



# wwPDB X-ray Structure Validation Summary Report

Mar 15, 2026 – 02:02 AM UTC

PDB ID : 4F86 / pdb\_00004f86  
Title : Structure analysis of Geranyl diphosphate methyltransferase in complex with GPP and sinefungin  
Authors : Ariyawutthiphan, O.; Ose, T.; Minami, A.; Gao, Y.G.; Yao, M.; Oikawa, H.; Tanaka, I.  
Deposited on : 2012-05-17  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

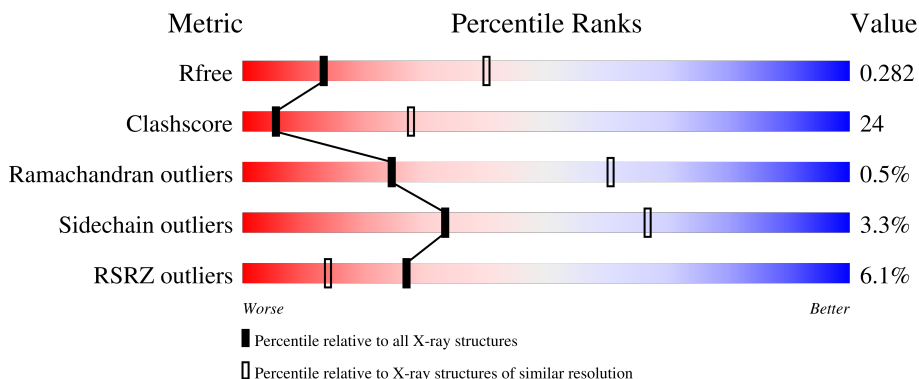
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	320	 6% 50% 33% 14%
1	B	320	 4% 51% 31% 15%
1	C	320	 6% 51% 32% 14%
1	D	320	 7% 52% 30% 15%

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Mol	Chain	Length	Quality of chain
1	E	320	
1	F	320	
1	G	320	
1	H	320	
1	I	320	
1	J	320	
1	K	320	
1	L	320	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SFG	A	501	-	-	X	-
2	SFG	I	501	-	-	X	-
2	SFG	K	501	-	-	X	-
3	GPP	A	502	-	-	X	-
3	GPP	B	502	-	-	X	-
3	GPP	C	502	-	-	X	-
3	GPP	D	502	-	-	X	-
3	GPP	H	502	-	-	X	-
3	GPP	I	502	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26078 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 Geranyl diphosphate 2-C-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2155	1345	392	408	10	0	0	0
1	B	273	2147	1340	393	404	10	0	0	0
1	C	274	2142	1338	390	404	10	0	0	0
1	D	273	2146	1341	392	403	10	0	0	0
1	E	272	2142	1337	392	403	10	0	0	0
1	F	269	2113	1321	388	394	10	0	0	0
1	G	269	2119	1326	386	397	10	0	0	0
1	H	268	2096	1310	383	393	10	0	0	0
1	I	273	2143	1338	390	405	10	0	0	0
1	J	272	2148	1341	392	405	10	0	0	0
1	K	258	2013	1256	368	379	10	0	0	0
1	L	273	2150	1343	392	405	10	0	0	0

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP D3KYU3
A	-18	GLY	-	expression tag	UNP D3KYU3
A	-17	SER	-	expression tag	UNP D3KYU3
A	-16	SER	-	expression tag	UNP D3KYU3
A	-15	HIS	-	expression tag	UNP D3KYU3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP D3KYU3
A	-13	HIS	-	expression tag	UNP D3KYU3
A	-12	HIS	-	expression tag	UNP D3KYU3
A	-11	HIS	-	expression tag	UNP D3KYU3
A	-10	HIS	-	expression tag	UNP D3KYU3
A	-9	SER	-	expression tag	UNP D3KYU3
A	-8	SER	-	expression tag	UNP D3KYU3
A	-7	GLY	-	expression tag	UNP D3KYU3
A	-6	LEU	-	expression tag	UNP D3KYU3
A	-5	VAL	-	expression tag	UNP D3KYU3
A	-4	PRO	-	expression tag	UNP D3KYU3
A	-3	ARG	-	expression tag	UNP D3KYU3
A	-2	GLY	-	expression tag	UNP D3KYU3
A	-1	SER	-	expression tag	UNP D3KYU3
A	0	HIS	-	expression tag	UNP D3KYU3
B	-19	MET	-	expression tag	UNP D3KYU3
B	-18	GLY	-	expression tag	UNP D3KYU3
B	-17	SER	-	expression tag	UNP D3KYU3
B	-16	SER	-	expression tag	UNP D3KYU3
B	-15	HIS	-	expression tag	UNP D3KYU3
B	-14	HIS	-	expression tag	UNP D3KYU3
B	-13	HIS	-	expression tag	UNP D3KYU3
B	-12	HIS	-	expression tag	UNP D3KYU3
B	-11	HIS	-	expression tag	UNP D3KYU3
B	-10	HIS	-	expression tag	UNP D3KYU3
B	-9	SER	-	expression tag	UNP D3KYU3
B	-8	SER	-	expression tag	UNP D3KYU3
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B	-4	PRO	-	expression tag	UNP D3KYU3
B	-3	ARG	-	expression tag	UNP D3KYU3
B	-2	GLY	-	expression tag	UNP D3KYU3
B	-1	SER	-	expression tag	UNP D3KYU3
B	0	HIS	-	expression tag	UNP D3KYU3
C	-19	MET	-	expression tag	UNP D3KYU3
C	-18	GLY	-	expression tag	UNP D3KYU3
C	-17	SER	-	expression tag	UNP D3KYU3
C	-16	SER	-	expression tag	UNP D3KYU3
C	-15	HIS	-	expression tag	UNP D3KYU3
C	-14	HIS	-	expression tag	UNP D3KYU3
C	-13	HIS	-	expression tag	UNP D3KYU3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP D3KYU3
C	-11	HIS	-	expression tag	UNP D3KYU3
C	-10	HIS	-	expression tag	UNP D3KYU3
C	-9	SER	-	expression tag	UNP D3KYU3
C	-8	SER	-	expression tag	UNP D3KYU3
C	-7	GLY	-	expression tag	UNP D3KYU3
C	-6	LEU	-	expression tag	UNP D3KYU3
C	-5	VAL	-	expression tag	UNP D3KYU3
C	-4	PRO	-	expression tag	UNP D3KYU3
C	-3	ARG	-	expression tag	UNP D3KYU3
C	-2	GLY	-	expression tag	UNP D3KYU3
C	-1	SER	-	expression tag	UNP D3KYU3
C	0	HIS	-	expression tag	UNP D3KYU3
D	-19	MET	-	expression tag	UNP D3KYU3
D	-18	GLY	-	expression tag	UNP D3KYU3
D	-17	SER	-	expression tag	UNP D3KYU3
D	-16	SER	-	expression tag	UNP D3KYU3
D	-15	HIS	-	expression tag	UNP D3KYU3
D	-14	HIS	-	expression tag	UNP D3KYU3
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D	-2	GLY	-	expression tag	UNP D3KYU3
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E	-18	GLY	-	expression tag	UNP D3KYU3
E	-17	SER	-	expression tag	UNP D3KYU3
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E	-15	HIS	-	expression tag	UNP D3KYU3
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E	-13	HIS	-	expression tag	UNP D3KYU3
E	-12	HIS	-	expression tag	UNP D3KYU3
E	-11	HIS	-	expression tag	UNP D3KYU3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP D3KYU3
E	-9	SER	-	expression tag	UNP D3KYU3
E	-8	SER	-	expression tag	UNP D3KYU3
E	-7	GLY	-	expression tag	UNP D3KYU3
E	-6	LEU	-	expression tag	UNP D3KYU3
E	-5	VAL	-	expression tag	UNP D3KYU3
E	-4	PRO	-	expression tag	UNP D3KYU3
E	-3	ARG	-	expression tag	UNP D3KYU3
E	-2	GLY	-	expression tag	UNP D3KYU3
E	-1	SER	-	expression tag	UNP D3KYU3
E	0	HIS	-	expression tag	UNP D3KYU3
F	-19	MET	-	expression tag	UNP D3KYU3
F	-18	GLY	-	expression tag	UNP D3KYU3
F	-17	SER	-	expression tag	UNP D3KYU3
F	-16	SER	-	expression tag	UNP D3KYU3
F	-15	HIS	-	expression tag	UNP D3KYU3
F	-14	HIS	-	expression tag	UNP D3KYU3
F	-13	HIS	-	expression tag	UNP D3KYU3
F	-12	HIS	-	expression tag	UNP D3KYU3
F	-11	HIS	-	expression tag	UNP D3KYU3
F	-10	HIS	-	expression tag	UNP D3KYU3
F	-9	SER	-	expression tag	UNP D3KYU3
F	-8	SER	-	expression tag	UNP D3KYU3
F	-7	GLY	-	expression tag	UNP D3KYU3
F	-6	LEU	-	expression tag	UNP D3KYU3
F	-5	VAL	-	expression tag	UNP D3KYU3
F	-4	PRO	-	expression tag	UNP D3KYU3
F	-3	ARG	-	expression tag	UNP D3KYU3
F	-2	GLY	-	expression tag	UNP D3KYU3
F	-1	SER	-	expression tag	UNP D3KYU3
F	0	HIS	-	expression tag	UNP D3KYU3
G	-19	MET	-	expression tag	UNP D3KYU3
G	-18	GLY	-	expression tag	UNP D3KYU3
G	-17	SER	-	expression tag	UNP D3KYU3
G	-16	SER	-	expression tag	UNP D3KYU3
G	-15	HIS	-	expression tag	UNP D3KYU3
G	-14	HIS	-	expression tag	UNP D3KYU3
G	-13	HIS	-	expression tag	UNP D3KYU3
G	-12	HIS	-	expression tag	UNP D3KYU3
G	-11	HIS	-	expression tag	UNP D3KYU3
G	-10	HIS	-	expression tag	UNP D3KYU3
G	-9	SER	-	expression tag	UNP D3KYU3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	expression tag	UNP D3KYU3
G	-7	GLY	-	expression tag	UNP D3KYU3
G	-6	LEU	-	expression tag	UNP D3KYU3
G	-5	VAL	-	expression tag	UNP D3KYU3
G	-4	PRO	-	expression tag	UNP D3KYU3
G	-3	ARG	-	expression tag	UNP D3KYU3
G	-2	GLY	-	expression tag	UNP D3KYU3
G	-1	SER	-	expression tag	UNP D3KYU3
G	0	HIS	-	expression tag	UNP D3KYU3
H	-19	MET	-	expression tag	UNP D3KYU3
H	-18	GLY	-	expression tag	UNP D3KYU3
H	-17	SER	-	expression tag	UNP D3KYU3
H	-16	SER	-	expression tag	UNP D3KYU3
H	-15	HIS	-	expression tag	UNP D3KYU3
H	-14	HIS	-	expression tag	UNP D3KYU3
H	-13	HIS	-	expression tag	UNP D3KYU3
H	-12	HIS	-	expression tag	UNP D3KYU3
H	-11	HIS	-	expression tag	UNP D3KYU3
H	-10	HIS	-	expression tag	UNP D3KYU3
H	-9	SER	-	expression tag	UNP D3KYU3
H	-8	SER	-	expression tag	UNP D3KYU3
H	-7	GLY	-	expression tag	UNP D3KYU3
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I	-15	HIS	-	expression tag	UNP D3KYU3
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I	-9	SER	-	expression tag	UNP D3KYU3
I	-8	SER	-	expression tag	UNP D3KYU3
I	-7	GLY	-	expression tag	UNP D3KYU3

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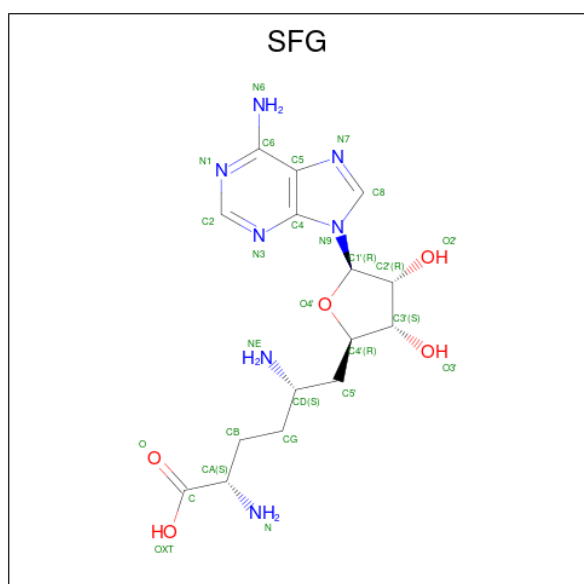
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I	-5	VAL	-	expression tag	UNP D3KYU3
I	-4	PRO	-	expression tag	UNP D3KYU3
I	-3	ARG	-	expression tag	UNP D3KYU3
I	-2	GLY	-	expression tag	UNP D3KYU3
I	-1	SER	-	expression tag	UNP D3KYU3
I	0	HIS	-	expression tag	UNP D3KYU3
J	-19	MET	-	expression tag	UNP D3KYU3
J	-18	GLY	-	expression tag	UNP D3KYU3
J	-17	SER	-	expression tag	UNP D3KYU3
J	-16	SER	-	expression tag	UNP D3KYU3
J	-15	HIS	-	expression tag	UNP D3KYU3
J	-14	HIS	-	expression tag	UNP D3KYU3
J	-13	HIS	-	expression tag	UNP D3KYU3
J	-12	HIS	-	expression tag	UNP D3KYU3
J	-11	HIS	-	expression tag	UNP D3KYU3
J	-10	HIS	-	expression tag	UNP D3KYU3
J	-9	SER	-	expression tag	UNP D3KYU3
J	-8	SER	-	expression tag	UNP D3KYU3
J	-7	GLY	-	expression tag	UNP D3KYU3
J	-6	LEU	-	expression tag	UNP D3KYU3
J	-5	VAL	-	expression tag	UNP D3KYU3
J	-4	PRO	-	expression tag	UNP D3KYU3
J	-3	ARG	-	expression tag	UNP D3KYU3
J	-2	GLY	-	expression tag	UNP D3KYU3
J	-1	SER	-	expression tag	UNP D3KYU3
J	0	HIS	-	expression tag	UNP D3KYU3
K	-19	MET	-	expression tag	UNP D3KYU3
K	-18	GLY	-	expression tag	UNP D3KYU3
K	-17	SER	-	expression tag	UNP D3KYU3
K	-16	SER	-	expression tag	UNP D3KYU3
K	-15	HIS	-	expression tag	UNP D3KYU3
K	-14	HIS	-	expression tag	UNP D3KYU3
K	-13	HIS	-	expression tag	UNP D3KYU3
K	-12	HIS	-	expression tag	UNP D3KYU3
K	-11	HIS	-	expression tag	UNP D3KYU3
K	-10	HIS	-	expression tag	UNP D3KYU3
K	-9	SER	-	expression tag	UNP D3KYU3
K	-8	SER	-	expression tag	UNP D3KYU3
K	-7	GLY	-	expression tag	UNP D3KYU3
K	-6	LEU	-	expression tag	UNP D3KYU3
K	-5	VAL	-	expression tag	UNP D3KYU3

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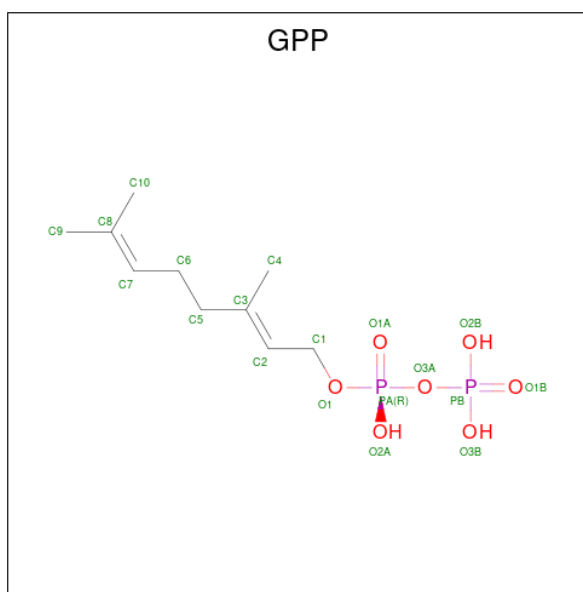
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP D3KYU3
K	-3	ARG	-	expression tag	UNP D3KYU3
K	-2	GLY	-	expression tag	UNP D3KYU3
K	-1	SER	-	expression tag	UNP D3KYU3
K	0	HIS	-	expression tag	UNP D3KYU3
L	-19	MET	-	expression tag	UNP D3KYU3
L	-18	GLY	-	expression tag	UNP D3KYU3
L	-17	SER	-	expression tag	UNP D3KYU3
L	-16	SER	-	expression tag	UNP D3KYU3
L	-15	HIS	-	expression tag	UNP D3KYU3
L	-14	HIS	-	expression tag	UNP D3KYU3
L	-13	HIS	-	expression tag	UNP D3KYU3
L	-12	HIS	-	expression tag	UNP D3KYU3
L	-11	HIS	-	expression tag	UNP D3KYU3
L	-10	HIS	-	expression tag	UNP D3KYU3
L	-9	SER	-	expression tag	UNP D3KYU3
L	-8	SER	-	expression tag	UNP D3KYU3
L	-7	GLY	-	expression tag	UNP D3KYU3
L	-6	LEU	-	expression tag	UNP D3KYU3
L	-5	VAL	-	expression tag	UNP D3KYU3
L	-4	PRO	-	expression tag	UNP D3KYU3
L	-3	ARG	-	expression tag	UNP D3KYU3
L	-2	GLY	-	expression tag	UNP D3KYU3
L	-1	SER	-	expression tag	UNP D3KYU3
L	0	HIS	-	expression tag	UNP D3KYU3

- Molecule 2 is SINEFUNGIN (CCD ID: SFG) (formula:  $C_{15}H_{23}N_7O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	15	7	5		
2	B	1	Total	C	N	O	0	0
			27	15	7	5		
2	C	1	Total	C	N	O	0	0
			27	15	7	5		
2	D	1	Total	C	N	O	0	0
			27	15	7	5		
2	E	1	Total	C	N	O	0	0
			27	15	7	5		
2	F	1	Total	C	N	O	0	0
			27	15	7	5		
2	G	1	Total	C	N	O	0	0
			27	15	7	5		
2	H	1	Total	C	N	O	0	0
			27	15	7	5		
2	I	1	Total	C	N	O	0	0
			27	15	7	5		
2	J	1	Total	C	N	O	0	0
			27	15	7	5		
2	K	1	Total	C	N	O	0	0
			27	15	7	5		
2	L	1	Total	C	N	O	0	0
			27	15	7	5		

