



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:02 am BST

PDB ID : 5Y4Q  
Title : Crystal structure of Trypanosoma cruzi spermidine synthase in complex with N-(4-methoxyphenyl)quinolin-4-amine  
Authors : Amano, Y.; Tateishi, Y.  
Deposited on : 2017-08-04  
Resolution : 2.07 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

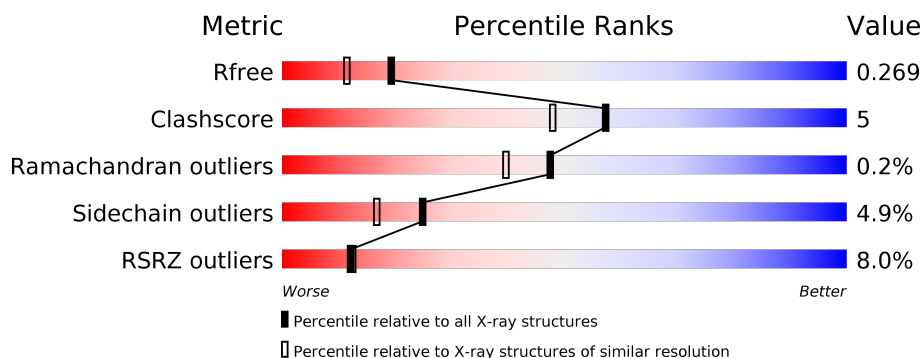
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	304	<div> <div>9%</div> <div>74%</div> <div>13%</div> <div>•</div> <div>10%</div> </div>
1	B	304	<div> <div>9%</div> <div>80%</div> <div>11%</div> <div>•</div> <div>8%</div> </div>
1	C	304	<div> <div>8%</div> <div>76%</div> <div>12%</div> <div>•</div> <div>11%</div> </div>
1	D	304	<div> <div>4%</div> <div>79%</div> <div>9%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8991 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	273	Total	C	N	O	S	0	0	0
			2163	1374	371	404	14			
1	B	279	Total	C	N	O	S	0	0	0
			2209	1404	378	414	13			
1	C	272	Total	C	N	O	S	0	0	0
			2149	1363	369	403	14			
1	D	270	Total	C	N	O	S	0	0	0
			2140	1360	366	401	13			

There are 32 discrepancies between the modelled and reference sequences:

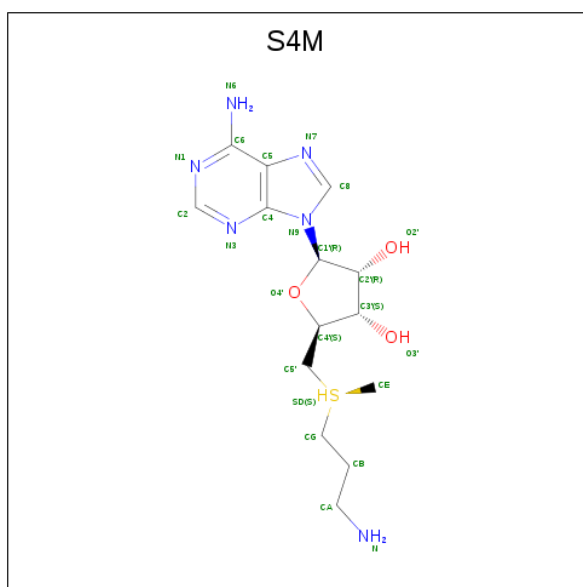
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q4DA73
A	-6	ALA	-	expression tag	UNP Q4DA73
A	-5	HIS	-	expression tag	UNP Q4DA73
A	-4	HIS	-	expression tag	UNP Q4DA73
A	-3	HIS	-	expression tag	UNP Q4DA73
A	-2	HIS	-	expression tag	UNP Q4DA73
A	-1	HIS	-	expression tag	UNP Q4DA73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

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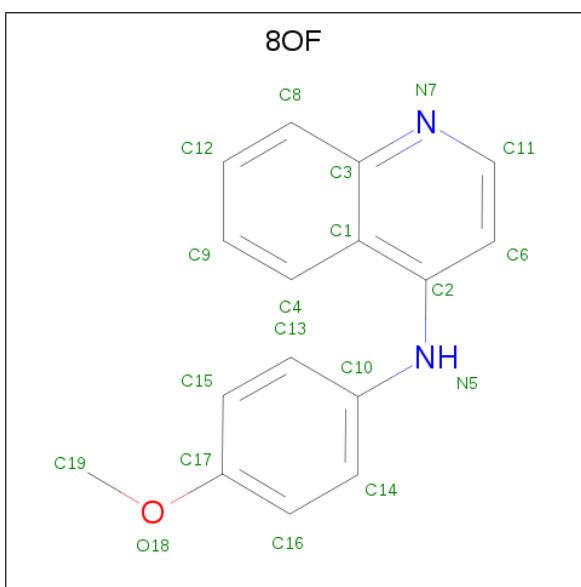
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q4DA73
C	-1	HIS	-	expression tag	UNP Q4DA73
C	0	HIS	-	expression tag	UNP Q4DA73
D	-7	MET	-	expression tag	UNP Q4DA73
D	-6	ALA	-	expression tag	UNP Q4DA73
D	-5	HIS	-	expression tag	UNP Q4DA73
D	-4	HIS	-	expression tag	UNP Q4DA73
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 (three-letter code: S4M) (formula: C<sub>14</sub>H<sub>24</sub>N<sub>6</sub>O<sub>3</sub>S).



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

- Molecule 3 is N-(4-methoxyphenyl)quinolin-4-amine (three-letter code: 8OF) (formula: C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	16	2	1		
3	B	1	Total	C	N	O	0	0
			19	16	2	1		
3	C	1	Total	C	N	O	0	0
			19	16	2	1		
3	D	1	Total	C	N	O	0	0
			19	16	2	1		

- Molecule 4 is water.

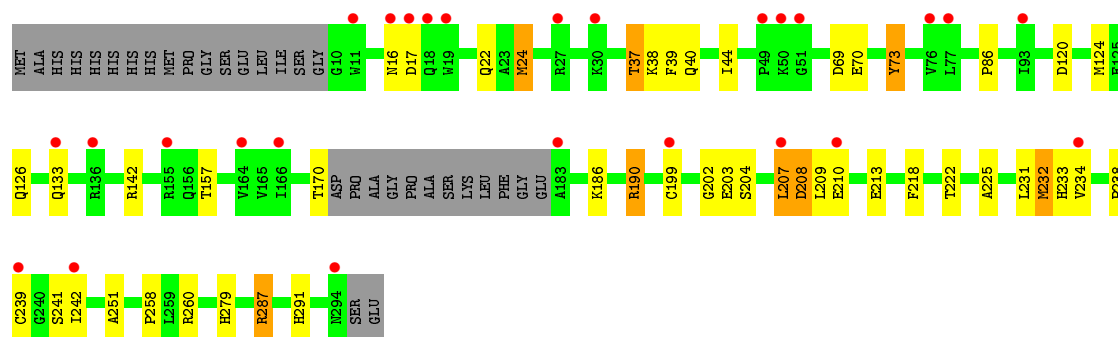
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	39	Total	O	0	0
			39	39		
4	C	52	Total	O	0	0
			52	52		
4	D	35	Total	O	0	0
			35	35		

### 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.

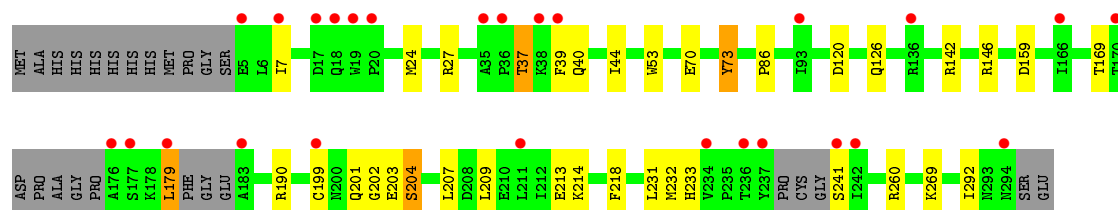
- Molecule 1: Spermidine synthase, putative

Chain A: 




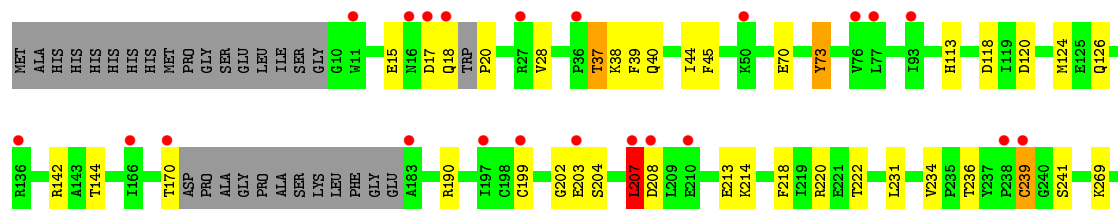
- Molecule 1: Spermidine synthase, putative

