



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:08 PM BST

PDB ID : 4HZ5  
Title : Pyrrolopyrimidine inhibitors of dna gyrase b and topoisomerase iv, part i: structure guided discovery and optimization of dual targeting agents with potent, broad-spectrum enzymatic activity  
Authors : Bensen, D.C.; Creighton, C.J.; Tari, L.W.  
Deposited on : 2012-11-14  
Resolution : 2.70 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 : 2.13.1  
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) : 2.13.1

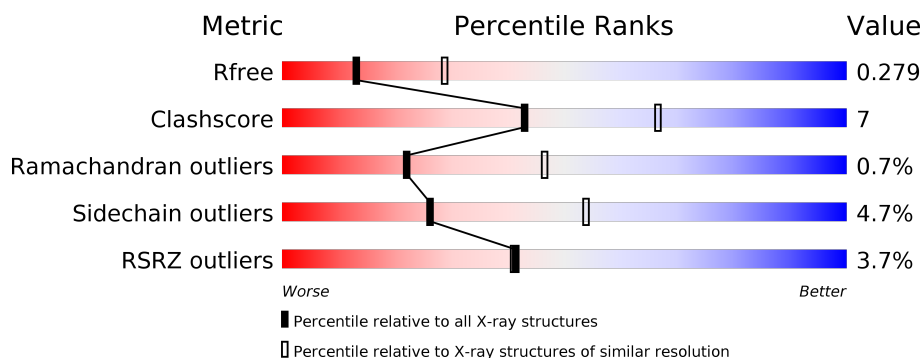
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	216	
1	B	216	
1	C	216	
1	D	216	
1	E	216	
1	F	216	

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Mol	Chain	Length	Quality of chain
1	G	216	<div><div></div><div>7%</div><div>71%</div><div>16%</div><div>•</div><div>12%</div></div>
1	H	216	<div><div></div><div>11%</div><div>78%</div><div>10%</div><div>•</div><div>12%</div></div>
1	J	216	<div><div></div><div>7%</div><div>74%</div><div>11%</div><div></div><div>14%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13507 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 DNA topoisomerase IV, B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1483	933	256	289	5			
1	B	190	Total	C	N	O	S	0	0	0
			1474	928	255	286	5			
1	C	191	Total	C	N	O	S	0	0	0
			1483	933	256	289	5			
1	D	190	Total	C	N	O	S	0	0	0
			1478	930	255	288	5			
1	E	191	Total	C	N	O	S	0	0	0
			1483	933	256	289	5			
1	F	191	Total	C	N	O	S	0	0	0
			1483	933	256	289	5			
1	G	190	Total	C	N	O	S	0	0	0
			1474	928	255	286	5			
1	H	191	Total	C	N	O	S	0	0	0
			1483	933	256	289	5			
1	J	185	Total	C	N	O	S	0	0	0
			1431	901	243	282	5			

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	EXPRESSION TAG	UNP H7C794
A	226	LEU	-	EXPRESSION TAG	UNP H7C794
A	227	GLU	-	EXPRESSION TAG	UNP H7C794
A	228	HIS	-	EXPRESSION TAG	UNP H7C794
A	229	HIS	-	EXPRESSION TAG	UNP H7C794
A	230	HIS	-	EXPRESSION TAG	UNP H7C794
A	231	HIS	-	EXPRESSION TAG	UNP H7C794
A	232	HIS	-	EXPRESSION TAG	UNP H7C794
A	233	HIS	-	EXPRESSION TAG	UNP H7C794
B	18	MET	-	EXPRESSION TAG	UNP H7C794
B	226	LEU	-	EXPRESSION TAG	UNP H7C794

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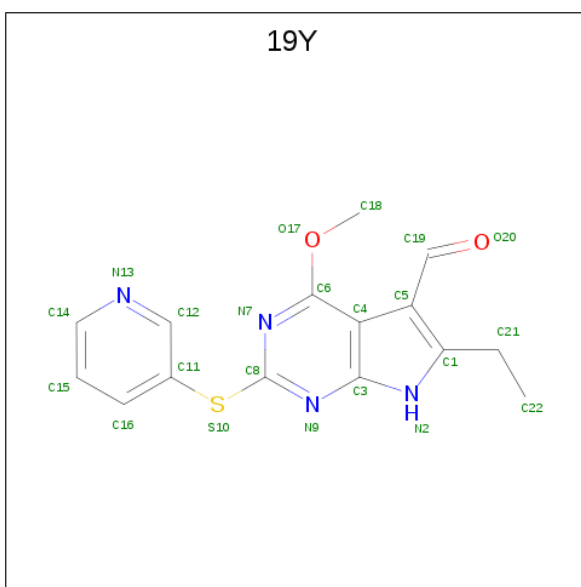
Chain	Residue	Modelled	Actual	Comment	Reference
B	227	GLU	-	EXPRESSION TAG	UNP H7C794
B	228	HIS	-	EXPRESSION TAG	UNP H7C794
B	229	HIS	-	EXPRESSION TAG	UNP H7C794
B	230	HIS	-	EXPRESSION TAG	UNP H7C794
B	231	HIS	-	EXPRESSION TAG	UNP H7C794
B	232	HIS	-	EXPRESSION TAG	UNP H7C794
B	233	HIS	-	EXPRESSION TAG	UNP H7C794
C	18	MET	-	EXPRESSION TAG	UNP H7C794
C	226	LEU	-	EXPRESSION TAG	UNP H7C794
C	227	GLU	-	EXPRESSION TAG	UNP H7C794
C	228	HIS	-	EXPRESSION TAG	UNP H7C794
C	229	HIS	-	EXPRESSION TAG	UNP H7C794
C	230	HIS	-	EXPRESSION TAG	UNP H7C794
C	231	HIS	-	EXPRESSION TAG	UNP H7C794
C	232	HIS	-	EXPRESSION TAG	UNP H7C794
C	233	HIS	-	EXPRESSION TAG	UNP H7C794
D	18	MET	-	EXPRESSION TAG	UNP H7C794
D	226	LEU	-	EXPRESSION TAG	UNP H7C794
D	227	GLU	-	EXPRESSION TAG	UNP H7C794
D	228	HIS	-	EXPRESSION TAG	UNP H7C794
D	229	HIS	-	EXPRESSION TAG	UNP H7C794
D	230	HIS	-	EXPRESSION TAG	UNP H7C794
D	231	HIS	-	EXPRESSION TAG	UNP H7C794
D	232	HIS	-	EXPRESSION TAG	UNP H7C794
D	233	HIS	-	EXPRESSION TAG	UNP H7C794
E	18	MET	-	EXPRESSION TAG	UNP H7C794
E	226	LEU	-	EXPRESSION TAG	UNP H7C794
E	227	GLU	-	EXPRESSION TAG	UNP H7C794
E	228	HIS	-	EXPRESSION TAG	UNP H7C794
E	229	HIS	-	EXPRESSION TAG	UNP H7C794
E	230	HIS	-	EXPRESSION TAG	UNP H7C794
E	231	HIS	-	EXPRESSION TAG	UNP H7C794
E	232	HIS	-	EXPRESSION TAG	UNP H7C794
E	233	HIS	-	EXPRESSION TAG	UNP H7C794
F	18	MET	-	EXPRESSION TAG	UNP H7C794
F	226	LEU	-	EXPRESSION TAG	UNP H7C794
F	227	GLU	-	EXPRESSION TAG	UNP H7C794
F	228	HIS	-	EXPRESSION TAG	UNP H7C794
F	229	HIS	-	EXPRESSION TAG	UNP H7C794
F	230	HIS	-	EXPRESSION TAG	UNP H7C794
F	231	HIS	-	EXPRESSION TAG	UNP H7C794
F	232	HIS	-	EXPRESSION TAG	UNP H7C794

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Chain	Residue	Modelled	Actual	Comment	Reference
F	233	HIS	-	EXPRESSION TAG	UNP H7C794
G	18	MET	-	EXPRESSION TAG	UNP H7C794
G	226	LEU	-	EXPRESSION TAG	UNP H7C794
G	227	GLU	-	EXPRESSION TAG	UNP H7C794
G	228	HIS	-	EXPRESSION TAG	UNP H7C794
G	229	HIS	-	EXPRESSION TAG	UNP H7C794
G	230	HIS	-	EXPRESSION TAG	UNP H7C794
G	231	HIS	-	EXPRESSION TAG	UNP H7C794
G	232	HIS	-	EXPRESSION TAG	UNP H7C794
G	233	HIS	-	EXPRESSION TAG	UNP H7C794
H	18	MET	-	EXPRESSION TAG	UNP H7C794
H	226	LEU	-	EXPRESSION TAG	UNP H7C794
H	227	GLU	-	EXPRESSION TAG	UNP H7C794
H	228	HIS	-	EXPRESSION TAG	UNP H7C794
H	229	HIS	-	EXPRESSION TAG	UNP H7C794
H	230	HIS	-	EXPRESSION TAG	UNP H7C794
H	231	HIS	-	EXPRESSION TAG	UNP H7C794
H	232	HIS	-	EXPRESSION TAG	UNP H7C794
H	233	HIS	-	EXPRESSION TAG	UNP H7C794
J	18	MET	-	EXPRESSION TAG	UNP H7C794
J	226	LEU	-	EXPRESSION TAG	UNP H7C794
J	227	GLU	-	EXPRESSION TAG	UNP H7C794
J	228	HIS	-	EXPRESSION TAG	UNP H7C794
J	229	HIS	-	EXPRESSION TAG	UNP H7C794
J	230	HIS	-	EXPRESSION TAG	UNP H7C794
J	231	HIS	-	EXPRESSION TAG	UNP H7C794
J	232	HIS	-	EXPRESSION TAG	UNP H7C794
J	233	HIS	-	EXPRESSION TAG	UNP H7C794

- Molecule 2 is 6-ethyl-4-methoxy-2-(pyridin-3-ylsulfanyl)-7H-pyrrolo[2,3-d]pyrimidine-5-carb aldehyde (three-letter code: 19Y) (formula: C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
2	B	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
2	C	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
2	D	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
2	E	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
2	F	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
2	G	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
2	J	1	Total	C	N	O	S	0	0
			22	15	4	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	2	Total	O	0	0
			2	2		
3	C	10	Total	O	0	0
			10	10		
3	D	8	Total	O	0	0
			8	8		

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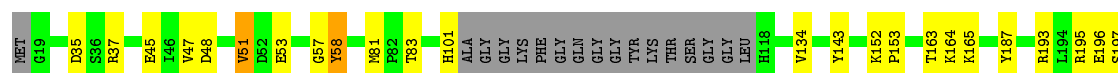
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	3	Total 3	O 3	0	0
3	F	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	J	4	Total 4	O 4	0	0



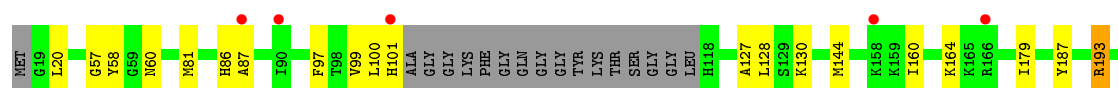




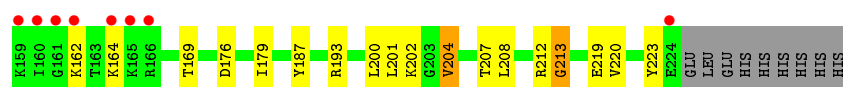
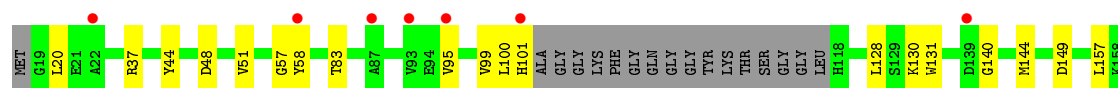
- Molecule 1: DNA topoisomerase IV, B subunit



