wwPDB X-ray Structure Validation Summary Report (i)

Dec 2, 2024 – 01:59 PM JST

PDB ID	:	8ZMQ
Title	:	Crystal Structure of the second bromodomain of human BRD4 BD2 in complex with the inhibitor Y13190
Authors	:	Li, J.; Hu, Q.; Xu, H.; Zhao, X.; Zhang, C.; Zhu, R.; Wu, X.; Zhang, Y.; Xu, Y.
Deposited on	:	2024-05-23
Resolution	:	2.20 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

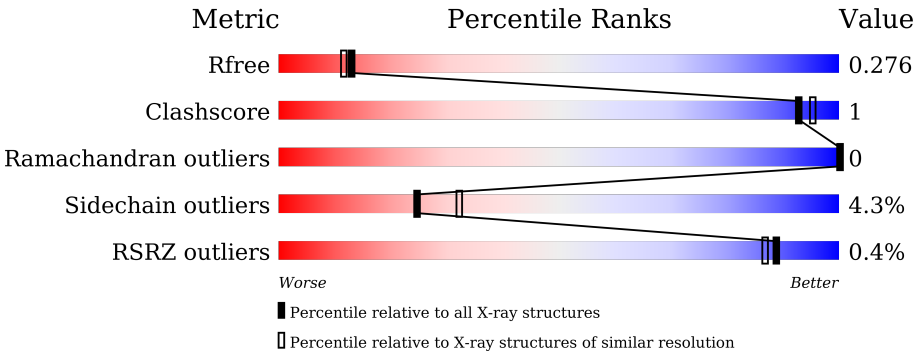
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (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 of 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 <=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	147	70% 5% 25%
1	B	147	69% 5% • 25%
1	C	147	70% 5% • 24%
1	D	147	71% • 24%
1	E	147	69% 5% • 25%

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Mol	Chain	Length	Quality of chain
1	F	147	71% 5% 24%
1	G	147	71% 5% 24%
1	H	147	70% 5% 24%
1	I	147	% 72% 26%
1	J	147	% 70% 25%
1	K	147	% 70% 5% 25%
1	L	147	69% 5% 25%
1	M	147	72% 25%
1	N	147	71% 25%
1	O	147	% 66% 7% 25%
1	P	147	69% 5% 25%
1	Q	147	% 63% 10% 26%
1	R	147	% 70% 26%
1	S	147	69% 5% 25%
1	T	147	% 70% 26%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19095 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 BRD4_HUMAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	1	0
			906	581	152	162	11			
1	B	110	Total	C	N	O	S	0	2	0
			910	585	153	161	11			
1	C	111	Total	C	N	O	S	0	0	0
			905	580	152	162	11			
1	D	111	Total	C	N	O	S	0	0	0
			905	580	152	162	11			
1	E	110	Total	C	N	O	S	0	1	0
			903	580	151	161	11			
1	F	111	Total	C	N	O	S	0	1	0
			911	584	152	164	11			
1	G	111	Total	C	N	O	S	0	0	0
			905	580	152	162	11			
1	H	111	Total	C	N	O	S	0	1	0
			911	584	152	164	11			
1	I	109	Total	C	N	O	S	0	0	0
			888	570	149	158	11			
1	J	110	Total	C	N	O	S	0	1	0
			902	578	150	163	11			
1	K	110	Total	C	N	O	S	0	1	0
			903	580	151	161	11			
1	L	110	Total	C	N	O	S	0	0	0
			897	576	151	159	11			
1	M	110	Total	C	N	O	S	0	0	0
			896	574	150	161	11			
1	N	110	Total	C	N	O	S	0	0	0
			894	572	150	161	11			
1	O	110	Total	C	N	O	S	0	0	0
			896	574	150	161	11			
1	P	110	Total	C	N	O	S	0	0	0
			896	574	150	161	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	109	Total	C	N	O	S	0	0	0
			888	570	149	158	11			
1	R	109	Total	C	N	O	S	0	0	0
			888	570	149	158	11			
1	S	110	Total	C	N	O	S	0	0	0
			897	576	151	159	11			
1	T	109	Total	C	N	O	S	0	0	0
			885	568	148	158	11			

There are 380 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	MET	-	initiating methionine	UNP O60885
A	315	LYS	-	expression tag	UNP O60885
A	316	LYS	-	expression tag	UNP O60885
A	317	GLY	-	expression tag	UNP O60885
A	318	HIS	-	expression tag	UNP O60885
A	319	HIS	-	expression tag	UNP O60885
A	320	HIS	-	expression tag	UNP O60885
A	321	HIS	-	expression tag	UNP O60885
A	322	HIS	-	expression tag	UNP O60885
A	323	HIS	-	expression tag	UNP O60885
A	324	GLU	-	expression tag	UNP O60885
A	325	ASN	-	expression tag	UNP O60885
A	326	LEU	-	expression tag	UNP O60885
A	327	TYR	-	expression tag	UNP O60885
A	328	PHE	-	expression tag	UNP O60885
A	329	GLN	-	expression tag	UNP O60885
A	330	GLY	-	expression tag	UNP O60885
A	331	GLY	-	expression tag	UNP O60885
A	332	SER	-	expression tag	UNP O60885
B	314	MET	-	initiating methionine	UNP O60885
B	315	LYS	-	expression tag	UNP O60885
B	316	LYS	-	expression tag	UNP O60885
B	317	GLY	-	expression tag	UNP O60885
B	318	HIS	-	expression tag	UNP O60885
B	319	HIS	-	expression tag	UNP O60885
B	320	HIS	-	expression tag	UNP O60885
B	321	HIS	-	expression tag	UNP O60885
B	322	HIS	-	expression tag	UNP O60885
B	323	HIS	-	expression tag	UNP O60885
B	324	GLU	-	expression tag	UNP O60885
B	325	ASN	-	expression tag	UNP O60885

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Chain	Residue	Modelled	Actual	Comment	Reference
B	326	LEU	-	expression tag	UNP O60885
B	327	TYR	-	expression tag	UNP O60885
B	328	PHE	-	expression tag	UNP O60885
B	329	GLN	-	expression tag	UNP O60885
B	330	GLY	-	expression tag	UNP O60885
B	331	GLY	-	expression tag	UNP O60885
B	332	SER	-	expression tag	UNP O60885
C	314	MET	-	initiating methionine	UNP O60885
C	315	LYS	-	expression tag	UNP O60885
C	316	LYS	-	expression tag	UNP O60885
C	317	GLY	-	expression tag	UNP O60885
C	318	HIS	-	expression tag	UNP O60885
C	319	HIS	-	expression tag	UNP O60885
C	320	HIS	-	expression tag	UNP O60885
C	321	HIS	-	expression tag	UNP O60885
C	322	HIS	-	expression tag	UNP O60885
C	323	HIS	-	expression tag	UNP O60885
C	324	GLU	-	expression tag	UNP O60885
C	325	ASN	-	expression tag	UNP O60885
C	326	LEU	-	expression tag	UNP O60885
C	327	TYR	-	expression tag	UNP O60885
C	328	PHE	-	expression tag	UNP O60885
C	329	GLN	-	expression tag	UNP O60885
C	330	GLY	-	expression tag	UNP O60885
C	331	GLY	-	expression tag	UNP O60885
C	332	SER	-	expression tag	UNP O60885
D	314	MET	-	initiating methionine	UNP O60885
D	315	LYS	-	expression tag	UNP O60885
D	316	LYS	-	expression tag	UNP O60885
D	317	GLY	-	expression tag	UNP O60885
D	318	HIS	-	expression tag	UNP O60885
D	319	HIS	-	expression tag	UNP O60885
D	320	HIS	-	expression tag	UNP O60885
D	321	HIS	-	expression tag	UNP O60885
D	322	HIS	-	expression tag	UNP O60885
D	323	HIS	-	expression tag	UNP O60885
D	324	GLU	-	expression tag	UNP O60885
D	325	ASN	-	expression tag	UNP O60885
D	326	LEU	-	expression tag	UNP O60885
D	327	TYR	-	expression tag	UNP O60885
D	328	PHE	-	expression tag	UNP O60885
D	329	GLN	-	expression tag	UNP O60885

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Chain	Residue	Modelled	Actual	Comment	Reference
D	330	GLY	-	expression tag	UNP O60885
D	331	GLY	-	expression tag	UNP O60885
D	332	SER	-	expression tag	UNP O60885
E	314	MET	-	initiating methionine	UNP O60885
E	315	LYS	-	expression tag	UNP O60885
E	316	LYS	-	expression tag	UNP O60885
E	317	GLY	-	expression tag	UNP O60885
E	318	HIS	-	expression tag	UNP O60885
E	319	HIS	-	expression tag	UNP O60885
E	320	HIS	-	expression tag	UNP O60885
E	321	HIS	-	expression tag	UNP O60885
E	322	HIS	-	expression tag	UNP O60885
E	323	HIS	-	expression tag	UNP O60885
E	324	GLU	-	expression tag	UNP O60885
E	325	ASN	-	expression tag	UNP O60885
E	326	LEU	-	expression tag	UNP O60885
E	327	TYR	-	expression tag	UNP O60885
E	328	PHE	-	expression tag	UNP O60885
E	329	GLN	-	expression tag	UNP O60885
E	330	GLY	-	expression tag	UNP O60885
E	331	GLY	-	expression tag	UNP O60885
E	332	SER	-	expression tag	UNP O60885
F	314	MET	-	initiating methionine	UNP O60885
F	315	LYS	-	expression tag	UNP O60885
F	316	LYS	-	expression tag	UNP O60885
F	317	GLY	-	expression tag	UNP O60885
F	318	HIS	-	expression tag	UNP O60885
F	319	HIS	-	expression tag	UNP O60885
F	320	HIS	-	expression tag	UNP O60885
F	321	HIS	-	expression tag	UNP O60885
F	322	HIS	-	expression tag	UNP O60885
F	323	HIS	-	expression tag	UNP O60885
F	324	GLU	-	expression tag	UNP O60885
F	325	ASN	-	expression tag	UNP O60885
F	326	LEU	-	expression tag	UNP O60885
F	327	TYR	-	expression tag	UNP O60885
F	328	PHE	-	expression tag	UNP O60885
F	329	GLN	-	expression tag	UNP O60885
F	330	GLY	-	expression tag	UNP O60885
F	331	GLY	-	expression tag	UNP O60885
F	332	SER	-	expression tag	UNP O60885
G	314	MET	-	initiating methionine	UNP O60885

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Chain	Residue	Modelled	Actual	Comment	Reference
G	315	LYS	-	expression tag	UNP O60885
G	316	LYS	-	expression tag	UNP O60885
G	317	GLY	-	expression tag	UNP O60885
G	318	HIS	-	expression tag	UNP O60885
G	319	HIS	-	expression tag	UNP O60885
G	320	HIS	-	expression tag	UNP O60885
G	321	HIS	-	expression tag	UNP O60885
G	322	HIS	-	expression tag	UNP O60885
G	323	HIS	-	expression tag	UNP O60885
G	324	GLU	-	expression tag	UNP O60885
G	325	ASN	-	expression tag	UNP O60885
G	326	LEU	-	expression tag	UNP O60885
G	327	TYR	-	expression tag	UNP O60885
G	328	PHE	-	expression tag	UNP O60885
G	329	GLN	-	expression tag	UNP O60885
G	330	GLY	-	expression tag	UNP O60885
G	331	GLY	-	expression tag	UNP O60885
G	332	SER	-	expression tag	UNP O60885
H	314	MET	-	initiating methionine	UNP O60885
H	315	LYS	-	expression tag	UNP O60885
H	316	LYS	-	expression tag	UNP O60885
H	317	GLY	-	expression tag	UNP O60885
H	318	HIS	-	expression tag	UNP O60885
H	319	HIS	-	expression tag	UNP O60885
H	320	HIS	-	expression tag	UNP O60885
H	321	HIS	-	expression tag	UNP O60885
H	322	HIS	-	expression tag	UNP O60885
H	323	HIS	-	expression tag	UNP O60885
H	324	GLU	-	expression tag	UNP O60885
H	325	ASN	-	expression tag	UNP O60885
H	326	LEU	-	expression tag	UNP O60885
H	327	TYR	-	expression tag	UNP O60885
H	328	PHE	-	expression tag	UNP O60885
H	329	GLN	-	expression tag	UNP O60885
H	330	GLY	-	expression tag	UNP O60885
H	331	GLY	-	expression tag	UNP O60885
H	332	SER	-	expression tag	UNP O60885
I	314	MET	-	initiating methionine	UNP O60885
I	315	LYS	-	expression tag	UNP O60885
I	316	LYS	-	expression tag	UNP O60885
I	317	GLY	-	expression tag	UNP O60885
I	318	HIS	-	expression tag	UNP O60885

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Chain	Residue	Modelled	Actual	Comment	Reference
I	319	HIS	-	expression tag	UNP O60885
I	320	HIS	-	expression tag	UNP O60885
I	321	HIS	-	expression tag	UNP O60885
I	322	HIS	-	expression tag	UNP O60885
I	323	HIS	-	expression tag	UNP O60885
I	324	GLU	-	expression tag	UNP O60885
I	325	ASN	-	expression tag	UNP O60885
I	326	LEU	-	expression tag	UNP O60885
I	327	TYR	-	expression tag	UNP O60885
I	328	PHE	-	expression tag	UNP O60885
I	329	GLN	-	expression tag	UNP O60885
I	330	GLY	-	expression tag	UNP O60885
I	331	GLY	-	expression tag	UNP O60885
I	332	SER	-	expression tag	UNP O60885
J	314	MET	-	initiating methionine	UNP O60885
J	315	LYS	-	expression tag	UNP O60885
J	316	LYS	-	expression tag	UNP O60885
J	317	GLY	-	expression tag	UNP O60885
J	318	HIS	-	expression tag	UNP O60885
J	319	HIS	-	expression tag	UNP O60885
J	320	HIS	-	expression tag	UNP O60885
J	321	HIS	-	expression tag	UNP O60885
J	322	HIS	-	expression tag	UNP O60885
J	323	HIS	-	expression tag	UNP O60885
J	324	GLU	-	expression tag	UNP O60885
J	325	ASN	-	expression tag	UNP O60885
J	326	LEU	-	expression tag	UNP O60885
J	327	TYR	-	expression tag	UNP O60885
J	328	PHE	-	expression tag	UNP O60885
J	329	GLN	-	expression tag	UNP O60885
J	330	GLY	-	expression tag	UNP O60885
J	331	GLY	-	expression tag	UNP O60885
J	332	SER	-	expression tag	UNP O60885
K	314	MET	-	initiating methionine	UNP O60885
K	315	LYS	-	expression tag	UNP O60885
K	316	LYS	-	expression tag	UNP O60885
K	317	GLY	-	expression tag	UNP O60885
K	318	HIS	-	expression tag	UNP O60885
K	319	HIS	-	expression tag	UNP O60885
K	320	HIS	-	expression tag	UNP O60885
K	321	HIS	-	expression tag	UNP O60885
K	322	HIS	-	expression tag	UNP O60885

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Chain	Residue	Modelled	Actual	Comment	Reference
K	323	HIS	-	expression tag	UNP O60885
K	324	GLU	-	expression tag	UNP O60885
K	325	ASN	-	expression tag	UNP O60885
K	326	LEU	-	expression tag	UNP O60885
K	327	TYR	-	expression tag	UNP O60885
K	328	PHE	-	expression tag	UNP O60885
K	329	GLN	-	expression tag	UNP O60885
K	330	GLY	-	expression tag	UNP O60885
K	331	GLY	-	expression tag	UNP O60885
K	332	SER	-	expression tag	UNP O60885
L	314	MET	-	initiating methionine	UNP O60885
L	315	LYS	-	expression tag	UNP O60885
L	316	LYS	-	expression tag	UNP O60885
L	317	GLY	-	expression tag	UNP O60885
L	318	HIS	-	expression tag	UNP O60885
L	319	HIS	-	expression tag	UNP O60885
L	320	HIS	-	expression tag	UNP O60885
L	321	HIS	-	expression tag	UNP O60885
L	322	HIS	-	expression tag	UNP O60885
L	323	HIS	-	expression tag	UNP O60885
L	324	GLU	-	expression tag	UNP O60885
L	325	ASN	-	expression tag	UNP O60885
L	326	LEU	-	expression tag	UNP O60885
L	327	TYR	-	expression tag	UNP O60885
L	328	PHE	-	expression tag	UNP O60885
L	329	GLN	-	expression tag	UNP O60885
L	330	GLY	-	expression tag	UNP O60885
L	331	GLY	-	expression tag	UNP O60885
L	332	SER	-	expression tag	UNP O60885
M	314	MET	-	initiating methionine	UNP O60885
M	315	LYS	-	expression tag	UNP O60885
M	316	LYS	-	expression tag	UNP O60885
M	317	GLY	-	expression tag	UNP O60885
M	318	HIS	-	expression tag	UNP O60885
M	319	HIS	-	expression tag	UNP O60885
M	320	HIS	-	expression tag	UNP O60885
M	321	HIS	-	expression tag	UNP O60885
M	322	HIS	-	expression tag	UNP O60885
M	323	HIS	-	expression tag	UNP O60885
M	324	GLU	-	expression tag	UNP O60885
M	325	ASN	-	expression tag	UNP O60885
M	326	LEU	-	expression tag	UNP O60885

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Chain	Residue	Modelled	Actual	Comment	Reference
M	327	TYR	-	expression tag	UNP O60885
M	328	PHE	-	expression tag	UNP O60885
M	329	GLN	-	expression tag	UNP O60885
M	330	GLY	-	expression tag	UNP O60885
M	331	GLY	-	expression tag	UNP O60885
M	332	SER	-	expression tag	UNP O60885
N	314	MET	-	initiating methionine	UNP O60885
N	315	LYS	-	expression tag	UNP O60885
N	316	LYS	-	expression tag	UNP O60885
N	317	GLY	-	expression tag	UNP O60885
N	318	HIS	-	expression tag	UNP O60885
N	319	HIS	-	expression tag	UNP O60885
N	320	HIS	-	expression tag	UNP O60885
N	321	HIS	-	expression tag	UNP O60885
N	322	HIS	-	expression tag	UNP O60885
N	323	HIS	-	expression tag	UNP O60885
N	324	GLU	-	expression tag	UNP O60885
N	325	ASN	-	expression tag	UNP O60885
N	326	LEU	-	expression tag	UNP O60885
N	327	TYR	-	expression tag	UNP O60885
N	328	PHE	-	expression tag	UNP O60885
N	329	GLN	-	expression tag	UNP O60885
N	330	GLY	-	expression tag	UNP O60885
N	331	GLY	-	expression tag	UNP O60885
N	332	SER	-	expression tag	UNP O60885
O	314	MET	-	initiating methionine	UNP O60885
O	315	LYS	-	expression tag	UNP O60885
O	316	LYS	-	expression tag	UNP O60885
O	317	GLY	-	expression tag	UNP O60885
O	318	HIS	-	expression tag	UNP O60885
O	319	HIS	-	expression tag	UNP O60885
O	320	HIS	-	expression tag	UNP O60885
O	321	HIS	-	expression tag	UNP O60885
O	322	HIS	-	expression tag	UNP O60885
O	323	HIS	-	expression tag	UNP O60885
O	324	GLU	-	expression tag	UNP O60885
O	325	ASN	-	expression tag	UNP O60885
O	326	LEU	-	expression tag	UNP O60885
O	327	TYR	-	expression tag	UNP O60885
O	328	PHE	-	expression tag	UNP O60885
O	329	GLN	-	expression tag	UNP O60885
O	330	GLY	-	expression tag	UNP O60885

