



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:38 pm BST

PDB ID : 5XMQ
Title : Plasmodium vivax SHMT(C346A) bound with PLP-glycine and MF011
Authors : Chitnumsub, P.; Jaruwat, A.; Leartsakulpanich, U.; Schwertz, G.; Diederich, F.
Deposited on : 2017-05-16
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

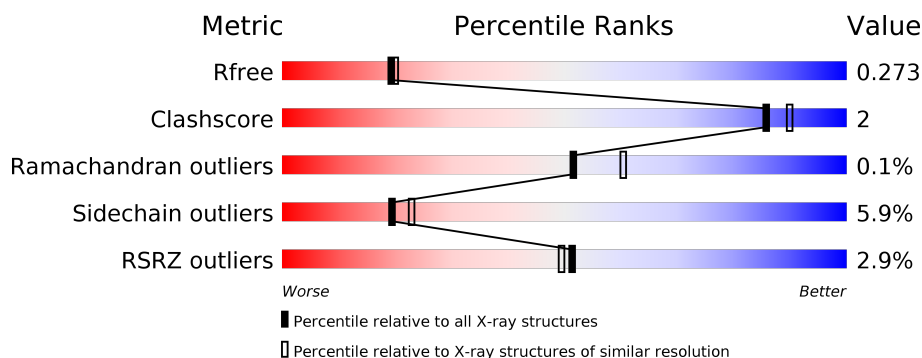
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 ≥ 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>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> <div>•</div> </div>
1	B	442	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> <div>•</div> </div>
1	C	442	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> <div>•</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11030 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.

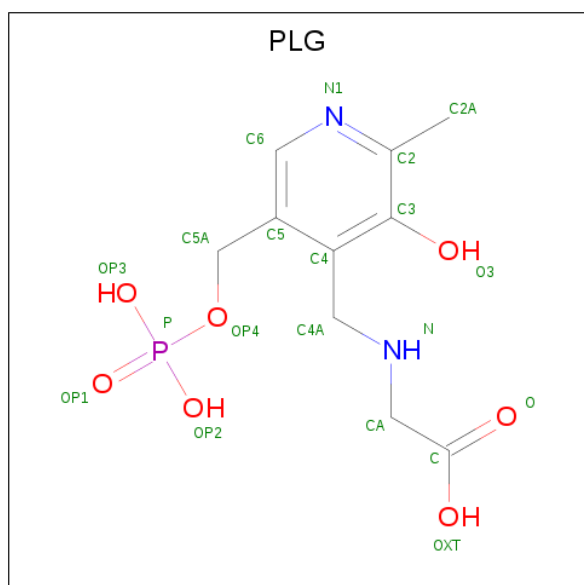
- Molecule 1 is a protein called Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3457	2186	600	655	16			
1	B	442	Total	C	N	O	S	0	0	0
			3457	2186	600	655	16			
1	C	442	Total	C	N	O	S	0	0	0
			3457	2186	600	655	16			

There are 3 discrepancies between the modelled and reference sequences:

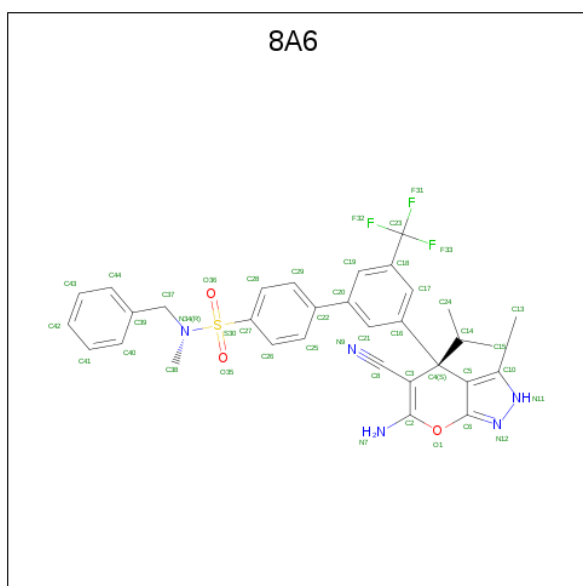
Chain	Residue	Modelled	Actual	Comment	Reference
A	364	ALA	CYS	engineered mutation	UNP A0A1G4H5I1
B	364	ALA	CYS	engineered mutation	UNP A0A1G4H5I1
C	364	ALA	CYS	engineered mutation	UNP A0A1G4H5I1

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: C₁₀H₁₅N₂O₇P).



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 4-[3-[(4 {S})-6-azanyl-5-cyano-3-methyl-4-propan-2-yl-2 {H}-pyrano[2,3-c]pyrazol-4-yl]-5-(trifluoromethyl)phenyl]- {N}-methyl- {N}-(phenylmethyl)benzenesulfonamide (three-letter code: 8A6) (formula: C₃₂H₃₀F₃N₅O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 44	C 32	F 3	N 5	O 3	S 1	0	0
3	B	1	Total 44	C 32	F 3	N 5	O 3	S 1	0	0
3	C	1	Total 44	C 32	F 3	N 5	O 3	S 1	0	0

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

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

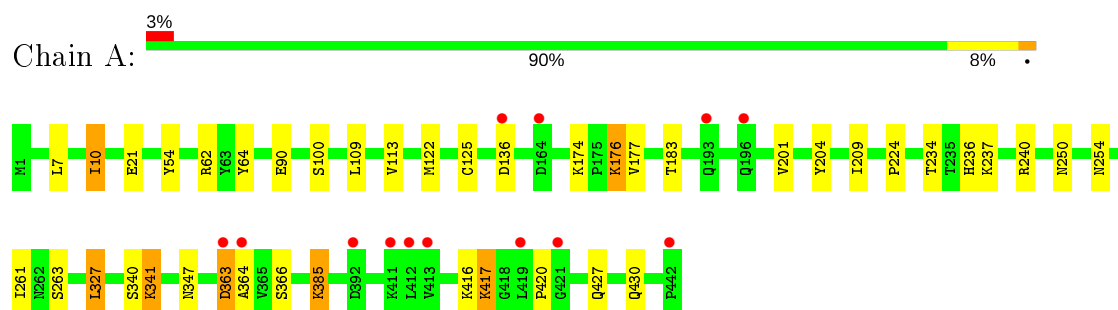
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	153	Total 153	O 153	0	0
5	B	158	Total 158	O 158	0	0
5	C	154	Total 154	O 154	0	0

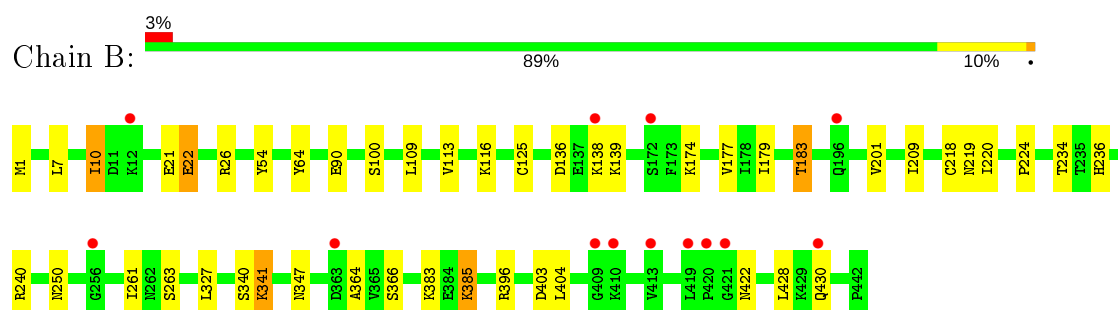
3 Residue-property plots [i](#)

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.

