



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2026 – 06:57 PM JST

PDB ID : 9VF9 / pdb\_00009vf9  
Title : GSTM1 in complex with bithionol  
Authors : Sun, Q.  
Deposited on : 2025-06-10  
Resolution : 2.50 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.

The types of validation reports are described at

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

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

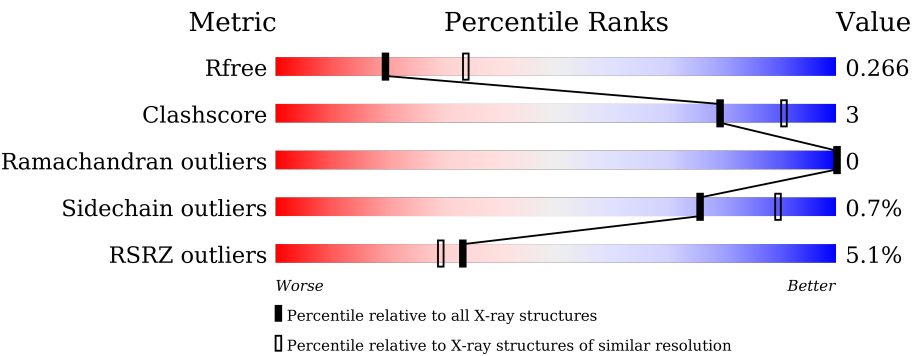
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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	218	<div><div>2%</div><div>93%</div><div>7%</div></div>
1	B	218	<div><div>2%</div><div>91%</div><div>9%</div></div>
1	C	218	<div><div>4%</div><div>93%</div><div>6%</div></div>
1	D	218	<div><div>6%</div><div>92%</div><div>7%</div></div>
1	E	218	<div><div>6%</div><div>93%</div><div>7%</div></div>
1	F	218	<div><div>8%</div><div>93%</div><div>7%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	218	<div><div>5%</div><div><div></div><div>94%</div><div>6%</div></div></div>
1	H	218	<div><div>9%</div><div><div></div><div>96%</div><div></div></div></div>

## 2 Entry composition

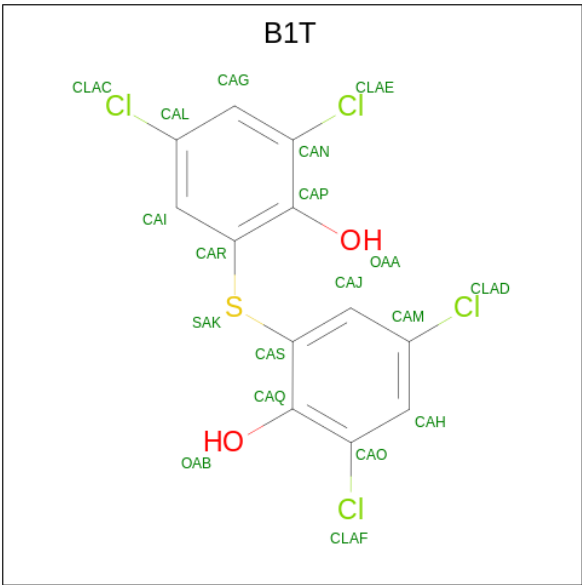
There are 5 unique types of molecules in this entry. The entry contains 14827 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutathione S-transferase Mu 1.

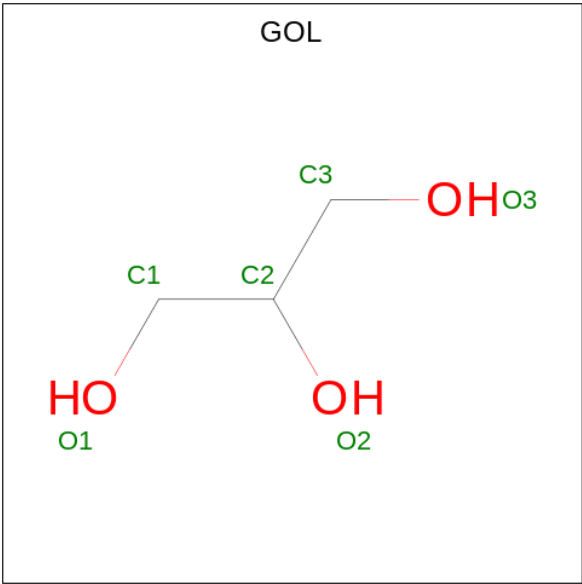
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1812	1179	296	325	12			
1	B	218	Total	C	N	O	S	0	0	0
			1812	1179	296	325	12			
1	C	218	Total	C	N	O	S	0	0	0
			1812	1179	296	325	12			
1	D	218	Total	C	N	O	S	0	0	0
			1812	1179	296	325	12			
1	E	218	Total	C	N	O	S	0	0	0
			1812	1179	296	325	12			
1	F	218	Total	C	N	O	S	0	0	0
			1812	1179	296	325	12			
1	G	218	Total	C	N	O	S	0	0	0
			1812	1179	296	325	12			
1	H	218	Total	C	N	O	S	0	0	0
			1812	1179	296	325	12			

- Molecule 2 is 2,2'-sulfanediylbis(4,6-dichlorophenol) (CCD ID: B1T) (formula: C<sub>12</sub>H<sub>6</sub>Cl<sub>4</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		
2	B	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		
2	C	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		
2	G	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	27	Total O 27 27	0	0
5	B	41	Total O 41 41	0	0
5	C	48	Total O 48 48	0	0
5	D	30	Total O 30 30	0	0
5	E	21	Total O 21 21	0	0
5	F	30	Total O 30 30	0	0
5	G	11	Total O 11 11	0	0
5	H	16	Total O 16 16	0	0

### 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: Glutathione S-transferase Mu 1



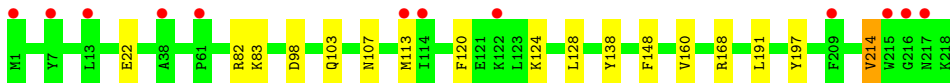
- Molecule 1: Glutathione S-transferase Mu 1