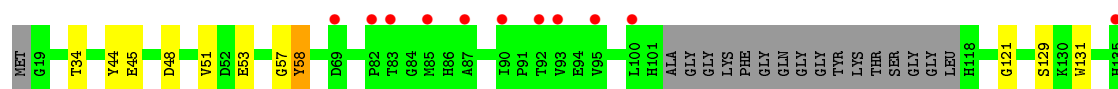
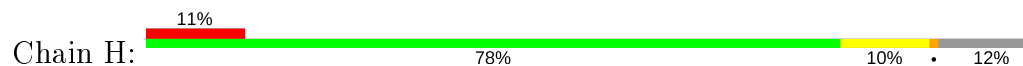
- Molecule 1: DNA topoisomerase IV, B subunit



- Molecule 1: DNA topoisomerase IV, B subunit

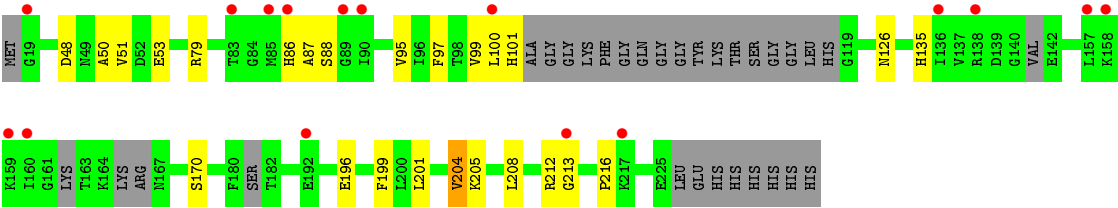


- Molecule 1: DNA topoisomerase IV, B subunit



- Molecule 1: DNA topoisomerase IV, B subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.21 Å   144.21 Å   84.17 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 2.70 47.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.70) 97.8 (47.20-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.231 , 0.280 0.231 , 0.279	Depositor DCC
$R_{free}$ test set	2663 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 35.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l 0.022 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 19Y

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	0.42	0/1509	0.59	0/2036
1	B	0.42	1/1500 (0.1%)	0.55	0/2024
1	C	0.42	0/1509	0.55	0/2036
1	D	0.42	0/1503	0.56	0/2026
1	E	0.40	0/1509	0.53	0/2036
1	F	0.42	0/1509	0.54	0/2036
1	G	0.41	1/1500 (0.1%)	0.53	0/2024
1	H	0.41	1/1509 (0.1%)	0.50	0/2036
1	J	0.40	0/1452	0.49	0/1955
All	All	0.41	3/13500 (0.0%)	0.54	0/18209

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	131	TRP	CD2-CE2	5.10	1.47	1.41
1	B	131	TRP	CD2-CE2	5.05	1.47	1.41
1	G	131	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

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	1483	0	1467	28	0
1	B	1474	0	1461	20	0
1	C	1483	0	1467	25	0
1	D	1478	0	1461	19	0
1	E	1483	0	1467	23	0
1	F	1483	0	1467	21	0
1	G	1474	0	1461	21	0
1	H	1483	0	1467	14	0
1	J	1431	0	1403	15	0
2	A	22	0	14	0	0
2	B	22	0	14	0	0
2	C	22	0	14	0	0
2	D	22	0	14	0	0
2	E	22	0	14	0	0
2	F	22	0	14	0	0
2	G	22	0	14	0	0
2	J	22	0	14	1	0
3	A	29	0	0	0	0
3	B	2	0	0	0	0
3	C	10	0	0	0	0
3	D	8	0	0	0	0
3	E	3	0	0	0	0
3	F	2	0	0	0	0
3	H	1	0	0	0	0
3	J	4	0	0	0	0
All	All	13507	0	13233	180	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 7.

