



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:42 am BST

PDB ID : 5YG3  
Title : Plasmodium vivax SHMT bound with PLP-glycine and S-GS834  
Authors : Chitnumsub, P.; Jaruwat, A.; Leartsakulpanich, U.; Schwertz, G.; Diederich, F.  
Deposited on : 2017-09-22  
Resolution : 2.40 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

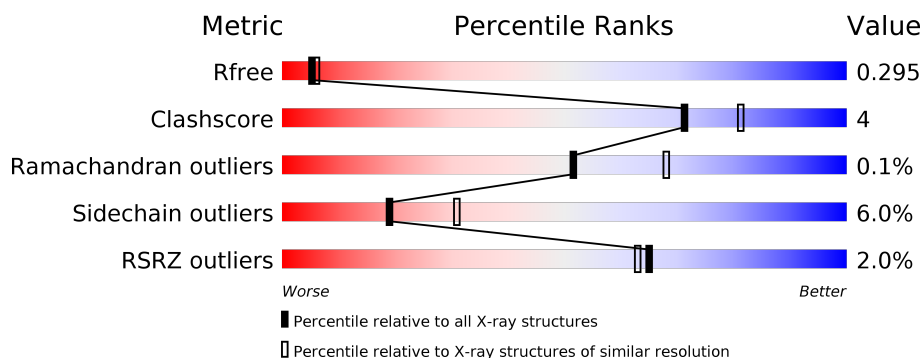
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	442	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> </div>
1	B	442	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
1	C	442	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>

## 2 Entry composition [i](#)

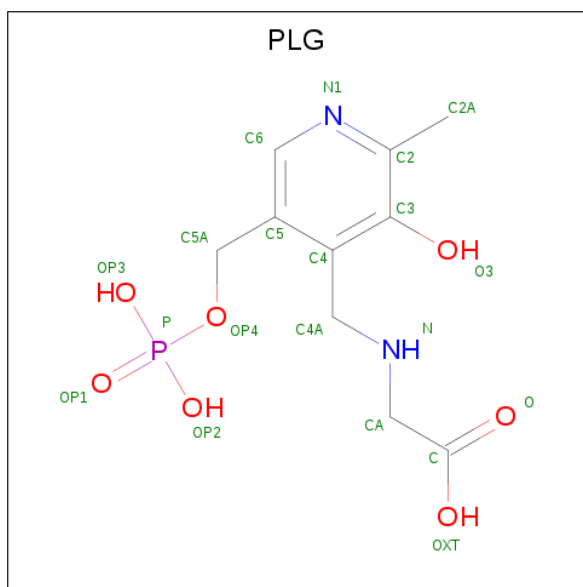
There are 5 unique types of molecules in this entry. The entry contains 10765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine hydroxymethyltransferase.

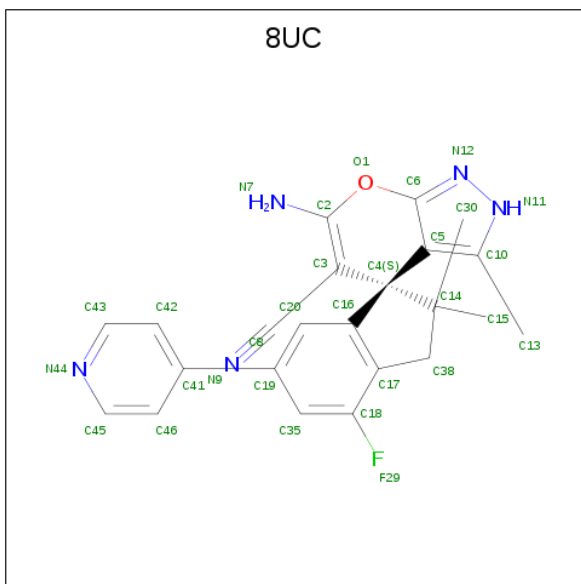
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3458	2186	600	655	17			
1	B	442	Total	C	N	O	S	0	0	0
			3458	2186	600	655	17			
1	C	442	Total	C	N	O	S	0	0	0
			3458	2186	600	655	17			

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula:  $C_{10}H_{15}N_2O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is (3 {S})-6'-azanyl-7-fluoranyl-2,2,3'-trimethyl-5-pyridin-4-yl-spiro[1 {H}-indene-3,4'-2 {H}-pyrano[2,3-c]pyrazole]-5'-carbonitrile (three-letter code: 8UC) (formula: C<sub>23</sub>H<sub>20</sub>FN<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			30	23	1	5	1		
3	B	1	Total	C	F	N	O	0	0
			30	23	1	5	1		
3	C	1	Total	C	F	N	O	0	0
			30	23	1	5	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

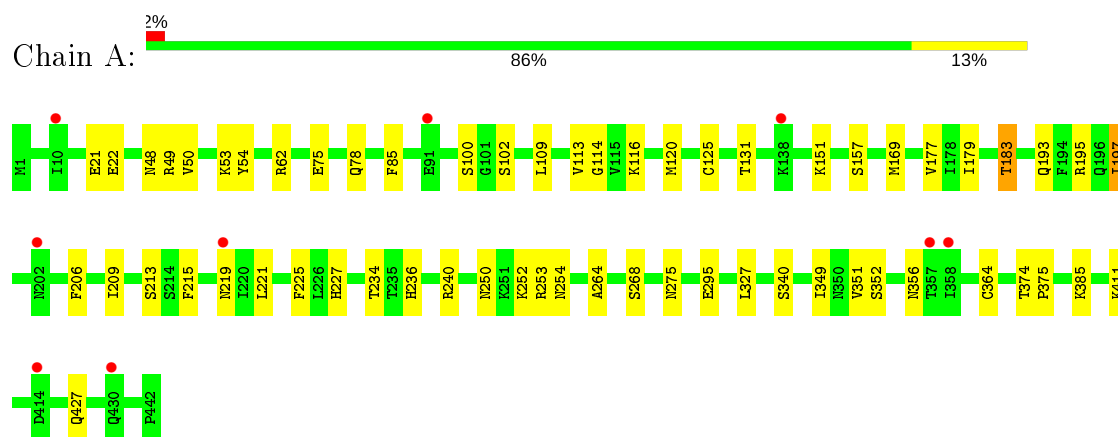
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		
5	B	82	Total	O	0	0
			82	82		
5	C	81	Total	O	0	0
			81	81		

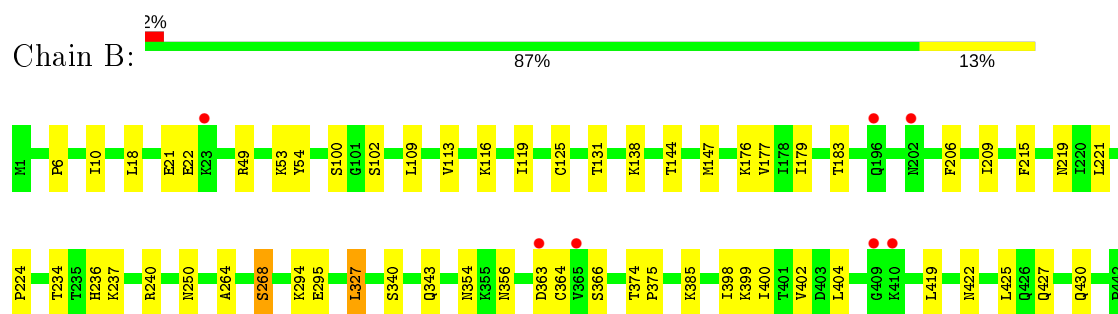
### 3 Residue-property plots [i](#)

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.