Chain B: 



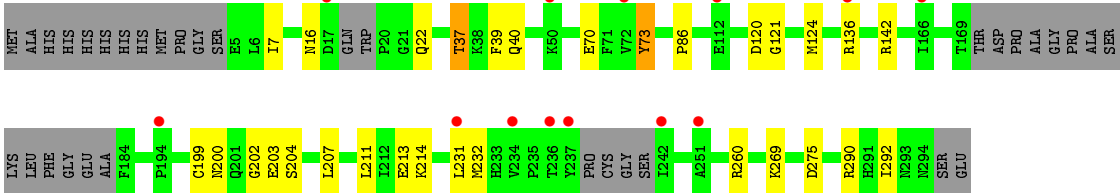
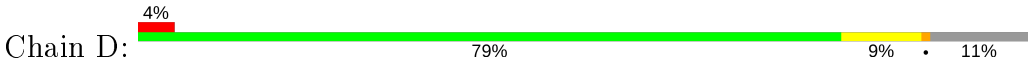
- Molecule 1: Spermidine synthase, putative

Chain C: 





● 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, $\alpha$ , $\beta$ , $\gamma$	43.98Å 99.67Å 134.50Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	50.00 – 2.07 30.85 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.07) 99.0 (30.85-2.07)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.13 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.241 , 0.269 0.241 , 0.269	Depositor DCC
$R_{free}$ test set	3524 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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 72.80 % 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 2.0643e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 8OF, S4M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.71	0/2216	0.95	9/3005 (0.3%)
1	B	0.70	0/2259	0.83	8/3058 (0.3%)
1	C	0.73	0/2199	0.97	8/2978 (0.3%)
1	D	0.69	0/2188	0.84	5/2960 (0.2%)
All	All	0.71	0/8862	0.90	30/12001 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	ARG	NE-CZ-NH2	-20.30	110.15	120.30
1	A	190	ARG	NE-CZ-NH2	-18.20	111.20	120.30
1	C	190	ARG	NE-CZ-NH1	17.74	129.17	120.30
1	A	190	ARG	NE-CZ-NH1	15.24	127.92	120.30
1	D	142	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	C	190	ARG	CD-NE-CZ	7.23	133.72	123.60
1	D	142	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	B	142	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	190	ARG	CD-NE-CZ	6.36	132.51	123.60
1	B	207	LEU	CA-CB-CG	6.29	129.77	115.30
1	C	190	ARG	CG-CD-NE	-6.26	98.66	111.80
1	C	142	ARG	NE-CZ-NH2	-5.95	117.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ARG	CG-CD-NE	-5.93	99.34	111.80
1	D	275	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	287	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	231	LEU	CA-CB-CG	5.66	128.31	115.30
1	C	231	LEU	CA-CB-CG	5.57	128.10	115.30
1	B	190	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	142	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	142	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	142	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	207	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	190	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	207	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	142	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	231	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	A	69	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	231	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	159	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	231	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	15	GLU	Peptide

## 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	2163	0	2115	31	0
1	B	2209	0	2168	20	0
1	C	2149	0	2105	25	0
1	D	2140	0	2100	15	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0
2	C	24	0	24	0	0
2	D	24	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	19	0	0	1	0
3	B	19	0	0	0	0
3	C	19	0	0	1	0
3	D	19	0	0	0	0
4	A	32	0	0	2	0
4	B	39	0	0	0	0
4	C	52	0	0	1	0
4	D	35	0	0	0	0
All	All	8991	0	8584	86	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 (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:HG21	1:A:120:ASP:OD2	1.57	1.05
1:B:37:THR:HG21	1:B:120:ASP:OD2	1.56	1.03
1:C:37:THR:HG21	1:C:120:ASP:OD2	1.61	1.00
1:D:37:THR:HG21	1:D:120:ASP:OD2	1.70	0.91
1:C:37:THR:HG22	1:C:39:PHE:H	1.38	0.86
1:C:236:THR:HG21	1:D:22:GLN:HE22	1.42	0.84
1:A:37:THR:HG22	1:A:39:PHE:H	1.45	0.81
1:A:37:THR:CG2	1:A:39:PHE:H	1.97	0.78
1:B:37:THR:HG22	1:B:39:PHE:H	1.48	0.78
1:D:37:THR:HG22	1:D:39:PHE:H	1.52	0.75
1:C:18:GLN:O	1:C:20:PRO:HD3	1.89	0.73
1:A:37:THR:HG22	1:A:40:GLN:H	1.53	0.72
1:B:37:THR:HG22	1:B:40:GLN:H	1.55	0.71
1:C:37:THR:CG2	1:C:39:PHE:H	2.03	0.70
1:A:234:VAL:HG12	4:A:405:HOH:O	1.91	0.69
1:A:204:SER:O	1:A:208:ASP:HB3	1.92	0.69
1:A:86:PRO:O	1:A:260:ARG:HD3	1.93	0.68
1:D:37:THR:HG22	1:D:40:GLN:H	1.58	0.68
1:B:37:THR:CG2	1:B:39:PHE:H	2.07	0.67
1:A:218:PHE:O	1:A:222:THR:HG23	1.95	0.67
1:C:37:THR:HG22	1:C:40:GLN:H	1.60	0.67
1:D:37:THR:CG2	1:D:39:PHE:H	2.08	0.67
1:A:24:MET:HG2	1:B:24:MET:HE2	1.77	0.66
1:B:169:THR:HG21	1:B:179:LEU:HD23	1.78	0.65
1:C:37:THR:HB	1:C:40:GLN:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HG	1:C:239:CYS:O	2.00	0.61
1:D:86:PRO:O	1:D:260:ARG:HD3	2.02	0.60
1:D:70:GLU:HA	1:D:73:TYR:CZ	2.37	0.59
1:D:121:GLY:HA2	1:D:124:MET:HE3	1.83	0.59
1:C:234:VAL:HG12	4:C:406:HOH:O	2.03	0.58
1:D:202:GLY:O	1:D:203:GLU:HB2	2.05	0.57
1:A:37:THR:HG22	1:A:39:PHE:N	2.17	0.57
1:C:70:GLU:HA	1:C:73:TYR:CZ	2.40	0.57
1:B:70:GLU:HA	1:B:73:TYR:CZ	2.41	0.56
1:A:186:LYS:HG3	1:A:222:THR:HB	1.88	0.56
1:A:234:VAL:CG1	4:A:405:HOH:O	2.52	0.56
1:C:204:SER:HB2	1:C:241:SER:H	1.72	0.55
1:A:232:MET:HG3	1:A:242:ILE:HG23	1.87	0.55
1:C:37:THR:HG22	1:C:39:PHE:N	2.16	0.55
1:C:218:PHE:O	1:C:222:THR:HG23	2.08	0.54
1:D:37:THR:HB	1:D:40:GLN:O	2.08	0.54
1:C:213:GLU:OE2	1:C:291:HIS:CD2	2.61	0.53
1:A:204:SER:HB2	1:A:241:SER:H	1.73	0.53
1:B:86:PRO:O	1:B:260:ARG:HD3	2.09	0.53
1:A:24:MET:HG3	1:A:238:PRO:HG3	1.92	0.52
1:A:157:THR:O	1:A:190:ARG:NH2	2.28	0.52
1:A:70:GLU:HA	1:A:73:TYR:CZ	2.45	0.52
1:A:233:HIS:CE1	1:B:233:HIS:CE1	2.99	0.50
1:D:213:GLU:HG2	1:D:292:ILE:HD11	1.92	0.50
1:A:24:MET:HG2	1:B:24:MET:CE	2.42	0.49
1:A:44:ILE:CD1	1:A:126:GLN:HB3	2.43	0.49
1:B:204:SER:HB2	1:B:241:SER:O	2.13	0.49
1:A:202:GLY:O	1:A:203:GLU:HB2	2.14	0.48
1:A:22:GLN:NE2	1:B:53:TRP:HE1	2.11	0.48
1:C:203:GLU:HB3	1:C:208:ASP:OD1	2.14	0.48
1:A:44:ILE:HD12	1:A:126:GLN:HB3	1.96	0.47
1:D:213:GLU:HG2	1:D:292:ILE:CD1	2.46	0.46
1:B:213:GLU:HG2	1:B:292:ILE:CD1	2.46	0.46
1:B:213:GLU:HG2	1:B:292:ILE:HD11	1.97	0.46
1:A:37:THR:HB	1:A:40:GLN:O	2.16	0.46
1:B:202:GLY:O	1:B:203:GLU:HB2	2.16	0.46
1:B:37:THR:HB	1:B:40:GLN:O	2.16	0.45
1:D:37:THR:HG22	1:D:39:PHE:N	2.26	0.45
1:B:37:THR:CG2	1:B:120:ASP:OD2	2.47	0.45
1:A:213:GLU:OE1	1:A:291:HIS:HD2	2.00	0.45
1:D:200:ASN:C	1:D:200:ASN:OD1	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:HG22	1:B:39:PHE:N	2.25	0.44
1:A:207:LEU:C	1:A:209:LEU:H	2.20	0.44
1:B:209:LEU:O	1:B:213:GLU:HG3	2.18	0.43
1:C:202:GLY:O	1:C:203:GLU:HB2	2.19	0.43
1:A:225:ALA:HB1	1:A:251:ALA:HA	2.01	0.42
1:C:120:ASP:O	1:C:124:MET:HE3	2.19	0.42
1:C:28:VAL:HG13	1:C:45:PHE:HB2	2.01	0.42
1:A:38:LYS:HE3	1:A:39:PHE:CZ	2.55	0.42
1:A:37:THR:HG23	1:A:38:LYS:N	2.36	0.41
1:C:113:HIS:HE1	1:C:144:THR:OG1	2.03	0.41
1:C:204:SER:HB2	1:C:241:SER:O	2.21	0.41
1:A:73:TYR:CD1	3:A:302:8OF:C15	3.04	0.41
1:B:44:ILE:CD1	1:B:126:GLN:HB3	2.50	0.41
1:C:118:ASP:HB3	1:C:124:MET:CE	2.51	0.41
1:A:258:PRO:HG3	1:A:279:HIS:CG	2.56	0.41
1:C:37:THR:HG23	1:C:38:LYS:N	2.36	0.41
1:C:118:ASP:HB3	1:C:124:MET:HE1	2.03	0.40
1:D:203:GLU:HG3	1:D:211:LEU:HD23	2.02	0.40
1:C:73:TYR:CD1	3:C:302:8OF:C15	3.05	0.40
1:C:44:ILE:CD1	1:C:126:GLN:HB3	2.52	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	269/304 (88%)	259 (96%)	8 (3%)	2 (1%)	22	11
1	B	271/304 (89%)	262 (97%)	9 (3%)	0	100	100
1	C	266/304 (88%)	258 (97%)	8 (3%)	0	100	100
1	D	262/304 (86%)	252 (96%)	10 (4%)	0	100	100
All	All	1068/1216 (88%)	1031 (96%)	35 (3%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	A	207	LEU