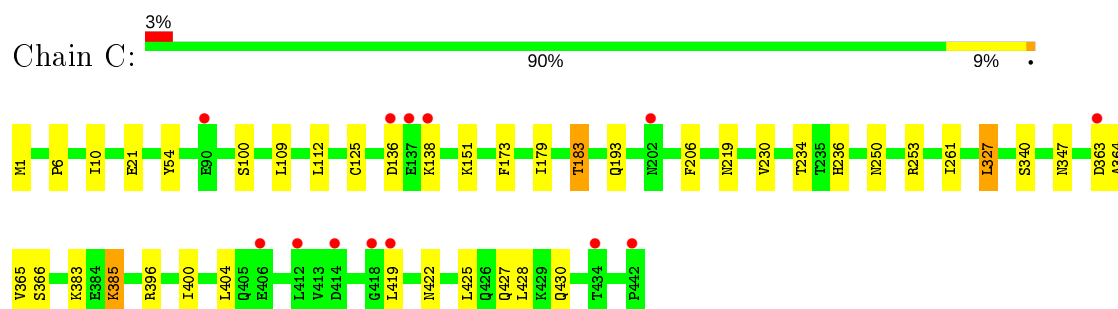
- Molecule 1: Serine hydroxymethyltransferase



- 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, α , β , γ	101.32Å 58.36Å 236.45Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.00-2.20) 93.7 (29.56-2.20)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.39 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.216 , 0.276 0.217 , 0.273	Depositor DCC
R_{free} test set	6558 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 13.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.021 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.460 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.457 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11030	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLG, 8A6, 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	0.55	0/3520	0.70	2/4753 (0.0%)
1	B	0.54	0/3520	0.70	2/4753 (0.0%)
1	C	0.54	0/3520	0.70	1/4753 (0.0%)
All	All	0.54	0/10560	0.70	5/14259 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	327	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	240	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	240	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	327	LEU	CA-CB-CG	5.14	127.12	115.30
1	B	327	LEU	CA-CB-CG	5.04	126.88	115.30

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	3457	0	3477	15	0
1	B	3457	0	3477	17	0
1	C	3457	0	3477	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	11	0	0
2	B	20	0	11	1	0
2	C	20	0	11	1	0
3	A	44	0	0	1	0
3	B	44	0	0	2	0
3	C	44	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	153	0	0	2	0
5	B	158	0	0	3	0
5	C	154	0	0	0	0
All	All	11030	0	10464	47	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 2.

All (47) 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:417:LYS:O	5:A:601:HOH:O	2.02	0.76
1:B:403:ASP:OD2	5:B:601:HOH:O	2.12	0.66
1:C:125:CYS:SG	1:C:364:ALA:HB2	2.39	0.62
1:B:341:LYS:NZ	5:B:602:HOH:O	2.33	0.61
1:A:113:VAL:HG12	1:A:176:LYS:HB3	1.85	0.58
1:B:7:LEU:HA	1:B:10:ILE:HG22	1.87	0.57
1:C:363:ASP:HB3	1:C:365:VAL:HG23	1.89	0.54
1:C:6:PRO:O	1:C:10:ILE:HG22	2.08	0.53
1:B:218:CYS:HB2	1:B:220:ILE:HD12	1.91	0.52
1:C:109:LEU:HD21	1:C:179:ILE:HD11	1.93	0.50
1:B:109:LEU:HD21	1:B:179:ILE:HD11	1.94	0.49
1:B:22:GLU:OE2	1:B:26:ARG:NH2	2.47	0.47
1:A:341:LYS:NZ	5:A:605:HOH:O	2.47	0.47
1:C:383:LYS:HB2	1:C:385:LYS:HE2	1.95	0.47
1:A:109:LEU:O	1:A:113:VAL:HG22	2.15	0.46
1:A:363:ASP:O	1:A:364:ALA:HB3	2.15	0.46
1:A:174:LYS:HD3	1:A:201:VAL:HG13	1.97	0.46
1:A:7:LEU:HA	1:A:10:ILE:HG22	1.97	0.46
1:B:125:CYS:SG	1:B:364:ALA:HB2	2.56	0.46
3:A:502:8A6:C15	1:B:64:TYR:HE1	2.30	0.45
1:C:234:THR:HB	1:C:236:HIS:CE1	2.52	0.45
1:C:400:ILE:HG21	1:C:425:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:THR:HB	1:B:236:HIS:CE1	2.52	0.44
1:C:363:ASP:O	1:C:364:ALA:HB3	2.18	0.44
1:B:183:THR:HB	2:B:501:PLG:O3	2.18	0.44
1:C:404:LEU:HD21	1:C:422:ASN:HD22	1.83	0.44
1:A:209:ILE:HG21	1:A:224:PRO:HG3	2.00	0.43
1:B:383:LYS:HB2	1:B:385:LYS:HE2	1.99	0.43
3:B:502:8A6:C17	3:B:502:8A6:C8	2.96	0.43
1:A:177:VAL:HG22	1:A:204:TYR:HB2	2.01	0.43
1:B:404:LEU:HD21	1:B:422:ASN:HD22	1.84	0.42
1:C:383:LYS:CB	1:C:385:LYS:HE2	2.49	0.42
1:A:234:THR:HB	1:A:236:HIS:CE1	2.55	0.42
1:B:113:VAL:CG1	1:B:177:VAL:HG23	2.50	0.41
1:A:64:TYR:HE1	3:B:502:8A6:C15	2.33	0.41
1:B:209:ILE:HG21	1:B:224:PRO:HG3	2.02	0.41
1:B:396:ARG:CZ	1:B:428:LEU:HD13	2.51	0.41
1:A:125:CYS:SG	1:A:364:ALA:HB2	2.60	0.41
1:C:112:LEU:HD11	1:C:230:VAL:HG21	2.02	0.41
1:A:385:LYS:H	1:A:385:LYS:CE	2.34	0.41
1:A:416:LYS:O	1:A:420:PRO:HD3	2.21	0.41
1:A:10:ILE:HD12	5:B:609:HOH:O	2.21	0.41
1:B:383:LYS:HB2	1:B:385:LYS:CE	2.52	0.40
1:C:151:LYS:HD2	1:C:173:PHE:CD1	2.56	0.40
1:B:174:LYS:HD3	1:B:201:VAL:HG13	2.02	0.40
1:C:183:THR:HB	2:C:501:PLG:O3	2.22	0.40
1:C:396:ARG:CZ	1:C:428:LEU:HD13	2.51	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%)	425 (97%)	14 (3%)	1 (0%)	47 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	440/442 (100%)	428 (97%)	12 (3%)	0	100	100
1	C	440/442 (100%)	428 (97%)	12 (3%)	0	100	100
All	All	1320/1326 (100%)	1281 (97%)	38 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	LYS

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	380/380 (100%)	356 (94%)	24 (6%)	18	20
1	B	380/380 (100%)	358 (94%)	22 (6%)	20	23
1	C	380/380 (100%)	359 (94%)	21 (6%)	21	26
All	All	1140/1140 (100%)	1073 (94%)	67 (6%)	19	23

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	21	GLU
1	A	54	TYR
1	A	62	ARG
1	A	90	GLU
1	A	100	SER
1	A	122	MET
1	A	136	ASP
1	A	176	LYS
1	A	183	THR
1	A	250	ASN
1	A	254	ASN
1	A	261	ILE

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Mol	Chain	Res	Type
1	A	263	SER
1	A	327	LEU
1	A	340	SER
1	A	341	LYS
1	A	347	ASN
1	A	363	ASP
1	A	366	SER
1	A	385	LYS
1	A	417	LYS
1	A	427	GLN
1	A	430	GLN
1	B	1	MET
1	B	10	ILE
1	B	21	GLU
1	B	22	GLU
1	B	54	TYR
1	B	90	GLU
1	B	100	SER
1	B	116	LYS
1	B	136	ASP
1	B	138	LYS
1	B	139	LYS
1	B	183	THR
1	B	219	ASN
1	B	250	ASN
1	B	261	ILE
1	B	263	SER
1	B	340	SER
1	B	341	LYS
1	B	347	ASN
1	B	366	SER
1	B	385	LYS
1	B	430	GLN
1	C	1	MET
1	C	21	GLU
1	C	54	TYR
1	C	100	SER
1	C	136	ASP
1	C	138	LYS
1	C	183	THR
1	C	193	GLN
1	C	206	PHE

