1:C:203:GLU:HG3	1:C:211:LEU:HD23	1.97	0.47
1:C:265:MET:HE2	1:C:267:PHE:HE2	1.79	0.47
1:C:265:MET:HE2	1:C:267:PHE:CE2	2.50	0.46
1:B:262:VAL:HA	1:B:265:MET:HE2	1.96	0.46
1:C:37:THR:HG22	1:C:39:PHE:H	1.80	0.46
1:A:259:LEU:CD1	1:D:146:ARG:HG3	2.46	0.46
1:D:182:GLU:HB2	1:D:218:PHE:CZ	2.51	0.46
1:C:70:GLU:HA	1:C:73:TYR:CZ	2.51	0.45
1:B:215:MET:HE3	1:B:218:PHE:CZ	2.51	0.45
1:C:238:PRO:HB2	4:C:427:HOH:O	2.15	0.45
1:C:265:MET:CE	4:C:410:HOH:O	2.64	0.45
1:C:37:THR:CG2	1:C:120:ASP:OD2	2.60	0.45
1:B:37:THR:HG23	1:B:39:PHE:H	1.82	0.45
1:B:131:PHE:HB3	1:B:134:ILE:HD12	1.98	0.45
1:C:265:MET:HE3	4:C:410:HOH:O	2.16	0.44
1:A:108:HIS:ND1	1:A:265:MET:HE1	2.33	0.43
1:A:22:GLN:NE2	1:B:53:TRP:NE1	2.62	0.42
1:A:265:MET:HE2	4:A:415:HOH:O	2.18	0.42
1:C:64:GLN:HB3	2:C:301:S4M:HE2	2.01	0.42
1:C:187:ASP:OD1	1:C:190:ARG:NH1	2.51	0.42
1:A:262:VAL:O	1:A:268:ALA:HB2	2.19	0.42
1:A:22:GLN:HE22	1:B:53:TRP:NE1	2.16	0.42
1:A:213:GLU:HG2	1:A:292:ILE:CD1	2.49	0.42
1:B:187:ASP:OD1	1:B:190:ARG:NH1	2.52	0.42
1:A:267:PHE:O	1:A:270:ASP:HB2	2.19	0.42
1:A:160:ASN:OD1	1:A:194:PRO:HD3	2.20	0.41
1:D:113:HIS:CE1	1:D:144:THR:OG1	2.73	0.41
1:C:101:VAL:HG11	1:C:166:ILE:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:MET:HE3	1:B:267:PHE:HZ	1.78	0.41
1:B:71:PHE:O	1:B:75:GLU:HG3	2.21	0.41
1:D:131:PHE:HA	1:D:133:GLN:HE22	1.86	0.41
1:D:199:CYS:HA	1:D:245:LEU:O	2.21	0.41
1:A:70:GLU:HG2	1:A:134:ILE:HD11	2.02	0.40
1:B:230:ALA:HB2	1:B:283:PHE:CE1	2.55	0.40
1:A:38:LYS:HB3	1:A:39:PHE:CD2	2.57	0.40
1:A:259:LEU:HD11	1:D:146:ARG:HG3	2.03	0.40
1:A:18:GLN:O	1:A:20:PRO:HD3	2.17	0.40
1:C:37:THR:HG23	1:C:39:PHE:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/304 (85%)	250 (97%)	8 (3%)	0	100	100
1	B	274/304 (90%)	263 (96%)	11 (4%)	0	100	100
1	C	269/304 (88%)	259 (96%)	10 (4%)	0	100	100
1	D	268/304 (88%)	259 (97%)	9 (3%)	0	100	100
All	All	1069/1216 (88%)	1031 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	232/262 (88%)	224 (97%)	8 (3%)	32	33
1	B	242/262 (92%)	228 (94%)	14 (6%)	18	14
1	C	238/262 (91%)	225 (94%)	13 (6%)	19	15
1	D	239/262 (91%)	228 (95%)	11 (5%)	24	22
All	All	951/1048 (91%)	905 (95%)	46 (5%)	23	20