- Molecule 3 is GERANYL DIPHOSPHATE (CCD ID: GPP) (formula:  $C_{10}H_{20}O_7P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			19	10	7	2		
3	B	1	Total	C	O	P	0	0
			19	10	7	2		
3	C	1	Total	C	O	P	0	0
			19	10	7	2		
3	D	1	Total	C	O	P	0	0
			19	10	7	2		
3	E	1	Total	C	O	P	0	0
			19	10	7	2		
3	F	1	Total	C	O	P	0	0
			19	10	7	2		
3	G	1	Total	C	O	P	0	0
			19	10	7	2		
3	H	1	Total	C	O	P	0	0
			19	10	7	2		
3	I	1	Total	C	O	P	0	0
			19	10	7	2		
3	J	1	Total	C	O	P	0	0
			19	10	7	2		
3	K	1	Total	C	O	P	0	0
			19	10	7	2		
3	L	1	Total	C	O	P	0	0
			19	10	7	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		

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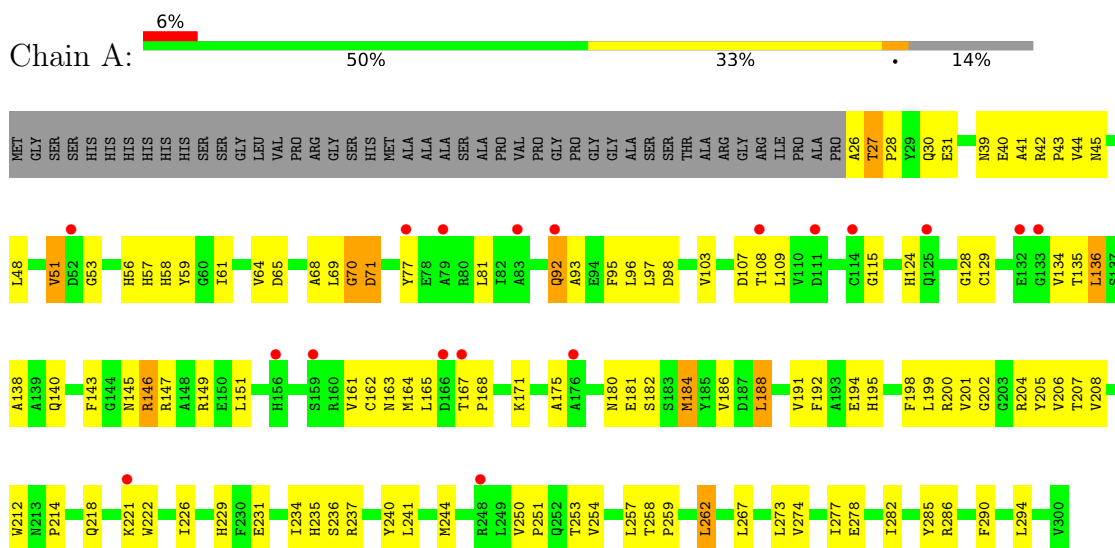
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	I	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0

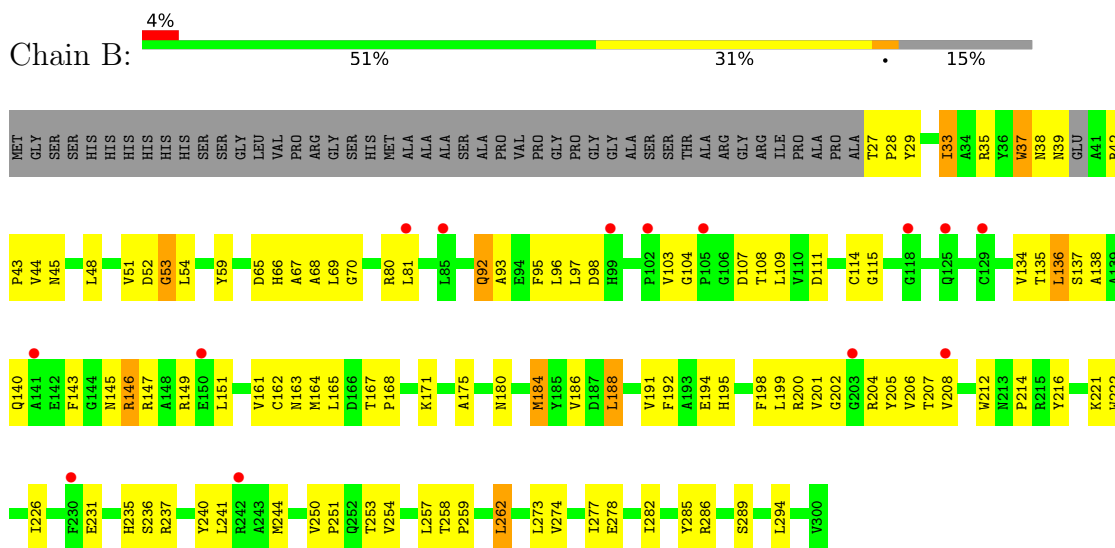
### 3 Residue-property plots [i](#)

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: Geranyl diphosphate 2-C-methyltransferase

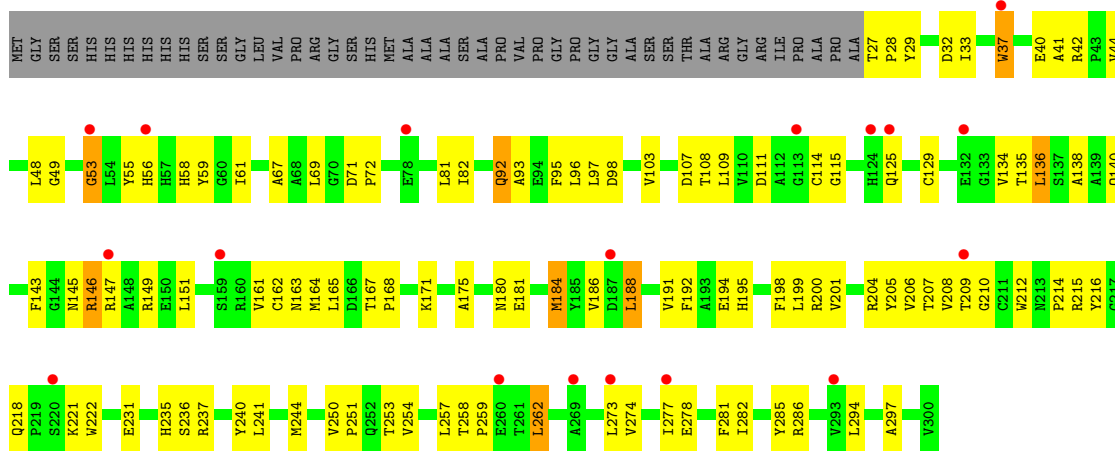


- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

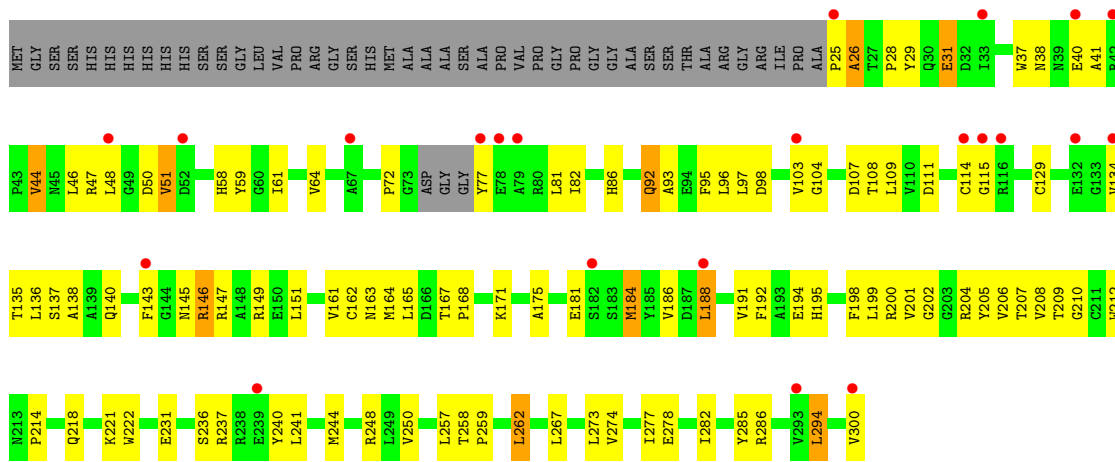


- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

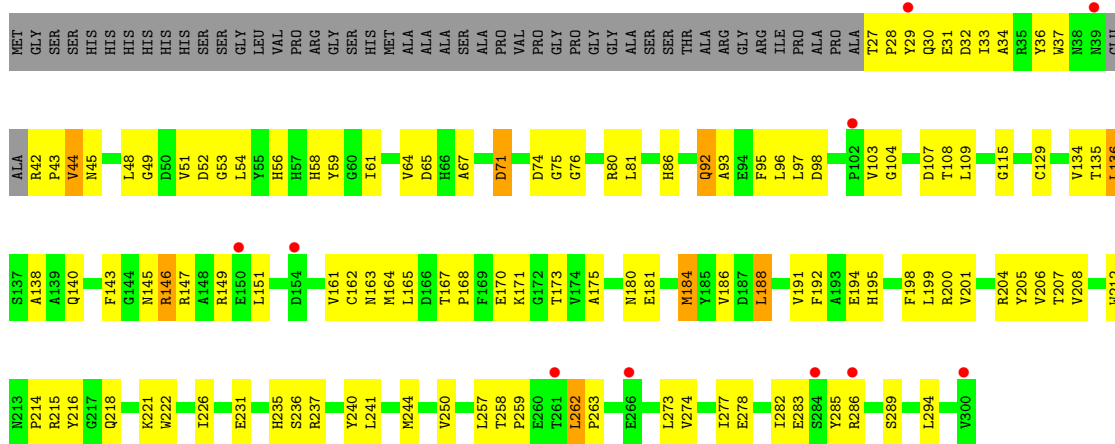




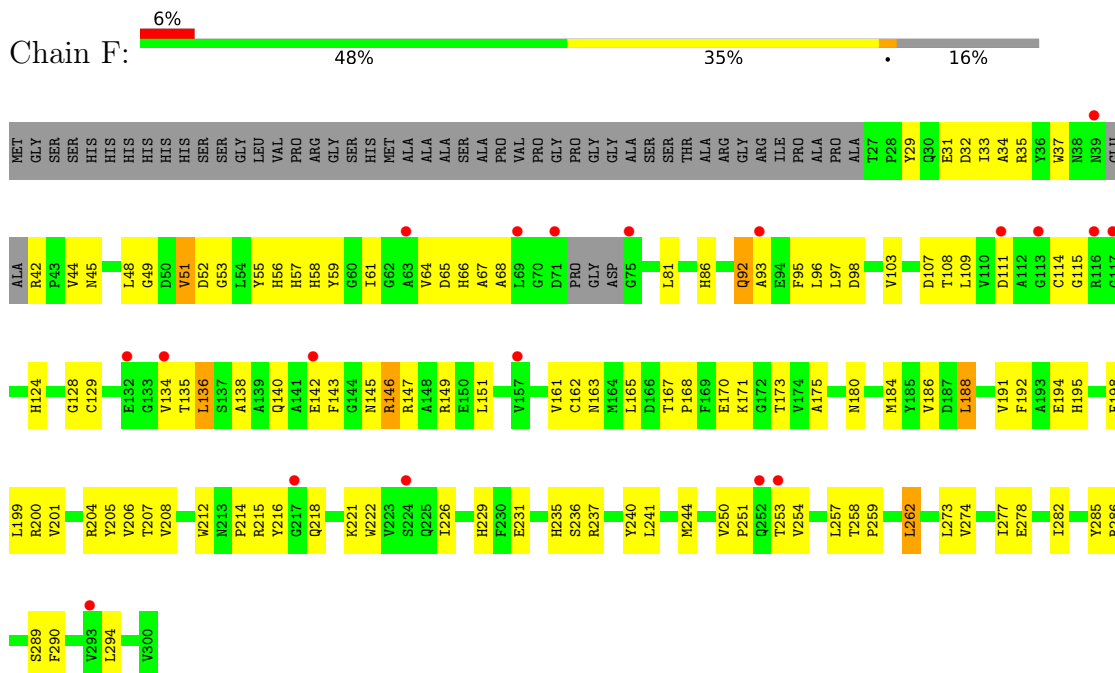
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase



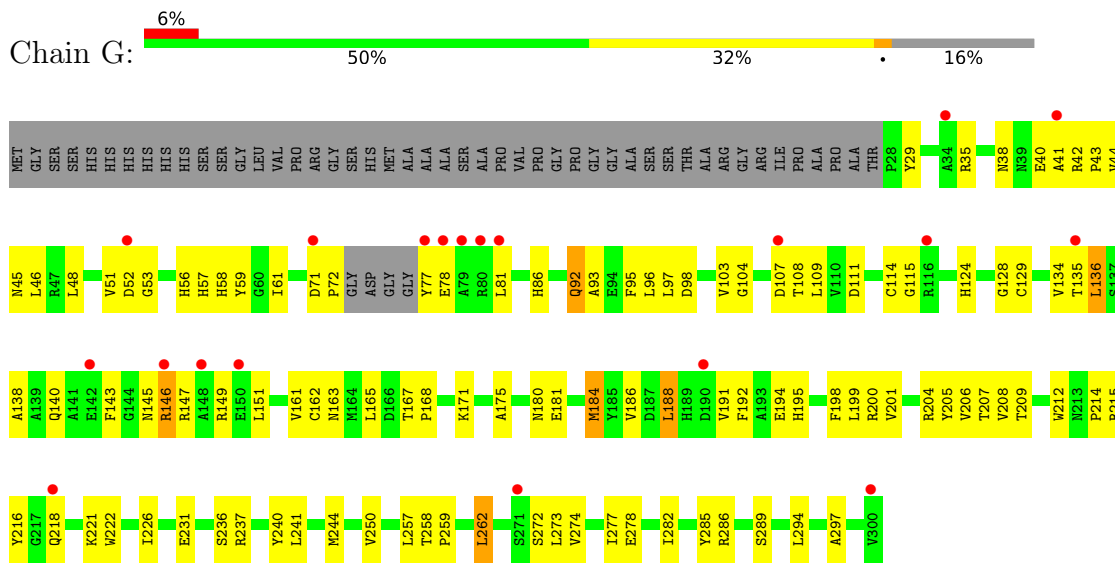
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase



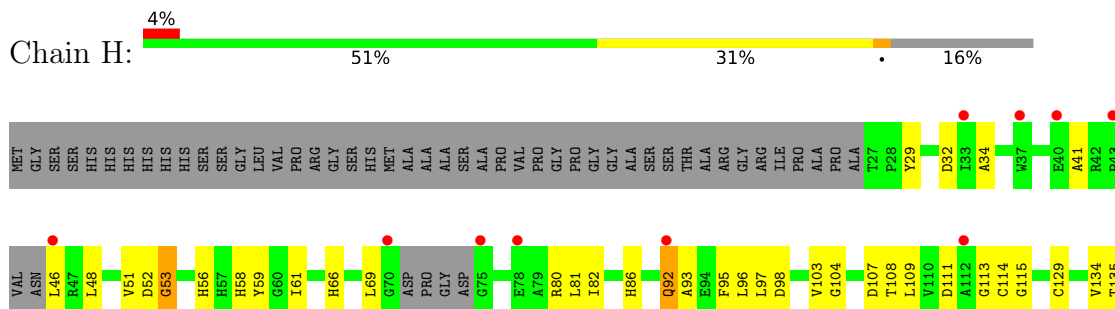
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

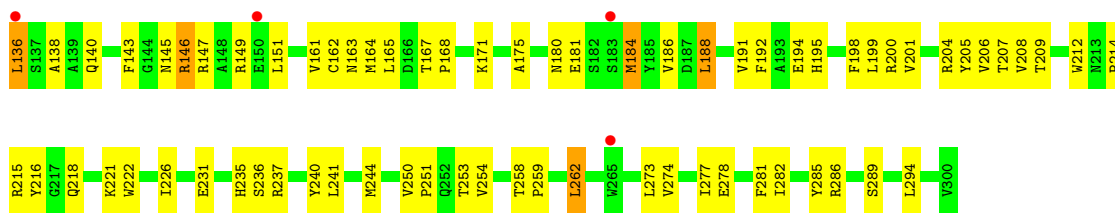


- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

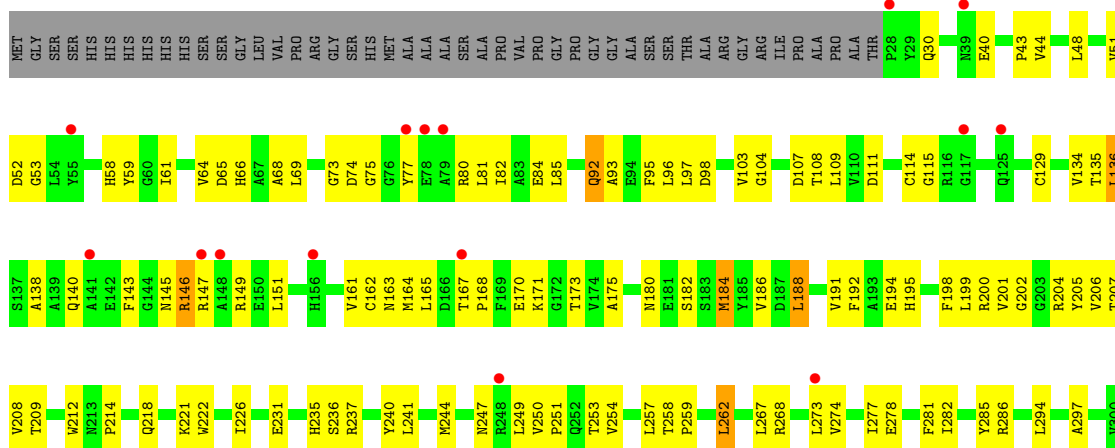


- Molecule 1: Geranyl diphosphate 2-C-methyltransferase





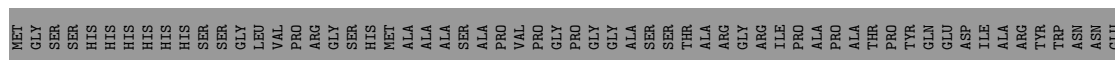
● Molecule 1: Geranyl diphosphate 2-C-methyltransferase