All (180) 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:57:GLY:HA3	1:A:58:TYR:CG	1.86	1.10
1:A:57:GLY:HA3	1:A:58:TYR:CD2	1.98	0.96
1:G:212:ARG:N	1:G:213:GLY:HA3	1.80	0.96
1:C:201:LEU:HB3	1:C:204:VAL:HG13	1.54	0.89
1:D:212:ARG:N	1:D:213:GLY:HA3	1.87	0.89
1:B:212:ARG:N	1:B:213:GLY:HA3	1.91	0.86
1:J:212:ARG:N	1:J:213:GLY:HA3	1.91	0.86
1:E:212:ARG:N	1:E:213:GLY:HA3	1.92	0.85
1:B:201:LEU:HB3	1:B:204:VAL:HG13	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HB2	1:B:101:HIS:C	1.99	0.82
1:C:100:LEU:CB	1:C:101:HIS:HB2	2.10	0.81
1:D:201:LEU:HB3	1:D:204:VAL:HG13	1.64	0.79
1:G:201:LEU:HB3	1:G:204:VAL:HG13	1.63	0.79
1:J:212:ARG:H	1:J:213:GLY:HA3	1.48	0.78
1:A:201:LEU:HB3	1:A:204:VAL:HG13	1.65	0.78
1:A:100:LEU:HB2	1:A:101:HIS:C	2.06	0.76
1:E:201:LEU:HB3	1:E:204:VAL:HG13	1.66	0.76
1:F:212:ARG:N	1:F:213:GLY:HA3	2.01	0.76
1:G:100:LEU:HB2	1:G:101:HIS:HB2	1.71	0.73
1:A:212:ARG:N	1:A:213:GLY:HA3	2.03	0.73
1:A:57:GLY:HA3	1:A:58:TYR:CB	2.19	0.73
1:F:57:GLY:HA2	1:F:58:TYR:CD2	2.23	0.73
1:H:57:GLY:CA	1:H:58:TYR:HB2	2.20	0.71
1:H:207:THR:HG22	1:H:220:VAL:HG12	1.73	0.71
1:C:100:LEU:HB3	1:C:101:HIS:HB2	1.71	0.71
1:F:207:THR:HG22	1:F:220:VAL:HG12	1.73	0.70
1:F:193:ARG:HH21	1:F:193:ARG:HG2	1.55	0.70
1:F:201:LEU:HB3	1:F:204:VAL:HG13	1.73	0.70
1:G:212:ARG:H	1:G:213:GLY:HA3	1.57	0.69
1:G:207:THR:HG22	1:G:220:VAL:HG12	1.75	0.68
1:A:223:TYR:HB3	1:A:224:GLU:HB2	1.78	0.65
1:F:100:LEU:HB2	1:F:101:HIS:C	2.17	0.65
1:E:193:ARG:HG3	1:E:193:ARG:HH21	1.63	0.64
1:E:212:ARG:H	1:E:213:GLY:HA3	1.60	0.63
1:A:48:ASP:HA	1:A:51:VAL:HG13	1.80	0.63
1:C:100:LEU:HB2	1:C:101:HIS:HB2	1.79	0.63
1:C:201:LEU:HB3	1:C:204:VAL:CG1	2.25	0.63
1:G:202:LYS:HA	1:G:223:TYR:O	1.99	0.63
1:D:57:GLY:HA2	1:D:58:TYR:HB2	1.81	0.63
1:H:53:GLU:O	1:H:57:GLY:HA3	1.99	0.63
1:G:212:ARG:N	1:G:213:GLY:CA	2.60	0.62
1:J:201:LEU:HB3	1:J:204:VAL:HG13	1.82	0.62
1:C:192:GLU:OE2	1:D:45:GLU:HG2	2.00	0.61
1:F:193:ARG:HG2	1:F:193:ARG:NH2	2.11	0.61
1:G:100:LEU:CB	1:G:101:HIS:HB2	2.30	0.61
1:F:212:ARG:H	1:F:213:GLY:HA3	1.66	0.61
1:A:223:TYR:CA	1:A:224:GLU:HB2	2.33	0.59
1:G:201:LEU:HB3	1:G:204:VAL:CG1	2.32	0.59
1:G:44:TYR:CE2	1:G:193:ARG:HG2	2.37	0.59
1:H:57:GLY:CA	1:H:58:TYR:CB	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:GLY:HA3	1:H:58:TYR:HB2	1.83	0.58
1:C:195:ARG:HD2	1:C:199:PHE:CZ	2.38	0.58
1:C:212:ARG:N	1:C:213:GLY:HA3	2.18	0.58
1:C:57:GLY:HA2	1:C:58:TYR:HB2	1.85	0.57
1:H:201:LEU:HB3	1:H:204:VAL:HG13	1.86	0.57
1:F:201:LEU:HB3	1:F:204:VAL:CG1	2.34	0.56
1:F:81:MET:HE1	1:F:97:PHE:HE1	1.71	0.56
1:H:57:GLY:HA2	1:H:58:TYR:HB2	1.86	0.56
1:J:48:ASP:HA	1:J:51:VAL:HG22	1.87	0.56
1:D:100:LEU:HB2	1:D:101:HIS:C	2.25	0.56
1:F:99:VAL:HG12	1:F:101:HIS:HA	1.87	0.56
1:E:48:ASP:HA	1:E:51:VAL:CG1	2.36	0.56
1:A:223:TYR:HA	1:A:224:GLU:HB2	1.89	0.55
1:B:196:GLU:HA	1:B:199:PHE:CD1	2.40	0.55
1:J:100:LEU:N	1:J:101:HIS:HA	2.22	0.55
1:H:57:GLY:HA2	1:H:58:TYR:CD2	2.42	0.54
1:B:207:THR:HG22	1:B:220:VAL:HG12	1.88	0.54
1:C:57:GLY:HA2	1:C:58:TYR:CB	2.38	0.54
1:C:81:MET:HE2	1:C:134:VAL:HG21	1.88	0.54
1:D:57:GLY:HA2	1:D:58:TYR:CB	2.36	0.54
1:F:57:GLY:HA2	1:F:58:TYR:CG	2.43	0.54
1:F:20:LEU:HD22	1:F:127:ALA:HB2	1.90	0.54
1:A:201:LEU:HB3	1:A:204:VAL:CG1	2.36	0.53
1:B:128:LEU:HD22	1:B:179:ILE:HG21	1.88	0.53
1:C:100:LEU:HB3	1:C:101:HIS:CB	2.38	0.53
1:B:187:TYR:OH	1:B:219:GLU:HG2	2.08	0.53
1:A:57:GLY:CA	1:A:58:TYR:CD2	2.85	0.53
1:A:100:LEU:CB	1:A:101:HIS:C	2.77	0.52
1:D:48:ASP:HA	1:D:51:VAL:HG22	1.93	0.51
1:J:95:VAL:O	1:J:99:VAL:HG22	2.11	0.51
1:A:137:VAL:HG22	1:A:142:GLU:HG3	1.93	0.51
1:D:97:PHE:HB3	1:D:126:ASN:HD22	1.75	0.51
1:A:223:TYR:CB	1:A:224:GLU:HB2	2.40	0.51
1:D:53:GLU:O	1:D:57:GLY:CA	2.59	0.51
1:B:48:ASP:HA	1:B:51:VAL:HG13	1.94	0.50
1:B:142:GLU:HG2	1:B:160:ILE:HD12	1.93	0.50
1:E:193:ARG:CG	1:E:193:ARG:HH21	2.21	0.50
1:G:95:VAL:O	1:G:99:VAL:HG22	2.12	0.50
1:H:44:TYR:CE2	1:H:193:ARG:HG2	2.45	0.50
1:A:72:ILE:O	1:A:172:THR:HA	2.11	0.50
1:F:193:ARG:CG	1:F:193:ARG:HH21	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:TYR:CZ	1:G:193:ARG:HG2	2.46	0.49
1:E:57:GLY:HA2	1:E:58:TYR:CD2	2.47	0.49
1:H:57:GLY:HA2	1:H:58:TYR:CB	2.43	0.49
1:G:187:TYR:OH	1:G:219:GLU:HG2	2.13	0.49
1:E:212:ARG:N	1:E:213:GLY:CA	2.72	0.48
1:J:196:GLU:HA	1:J:199:PHE:CD1	2.48	0.48
1:B:81:MET:HE1	1:B:97:PHE:HE1	1.79	0.47
1:A:212:ARG:H	1:A:213:GLY:HA3	1.76	0.47
1:B:100:LEU:CB	1:B:101:HIS:C	2.79	0.47
1:A:205:LYS:HD3	1:A:207:THR:HG23	1.97	0.47
1:B:201:LEU:HB3	1:B:204:VAL:CG1	2.38	0.47
1:F:196:GLU:HA	1:F:199:PHE:CD1	2.50	0.47
1:E:196:GLU:HA	1:E:199:PHE:CD1	2.50	0.47
1:D:194:LEU:HD12	1:D:208:LEU:HG	1.97	0.47
1:C:137:VAL:HG22	1:C:142:GLU:HG3	1.97	0.46
1:F:57:GLY:CA	1:F:58:TYR:CB	2.93	0.46
1:J:212:ARG:N	1:J:213:GLY:CA	2.71	0.46
1:E:195:ARG:HD2	1:E:199:PHE:CZ	2.51	0.46
1:C:81:MET:HB2	1:C:136:ILE:HG12	1.97	0.46
1:J:97:PHE:HB3	1:J:126:ASN:HD22	1.81	0.46
1:A:57:GLY:CA	1:A:58:TYR:CB	2.92	0.46
1:B:212:ARG:N	1:B:213:GLY:CA	2.73	0.46
1:E:57:GLY:HA2	1:E:58:TYR:CB	2.45	0.46
1:G:48:ASP:HA	1:G:51:VAL:HG22	1.98	0.46
1:F:60:ASN:HA	1:F:204:VAL:HB	1.98	0.46
1:H:187:TYR:OH	1:H:219:GLU:HG2	2.15	0.46
1:F:187:TYR:OH	1:F:219:GLU:HG2	2.16	0.45
1:H:48:ASP:HA	1:H:51:VAL:HG22	1.98	0.45
1:F:144:MET:HB2	1:F:160:ILE:HD11	1.98	0.45
1:D:212:ARG:N	1:D:213:GLY:CA	2.71	0.45
1:E:163:THR:HB	1:E:165:LYS:HG2	1.97	0.45
1:G:130:LYS:HG3	1:G:176:ASP:HA	1.99	0.45
1:B:208:LEU:O	1:B:218:GLU:HA	2.16	0.45
1:F:86:HIS:CG	1:F:87:ALA:N	2.85	0.45
1:A:207:THR:HG22	1:A:220:VAL:HG22	1.99	0.44
1:B:57:GLY:HA2	1:B:58:TYR:HB2	2.00	0.44
1:D:20:LEU:HD22	1:D:127:ALA:HB2	1.99	0.44
1:E:53:GLU:O	1:E:57:GLY:CA	2.65	0.44
1:A:81:MET:HE3	1:A:93:VAL:HG22	1.99	0.44
1:C:72:ILE:O	1:C:172:THR:HA	2.17	0.44
1:F:128:LEU:HD22	1:F:179:ILE:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ARG:HD2	1:B:199:PHE:CZ	2.53	0.44
1:H:45:GLU:HG2	1:H:121:GLY:HA3	2.00	0.44
1:E:57:GLY:HA2	1:E:58:TYR:HB2	2.00	0.43
1:C:199:PHE:HB3	1:D:200:LEU:HG	2.00	0.43
1:J:135:HIS:HB2	1:J:170:SER:HB3	1.99	0.43
1:C:53:GLU:O	1:C:57:GLY:CA	2.67	0.43
1:D:187:TYR:CD2	1:D:210:ASP:HB2	2.54	0.43
1:E:51:VAL:HG23	1:E:201:LEU:HD21	1.99	0.43
1:D:136:ILE:HG13	1:D:169:THR:HG23	2.00	0.43
1:G:83:THR:HG23	1:G:157:LEU:HD21	2.01	0.43
1:C:164:LYS:H	1:C:164:LYS:HE2	1.83	0.43
1:A:144:MET:HG2	1:A:145:GLU:N	2.34	0.42
1:A:192:GLU:HG3	1:C:45:GLU:OE2	2.18	0.42
1:B:81:MET:HE3	1:B:93:VAL:HG22	1.99	0.42
1:E:195:ARG:HG3	1:E:221:PHE:CD2	2.53	0.42
1:C:163:THR:HG22	1:C:164:LYS:HE2	2.02	0.42
1:E:47:VAL:O	1:E:51:VAL:HG12	2.19	0.42
1:G:200:LEU:HD23	1:J:199:PHE:CB	2.49	0.42
1:G:200:LEU:HD23	1:J:199:PHE:HB3	2.02	0.42
1:G:57:GLY:HA2	1:G:58:TYR:CB	2.49	0.42
1:H:201:LEU:HB3	1:H:204:VAL:CG1	2.50	0.42
1:A:81:MET:HG3	1:A:169:THR:HG21	2.00	0.42
1:E:83:THR:HG21	1:E:143:TYR:CD1	2.54	0.42
1:A:215:GLU:HA	1:A:216:PRO:HD3	1.95	0.42
1:E:193:ARG:CG	1:E:193:ARG:NH2	2.81	0.42
1:C:135:HIS:CE1	1:C:144:MET:HG3	2.55	0.42
1:D:214:GLU:CD	1:D:214:GLU:H	2.22	0.42
1:G:128:LEU:HD22	1:G:179:ILE:HG21	2.02	0.41
1:J:50:ALA:HB2	2:J:301:19Y:H2	2.02	0.41
1:J:86:HIS:C	1:J:88:SER:H	2.23	0.41
1:D:208:LEU:O	1:D:218:GLU:HA	2.20	0.41
1:E:81:MET:HE2	1:E:134:VAL:HG21	2.02	0.41
1:J:201:LEU:HB3	1:J:204:VAL:CG1	2.49	0.41
1:A:81:MET:CE	1:A:93:VAL:HG13	2.51	0.41
1:C:81:MET:HE1	1:C:97:PHE:HE1	1.85	0.41
1:E:152:LYS:HA	1:E:153:PRO:HD3	1.92	0.41
1:G:57:GLY:HA2	1:G:58:TYR:HB2	2.02	0.41
1:B:187:TYR:CD2	1:B:210:ASP:HB2	2.56	0.41
1:B:48:ASP:HA	1:B:51:VAL:CG1	2.51	0.41
1:A:200:LEU:HG	1:D:199:PHE:HB3	2.02	0.41
1:E:187:TYR:CD2	1:E:210:ASP:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:SER:HA	1:E:200:LEU:HD22	2.03	0.41
1:B:86:HIS:CD2	1:B:88:SER:H	2.39	0.40
1:C:195:ARG:HG3	1:C:221:PHE:CD2	2.55	0.40
1:C:62:ILE:HB	1:C:206:ILE:HG12	2.03	0.40
1:C:47:VAL:O	1:C:51:VAL:HG13	2.21	0.40
1:A:208:LEU:O	1:A:218:GLU:HB2	2.21	0.40
1:D:44:TYR:CE2	1:D:193:ARG:HG2	2.56	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	187/216 (87%)	178 (95%)	6 (3%)	3 (2%)	9	24
1	B	186/216 (86%)	180 (97%)	6 (3%)	0	100	100
1	C	187/216 (87%)	179 (96%)	8 (4%)	0	100	100
1	D	184/216 (85%)	173 (94%)	10 (5%)	1 (0%)	29	54
1	E	187/216 (87%)	179 (96%)	7 (4%)	1 (0%)	29	54
1	F	187/216 (87%)	176 (94%)	11 (6%)	0	100	100
1	G	186/216 (86%)	166 (89%)	17 (9%)	3 (2%)	9	24
1	H	187/216 (87%)	178 (95%)	7 (4%)	2 (1%)	14	34
1	J	173/216 (80%)	153 (88%)	18 (10%)	2 (1%)	13	32
All	All	1664/1944 (86%)	1562 (94%)	90 (5%)	12 (1%)	22	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	TYR

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Mol	Chain	Res	Type
1	A	224	GLU
1	G	140	GLY
1	H	214	GLU
1	G	149	ASP
1	H	58	TYR
1	J	87	ALA
1	J	216	PRO
1	A	216	PRO
1	G	213	GLY
1	E	213	GLY
1	D	120	VAL

### 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	162/179 (90%)	152 (94%)	10 (6%)	18	40
1	B	161/179 (90%)	154 (96%)	7 (4%)	29	57
1	C	162/179 (90%)	155 (96%)	7 (4%)	29	57
1	D	162/179 (90%)	155 (96%)	7 (4%)	29	57
1	E	162/179 (90%)	151 (93%)	11 (7%)	16	36
1	F	162/179 (90%)	156 (96%)	6 (4%)	34	63
1	G	161/179 (90%)	153 (95%)	8 (5%)	24	51
1	H	162/179 (90%)	155 (96%)	7 (4%)	29	57
1	J	156/179 (87%)	151 (97%)	5 (3%)	39	68
All	All	1450/1611 (90%)	1382 (95%)	68 (5%)	26	54

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
1	A	144	MET
1	A	159	LYS

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Mol	Chain	Res	Type
1	A	166	ARG
1	A	193	ARG
1	A	200	LEU
1	A	204	VAL
1	A	205	LYS
1	A	208	LEU
1	A	225	GLU
1	B	37	ARG
1	B	51	VAL
1	B	164	LYS
1	B	195	ARG
1	B	204	VAL
1	B	205	LYS
1	B	208	LEU
1	C	51	VAL
1	C	158	LYS
1	C	163	THR
1	C	164	LYS
1	C	195	ARG
1	C	204	VAL
1	C	208	LEU
1	D	36	SER
1	D	70	ASN
1	D	160	ILE
1	D	162	LYS
1	D	200	LEU
1	D	204	VAL
1	D	208	LEU
1	E	35	ASP
1	E	37	ARG
1	E	45	GLU
1	E	51	VAL
1	E	58	TYR
1	E	101	HIS
1	E	164	LYS
1	E	200	LEU
1	E	204	VAL
1	E	208	LEU
1	E	224	GLU
1	F	130	LYS
1	F	164	LYS
1	F	193	ARG