### 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	238/262 (91%)	225 (94%)	13 (6%)	21	13
1	B	243/262 (93%)	230 (95%)	13 (5%)	22	14
1	C	237/262 (90%)	227 (96%)	10 (4%)	30	23
1	D	236/262 (90%)	225 (95%)	11 (5%)	26	18
All	All	954/1048 (91%)	907 (95%)	47 (5%)	25	17

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	17	ASP
1	A	24	MET
1	A	37	THR
1	A	73	TYR
1	A	124	MET
1	A	133	GLN
1	A	170	THR
1	A	199	CYS
1	A	210	GLU
1	A	232	MET
1	A	239	CYS
1	A	287	ARG
1	B	7	ILE
1	B	27	ARG
1	B	37	THR
1	B	73	TYR
1	B	146	ARG

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Mol	Chain	Res	Type
1	B	179	LEU
1	B	199	CYS
1	B	201	GLN
1	B	204	SER
1	B	214	LYS
1	B	218	PHE
1	B	232	MET
1	B	269	LYS
1	C	17	ASP
1	C	37	THR
1	C	73	TYR
1	C	170	THR
1	C	199	CYS
1	C	207	LEU
1	C	214	LYS
1	C	220	ARG
1	C	239	CYS
1	C	269	LYS
1	D	7	ILE
1	D	16	ASN
1	D	37	THR
1	D	73	TYR
1	D	136	ARG
1	D	199	CYS
1	D	204	SER
1	D	214	LYS
1	D	232	MET
1	D	269	LYS
1	D	290	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	129	GLN
1	A	233	HIS
1	A	291	HIS
1	B	22	GLN
1	B	129	GLN
1	B	233	HIS
1	C	113	HIS
1	C	129	GLN

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Mol	Chain	Res	Type
1	C	201	GLN
1	D	22	GLN
1	D	113	HIS
1	D	129	GLN

### 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 carbohydrates 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	8OF	C	302	-	21,21,21	1.08	4 (19%)	28,28,28	2.17	6 (21%)
3	8OF	B	302	-	21,21,21	0.99	2 (9%)	28,28,28	1.69	4 (14%)
3	8OF	D	302	-	21,21,21	0.99	1 (4%)	28,28,28	1.92	5 (17%)
2	S4M	B	301	-	22,26,26	0.87	0	21,37,37	1.16	3 (14%)
2	S4M	D	301	-	22,26,26	0.94	0	21,37,37	1.31	4 (19%)
2	S4M	C	301	-	22,26,26	0.88	0	21,37,37	0.96	0
2	S4M	A	301	-	22,26,26	0.95	1 (4%)	21,37,37	1.30	1 (4%)
3	8OF	A	302	-	21,21,21	1.03	2 (9%)	28,28,28	2.59	9 (32%)



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	8OF	C	302	-	-	2/6/6/6	0/3/3/3
3	8OF	B	302	-	-	4/6/6/6	0/3/3/3
3	8OF	D	302	-	-	1/6/6/6	0/3/3/3
2	S4M	B	301	-	-	4/7/28/28	0/3/3/3
2	S4M	D	301	-	-	4/7/28/28	0/3/3/3
2	S4M	C	301	-	-	4/7/28/28	0/3/3/3
2	S4M	A	301	-	-	5/7/28/28	0/3/3/3
3	8OF	A	302	-	-	0/6/6/6	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	8OF	C2-C1	-2.21	1.38	1.43
3	C	302	8OF	C3-N7	-2.19	1.33	1.37
3	C	302	8OF	C4-C1	-2.19	1.37	1.42
2	A	301	S4M	C2'-C1'	-2.18	1.50	1.53
3	C	302	8OF	C2-C1	-2.15	1.38	1.43
3	D	302	8OF	C2-C1	-2.06	1.39	1.43
3	A	302	8OF	C2-C1	-2.05	1.39	1.43
3	A	302	8OF	C3-N7	-2.05	1.33	1.37
3	B	302	8OF	C8-C3	-2.04	1.38	1.41
3	C	302	8OF	C8-C3	-2.04	1.38	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	8OF	C1-C2-N5	8.02	134.49	118.60
3	A	302	8OF	C6-C2-N5	-6.59	105.96	123.92
3	C	302	8OF	C1-C2-N5	6.37	131.22	118.60
3	C	302	8OF	C6-C2-N5	-5.21	109.70	123.92
3	A	302	8OF	C10-N5-C2	4.97	139.05	126.71
3	B	302	8OF	C19-O18-C17	-4.59	107.54	117.51
3	D	302	8OF	C19-O18-C17	-4.49	107.77	117.51
3	D	302	8OF	C1-C2-N5	4.38	127.27	118.60
3	D	302	8OF	C6-C2-N5	-4.08	112.80	123.92
3	C	302	8OF	C10-N5-C2	4.07	136.81	126.71
2	A	301	S4M	C5'-SD-CG	-3.75	93.83	103.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	8OF	C19-O18-C17	-3.72	109.44	117.51
3	B	302	8OF	C1-C2-N5	3.66	125.86	118.60
3	B	302	8OF	C6-C2-N5	-3.38	114.71	123.92
3	D	302	8OF	C10-N5-C2	3.37	135.07	126.71
2	D	301	S4M	C5'-SD-CG	-3.24	95.15	103.40
3	A	302	8OF	C13-C10-N5	-2.84	111.13	120.64
3	B	302	8OF	C10-N5-C2	2.84	133.76	126.71
2	D	301	S4M	O4'-C1'-C2'	-2.77	102.88	106.93
3	D	302	8OF	C13-C10-N5	-2.52	112.19	120.64
3	A	302	8OF	C6-C11-N7	-2.46	120.77	124.58
3	A	302	8OF	C2-C1-C3	-2.42	116.53	118.06
3	A	302	8OF	C14-C10-N5	2.32	128.41	120.64
2	B	301	S4M	C1'-N9-C4	-2.28	122.64	126.64
3	C	302	8OF	C13-C10-N5	-2.23	113.17	120.64
3	A	302	8OF	C19-O18-C17	-2.22	112.69	117.51
2	B	301	S4M	C5'-SD-CG	-2.22	97.75	103.40
2	D	301	S4M	O3'-C3'-C4'	-2.10	104.97	111.05
3	A	302	8OF	C11-C6-C2	2.08	120.64	119.60
2	D	301	S4M	O4'-C4'-C5'	2.07	114.12	108.88
3	C	302	8OF	C12-C9-C4	2.02	123.28	120.44
2	B	301	S4M	C2'-C3'-C4'	2.01	106.54	102.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	S4M	O4'-C4'-C5'-SD
2	B	301	S4M	C3'-C4'-C5'-SD
2	D	301	S4M	O4'-C4'-C5'-SD
2	D	301	S4M	C3'-C4'-C5'-SD
2	C	301	S4M	CA-CB-CG-SD
2	C	301	S4M	O4'-C4'-C5'-SD
2	C	301	S4M	C3'-C4'-C5'-SD
2	A	301	S4M	CB-CG-SD-CE
2	A	301	S4M	O4'-C4'-C5'-SD
2	A	301	S4M	C3'-C4'-C5'-SD
3	C	302	8OF	C15-C17-O18-C19
3	B	302	8OF	C15-C17-O18-C19
3	C	302	8OF	C16-C17-O18-C19
3	B	302	8OF	C16-C17-O18-C19
2	D	301	S4M	N-CA-CB-CG
2	B	301	S4M	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	A	301	S4M	CB-CG-SD-C5'
3	B	302	8OF	C6-C2-N5-C10
2	A	301	S4M	N-CA-CB-CG
3	D	302	8OF	C6-C2-N5-C10
3	B	302	8OF	C1-C2-N5-C10
2	B	301	S4M	CA-CB-CG-SD
2	D	301	S4M	CA-CB-CG-SD
2	C	301	S4M	CB-CG-SD-C5'