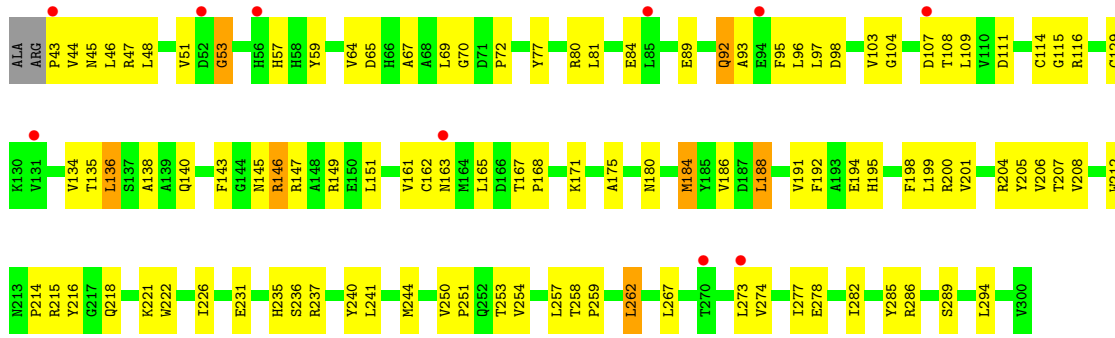


● Molecule 1: Geranyl diphosphate 2-C-methyltransferase

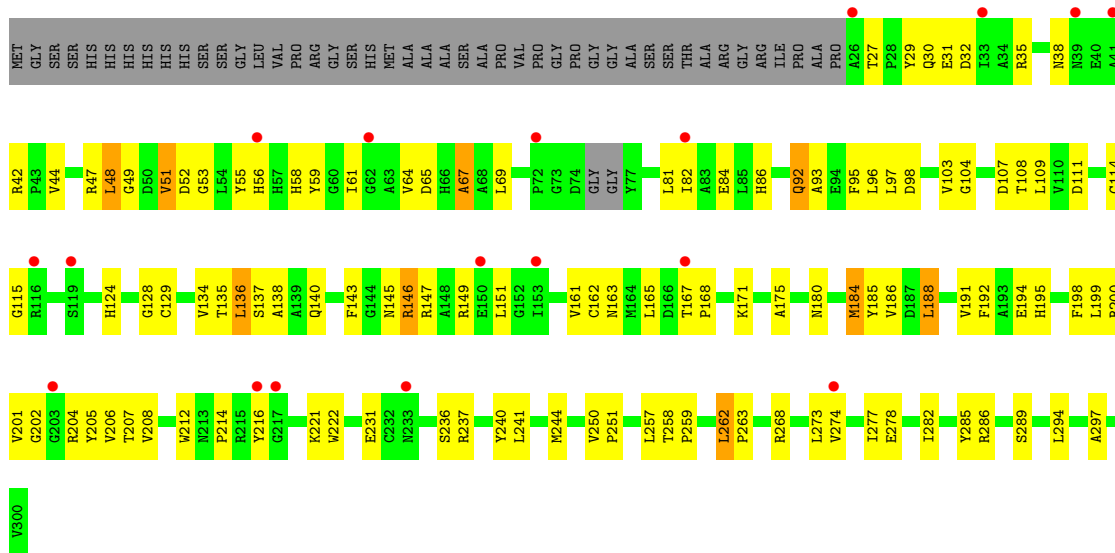


● Molecule 1: Geranyl diphosphate 2-C-methyltransferase





• Molecule 1: Geranyl diphosphate 2-C-methyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.94Å 87.73Å 160.22Å 100.01° 96.65° 90.89°	Depositor
Resolution (Å)	46.51 – 3.00 46.51 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.51-3.00) 95.7 (46.51-3.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.96Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.279 , 0.298 0.280 , 0.282	Depositor DCC
$R_{free}$ test set	4112 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.3	Xtrriage
Anisotropy	0.891	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 29.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	26078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.70% 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: GPP, SFG, MG

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	0.31	0/2208	0.81	2/2999 (0.1%)
1	B	0.31	0/2199	0.83	7/2984 (0.2%)
1	C	0.31	0/2195	0.81	2/2982 (0.1%)
1	D	0.32	0/2199	0.81	4/2985 (0.1%)
1	E	0.31	0/2194	0.82	6/2977 (0.2%)
1	F	0.30	0/2163	0.80	2/2933 (0.1%)
1	G	0.31	0/2171	0.80	3/2947 (0.1%)
1	H	0.29	0/2146	0.80	3/2910 (0.1%)
1	I	0.31	0/2196	0.82	4/2981 (0.1%)
1	J	0.31	0/2200	0.81	3/2986 (0.1%)
1	K	0.31	0/2061	0.80	4/2795 (0.1%)
1	L	0.30	0/2202	0.81	4/2989 (0.1%)
All	All	0.31	0/26134	0.81	44/35468 (0.1%)

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	53	GLY	N-CA-C	-7.79	103.73	114.64
1	B	53	GLY	N-CA-C	-7.29	105.15	115.43
1	I	53	GLY	N-CA-C	-6.63	105.45	115.00
1	B	33	ILE	N-CA-C	-6.45	103.55	113.16
1	C	53	GLY	N-CA-C	-6.11	106.97	114.92

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2155	0	2038	112	0
1	B	2147	0	2037	102	0
1	C	2142	0	2023	103	3
1	D	2146	0	2033	100	0
1	E	2142	0	2032	105	0
1	F	2113	0	2002	104	3
1	G	2119	0	2009	104	0
1	H	2096	0	1978	102	0
1	I	2143	0	2027	110	0
1	J	2148	0	2037	95	0
1	K	2013	0	1920	102	0
1	L	2150	0	2038	98	0
2	A	27	0	22	10	0
2	B	27	0	22	8	0
2	C	27	0	22	5	0
2	D	27	0	22	2	0
2	E	27	0	22	7	0
2	F	27	0	22	8	0
2	G	27	0	22	5	0
2	H	27	0	22	7	0
2	I	27	0	22	9	0
2	J	27	0	22	7	0
2	K	27	0	22	10	0
2	L	27	0	22	6	0
3	A	19	0	17	8	0
3	B	19	0	17	12	0
3	C	19	0	17	9	0
3	D	19	0	17	10	0
3	E	19	0	17	4	0
3	F	19	0	17	4	0
3	G	19	0	17	6	0
3	H	19	0	17	11	0
3	I	19	0	17	9	0
3	J	19	0	17	5	0
3	K	19	0	17	6	0
3	L	19	0	17	4	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
All	All	26078	0	24642	1207	3

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 24.

The worst 5 of 1207 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:H:180:ASN:HB3	2:H:501:SFG:HN1	1.24	1.02
1:C:171:LYS:H	1:C:171:LYS:HD2	1.28	0.98
1:J:171:LYS:H	1:J:171:LYS:HD2	1.28	0.98
1:K:171:LYS:HD2	1:K:171:LYS:H	1.28	0.98
1:A:171:LYS:H	1:A:171:LYS:HD2	1.28	0.97

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLN:O	1:F:142:GLU:OE1[1_565]	2.05	0.15
1:C:125:GLN:O	1:F:142:GLU:OE2[1_565]	2.07	0.13
1:C:125:GLN:O	1:F:142:GLU:CD[1_565]	2.19	0.01

## 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	273/320 (85%)	249 (91%)	21 (8%)	3 (1%)	11	43
1	B	269/320 (84%)	251 (93%)	17 (6%)	1 (0%)	30	65
1	C	272/320 (85%)	249 (92%)	23 (8%)	0	100	100
1	D	269/320 (84%)	248 (92%)	20 (7%)	1 (0%)	30	65
1	E	268/320 (84%)	246 (92%)	20 (8%)	2 (1%)	18	53
1	F	263/320 (82%)	240 (91%)	21 (8%)	2 (1%)	16	50
1	G	265/320 (83%)	247 (93%)	17 (6%)	1 (0%)	30	65
1	H	262/320 (82%)	238 (91%)	23 (9%)	1 (0%)	30	65
1	I	271/320 (85%)	254 (94%)	17 (6%)	0	100	100
1	J	268/320 (84%)	245 (91%)	19 (7%)	4 (2%)	8	35
1	K	256/320 (80%)	237 (93%)	19 (7%)	0	100	100
1	L	269/320 (84%)	244 (91%)	23 (9%)	2 (1%)	18	53
All	All	3205/3840 (84%)	2948 (92%)	240 (8%)	17 (0%)	24	60

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	B	67	ALA
1	D	26	ALA
1	F	67	ALA
1	J	41	ALA

### 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	222/254 (87%)	215 (97%)	7 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	222/254 (87%)	215 (97%)	7 (3%)	34	67
1	C	220/254 (87%)	213 (97%)	7 (3%)	34	67
1	D	221/254 (87%)	211 (96%)	10 (4%)	24	59
1	E	222/254 (87%)	215 (97%)	7 (3%)	34	67
1	F	217/254 (85%)	211 (97%)	6 (3%)	38	70
1	G	219/254 (86%)	211 (96%)	8 (4%)	30	64
1	H	214/254 (84%)	208 (97%)	6 (3%)	38	70
1	I	221/254 (87%)	213 (96%)	8 (4%)	31	65
1	J	223/254 (88%)	215 (96%)	8 (4%)	31	65
1	K	209/254 (82%)	203 (97%)	6 (3%)	37	70
1	L	222/254 (87%)	215 (97%)	7 (3%)	34	67
All	All	2632/3048 (86%)	2545 (97%)	87 (3%)	33	67

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	262	LEU
1	J	184	MET
1	I	52	ASP
1	I	262	LEU
1	K	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	252	GLN
1	I	189	HIS
1	H	38	ASN
1	H	252	GLN
1	J	38	ASN

### 5.3.3 RNA ⓘ

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 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	GPP	H	502	4	17,18,18	2.00	5 (29%)	21,25,25	1.14	3 (14%)
2	SFG	I	501	-	28,29,29	1.00	3 (10%)	34,42,42	1.97	10 (29%)
2	SFG	D	501	-	28,29,29	1.01	3 (10%)	34,42,42	1.96	9 (26%)
3	GPP	F	502	4	17,18,18	2.00	5 (29%)	21,25,25	1.19	3 (14%)
2	SFG	F	501	-	28,29,29	1.01	3 (10%)	34,42,42	2.08	10 (29%)
3	GPP	B	502	4	17,18,18	2.00	5 (29%)	21,25,25	1.23	4 (19%)
2	SFG	E	501	-	28,29,29	1.01	3 (10%)	34,42,42	1.97	9 (26%)
2	SFG	B	501	-	28,29,29	1.00	3 (10%)	34,42,42	1.97	10 (29%)
3	GPP	E	502	4	17,18,18	2.01	5 (29%)	21,25,25	1.19	3 (14%)
3	GPP	A	502	4	17,18,18	2.00	5 (29%)	21,25,25	1.15	3 (14%)
3	GPP	I	502	4	17,18,18	2.00	5 (29%)	21,25,25	1.16	3 (14%)
2	SFG	L	501	-	28,29,29	1.01	3 (10%)	34,42,42	1.97	10 (29%)
3	GPP	J	502	4	17,18,18	2.01	5 (29%)	21,25,25	1.14	3 (14%)
3	GPP	G	502	4	17,18,18	2.00	5 (29%)	21,25,25	1.23	3 (14%)
3	GPP	L	502	4	17,18,18	2.01	5 (29%)	21,25,25	1.22	3 (14%)
2	SFG	J	501	-	28,29,29	1.01	3 (10%)	34,42,42	1.97	10 (29%)
2	SFG	K	501	-	28,29,29	1.00	3 (10%)	34,42,42	2.01	10 (29%)
2	SFG	H	501	-	28,29,29	1.01	3 (10%)	34,42,42	1.97	10 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SFG	A	501	-	28,29,29	1.01	3 (10%)	34,42,42	1.98	10 (29%)
2	SFG	C	501	-	28,29,29	1.00	3 (10%)	34,42,42	1.98	10 (29%)
3	GPP	K	502	4	17,18,18	2.01	5 (29%)	21,25,25	1.20	3 (14%)
3	GPP	C	502	4	17,18,18	2.00	5 (29%)	21,25,25	1.25	3 (14%)
3	GPP	D	502	4	17,18,18	2.01	6 (35%)	21,25,25	1.19	3 (14%)
2	SFG	G	501	-	28,29,29	1.01	3 (10%)	34,42,42	1.95	9 (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	GPP	H	502	4	-	2/19/19/19	-
2	SFG	I	501	-	-	1/17/33/33	0/3/3/3
2	SFG	D	501	-	-	3/17/33/33	0/3/3/3
3	GPP	F	502	4	-	9/19/19/19	-
2	SFG	F	501	-	-	0/17/33/33	0/3/3/3
3	GPP	B	502	4	-	3/19/19/19	-
2	SFG	E	501	-	-	1/17/33/33	0/3/3/3
2	SFG	B	501	-	-	0/17/33/33	0/3/3/3
3	GPP	E	502	4	-	2/19/19/19	-
3	GPP	A	502	4	-	0/19/19/19	-
3	GPP	I	502	4	-	4/19/19/19	-
2	SFG	L	501	-	-	1/17/33/33	0/3/3/3
3	GPP	J	502	4	-	3/19/19/19	-
3	GPP	G	502	4	-	0/19/19/19	-
3	GPP	L	502	4	-	3/19/19/19	-
2	SFG	J	501	-	-	1/17/33/33	0/3/3/3
2	SFG	K	501	-	-	1/17/33/33	0/3/3/3
2	SFG	H	501	-	-	0/17/33/33	0/3/3/3
2	SFG	A	501	-	-	0/17/33/33	0/3/3/3
2	SFG	C	501	-	-	2/17/33/33	0/3/3/3
3	GPP	K	502	4	-	3/19/19/19	-
3	GPP	C	502	4	-	1/19/19/19	-
3	GPP	D	502	4	-	5/19/19/19	-
2	SFG	G	501	-	-	1/17/33/33	0/3/3/3

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	GPP	C6-C7	-3.66	1.39	1.50
3	D	502	GPP	C6-C7	-3.66	1.39	1.50
3	K	502	GPP	C6-C7	-3.65	1.39	1.50
3	C	502	GPP	C6-C7	-3.65	1.39	1.50
3	B	502	GPP	C6-C7	-3.64	1.39	1.50

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	SFG	C5-C4-N3	-5.40	119.28	126.72
2	B	501	SFG	C5-C4-N3	-5.35	119.34	126.72
2	G	501	SFG	C5-C4-N3	-5.33	119.37	126.72
2	I	501	SFG	C5-C4-N3	-5.33	119.37	126.72
2	H	501	SFG	C5-C4-N3	-5.33	119.38	126.72

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	GPP	O1-C1-C2-C3
3	D	502	GPP	PA-O3A-PB-O2B
3	F	502	GPP	C1-O1-PA-O1A
3	F	502	GPP	C1-O1-PA-O2A
3	F	502	GPP	C1-O1-PA-O3A

There are no ring outliers.

24 monomers are involved in 157 short contacts:

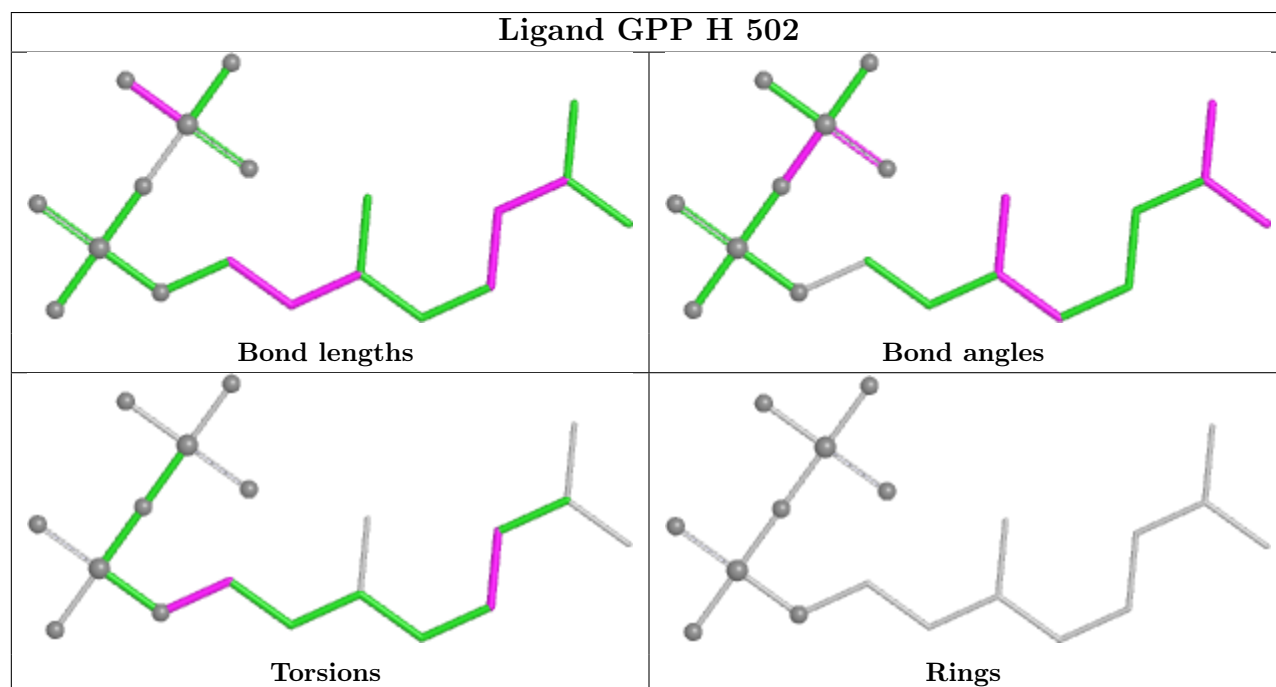
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	502	GPP	11	0
2	I	501	SFG	9	0
2	D	501	SFG	2	0
3	F	502	GPP	4	0
2	F	501	SFG	8	0
3	B	502	GPP	12	0
2	E	501	SFG	7	0
2	B	501	SFG	8	0
3	E	502	GPP	4	0
3	A	502	GPP	8	0
3	I	502	GPP	9	0
2	L	501	SFG	6	0
3	J	502	GPP	5	0