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Mol	Chain	Res	Type
1	F	200	LEU
1	F	204	VAL
1	F	208	LEU
1	G	20	LEU
1	G	37	ARG
1	G	144	MET
1	G	162	LYS
1	G	164	LYS
1	G	169	THR
1	G	204	VAL
1	G	208	LEU
1	H	34	THR
1	H	129	SER
1	H	149	ASP
1	H	182	THR
1	H	204	VAL
1	H	208	LEU
1	H	212	ARG
1	J	53	GLU
1	J	79	ARG
1	J	204	VAL
1	J	205	LYS
1	J	208	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	86	HIS
1	B	86	HIS
1	B	135	HIS
1	E	86	HIS
1	F	67	GLN
1	F	86	HIS
1	H	67	GLN
1	H	86	HIS
1	J	49	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	19Y	F	301	-	22,24,24	2.82	7 (31%)	20,33,33	3.42	8 (40%)
2	19Y	D	301	-	22,24,24	2.74	7 (31%)	20,33,33	3.42	9 (45%)
2	19Y	E	301	-	22,24,24	2.79	7 (31%)	20,33,33	3.42	8 (40%)
2	19Y	C	301	-	22,24,24	2.75	7 (31%)	20,33,33	3.41	10 (50%)
2	19Y	G	301	-	22,24,24	2.81	7 (31%)	20,33,33	3.36	9 (45%)
2	19Y	J	301	-	22,24,24	2.80	7 (31%)	20,33,33	3.33	8 (40%)
2	19Y	A	301	-	22,24,24	2.76	6 (27%)	20,33,33	3.33	8 (40%)
2	19Y	B	301	-	22,24,24	2.74	7 (31%)	20,33,33	3.37	9 (45%)

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
2	19Y	F	301	-	-	1/7/10/10	0/3/3/3
2	19Y	D	301	-	-	4/7/10/10	0/3/3/3
2	19Y	E	301	-	-	2/7/10/10	0/3/3/3
2	19Y	C	301	-	-	3/7/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	19Y	G	301	-	-	2/7/10/10	0/3/3/3
2	19Y	J	301	-	-	4/7/10/10	0/3/3/3
2	19Y	A	301	-	-	2/7/10/10	0/3/3/3
2	19Y	B	301	-	-	2/7/10/10	0/3/3/3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	19Y	C5-C1	9.48	1.48	1.38
2	G	301	19Y	C5-C1	9.41	1.48	1.38
2	J	301	19Y	C5-C1	9.34	1.48	1.38
2	E	301	19Y	C5-C1	9.30	1.48	1.38
2	C	301	19Y	C5-C1	9.23	1.48	1.38
2	D	301	19Y	C5-C1	9.16	1.48	1.38
2	B	301	19Y	C5-C1	9.06	1.48	1.38
2	A	301	19Y	C5-C1	9.06	1.48	1.38
2	E	301	19Y	C8-S10	-4.67	1.69	1.75
2	A	301	19Y	C8-S10	-4.64	1.69	1.75
2	G	301	19Y	C8-S10	-4.53	1.69	1.75
2	F	301	19Y	C8-S10	-4.36	1.69	1.75
2	C	301	19Y	C8-S10	-4.34	1.70	1.75
2	B	301	19Y	C8-S10	-4.34	1.70	1.75
2	D	301	19Y	C8-S10	-4.21	1.70	1.75
2	A	301	19Y	C5-C4	4.20	1.48	1.40
2	J	301	19Y	C8-S10	-4.20	1.70	1.75
2	F	301	19Y	C6-C4	4.15	1.49	1.43
2	B	301	19Y	C6-C4	4.15	1.49	1.43
2	G	301	19Y	C6-C4	4.10	1.48	1.43
2	J	301	19Y	C6-C4	4.09	1.48	1.43
2	E	301	19Y	C6-C4	4.07	1.48	1.43
2	A	301	19Y	C6-C4	3.97	1.48	1.43
2	D	301	19Y	C6-C4	3.96	1.48	1.43
2	J	301	19Y	C5-C4	3.92	1.47	1.40
2	G	301	19Y	C5-C4	3.86	1.47	1.40
2	F	301	19Y	C11-S10	-3.83	1.70	1.77
2	C	301	19Y	C11-S10	-3.83	1.70	1.77
2	E	301	19Y	C11-S10	-3.82	1.70	1.77
2	C	301	19Y	C6-C4	3.81	1.48	1.43
2	D	301	19Y	C5-C4	3.79	1.47	1.40
2	F	301	19Y	C5-C4	3.78	1.47	1.40
2	E	301	19Y	C5-C4	3.78	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	19Y	C5-C4	3.76	1.47	1.40
2	C	301	19Y	C5-C4	3.74	1.47	1.40
2	D	301	19Y	C11-S10	-3.73	1.70	1.77
2	A	301	19Y	C11-S10	-3.70	1.70	1.77
2	G	301	19Y	C11-S10	-3.67	1.70	1.77
2	J	301	19Y	C11-S10	-3.64	1.70	1.77
2	B	301	19Y	C11-S10	-3.55	1.70	1.77
2	B	301	19Y	C6-N7	2.57	1.36	1.31
2	J	301	19Y	C6-N7	2.49	1.35	1.31
2	E	301	19Y	C6-N7	2.34	1.35	1.31
2	F	301	19Y	C6-N7	2.34	1.35	1.31
2	C	301	19Y	C6-N7	2.32	1.35	1.31
2	D	301	19Y	C6-N7	2.25	1.35	1.31
2	G	301	19Y	C4-C3	2.24	1.48	1.43
2	D	301	19Y	C4-C3	2.17	1.48	1.43
2	J	301	19Y	C4-C3	2.17	1.48	1.43
2	A	301	19Y	C6-N7	2.14	1.35	1.31
2	G	301	19Y	C6-N7	2.14	1.35	1.31
2	F	301	19Y	C4-C3	2.11	1.48	1.43
2	C	301	19Y	C4-C3	2.03	1.48	1.43
2	E	301	19Y	C4-C3	2.03	1.48	1.43
2	B	301	19Y	C4-C3	2.01	1.48	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	19Y	C4-C6-N7	-9.73	116.72	124.53
2	G	301	19Y	C4-C6-N7	-9.57	116.84	124.53
2	F	301	19Y	C4-C6-N7	-9.52	116.88	124.53
2	E	301	19Y	C4-C6-N7	-9.51	116.90	124.53
2	D	301	19Y	C4-C6-N7	-9.33	117.04	124.53
2	B	301	19Y	C4-C6-N7	-9.23	117.12	124.53
2	J	301	19Y	C4-C6-N7	-8.98	117.32	124.53
2	A	301	19Y	C4-C6-N7	-8.84	117.44	124.53
2	F	301	19Y	C5-C4-C3	-6.22	102.58	107.54
2	A	301	19Y	C5-C4-C3	-6.15	102.63	107.54
2	E	301	19Y	C5-C4-C3	-6.10	102.67	107.54
2	G	301	19Y	C5-C4-C3	-5.89	102.84	107.54
2	D	301	19Y	C5-C4-C3	-5.87	102.85	107.54
2	B	301	19Y	C5-C4-C3	-5.87	102.85	107.54
2	C	301	19Y	C5-C4-C3	-5.83	102.89	107.54
2	G	301	19Y	C8-N7-C6	5.76	122.64	115.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	19Y	C8-N7-C6	5.74	122.61	115.85
2	J	301	19Y	C5-C4-C3	-5.71	102.98	107.54
2	D	301	19Y	C8-N7-C6	5.68	122.54	115.85
2	E	301	19Y	C8-N7-C6	5.67	122.53	115.85
2	B	301	19Y	C8-N7-C6	5.60	122.45	115.85
2	A	301	19Y	C8-N7-C6	5.52	122.35	115.85
2	F	301	19Y	C8-N7-C6	5.41	122.22	115.85
2	J	301	19Y	C8-N7-C6	5.35	122.16	115.85
2	D	301	19Y	C8-S10-C11	5.07	112.03	103.18
2	J	301	19Y	C8-S10-C11	5.04	111.98	103.18
2	B	301	19Y	C8-N9-C3	4.81	121.96	115.32
2	A	301	19Y	C8-S10-C11	4.78	111.53	103.18
2	A	301	19Y	C8-N9-C3	4.77	121.89	115.32
2	J	301	19Y	C8-N9-C3	4.75	121.88	115.32
2	F	301	19Y	C8-N9-C3	4.72	121.83	115.32
2	D	301	19Y	C8-N9-C3	4.67	121.77	115.32
2	E	301	19Y	C8-N9-C3	4.67	121.77	115.32
2	C	301	19Y	C8-N9-C3	4.56	121.60	115.32
2	E	301	19Y	C8-S10-C11	4.52	111.07	103.18
2	G	301	19Y	C8-N9-C3	4.41	121.40	115.32
2	B	301	19Y	C8-S10-C11	4.31	110.70	103.18
2	F	301	19Y	C8-S10-C11	4.29	110.67	103.18
2	C	301	19Y	C8-S10-C11	3.96	110.10	103.18
2	G	301	19Y	C8-S10-C11	3.68	109.61	103.18
2	C	301	19Y	C14-N13-C12	2.76	121.61	116.85
2	F	301	19Y	C14-N13-C12	2.75	121.60	116.85
2	G	301	19Y	C14-N13-C12	2.73	121.57	116.85
2	E	301	19Y	C5-C1-N2	-2.65	105.74	110.29
2	J	301	19Y	C14-N13-C12	2.64	121.41	116.85
2	B	301	19Y	C14-N13-C12	2.57	121.29	116.85
2	A	301	19Y	C14-N13-C12	2.57	121.29	116.85
2	A	301	19Y	C5-C1-N2	-2.52	105.97	110.29
2	B	301	19Y	N9-C8-N7	-2.52	122.36	126.98
2	E	301	19Y	C14-N13-C12	2.50	121.18	116.85
2	D	301	19Y	C14-N13-C12	2.49	121.15	116.85
2	B	301	19Y	C5-C1-N2	-2.46	106.06	110.29
2	D	301	19Y	C5-C1-N2	-2.46	106.06	110.29
2	G	301	19Y	C5-C1-N2	-2.46	106.07	110.29
2	J	301	19Y	C5-C1-N2	-2.44	106.10	110.29
2	A	301	19Y	N9-C8-N7	-2.43	122.50	126.98
2	F	301	19Y	C5-C1-N2	-2.42	106.14	110.29
2	C	301	19Y	C5-C1-N2	-2.38	106.21	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	19Y	N9-C8-N7	-2.37	122.63	126.98
2	J	301	19Y	N9-C8-N7	-2.33	122.69	126.98
2	E	301	19Y	N9-C8-N7	-2.33	122.70	126.98
2	C	301	19Y	N9-C8-N7	-2.32	122.71	126.98
2	F	301	19Y	N9-C8-N7	-2.24	122.87	126.98
2	B	301	19Y	C22-C21-C1	-2.23	109.39	114.88
2	D	301	19Y	C21-C1-C5	-2.22	126.55	130.34
2	C	301	19Y	C21-C1-C5	-2.21	126.56	130.34
2	G	301	19Y	N9-C8-N7	-2.20	122.94	126.98
2	G	301	19Y	C21-C1-C5	-2.09	126.78	130.34
2	C	301	19Y	C11-C12-N13	-2.07	120.02	123.26

There are no chirality outliers.