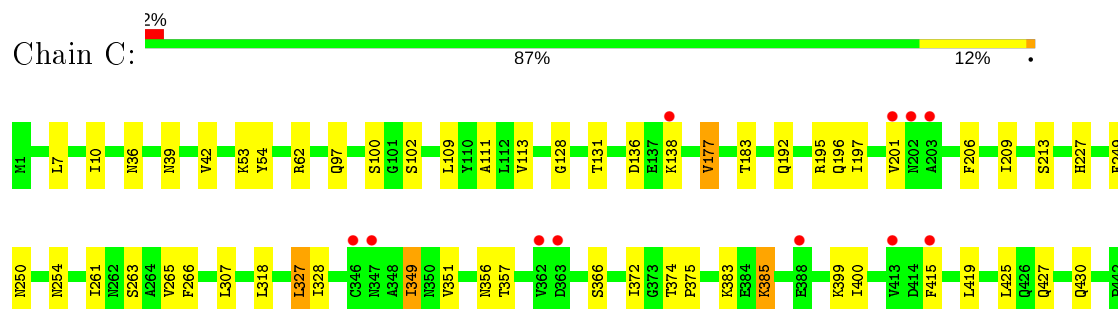
#### • Molecule 1: Serine hydroxymethyltransferase



#### • Molecule 1: Serine hydroxymethyltransferase



#### • Molecule 1: Serine hydroxymethyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.62Å 58.73Å 236.14Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	19.81 – 2.40 20.33 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.8 (19.81-2.40) 94.6 (20.33-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.222 , 0.300 0.223 , 0.295	Depositor DCC
$R_{free}$ test set	5468 reflections (10.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.876	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 19.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.043 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.044 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.470 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.477 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.038 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PLG, CL, 8UC

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	0.59	0/3521	0.74	0/4754
1	B	0.58	0/3521	0.74	0/4754
1	C	0.57	0/3521	0.73	0/4754
All	All	0.58	0/10563	0.74	0/14262

There are no bond length outliers.

There are no bond angle outliers.

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	3458	0	3477	27	0
1	B	3458	0	3477	25	0
1	C	3458	0	3477	26	0
2	A	20	0	11	1	0
2	B	20	0	11	0	0
2	C	20	0	11	0	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
3	C	30	0	0	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
5	A	76	0	0	1	0
5	B	82	0	0	1	0
5	C	81	0	0	1	0
All	All	10765	0	10464	74	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 4.

All (74) 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:85:PHE:HB3	1:A:225:PHE:CE2	2.23	0.74
1:C:109:LEU:O	1:C:113:VAL:HG22	1.90	0.72
1:C:53:LYS:NZ	5:C:601:HOH:O	2.25	0.68
1:A:85:PHE:HB3	1:A:225:PHE:HE2	1.57	0.68
1:C:383:LYS:HB2	1:C:385:LYS:HE2	1.77	0.64
1:A:109:LEU:HD21	1:A:179:ILE:HD11	1.79	0.64
1:A:125:CYS:HG	1:A:364:CYS:HG	1.47	0.62
1:B:404:LEU:HD21	1:B:422:ASN:HD22	1.69	0.57
1:B:109:LEU:O	1:B:113:VAL:HG22	2.04	0.56
5:A:609:HOH:O	1:B:53:LYS:HE3	2.04	0.56
1:C:209:ILE:HD12	1:C:213:SER:HA	1.88	0.55
1:A:374:THR:N	1:A:375:PRO:CD	2.70	0.55
1:C:195:ARG:NH1	1:C:227:HIS:O	2.39	0.54
1:A:374:THR:N	1:A:375:PRO:HD3	2.24	0.52
1:B:125:CYS:HG	1:B:364:CYS:HG	1.55	0.52
1:A:209:ILE:HD12	1:A:213:SER:HA	1.93	0.51
1:C:102:SER:HA	1:C:131:THR:HG21	1.93	0.51
1:B:404:LEU:HD21	1:B:422:ASN:ND2	2.26	0.51
1:C:195:ARG:HB2	1:C:227:HIS:HB3	1.93	0.51
1:C:263:SER:HA	1:C:266:PHE:O	2.11	0.51
1:C:7:LEU:HA	1:C:10:ILE:HG22	1.93	0.50
1:A:125:CYS:SG	1:A:364:CYS:SG	3.01	0.50
1:C:383:LYS:CB	1:C:385:LYS:HE2	2.41	0.50
1:C:400:ILE:HG21	1:C:425:LEU:HD21	1.94	0.49
1:C:374:THR:N	1:C:375:PRO:CD	2.76	0.48
1:B:109:LEU:HD22	1:B:119:ILE:HG21	1.96	0.47
1:A:193:GLN:O	1:A:197:ILE:HG13	2.15	0.47
1:B:343:GLN:OE1	1:B:354:ASN:HA	2.15	0.47
1:A:53:LYS:HE3	5:B:602:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG22	1:A:275:ASN:HB3	1.97	0.46
1:C:327:LEU:C	1:C:327:LEU:HD12	2.36	0.46
1:C:318:LEU:HD22	1:C:328:ILE:CG2	2.45	0.46
1:A:109:LEU:O	1:A:113:VAL:HG22	2.15	0.46
1:A:113:VAL:CG1	1:A:177:VAL:HG23	2.45	0.46
1:B:102:SER:HA	1:B:131:THR:HG21	1.96	0.46
1:A:22:GLU:OE2	1:B:49:ARG:NH1	2.48	0.46
1:B:119:ILE:HG22	1:B:177:VAL:HB	1.97	0.46
1:C:349:ILE:HG13	1:C:351:VAL:HG23	1.97	0.46
1:C:97:GLN:HB2	1:C:265:VAL:HG11	1.98	0.46
1:A:183:THR:HB	2:A:501:PLG:O3	2.16	0.46
1:A:264:ALA:HA	1:A:268:SER:HB2	1.98	0.45
1:B:400:ILE:HG21	1:B:425:LEU:HD21	1.98	0.45
1:B:109:LEU:HD21	1:B:179:ILE:HD11	1.99	0.45
1:B:327:LEU:HD12	1:B:327:LEU:C	2.37	0.44
1:B:374:THR:N	1:B:375:PRO:CD	2.80	0.44
1:C:111:ALA:CB	1:C:261:ILE:HD12	2.48	0.44
1:A:113:VAL:HG23	1:A:114:GLY:O	2.18	0.44
1:A:195:ARG:HB2	1:A:227:HIS:HB3	2.00	0.44
1:C:113:VAL:HG11	1:C:177:VAL:HG23	1.99	0.44
1:B:209:ILE:HG21	1:B:224:PRO:HG3	1.99	0.44
1:C:307:LEU:HD21	1:C:372:ILE:HD12	1.99	0.43
1:A:116:LYS:HE3	1:B:116:LYS:HE2	1.99	0.43
1:A:215:PHE:HB3	1:A:221:LEU:HG	1.99	0.43
1:A:75:GLU:HA	1:A:78:GLN:OE1	2.18	0.43
1:B:398:ILE:O	1:B:402:VAL:HG23	2.18	0.43
1:C:374:THR:N	1:C:375:PRO:HD3	2.34	0.42
1:C:415:PHE:CE2	1:C:419:LEU:HD11	2.54	0.42
1:A:102:SER:HA	1:A:131:THR:HG21	2.01	0.42
1:C:249:PHE:CD1	1:C:261:ILE:HG21	2.55	0.42
1:B:234:THR:HB	1:B:236:HIS:CE1	2.54	0.42
1:A:234:THR:HB	1:A:236:HIS:CE1	2.55	0.42
1:A:120:MET:SD	1:A:169:MET:HE3	2.59	0.42
1:C:201:VAL:HG12	1:C:201:VAL:O	2.20	0.42
1:C:39:ASN:OD1	1:C:42:VAL:HG23	2.20	0.41
1:A:349:ILE:HG13	1:A:351:VAL:HG23	2.02	0.41
1:C:192:GLN:HG3	1:C:227:HIS:CE1	2.56	0.41
1:B:131:THR:O	1:B:144:THR:HG21	2.21	0.41
1:A:48:ASN:OD1	1:B:18:LEU:HD22	2.21	0.41
1:B:215:PHE:HB3	1:B:221:LEU:HG	2.01	0.41
1:B:374:THR:N	1:B:375:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:PRO:O	1:B:10:ILE:HG22	2.20	0.41
1:C:128:GLY:O	3:C:502:8UC:N7	2.54	0.40
1:A:49:ARG:NH1	1:B:22:GLU:OE2	2.55	0.40
1:B:264:ALA:HA	1:B:268:SER:HB2	2.02	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	440/442 (100%)	424 (96%)	16 (4%)	0	100	100
1	B	440/442 (100%)	426 (97%)	13 (3%)	1 (0%)	47	62
1	C	440/442 (100%)	427 (97%)	13 (3%)	0	100	100
All	All	1320/1326 (100%)	1277 (97%)	42 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	LYS

### 5.3.2 Protein sidechains [i](#)

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	381/381 (100%)	358 (94%)	23 (6%)	19	31
1	B	381/381 (100%)	357 (94%)	24 (6%)	18	28
1	C	381/381 (100%)	359 (94%)	22 (6%)	20	32
All	All	1143/1143 (100%)	1074 (94%)	69 (6%)	19	31