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Mol	Chain	Res	Type
1	C	219	ASN
1	C	250	ASN
1	C	253	ARG
1	C	261	ILE
1	C	327	LEU
1	C	340	SER
1	C	347	ASN
1	C	366	SER
1	C	385	LYS
1	C	419	LEU
1	C	427	GLN
1	C	430	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
1	A	192	GLN
1	A	227	HIS
1	A	254	ASN
1	B	158	GLN
1	B	299	GLN
1	B	321	ASN
1	B	427	GLN
1	C	158	GLN
1	C	193	GLN
1	C	347	ASN
1	C	427	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
3	8A6	B	502	-	42,48,48	2.73	3 (7%)	59,74,74	2.16	14 (23%)
2	PLG	C	501	-	17,20,20	2.56	3 (17%)	23,28,28	1.80	7 (30%)
2	PLG	A	501	-	17,20,20	2.58	3 (17%)	23,28,28	1.85	8 (34%)
3	8A6	C	502	-	42,48,48	2.93	5 (11%)	59,74,74	2.09	18 (30%)
3	8A6	A	502	-	42,48,48	2.80	4 (9%)	59,74,74	2.18	15 (25%)
2	PLG	B	501	-	17,20,20	2.81	3 (17%)	23,28,28	1.82	6 (26%)

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	8A6	B	502	-	-	3/38/60/60	0/5/5/5
2	PLG	C	501	-	-	5/10/12/12	0/1/1/1
2	PLG	A	501	-	-	4/10/12/12	0/1/1/1
3	8A6	C	502	-	-	5/38/60/60	0/5/5/5
3	8A6	A	502	-	-	3/38/60/60	0/5/5/5
2	PLG	B	501	-	-	6/10/12/12	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	8A6	C27-S30	-11.03	1.61	1.76
3	A	502	8A6	C27-S30	-10.77	1.61	1.76
3	C	502	8A6	C8-C3	-10.47	1.28	1.42
3	B	502	8A6	C27-S30	-10.41	1.62	1.76
3	A	502	8A6	C8-C3	-9.72	1.29	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	8A6	O1-C2	9.72	1.47	1.36
3	B	502	8A6	C8-C3	-9.55	1.29	1.42
3	A	502	8A6	O1-C2	9.41	1.47	1.36
3	B	502	8A6	O1-C2	9.02	1.47	1.36
2	B	501	PLG	C3-C2	7.52	1.48	1.40
2	A	501	PLG	C3-C2	6.94	1.47	1.40
2	C	501	PLG	C3-C2	6.37	1.47	1.40
2	B	501	PLG	C5-C4	6.34	1.49	1.40
2	C	501	PLG	C5-C4	5.63	1.48	1.40
2	A	501	PLG	C5-C4	5.49	1.48	1.40
2	C	501	PLG	C3-C4	5.36	1.48	1.40
2	B	501	PLG	C3-C4	4.93	1.47	1.40
2	A	501	PLG	C3-C4	4.80	1.47	1.40
3	C	502	8A6	C21-C16	2.43	1.43	1.39
3	A	502	8A6	N12-N11	2.04	1.41	1.37
3	C	502	8A6	N12-N11	2.03	1.41	1.37

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	8A6	O1-C2-N7	6.86	115.15	110.22
3	B	502	8A6	O35-S30-O36	-6.71	108.65	119.52
3	A	502	8A6	O1-C2-N7	6.62	114.98	110.22
3	A	502	8A6	O35-S30-O36	-6.49	109.01	119.52
3	C	502	8A6	O35-S30-O36	-6.46	109.05	119.52
3	B	502	8A6	C27-S30-N34	6.12	115.38	107.02
3	B	502	8A6	O1-C2-N7	6.02	114.55	110.22
3	C	502	8A6	C27-S30-N34	5.40	114.39	107.02
3	A	502	8A6	C27-S30-N34	5.11	114.01	107.02
2	B	501	PLG	OP4-C5A-C5	4.63	118.18	109.35
3	A	502	8A6	C3-C2-N7	-4.44	123.03	127.47
3	A	502	8A6	C14-C4-C3	-4.19	103.59	110.32
3	C	502	8A6	C3-C2-N7	-4.14	123.32	127.47
3	B	502	8A6	C3-C2-N7	-3.97	123.49	127.47
2	A	501	PLG	OP4-C5A-C5	3.95	116.88	109.35
3	A	502	8A6	C5-C4-C3	3.89	112.25	104.34
3	B	502	8A6	C5-C4-C3	3.77	112.01	104.34
3	B	502	8A6	C14-C4-C3	-3.71	104.37	110.32
2	C	501	PLG	OP4-C5A-C5	3.69	116.39	109.35
3	B	502	8A6	C39-C37-N34	3.56	119.64	113.21
3	B	502	8A6	C6-C5-C10	-3.50	100.31	104.01
3	B	502	8A6	F31-C23-C18	-3.42	105.41	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	8A6	C5-C4-C3	3.35	111.16	104.34
3	A	502	8A6	C6-C5-C10	-3.30	100.53	104.01
3	A	502	8A6	C19-C20-C22	-3.25	115.50	120.86
2	B	501	PLG	C4-C4A-N	3.23	117.62	111.58
3	B	502	8A6	C6-O1-C2	3.11	121.75	118.38
3	C	502	8A6	C19-C20-C22	-3.07	115.79	120.86
3	A	502	8A6	C6-O1-C2	3.05	121.69	118.38
3	A	502	8A6	C24-C14-C4	2.97	115.59	112.40
2	C	501	PLG	C6-N1-C2	2.94	124.62	119.17
3	C	502	8A6	C6-C5-C10	-2.90	100.94	104.01
2	C	501	PLG	OP2-P-OP4	-2.86	99.12	106.73
3	C	502	8A6	C14-C4-C3	-2.85	105.74	110.32
2	A	501	PLG	OP2-P-OP4	-2.82	99.22	106.73
2	B	501	PLG	C6-N1-C2	2.76	124.29	119.17
3	A	502	8A6	F31-C23-C18	-2.74	106.91	112.93
3	C	502	8A6	F31-C23-C18	-2.67	107.07	112.93
2	C	501	PLG	C2A-C2-N1	2.66	122.87	117.67
3	B	502	8A6	O35-S30-N34	-2.66	103.72	107.05
2	A	501	PLG	C4-C4A-N	2.62	116.47	111.58
3	C	502	8A6	C21-C16-C4	2.58	125.09	120.67
2	B	501	PLG	OP3-P-OP2	2.57	117.45	107.64
2	A	501	PLG	CA-N-C4A	2.55	118.97	112.54
2	C	501	PLG	C4-C4A-N	2.54	116.32	111.58
3	B	502	8A6	C24-C14-C4	2.54	115.12	112.40
2	A	501	PLG	C3-C4-C5	-2.50	116.32	118.72
3	C	502	8A6	O36-S30-N34	2.49	110.15	107.05
3	C	502	8A6	C6-O1-C2	2.48	121.07	118.38
2	C	501	PLG	CA-N-C4A	2.39	118.57	112.54
3	B	502	8A6	O36-S30-N34	2.34	109.97	107.05
3	C	502	8A6	C39-C37-N34	2.34	117.44	113.21
3	A	502	8A6	C17-C18-C23	2.30	122.69	119.58
2	B	501	PLG	C2A-C2-N1	2.27	122.11	117.67
2	B	501	PLG	CA-N-C4A	2.26	118.23	112.54
3	C	502	8A6	C24-C14-C4	2.24	114.80	112.40
3	C	502	8A6	F32-C23-C18	-2.22	108.06	112.93
2	A	501	PLG	C4A-C4-C5	2.20	122.15	119.71
2	A	501	PLG	C6-N1-C2	2.19	123.22	119.17
3	A	502	8A6	O36-S30-N34	2.15	109.73	107.05
2	C	501	PLG	C3-C2-N1	-2.11	118.05	120.77
3	C	502	8A6	O35-S30-N34	-2.10	104.42	107.05
3	B	502	8A6	C21-C16-C4	2.10	124.28	120.67
3	C	502	8A6	C38-N34-S30	-2.10	110.76	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLG	OP3-P-OP4	-2.09	101.17	106.73
3	A	502	8A6	C21-C20-C22	2.06	124.27	120.86
3	C	502	8A6	C21-C20-C22	2.04	124.23	120.86
3	A	502	8A6	O35-S30-N34	-2.03	104.51	107.05