All (20) torsion outliers are listed below:

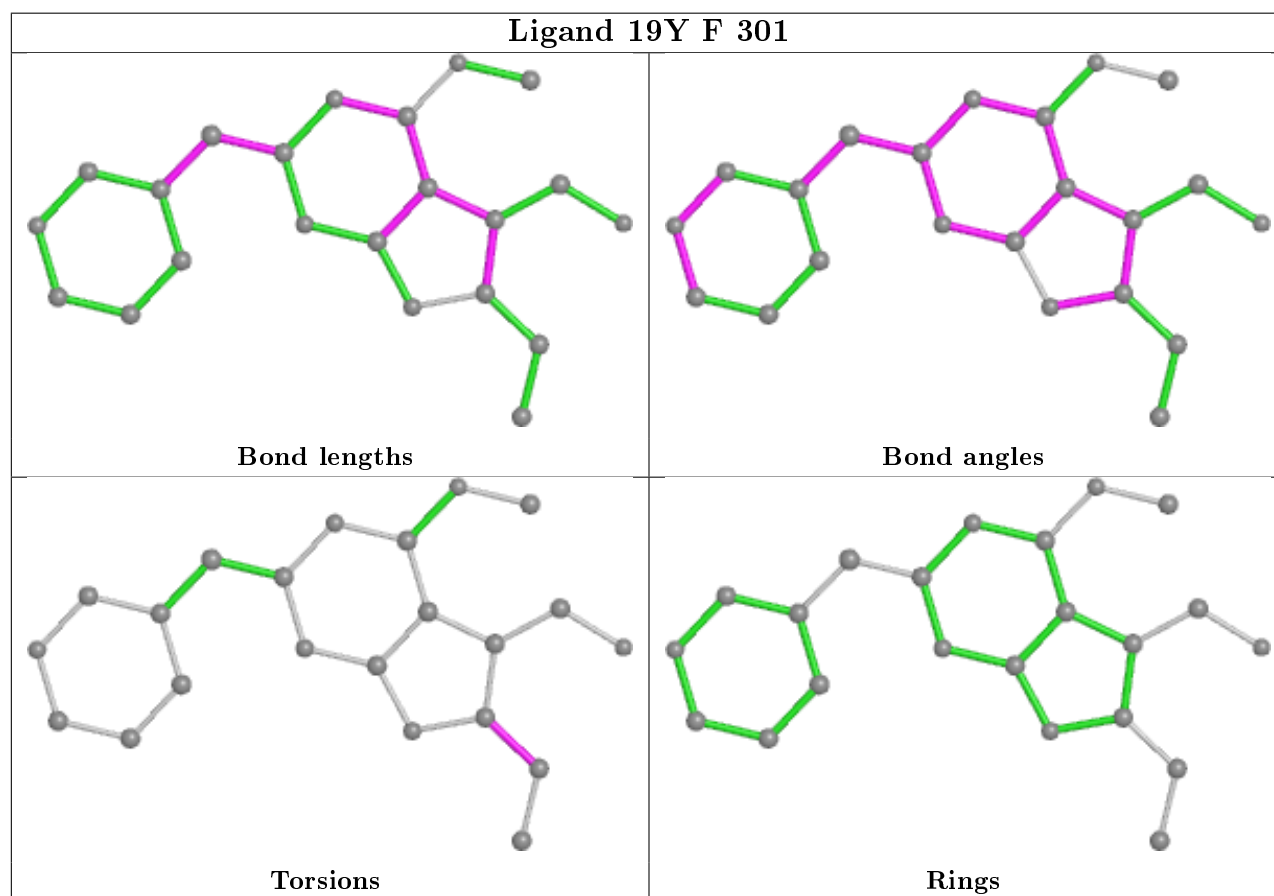
Mol	Chain	Res	Type	Atoms
2	D	301	19Y	C4-C6-O17-C18
2	E	301	19Y	N7-C6-O17-C18
2	C	301	19Y	N7-C6-O17-C18
2	G	301	19Y	C4-C6-O17-C18
2	J	301	19Y	C4-C6-O17-C18
2	J	301	19Y	N9-C8-S10-C11
2	B	301	19Y	C4-C6-O17-C18
2	G	301	19Y	N7-C6-O17-C18
2	B	301	19Y	N7-C6-O17-C18
2	J	301	19Y	N7-C8-S10-C11
2	C	301	19Y	C4-C6-O17-C18
2	D	301	19Y	N7-C6-O17-C18
2	J	301	19Y	N7-C6-O17-C18
2	E	301	19Y	C4-C6-O17-C18
2	A	301	19Y	N7-C6-O17-C18
2	A	301	19Y	C4-C6-O17-C18
2	F	301	19Y	C5-C1-C21-C22
2	D	301	19Y	C5-C1-C21-C22
2	C	301	19Y	C5-C1-C21-C22
2	D	301	19Y	C16-C11-S10-C8

There are no ring outliers.

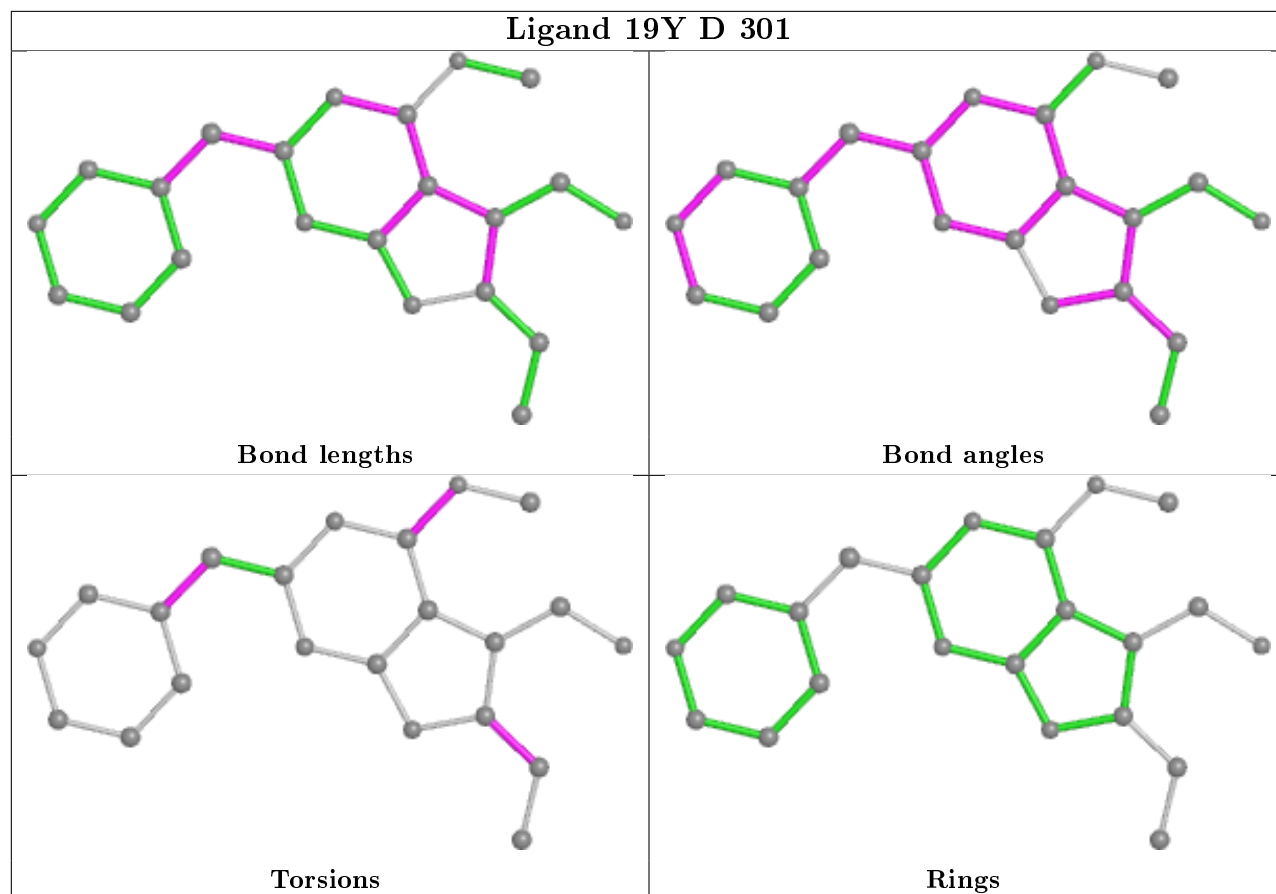
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301	19Y	1	0

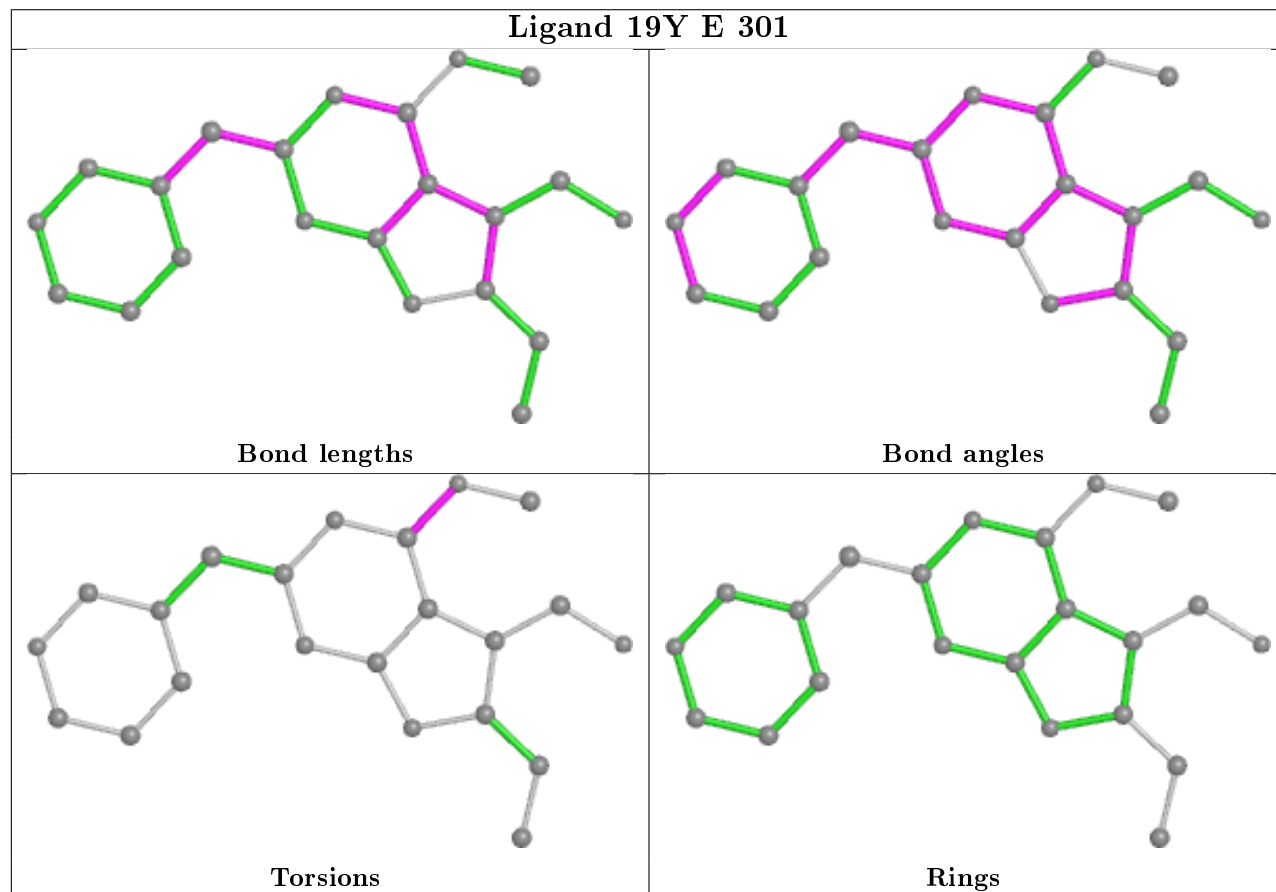
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