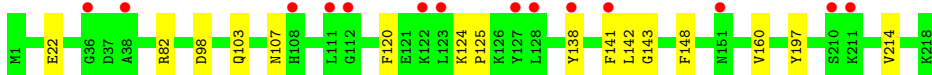
- Molecule 1: Glutathione S-transferase Mu 1



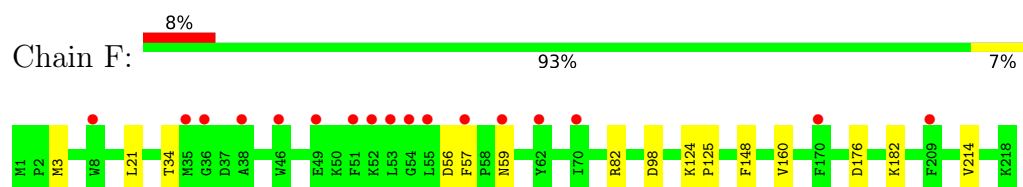
- Molecule 1: Glutathione S-transferase Mu 1



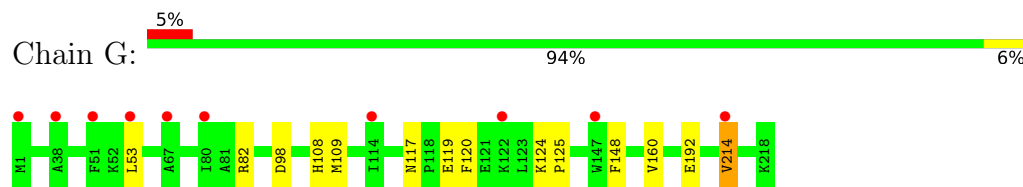
- Molecule 1: Glutathione S-transferase Mu 1



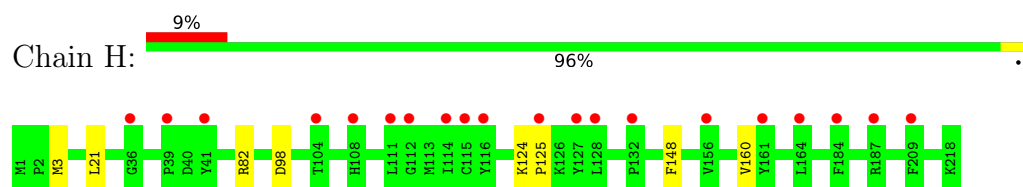
- Molecule 1: Glutathione S-transferase Mu 1



- Molecule 1: Glutathione S-transferase Mu 1



- Molecule 1: Glutathione S-transferase Mu 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.21Å 212.24Å 91.64Å 90.00° 95.82° 90.00°	Depositor
Resolution (Å)	45.63 – 2.50 45.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.63-2.50) 98.8 (45.63-2.50)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.238 , 0.267 0.239 , 0.266	Depositor DCC
$R_{free}$ test set	3290 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	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 33.50 % 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 7.9195e-04. 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, B1T, CL

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	0.47	0/1861	0.88	0/2508
1	B	0.47	0/1861	0.88	0/2508
1	C	0.47	0/1861	0.87	1/2508 (0.0%)
1	D	0.46	0/1861	0.88	0/2508
1	E	0.46	0/1861	0.88	0/2508
1	F	0.47	0/1861	0.87	0/2508
1	G	0.46	0/1861	0.87	0/2508
1	H	0.47	0/1861	0.87	0/2508
All	All	0.46	0/14888	0.87	1/20064 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	ARG	CG-CD-NE	5.68	124.49	112.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1812	0	1804	10	0
1	B	1812	0	1804	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1812	0	1804	10	0
1	D	1812	0	1804	10	0
1	E	1812	0	1804	15	0
1	F	1812	0	1804	11	0
1	G	1812	0	1804	10	0
1	H	1812	0	1804	9	0
2	A	19	0	6	2	0
2	B	19	0	6	3	0
2	C	19	0	5	2	0
2	G	19	0	6	1	0
3	A	12	0	16	0	0
3	C	6	0	8	0	0
3	E	12	0	16	0	0
4	H	1	0	0	0	0
5	A	27	0	0	0	0
5	B	41	0	0	1	0
5	C	48	0	0	1	0
5	D	30	0	0	0	0
5	E	21	0	0	0	0
5	F	30	0	0	1	0
5	G	11	0	0	1	0
5	H	16	0	0	0	0
All	All	14827	0	14495	77	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 3.