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	8A6	C39-C37-N34-C38
2	C	501	PLG	C5A-OP4-P-OP3
2	C	501	PLG	C-CA-N-C4A
2	A	501	PLG	C-CA-N-C4A
3	C	502	8A6	C39-C37-N34-C38
3	A	502	8A6	C39-C37-N34-C38
2	B	501	PLG	C5A-OP4-P-OP1
2	B	501	PLG	C-CA-N-C4A
2	C	501	PLG	C5-C4-C4A-N
2	A	501	PLG	C5-C4-C4A-N
2	B	501	PLG	C5-C4-C4A-N
2	A	501	PLG	C3-C4-C4A-N
2	B	501	PLG	C3-C4-C4A-N
3	C	502	8A6	C17-C16-C4-C5
2	C	501	PLG	C5A-OP4-P-OP2
2	B	501	PLG	C5A-OP4-P-OP3
2	C	501	PLG	C3-C4-C4A-N
3	C	502	8A6	C15-C14-C4-C3
3	A	502	8A6	C37-N34-S30-O36
3	B	502	8A6	C17-C16-C4-C5
3	B	502	8A6	C21-C16-C4-C5
3	C	502	8A6	C21-C16-C4-C5
3	A	502	8A6	C17-C16-C4-C5
3	C	502	8A6	C21-C16-C4-C14
2	A	501	PLG	C5A-OP4-P-OP3
2	B	501	PLG	C5A-OP4-P-OP2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

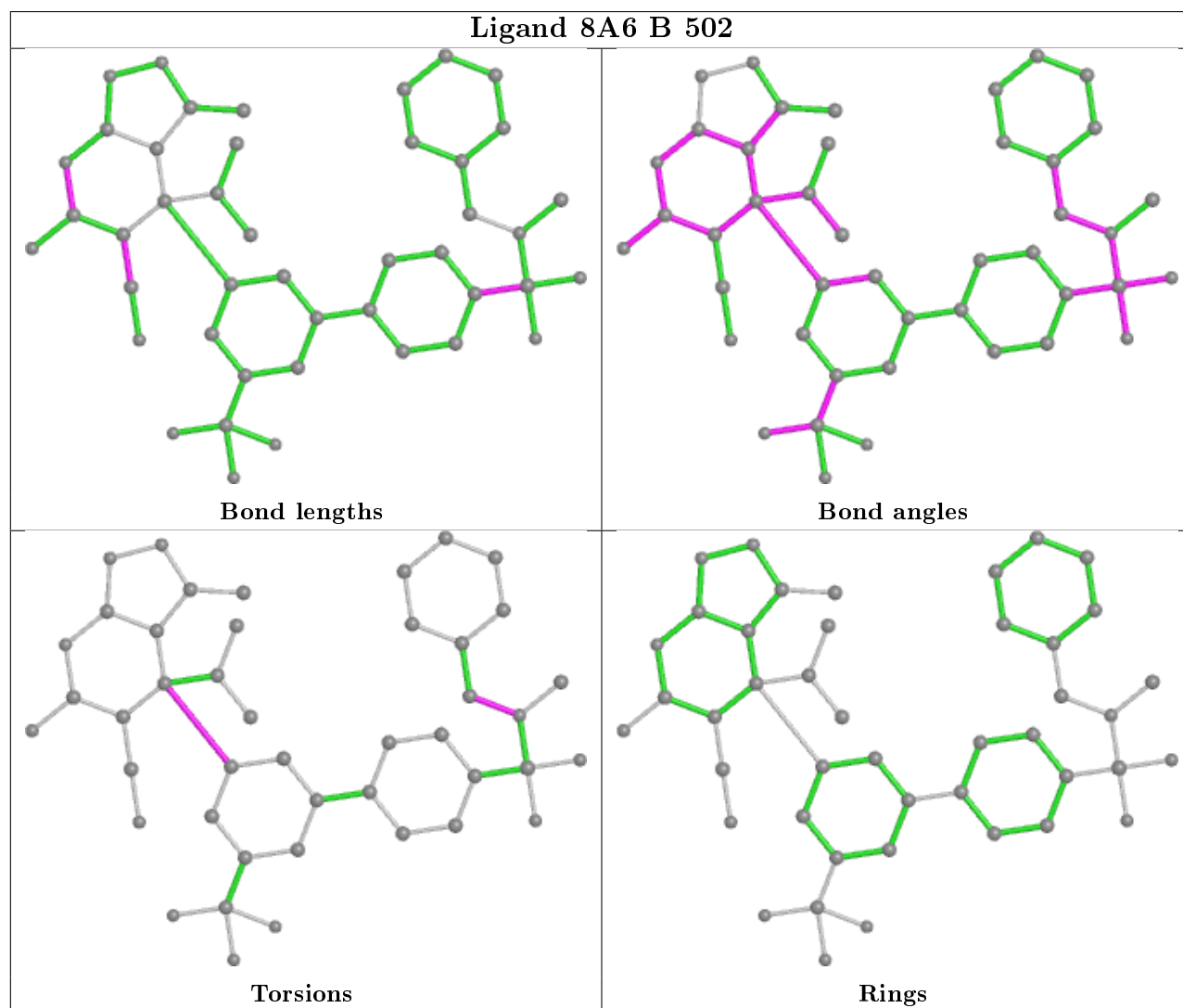
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	8A6	2	0