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Chain	Residue	Modelled	Actual	Comment	Reference
O	331	GLY	-	expression tag	UNP O60885
O	332	SER	-	expression tag	UNP O60885
P	314	MET	-	initiating methionine	UNP O60885
P	315	LYS	-	expression tag	UNP O60885
P	316	LYS	-	expression tag	UNP O60885
P	317	GLY	-	expression tag	UNP O60885
P	318	HIS	-	expression tag	UNP O60885
P	319	HIS	-	expression tag	UNP O60885
P	320	HIS	-	expression tag	UNP O60885
P	321	HIS	-	expression tag	UNP O60885
P	322	HIS	-	expression tag	UNP O60885
P	323	HIS	-	expression tag	UNP O60885
P	324	GLU	-	expression tag	UNP O60885
P	325	ASN	-	expression tag	UNP O60885
P	326	LEU	-	expression tag	UNP O60885
P	327	TYR	-	expression tag	UNP O60885
P	328	PHE	-	expression tag	UNP O60885
P	329	GLN	-	expression tag	UNP O60885
P	330	GLY	-	expression tag	UNP O60885
P	331	GLY	-	expression tag	UNP O60885
P	332	SER	-	expression tag	UNP O60885
Q	314	MET	-	initiating methionine	UNP O60885
Q	315	LYS	-	expression tag	UNP O60885
Q	316	LYS	-	expression tag	UNP O60885
Q	317	GLY	-	expression tag	UNP O60885
Q	318	HIS	-	expression tag	UNP O60885
Q	319	HIS	-	expression tag	UNP O60885
Q	320	HIS	-	expression tag	UNP O60885
Q	321	HIS	-	expression tag	UNP O60885
Q	322	HIS	-	expression tag	UNP O60885
Q	323	HIS	-	expression tag	UNP O60885
Q	324	GLU	-	expression tag	UNP O60885
Q	325	ASN	-	expression tag	UNP O60885
Q	326	LEU	-	expression tag	UNP O60885
Q	327	TYR	-	expression tag	UNP O60885
Q	328	PHE	-	expression tag	UNP O60885
Q	329	GLN	-	expression tag	UNP O60885
Q	330	GLY	-	expression tag	UNP O60885
Q	331	GLY	-	expression tag	UNP O60885
Q	332	SER	-	expression tag	UNP O60885
R	314	MET	-	initiating methionine	UNP O60885
R	315	LYS	-	expression tag	UNP O60885

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Chain	Residue	Modelled	Actual	Comment	Reference
R	316	LYS	-	expression tag	UNP O60885
R	317	GLY	-	expression tag	UNP O60885
R	318	HIS	-	expression tag	UNP O60885
R	319	HIS	-	expression tag	UNP O60885
R	320	HIS	-	expression tag	UNP O60885
R	321	HIS	-	expression tag	UNP O60885
R	322	HIS	-	expression tag	UNP O60885
R	323	HIS	-	expression tag	UNP O60885
R	324	GLU	-	expression tag	UNP O60885
R	325	ASN	-	expression tag	UNP O60885
R	326	LEU	-	expression tag	UNP O60885
R	327	TYR	-	expression tag	UNP O60885
R	328	PHE	-	expression tag	UNP O60885
R	329	GLN	-	expression tag	UNP O60885
R	330	GLY	-	expression tag	UNP O60885
R	331	GLY	-	expression tag	UNP O60885
R	332	SER	-	expression tag	UNP O60885
S	314	MET	-	initiating methionine	UNP O60885
S	315	LYS	-	expression tag	UNP O60885
S	316	LYS	-	expression tag	UNP O60885
S	317	GLY	-	expression tag	UNP O60885
S	318	HIS	-	expression tag	UNP O60885
S	319	HIS	-	expression tag	UNP O60885
S	320	HIS	-	expression tag	UNP O60885
S	321	HIS	-	expression tag	UNP O60885
S	322	HIS	-	expression tag	UNP O60885
S	323	HIS	-	expression tag	UNP O60885
S	324	GLU	-	expression tag	UNP O60885
S	325	ASN	-	expression tag	UNP O60885
S	326	LEU	-	expression tag	UNP O60885
S	327	TYR	-	expression tag	UNP O60885
S	328	PHE	-	expression tag	UNP O60885
S	329	GLN	-	expression tag	UNP O60885
S	330	GLY	-	expression tag	UNP O60885
S	331	GLY	-	expression tag	UNP O60885
S	332	SER	-	expression tag	UNP O60885
T	314	MET	-	initiating methionine	UNP O60885
T	315	LYS	-	expression tag	UNP O60885
T	316	LYS	-	expression tag	UNP O60885
T	317	GLY	-	expression tag	UNP O60885
T	318	HIS	-	expression tag	UNP O60885
T	319	HIS	-	expression tag	UNP O60885

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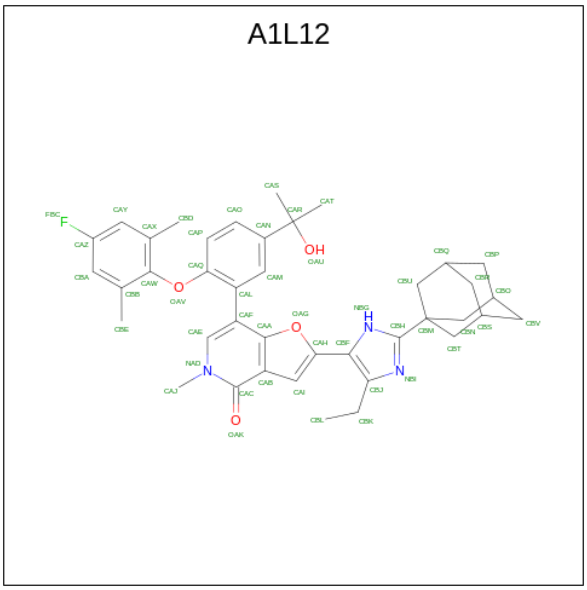
Chain	Residue	Modelled	Actual	Comment	Reference
T	320	HIS	-	expression tag	UNP O60885
T	321	HIS	-	expression tag	UNP O60885
T	322	HIS	-	expression tag	UNP O60885
T	323	HIS	-	expression tag	UNP O60885
T	324	GLU	-	expression tag	UNP O60885
T	325	ASN	-	expression tag	UNP O60885
T	326	LEU	-	expression tag	UNP O60885
T	327	TYR	-	expression tag	UNP O60885
T	328	PHE	-	expression tag	UNP O60885
T	329	GLN	-	expression tag	UNP O60885
T	330	GLY	-	expression tag	UNP O60885
T	331	GLY	-	expression tag	UNP O60885
T	332	SER	-	expression tag	UNP O60885

- Molecule 2 is 2-(2-(adamantan-1-yl)-4-ethyl-1H-imidazol-5-yl)-7-(2-(4-fluoro-2,6-dimethylphenoxy)-5-(2-hydroxypropan-2-yl)phenyl)-5-methylfuro[3,2-c]pyridin-4(5H)-one (three-letter code: A1L12) (formula: $C_{40}H_{44}FN_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	B	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	C	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	D	1	Total	C	F	N	O	0	0
			48	40	1	3	4		

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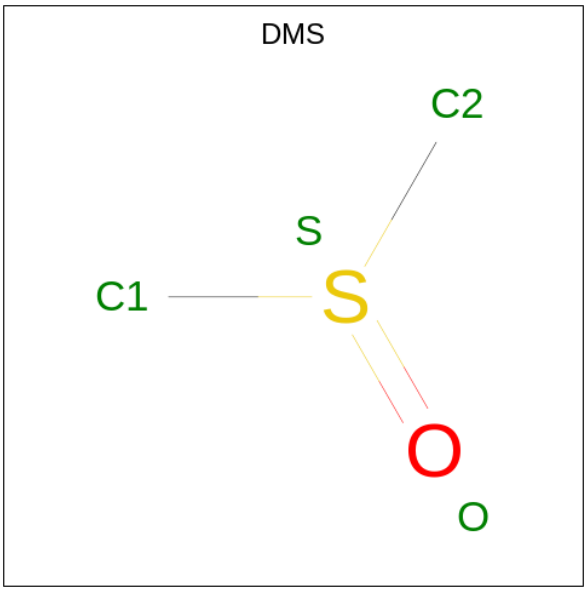
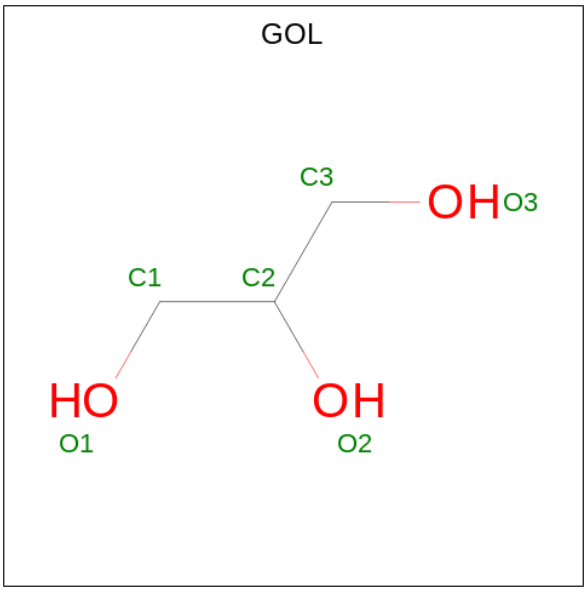
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	F	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	G	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	H	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	I	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	J	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	K	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	L	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	M	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	N	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	O	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	P	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	Q	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	R	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	S	1	Total	C	F	N	O	0	0
			48	40	1	3	4		
2	T	1	Total	C	F	N	O	0	0
			48	40	1	3	4		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	M	1	Total	C	O	S	0	0
			4	2	1	1		
3	N	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	15	Total O 15 15	0	0
5	B	13	Total O 13 13	0	0
5	C	9	Total O 9 9	0	0
5	D	7	Total O 7 7	0	0
5	E	15	Total O 15 15	0	0
5	F	9	Total O 9 9	0	0
5	G	8	Total O 8 8	0	0
5	H	5	Total O 5 5	0	0
5	I	8	Total O 8 8	0	0
5	J	12	Total O 12 12	0	0
5	K	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	11	Total O 11 11	0	0
5	M	2	Total O 2 2	0	0
5	N	3	Total O 3 3	0	0
5	S	2	Total O 2 2	0	0

3 Residue-property plots (i)

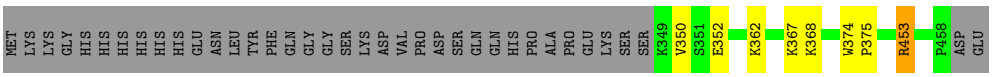
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BRD4_HUMAN

Chain A:

• Molecule 1: BRD4_HUMAN

Chain B:

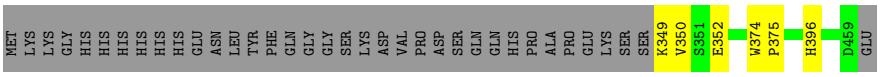


• Molecule 1: BRD4_HUMAN

Chain C:

• Molecule 1: BRD4_HUMAN

Chain D:



• Molecule 1: BRD4_HUMAN

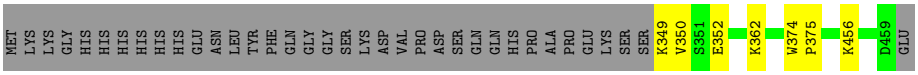
Chain E:

• Molecule 1: BRD4_HUMAN

Chain F:

• Molecule 1: BRD4_HUMAN

Chain G:

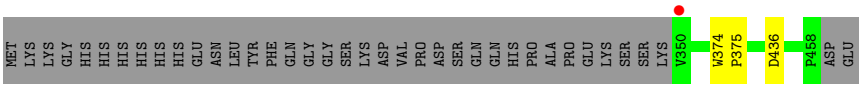


• Molecule 1: BRD4_HUMAN

Chain H:

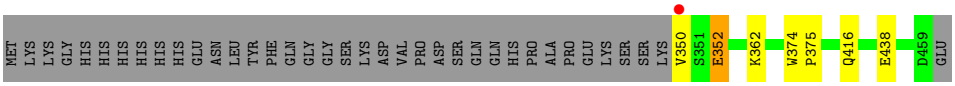
• Molecule 1: BRD4_HUMAN

Chain I:



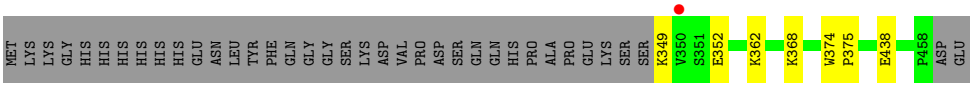
• Molecule 1: BRD4_HUMAN

Chain J:



• Molecule 1: BRD4_HUMAN

Chain K:

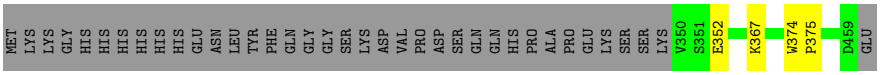


• Molecule 1: BRD4_HUMAN

Chain L:

• Molecule 1: BRD4_HUMAN

Chain M:

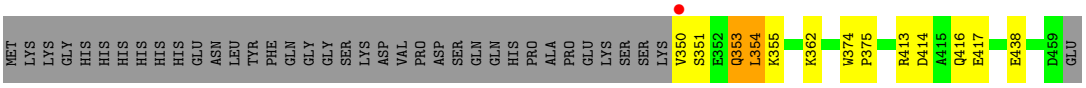


• Molecule 1: BRD4_HUMAN

Chain N:

• Molecule 1: BRD4_HUMAN

Chain O:

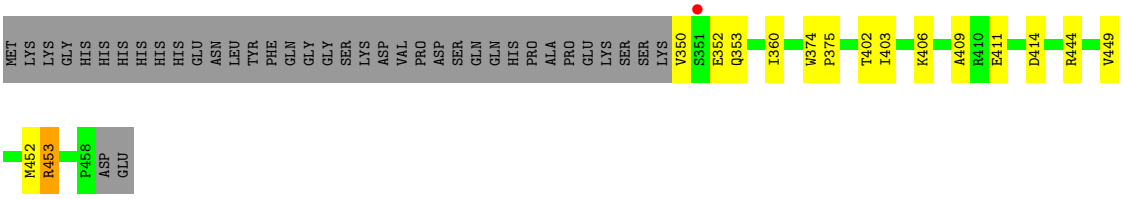


• Molecule 1: BRD4_HUMAN

Chain P:

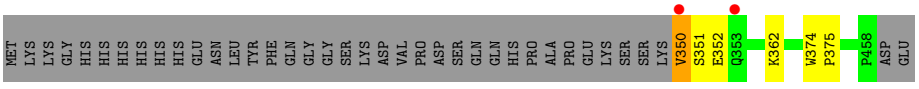
• Molecule 1: BRD4_HUMAN

Chain Q:



• Molecule 1: BRD4_HUMAN

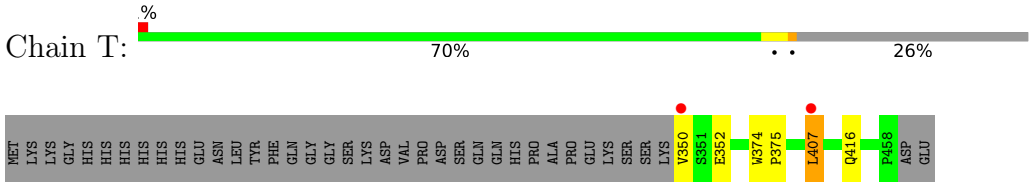
Chain R:



• Molecule 1: BRD4_HUMAN

Chain S:

• Molecule 1: BRD4_HUMAN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.91Å 125.11Å 300.35Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	300.35 – 2.20 300.35 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (300.35-2.20) 99.8 (300.35-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.256 , 0.274 0.259 , 0.276	Depositor DCC
R_{free} test set	10956 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19095	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: A1L12, DMS, GOL

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	0.65	0/929	0.72	0/1247
1	B	0.64	0/940	0.72	0/1263
1	C	0.68	0/928	0.78	1/1246 (0.1%)
1	D	0.64	0/928	0.71	0/1246
1	E	0.65	0/929	0.75	1/1247 (0.1%)
1	F	0.64	0/937	0.72	0/1258
1	G	0.65	0/928	0.72	0/1246
1	H	0.64	0/937	0.71	0/1258
1	I	0.65	0/911	0.69	0/1224
1	J	0.65	0/928	0.70	0/1247
1	K	0.65	0/929	0.71	0/1247
1	L	0.65	0/920	0.75	0/1235
1	M	0.64	0/919	0.71	0/1235
1	N	0.64	0/917	0.70	0/1232
1	O	0.66	0/919	0.73	1/1235 (0.1%)
1	P	0.65	0/919	0.74	0/1235
1	Q	0.71	0/911	0.77	1/1224 (0.1%)
1	R	0.66	0/911	0.72	0/1224
1	S	0.66	0/920	0.76	1/1235 (0.1%)
1	T	0.65	0/908	0.73	0/1221
All	All	0.65	0/18468	0.73	5/24805 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	353	GLN	CA-CB-CG	6.56	127.84	113.40
1	Q	453	ARG	CB-CG-CD	5.94	127.05	111.60
1	S	453	ARG	CG-CD-NE	5.83	124.04	111.80
1	C	349	LYS	CB-CA-C	5.63	121.66	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	368	LYS	CA-CB-CG	5.54	125.59	113.40

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	906	0	892	1	0
1	B	910	0	900	3	0
1	C	905	0	891	4	0
1	D	905	0	891	2	0
1	E	903	0	893	1	0
1	F	911	0	897	3	0
1	G	905	0	891	2	0
1	H	911	0	897	3	0
1	I	888	0	874	3	0
1	J	902	0	884	2	0
1	K	903	0	893	1	0
1	L	897	0	887	2	0
1	M	896	0	878	2	0
1	N	894	0	871	2	0
1	O	896	0	878	4	0
1	P	896	0	878	2	0
1	Q	888	0	874	11	0
1	R	888	0	874	2	0
1	S	897	0	887	2	0
1	T	885	0	865	2	0
2	A	48	0	0	0	0
2	B	48	0	0	0	0
2	C	48	0	0	0	0
2	D	48	0	0	0	0
2	E	48	0	0	0	0
2	F	48	0	0	0	0
2	G	48	0	0	0	0
2	H	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	48	0	0	0	0
2	J	48	0	0	0	0
2	K	48	0	0	0	0
2	L	48	0	0	0	0
2	M	48	0	0	0	0
2	N	48	0	0	0	0
2	O	48	0	0	0	0
2	P	48	0	0	0	0
2	Q	48	0	0	0	0
2	R	48	0	0	0	0
2	S	48	0	0	0	0
2	T	48	0	0	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	M	4	0	6	0	0
3	N	4	0	6	0	0
4	L	6	0	8	0	0
5	A	15	0	0	0	0
5	B	13	0	0	0	0
5	C	9	0	0	0	0
5	D	7	0	0	1	0
5	E	15	0	0	0	0
5	F	9	0	0	0	0
5	G	8	0	0	1	0
5	H	5	0	0	1	0
5	I	8	0	0	0	0
5	J	12	0	0	0	0
5	K	4	0	0	0	0
5	L	11	0	0	0	0
5	M	2	0	0	0	0
5	N	3	0	0	0	0
5	S	2	0	0	0	0
All	All	19095	0	17733	50	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 1.