All (77) 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:82:ARG:NH2	1:B:98:ASP:OD2	2.29	0.64
1:B:108:HIS:ND1	2:B:301:B1T:CLAC	2.69	0.62
1:E:141:PHE:CD1	1:F:56:ASP:HB3	2.37	0.59
1:G:117:ASN:OD1	1:G:119:GLU:HG2	2.03	0.59
1:G:82:ARG:NH2	1:H:98:ASP:OD2	2.36	0.58
1:E:142:LEU:C	1:E:142:LEU:HD13	2.29	0.58
1:H:124:LYS:HG2	1:H:125:PRO:HD3	1.87	0.56
1:C:108:HIS:ND1	2:C:301:B1T:CLAC	2.76	0.55
1:C:82:ARG:NH2	1:D:98:ASP:OD2	2.41	0.54
1:A:98:ASP:OD2	1:B:82:ARG:NH2	2.41	0.54
1:B:122:LYS:HB2	1:D:83:LYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ASN:ND2	1:D:138:TYR:OH	2.41	0.52
1:E:98:ASP:OD2	1:F:82:ARG:NH2	2.43	0.52
1:B:32:LYS:NZ	5:B:402:HOH:O	2.44	0.51
1:B:107:ASN:ND2	1:B:138:TYR:OH	2.41	0.50
1:C:98:ASP:OD2	1:D:82:ARG:NH2	2.45	0.50
1:F:148:PHE:CZ	1:F:160:VAL:HG11	2.47	0.50
1:B:184:PHE:HA	1:B:187:ARG:NH1	2.28	0.49
1:E:107:ASN:ND2	1:E:138:TYR:OH	2.42	0.49
1:C:148:PHE:CZ	1:C:160:VAL:HG11	2.47	0.49
1:H:148:PHE:CZ	1:H:160:VAL:HG11	2.48	0.49
1:E:148:PHE:CZ	1:E:160:VAL:HG11	2.48	0.49
1:B:148:PHE:CZ	1:B:160:VAL:HG11	2.48	0.48
1:A:148:PHE:CZ	1:A:160:VAL:HG11	2.49	0.48
1:G:148:PHE:CZ	1:G:160:VAL:HG11	2.48	0.48
1:C:107:ASN:ND2	1:C:138:TYR:OH	2.41	0.47
1:D:148:PHE:CZ	1:D:160:VAL:HG11	2.49	0.47
1:G:108:HIS:ND1	2:G:301:B1T:CLAC	2.85	0.47
1:E:142:LEU:CD1	1:E:143:GLY:O	2.63	0.47
1:G:53:LEU:HB2	5:G:401:HOH:O	2.16	0.46
1:C:124:LYS:NZ	5:C:403:HOH:O	2.48	0.45
1:G:98:ASP:OD2	1:H:82:ARG:NH2	2.49	0.45
1:A:108:HIS:ND1	2:A:301:B1T:CLAC	2.87	0.45
1:A:143:GLY:C	1:A:144:LYS:HE2	2.42	0.45
1:B:109:MET:HE1	2:B:301:B1T:OAB	2.17	0.45
1:A:124:LYS:HE2	1:A:128:LEU:HD11	1.99	0.44
1:D:191:LEU:HA	1:G:192:GLU:HB2	1.99	0.44
1:C:120:PHE:HB3	1:C:214:VAL:HG21	1.98	0.44
1:F:59:ASN:HA	5:F:308:HOH:O	2.18	0.44
1:E:142:LEU:HD13	1:E:143:GLY:O	2.17	0.43
1:G:120:PHE:HB3	1:G:214:VAL:HG21	2.00	0.43
1:E:120:PHE:CZ	1:E:124:LYS:CE	3.01	0.42
1:H:3:MET:HE1	1:H:21:LEU:CD2	2.49	0.42
1:B:108:HIS:CE1	2:B:301:B1T:CLAC	3.09	0.42
1:G:148:PHE:CE2	1:G:160:VAL:HG11	2.55	0.42
1:H:124:LYS:CG	1:H:125:PRO:HD3	2.49	0.42
1:D:120:PHE:HB3	1:D:214:VAL:HG21	2.01	0.42
1:C:212:MET:HE3	2:C:301:B1T:CLAD	2.56	0.42
1:D:124:LYS:HE2	1:D:128:LEU:HD11	2.02	0.42
1:E:148:PHE:CE2	1:E:160:VAL:HG11	2.54	0.42
1:E:141:PHE:CD2	1:F:57:PHE:CE1	3.08	0.42
1:B:4:ILE:HD13	1:B:29:GLU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:PHE:CE2	1:F:160:VAL:HG11	2.55	0.41
1:F:176:ASP:HA	1:F:182:LYS:HE3	2.03	0.41
1:B:148:PHE:CE2	1:B:160:VAL:HG11	2.56	0.41
1:E:120:PHE:CZ	1:E:124:LYS:HE3	2.55	0.41
1:A:22:GLU:HG3	1:A:197:TYR:CD1	2.56	0.41
1:B:124:LYS:N	1:B:125:PRO:CD	2.84	0.41
1:C:124:LYS:N	1:C:125:PRO:CD	2.84	0.41
1:F:3:MET:HE1	1:F:21:LEU:CD2	2.50	0.41
1:H:148:PHE:CE2	1:H:160:VAL:HG11	2.56	0.41
1:H:3:MET:CE	1:H:21:LEU:CD2	2.98	0.41
1:H:124:LYS:N	1:H:125:PRO:CD	2.84	0.41
1:A:124:LYS:N	1:A:125:PRO:CD	2.84	0.41
1:E:124:LYS:N	1:E:125:PRO:CD	2.84	0.41
1:C:22:GLU:HG3	1:C:197:TYR:CD1	2.56	0.40
1:F:124:LYS:N	1:F:125:PRO:CD	2.84	0.40
1:G:124:LYS:N	1:G:125:PRO:CD	2.84	0.40
1:A:212:MET:SD	2:A:301:B1T:CLAD	3.16	0.40
1:D:22:GLU:HG3	1:D:197:TYR:CD1	2.56	0.40
1:B:71:THR:O	1:B:72:GLN:HB2	2.21	0.40
1:E:82:ARG:NH2	1:F:98:ASP:OD2	2.54	0.40
1:D:103:GLN:HE21	1:D:107:ASN:HD21	1.69	0.40
1:E:103:GLN:HE21	1:E:107:ASN:HD21	1.70	0.40
1:F:3:MET:CE	1:F:21:LEU:CD2	3.00	0.40
1:A:166:LEU:HD22	1:A:208:VAL:HG13	2.03	0.40
1:E:22:GLU:HG3	1:E:197:TYR:CD1	2.57	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	216/218 (99%)	212 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
1	C	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
1	D	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
1	E	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
1	F	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
1	G	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
1	H	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
All	All	1728/1744 (99%)	1696 (98%)	32 (2%)	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	197/197 (100%)	197 (100%)	0	100	100
1	B	197/197 (100%)	196 (100%)	1 (0%)	81	92
1	C	197/197 (100%)	195 (99%)	2 (1%)	68	86
1	D	197/197 (100%)	194 (98%)	3 (2%)	57	80
1	E	197/197 (100%)	196 (100%)	1 (0%)	81	92
1	F	197/197 (100%)	195 (99%)	2 (1%)	68	86
1	G	197/197 (100%)	195 (99%)	2 (1%)	68	86
1	H	197/197 (100%)	197 (100%)	0	100	100
All	All	1576/1576 (100%)	1565 (99%)	11 (1%)	76	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	214	VAL
1	C	168	ARG