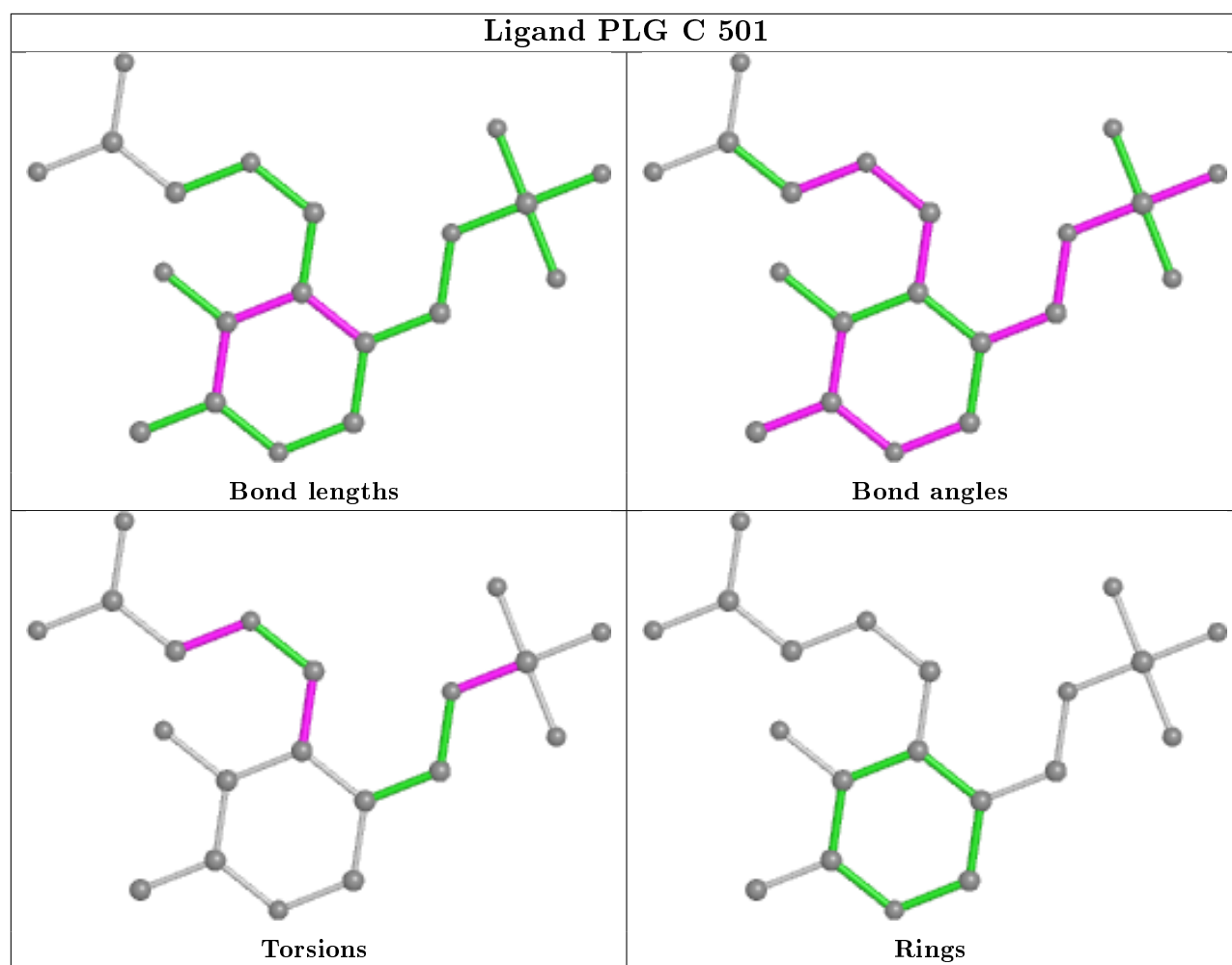
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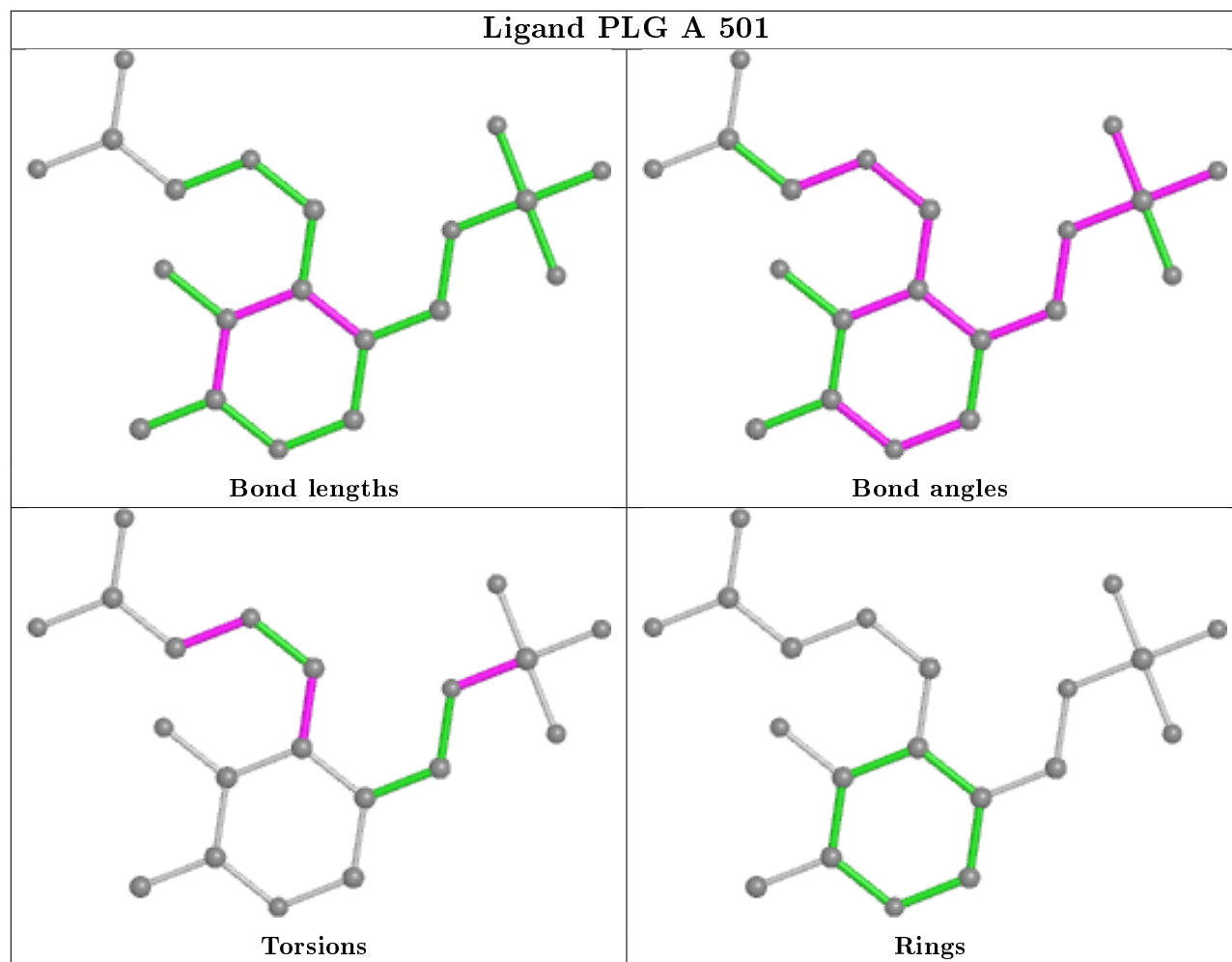
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PLG	1	0
3	A	502	8A6	1	0
2	B	501	PLG	1	0

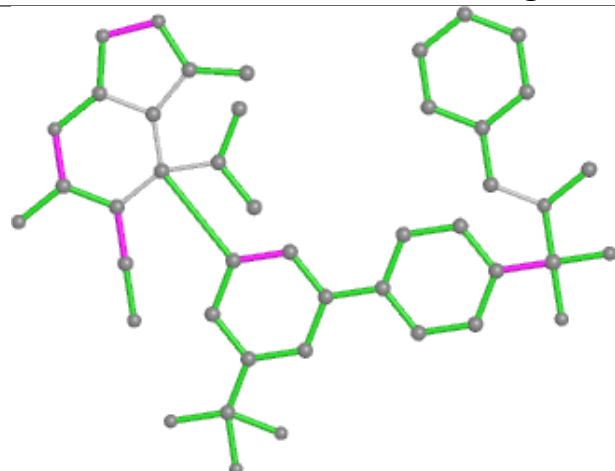
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