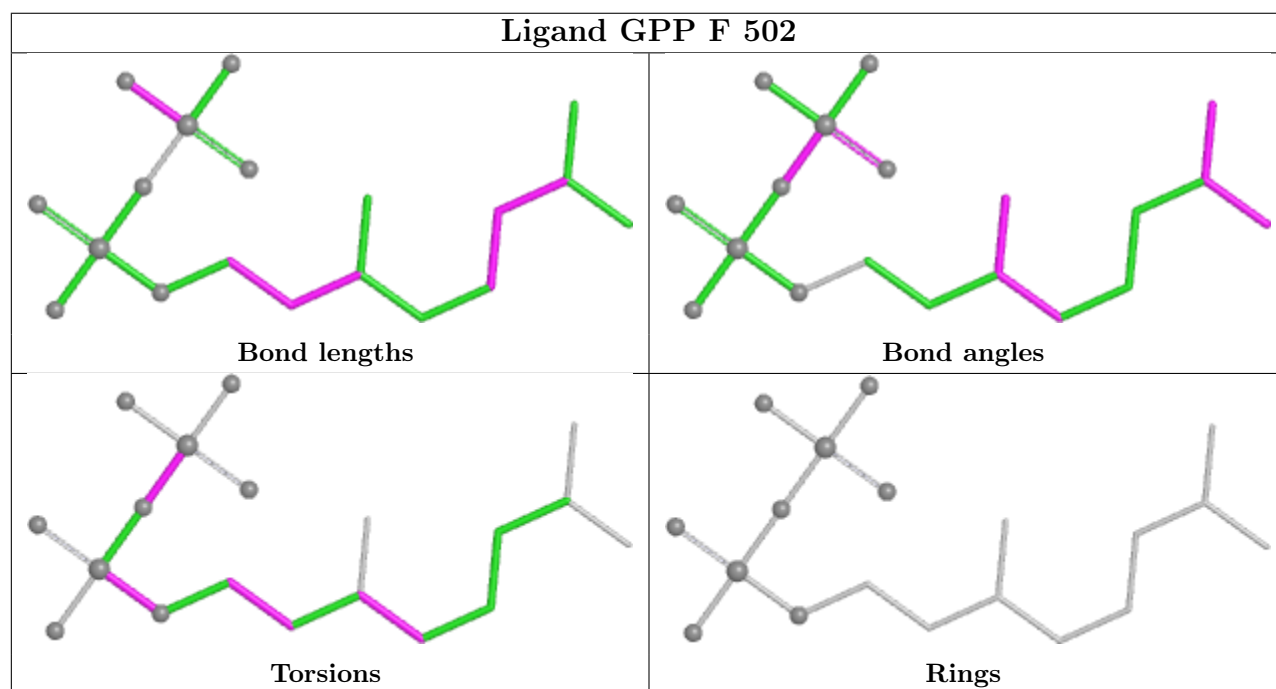
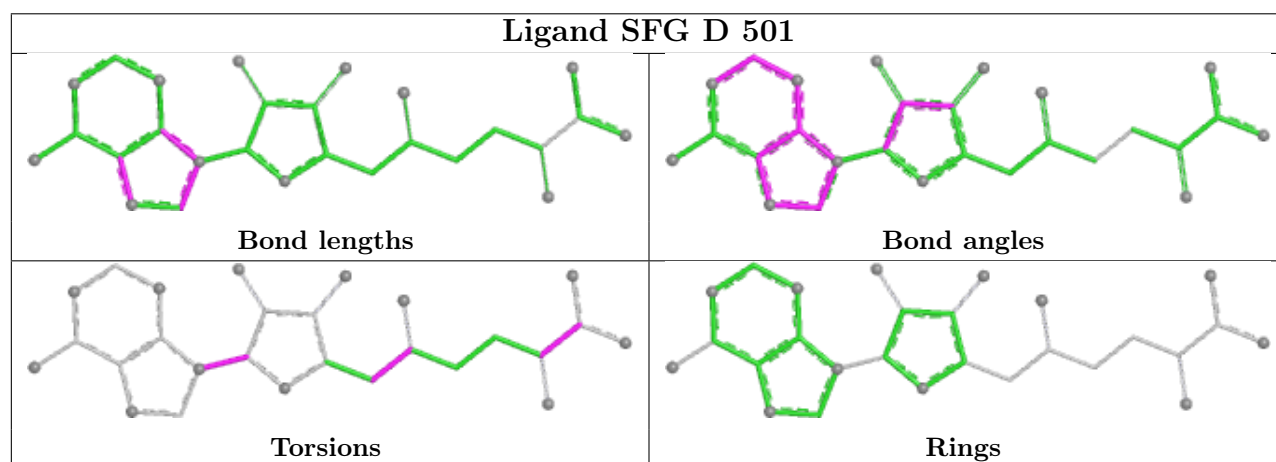
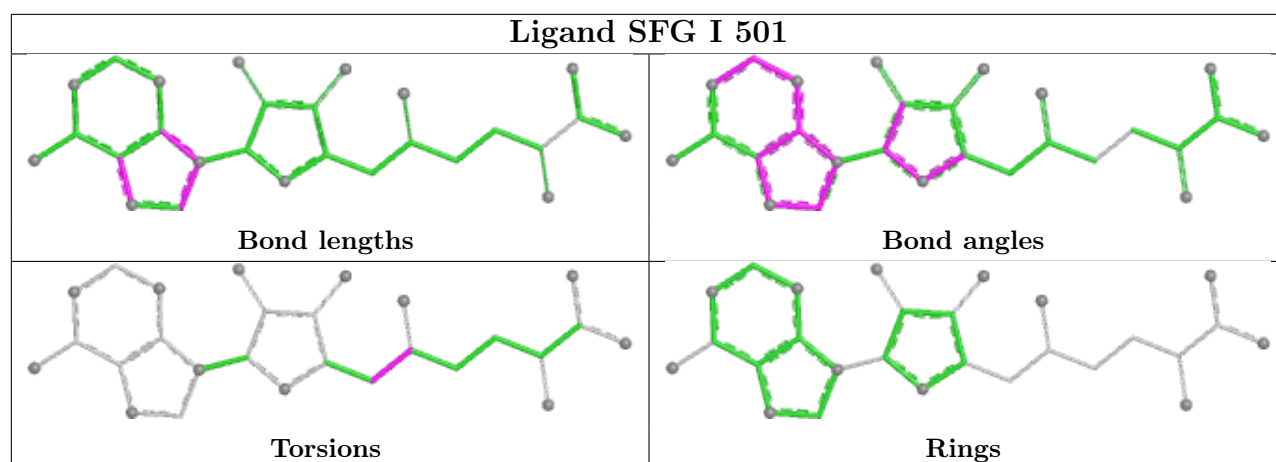
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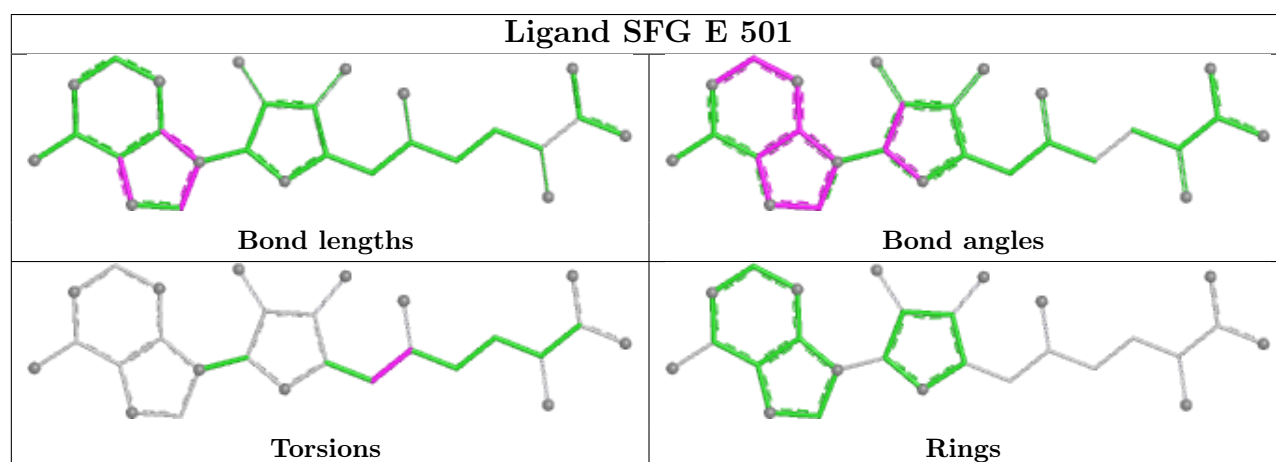
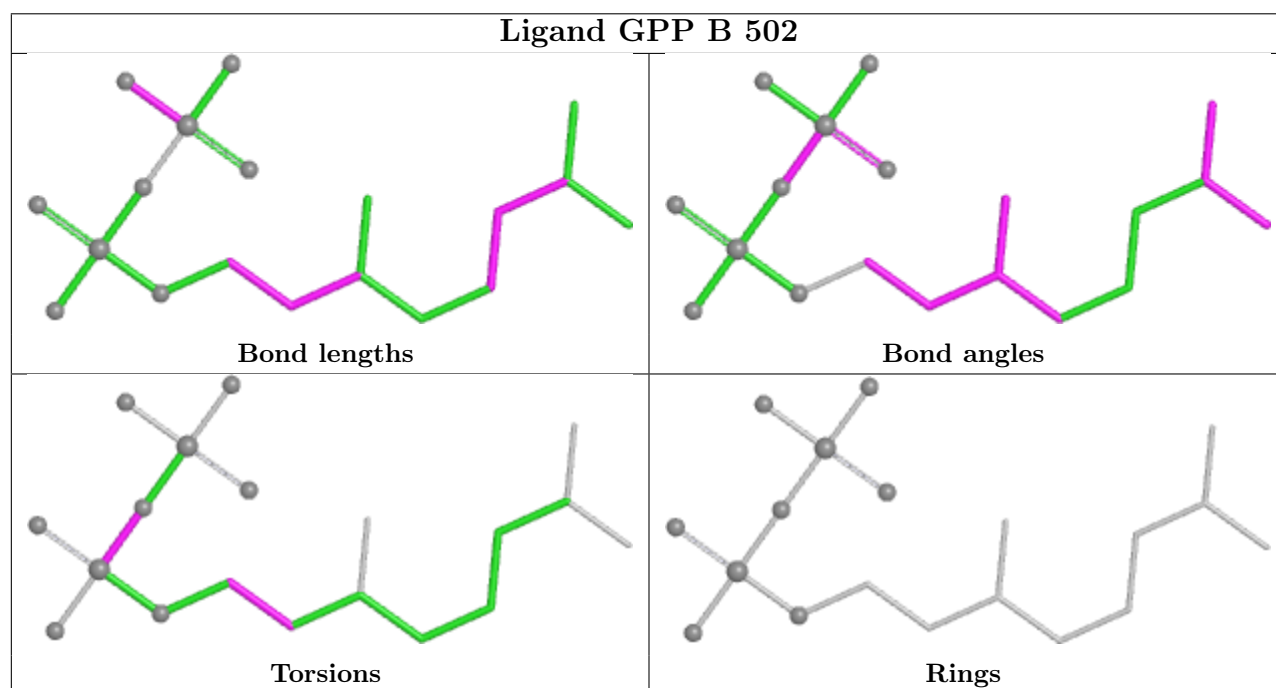
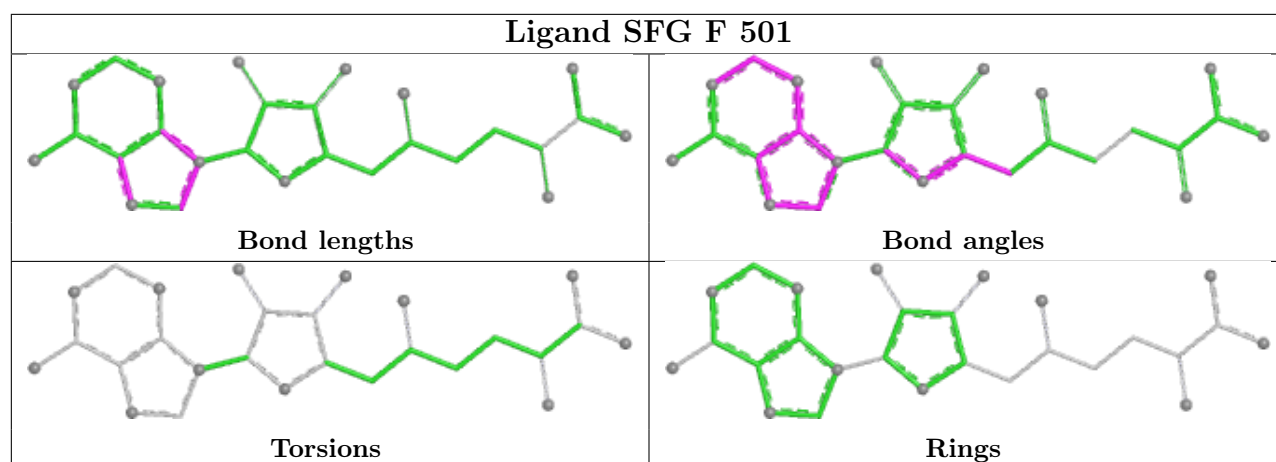
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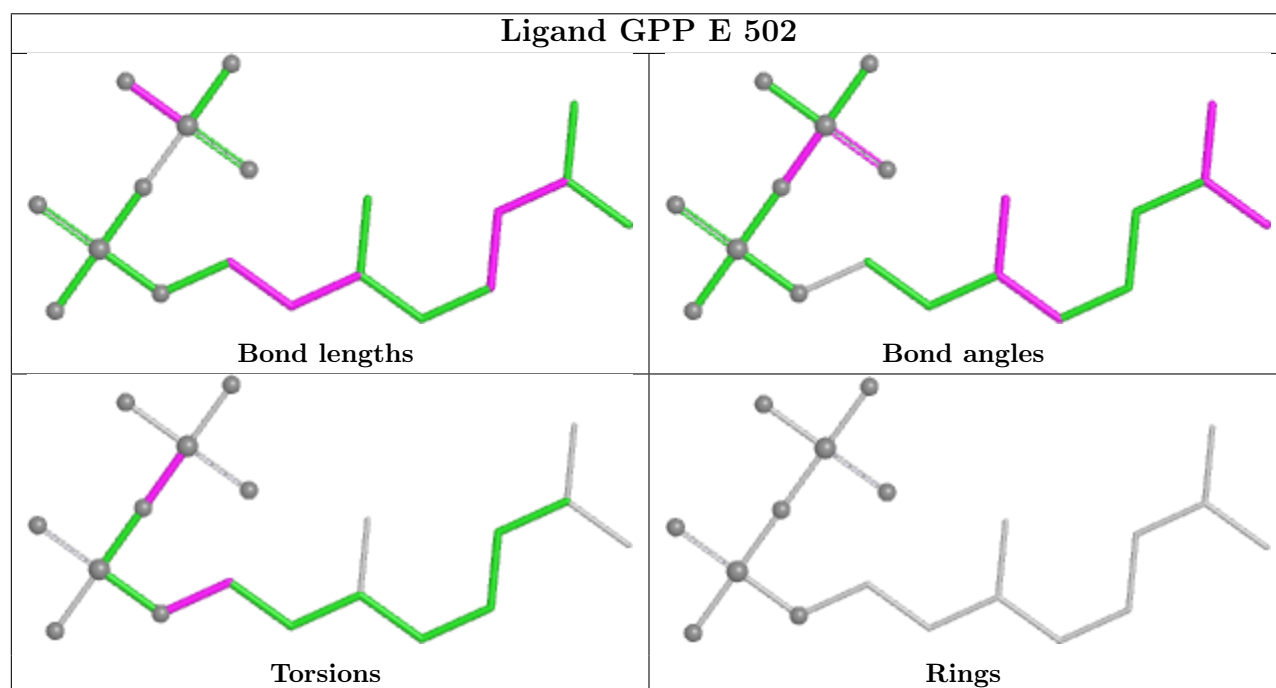
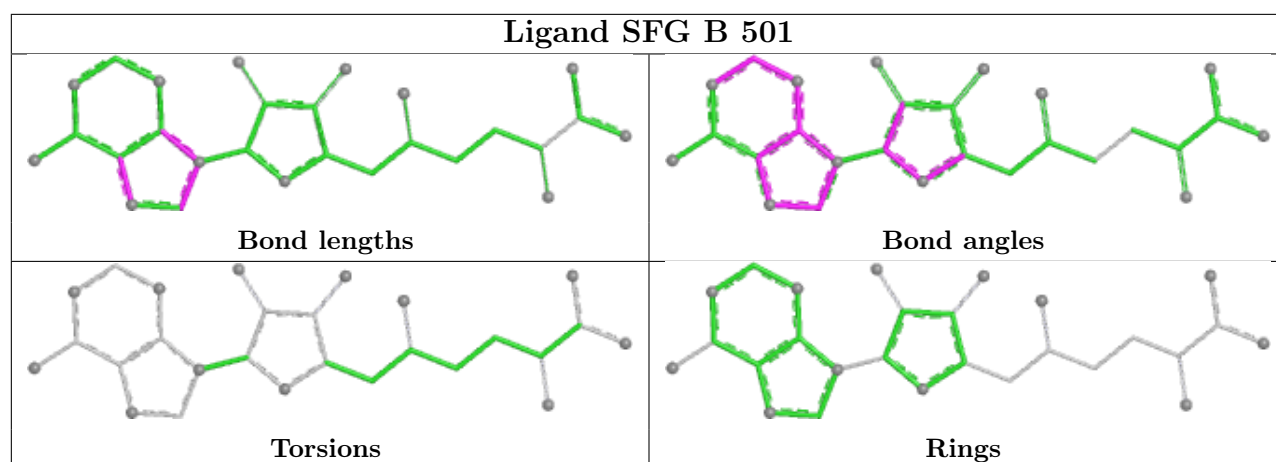
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	502	GPP	6	0
3	L	502	GPP	4	0
2	J	501	SFG	7	0
2	K	501	SFG	10	0
2	H	501	SFG	7	0
2	A	501	SFG	10	0
2	C	501	SFG	5	0
3	K	502	GPP	6	0
3	C	502	GPP	9	0
3	D	502	GPP	10	0
2	G	501	SFG	5	0