The worst 5 of 50 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:Q:402:THR:HG22	1:Q:406:LYS:HE3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:409:ALA:HB3	1:Q:411:GLU:OE1	1.85	0.77
1:Q:406:LYS:HA	1:Q:411:GLU:OE1	1.91	0.69
1:J:350:VAL:HG12	1:J:352:GLU:H	1.62	0.63
1:C:353:GLN:NE2	1:C:459:ASP:OD2	2.34	0.60

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	109/147 (74%)	109 (100%)	0	0	100	100
1	B	110/147 (75%)	110 (100%)	0	0	100	100
1	C	109/147 (74%)	109 (100%)	0	0	100	100
1	D	109/147 (74%)	109 (100%)	0	0	100	100
1	E	109/147 (74%)	109 (100%)	0	0	100	100
1	F	110/147 (75%)	110 (100%)	0	0	100	100
1	G	109/147 (74%)	109 (100%)	0	0	100	100
1	H	110/147 (75%)	110 (100%)	0	0	100	100
1	I	107/147 (73%)	107 (100%)	0	0	100	100
1	J	109/147 (74%)	109 (100%)	0	0	100	100
1	K	109/147 (74%)	109 (100%)	0	0	100	100
1	L	108/147 (74%)	108 (100%)	0	0	100	100
1	M	108/147 (74%)	108 (100%)	0	0	100	100
1	N	108/147 (74%)	108 (100%)	0	0	100	100
1	O	108/147 (74%)	107 (99%)	1 (1%)	0	100	100
1	P	108/147 (74%)	108 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	107/147 (73%)	107 (100%)	0	0	100	100
1	R	107/147 (73%)	106 (99%)	1 (1%)	0	100	100
1	S	108/147 (74%)	108 (100%)	0	0	100	100
1	T	107/147 (73%)	107 (100%)	0	0	100	100
All	All	2169/2940 (74%)	2167 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	97/129 (75%)	92 (95%)	5 (5%)	19	24
1	B	98/129 (76%)	92 (94%)	6 (6%)	15	18
1	C	97/129 (75%)	94 (97%)	3 (3%)	35	47
1	D	97/129 (75%)	94 (97%)	3 (3%)	35	47
1	E	97/129 (75%)	91 (94%)	6 (6%)	15	18
1	F	98/129 (76%)	95 (97%)	3 (3%)	35	47
1	G	97/129 (75%)	93 (96%)	4 (4%)	26	34
1	H	98/129 (76%)	94 (96%)	4 (4%)	26	34
1	I	95/129 (74%)	95 (100%)	0	100	100
1	J	97/129 (75%)	92 (95%)	5 (5%)	19	24
1	K	97/129 (75%)	91 (94%)	6 (6%)	15	18
1	L	96/129 (74%)	90 (94%)	6 (6%)	15	17
1	M	96/129 (74%)	94 (98%)	2 (2%)	48	63
1	N	95/129 (74%)	93 (98%)	2 (2%)	48	63
1	O	96/129 (74%)	87 (91%)	9 (9%)	7	7
1	P	96/129 (74%)	89 (93%)	7 (7%)	11	13
1	Q	95/129 (74%)	93 (98%)	2 (2%)	48	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	95/129 (74%)	92 (97%)	3 (3%)	34 45
1	S	96/129 (74%)	91 (95%)	5 (5%)	19 24
1	T	94/129 (73%)	90 (96%)	4 (4%)	25 32
All	All	1927/2580 (75%)	1842 (96%)	85 (4%)	25 31

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	355	LYS
1	Q	352	GLU
1	O	413	ARG
1	P	351	SER
1	R	362	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	353	GLN
1	S	353	GLN
1	S	447	GLN
1	H	353	GLN
1	I	353	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A1L12	O	501	-	44,55,55	3.44	17 (38%)	61,87,87	4.45	9 (14%)
2	A1L12	K	501	-	44,55,55	3.25	14 (31%)	61,87,87	4.53	10 (16%)
4	GOL	L	502	-	5,5,5	0.12	0	5,5,5	0.29	0
2	A1L12	C	501	-	44,55,55	3.19	17 (38%)	61,87,87	4.44	11 (18%)
2	A1L12	I	501	-	44,55,55	3.44	15 (34%)	61,87,87	4.52	8 (13%)
2	A1L12	T	501	-	44,55,55	3.46	15 (34%)	61,87,87	4.53	9 (14%)
2	A1L12	Q	501	-	44,55,55	3.54	16 (36%)	61,87,87	4.47	10 (16%)
2	A1L12	F	501	-	44,55,55	3.38	18 (40%)	61,87,87	4.33	9 (14%)
2	A1L12	B	502	-	44,55,55	3.41	18 (40%)	61,87,87	4.40	12 (19%)
3	DMS	B	503	-	3,3,3	0.26	0	3,3,3	0.09	0
2	A1L12	A	501	-	44,55,55	3.24	16 (36%)	61,87,87	4.39	8 (13%)
3	DMS	A	502	-	3,3,3	0.26	0	3,3,3	0.05	0
3	DMS	M	502	-	3,3,3	0.23	0	3,3,3	0.08	0
3	DMS	N	502	-	3,3,3	0.23	0	3,3,3	0.07	0
3	DMS	B	501	-	3,3,3	0.25	0	3,3,3	0.06	0
2	A1L12	G	501	-	44,55,55	3.05	14 (31%)	61,87,87	4.54	11 (18%)
2	A1L12	H	501	-	44,55,55	3.42	15 (34%)	61,87,87	4.34	8 (13%)
2	A1L12	P	501	-	44,55,55	3.43	15 (34%)	61,87,87	4.21	9 (14%)
2	A1L12	M	501	-	44,55,55	3.39	17 (38%)	61,87,87	4.41	9 (14%)
2	A1L12	S	501	-	44,55,55	3.62	15 (34%)	61,87,87	4.50	9 (14%)
2	A1L12	D	501	-	44,55,55	3.32	14 (31%)	61,87,87	4.58	8 (13%)
2	A1L12	N	501	-	44,55,55	3.33	18 (40%)	61,87,87	4.46	10 (16%)
2	A1L12	R	501	-	44,55,55	3.41	14 (31%)	61,87,87	4.52	9 (14%)
2	A1L12	L	501	-	44,55,55	3.40	16 (36%)	61,87,87	4.36	9 (14%)
2	A1L12	E	501	-	44,55,55	3.17	17 (38%)	61,87,87	4.39	12 (19%)
2	A1L12	J	501	-	44,55,55	3.22	16 (36%)	61,87,87	4.40	10 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1L12	O	501	-	-	4/21/53/53	0/9/8/8
2	A1L12	K	501	-	-	5/21/53/53	0/9/8/8
4	GOL	L	502	-	-	2/4/4/4	-
2	A1L12	C	501	-	-	4/21/53/53	0/9/8/8
2	A1L12	I	501	-	-	4/21/53/53	0/9/8/8
2	A1L12	T	501	-	-	3/21/53/53	0/9/8/8
2	A1L12	Q	501	-	-	4/21/53/53	0/9/8/8
2	A1L12	F	501	-	-	6/21/53/53	0/9/8/8
2	A1L12	B	502	-	-	6/21/53/53	0/9/8/8
2	A1L12	A	501	-	-	5/21/53/53	0/9/8/8
2	A1L12	G	501	-	-	4/21/53/53	0/9/8/8
2	A1L12	H	501	-	-	2/21/53/53	0/9/8/8
2	A1L12	P	501	-	-	2/21/53/53	0/9/8/8
2	A1L12	M	501	-	-	4/21/53/53	0/9/8/8
2	A1L12	S	501	-	-	4/21/53/53	0/9/8/8
2	A1L12	D	501	-	-	1/21/53/53	0/9/8/8
2	A1L12	N	501	-	-	4/21/53/53	0/9/8/8
2	A1L12	R	501	-	-	6/21/53/53	0/9/8/8
2	A1L12	L	501	-	-	5/21/53/53	0/9/8/8
2	A1L12	E	501	-	-	4/21/53/53	0/9/8/8
2	A1L12	J	501	-	-	5/21/53/53	0/9/8/8

The worst 5 of 317 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	501	A1L12	CAR-CAN	-16.81	1.41	1.53
2	Q	501	A1L12	CAR-CAN	-15.77	1.42	1.53
2	T	501	A1L12	CAR-CAN	-15.58	1.42	1.53
2	R	501	A1L12	CAR-CAN	-15.02	1.43	1.53
2	O	501	A1L12	CAR-CAN	-14.82	1.43	1.53

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	A1L12	CBM-CBU-CBQ	-30.57	84.42	110.98
2	I	501	A1L12	CBM-CBU-CBQ	-30.23	84.72	110.98
2	T	501	A1L12	CBM-CBU-CBQ	-30.16	84.78	110.98
2	G	501	A1L12	CBM-CBU-CBQ	-30.06	84.87	110.98
2	K	501	A1L12	CBM-CBU-CBQ	-30.05	84.88	110.98

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

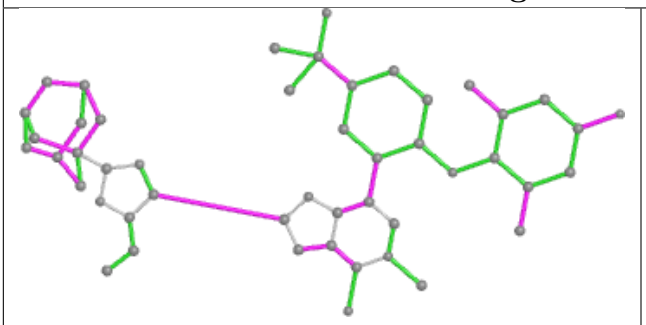
Mol	Chain	Res	Type	Atoms
2	A	501	A1L12	CBF-CBJ-CBK-CBL
2	B	502	A1L12	CBF-CBJ-CBK-CBL
2	C	501	A1L12	CBF-CBJ-CBK-CBL
2	D	501	A1L12	CBF-CBJ-CBK-CBL
2	E	501	A1L12	CBF-CBJ-CBK-CBL

There are no ring outliers.

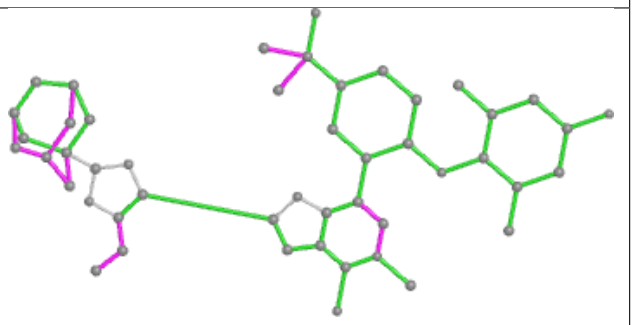
No monomer is involved in short contacts.

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 then 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.

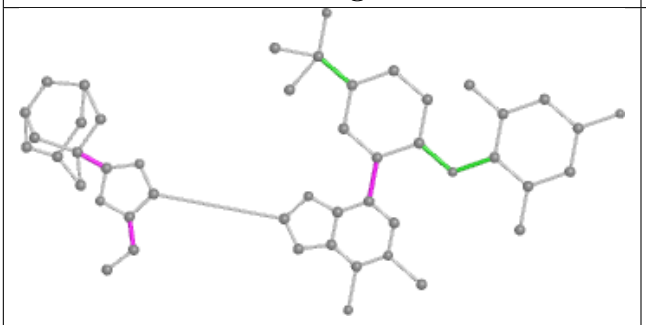
Ligand A1L12 O 501



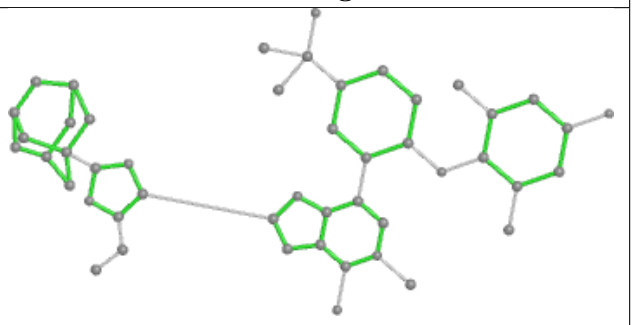
Bond lengths



Bond angles

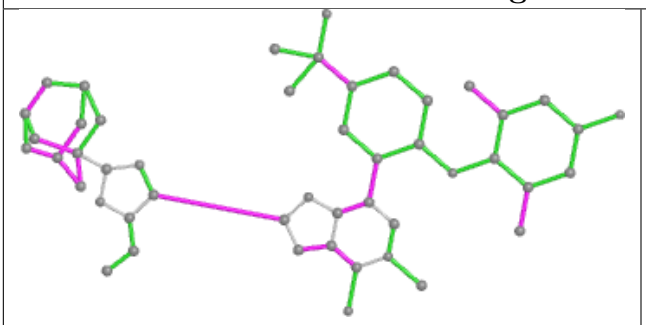


Torsions



Rings

Ligand A1L12 K 501



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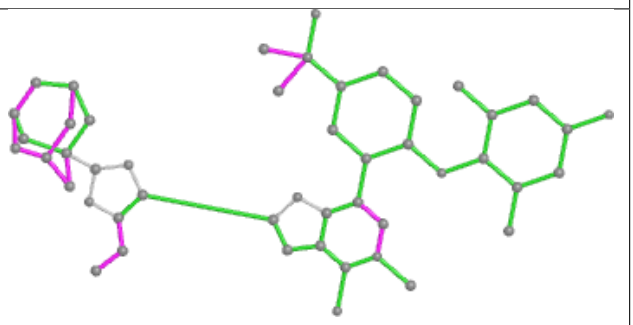

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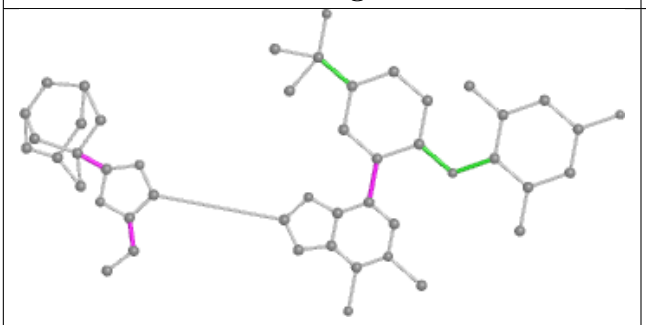

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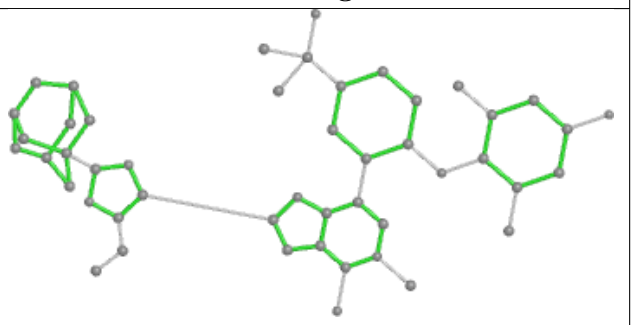
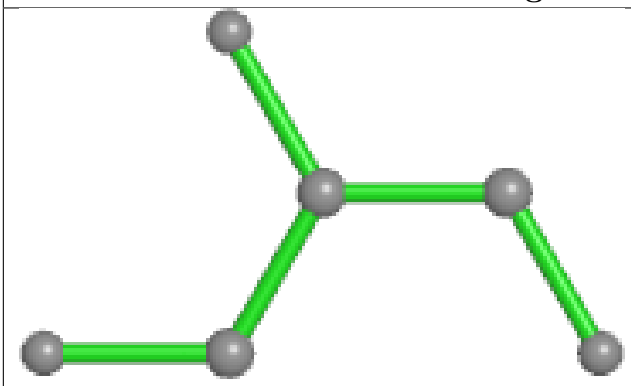


Rings

Ligand GOL L 502



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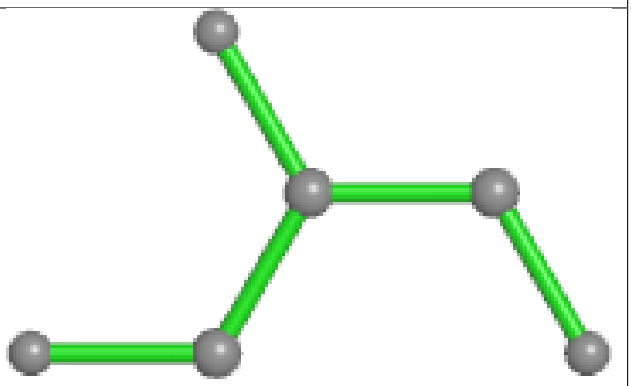

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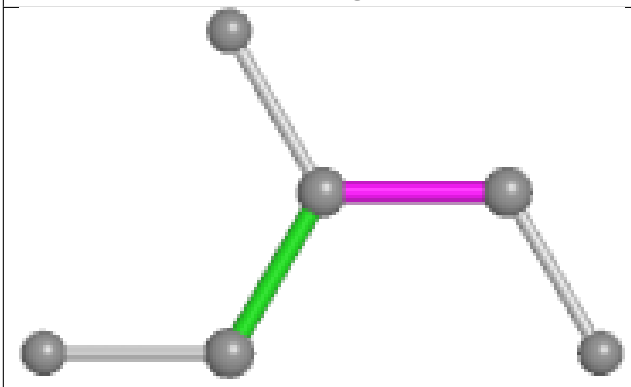

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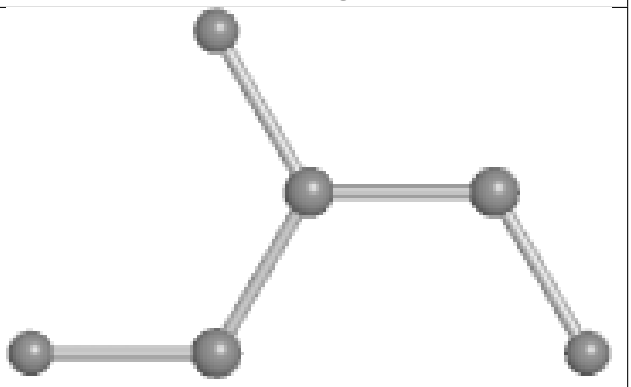
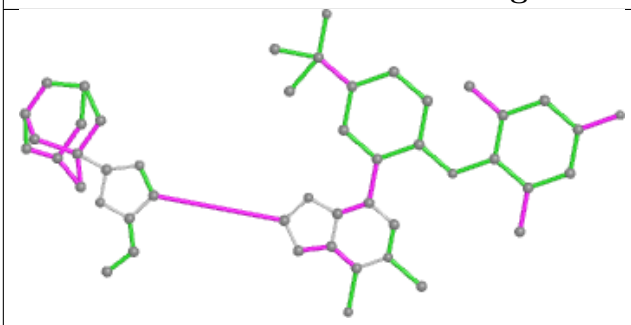


Rings

Ligand A1L12 C 501



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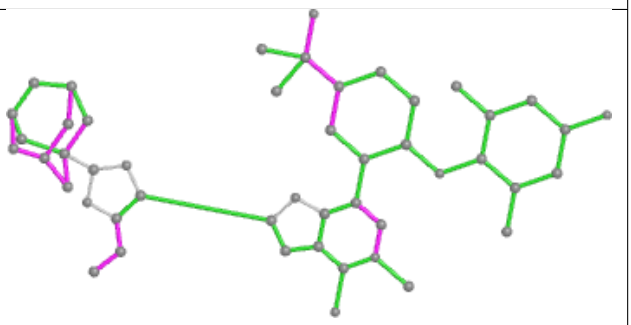

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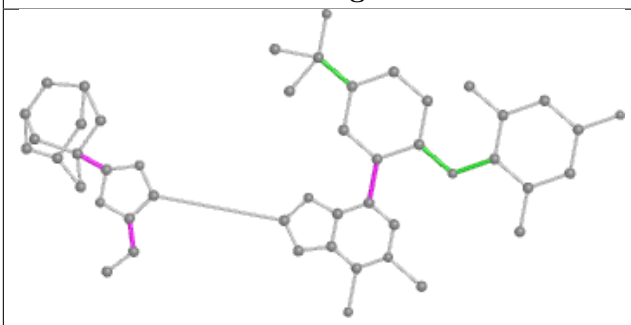

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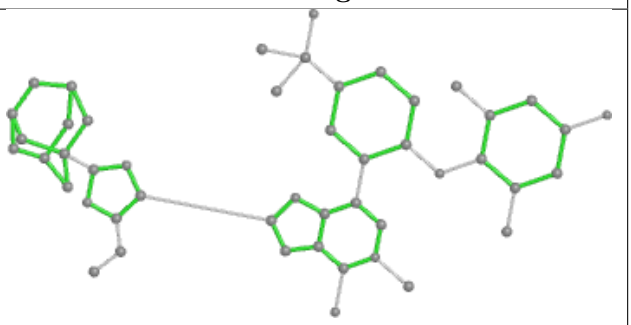
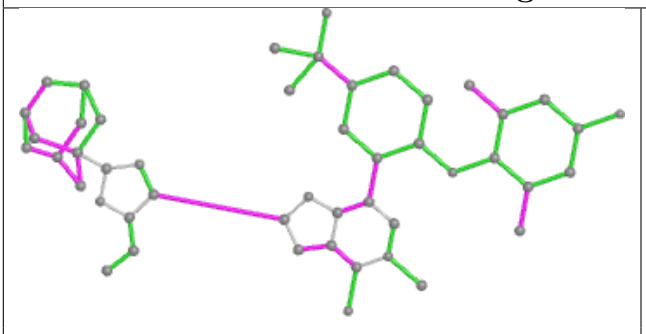