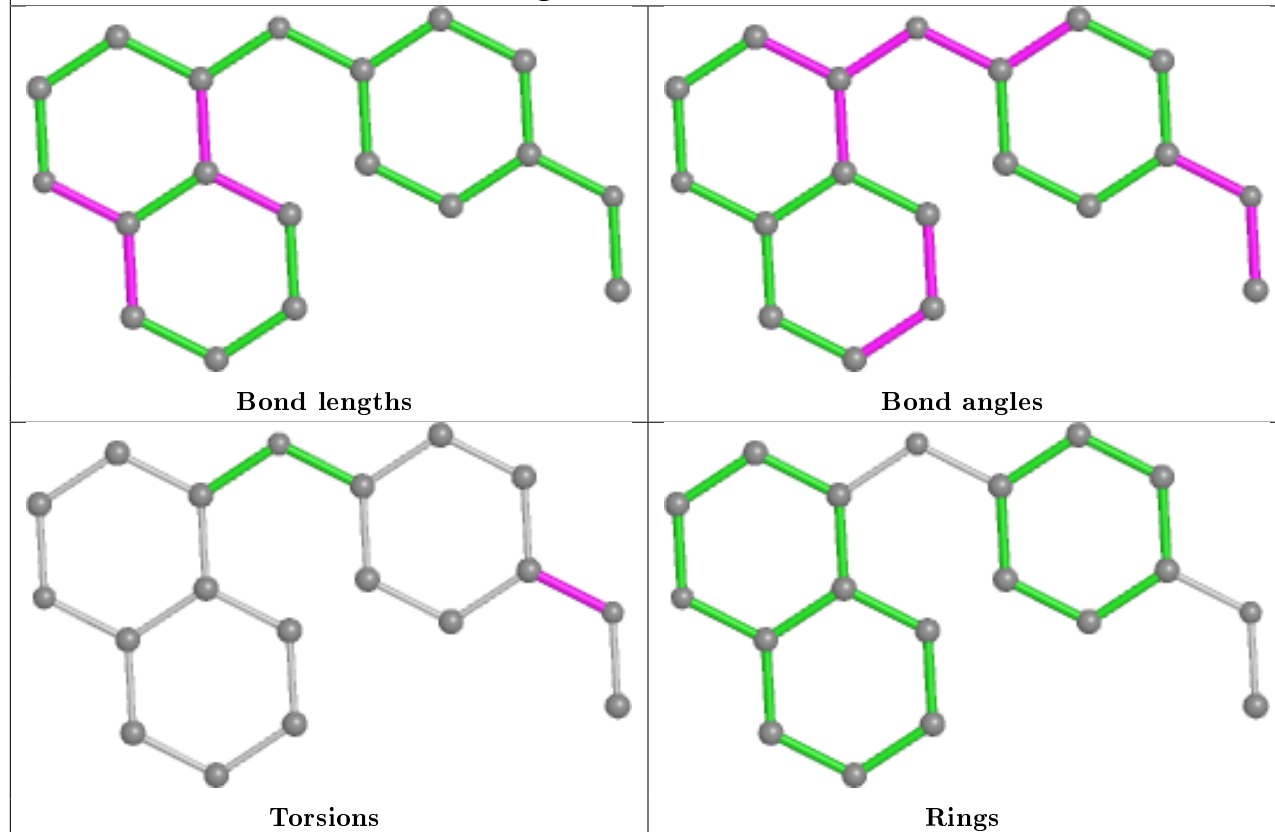
There are no ring outliers.

2 monomers are involved in 2 short contacts:

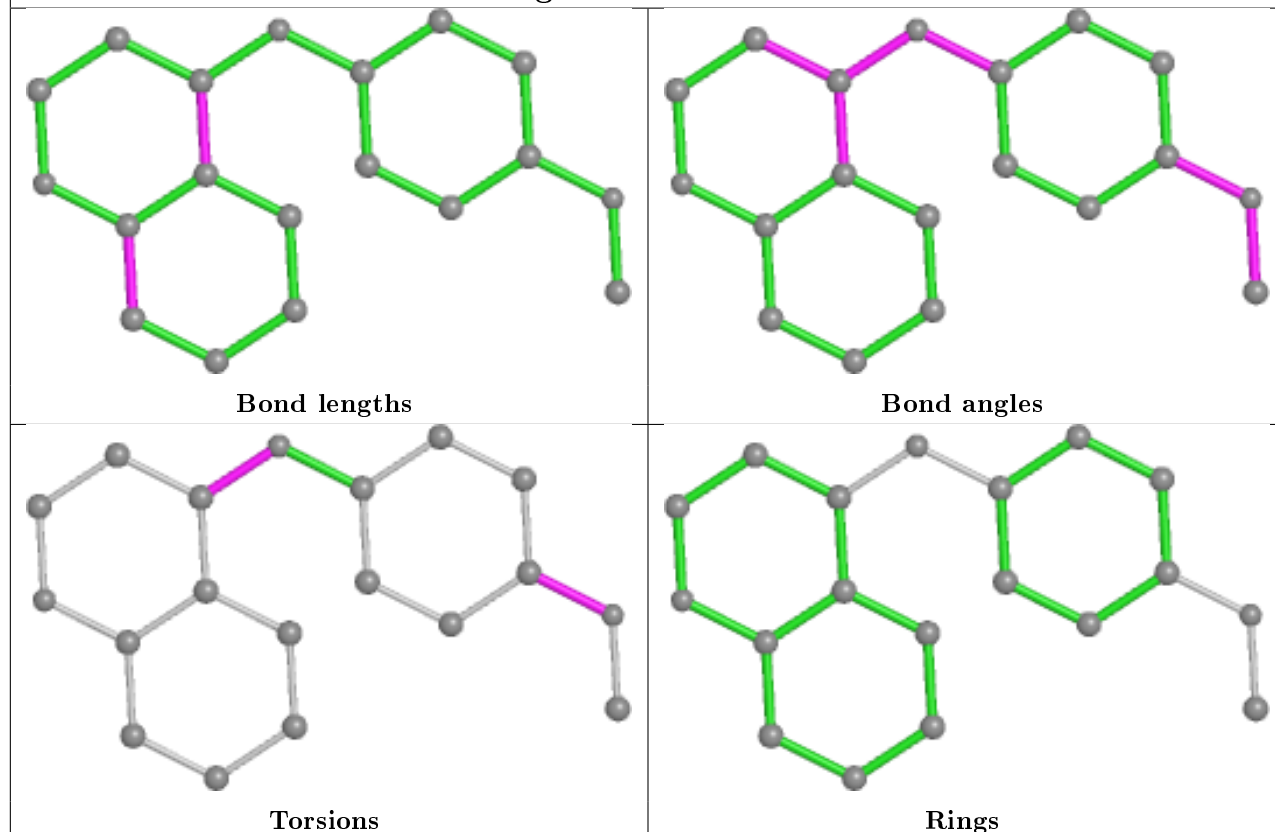
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	8OF	1	0
3	A	302	8OF	1	0

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.