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Mol	Chain	Res	Type
1	C	214	VAL
1	D	113	MET
1	D	168	ARG
1	D	214	VAL
1	E	214	VAL
1	F	34	THR
1	F	214	VAL
1	G	109	MET
1	G	214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	103	GLN
1	C	107	ASN
1	D	72	GLN
1	D	85	ASN
1	D	107	ASN
1	E	102	ASN
1	E	107	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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	GOL	A	302	-	5,5,5	0.11	0	5,5,5	0.30	0
2	B1T	G	301	-	20,20,20	1.92	4 (20%)	29,29,29	0.84	0
2	B1T	C	301	-	20,20,20	1.75	4 (20%)	29,29,29	1.16	3 (10%)
3	GOL	E	301	-	5,5,5	0.13	0	5,5,5	0.29	0
3	GOL	A	303	-	5,5,5	0.14	0	5,5,5	0.38	0
3	GOL	E	302	-	5,5,5	0.11	0	5,5,5	0.33	0
2	B1T	A	301	-	20,20,20	1.78	4 (20%)	29,29,29	0.87	1 (3%)
2	B1T	B	301	-	20,20,20	2.00	4 (20%)	29,29,29	1.03	1 (3%)
3	GOL	C	302	-	5,5,5	0.11	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	302	-	-	4/4/4/4	-
2	B1T	G	301	-	-	0/4/4/4	0/2/2/2
2	B1T	C	301	-	-	0/4/4/4	0/2/2/2
3	GOL	E	301	-	-	0/4/4/4	-
3	GOL	A	303	-	-	2/4/4/4	-
3	GOL	E	302	-	-	2/4/4/4	-
2	B1T	A	301	-	-	0/4/4/4	0/2/2/2
2	B1T	B	301	-	-	0/4/4/4	0/2/2/2
3	GOL	C	302	-	-	4/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	B1T	CAS-SAK	6.25	1.87	1.78
2	G	301	B1T	CAS-SAK	5.77	1.87	1.78
2	A	301	B1T	CAS-SAK	4.98	1.85	1.78
2	C	301	B1T	CAS-SAK	4.94	1.85	1.78
2	G	301	B1T	OAB-CAQ	4.57	1.47	1.37
2	A	301	B1T	OAB-CAQ	4.52	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	B1T	OAB-CAQ	4.38	1.47	1.37
2	B	301	B1T	OAB-CAQ	4.34	1.47	1.37
2	B	301	B1T	CAO-CLAF	2.75	1.80	1.73
2	C	301	B1T	CAP-CAR	-2.39	1.37	1.40
2	A	301	B1T	CAP-CAR	-2.35	1.37	1.40
2	G	301	B1T	CAP-CAR	-2.31	1.37	1.40
2	A	301	B1T	CAO-CLAF	2.30	1.79	1.73
2	B	301	B1T	CAP-CAR	-2.22	1.37	1.40
2	C	301	B1T	CAO-CLAF	2.08	1.78	1.73
2	G	301	B1T	CAO-CLAF	2.02	1.78	1.73

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	B1T	CAG-CAL-CLAC	3.60	123.65	119.15
2	A	301	B1T	CAS-SAK-CAR	2.61	112.49	103.54
2	C	301	B1T	CAI-CAL-CLAC	-2.55	115.96	119.15
2	C	301	B1T	CAG-CAN-CLAE	2.13	121.92	118.49
2	B	301	B1T	CAS-SAK-CAR	2.12	110.81	103.54

There are no chirality outliers.

All (12) torsion outliers are listed below:

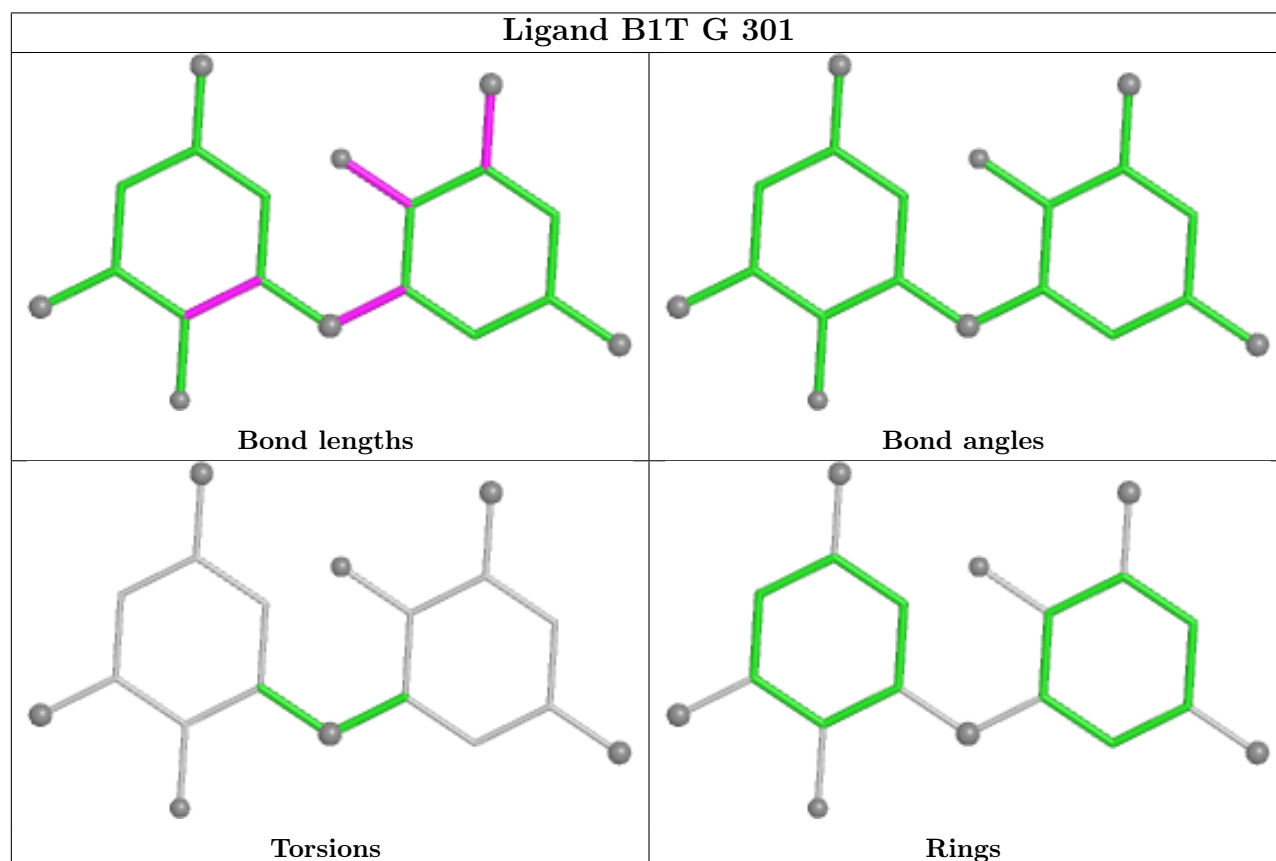
Mol	Chain	Res	Type	Atoms
3	A	303	GOL	C1-C2-C3-O3
3	C	302	GOL	O1-C1-C2-C3
3	C	302	GOL	C1-C2-C3-O3
3	E	302	GOL	C1-C2-C3-O3
3	E	302	GOL	O2-C2-C3-O3
3	C	302	GOL	O1-C1-C2-O2
3	C	302	GOL	O2-C2-C3-O3
3	A	303	GOL	O2-C2-C3-O3
3	A	302	GOL	O2-C2-C3-O3
3	A	302	GOL	C1-C2-C3-O3
3	A	302	GOL	O1-C1-C2-C3
3	A	302	GOL	O1-C1-C2-O2