Rings

Ligand A1L12 I 501



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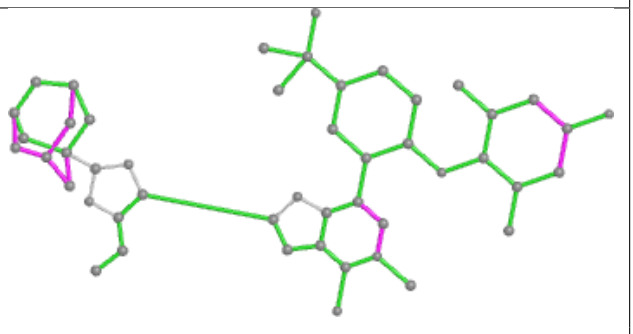
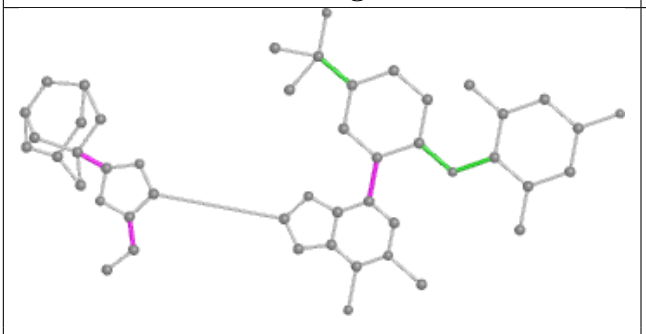


Bond angles



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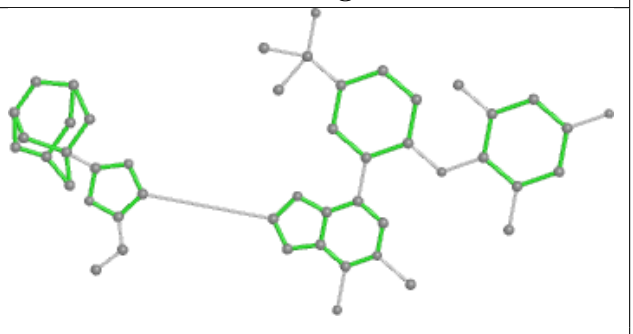
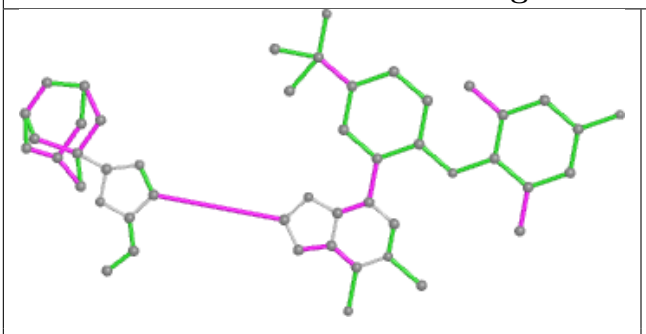
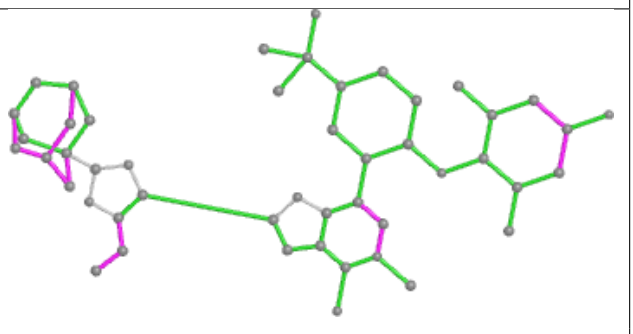


Rings

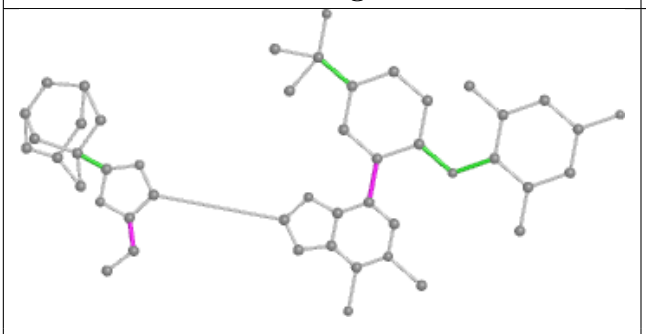
Ligand A1L12 T 501



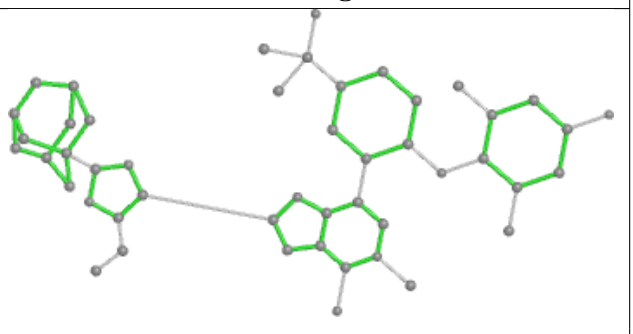
Bond lengths



Bond angles

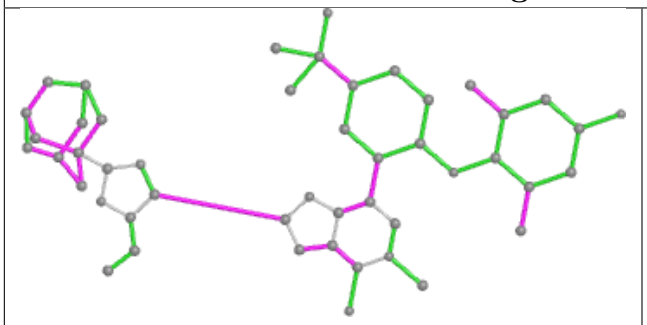


Torsions



Rings

Ligand A1L12 Q 501



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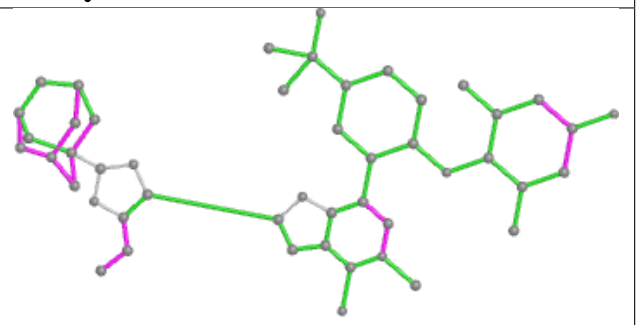

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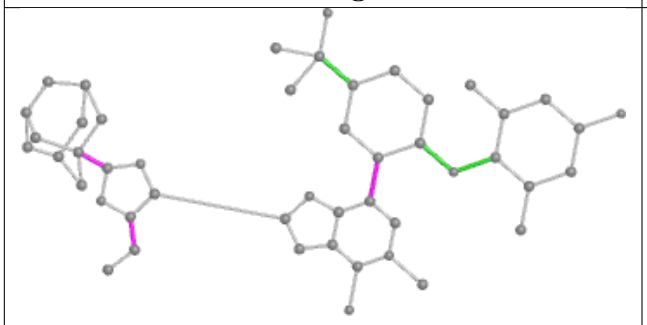

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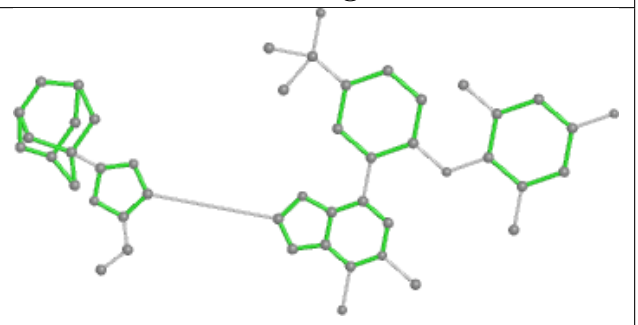
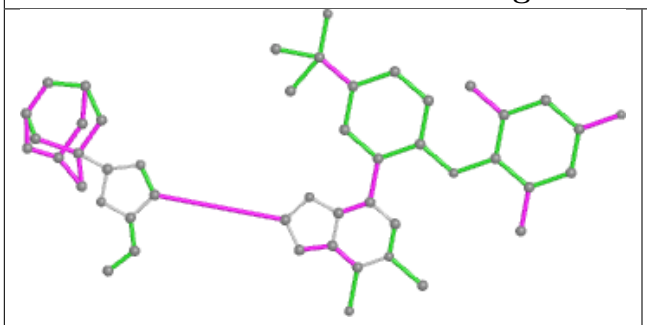


Rings

Ligand A1L12 F 501



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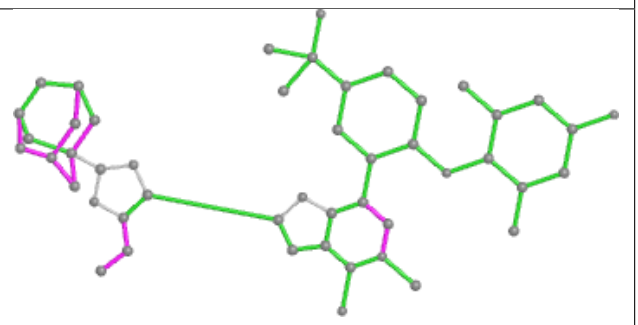

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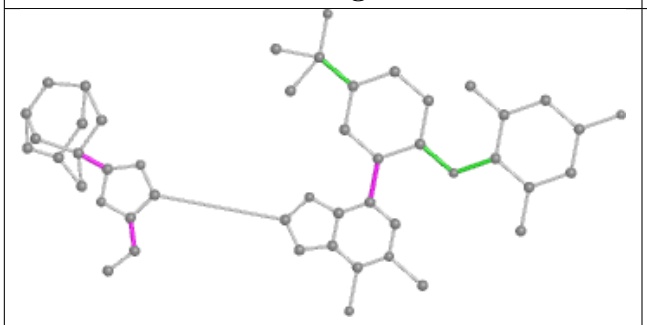

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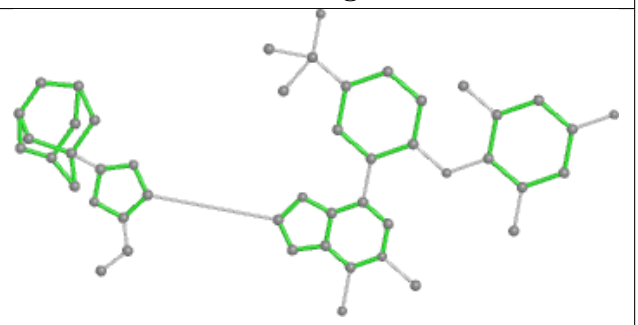
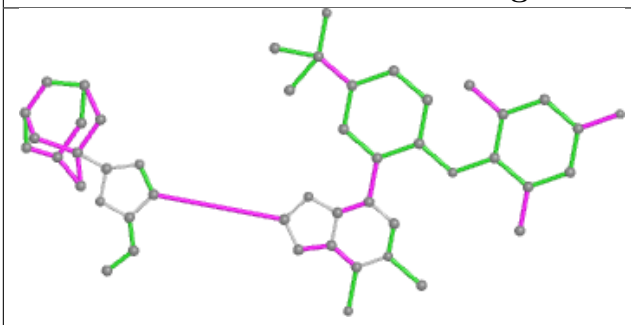


Rings

Ligand A1L12 B 502



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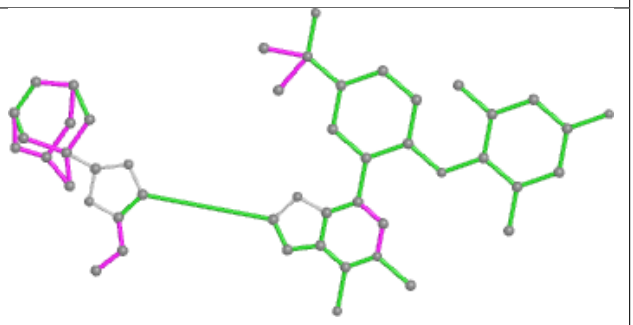

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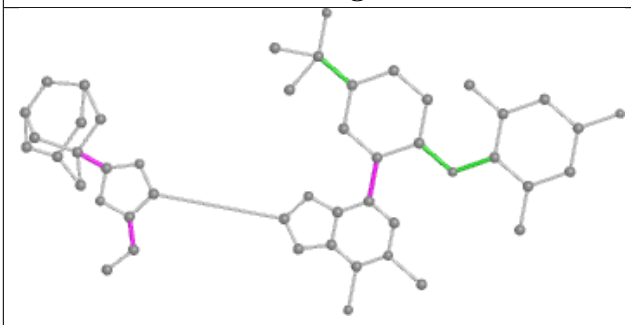

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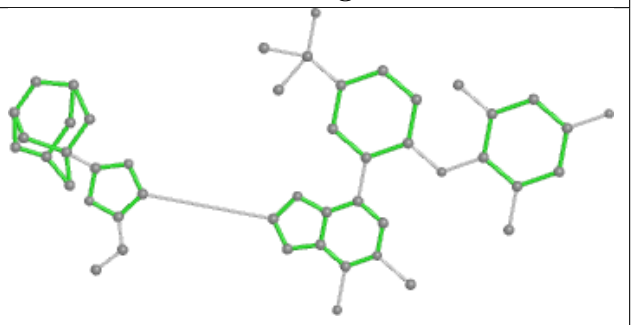
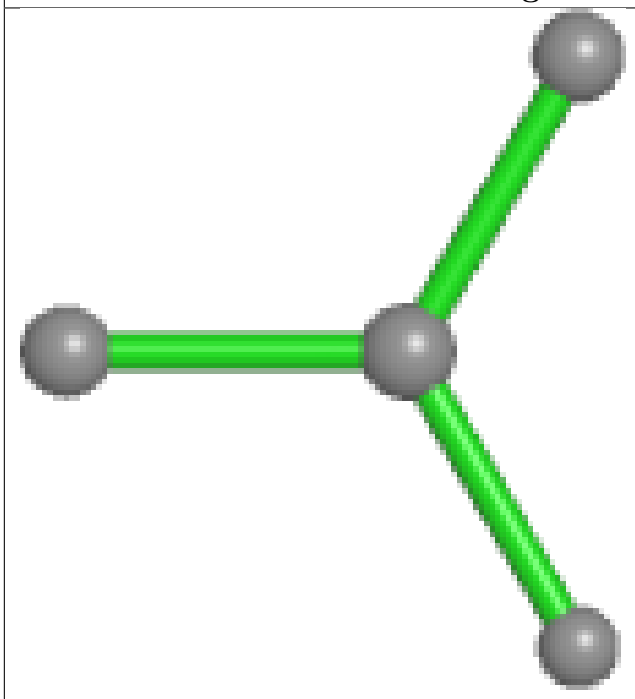


Rings

Ligand DMS B 503



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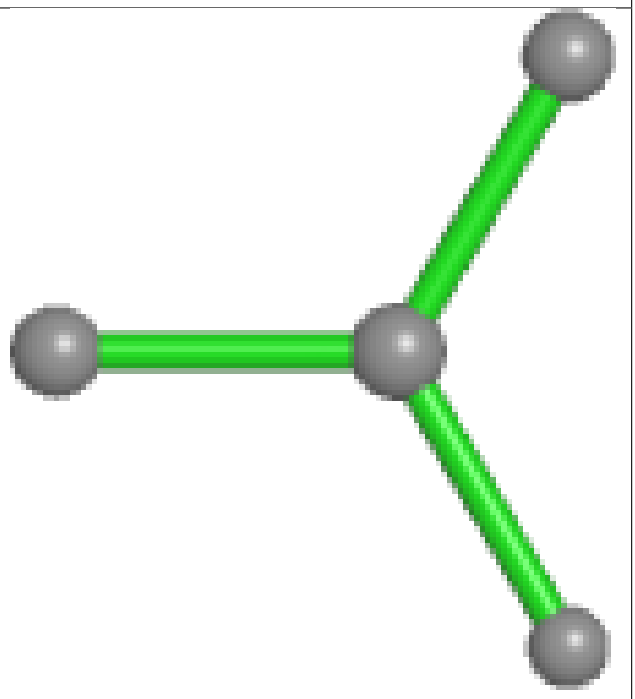

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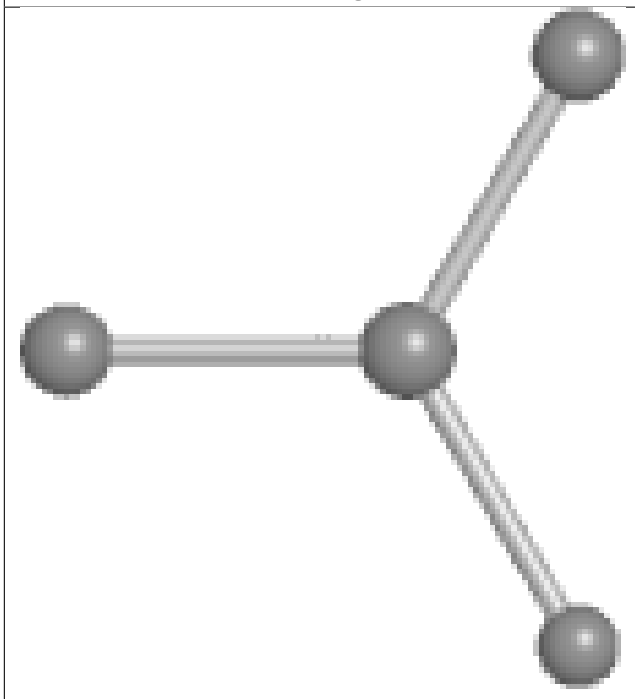

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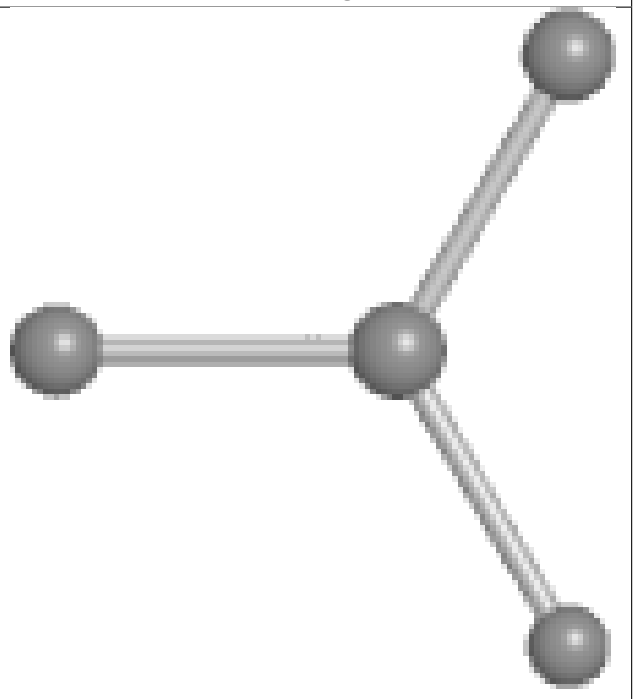
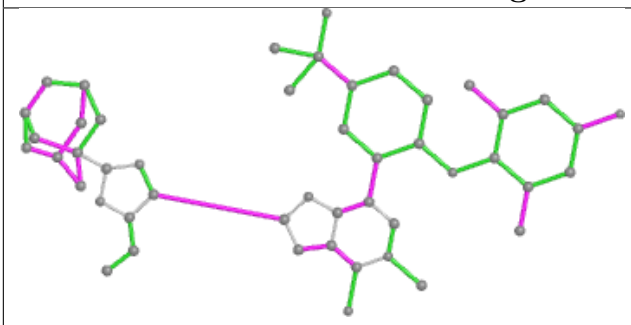