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	37	THR
1	A	133	GLN
1	A	221	GLU
1	A	236	THR
1	A	237	TYR
1	A	242	ILE
1	A	253	VAL
1	B	7	ILE
1	B	27	ARG
1	B	37	THR
1	B	50	LYS
1	B	133	GLN
1	B	151	LEU
1	B	208	ASP
1	B	213	GLU
1	B	215	MET
1	B	218	PHE
1	B	234	VAL
1	B	239	CYS
1	B	250	LYS
1	B	269	LYS
1	C	37	THR
1	C	50	LYS
1	C	73	TYR
1	C	129	GLN
1	C	133	GLN
1	C	151	LEU
1	C	170	THR
1	C	199	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	203	GLU
1	C	207	LEU
1	C	221	GLU
1	C	222	THR
1	C	239	CYS
1	D	6	LEU
1	D	7	ILE
1	D	30	LYS
1	D	38	LYS
1	D	133	GLN
1	D	182	GLU
1	D	199	CYS
1	D	207	LEU
1	D	208	ASP
1	D	236	THR
1	D	250	LYS

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

Mol	Chain	Res	Type
1	A	16	ASN
1	A	18	GLN
1	A	22	GLN
1	A	113	HIS
1	A	126	GLN
1	A	130	HIS
1	A	201	GLN
1	B	22	GLN
1	B	126	GLN
1	B	129	GLN
1	B	156	GLN
1	B	200	ASN
1	B	201	GLN
1	B	233	HIS
1	C	126	GLN
1	C	133	GLN
1	D	113	HIS
1	D	133	GLN
1	D	156	GLN
1	D	233	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	8QO	B	302	-	14,16,16	0.78	0	17,22,22	1.29	2 (11%)
3	8QO	C	302	-	14,16,16	0.79	0	17,22,22	1.40	3 (17%)
3	8QO	D	302	-	14,16,16	0.57	0	17,22,22	1.28	2 (11%)
3	8QO	A	302	-	14,16,16	0.65	0	17,22,22	1.30	1 (5%)
2	S4M	C	301	-	25,26,26	0.57	0	33,37,37	1.02	3 (9%)
2	S4M	A	301	-	25,26,26	0.68	1 (4%)	33,37,37	1.19	6 (18%)
2	S4M	D	301	-	25,26,26	0.66	1 (4%)	33,37,37	1.46	6 (18%)
2	S4M	B	301	-	25,26,26	0.62	0	33,37,37	1.07	3 (9%)

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	8QO	B	302	-	-	0/6/15/15	0/2/2/2
3	8QO	C	302	-	-	0/6/15/15	0/2/2/2
3	8QO	D	302	-	-	0/6/15/15	0/2/2/2
3	8QO	A	302	-	-	2/6/15/15	0/2/2/2
2	S4M	C	301	-	-	4/12/28/28	0/3/3/3
2	S4M	A	301	-	-	5/12/28/28	0/3/3/3
2	S4M	D	301	-	-	5/12/28/28	0/3/3/3
2	S4M	B	301	-	-	4/12/28/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	S4M	C6-N6	2.57	1.40	1.34
2	A	301	S4M	C6-N6	2.40	1.40	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	S4M	CG-SD-C5'	-4.97	91.28	103.43
3	D	302	8QO	C5-C2-C1	3.87	123.92	119.67
3	A	302	8QO	C15-O14-C13	-3.87	109.21	117.50
3	C	302	8QO	C15-O14-C13	-3.35	110.31	117.50
2	A	301	S4M	CG-SD-C5'	-2.94	96.25	103.43
3	B	302	8QO	C15-O14-C13	-2.83	111.43	117.50
2	A	301	S4M	O3'-C3'-C4'	-2.82	102.97	111.08
3	C	302	8QO	C5-C2-C1	2.81	122.76	119.67
2	A	301	S4M	O4'-C4'-C5'	2.48	115.15	108.88
2	D	301	S4M	C4'-O4'-C1'	-2.47	104.01	109.47
2	D	301	S4M	O4'-C4'-C5'	2.44	115.03	108.88
2	D	301	S4M	O3'-C3'-C4'	-2.34	104.36	111.08
3	B	302	8QO	C5-C2-C1	2.33	122.23	119.67
2	A	301	S4M	C4'-O4'-C1'	-2.32	104.35	109.47
3	D	302	8QO	C15-O14-C13	-2.30	112.56	117.50
2	D	301	S4M	O4'-C1'-C2'	-2.30	101.70	106.62
2	B	301	S4M	C4'-O4'-C1'	-2.25	104.50	109.47
2	A	301	S4M	O4'-C1'-N9	2.21	112.34	108.09
2	D	301	S4M	N9-C8-N7	-2.19	110.82	113.94
3	C	302	8QO	N4-C1-N3	-2.11	113.61	116.46
2	B	301	S4M	C4-N9-C8	2.10	107.94	105.74
2	C	301	S4M	CG-SD-C5'	-2.06	98.39	103.43
2	B	301	S4M	N9-C8-N7	-2.04	111.04	113.94
2	C	301	S4M	C4-N9-C8	2.03	107.87	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	S4M	O3'-C3'-C4'	-2.00	105.33	111.08
2	A	301	S4M	C2'-C3'-C4'	2.00	106.48	102.61