There are no ring outliers.

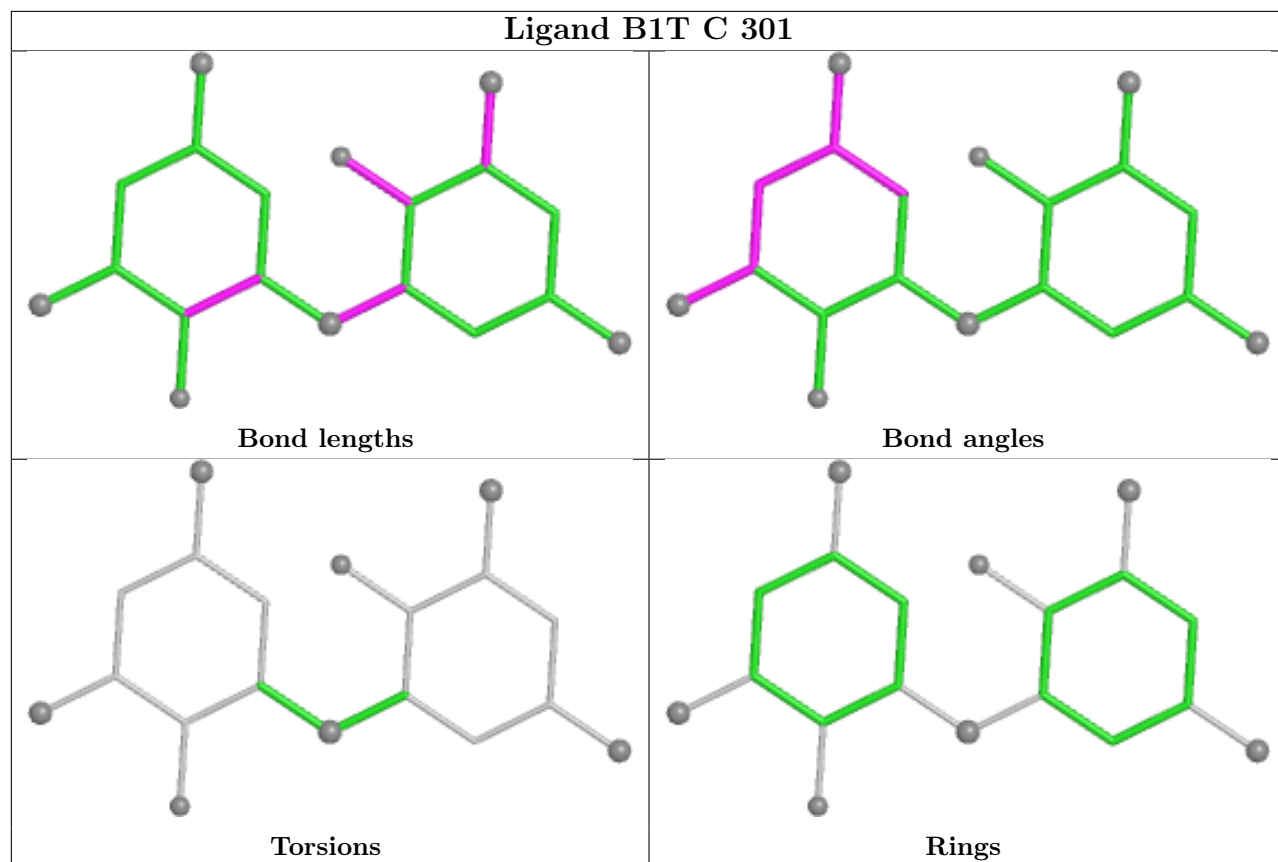
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	B1T	1	0
2	C	301	B1T	2	0
2	A	301	B1T	2	0
2	B	301	B1T	3	0