Rings

Ligand A1L12 A 501



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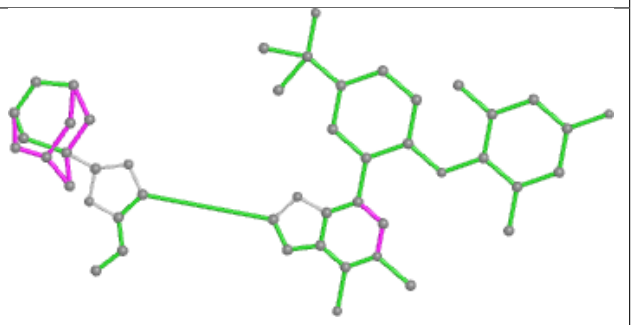

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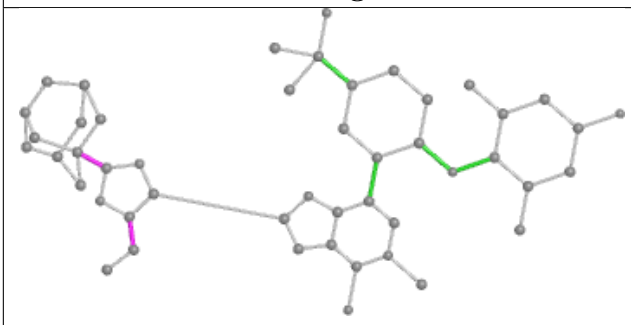

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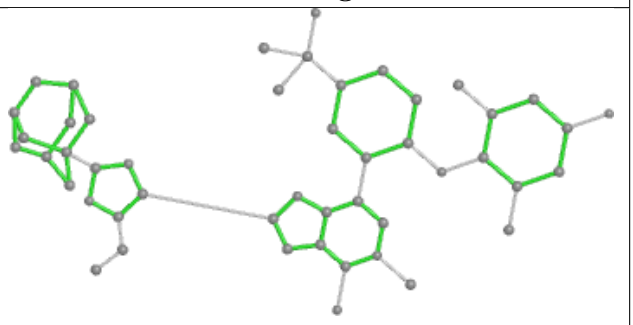

Rings

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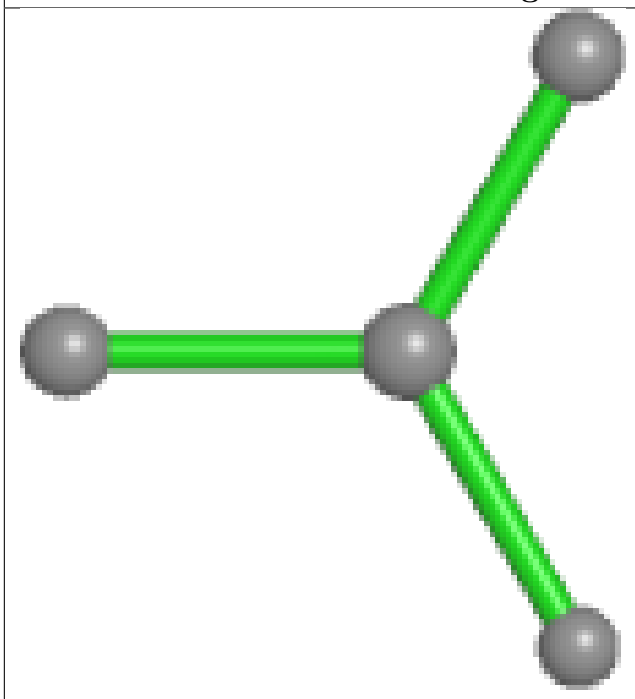

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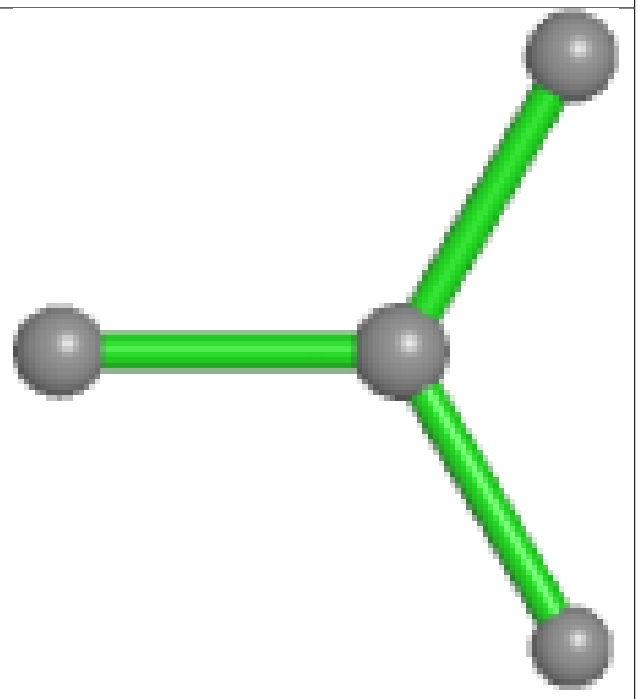

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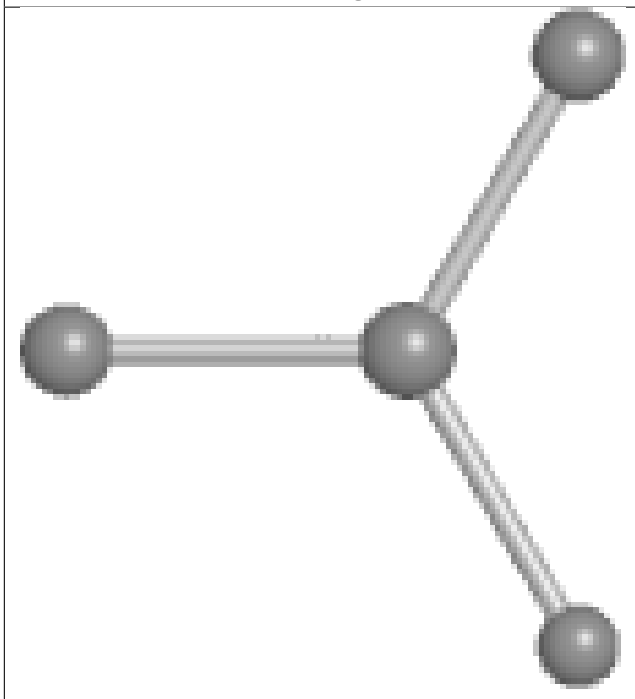

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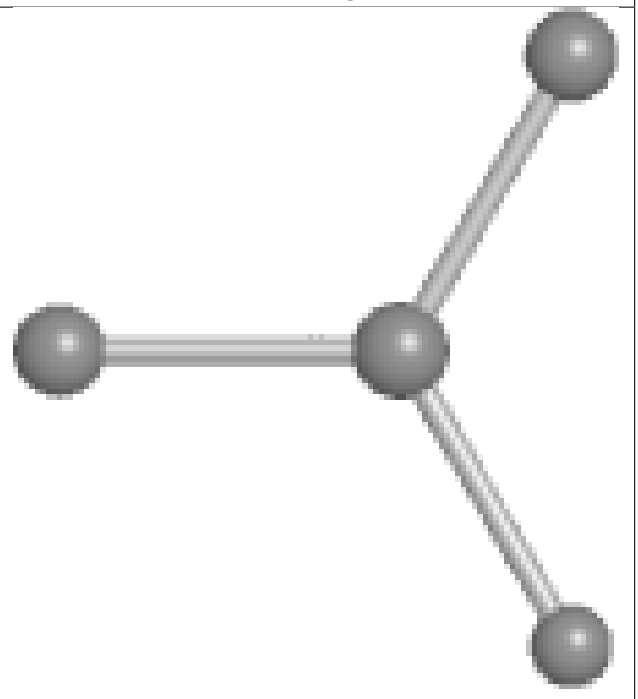

Rings

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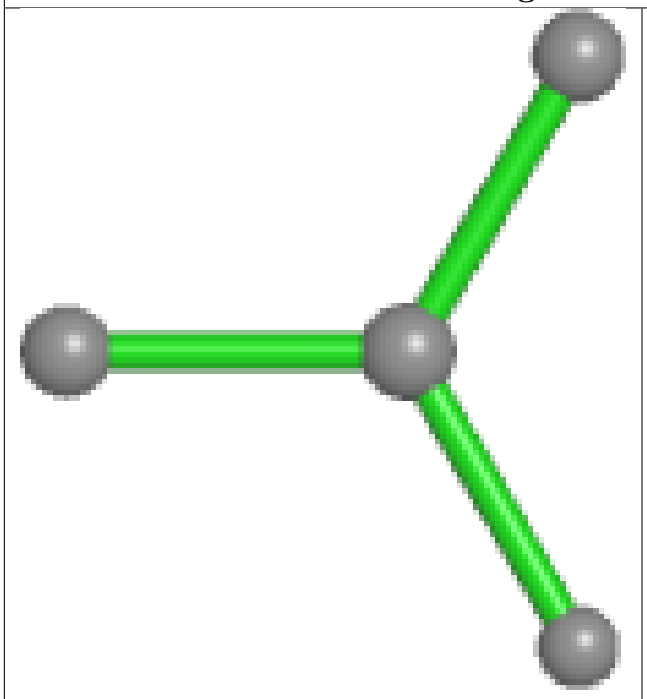

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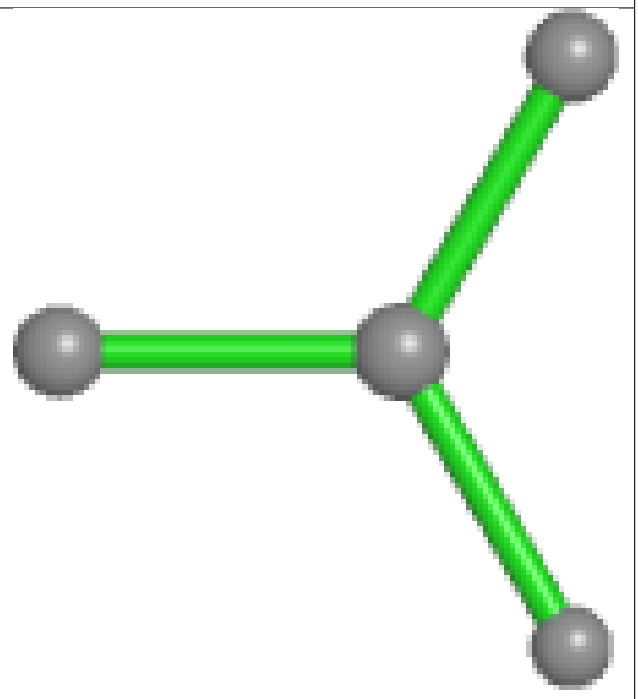

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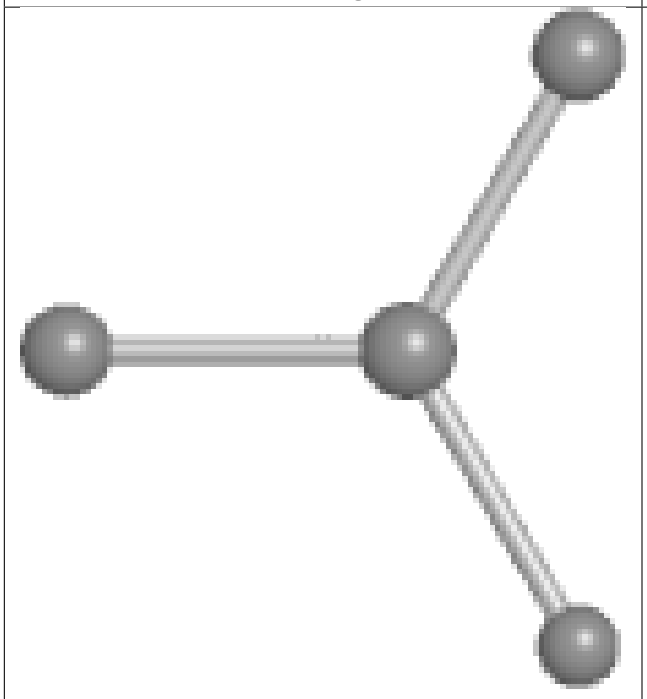

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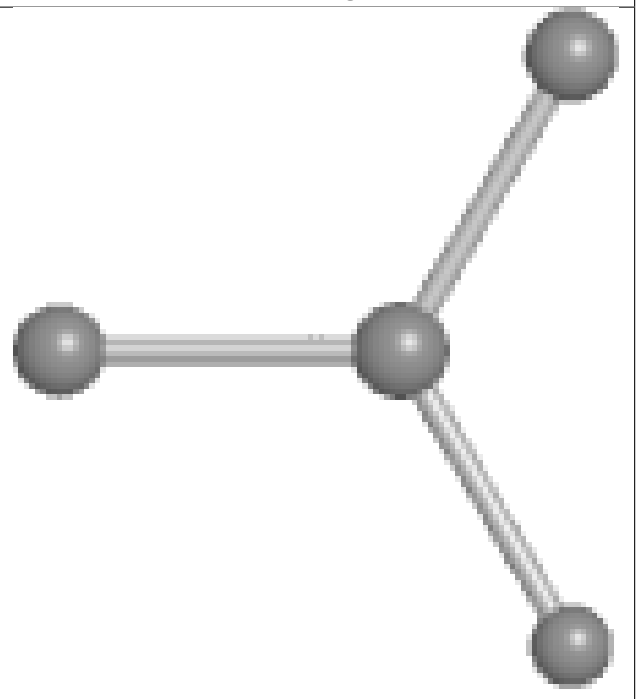

Rings

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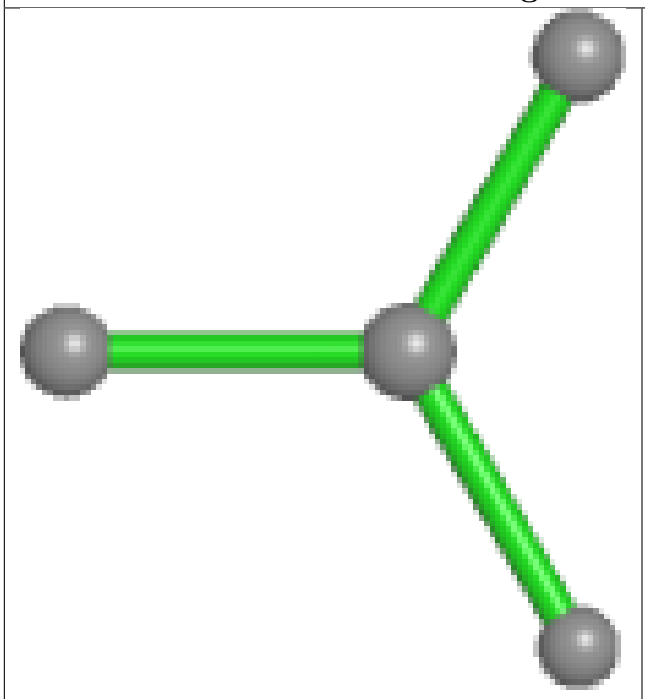

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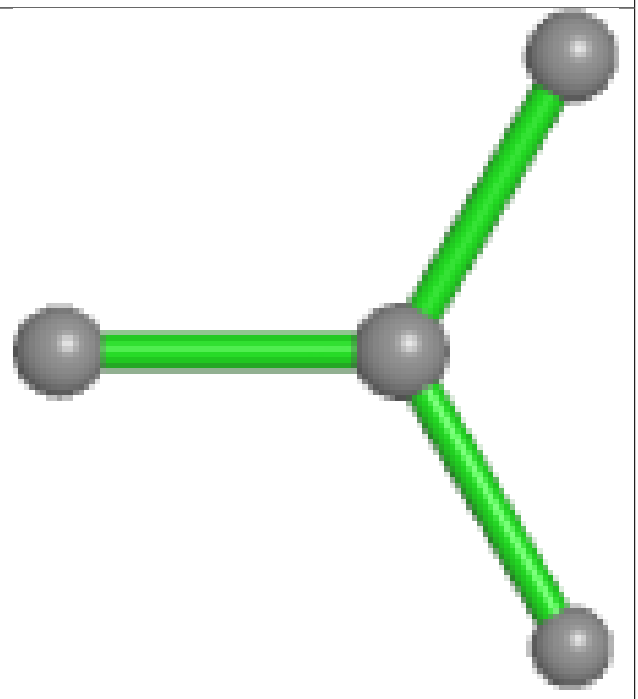

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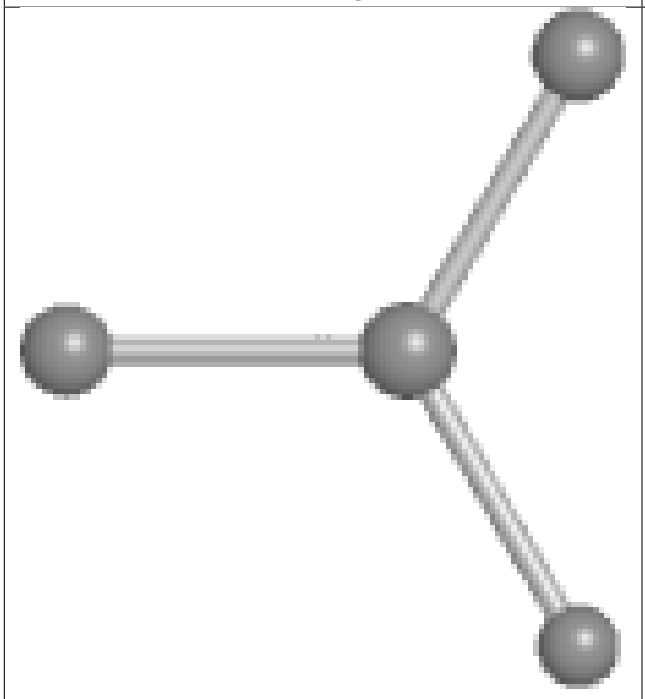

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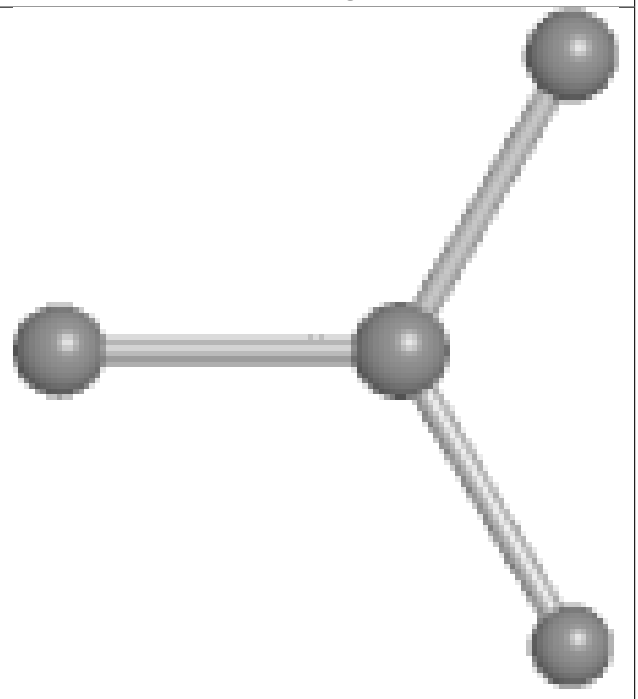