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	54	TYR
1	A	62	ARG
1	A	100	SER
1	A	151	LYS
1	A	157	SER
1	A	183	THR
1	A	197	ILE
1	A	206	PHE
1	A	219	ASN
1	A	240	ARG
1	A	250	ASN
1	A	252	LYS
1	A	253	ARG
1	A	254	ASN
1	A	295	GLU
1	A	327	LEU
1	A	340	SER
1	A	352	SER
1	A	356	ASN
1	A	385	LYS
1	A	411	LYS
1	A	427	GLN
1	B	21	GLU
1	B	54	TYR
1	B	100	SER
1	B	138	LYS
1	B	147	MET
1	B	176	LYS
1	B	183	THR
1	B	206	PHE
1	B	219	ASN
1	B	240	ARG
1	B	250	ASN

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Mol	Chain	Res	Type
1	B	268	SER
1	B	294	LYS
1	B	295	GLU
1	B	327	LEU
1	B	340	SER
1	B	356	ASN
1	B	363	ASP
1	B	366	SER
1	B	385	LYS
1	B	399	LYS
1	B	419	LEU
1	B	427	GLN
1	B	430	GLN
1	C	36	ASN
1	C	54	TYR
1	C	62	ARG
1	C	100	SER
1	C	136	ASP
1	C	138	LYS
1	C	177	VAL
1	C	183	THR
1	C	196	GLN
1	C	197	ILE
1	C	206	PHE
1	C	250	ASN
1	C	254	ASN
1	C	327	LEU
1	C	349	ILE
1	C	356	ASN
1	C	357	THR
1	C	366	SER
1	C	385	LYS
1	C	399	LYS
1	C	427	GLN
1	C	430	GLN

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

Mol	Chain	Res	Type
1	A	196	GLN
1	A	299	GLN
1	A	427	GLN

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Mol	Chain	Res	Type
1	B	299	GLN
1	B	427	GLN
1	C	227	HIS
1	C	299	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
2	PLG	B	501	-	17,20,20	2.93	3 (17%)	23,28,28	2.46	10 (43%)
3	8UC	A	502	-	31,34,34	2.72	4 (12%)	38,54,54	2.50	7 (18%)
2	PLG	C	501	-	17,20,20	3.04	4 (23%)	23,28,28	2.21	11 (47%)
2	PLG	A	501	-	17,20,20	2.77	4 (23%)	23,28,28	2.61	10 (43%)
3	8UC	C	502	-	31,34,34	2.79	5 (16%)	38,54,54	2.62	13 (34%)
3	8UC	B	502	-	31,34,34	2.66	4 (12%)	38,54,54	2.37	8 (21%)

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	PLG	B	501	-	-	6/10/12/12	0/1/1/1
3	8UC	A	502	-	-	4/4/46/46	0/5/5/5
2	PLG	C	501	-	-	7/10/12/12	0/1/1/1
2	PLG	A	501	-	-	5/10/12/12	0/1/1/1
3	8UC	C	502	-	-	4/4/46/46	0/5/5/5
3	8UC	B	502	-	-	0/4/46/46	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	8UC	C8-C3	-10.31	1.28	1.42
3	B	502	8UC	C8-C3	-10.27	1.28	1.42
3	A	502	8UC	C8-C3	-9.93	1.29	1.42
3	A	502	8UC	O1-C2	9.68	1.47	1.36
3	C	502	8UC	O1-C2	9.19	1.47	1.36
3	B	502	8UC	O1-C2	8.76	1.46	1.36
2	C	501	PLG	C3-C2	7.80	1.48	1.40
2	A	501	PLG	C5-C4	7.39	1.50	1.40
2	B	501	PLG	C3-C2	7.20	1.48	1.40
2	B	501	PLG	C5-C4	7.15	1.50	1.40
2	C	501	PLG	C5-C4	6.97	1.50	1.40
2	A	501	PLG	C3-C2	6.19	1.47	1.40
2	C	501	PLG	C3-C4	6.05	1.49	1.40
2	B	501	PLG	C3-C4	5.82	1.49	1.40
2	A	501	PLG	C3-C4	4.78	1.47	1.40
3	C	502	8UC	C35-C18	2.74	1.42	1.37
3	C	502	8UC	N11-N12	2.70	1.42	1.37
2	A	501	PLG	C4A-C4	2.55	1.55	1.51
3	B	502	8UC	C35-C18	2.42	1.41	1.37
2	C	501	PLG	C4A-C4	2.41	1.55	1.51
3	C	502	8UC	C4-C14	2.36	1.58	1.55
3	A	502	8UC	C8-N9	2.19	1.18	1.14
3	B	502	8UC	C4-C16	-2.10	1.50	1.52
3	A	502	8UC	C35-C18	2.03	1.41	1.37

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	8UC	C35-C18-C17	-8.86	118.37	124.59
3	A	502	8UC	O1-C2-N7	8.52	116.34	110.22
3	A	502	8UC	C35-C18-C17	-8.47	118.64	124.59
3	C	502	8UC	C35-C18-C17	-8.22	118.82	124.59
3	C	502	8UC	O1-C2-N7	7.40	115.53	110.22
3	B	502	8UC	O1-C2-N7	6.87	115.15	110.22
2	A	501	PLG	C4A-C4-C5	6.05	126.44	119.71
3	C	502	8UC	C3-C2-N7	-4.94	122.52	127.47
3	A	502	8UC	C3-C2-N7	-4.92	122.54	127.47
2	A	501	PLG	OP4-C5A-C5	4.76	118.42	109.35
2	A	501	PLG	C4-C4A-N	4.46	119.91	111.58
2	B	501	PLG	OP4-C5A-C5	4.42	117.77	109.35
2	A	501	PLG	C3-C4-C5	-4.39	114.51	118.72
2	B	501	PLG	OP3-P-OP4	-4.37	95.10	106.73
3	B	502	8UC	C3-C2-N7	-4.35	123.11	127.47
2	B	501	PLG	CA-N-C4A	4.25	123.27	112.54
2	B	501	PLG	C3-C4-C5	-3.86	115.01	118.72
2	B	501	PLG	C4A-C4-C5	3.70	123.82	119.71
2	C	501	PLG	C3-C4-C5	-3.64	115.22	118.72
3	C	502	8UC	C20-C19-C41	-3.58	114.94	120.86
3	C	502	8UC	C15-C14-C30	-3.56	102.55	108.42
3	C	502	8UC	C5-C4-C16	-3.37	104.11	112.30
2	C	501	PLG	CA-N-C4A	3.36	121.01	112.54
2	C	501	PLG	OP4-C5A-C5	3.35	115.73	109.35
2	C	501	PLG	C4-C4A-N	3.27	117.69	111.58
3	C	502	8UC	C13-C10-N11	3.21	126.70	119.65
3	C	502	8UC	C20-C16-C4	-3.17	125.92	131.32
2	B	501	PLG	C6-N1-C2	3.09	124.89	119.17
2	C	501	PLG	OP3-P-OP4	-3.06	98.59	106.73
2	B	501	PLG	OP3-P-OP2	3.06	119.32	107.64
2	A	501	PLG	CA-N-C4A	3.04	120.20	112.54
2	A	501	PLG	C6-N1-C2	2.98	124.68	119.17
3	C	502	8UC	C4-C3-C2	-2.94	121.28	125.00
3	B	502	8UC	C4-C3-C2	-2.93	121.29	125.00
2	C	501	PLG	C6-N1-C2	2.93	124.60	119.17
3	C	502	8UC	C35-C19-C41	2.91	125.67	120.86
2	C	501	PLG	C4A-C4-C5	2.85	122.88	119.71
2	C	501	PLG	OP3-P-OP1	2.84	121.79	110.68
3	A	502	8UC	C4-C3-C2	-2.80	121.46	125.00
2	A	501	PLG	C5A-C5-C6	-2.78	114.81	119.37
3	B	502	8UC	F29-C18-C35	2.76	124.09	118.61
2	B	501	PLG	C5A-C5-C6	-2.58	115.13	119.37
2	B	501	PLG	C6-C5-C4	2.58	119.94	118.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PLG	C5A-C5-C6	-2.50	115.27	119.37
3	A	502	8UC	C6-C5-C10	-2.49	101.38	104.01
2	A	501	PLG	OP2-P-OP4	-2.48	100.14	106.73
2	C	501	PLG	OP2-P-OP4	-2.44	100.23	106.73
3	A	502	8UC	C42-C43-N44	-2.42	119.41	123.62
2	C	501	PLG	C2A-C2-C3	2.42	123.87	120.89
3	B	502	8UC	C20-C19-C41	-2.42	116.87	120.86
3	A	502	8UC	C14-C4-C5	2.32	114.75	110.64
3	C	502	8UC	C42-C43-N44	-2.29	119.64	123.62
2	B	501	PLG	OP4-P-OP1	-2.18	100.35	106.47
3	B	502	8UC	C6-C5-C10	-2.16	101.73	104.01
3	C	502	8UC	C8-C3-C2	2.10	120.43	117.64
3	C	502	8UC	C42-C41-C19	-2.10	117.72	121.36
2	A	501	PLG	C6-C5-C4	2.10	119.60	118.12
3	B	502	8UC	C20-C16-C4	-2.07	127.80	131.32
2	A	501	PLG	OP3-P-OP4	-2.06	101.25	106.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PLG	C3-C4-C4A-N
2	B	501	PLG	C5-C4-C4A-N
2	B	501	PLG	C5A-OP4-P-OP1
2	C	501	PLG	C5A-OP4-P-OP1
2	C	501	PLG	C5A-OP4-P-OP2
2	C	501	PLG	C5A-OP4-P-OP3
2	A	501	PLG	C5A-OP4-P-OP2
2	A	501	PLG	C5A-OP4-P-OP3
2	C	501	PLG	C5-C4-C4A-N
2	C	501	PLG	C3-C4-C4A-N
3	C	502	8UC	C35-C19-C41-C46
2	B	501	PLG	C-CA-N-C4A
2	C	501	PLG	C-CA-N-C4A
2	A	501	PLG	C-CA-N-C4A
3	C	502	8UC	C35-C19-C41-C42
3	C	502	8UC	C20-C19-C41-C46
3	C	502	8UC	C20-C19-C41-C42
3	A	502	8UC	C35-C19-C41-C42
3	A	502	8UC	C35-C19-C41-C46
3	A	502	8UC	C20-C19-C41-C42
3	A	502	8UC	C20-C19-C41-C46