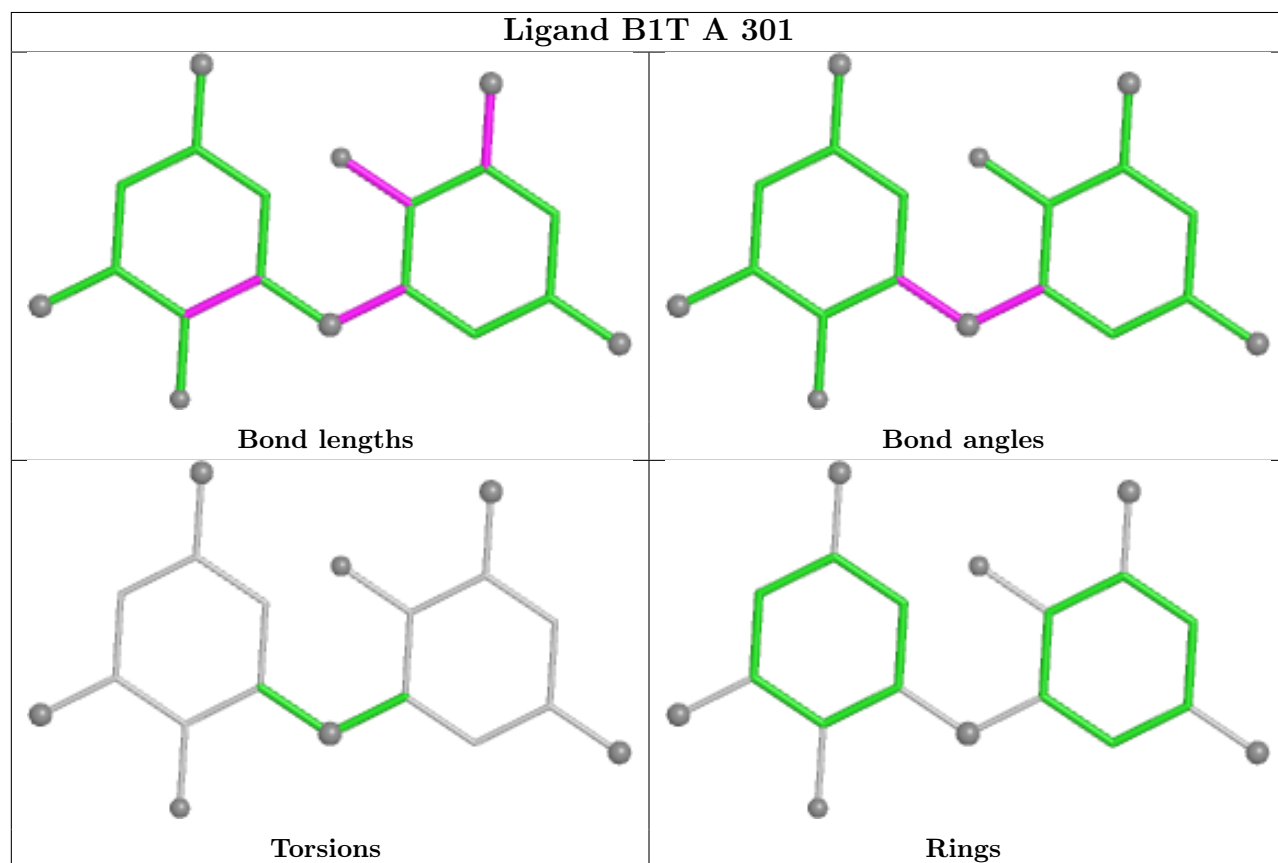
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