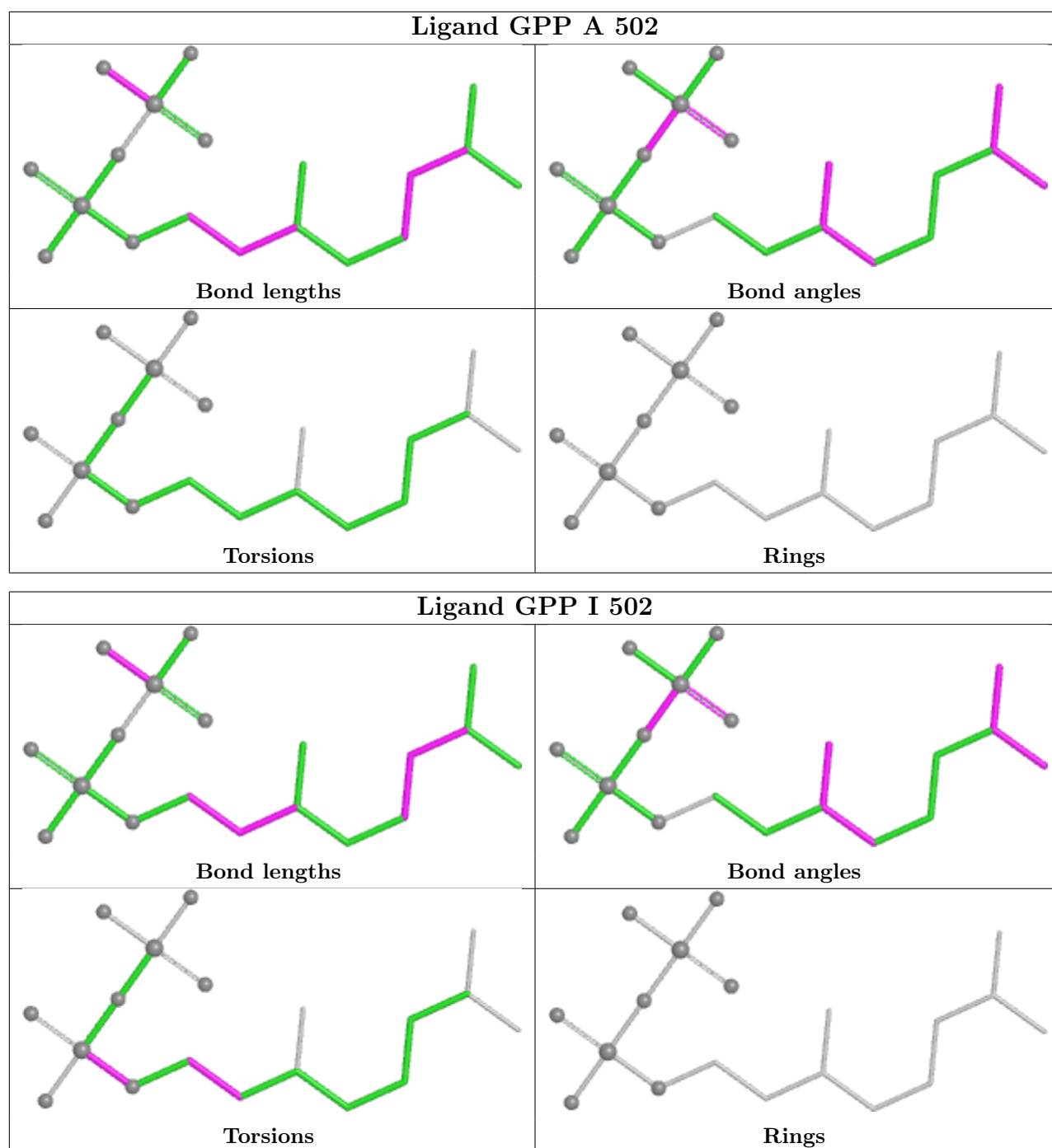
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

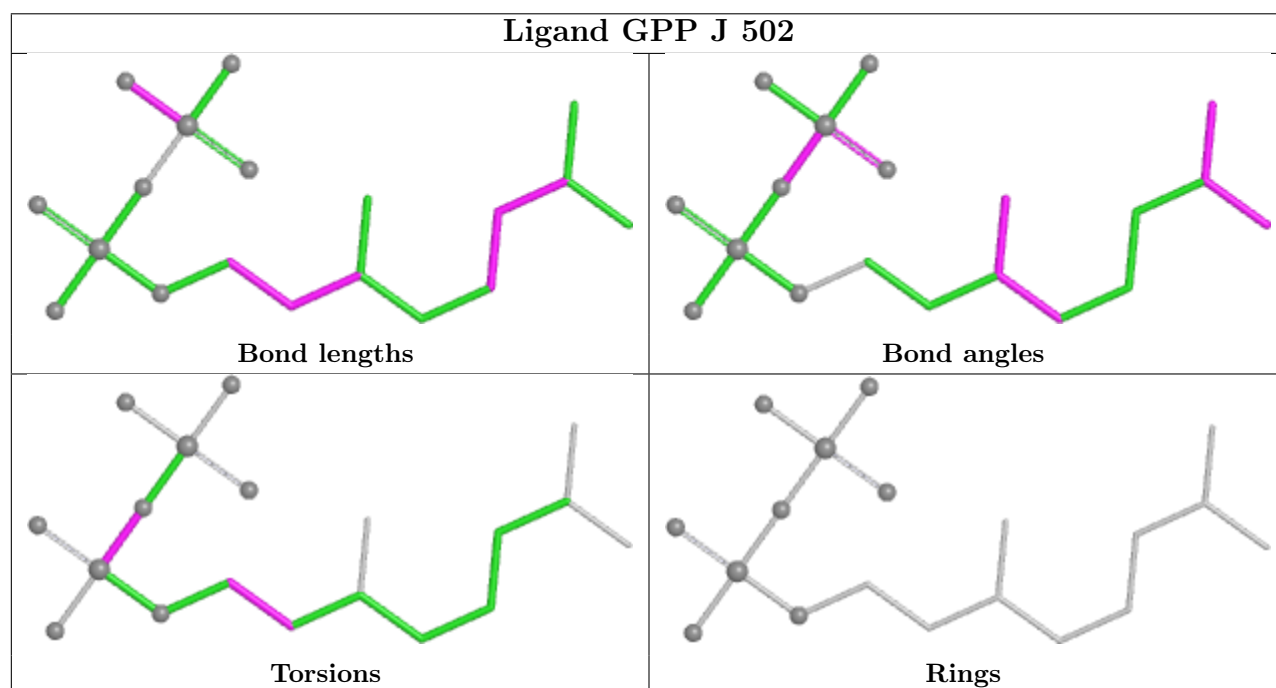
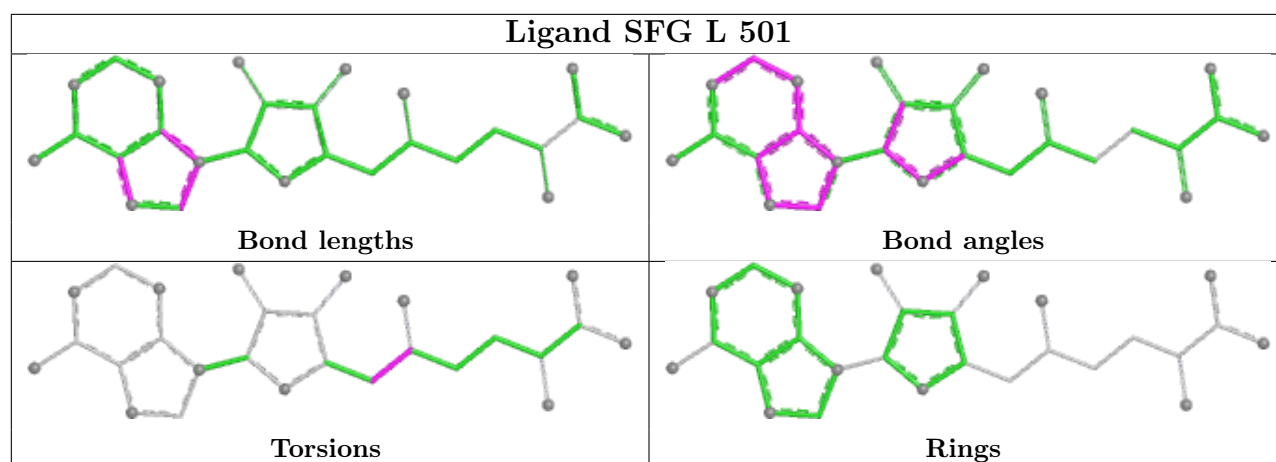


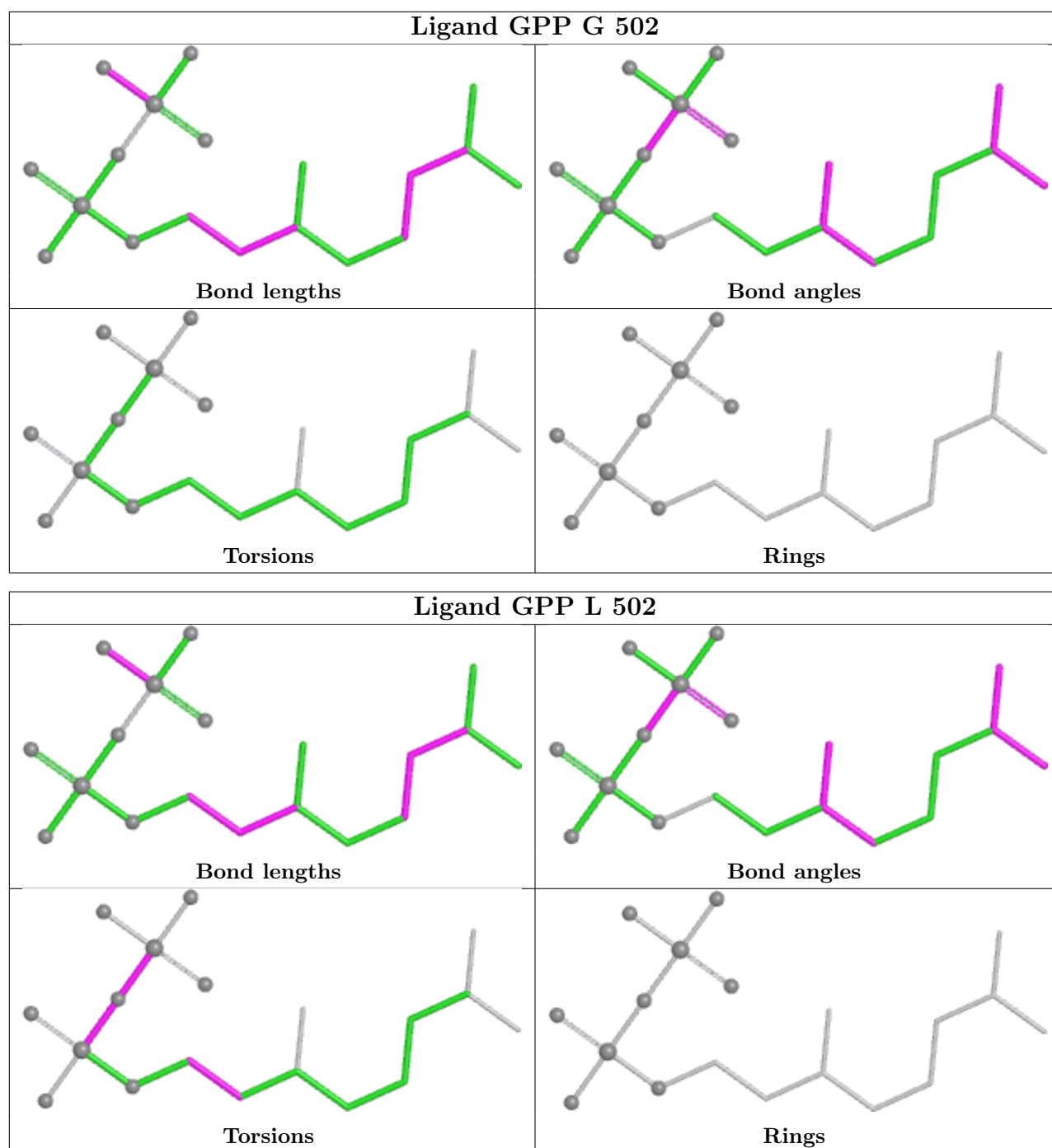


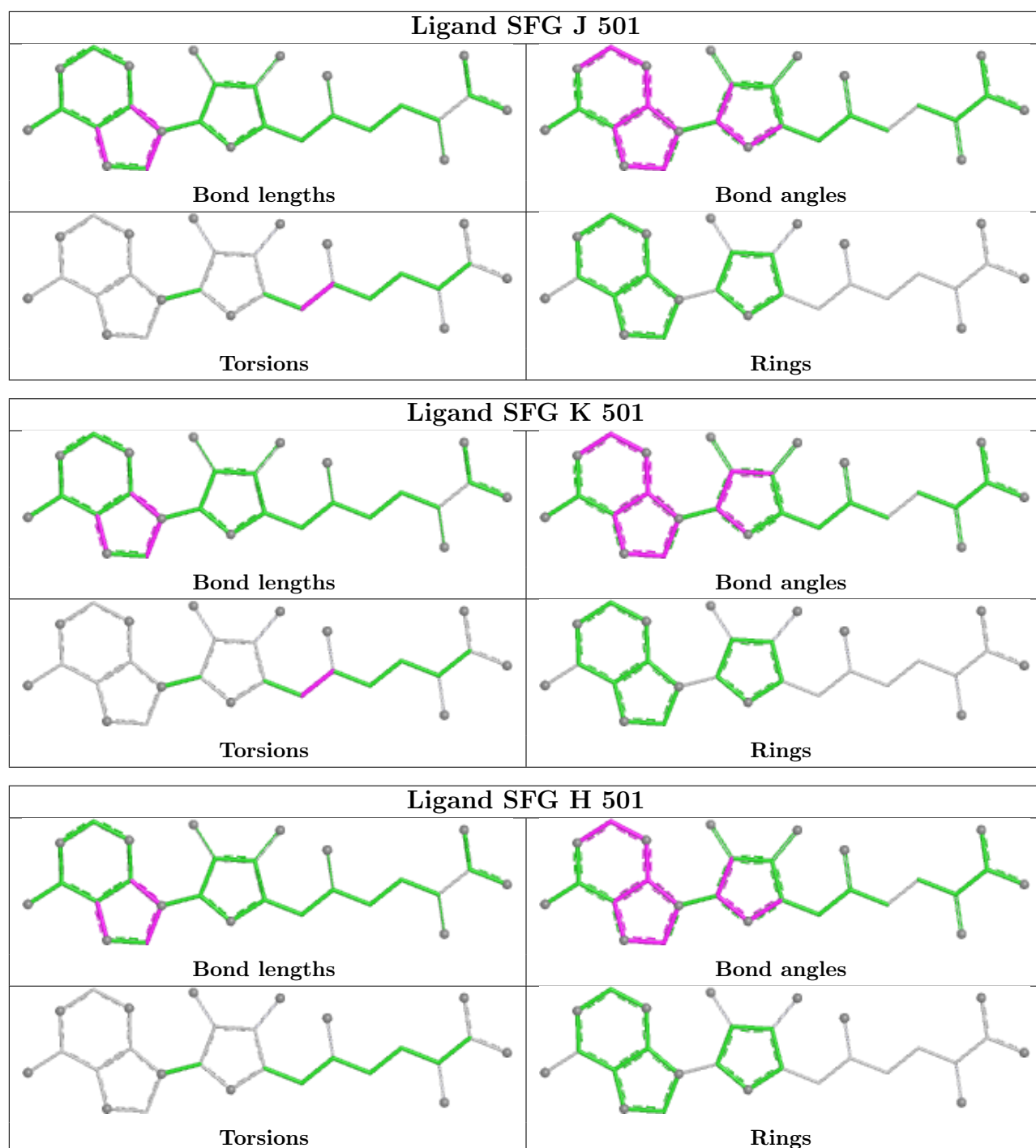


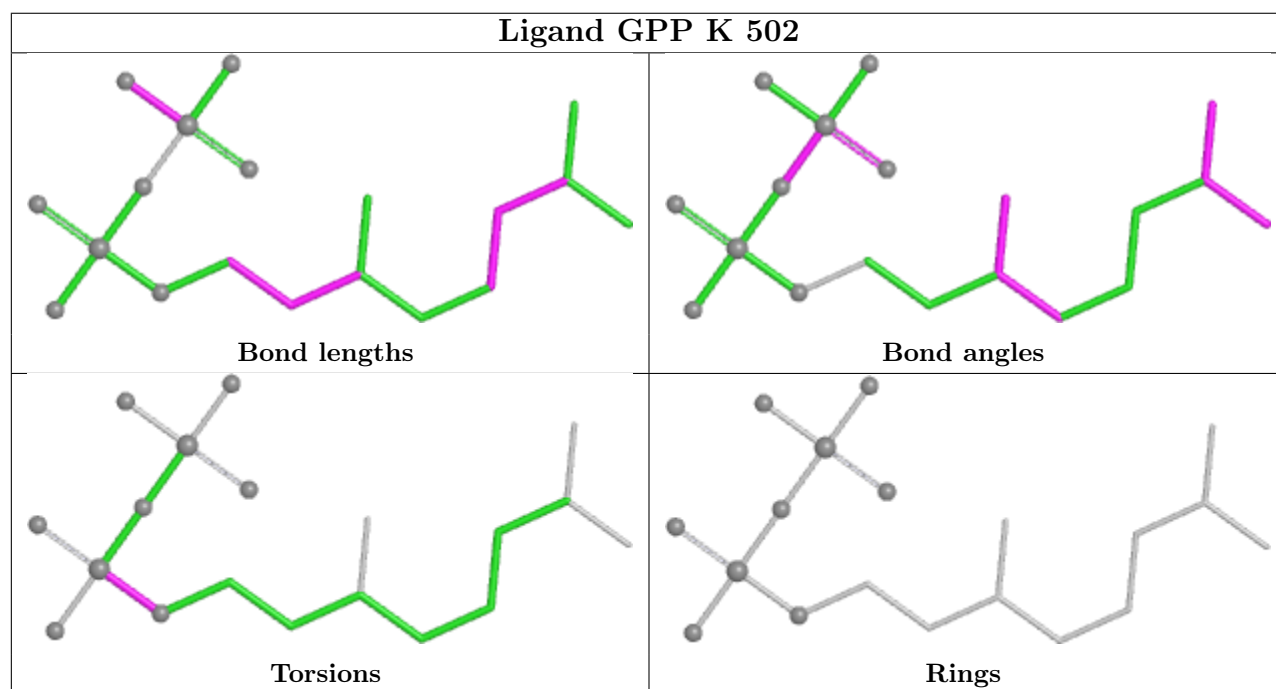
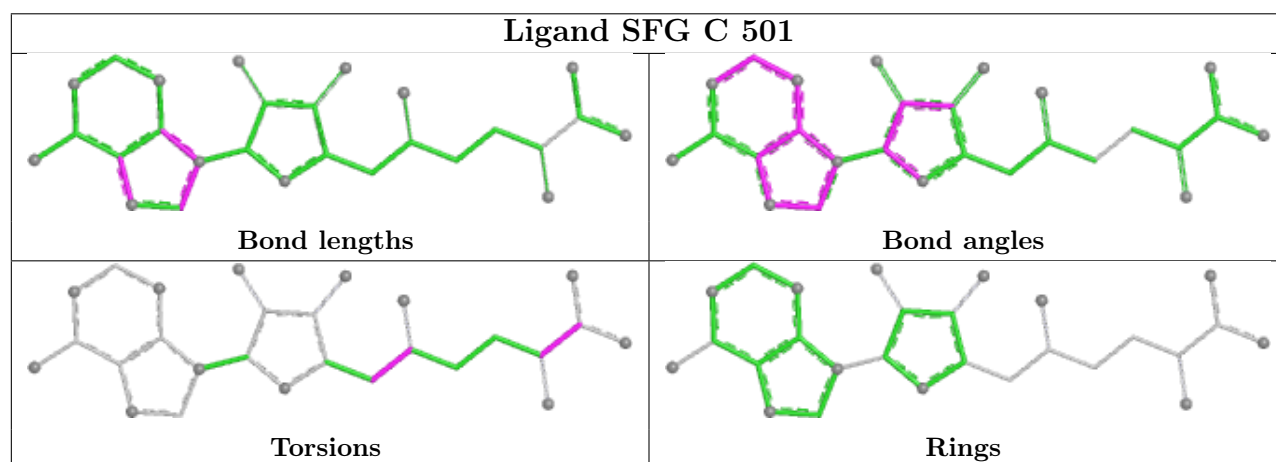
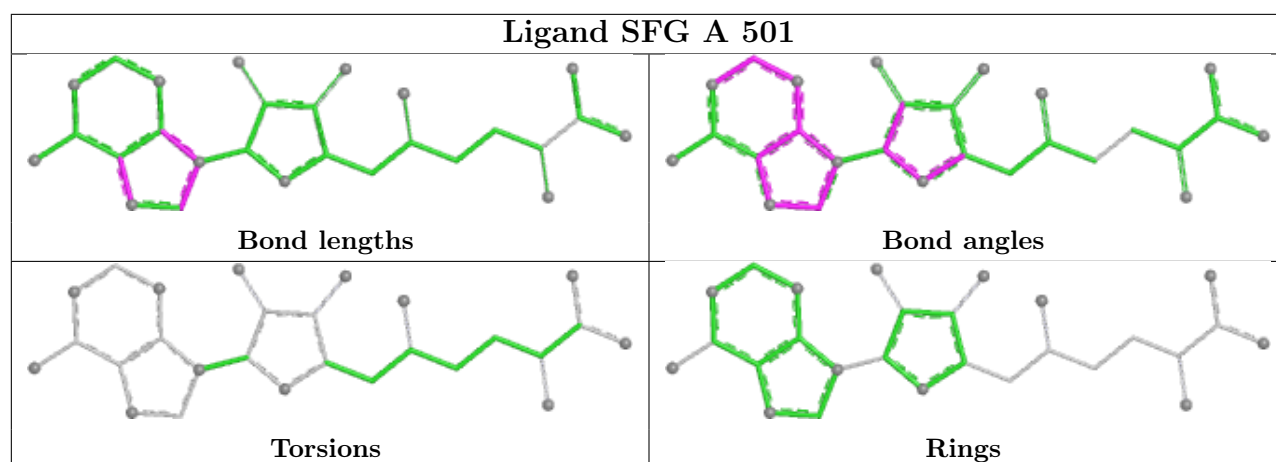