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	S4M	CA-CB-CG-SD
2	A	301	S4M	O4'-C4'-C5'-SD
2	A	301	S4M	C3'-C4'-C5'-SD
2	B	301	S4M	CA-CB-CG-SD
2	B	301	S4M	O4'-C4'-C5'-SD
2	B	301	S4M	C3'-C4'-C5'-SD
2	C	301	S4M	C4'-C5'-SD-CE
2	C	301	S4M	O4'-C4'-C5'-SD
2	C	301	S4M	C3'-C4'-C5'-SD
2	D	301	S4M	CA-CB-CG-SD
2	D	301	S4M	O4'-C4'-C5'-SD
2	D	301	S4M	C3'-C4'-C5'-SD
3	A	302	8QO	C11-C13-O14-C15
3	A	302	8QO	C9-C13-O14-C15
2	D	301	S4M	N-CA-CB-CG
2	B	301	S4M	N-CA-CB-CG
2	A	301	S4M	CB-CG-SD-C5'
2	D	301	S4M	CB-CG-SD-C5'
2	A	301	S4M	CB-CG-SD-CE
2	C	301	S4M	CB-CG-SD-C5'

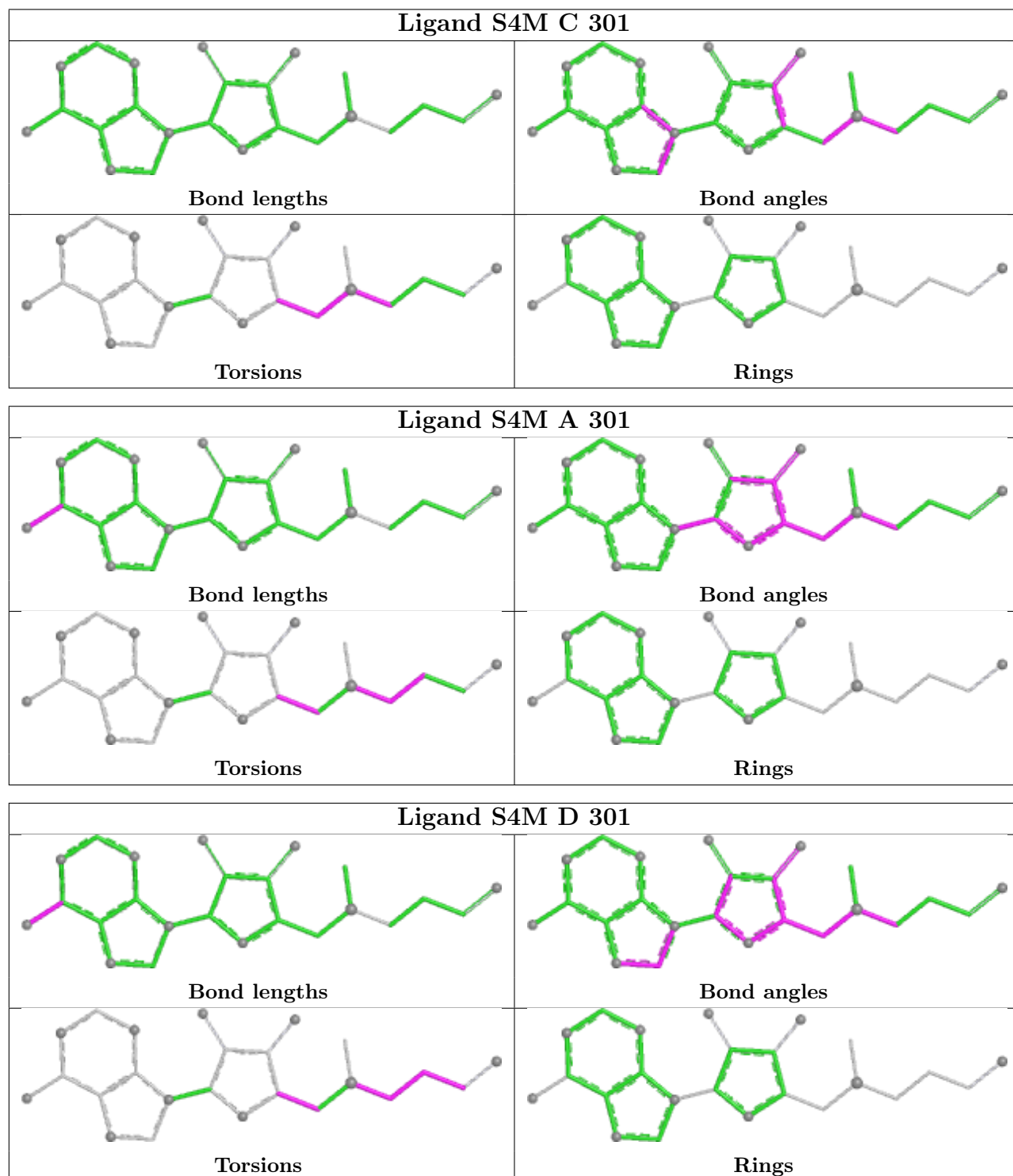
There are no ring outliers.