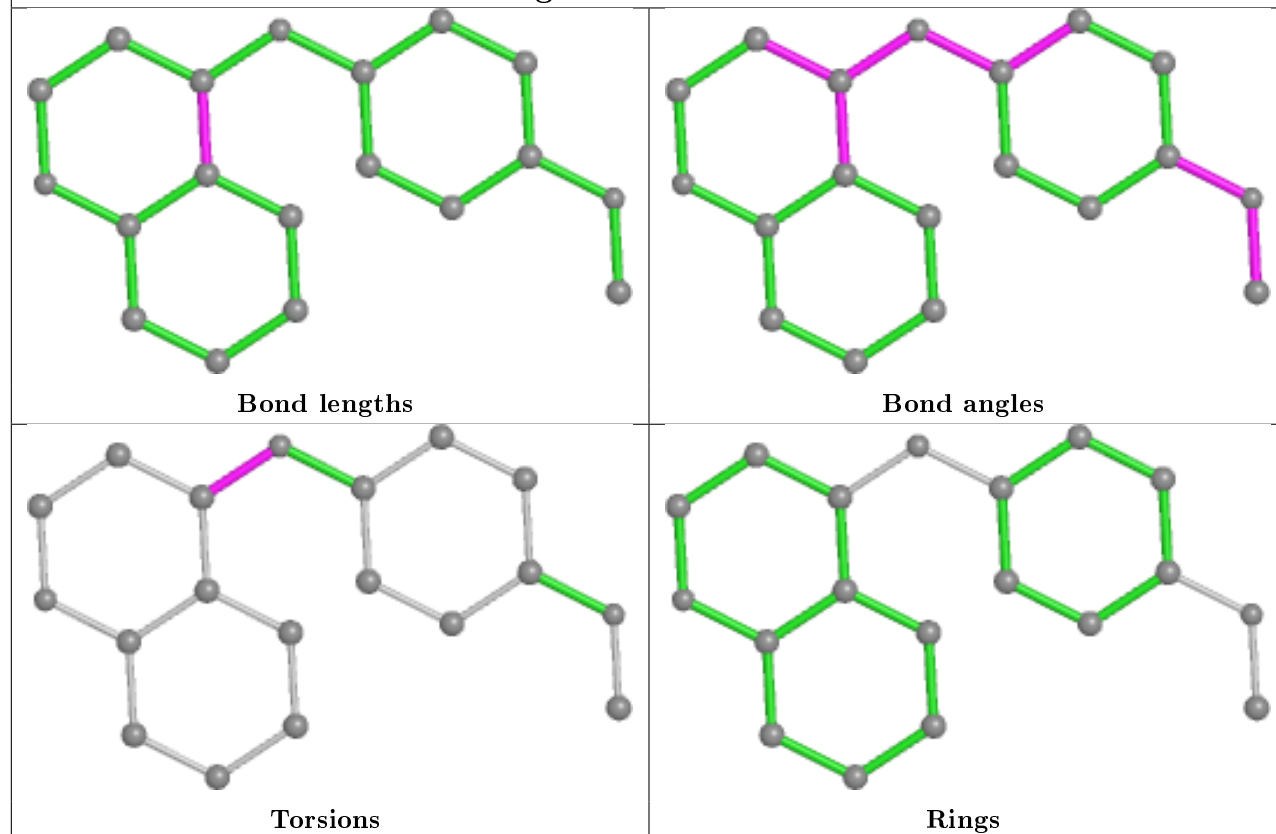
## Ligand 8OF C 302



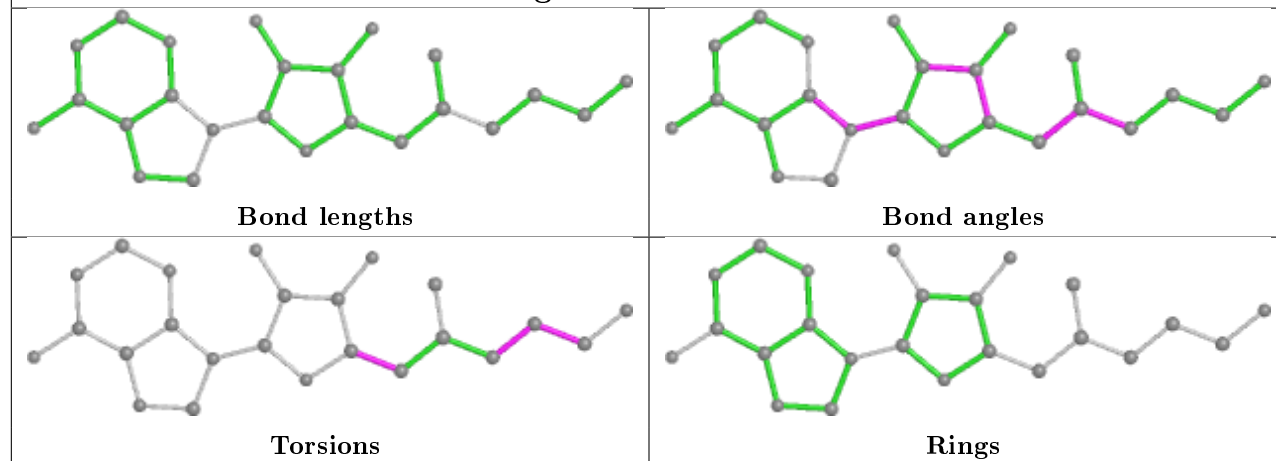
## Ligand 8OF B 302



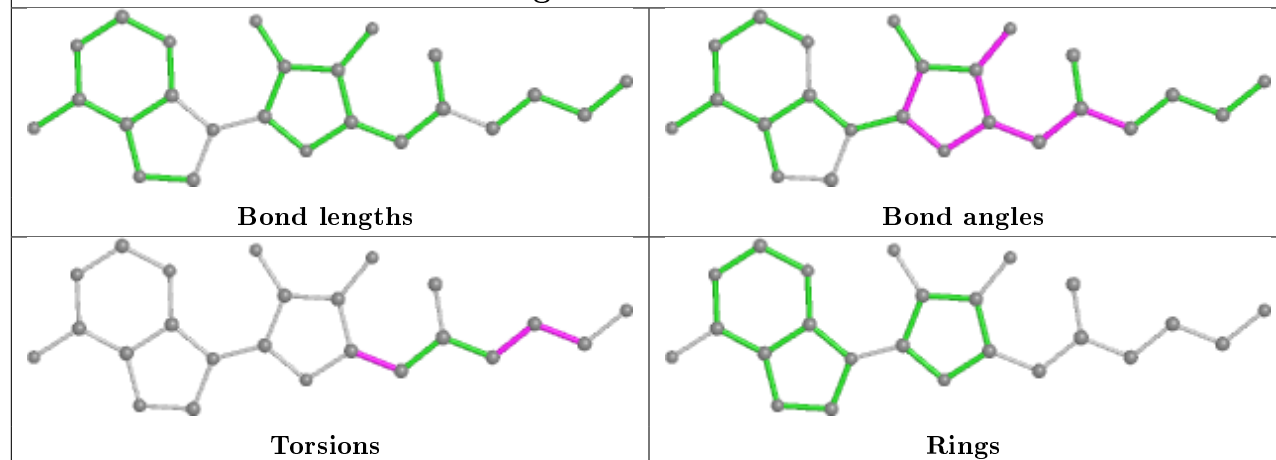
## Ligand 8OF D 302



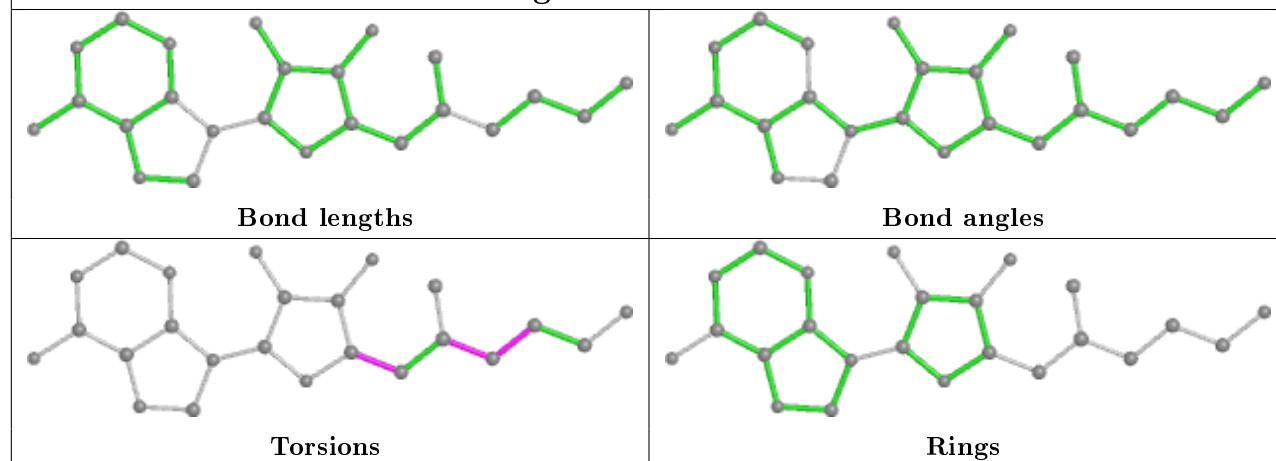
## Ligand S4M B 301



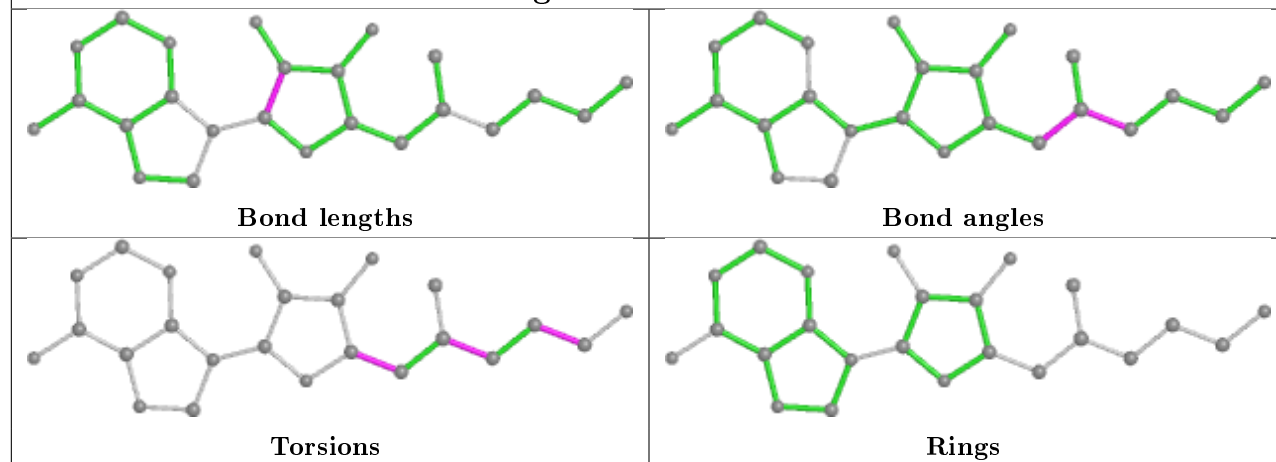
## Ligand S4M D 301

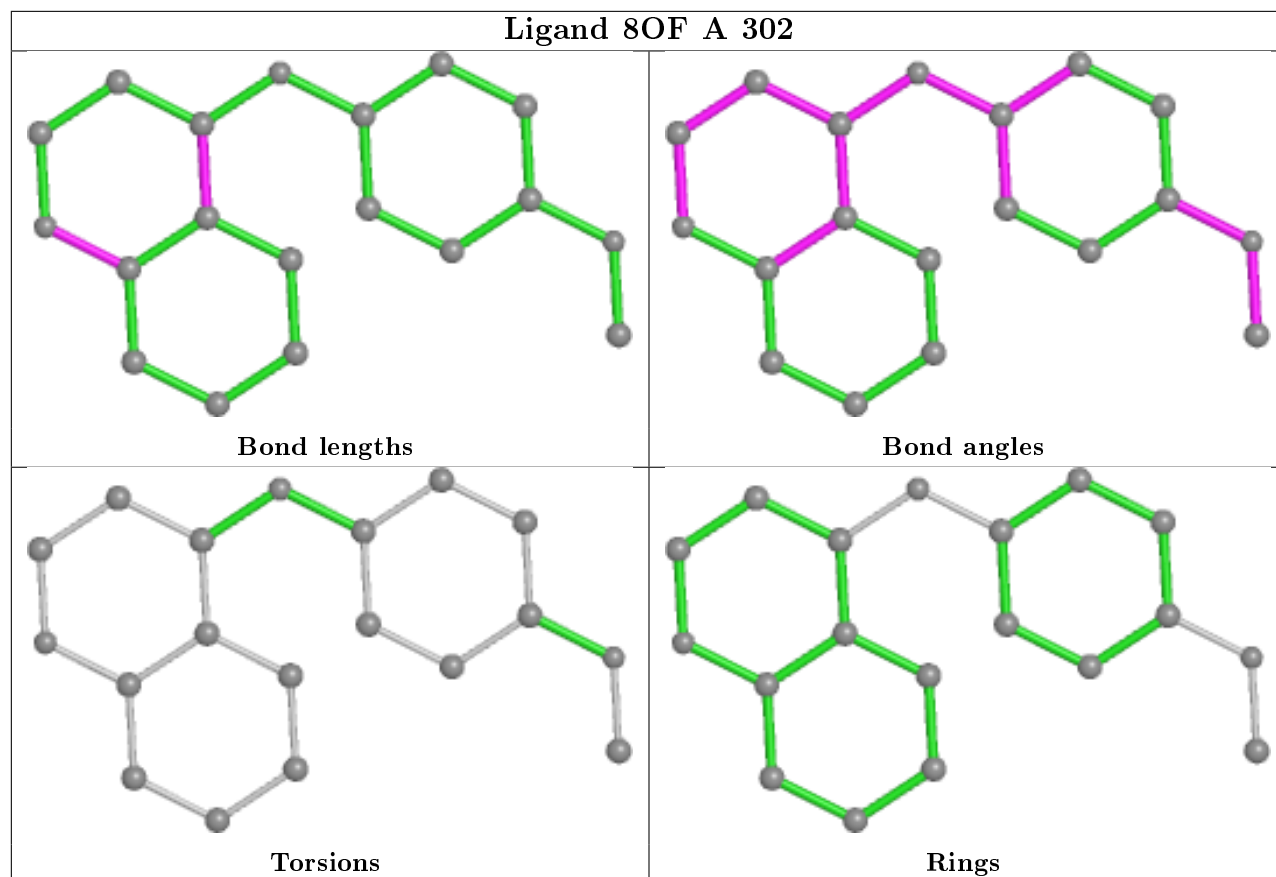


## Ligand S4M C 301



## Ligand S4M A 301





## 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	273/304 (89%)	0.69	26 (9%) 8 8	22, 35, 56, 73	0
1	B	279/304 (91%)	0.54	26 (9%) 8 9	21, 35, 59, 73	0
1	C	272/304 (89%)	0.52	23 (8%) 10 11	20, 32, 55, 81	0
1	D	270/304 (88%)	0.35	13 (4%) 30 31	19, 34, 51, 77	0
All	All	1094/1216 (89%)	0.53	88 (8%) 12 12	19, 34, 56, 81	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	177	SER	6.0
1	A	19	TRP	5.8
1	A	239	CYS	4.2
1	B	241	SER	4.1
1	A	294	ASN	4.0
1	A	51	GLY	4.0
1	D	242	ILE	4.0
1	A	27	ARG	3.9
1	B	237	TYR	3.8
1	C	11	TRP	3.8
1	C	207	LEU	3.5
1	D	17	ASP	3.4
1	B	19	TRP	3.4
1	B	176	ALA	3.4
1	C	239	CYS	3.3
1	C	294	ASN	3.3
1	D	237	TYR	3.2
1	B	242	ILE	3.2
1	C	136	ARG	3.1
1	B	17	ASP	3.1
1	C	17	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	166	ILE	3.1