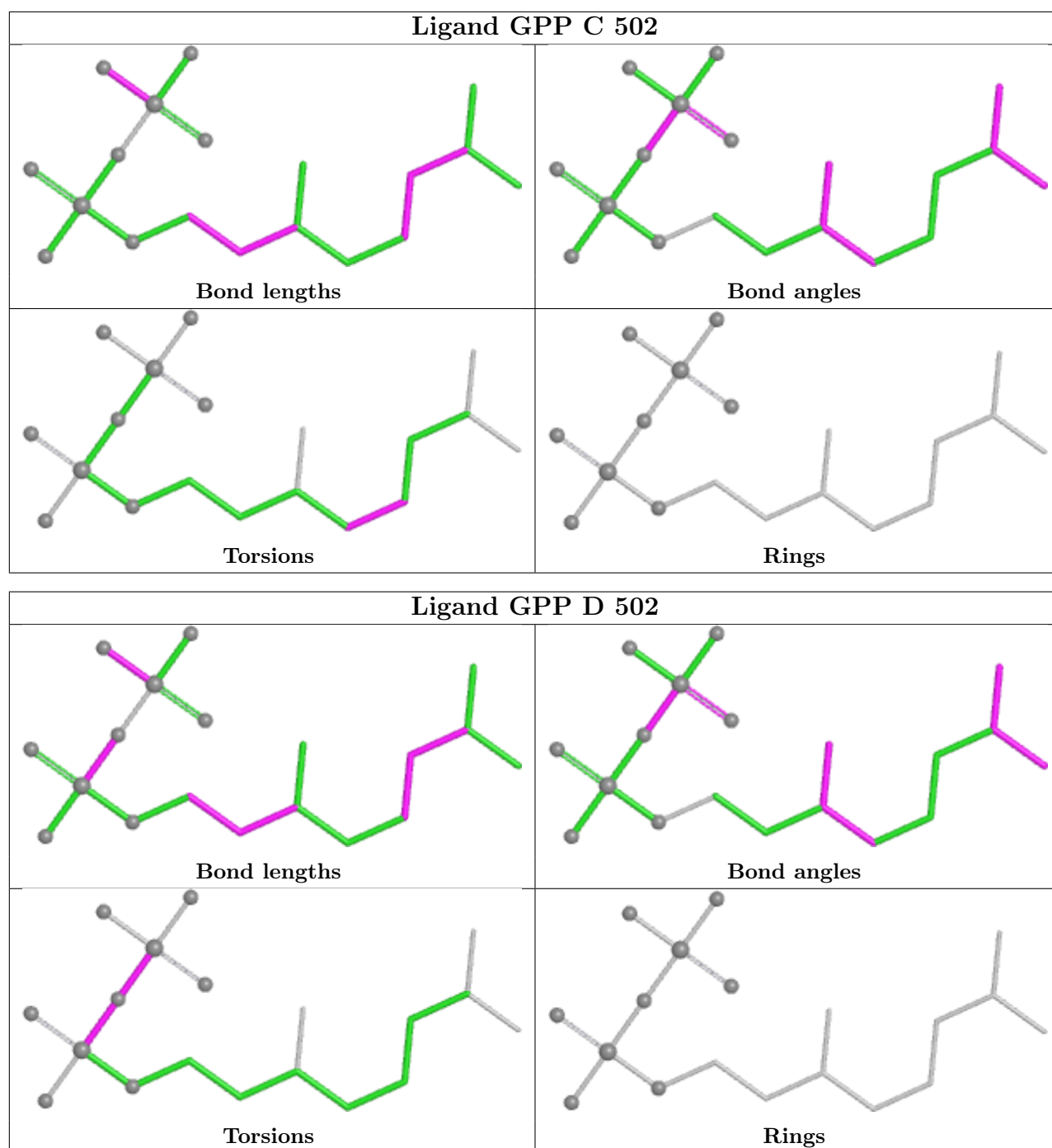


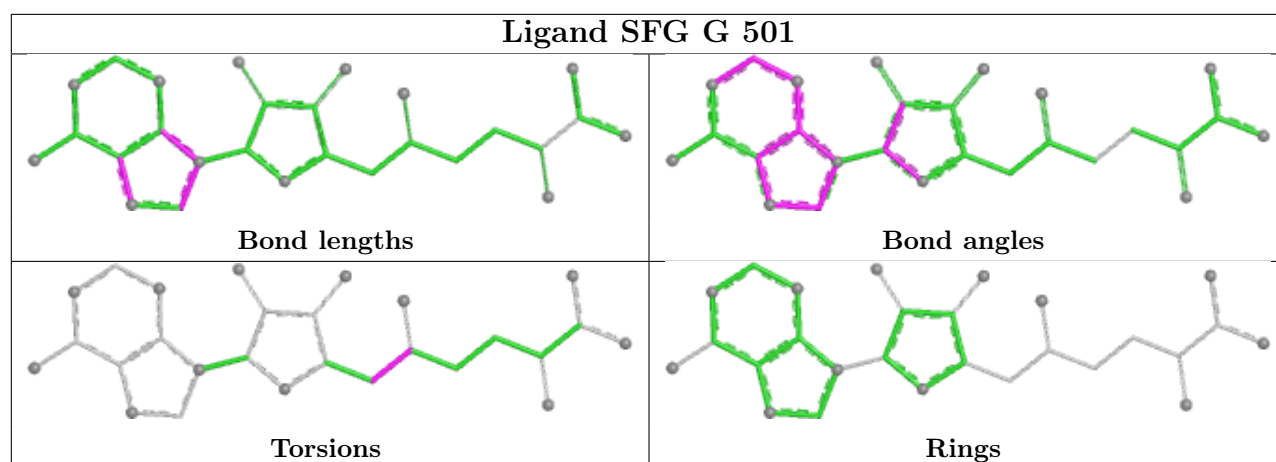












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	275/320 (85%)	0.89	18 (6%) 25 13	36, 47, 63, 77	0
1	B	273/320 (85%)	0.90	14 (5%) 33 17	30, 47, 72, 91	0
1	C	274/320 (85%)	0.93	18 (6%) 24 12	37, 50, 80, 93	0
1	D	273/320 (85%)	0.90	22 (8%) 18 9	34, 48, 65, 79	0
1	E	272/320 (85%)	0.80	10 (3%) 45 25	34, 49, 71, 87	0
1	F	269/320 (84%)	0.95	19 (7%) 22 11	37, 50, 74, 81	0
1	G	269/320 (84%)	0.88	20 (7%) 20 10	37, 47, 63, 81	0
1	H	268/320 (83%)	0.82	14 (5%) 33 17	38, 50, 76, 90	0
1	I	273/320 (85%)	0.85	15 (5%) 30 15	36, 48, 64, 77	0
1	J	272/320 (85%)	0.85	21 (7%) 19 10	31, 47, 67, 92	0
1	K	258/320 (80%)	0.83	10 (3%) 43 24	37, 49, 72, 90	0
1	L	273/320 (85%)	0.92	18 (6%) 24 12	38, 50, 80, 96	0
All	All	3249/3840 (84%)	0.88	199 (6%) 27 14	30, 48, 71, 96	0

The worst 5 of 199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	152	GLY	7.4
1	G	78	GLU	5.9
1	G	79	ALA	4.6
1	D	300	VAL	4.3
1	G	77	TYR	4.0

### 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 [i](#)

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

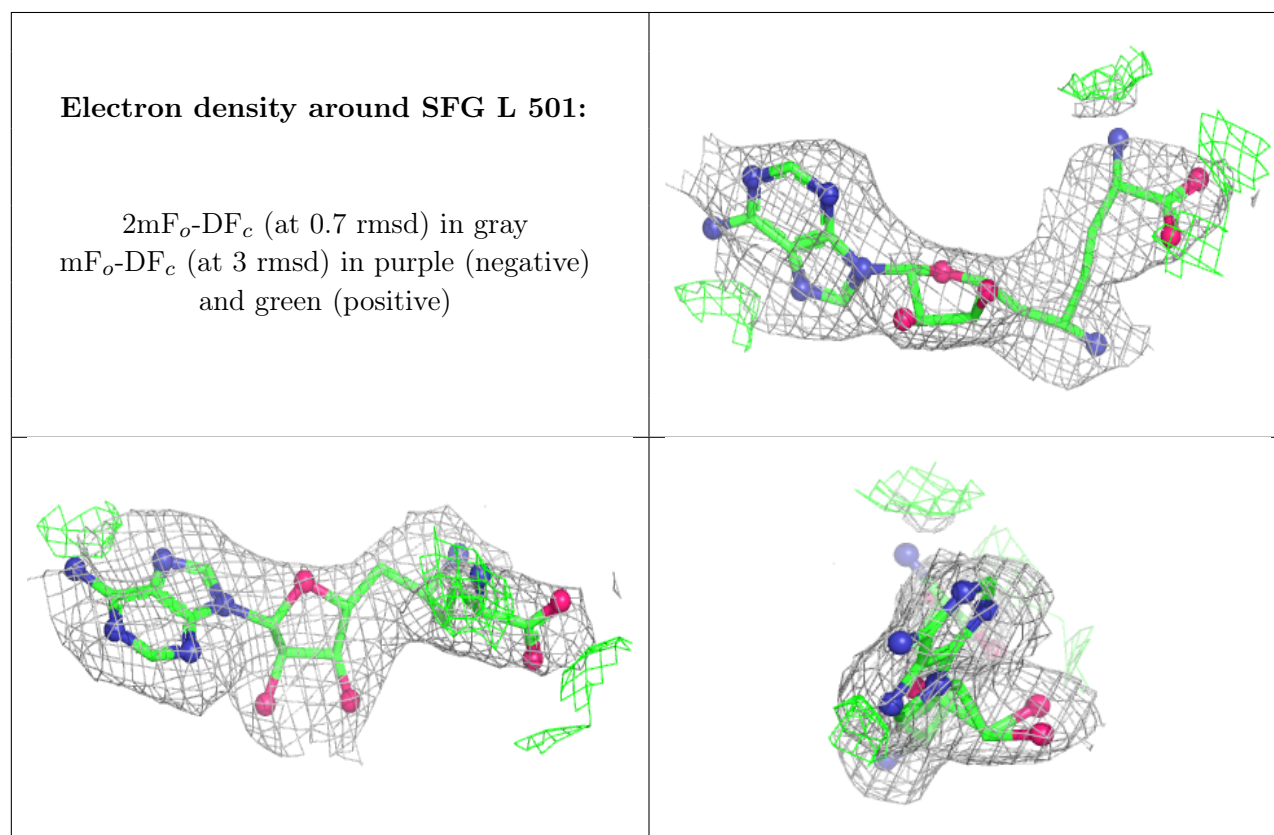
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SFG	L	501	27/27	0.77	0.19	64,66,70,71	0
4	MG	C	503	1/1	0.79	0.24	58,58,58,58	0
2	SFG	K	501	27/27	0.80	0.17	52,54,57,57	0
4	MG	K	503	1/1	0.80	0.23	49,49,49,49	0
2	SFG	D	501	27/27	0.81	0.17	37,45,47,49	0
4	MG	E	503	1/1	0.81	0.17	45,45,45,45	0
4	MG	G	503	1/1	0.81	0.18	38,38,38,38	0
2	SFG	F	501	27/27	0.81	0.18	57,59,69,71	0
4	MG	L	503	1/1	0.82	0.17	31,31,31,31	0
2	SFG	J	501	27/27	0.83	0.17	37,42,46,49	0
2	SFG	H	501	27/27	0.83	0.16	64,68,70,71	0
2	SFG	E	501	27/27	0.84	0.15	46,50,53,54	0
2	SFG	I	501	27/27	0.84	0.14	41,46,53,55	0
2	SFG	C	501	27/27	0.85	0.15	47,52,53,54	0
4	MG	F	503	1/1	0.86	0.13	36,36,36,36	0
2	SFG	G	501	27/27	0.86	0.14	40,47,52,54	0
2	SFG	B	501	27/27	0.87	0.16	42,43,45,46	0
2	SFG	A	501	27/27	0.89	0.14	34,40,50,50	0
3	GPP	F	502	19/19	0.90	0.14	50,56,61,61	0
3	GPP	B	502	19/19	0.91	0.19	54,56,62,63	0
4	MG	I	503	1/1	0.91	0.19	43,43,43,43	0
3	GPP	H	502	19/19	0.91	0.13	50,54,61,62	0
3	GPP	K	502	19/19	0.91	0.14	37,49,54,54	0
3	GPP	C	502	19/19	0.92	0.16	56,57,58,58	0
4	MG	J	503	1/1	0.92	0.10	21,21,21,21	0
3	GPP	I	502	19/19	0.92	0.17	44,47,53,53	0
4	MG	D	503	1/1	0.92	0.17	31,31,31,31	0
4	MG	B	503	1/1	0.93	0.16	9,9,9,9	0
3	GPP	E	502	19/19	0.93	0.16	49,57,61,61	0
3	GPP	D	502	19/19	0.93	0.16	34,43,48,48	0
3	GPP	G	502	19/19	0.93	0.16	34,39,42,42	0
3	GPP	L	502	19/19	0.93	0.14	58,68,71,71	0

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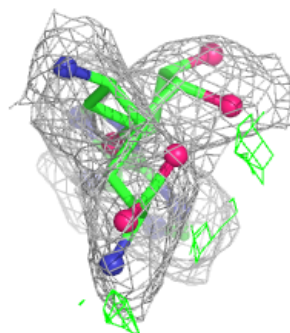
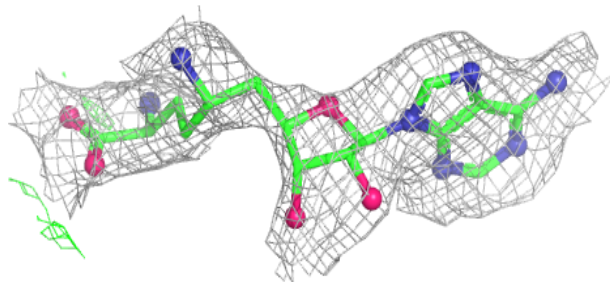
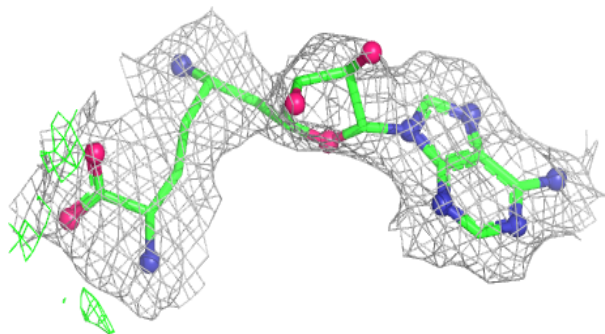
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	503	1/1	0.94	0.21	17,17,17,17	0
3	GPP	J	502	19/19	0.95	0.12	28,38,47,48	0
3	GPP	A	502	19/19	0.95	0.12	33,40,44,45	0
4	MG	H	503	1/1	0.96	0.06	35,35,35,35	0

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.