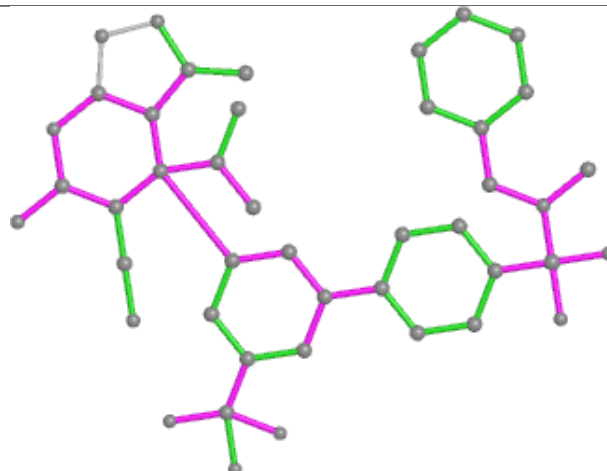




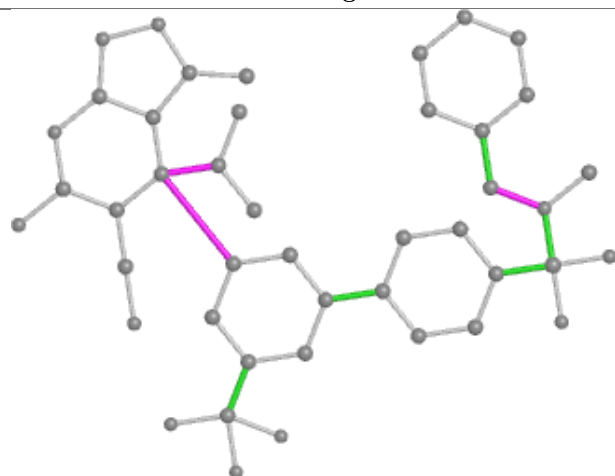
Ligand 8A6 C 502



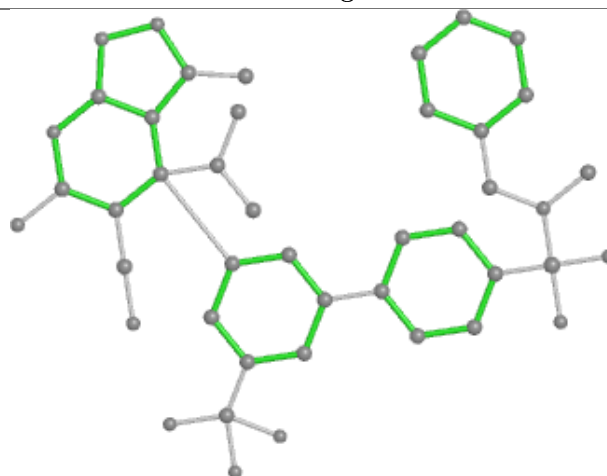
Bond lengths



Bond angles

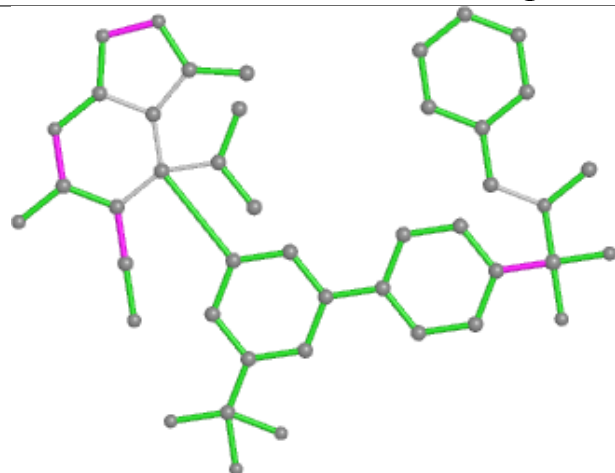


Torsions

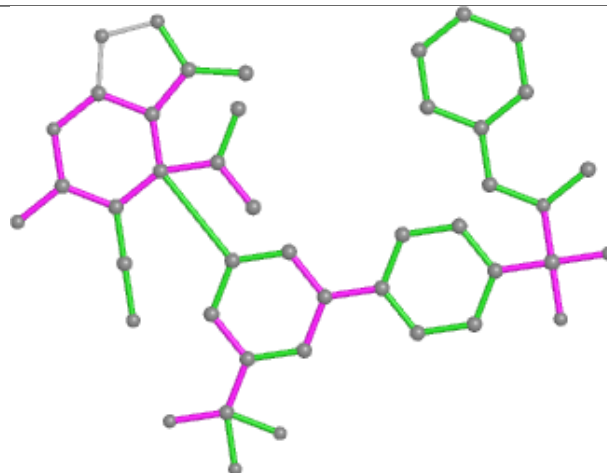


Rings

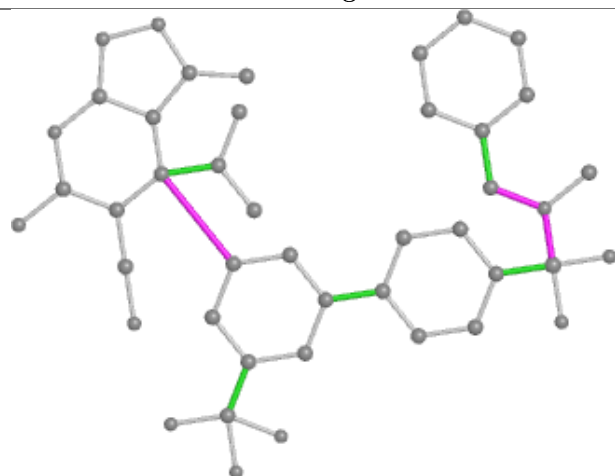
Ligand 8A6 A 502



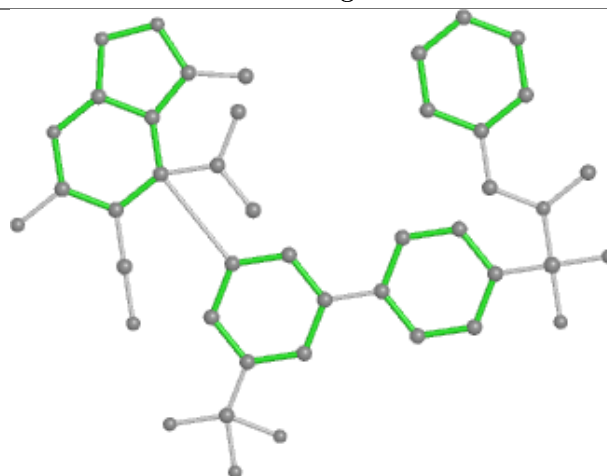
Bond lengths



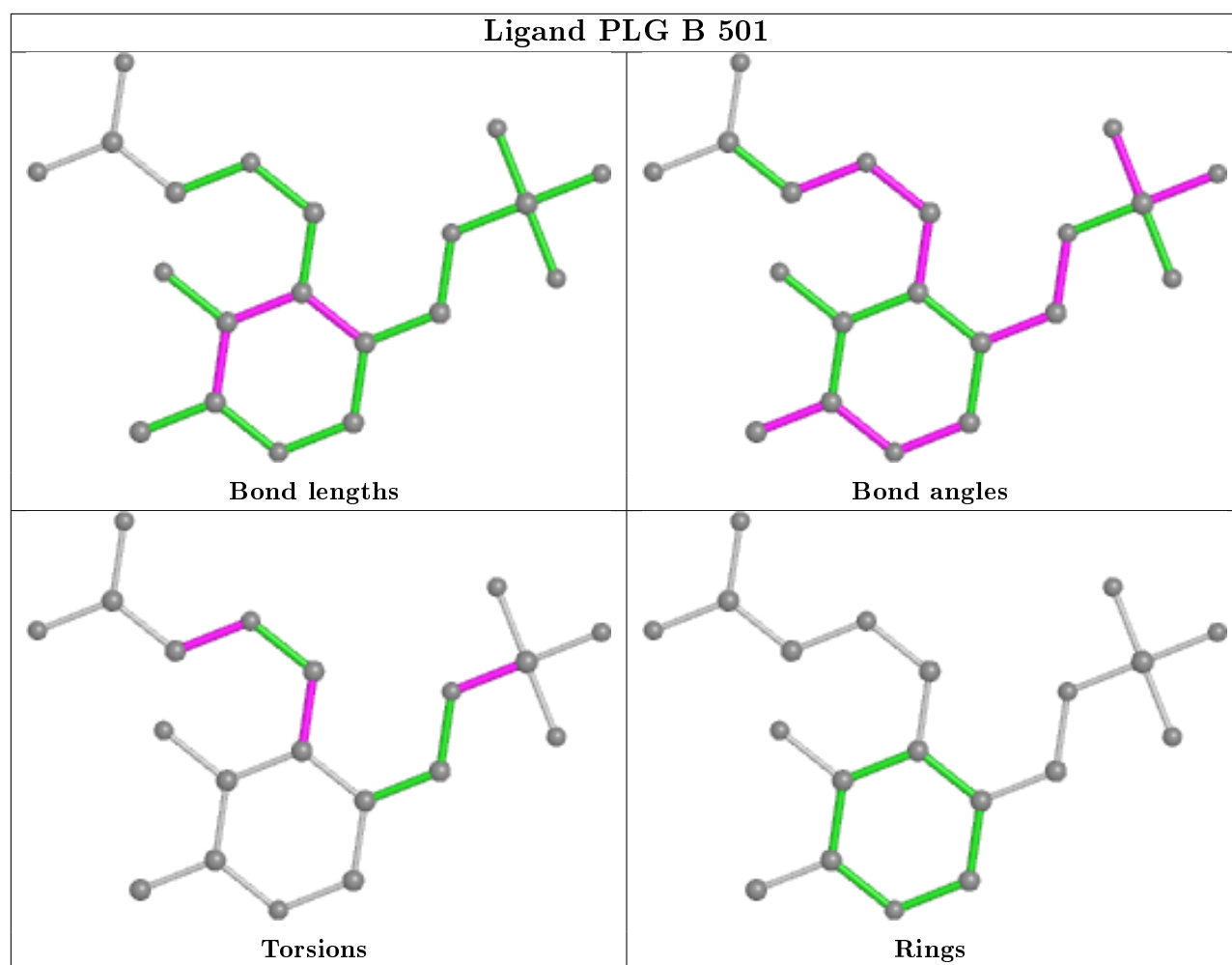
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	442/442 (100%)	0.16	13 (2%)	51	49	15, 28, 54, 84	0
1	B	442/442 (100%)	0.18	13 (2%)	51	49	15, 28, 52, 93	0
1	C	442/442 (100%)	0.15	13 (2%)	51	49	15, 28, 53, 99	0
All	All	1326/1326 (100%)	0.16	39 (2%)	51	49	15, 28, 54, 99	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	VAL	5.2
1	C	363	ASP	4.9
1	C	412	LEU	4.1
1	B	363	ASP	4.1
1	A	363	ASP	4.0
1	C	419	LEU	4.0
1	B	419	LEU	3.9
1	B	196	GLN	3.4
1	C	442	PRO	3.3
1	A	411	LYS	2.9
1	B	413	VAL	2.9
1	A	364	ALA	2.9
1	C	136	ASP	2.8
1	C	418	GLY	2.8
1	A	136	ASP	2.7
1	C	138	LYS	2.6
1	B	256	GLY	2.6
1	C	406	GLU	2.5
1	B	421	GLY	2.5
1	C	414	ASP	2.5
1	B	430	GLN	2.4
1	B	420	PRO	2.4
1	A	442	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	202	ASN	2.3
1	C	434	THR	2.2
1	B	138	LYS	2.2
1	A	421	GLY	2.2
1	B	409	GLY	2.2
1	C	137	GLU	2.2
1	B	410	LYS	2.1
1	C	90	GLU	2.1
1	A	412	LEU	2.1
1	B	12	LYS	2.1
1	A	164	ASP	2.1
1	A	193	GLN	2.1
1	A	419	LEU	2.0
1	A	196	GLN	2.0
1	A	392	ASP	2.0
1	B	172	SER	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	8A6	B	502	44/44	0.76	0.25	47,58,91,93	0
3	8A6	C	502	44/44	0.76	0.26	53,57,85,86	0
3	8A6	A	502	44/44	0.76	0.26	47,60,92,93	0
4	CL	A	503	1/1	0.76	0.10	38,38,38,38	0
4	CL	C	503	1/1	0.81	0.11	39,39,39,39	1
2	PLG	C	501	20/20	0.93	0.14	16,18,20,20	0
2	PLG	B	501	20/20	0.95	0.13	17,20,23,23	0