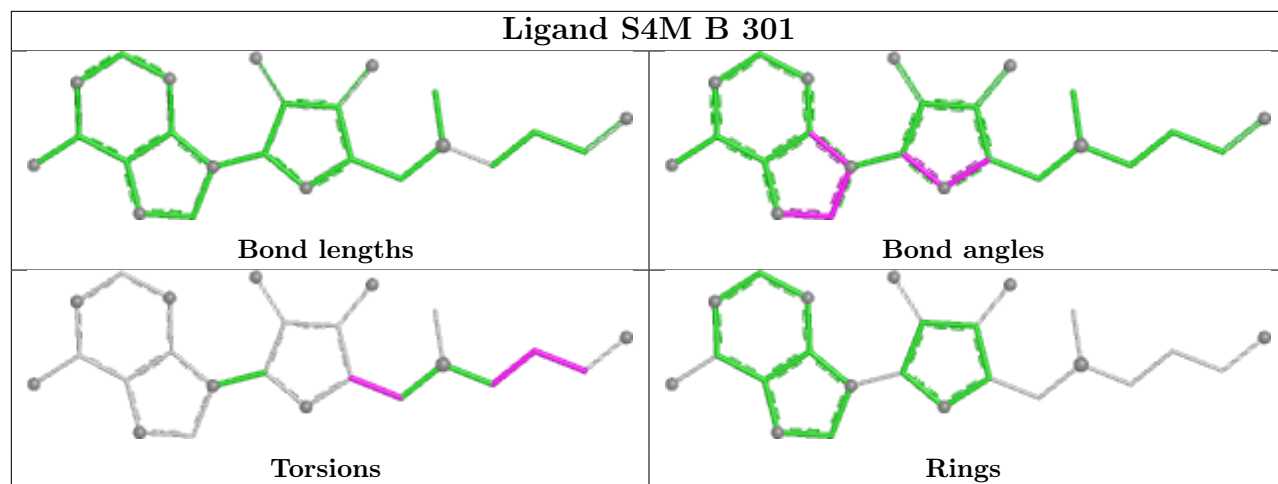
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	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	266/304 (87%)	0.53	13 (4%) 35 39	22, 39, 61, 76	0
1	B	278/304 (91%)	0.55	15 (5%) 31 35	24, 41, 63, 91	0
1	C	273/304 (89%)	0.37	16 (5%) 28 32	20, 34, 60, 87	0
1	D	274/304 (90%)	0.37	15 (5%) 30 34	21, 37, 57, 87	0
All	All	1091/1216 (89%)	0.46	59 (5%) 31 35	20, 38, 61, 91	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	VAL	5.0
1	A	237	TYR	4.3
1	B	218	PHE	4.2
1	D	37	THR	4.1
1	C	238	PRO	3.9
1	D	237	TYR	3.7
1	D	218	PHE	3.5
1	D	19	TRP	3.3
1	A	18	GLN	3.2
1	B	7	ILE	3.1
1	B	238	PRO	3.0
1	C	203	GLU	2.9
1	C	236	THR	2.9
1	C	237	TYR	2.9
1	B	169	THR	2.8
1	D	169	THR	2.8
1	C	170	THR	2.8
1	C	10	GLY	2.7
1	A	236	THR	2.7
1	C	11	TRP	2.7
1	C	207	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	183	ALA	2.6
1	D	236	THR	2.6
1	B	237	TYR	2.6
1	D	294	ASN	2.6
1	D	17	ASP	2.5
1	B	239	CYS	2.5
1	A	169	THR	2.5
1	C	202	GLY	2.4
1	C	18	GLN	2.4
1	C	294	ASN	2.3
1	C	169	THR	2.3
1	A	11	TRP	2.3
1	A	255	VAL	2.3
1	C	19	TRP	2.3
1	A	250	LYS	2.3
1	B	23	ALA	2.3
1	D	215	MET	2.3
1	C	218	PHE	2.2
1	B	236	THR	2.2
1	D	151	LEU	2.2
1	B	183	ALA	2.2
1	C	209	LEU	2.2
1	A	20	PRO	2.1
1	A	222	THR	2.2
1	D	20	PRO	2.1
1	B	207	LEU	2.1
1	B	200	ASN	2.1
1	D	182	GLU	2.1
1	A	31	VAL	2.1
1	B	252	GLY	2.1
1	A	151	LEU	2.1
1	D	207	LEU	2.1
1	A	252	GLY	2.1
1	B	225	ALA	2.1
1	B	241	SER	2.1
1	C	215	MET	2.0
1	D	204	SER	2.0
1	B	222	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