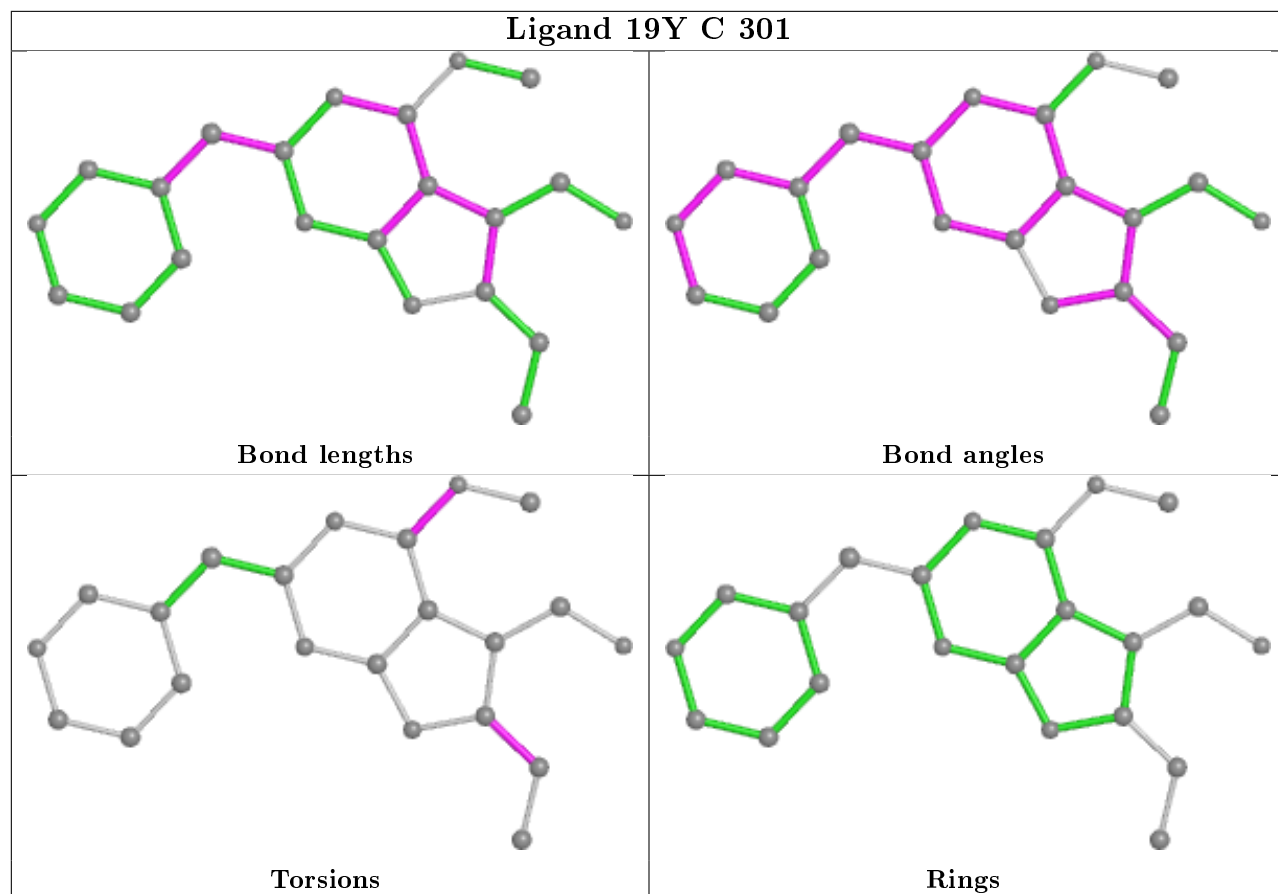
## Ligand 19Y D 301



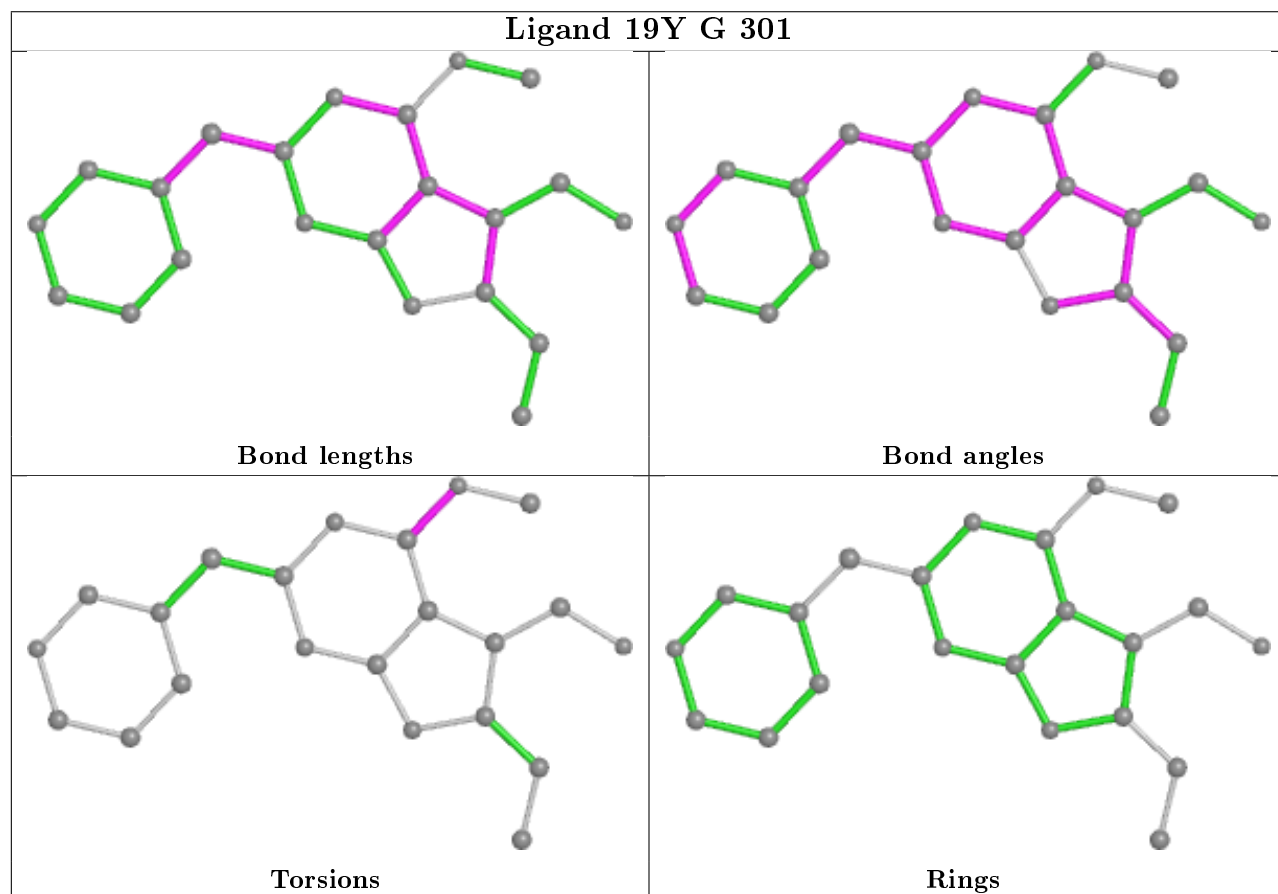
## Ligand 19Y E 301



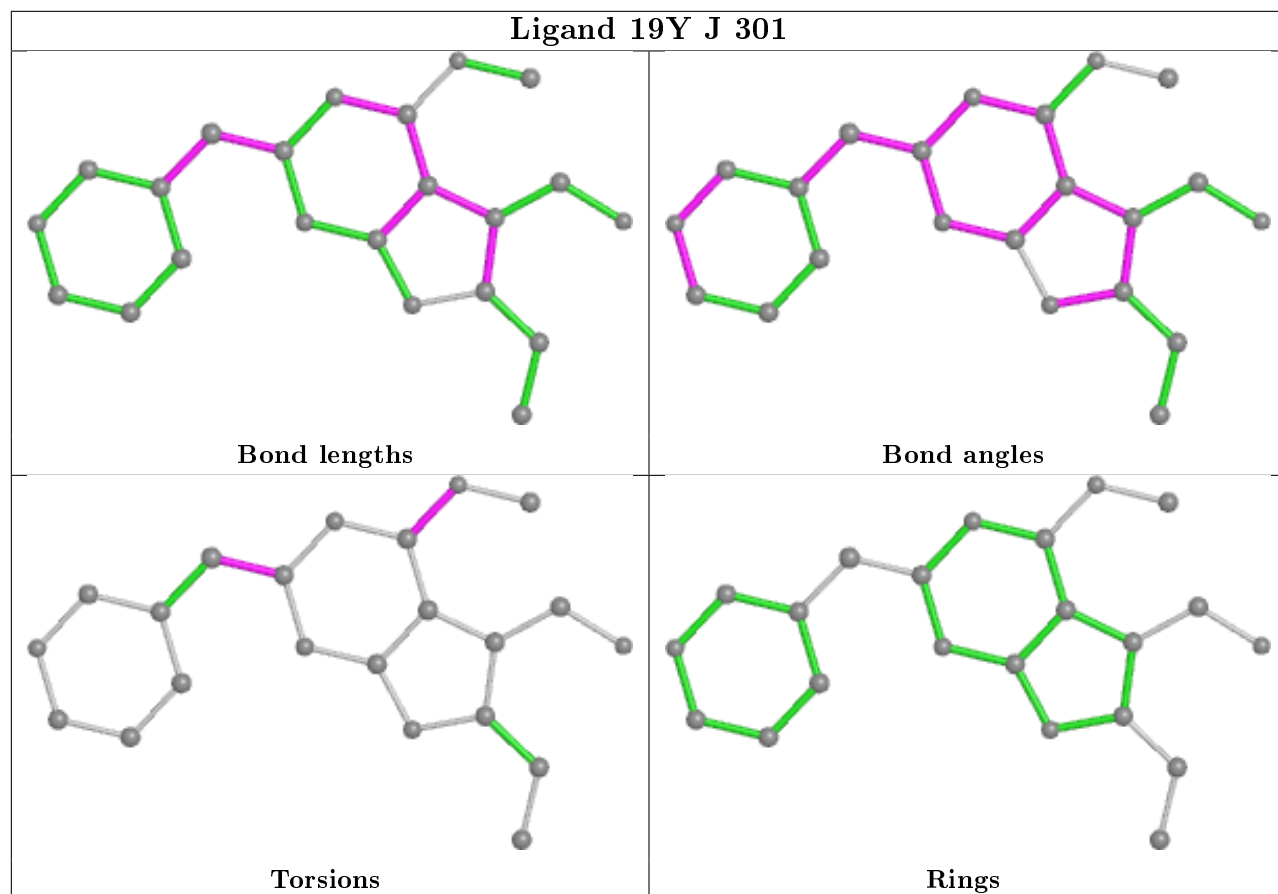
## Ligand 19Y C 301



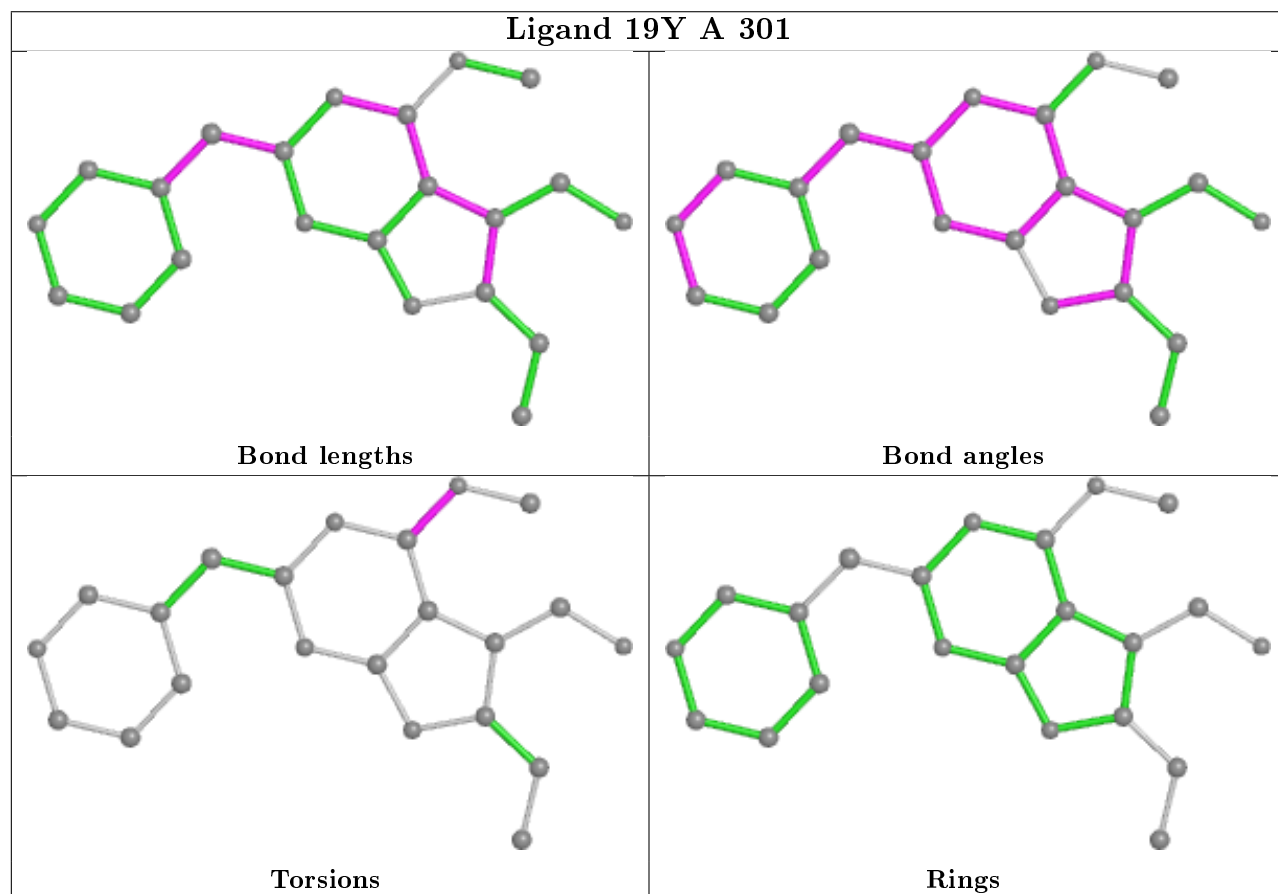
## Ligand 19Y G 301

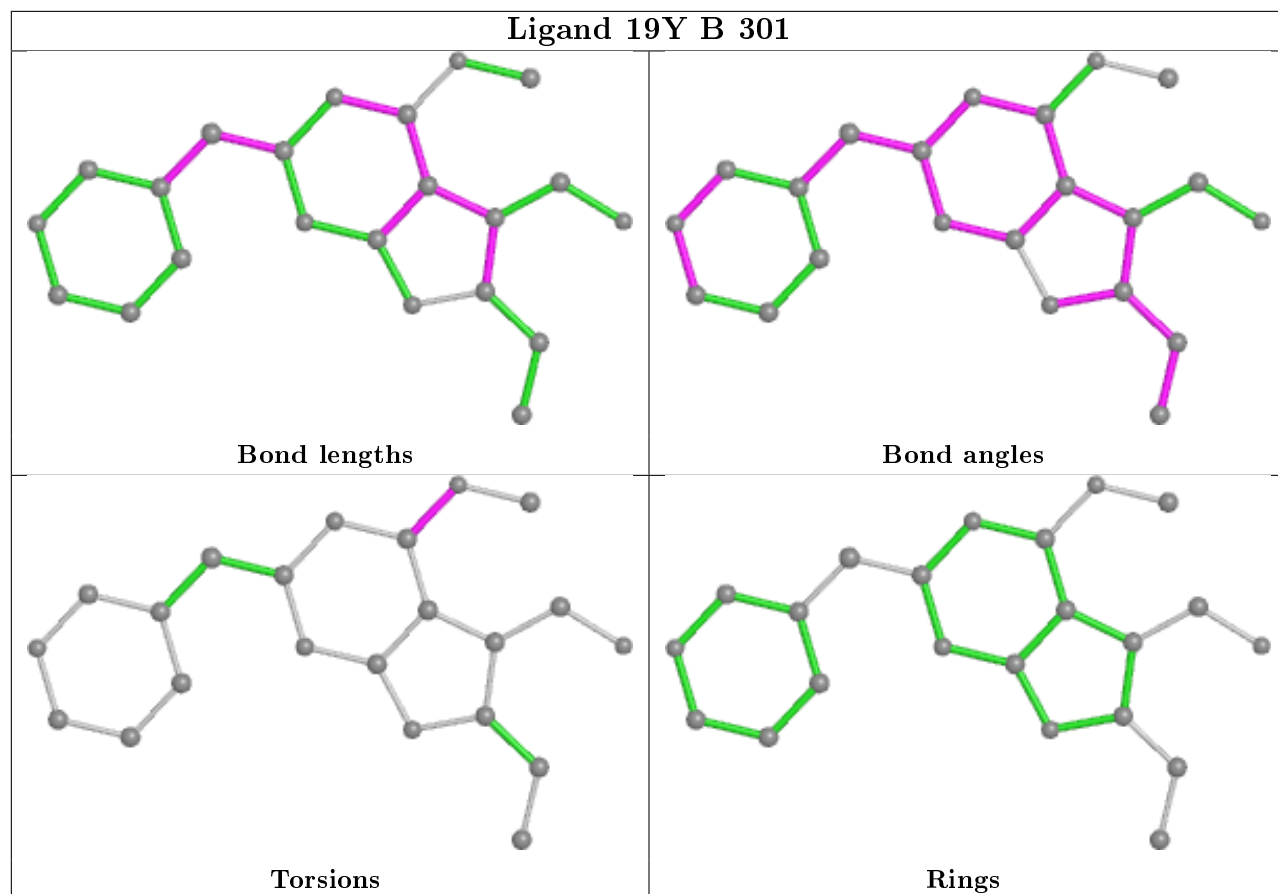


## Ligand 19Y J 301



## Ligand 19Y 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	191/216 (88%)	-0.31	0 100 100	17, 25, 48, 62	0
1	B	190/216 (87%)	-0.13	0 100 100	24, 37, 59, 75	0
1	C	191/216 (88%)	-0.16	1 (0%) 91 92	26, 38, 64, 78	0
1	D	190/216 (87%)	-0.03	1 (0%) 91 92	25, 40, 72, 86	0
1	E	191/216 (88%)	-0.12	1 (0%) 91 92	31, 42, 68, 86	0
1	F	191/216 (88%)	0.10	5 (2%) 56 57	38, 52, 75, 91	0
1	G	190/216 (87%)	0.47	15 (7%) 12 10	41, 75, 97, 112	0
1	H	191/216 (88%)	0.57	24 (12%) 3 3	41, 65, 106, 122	0
1	J	185/216 (85%)	0.51	16 (8%) 10 8	49, 75, 98, 112	0
All	All	1710/1944 (87%)	0.10	63 (3%) 41 41	17, 49, 90, 122	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	19	GLY	5.2
1	F	101	HIS	5.1
1	H	159	LYS	4.9
1	H	85	MET	4.8
1	J	89	GLY	4.4
1	G	224	GLU	4.2
1	J	86	HIS	4.2
1	H	164	LYS	4.1
1	H	139	ASP	4.0
1	H	87	ALA	3.8
1	G	161	GLY	3.7
1	G	165	LYS	3.7
1	H	160	ILE	3.6
1	G	139	ASP	3.6
1	G	160	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	93	VAL	3.4
1	H	141	VAL	3.4
1	H	90	ILE	3.3