Rings

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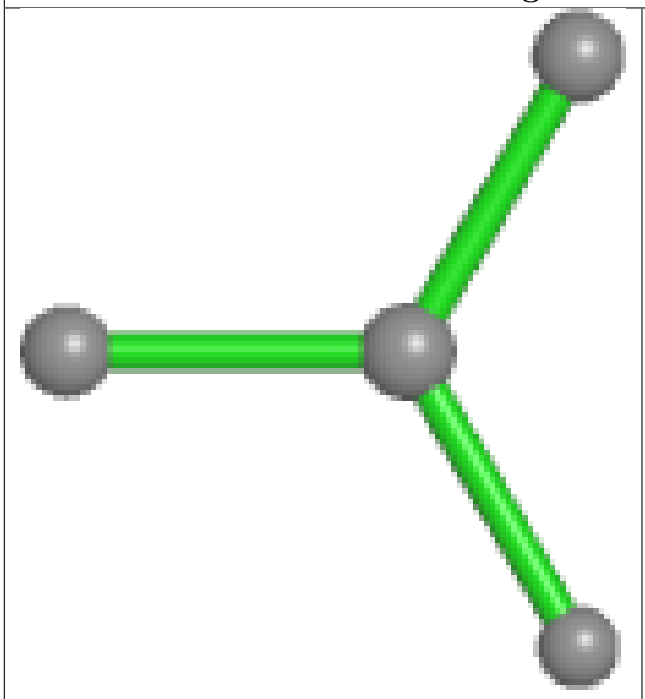

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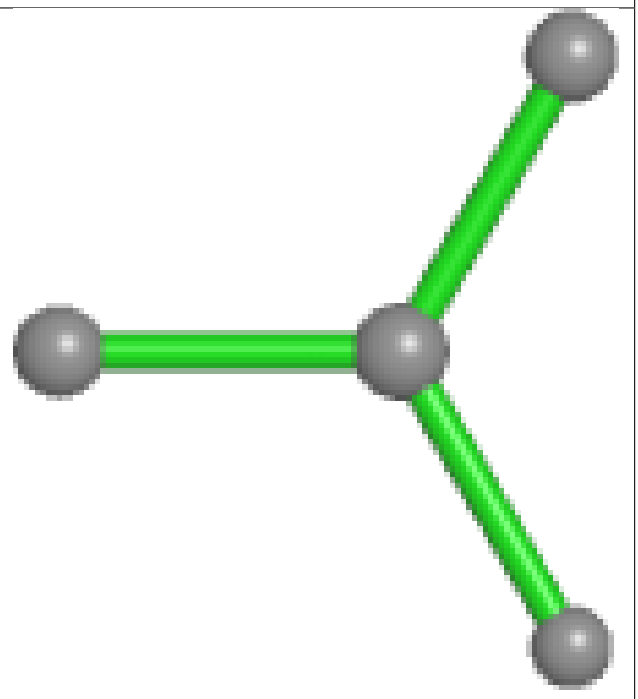

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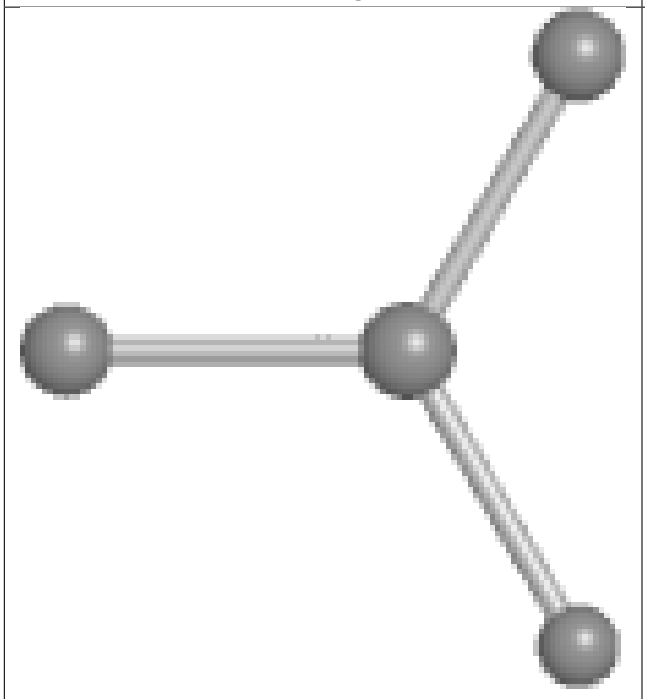

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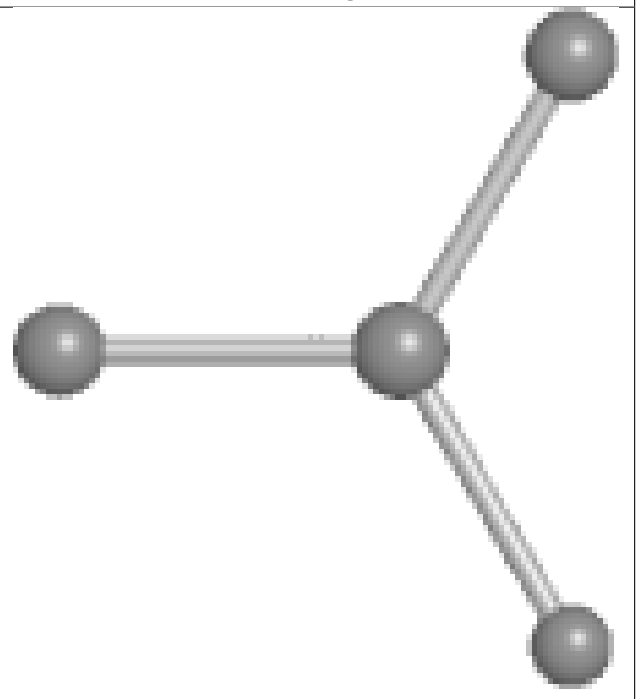
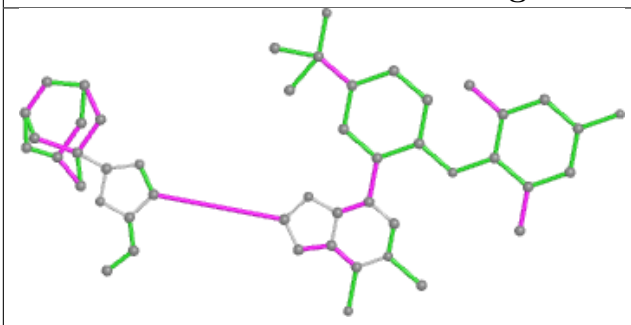


Rings

Ligand A1L12 G 501



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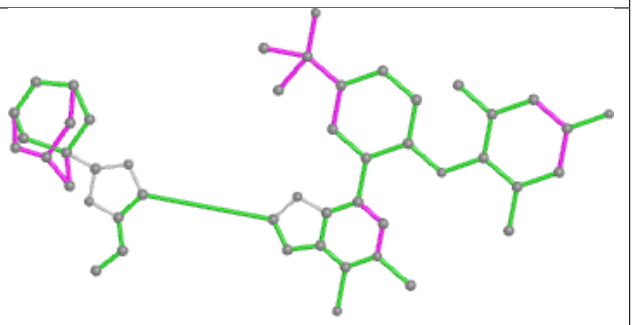

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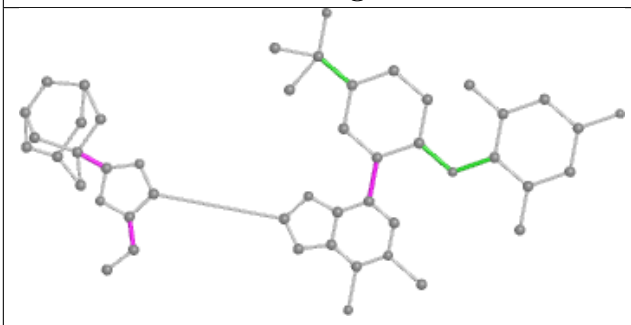

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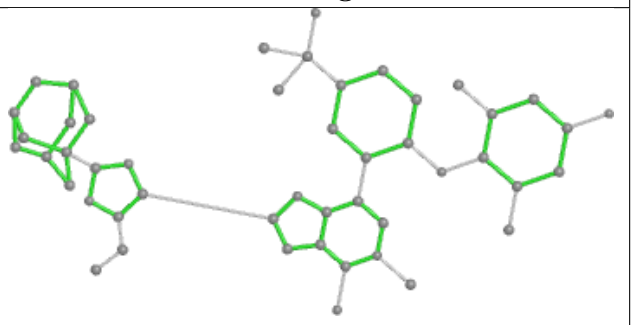
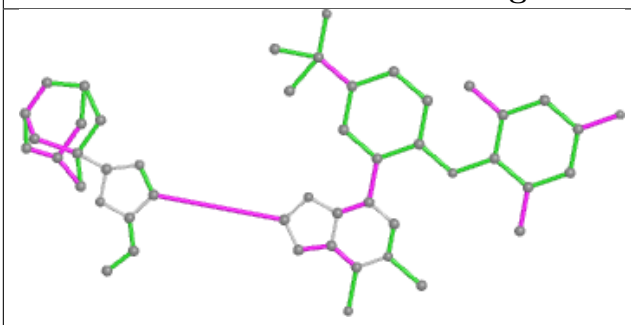


Rings

Ligand A1L12 H 501



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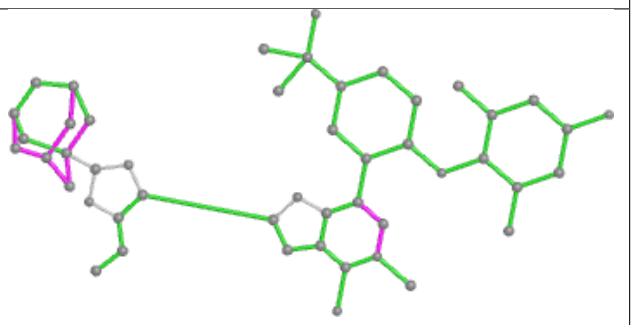
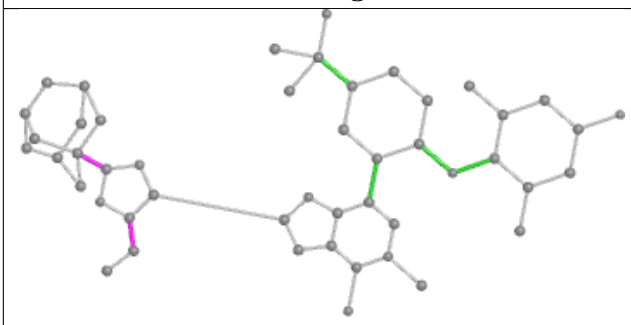


Bond angles



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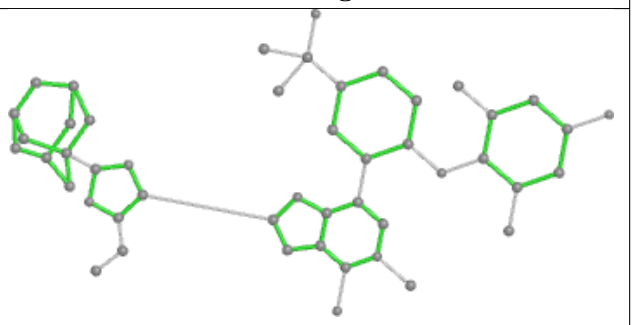
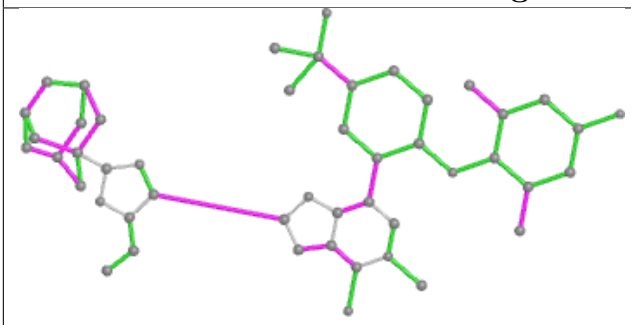


Rings

Ligand A1L12 P 501



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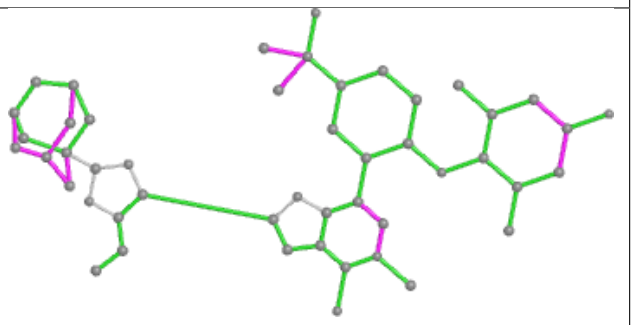
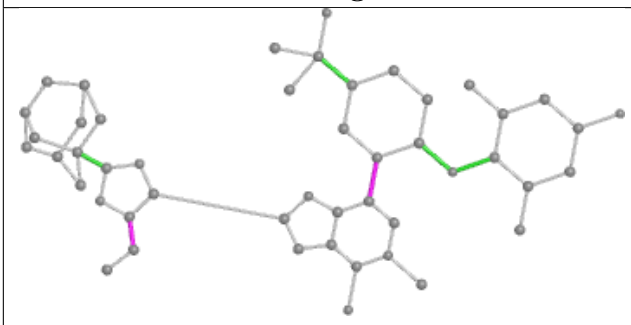


Bond angles



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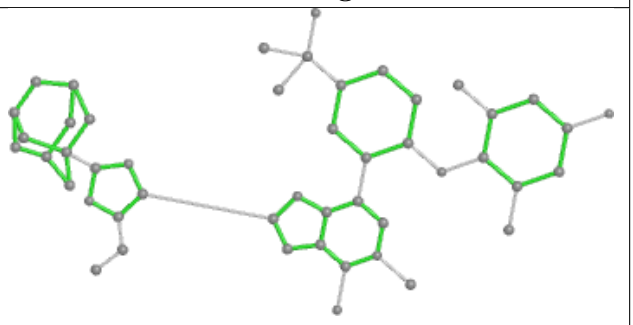
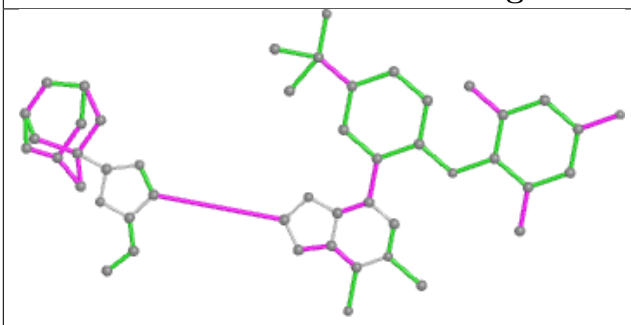


Rings

Ligand A1L12 M 501



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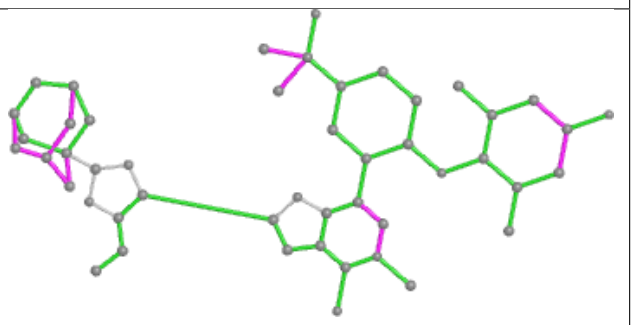
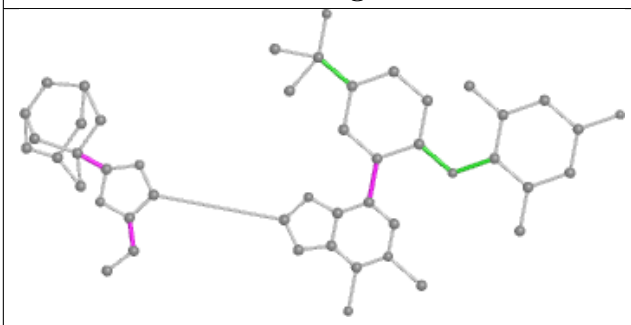


Bond angles



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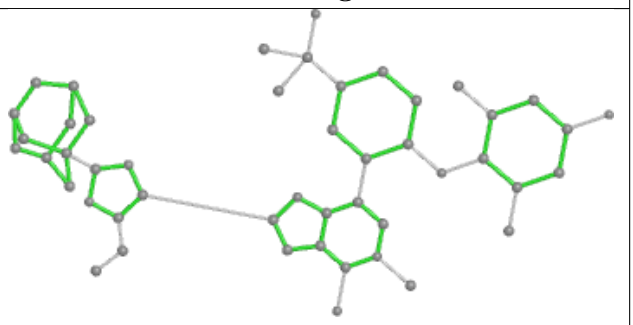
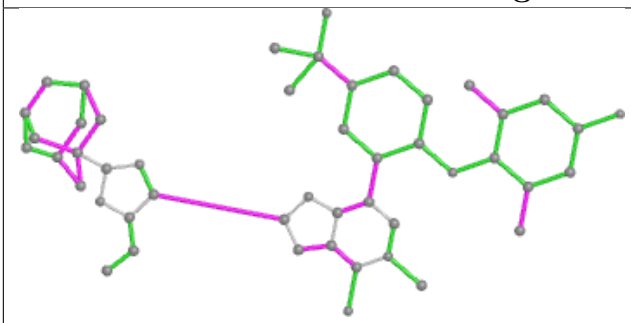
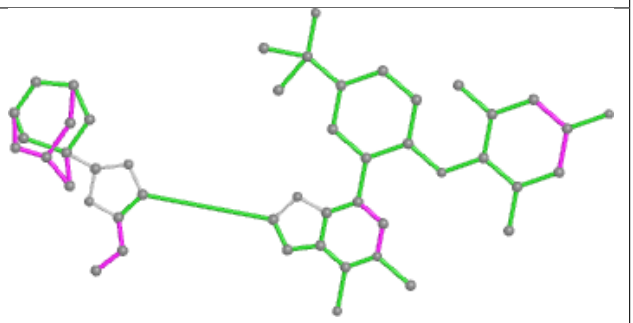