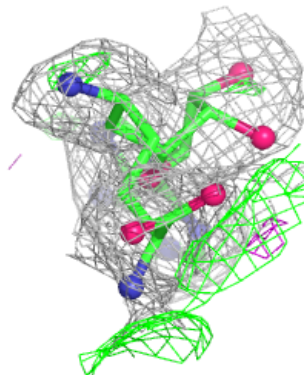
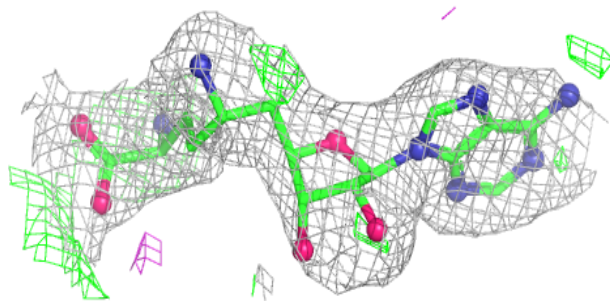
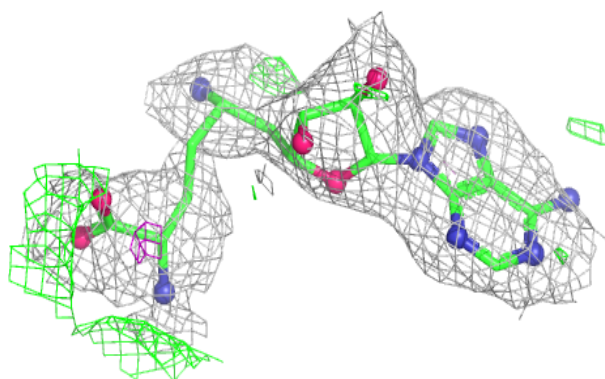


**Electron density around SFG K 501:**

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

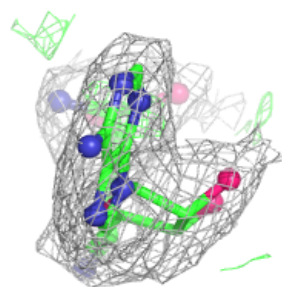
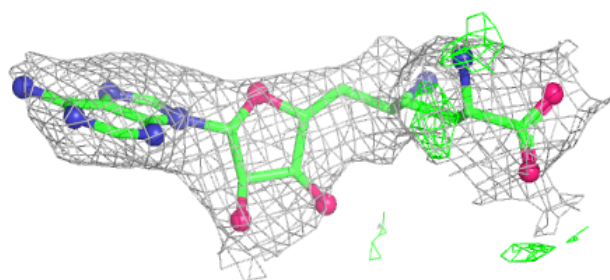
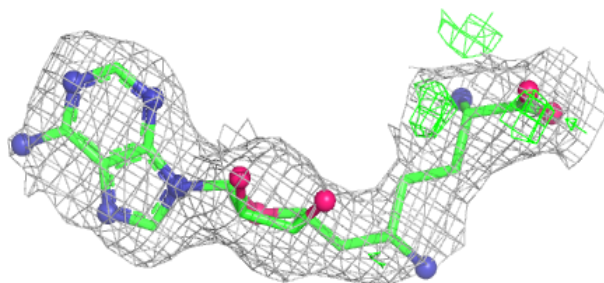
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and green (positive)

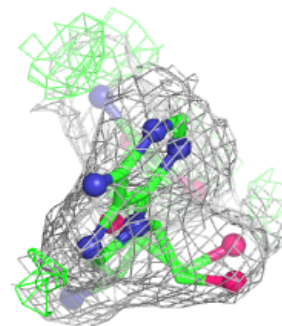
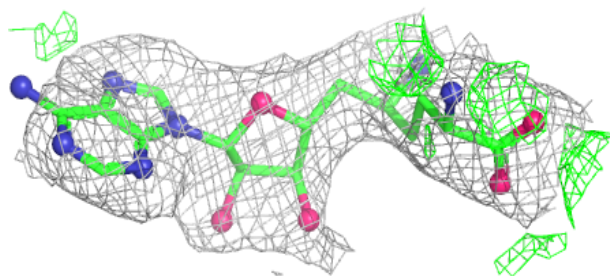
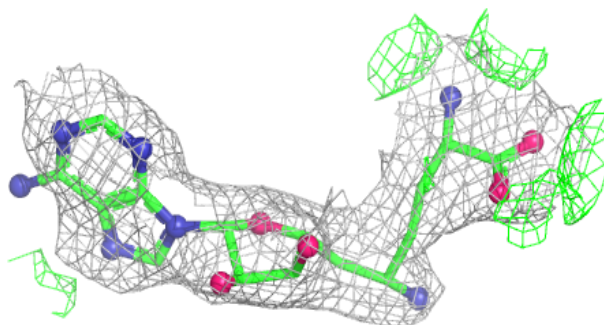


**Electron density around SFG F 501:**

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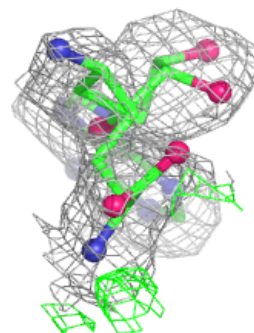
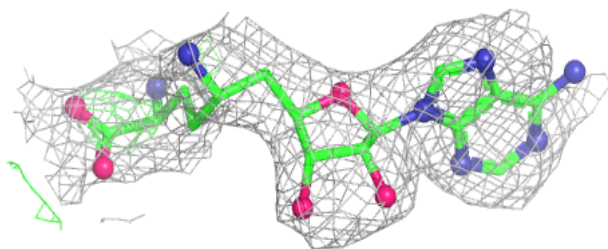
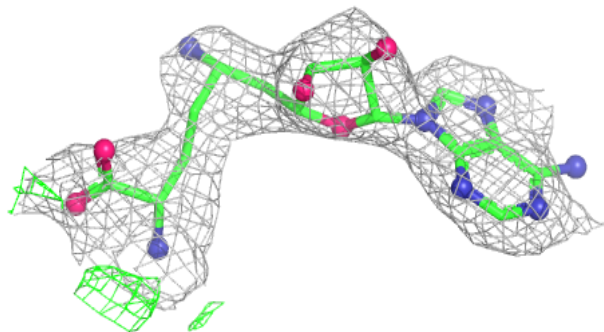
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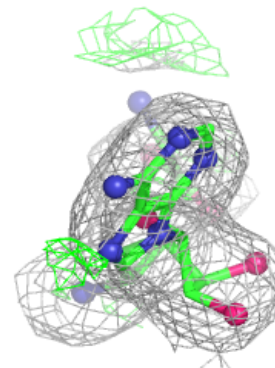
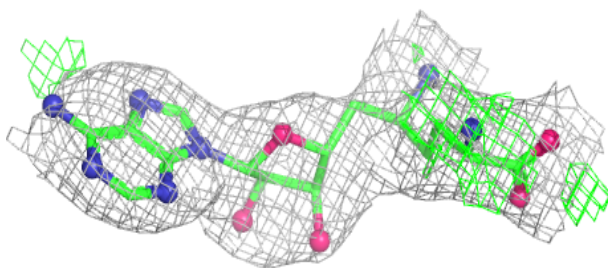
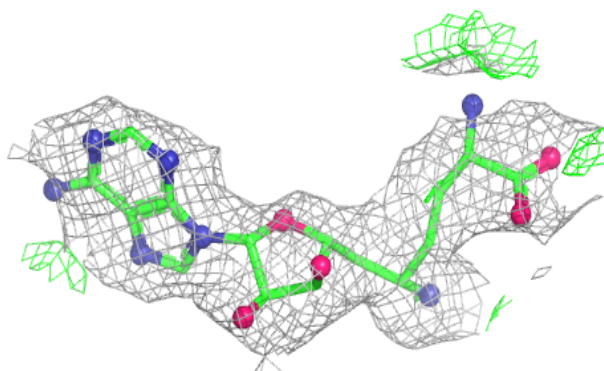


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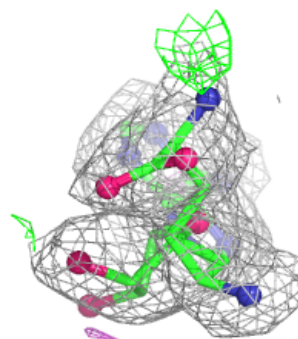
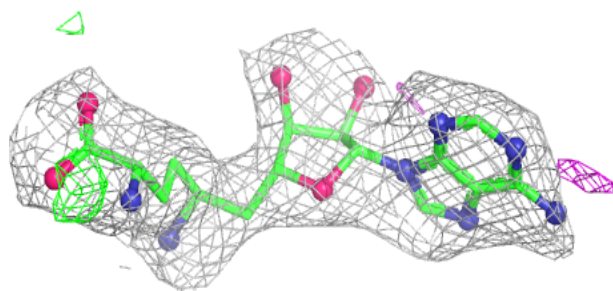
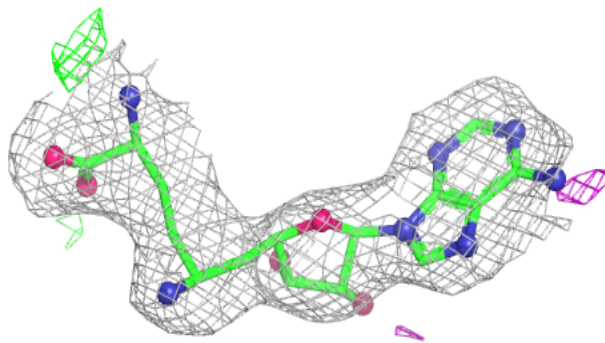
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and green (positive)

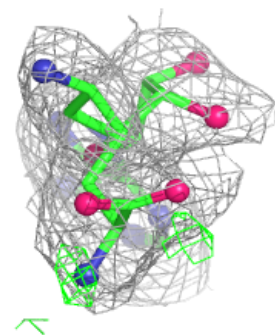
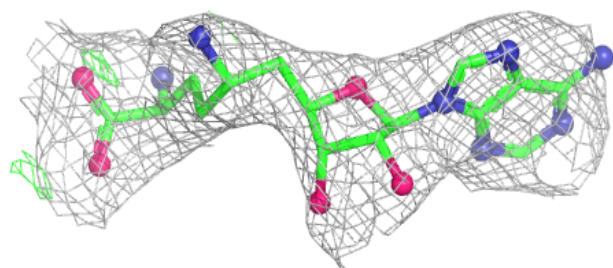
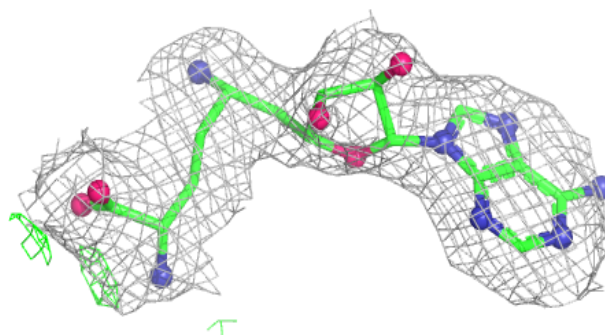


**Electron density around SFG I 501:**

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and green (positive)

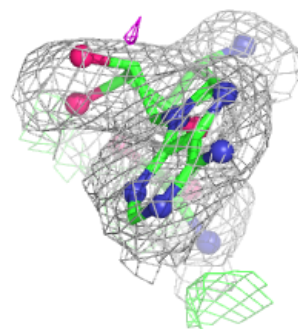
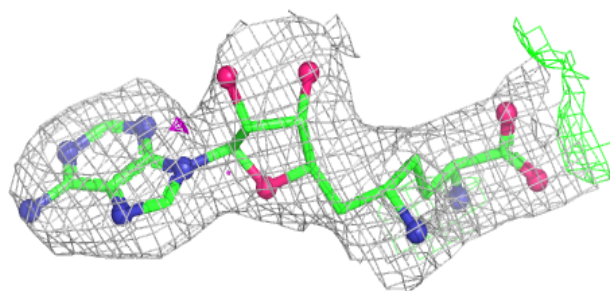
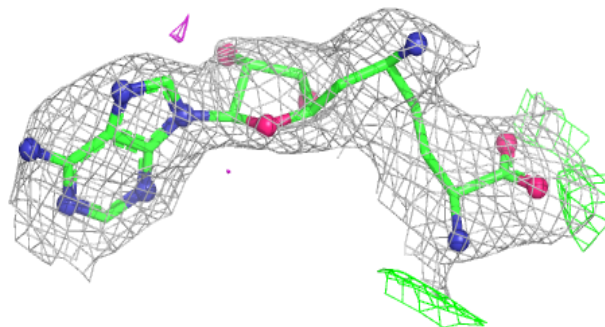
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and green (positive)

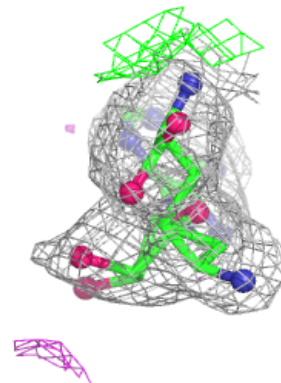
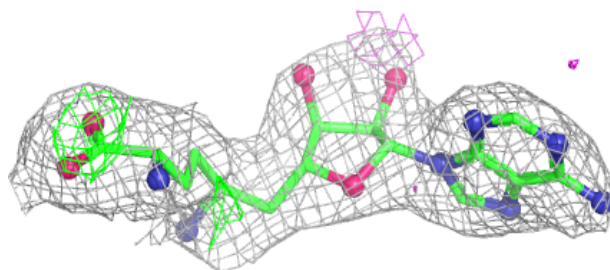
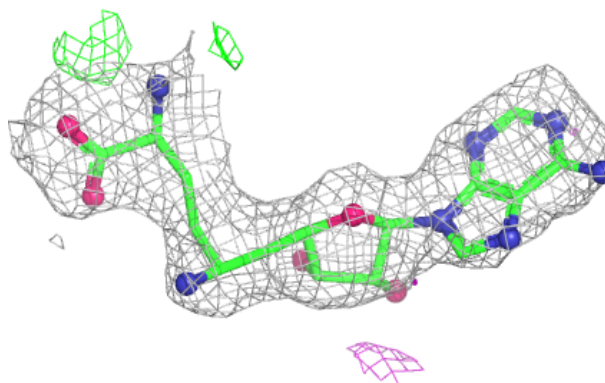


**Electron density around SFG G 501:**

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

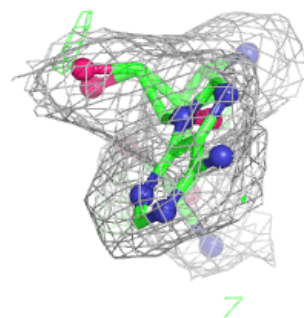
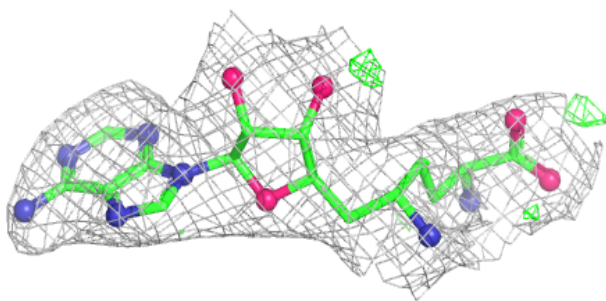
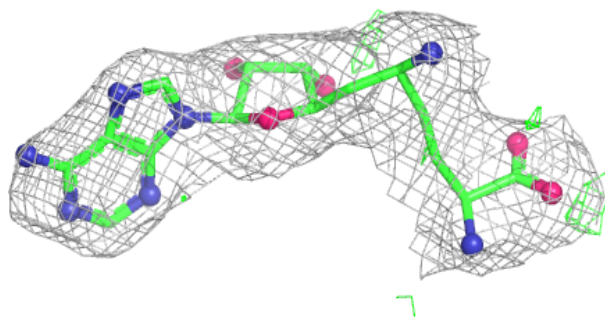
**Electron density around SFG B 501:**

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

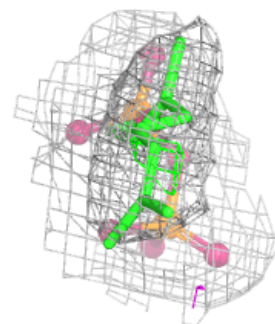
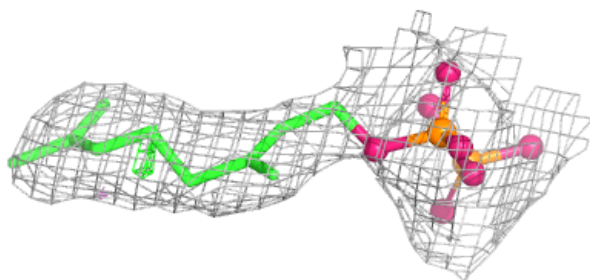
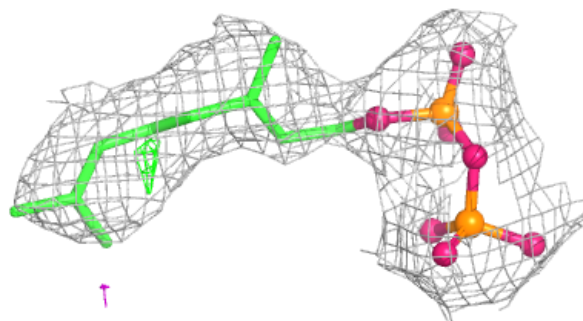


**Electron density around SFG A 501:**

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

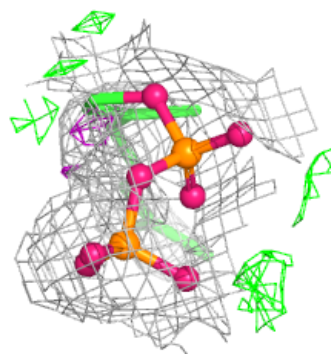
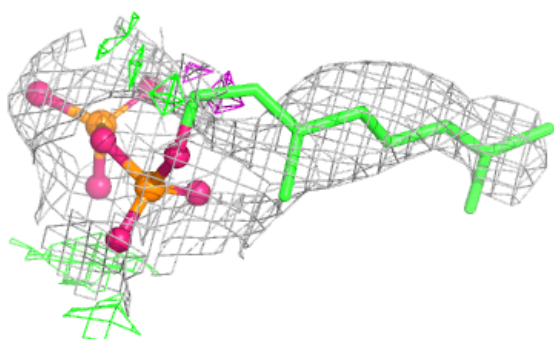
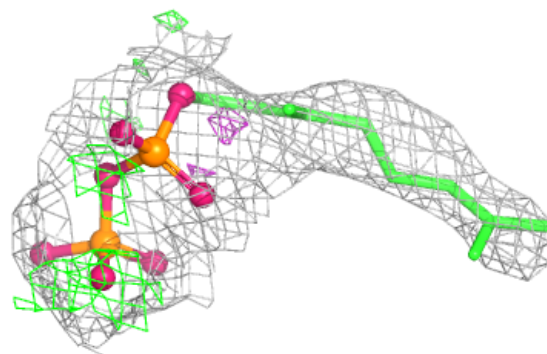
**Electron density around GPP F 502:**