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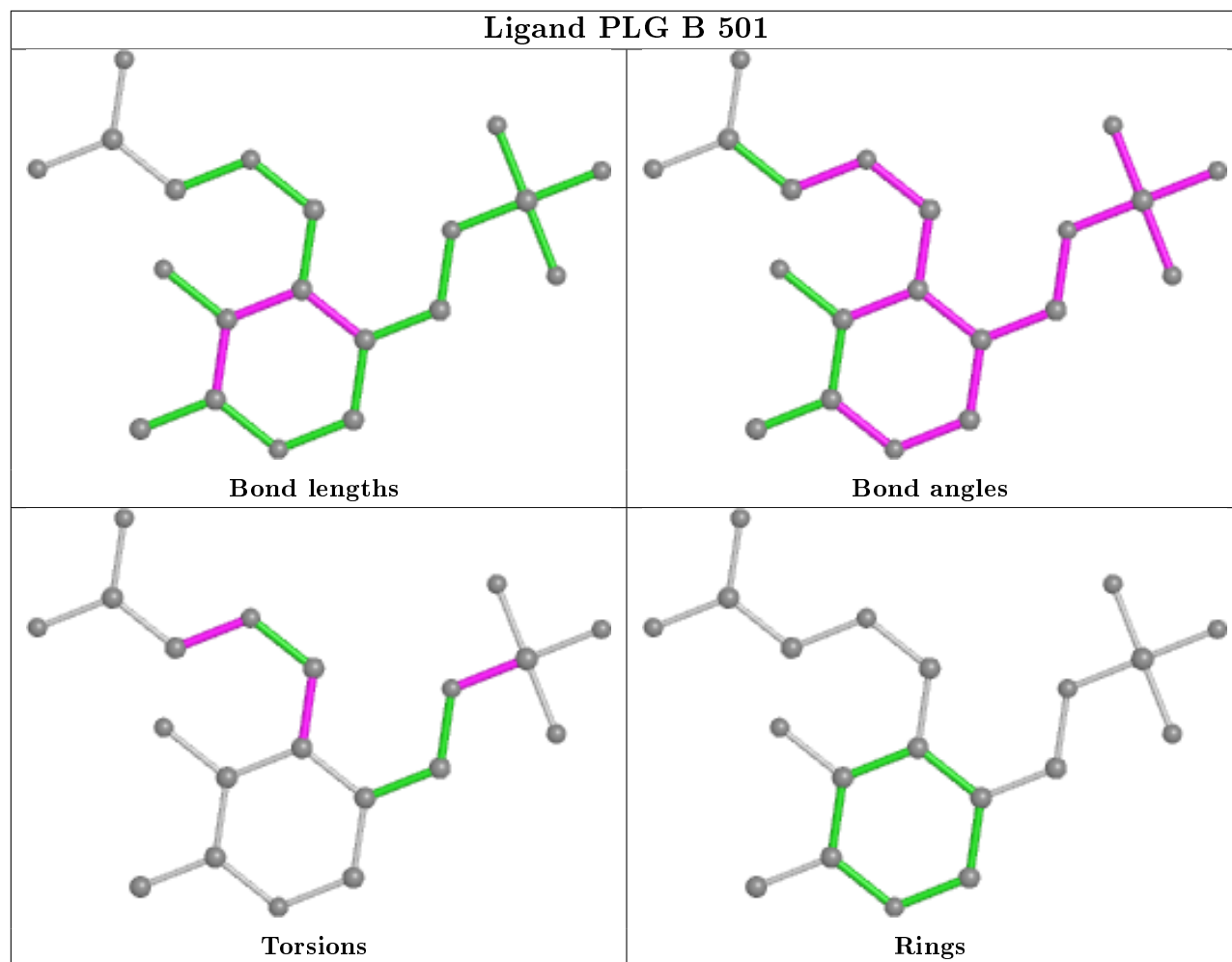
Mol	Chain	Res	Type	Atoms
2	C	501	PLG	C6-C5-C5A-OP4
2	B	501	PLG	C5A-OP4-P-OP2
2	B	501	PLG	C5A-OP4-P-OP3
2	A	501	PLG	C5-C4-C4A-N
2	A	501	PLG	C5A-OP4-P-OP1

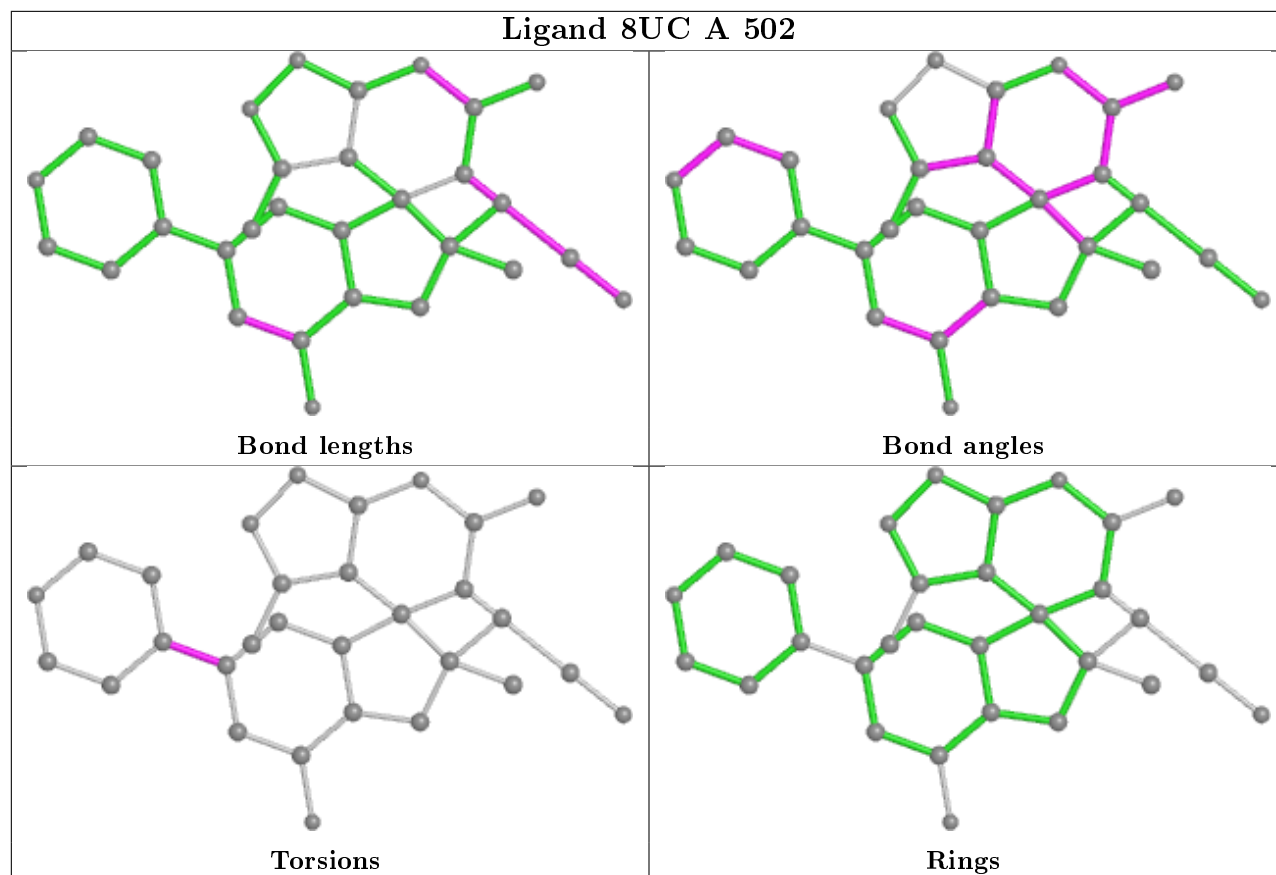
There are no ring outliers.