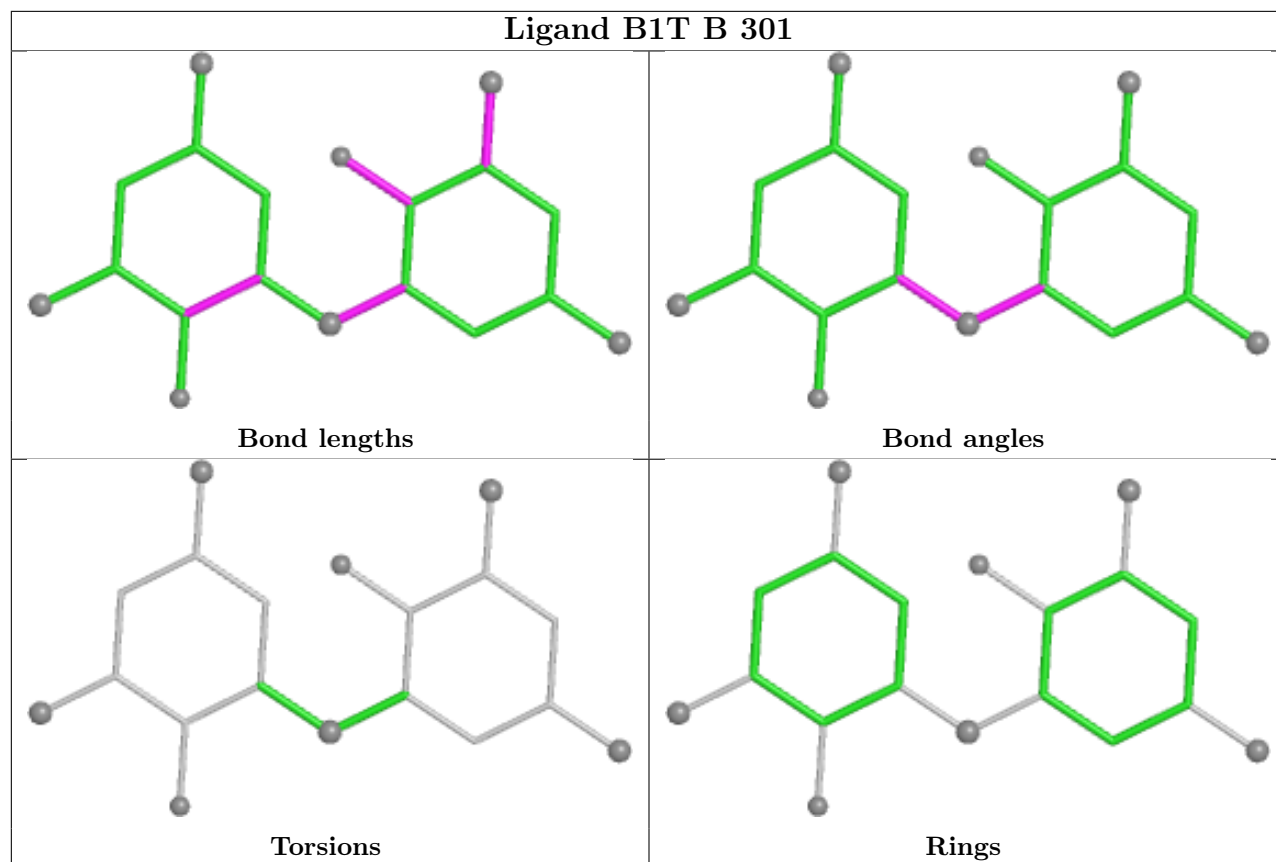


## Ligand B1T C 301



## Ligand B1T 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	218/218 (100%)	0.32	4 (1%) 67 64	31, 52, 101, 123	0
1	B	218/218 (100%)	0.24	4 (1%) 67 64	32, 50, 71, 120	0
1	C	218/218 (100%)	0.35	8 (3%) 45 40	33, 54, 81, 104	0
1	D	218/218 (100%)	0.52	12 (5%) 30 27	37, 58, 117, 151	0
1	E	218/218 (100%)	0.61	14 (6%) 25 22	35, 68, 136, 182	0
1	F	218/218 (100%)	0.60	17 (7%) 19 17	31, 61, 122, 154	0
1	G	218/218 (100%)	0.60	10 (4%) 37 33	48, 75, 126, 156	0
1	H	218/218 (100%)	0.80	20 (9%) 14 13	47, 77, 139, 156	0
All	All	1744/1744 (100%)	0.50	89 (5%) 33 29	31, 61, 122, 182	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	128	LEU	4.9
1	D	216	GLY	4.1
1	F	55	LEU	3.7
1	H	111	LEU	3.6
1	F	51	PHE	3.6
1	E	141	PHE	3.5
1	F	52	LYS	3.5
1	C	83	LYS	3.4
1	E	111	LEU	3.3
1	H	209	PHE	3.2
1	D	122	LYS	3.2
1	D	215	TRP	3.2
1	H	127	TYR	3.1
1	B	38	ALA	3.0
1	F	8	TRP	2.9
1	C	80	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	217	ASN	2.9
1	H	114	ILE	2.9
1	G	214	VAL	2.8
1	D	7	TYR	2.8
1	D	114	ILE	2.8
1	A	111	LEU	2.8
1	E	36	GLY	2.8
1	C	25	ASP	2.7
1	B	39	PRO	2.6
1	C	185	ILE	2.6
1	E	151	ASN	2.6
1	G	80	ILE	2.6
1	H	115	CYS	2.6
1	F	46	TRP	2.6
1	F	170	PHE	2.6
1	G	38	ALA	2.6
1	B	212	MET	2.5
1	A	183	ASP	2.5
1	F	70	ILE	2.5
1	D	1	MET	2.5
1	D	13	LEU	2.4
1	F	57	PHE	2.4
1	H	187	ARG	2.4
1	H	104	THR	2.4
1	F	54	GLY	2.4
1	H	41	TYR	2.4
1	C	188	PHE	2.4
1	E	38	ALA	2.4
1	H	116	TYR	2.4
1	D	61	PRO	2.4
1	E	112	GLY	2.4
1	F	36	GLY	2.4
1	H	112	GLY	2.4
1	E	123	LEU	2.4
1	D	113	MET	2.4
1	C	156	VAL	2.4
1	E	122	LYS	2.3
1	C	184	PHE	2.3
1	H	161	TYR	2.3
1	G	1	MET	2.3
1	H	108	HIS	2.2
1	F	53	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	184	PHE	2.2
1	D	38	ALA	2.2
1	E	108	HIS	2.2
1	F	35	MET	2.2
1	E	128	LEU	2.2
1	F	209	PHE	2.2
1	F	59	ASN	2.2
1	G	67	ALA	2.2
1	G	114	ILE	2.2
1	B	93	GLU	2.2
1	H	156	VAL	2.1
1	G	53	LEU	2.1
1	E	127	TYR	2.1
1	G	122	LYS	2.1
1	H	36	GLY	2.1
1	F	49	GLU	2.1
1	F	62	TYR	2.1
1	H	39	PRO	2.1
1	G	51	PHE	2.0
1	F	38	ALA	2.0
1	A	218	LYS	2.0
1	E	138	TYR	2.0
1	E	210	SER	2.0
1	D	209	PHE	2.0
1	H	164	LEU	2.0
1	E	211	LYS	2.0
1	C	114	ILE	2.0
1	G	147	TRP	2.0
1	A	113	MET	2.0
1	H	125	PRO	2.0
1	H	132	PRO	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 oligosaccharides 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.

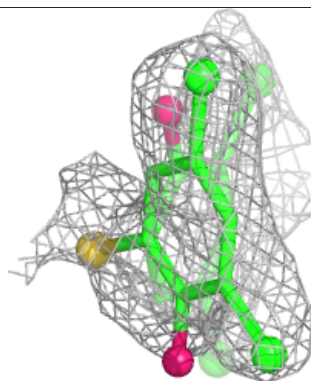
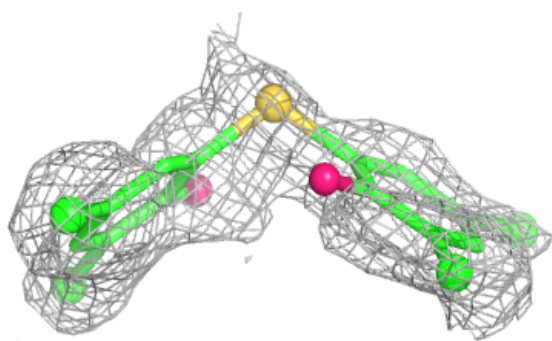
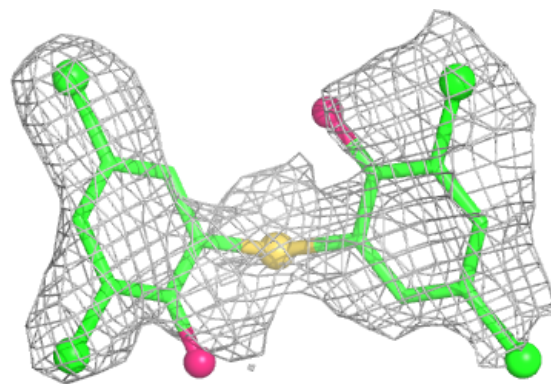
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	B1T	G	301	19/19	0.67	0.15	75,89,97,101	19
3	GOL	E	301	6/6	0.73	0.22	66,71,73,76	0
2	B1T	A	301	19/19	0.77	0.14	91,103,115,116	0
3	GOL	A	302	6/6	0.79	0.16	70,73,75,77	0
3	GOL	E	302	6/6	0.81	0.12	42,43,44,45	0
2	B1T	C	301	19/19	0.84	0.13	62,74,80,82	19
2	B1T	B	301	19/19	0.86	0.10	55,64,69,70	19
3	GOL	A	303	6/6	0.86	0.13	50,52,60,65	0
3	GOL	C	302	6/6	0.89	0.16	71,74,78,81	0
4	CL	H	301	1/1	0.92	0.14	73,73,73,73	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.