1	J	158	LYS	3.3
1	G	166	ARG	3.3
1	J	90	ILE	3.2
1	G	101	HIS	3.2
1	G	87	ALA	3.1
1	F	87	ALA	3.0
1	F	90	ILE	3.0
1	G	162	LYS	2.9
1	J	157	LEU	2.9
1	J	85	MET	2.9
1	H	135	HIS	2.7
1	H	224	GLU	2.7
1	H	165	LYS	2.7
1	G	164	LYS	2.7
1	H	157	LEU	2.7
1	F	166	ARG	2.6
1	J	159	LYS	2.5
1	C	87	ALA	2.5
1	H	166	ARG	2.5
1	H	83	THR	2.4
1	H	162	LYS	2.4
1	J	213	GLY	2.4
1	J	217	LYS	2.4
1	H	95	VAL	2.4
1	G	159	LYS	2.3
1	G	22	ALA	2.3
1	H	92	THR	2.3
1	J	160	ILE	2.3
1	G	95	VAL	2.3
1	J	100	LEU	2.2
1	H	69	ASP	2.2
1	G	93	VAL	2.2
1	G	58	TYR	2.2
1	J	136	ILE	2.2
1	H	82	PRO	2.2
1	E	222	HIS	2.2
1	J	138	ARG	2.2
1	H	136	ILE	2.1
1	H	145	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	83	THR	2.1
1	D	164	LYS	2.1
1	H	143	TYR	2.0
1	H	100	LEU	2.0
1	F	158	LYS	2.0
1	J	192	GLU	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](#)

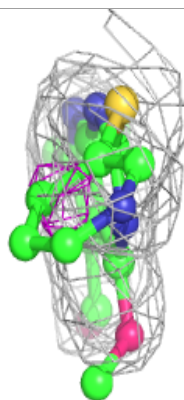
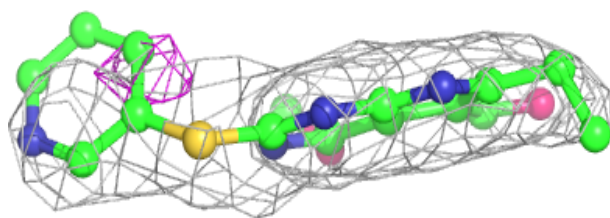
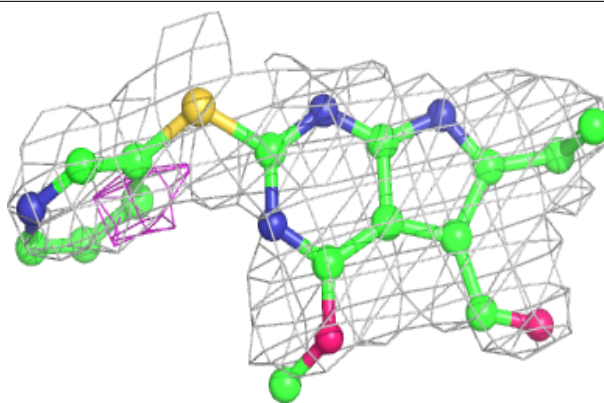
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	19Y	J	301	22/22	0.86	0.24	73,78,87,87	0
2	19Y	G	301	22/22	0.93	0.22	68,71,73,73	0
2	19Y	D	301	22/22	0.94	0.19	49,53,61,62	0
2	19Y	F	301	22/22	0.95	0.21	40,42,46,47	0
2	19Y	C	301	22/22	0.95	0.17	33,34,35,35	0
2	19Y	A	301	22/22	0.96	0.16	23,25,25,25	0
2	19Y	B	301	22/22	0.96	0.19	37,39,45,45	0
2	19Y	E	301	22/22	0.97	0.15	40,42,47,48	0