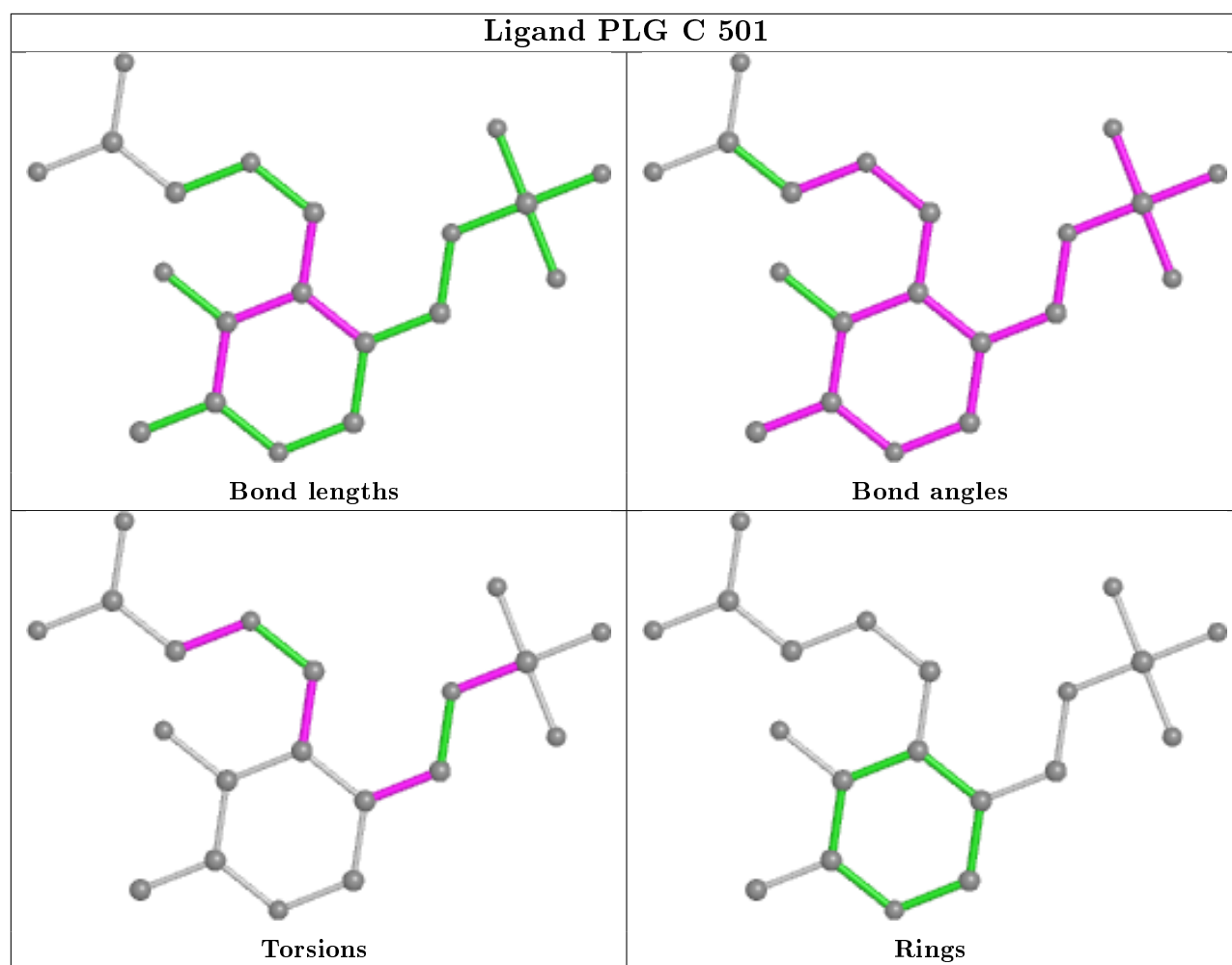
2 monomers are involved in 2 short contacts:

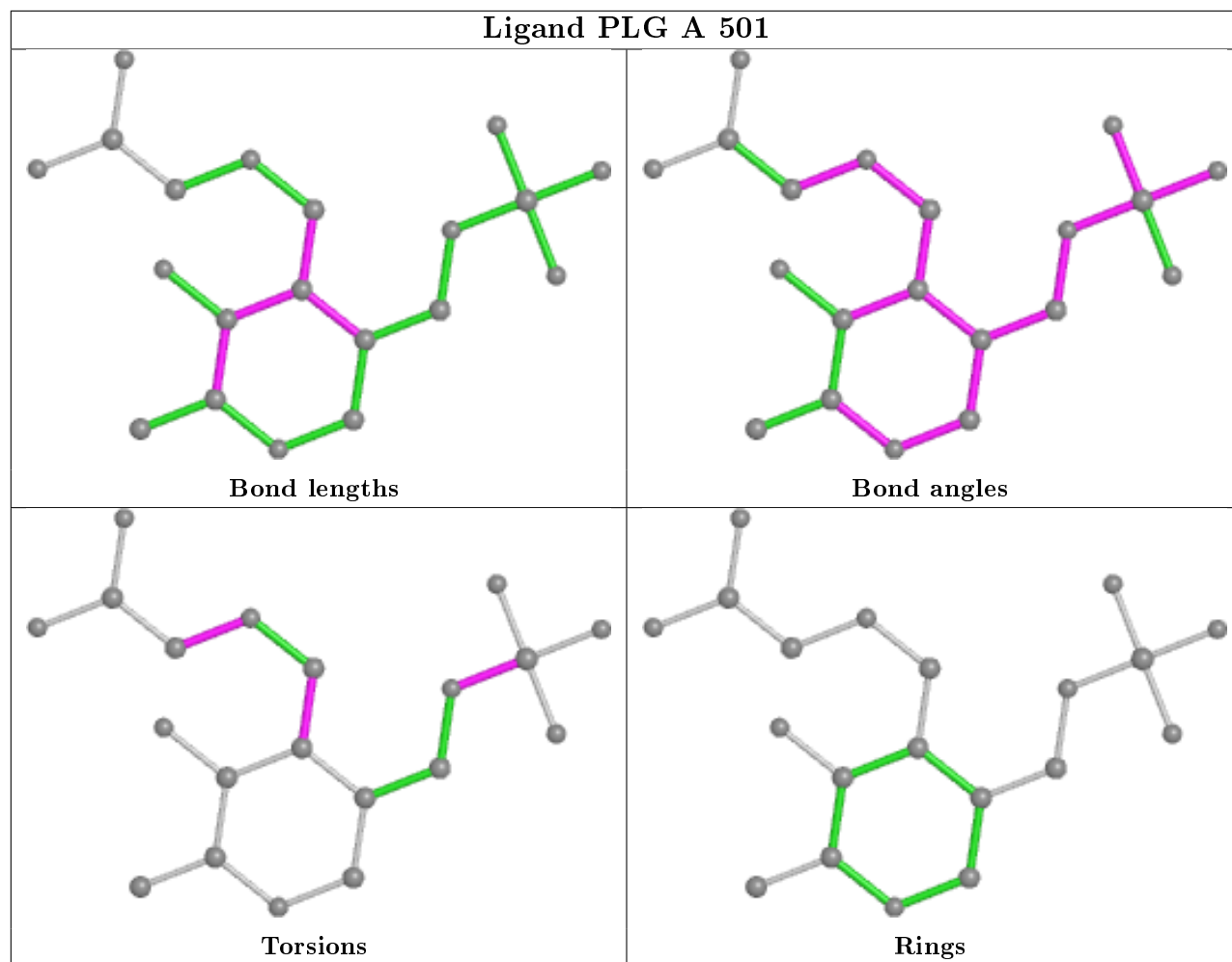
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLG	1	0
3	C	502	8UC	1	0

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.