Rings

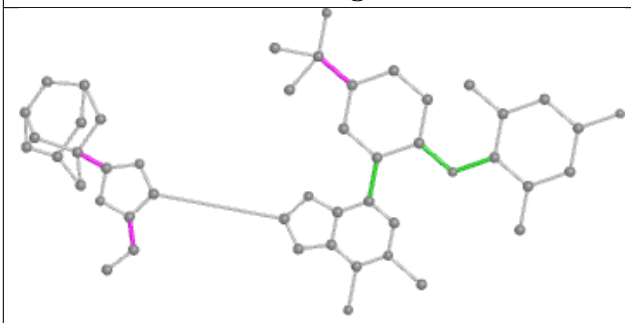
Ligand A1L12 S 501



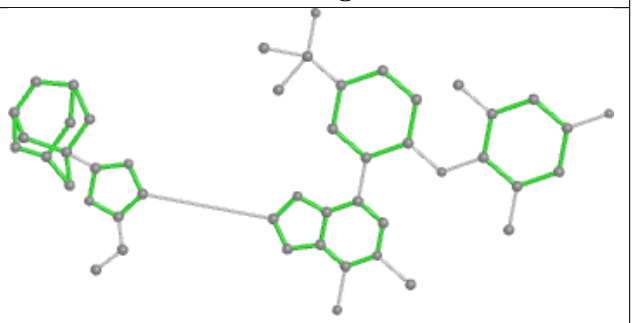
Bond lengths



Bond angles

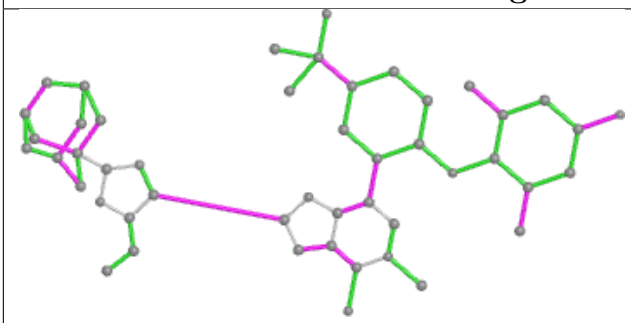


Torsions

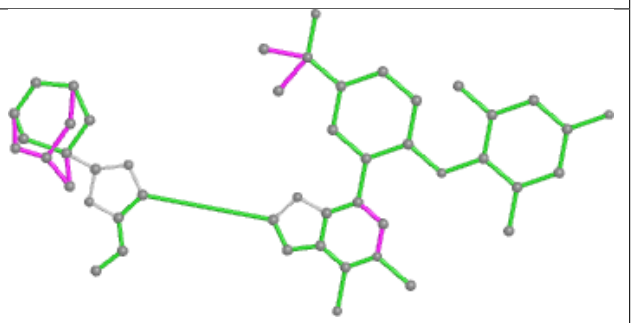


Rings

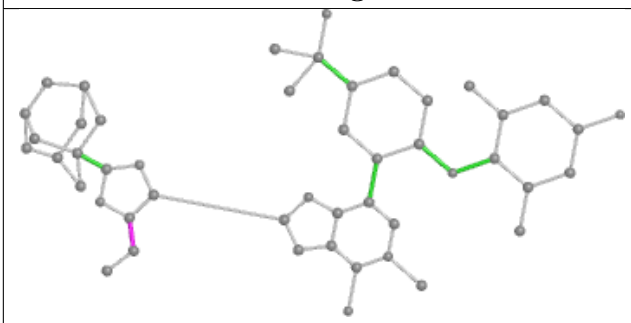
Ligand A1L12 D 501



Bond lengths



Bond angles



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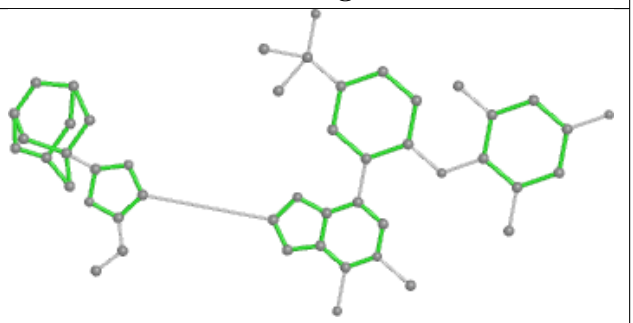
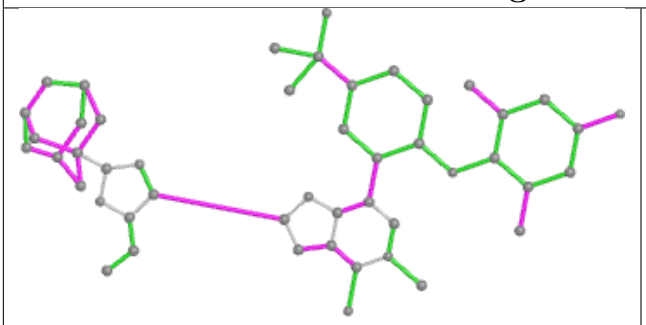
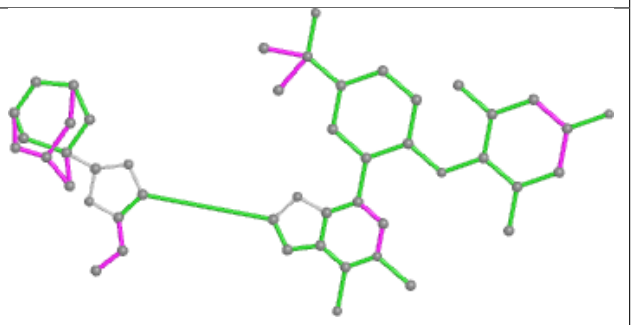


Rings

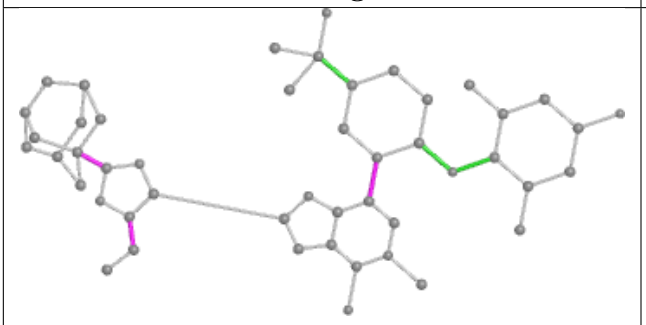
Ligand A1L12 N 501



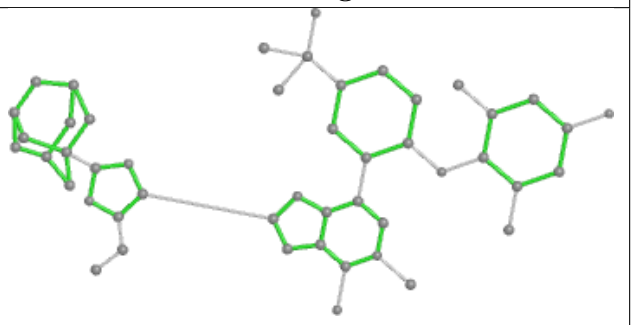
Bond lengths



Bond angles

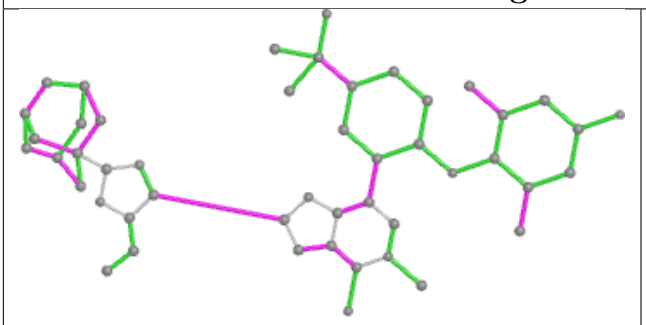


Torsions

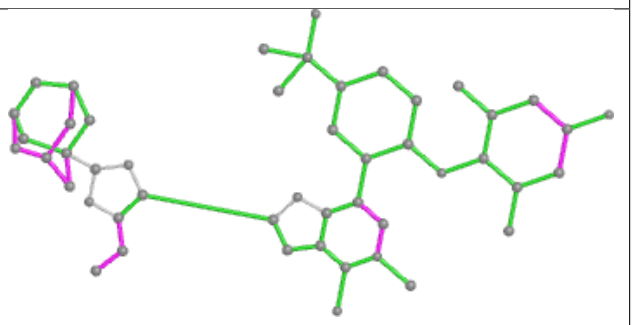


Rings

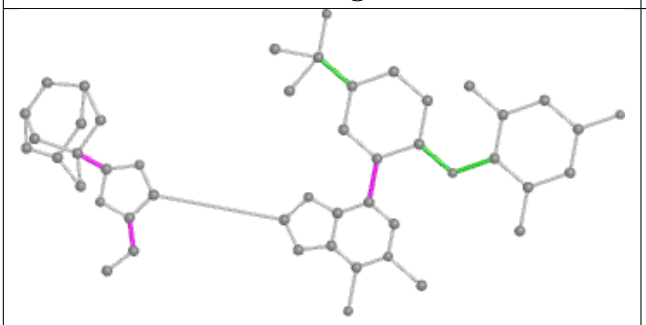
Ligand A1L12 R 501



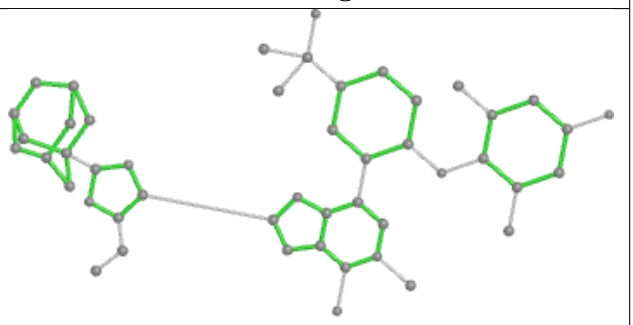
Bond lengths



Bond angles

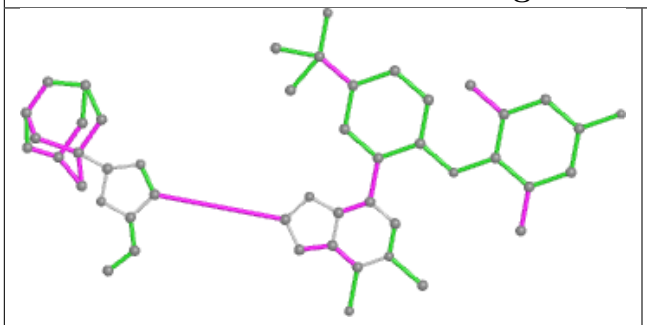


Torsions

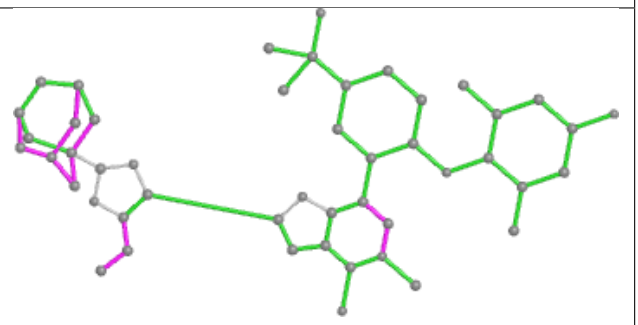


Rings

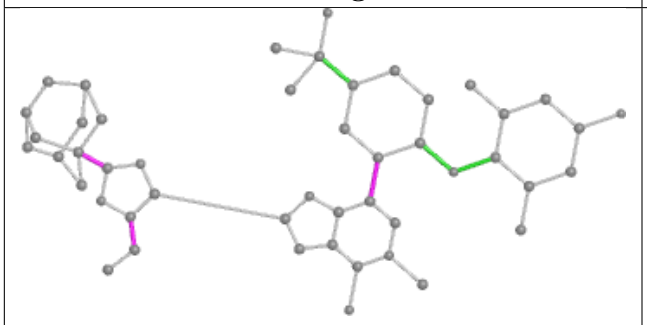
Ligand A1L12 L 501



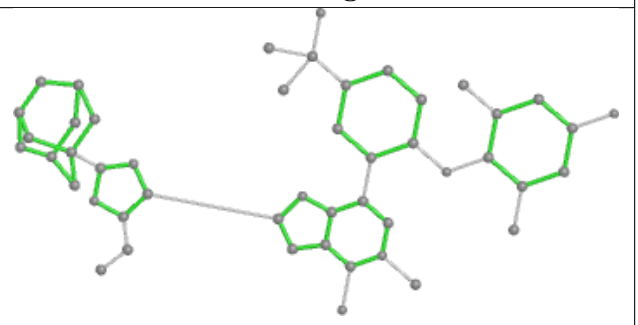
Bond lengths



Bond angles

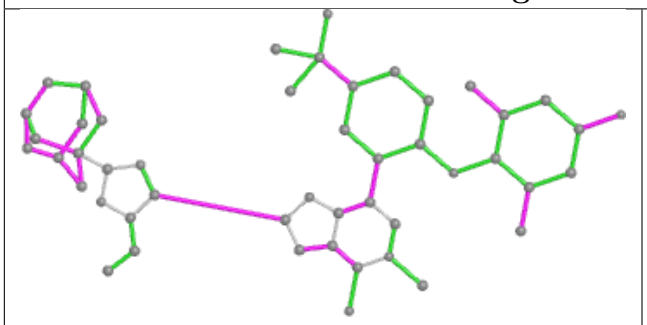


Torsions

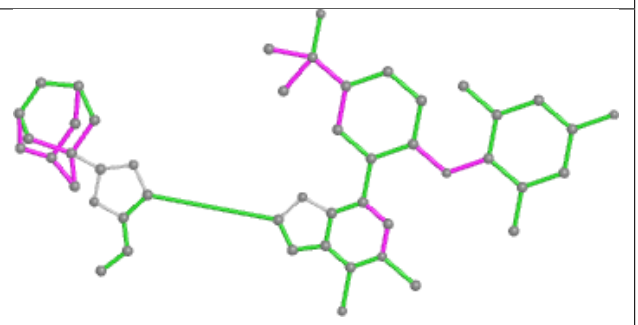


Rings

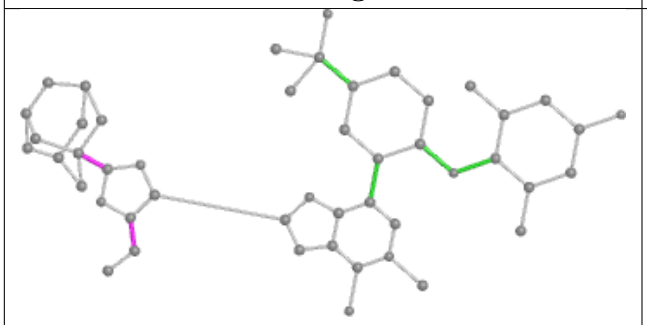
Ligand A1L12 E 501



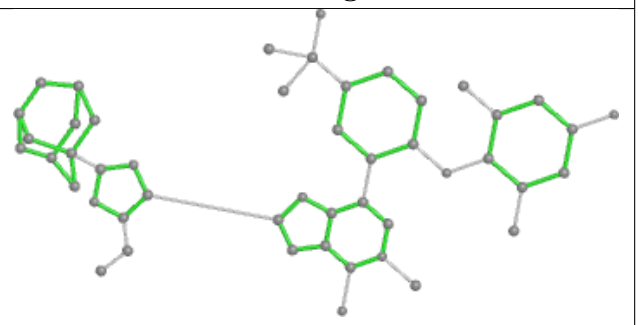
Bond lengths



Bond angles

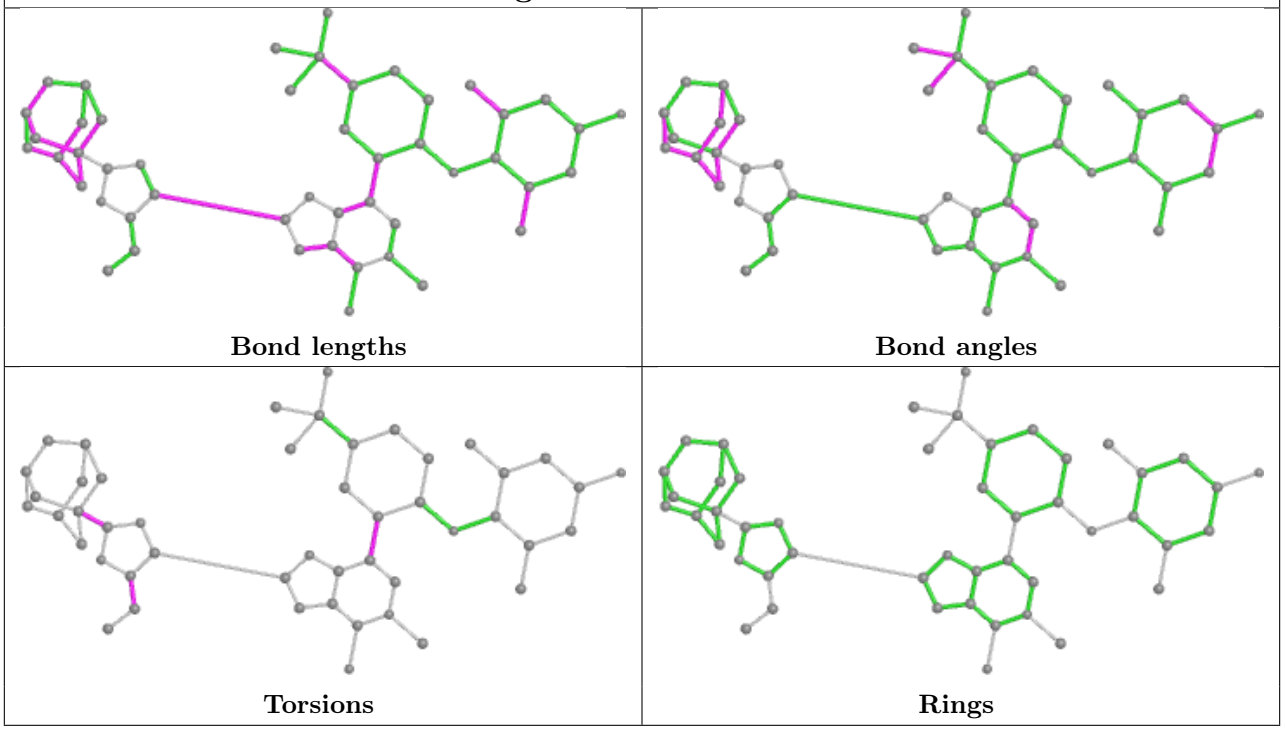


Torsions



Rings

Ligand A1L12 J 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	110/147 (74%)	-1.05	0 100 100	24, 46, 73, 112	1 (0%)
1	B	110/147 (74%)	-1.01	0 100 100	25, 47, 77, 115	2 (1%)
1	C	111/147 (75%)	-0.99	0 100 100	38, 52, 80, 119	0
1	D	111/147 (75%)	-0.88	0 100 100	40, 59, 89, 116	0
1	E	110/147 (74%)	-1.05	0 100 100	30, 46, 73, 116	1 (0%)
1	F	111/147 (75%)	-1.04	0 100 100	29, 47, 84, 114	1 (0%)
1	G	111/147 (75%)	-0.93	0 100 100	36, 53, 87, 121	0
1	H	111/147 (75%)	-0.85	0 100 100	34, 59, 92, 119	1 (0%)
1	I	109/147 (74%)	-0.89	1 (0%) 81 78	37, 59, 93, 117	0
1	J	110/147 (74%)	-0.90	1 (0%) 81 78	33, 57, 98, 111	1 (0%)
1	K	110/147 (74%)	-0.89	1 (0%) 81 78	35, 59, 96, 147	1 (0%)
1	L	110/147 (74%)	-0.83	0 100 100	37, 60, 101, 144	0
1	M	110/147 (74%)	-0.76	0 100 100	47, 64, 98, 132	0
1	N	110/147 (74%)	-0.91	0 100 100	47, 65, 101, 124	0
1	O	110/147 (74%)	-0.34	1 (0%) 81 78	62, 92, 131, 163	0
1	P	110/147 (74%)	-0.36	0 100 100	61, 91, 130, 144	0
1	Q	109/147 (74%)	-0.33	1 (0%) 81 78	73, 95, 131, 150	0
1	R	109/147 (74%)	-0.37	2 (1%) 67 64	66, 92, 128, 147	0
1	S	110/147 (74%)	-0.38	0 100 100	72, 94, 138, 148	0
1	T	109/147 (74%)	-0.27	2 (1%) 67 64	66, 92, 133, 149	0
All	All	2201/2940 (74%)	-0.75	9 (0%) 89 87	24, 64, 118, 163	8 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	350	VAL	3.7
1	T	350	VAL	3.2
1	R	353	GLN	2.8
1	I	350	VAL	2.7
1	R	350	VAL	2.5

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
3	DMS	A	502	4/4	0.97	0.12	102,103,106,108	0
3	DMS	B	501	4/4	0.97	0.12	128,128,129,130	0
3	DMS	M	502	4/4	0.97	0.12	123,127,127,130	0
3	DMS	N	502	4/4	0.97	0.09	113,117,121,123	0
3	DMS	B	503	4/4	0.98	0.10	109,120,121,121	0
2	A1L12	F	501	48/48	0.99	0.04	36,44,50,52	0
2	A1L12	G	501	48/48	0.99	0.04	44,51,58,63	0
2	A1L12	H	501	48/48	0.99	0.05	49,64,74,75	0
2	A1L12	I	501	48/48	0.99	0.04	45,49,55,56	0
2	A1L12	J	501	48/48	0.99	0.04	39,43,54,55	0
2	A1L12	K	501	48/48	0.99	0.04	40,45,50,51	0
2	A1L12	L	501	48/48	0.99	0.04	42,47,55,56	0
2	A1L12	M	501	48/48	0.99	0.05	47,52,65,66	0
2	A1L12	N	501	48/48	0.99	0.05	45,50,66,68	0
2	A1L12	O	501	48/48	0.99	0.05	52,58,71,71	0
2	A1L12	P	501	48/48	0.99	0.05	53,59,76,76	0
2	A1L12	Q	501	48/48	0.99	0.05	63,74,85,86	0
2	A1L12	R	501	48/48	0.99	0.08	66,81,100,100	0
2	A1L12	S	501	48/48	0.99	0.04	64,72,82,82	0