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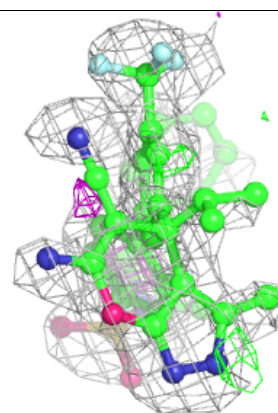
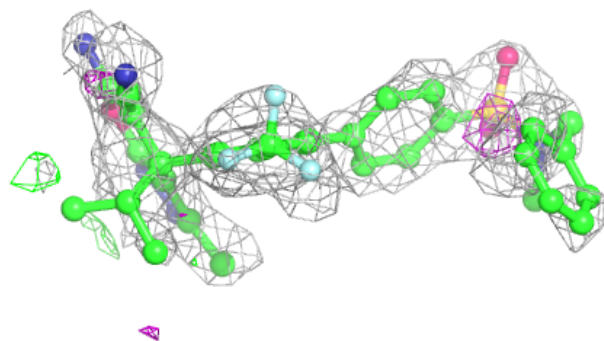
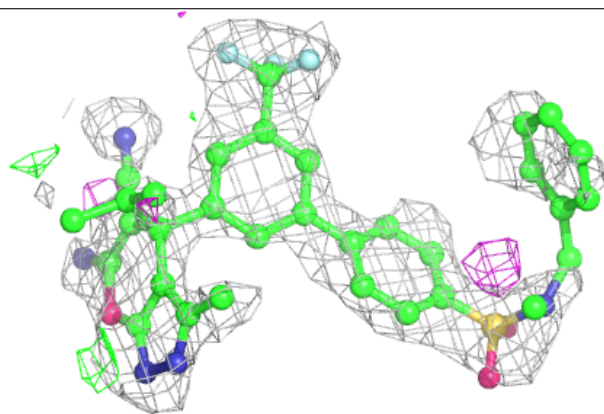
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PLG	A	501	20/20	0.95	0.11	16,19,20,20	0

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.

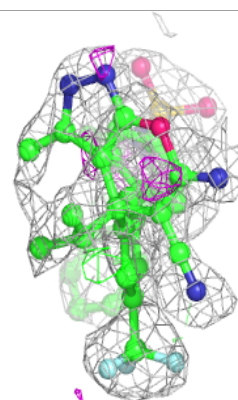
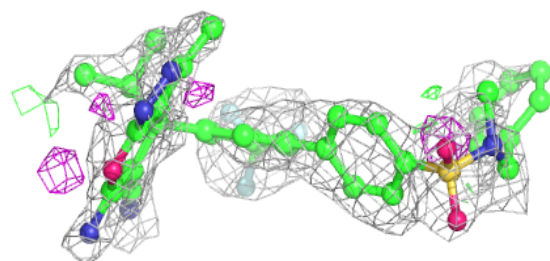
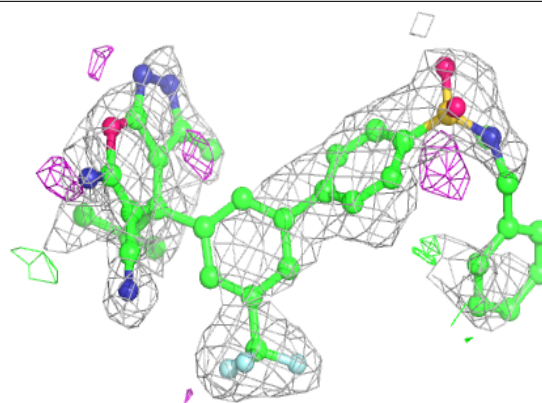
Electron density around 8A6 B 502:

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

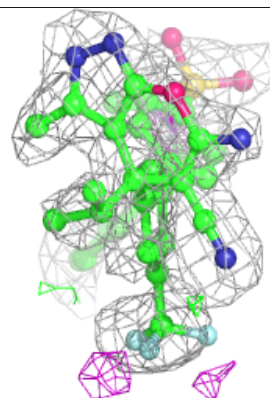
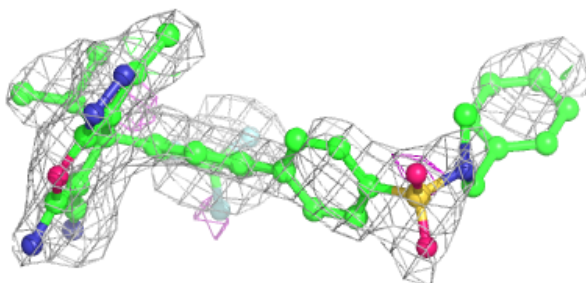
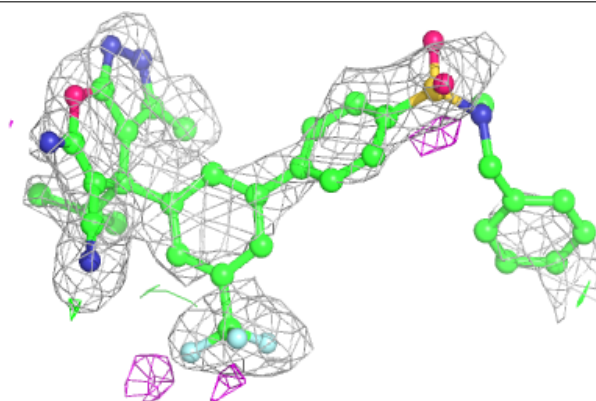


Electron density around 8A6 C 502:

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

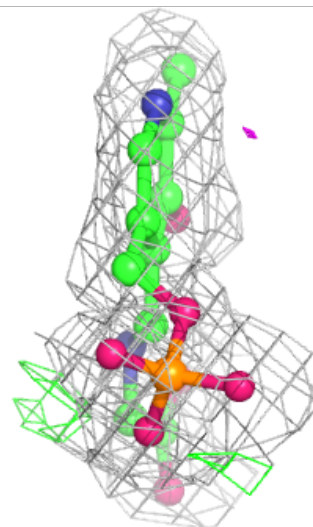
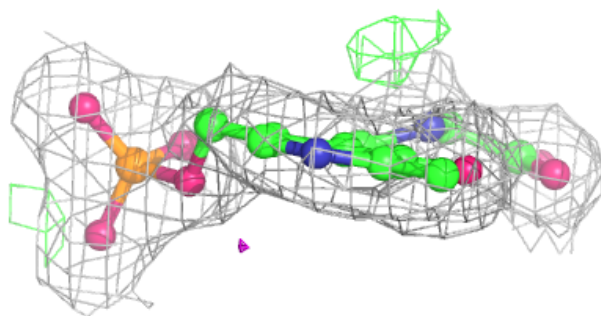
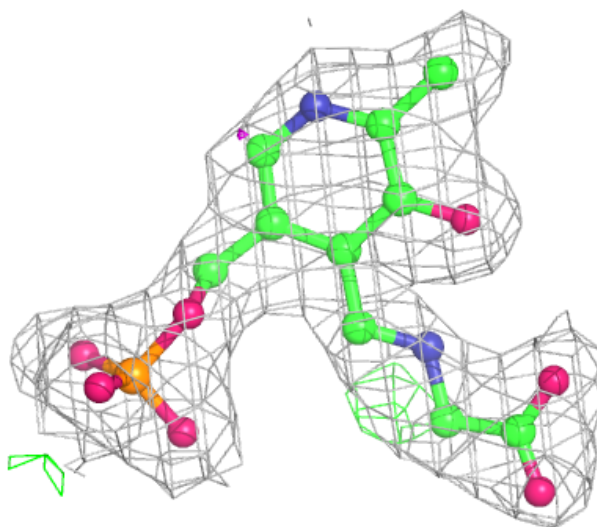
**Electron density around 8A6 A 502:**

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



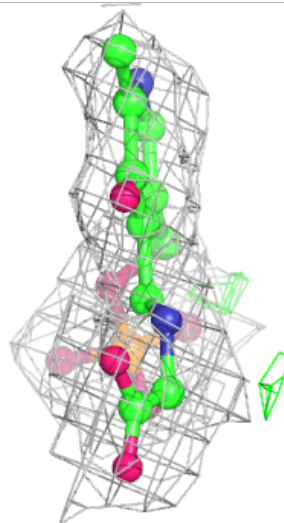
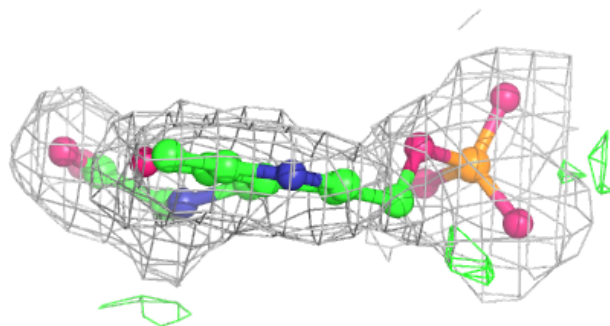
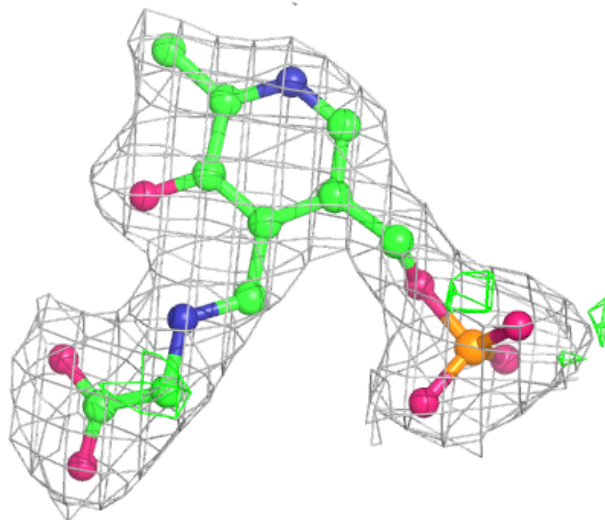
Electron density around PLG C 501:

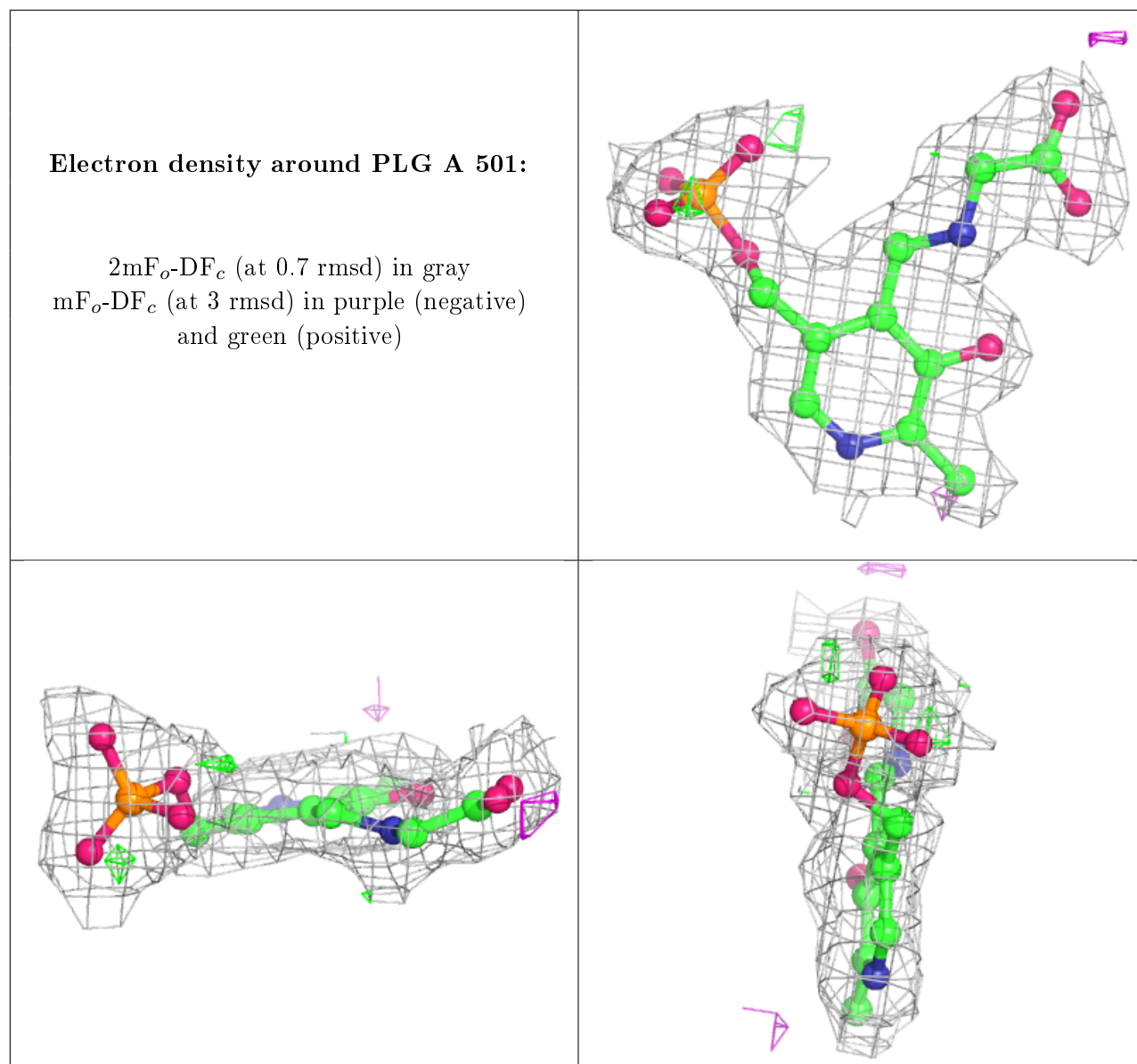
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.