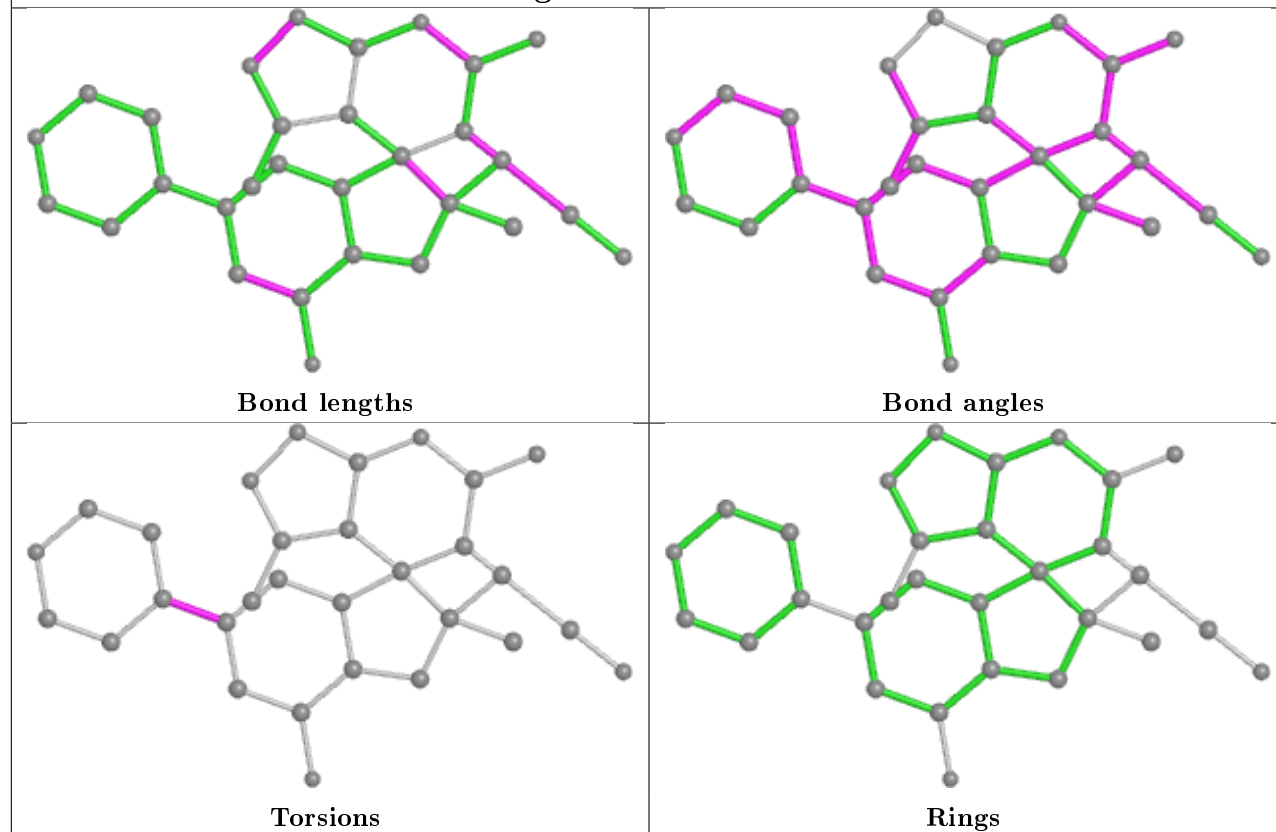




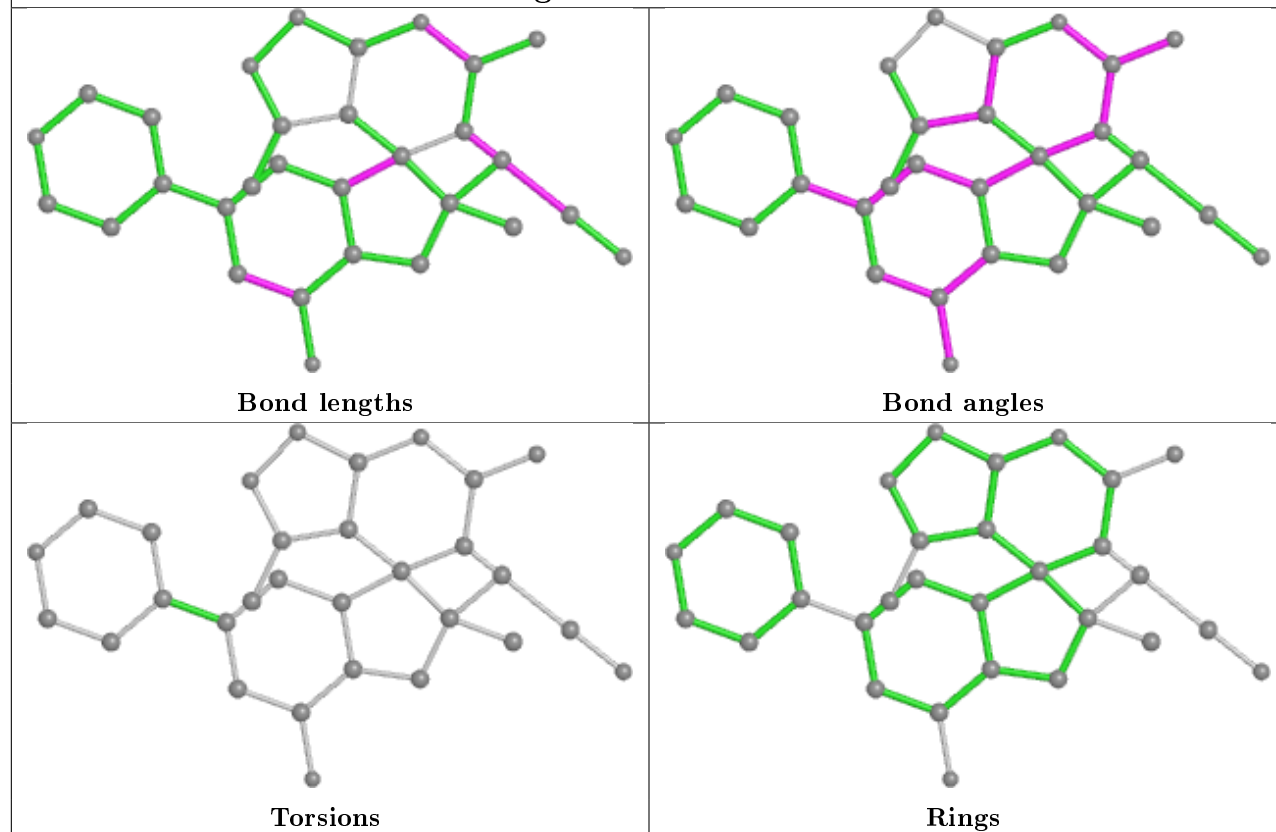




## Ligand 8UC C 502



## Ligand 8UC B 502



## 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	442/442 (100%)	0.00	9 (2%) 65 63	18, 35, 63, 92	0
1	B	442/442 (100%)	0.03	7 (1%) 72 70	18, 36, 64, 87	0
1	C	442/442 (100%)	0.02	11 (2%) 57 55	18, 36, 64, 96	0
All	All	1326/1326 (100%)	0.02	27 (2%) 65 63	18, 36, 64, 96	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	ASN	4.6
1	A	430	GLN	4.1
1	C	201	VAL	3.8
1	A	414	ASP	3.4
1	B	365	VAL	3.4
1	C	363	ASP	3.3
1	A	357	THR	3.1
1	A	138	LYS	3.1
1	C	203	ALA	2.9
1	C	346	CYS	2.8
1	B	409	GLY	2.8
1	B	410	LYS	2.7
1	C	202	ASN	2.5
1	A	10	ILE	2.4
1	C	415	PHE	2.4
1	B	23	LYS	2.4
1	B	363	ASP	2.3
1	C	413	VAL	2.3
1	A	91	GLU	2.3
1	C	138	LYS	2.2
1	A	358	ILE	2.1
1	A	219	ASN	2.1
1	C	347	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	196	GLN	2.1
1	C	388	GLU	2.1
1	C	362	VAL	2.0
1	A	202	ASN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