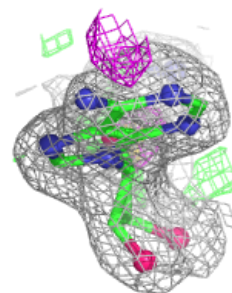
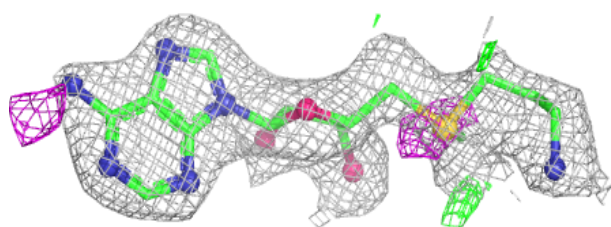
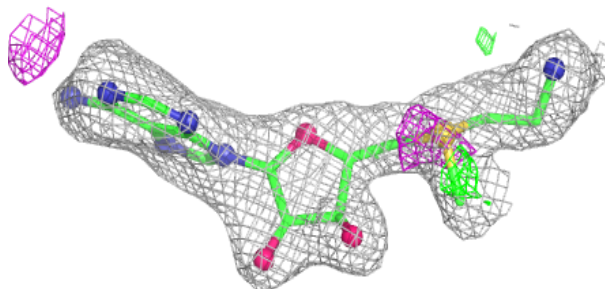
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	S4M	B	301	24/24	0.86	0.11	35,40,54,63	0
2	S4M	D	301	24/24	0.89	0.10	39,46,58,66	0
3	8QO	A	302	15/15	0.89	0.09	35,37,42,43	0
3	8QO	B	302	15/15	0.90	0.09	32,35,41,42	0
2	S4M	A	301	24/24	0.92	0.10	34,38,45,54	0
3	8QO	C	302	15/15	0.92	0.09	33,37,50,53	0
3	8QO	D	302	15/15	0.92	0.07	36,38,43,44	0
2	S4M	C	301	24/24	0.93	0.10	33,38,57,62	0