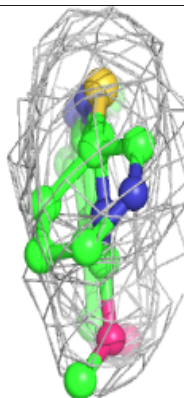
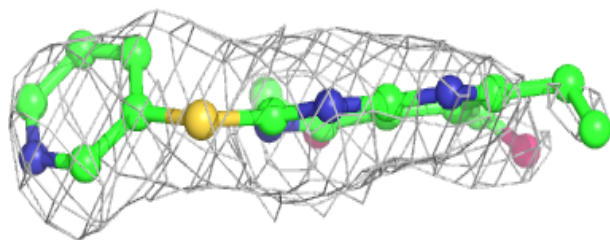
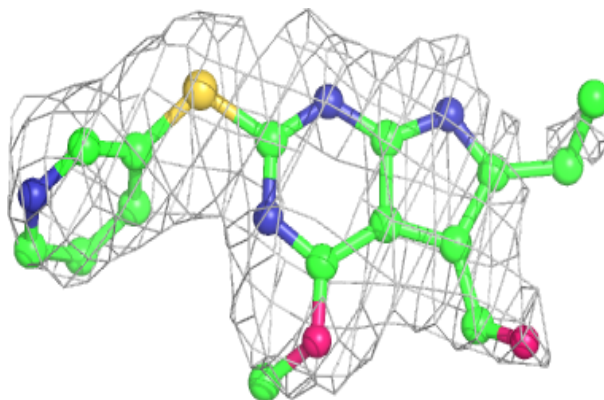
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 19Y J 301:**

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

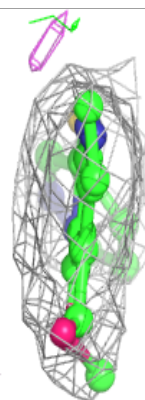
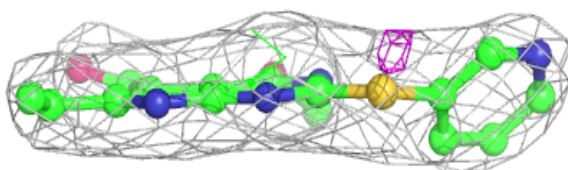
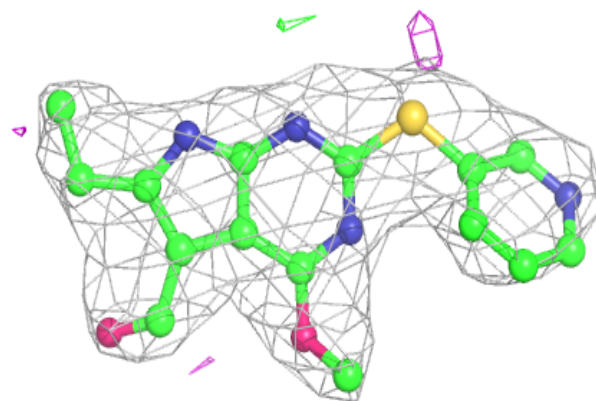
**Electron density around 19Y G 301:**

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

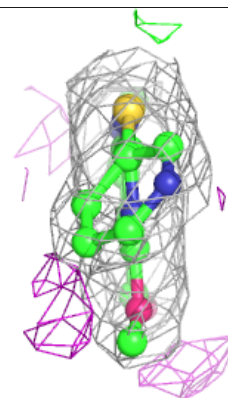
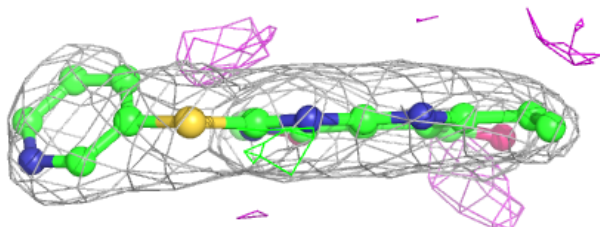
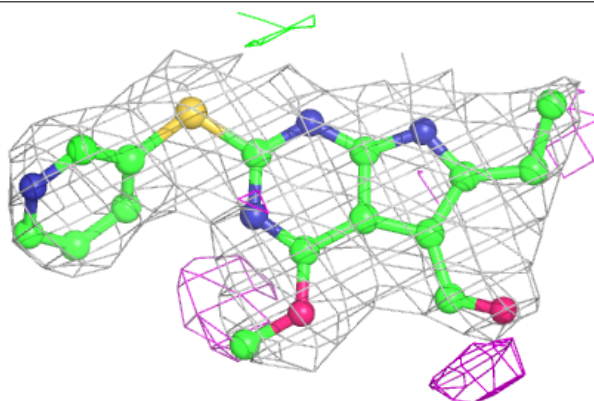


**Electron density around 19Y D 301:**

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

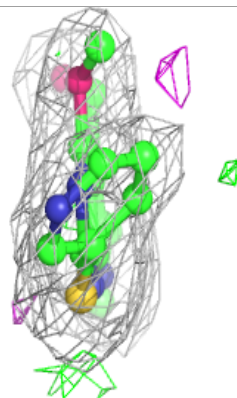
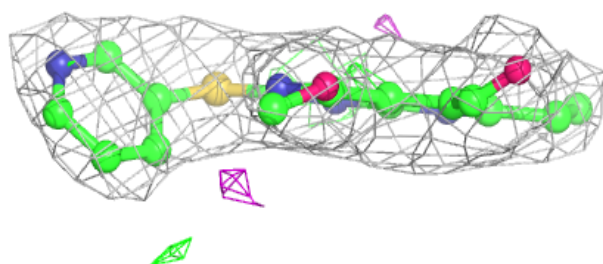
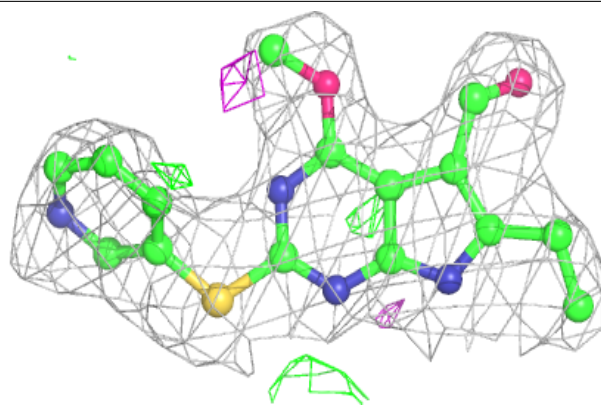
**Electron density around 19Y F 301:**

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

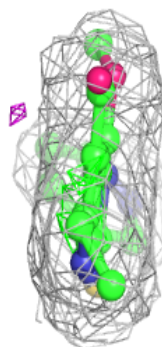
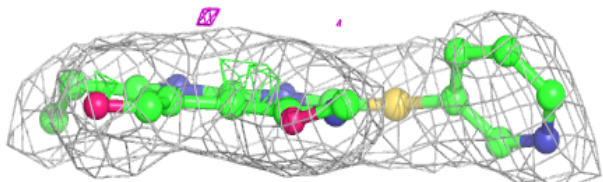
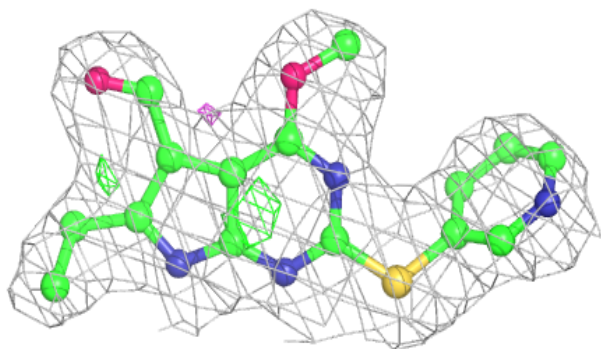


**Electron density around 19Y C 301:**

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

**Electron density around 19Y A 301:**

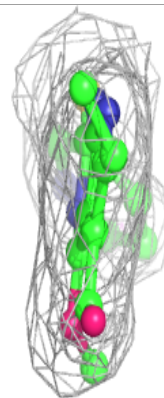
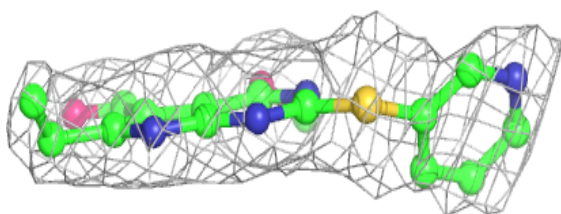
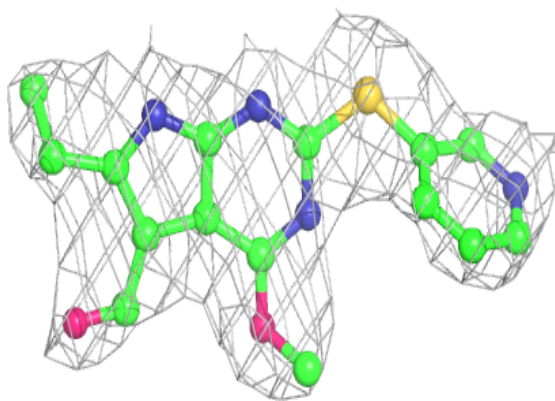
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



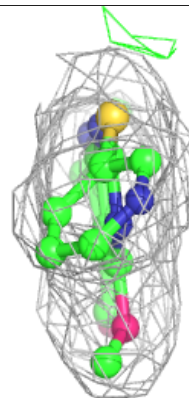
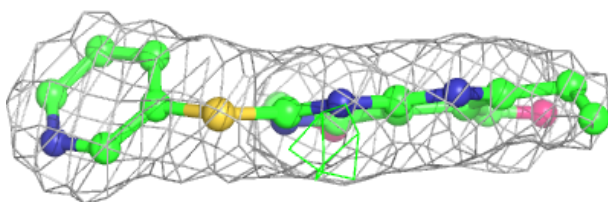
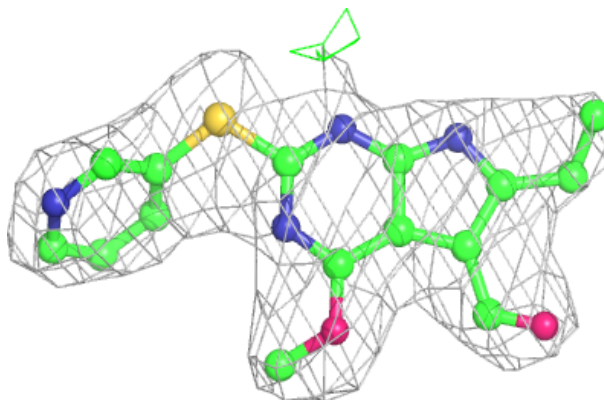


**Electron density around 19Y B 301:**

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

**Electron density around 19Y E 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

There are no such residues in this entry.