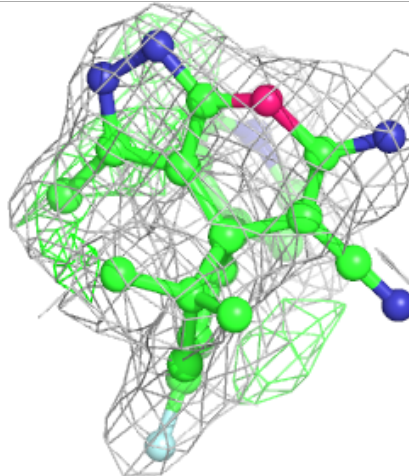
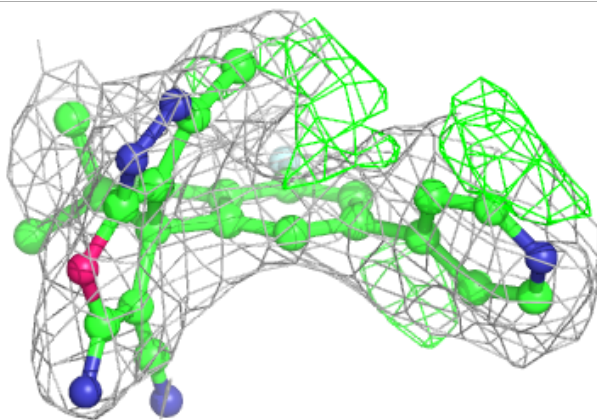
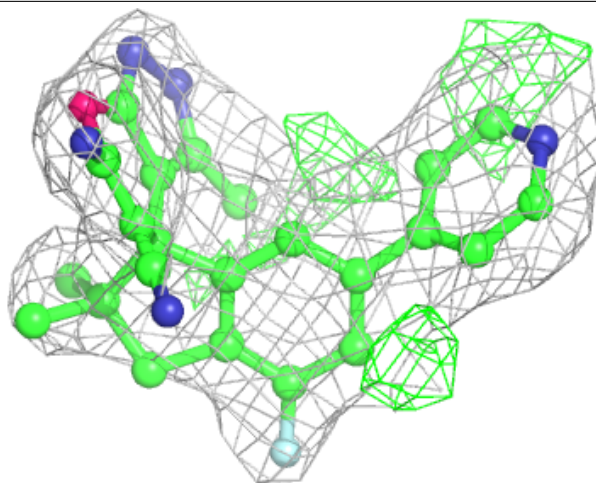
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	8UC	C	502	30/30	0.73	0.22	45,51,55,61	0
3	8UC	B	502	30/30	0.74	0.20	44,49,52,56	0
3	8UC	A	502	30/30	0.79	0.19	42,48,51,54	0
4	CL	A	503	1/1	0.95	0.09	30,30,30,30	0
2	PLG	C	501	20/20	0.95	0.22	22,29,32,33	0
4	CL	C	503	1/1	0.95	0.06	24,24,24,24	1
2	PLG	B	501	20/20	0.96	0.16	20,29,32,32	0
2	PLG	A	501	20/20	0.97	0.13	21,26,28,28	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.

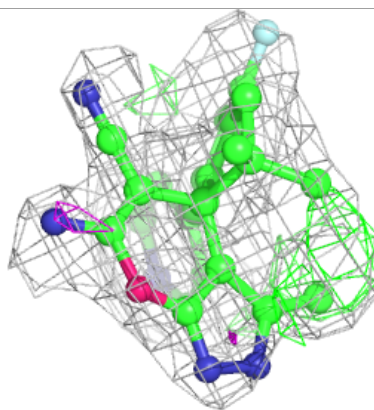
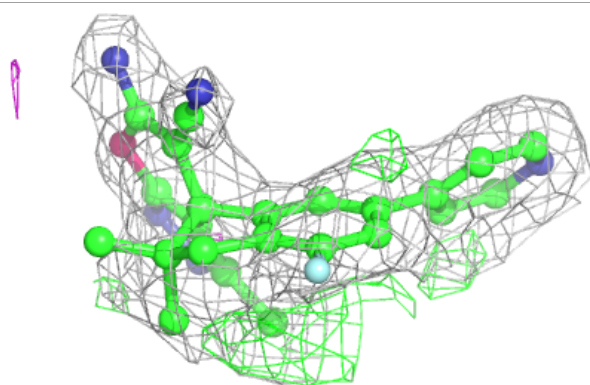
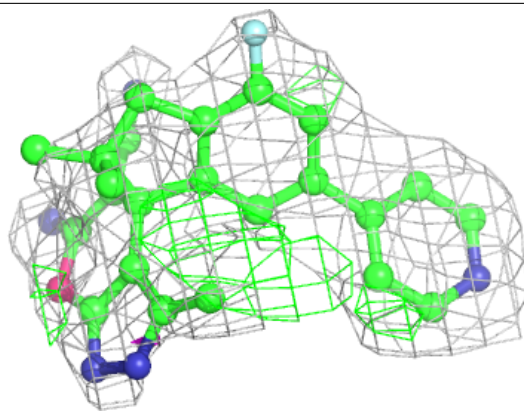
**Electron density around 8UC C 502:**

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



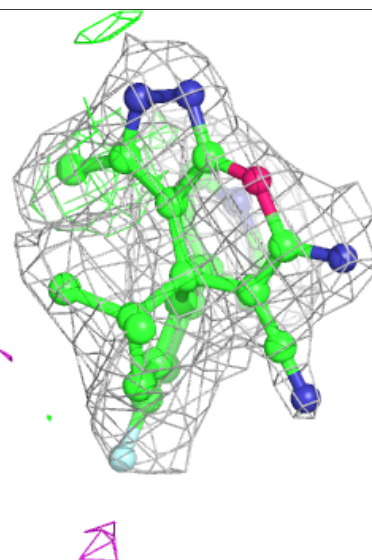
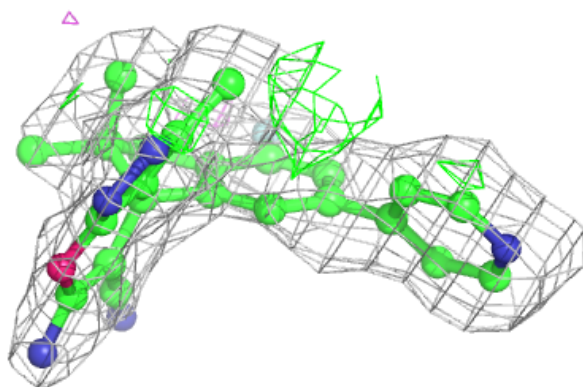
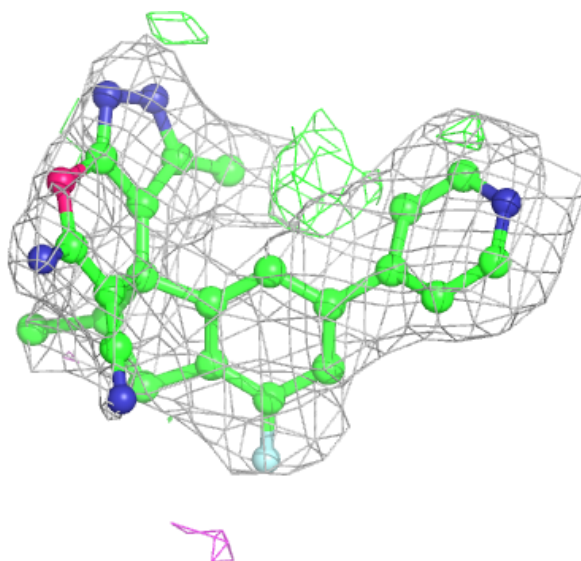
**Electron density around 8UC B 502:**