1	B	166	ILE	3.0
1	C	170	THR	3.0
1	A	207	LEU	3.0
1	C	27	ARG	3.0
1	A	210	GLU	2.9
1	C	18	GLN	2.9
1	A	18	GLN	2.9
1	A	30	LYS	2.9
1	A	49	PRO	2.9
1	C	16	ASN	2.9
1	B	20	PRO	2.9
1	D	50	LYS	2.8
1	A	17	ASP	2.8
1	C	166	ILE	2.8
1	A	136	ARG	2.8
1	B	183	ALA	2.8
1	A	77	LEU	2.8
1	C	199	CYS	2.7
1	A	16	ASN	2.7
1	D	236	THR	2.7
1	A	50	LYS	2.7
1	A	11	TRP	2.6
1	A	76	VAL	2.6
1	D	166	ILE	2.6
1	B	36	PRO	2.6
1	A	183	ALA	2.6
1	B	170	THR	2.6
1	C	210	GLU	2.6
1	B	236	THR	2.5
1	D	136	ARG	2.5
1	C	93	ILE	2.5
1	C	77	LEU	2.4
1	B	38	LYS	2.4
1	B	199	CYS	2.4
1	B	35	ALA	2.4
1	C	208	ASP	2.4
1	A	242	ILE	2.3
1	B	39	PHE	2.3
1	D	112	GLU	2.3
1	C	238	PRO	2.3
1	D	194	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	136	ARG	2.3
1	C	50	LYS	2.3
1	C	36	PRO	2.3
1	B	211	LEU	2.2
1	B	18	GLN	2.2
1	C	197	ILE	2.2
1	C	76	VAL	2.2
1	C	203	GLU	2.2
1	C	183	ALA	2.2
1	B	179	LEU	2.1
1	B	294	ASN	2.1
1	B	7	ILE	2.1
1	D	231	LEU	2.1
1	A	155	ARG	2.1
1	D	72	VAL	2.1
1	D	234	VAL	2.1
1	A	199	CYS	2.1
1	A	93	ILE	2.1
1	B	5	GLU	2.1
1	A	133	GLN	2.1
1	D	251	ALA	2.0
1	B	93	ILE	2.0
1	A	164	VAL	2.0
1	A	234	VAL	2.0
1	B	234	VAL	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