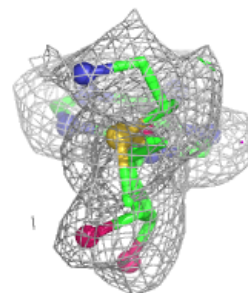
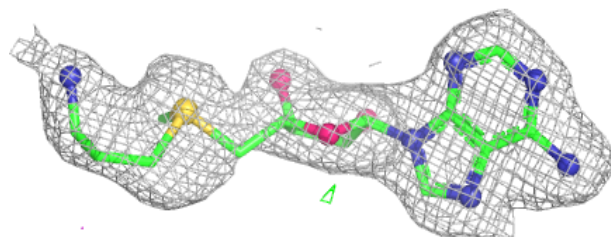
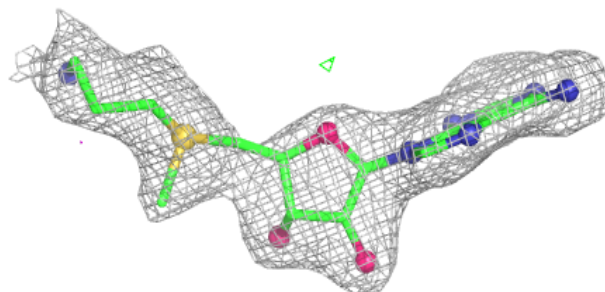
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around S4M B 301:

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

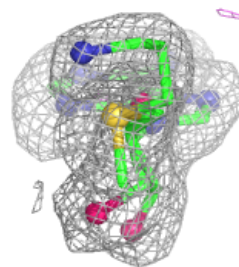
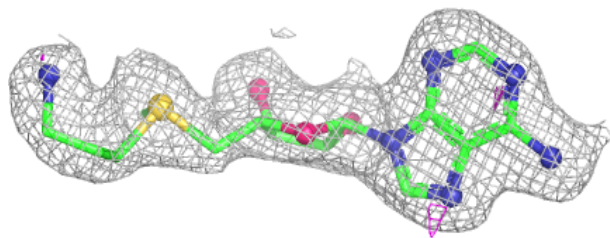
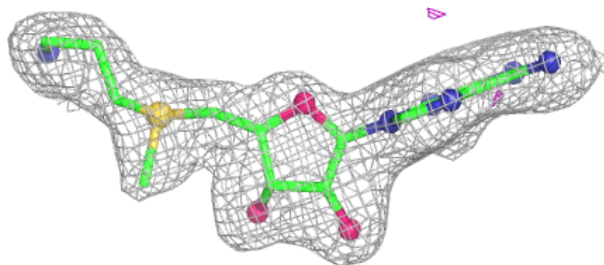
**Electron density around S4M D 301:**

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

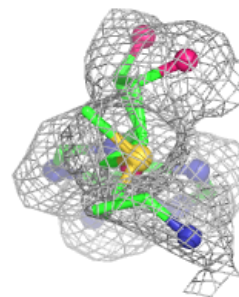
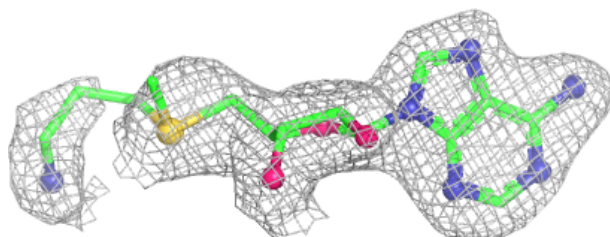
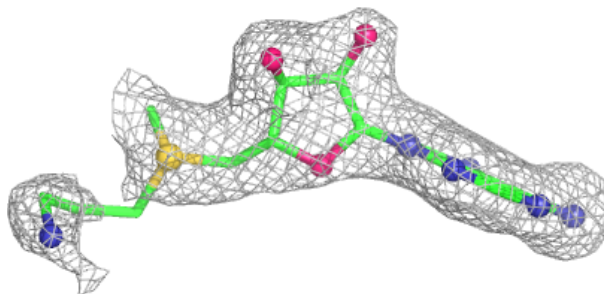


Electron density around S4M A 301:

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

**Electron density around S4M C 301:**

$2mF_o-DF_c$ (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.