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



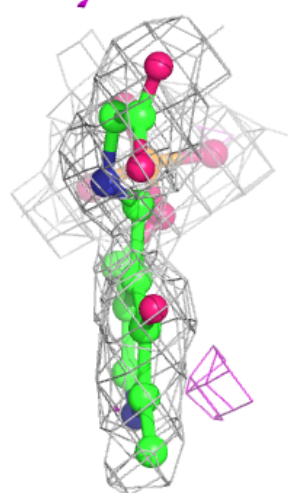
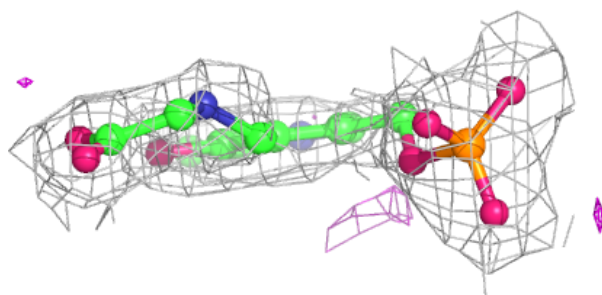
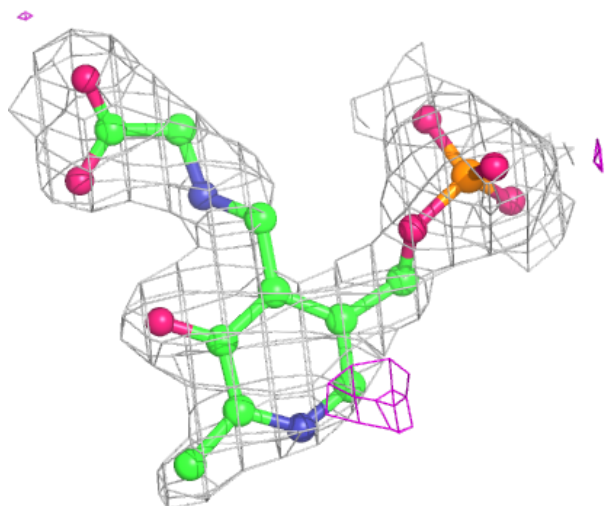
**Electron density around 8UC A 502:**

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



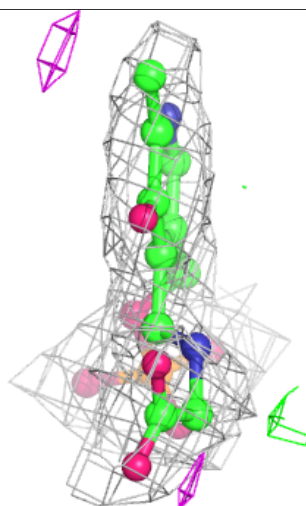
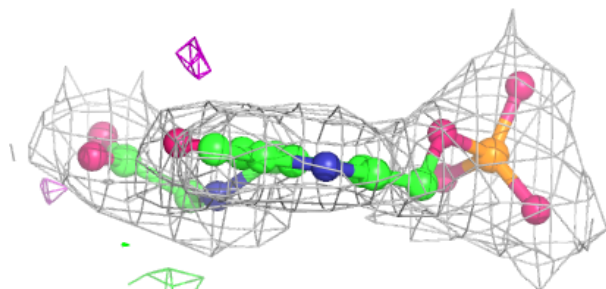
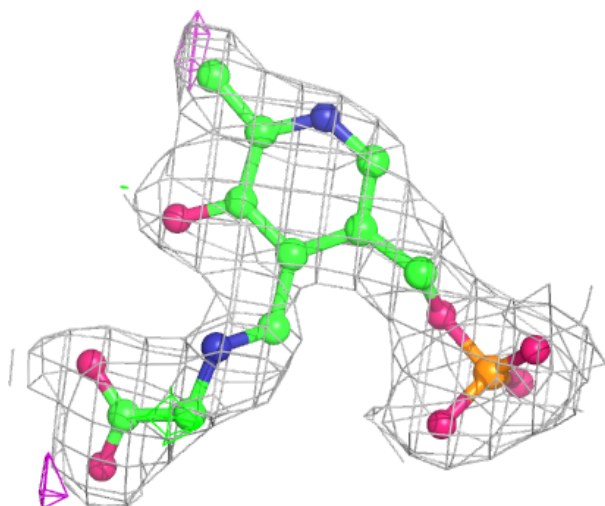
**Electron density around PLG C 501:**

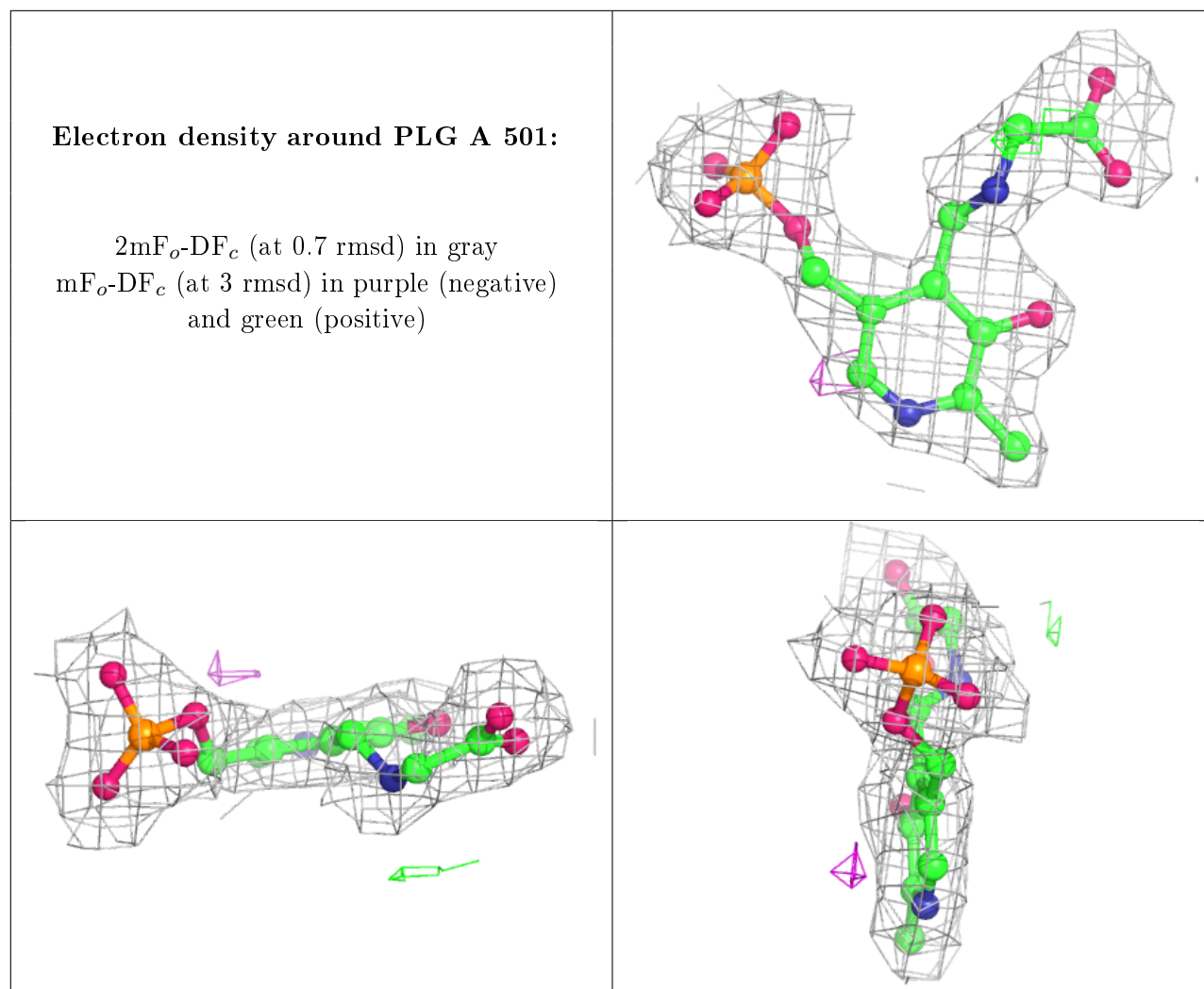
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PLG B 501:**

$2mF_o-DF_c$  (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.