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

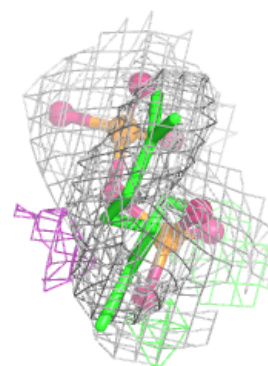
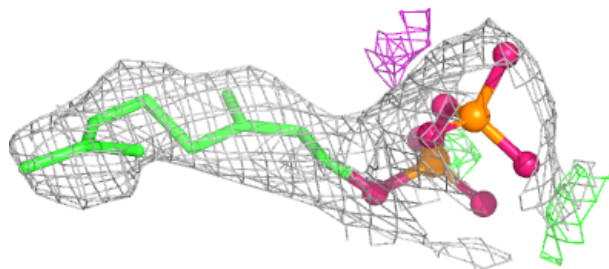
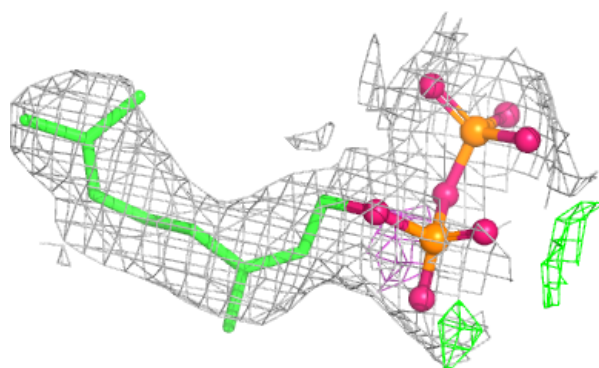


**Electron density around GPP B 502:**

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

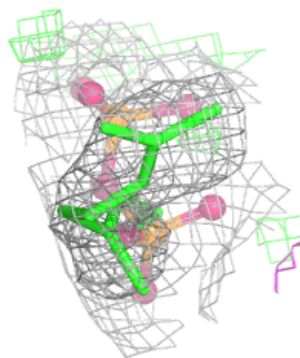
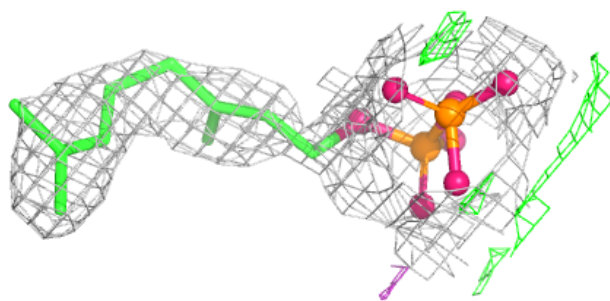
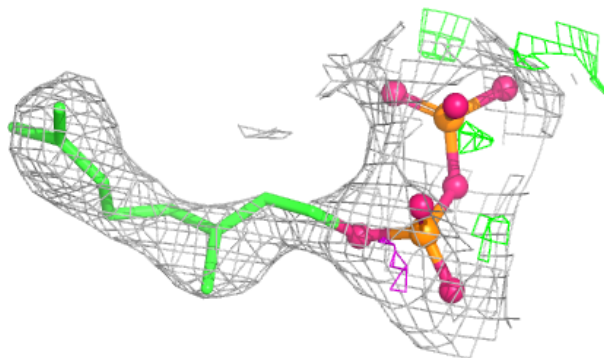
**Electron density around GPP H 502:**

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

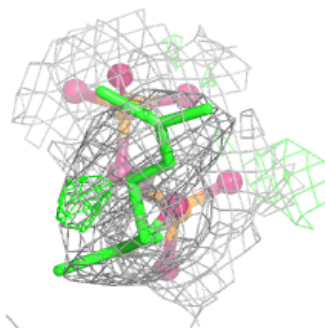
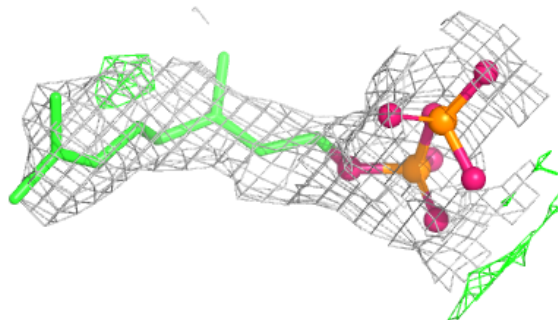
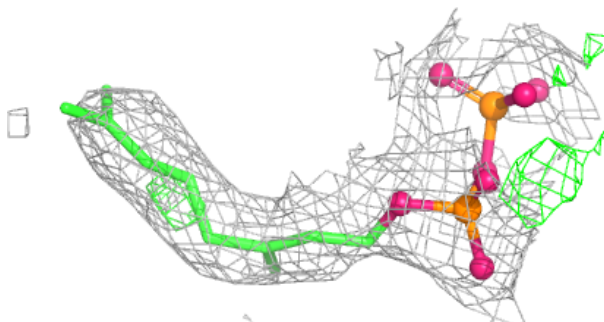


**Electron density around GPP K 502:**

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

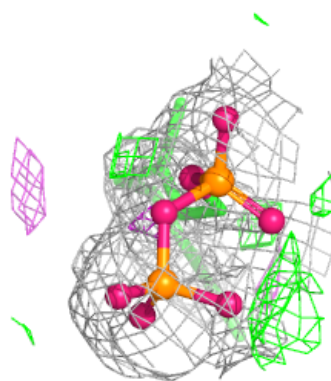
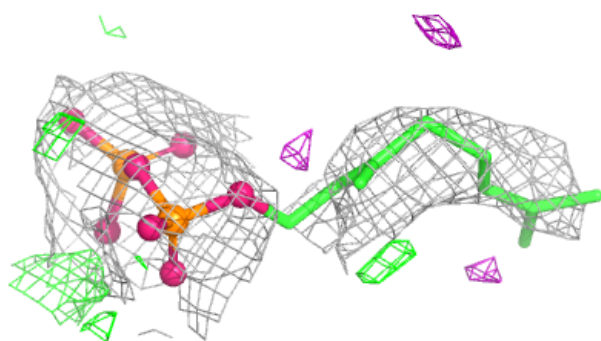
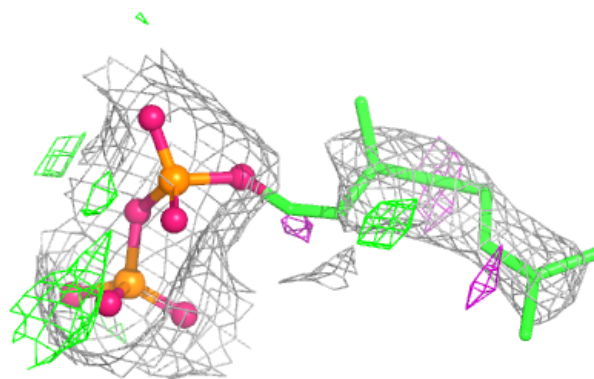
**Electron density around GPP C 502:**

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

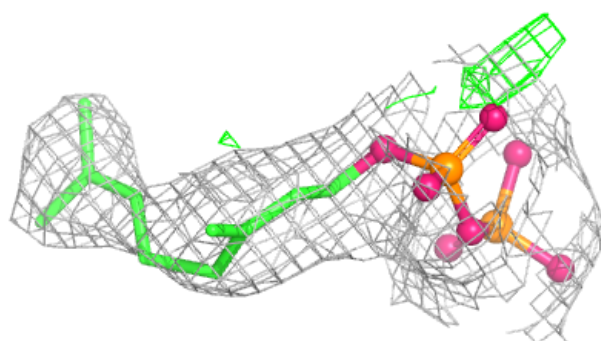
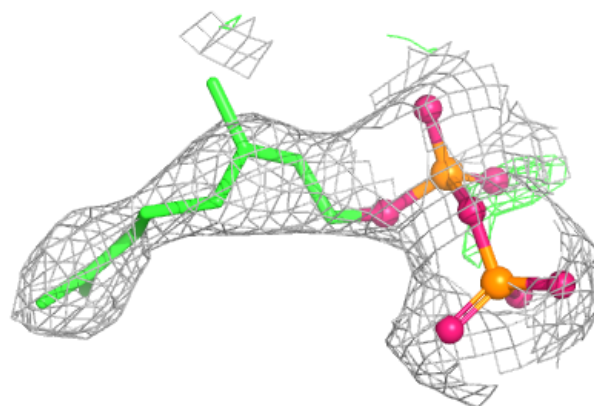


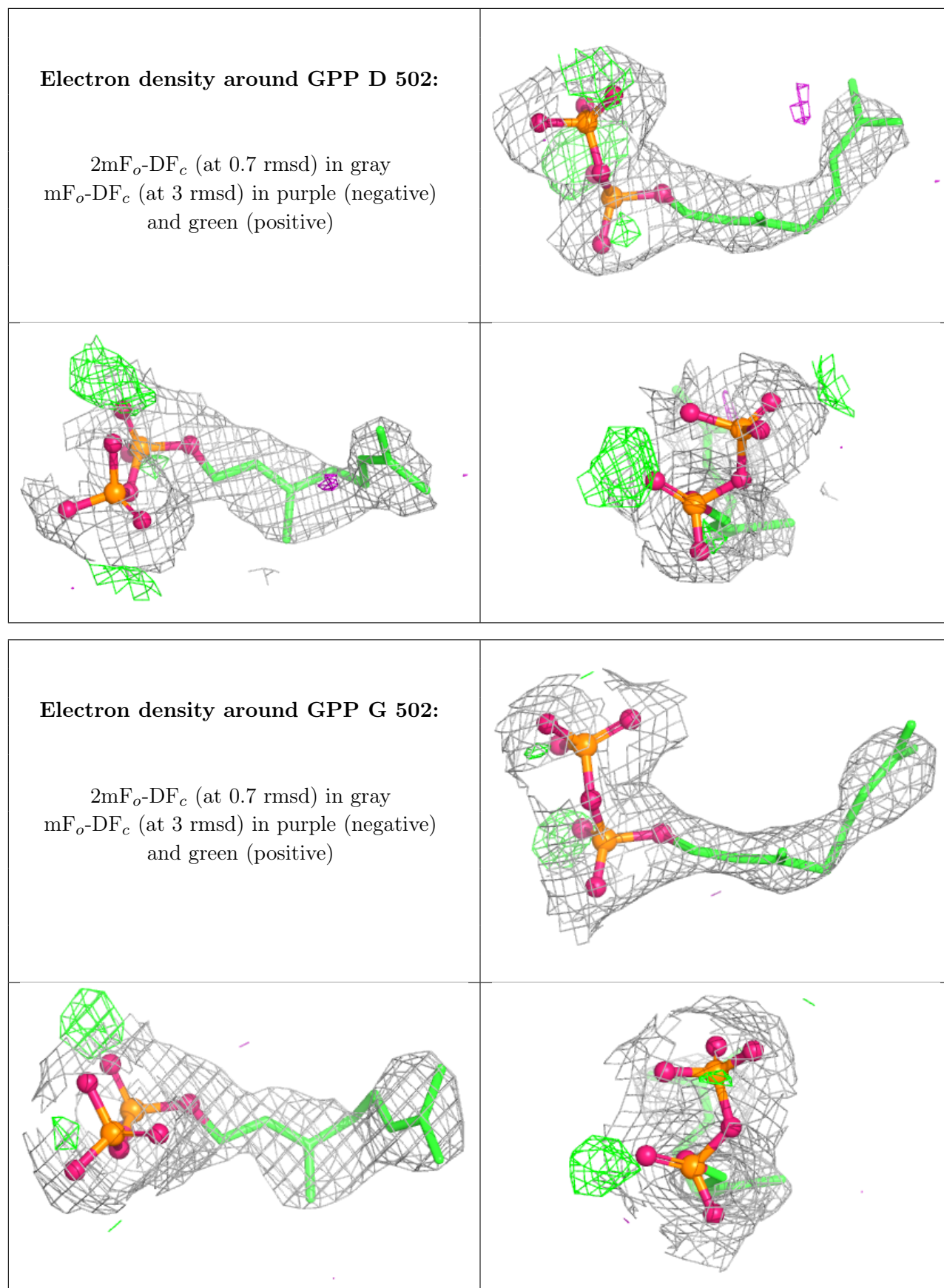
**Electron density around GPP I 502:**

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

**Electron density around GPP E 502:**

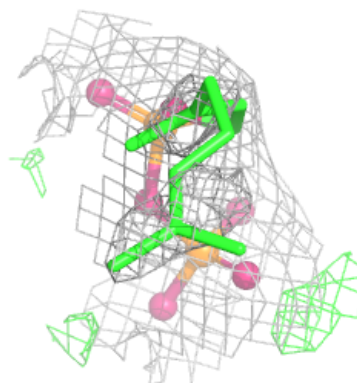
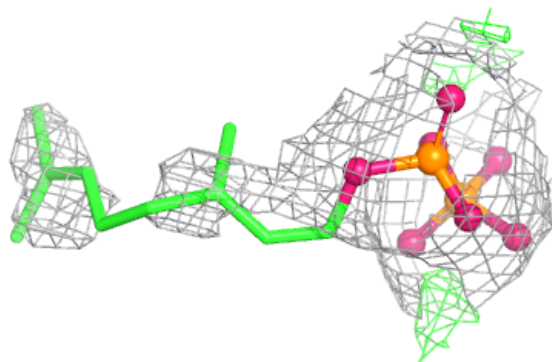
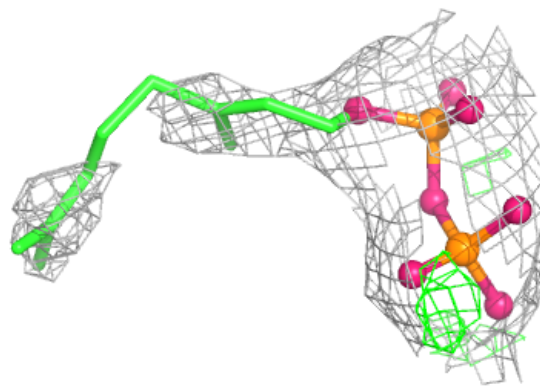
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



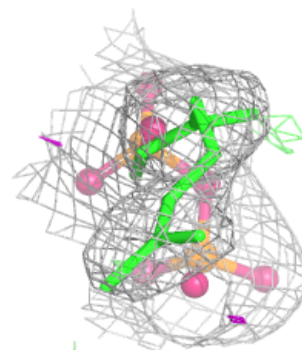
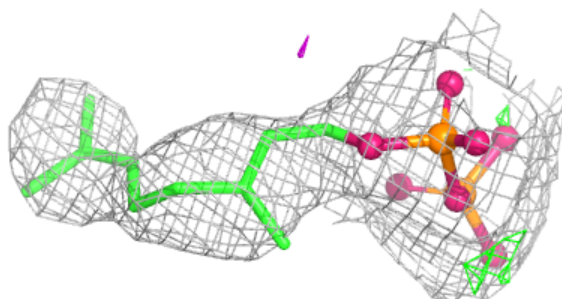
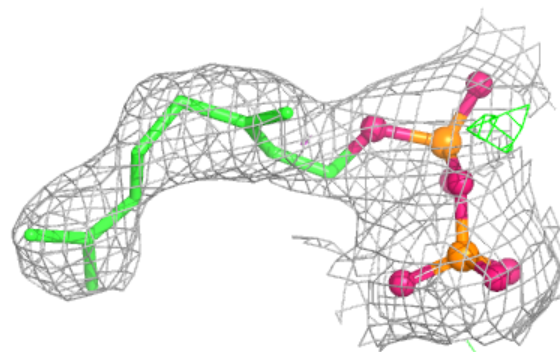


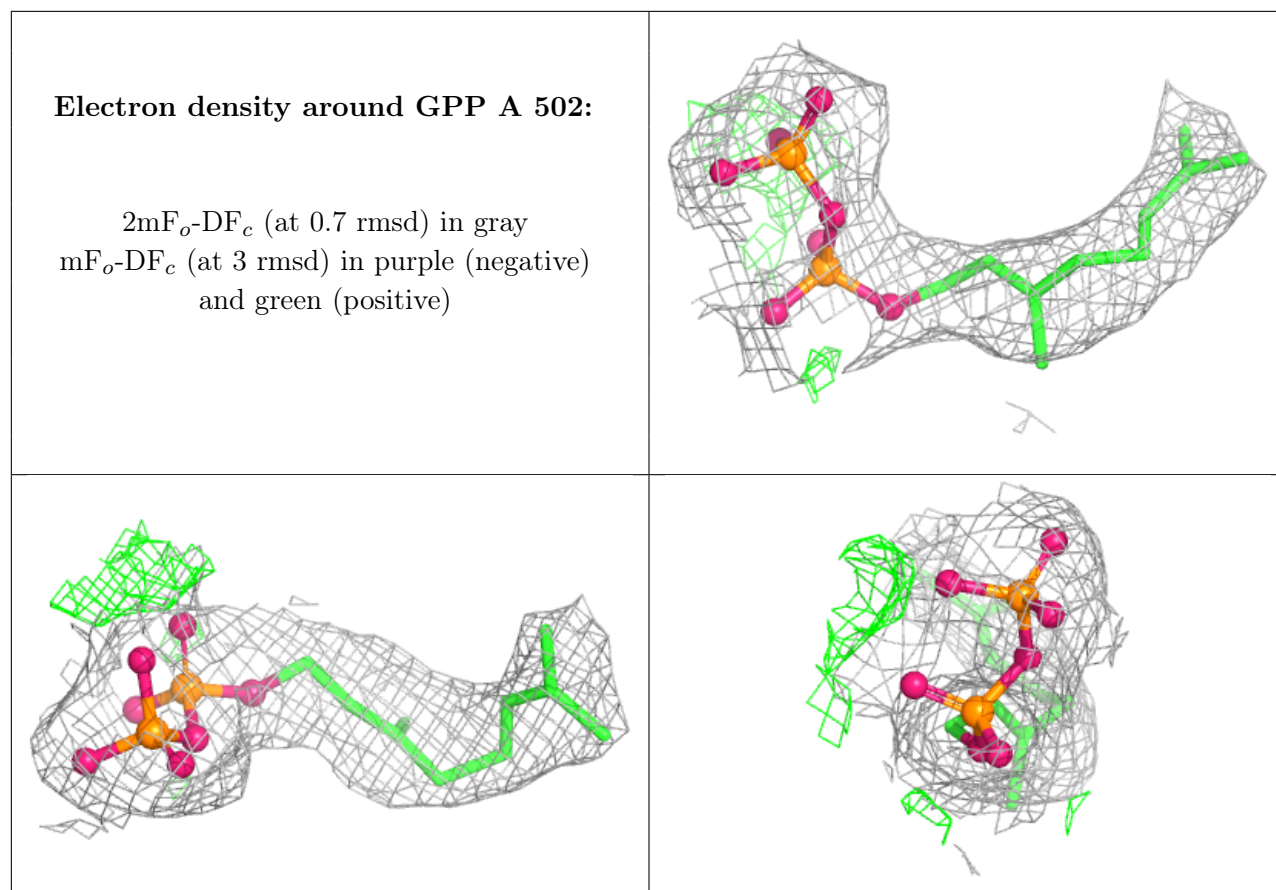
**Electron density around GPP L 502:**

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

**Electron density around GPP J 502:**

$2mF_o-DF_c$  (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.