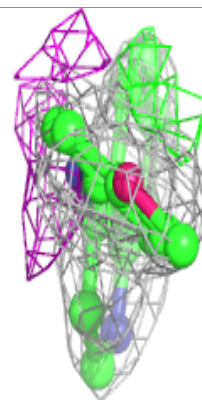
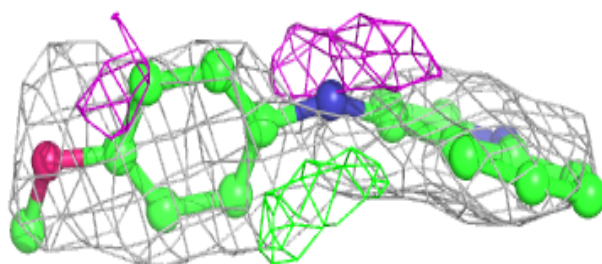
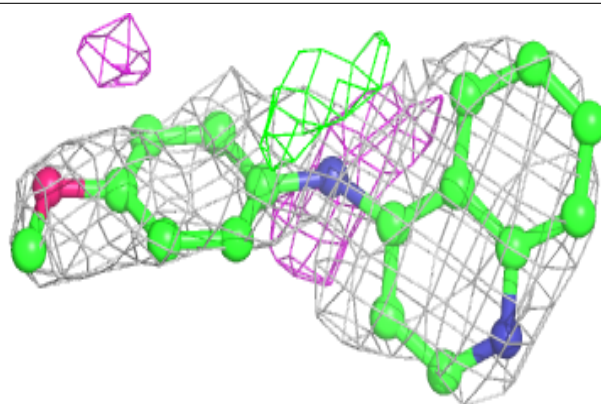
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	8OF	D	302	19/19	0.78	0.30	66,69,71,73	0
3	8OF	A	302	19/19	0.80	0.22	50,53,57,58	0
3	8OF	C	302	19/19	0.83	0.26	53,55,57,58	0
2	S4M	A	301	24/24	0.83	0.18	39,43,52,56	0
3	8OF	B	302	19/19	0.83	0.34	70,72,75,75	0
2	S4M	B	301	24/24	0.90	0.14	37,43,57,65	0
2	S4M	C	301	24/24	0.90	0.13	39,43,58,66	0
2	S4M	D	301	24/24	0.91	0.12	40,44,55,58	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.

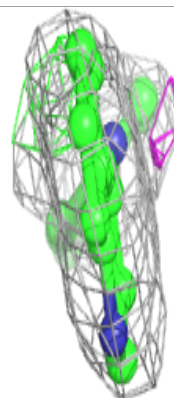
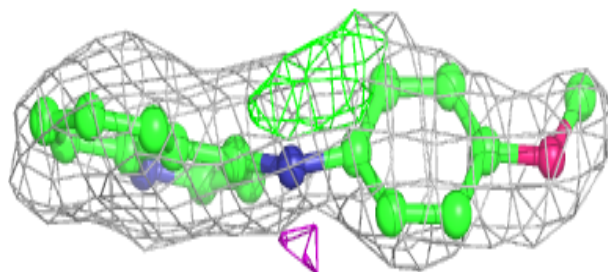
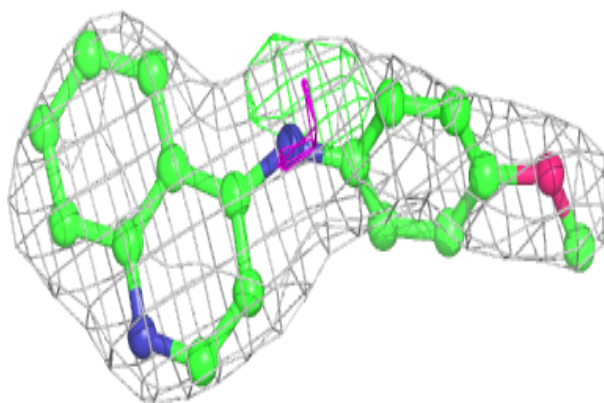
**Electron density around 8OF D 302:**

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)

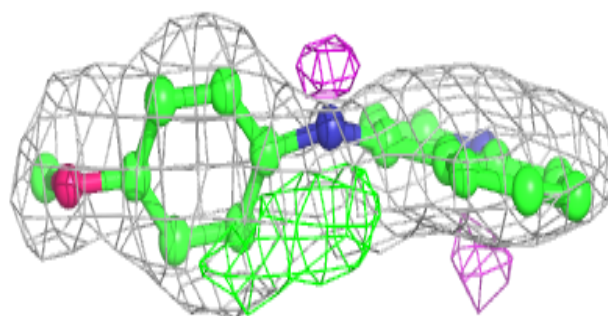
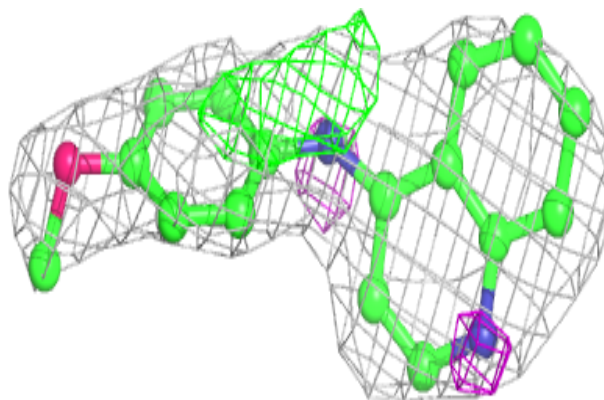


**Electron density around 8OF A 302:**

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

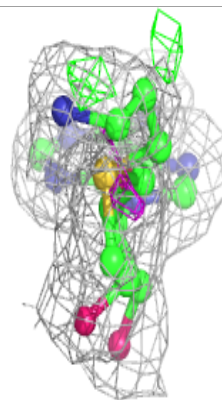
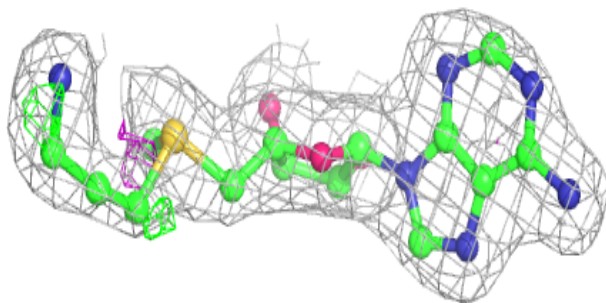
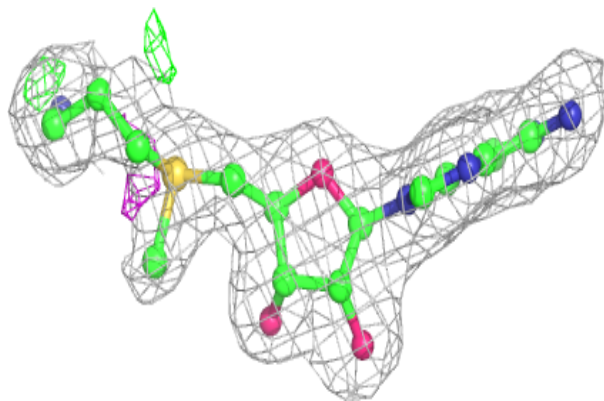
**Electron density around 8OF C 302:**