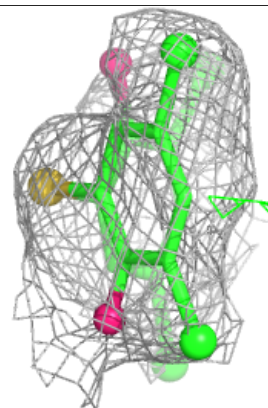
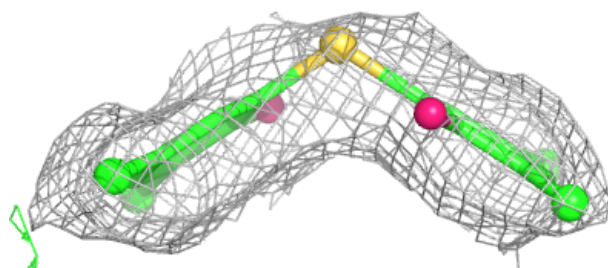
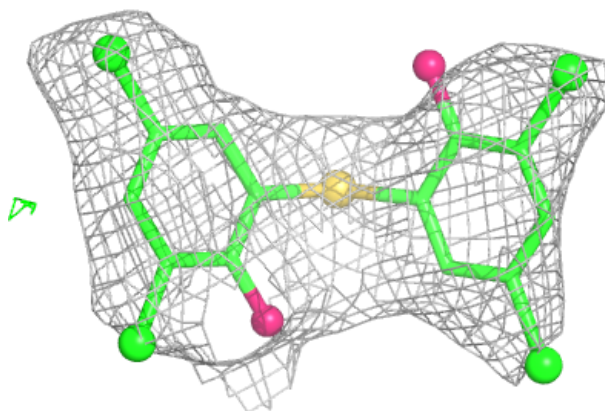
**Electron density around B1T G 301:**

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



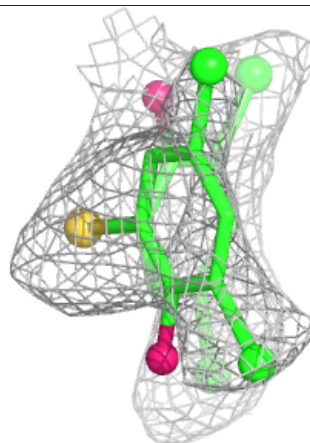
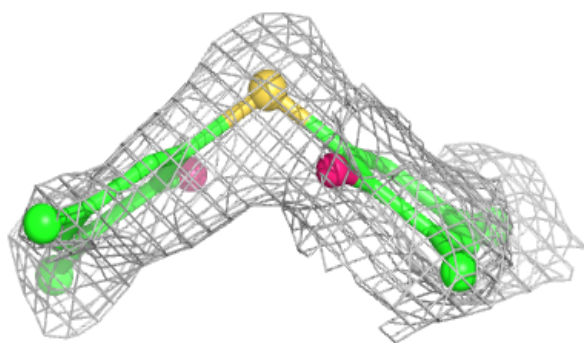
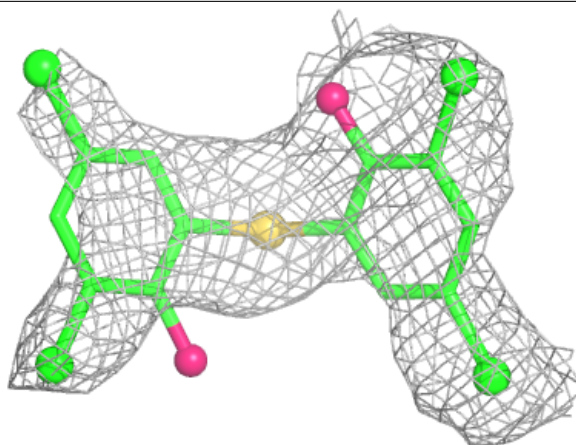
**Electron density around B1T A 301:**

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



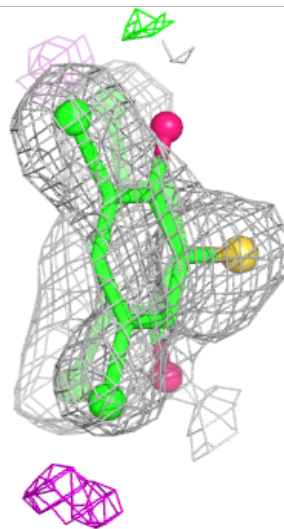
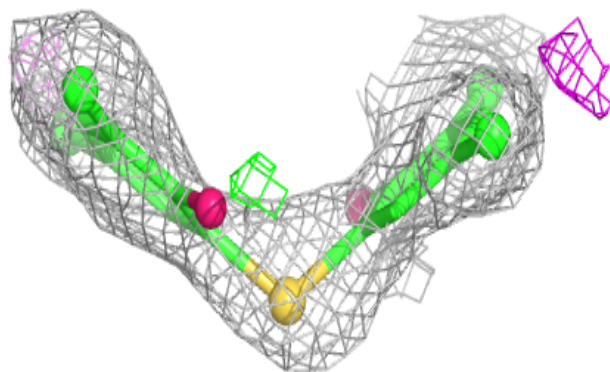
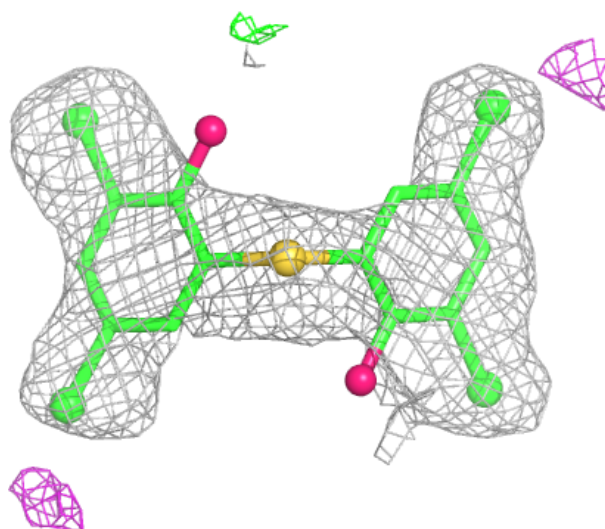
**Electron density around B1T C 301:**

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



**Electron density around B1T 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.