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

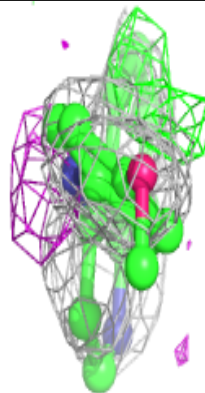
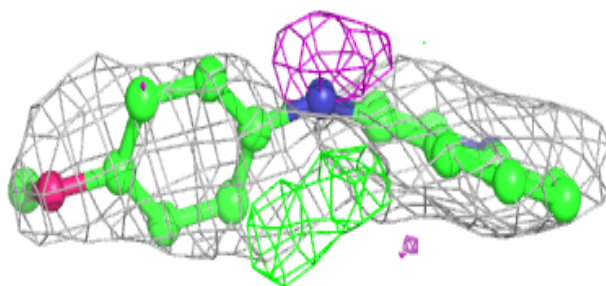
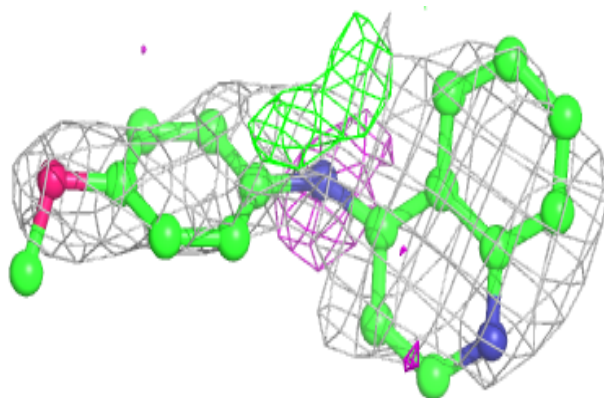


**Electron density around S4M A 301:**

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

**Electron density around 8OF B 302:**

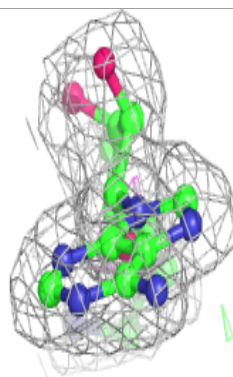
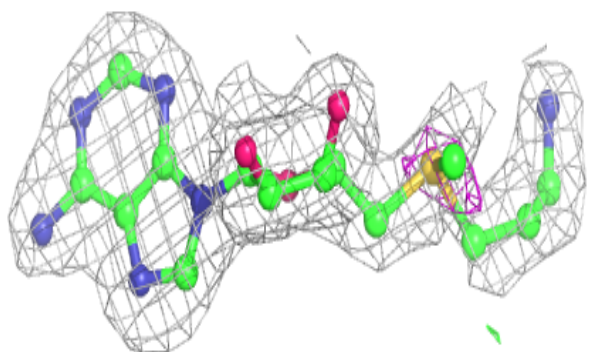
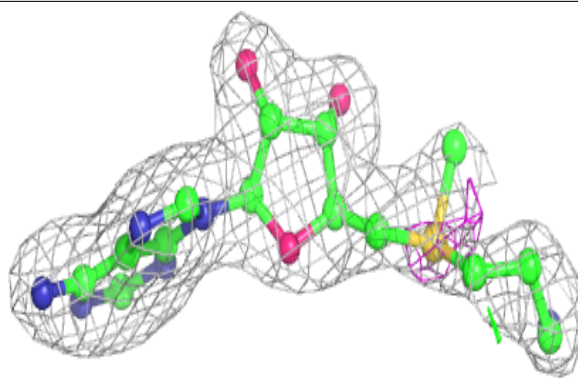
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



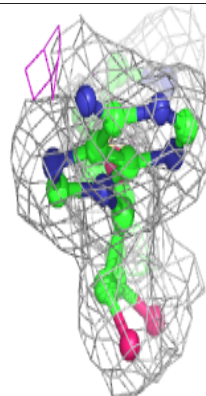
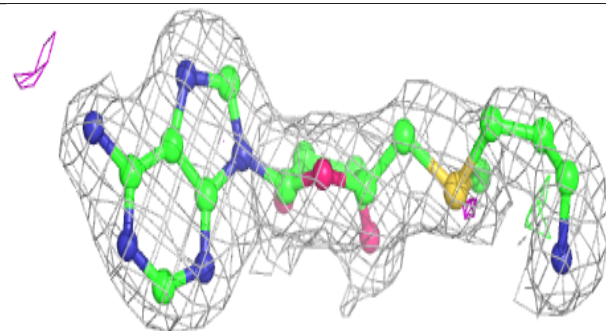
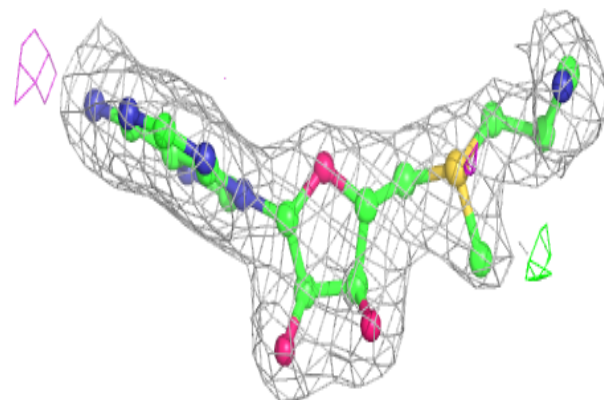


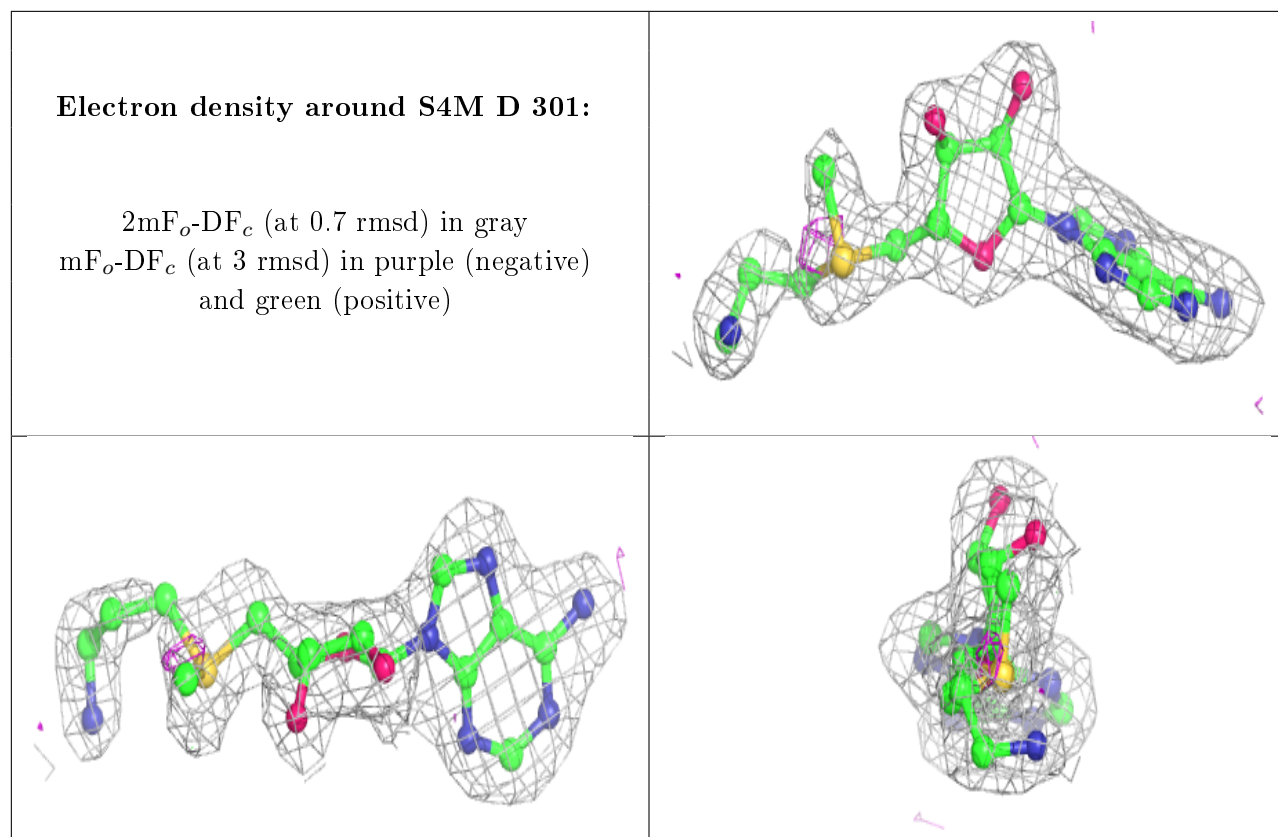
**Electron density around S4M B 301:**

$2mF_o-DF_c$  (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.