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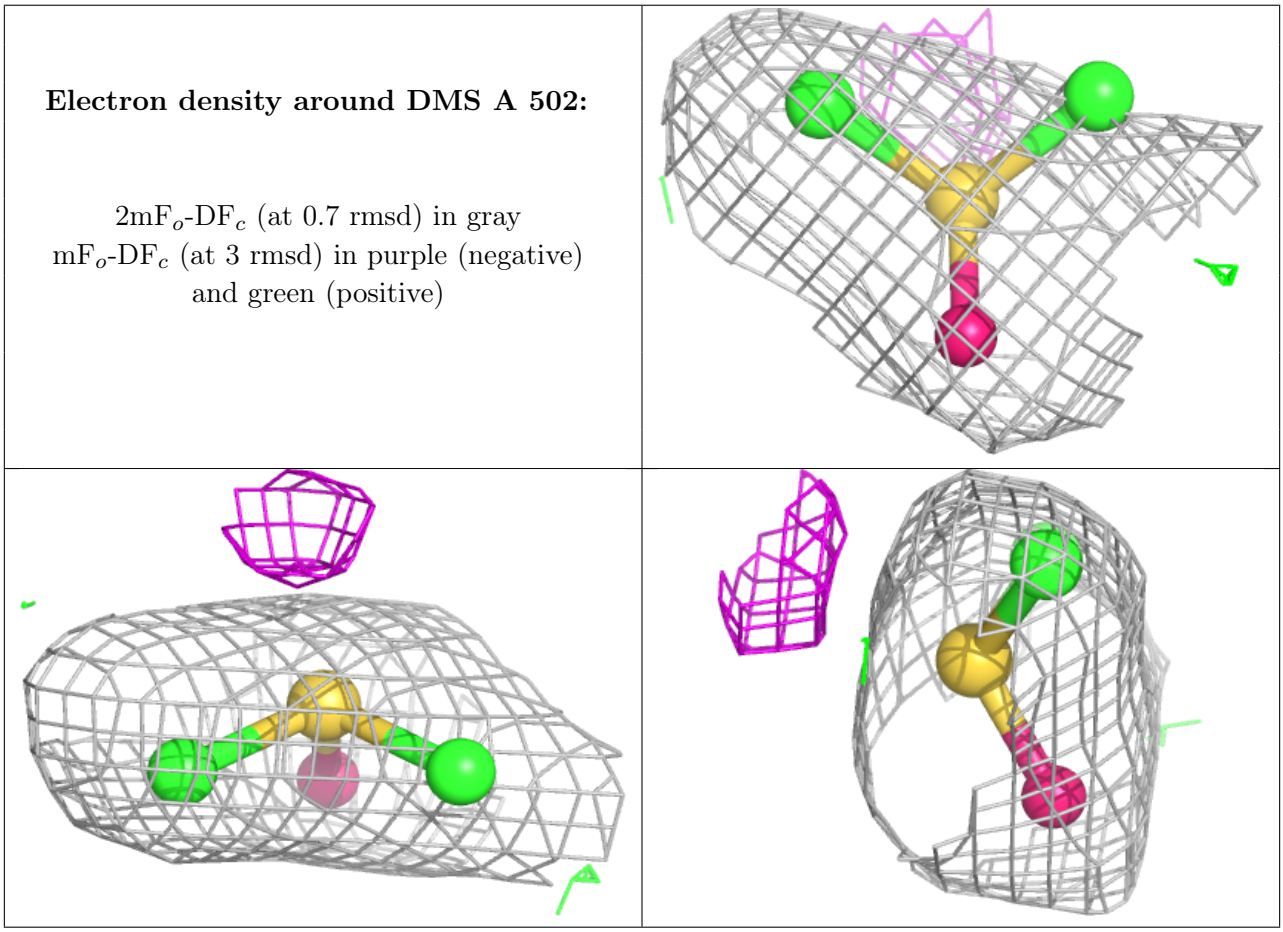
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1L12	T	501	48/48	0.99	0.07	63,80,98,99	0
2	A1L12	A	501	48/48	0.99	0.04	38,42,46,47	0
2	A1L12	B	502	48/48	0.99	0.04	39,43,48,50	0
2	A1L12	C	501	48/48	0.99	0.05	43,50,61,63	0
2	A1L12	D	501	48/48	0.99	0.05	47,63,72,73	0
2	A1L12	E	501	48/48	0.99	0.04	39,42,46,47	0
4	GOL	L	502	6/6	0.99	0.06	75,81,82,83	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.

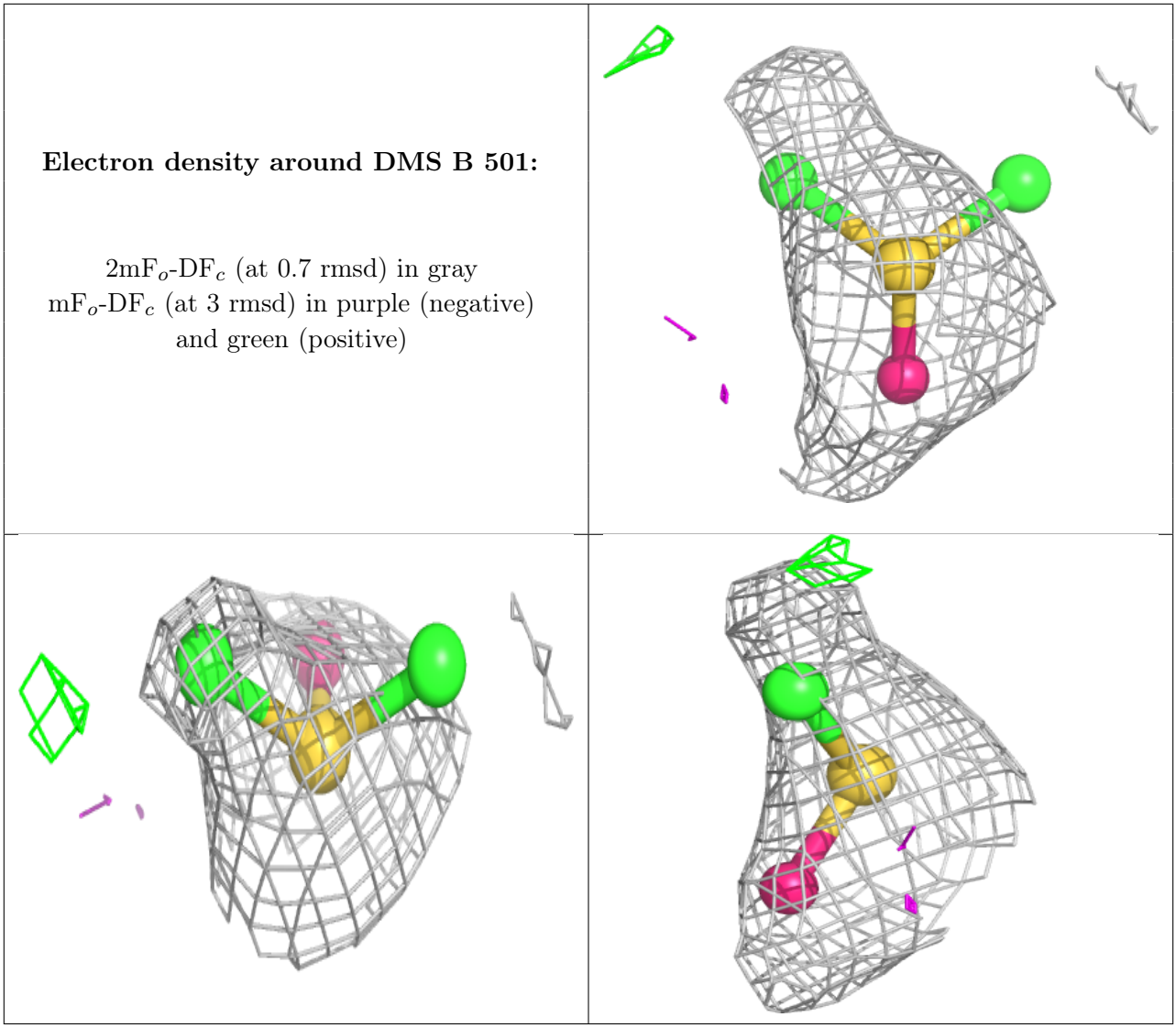
Electron density around DMS A 502:

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



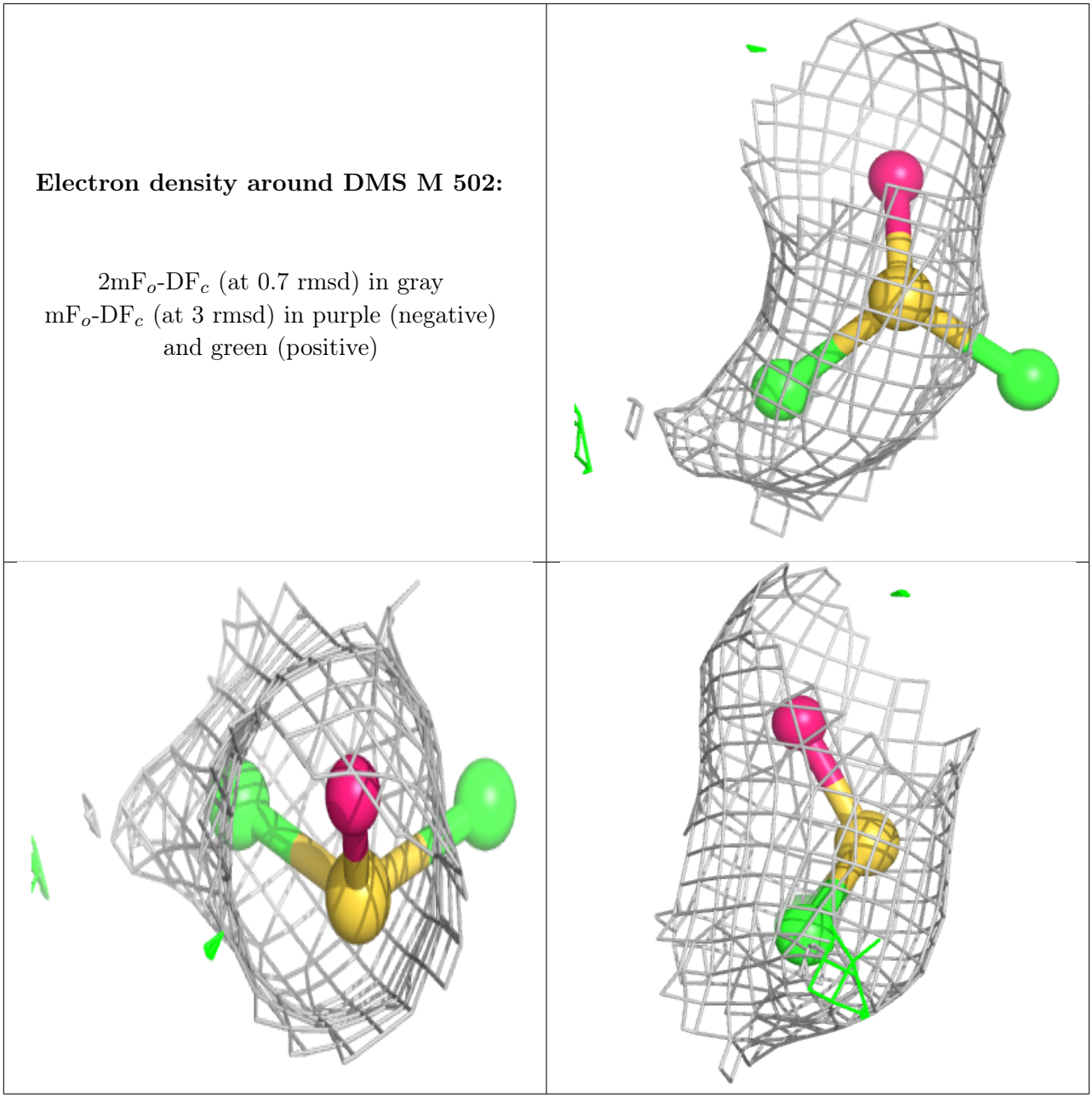
Electron density around DMS B 501:

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



Electron density around DMS M 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 DMS N 502:

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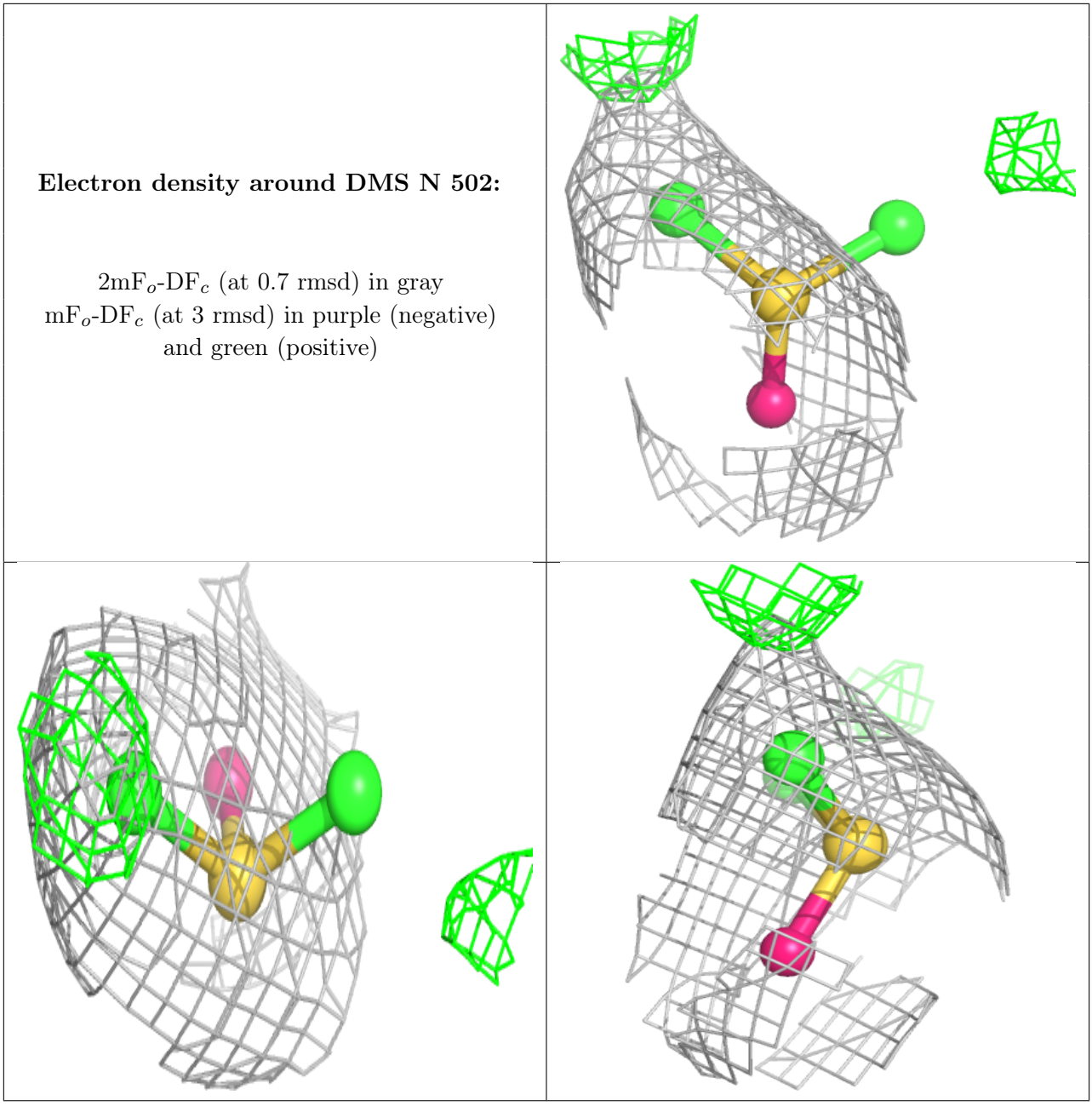
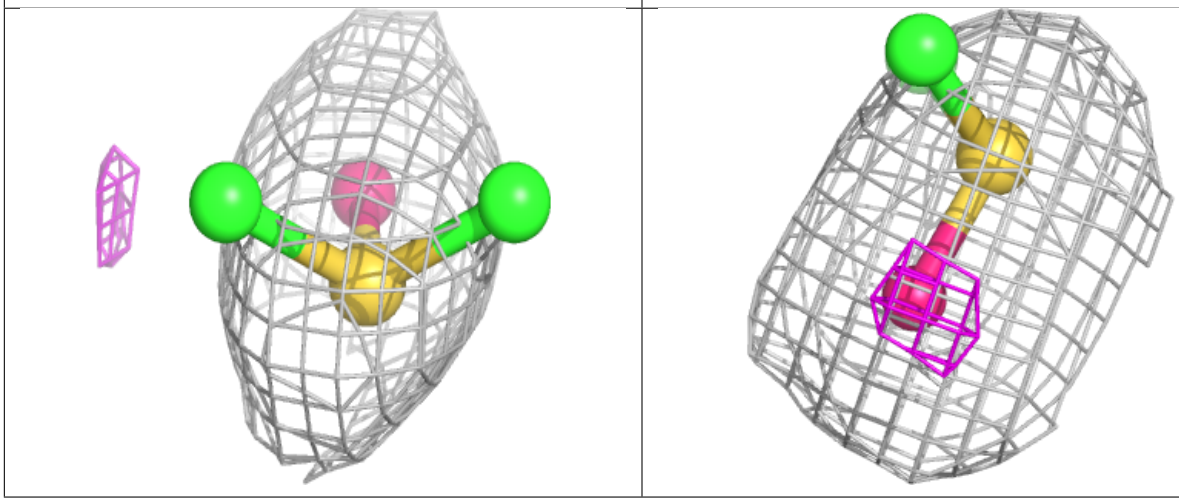
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



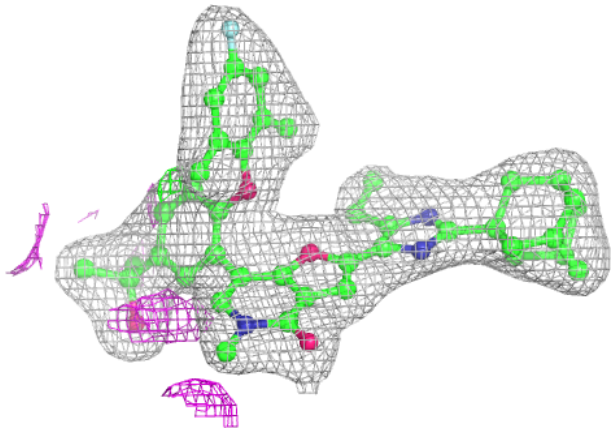
Electron density around DMS B 503:

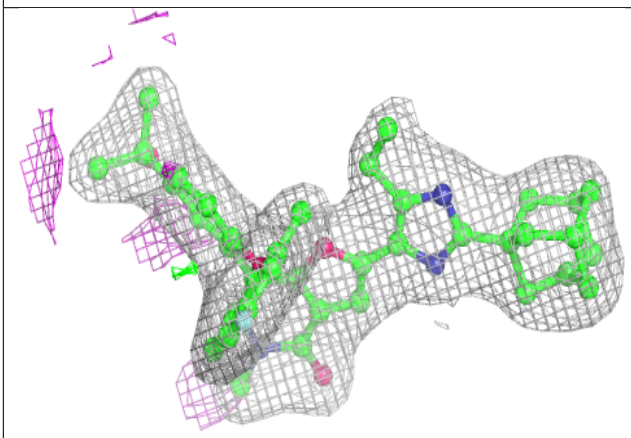
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

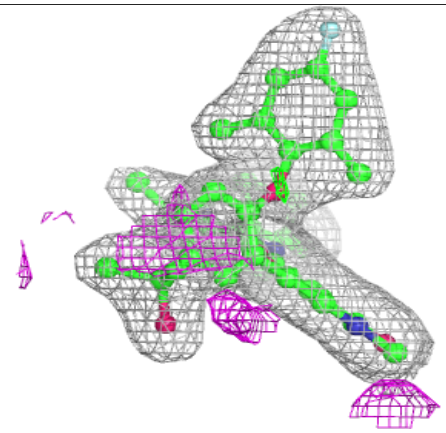


Electron density around A1L12 F 501:

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

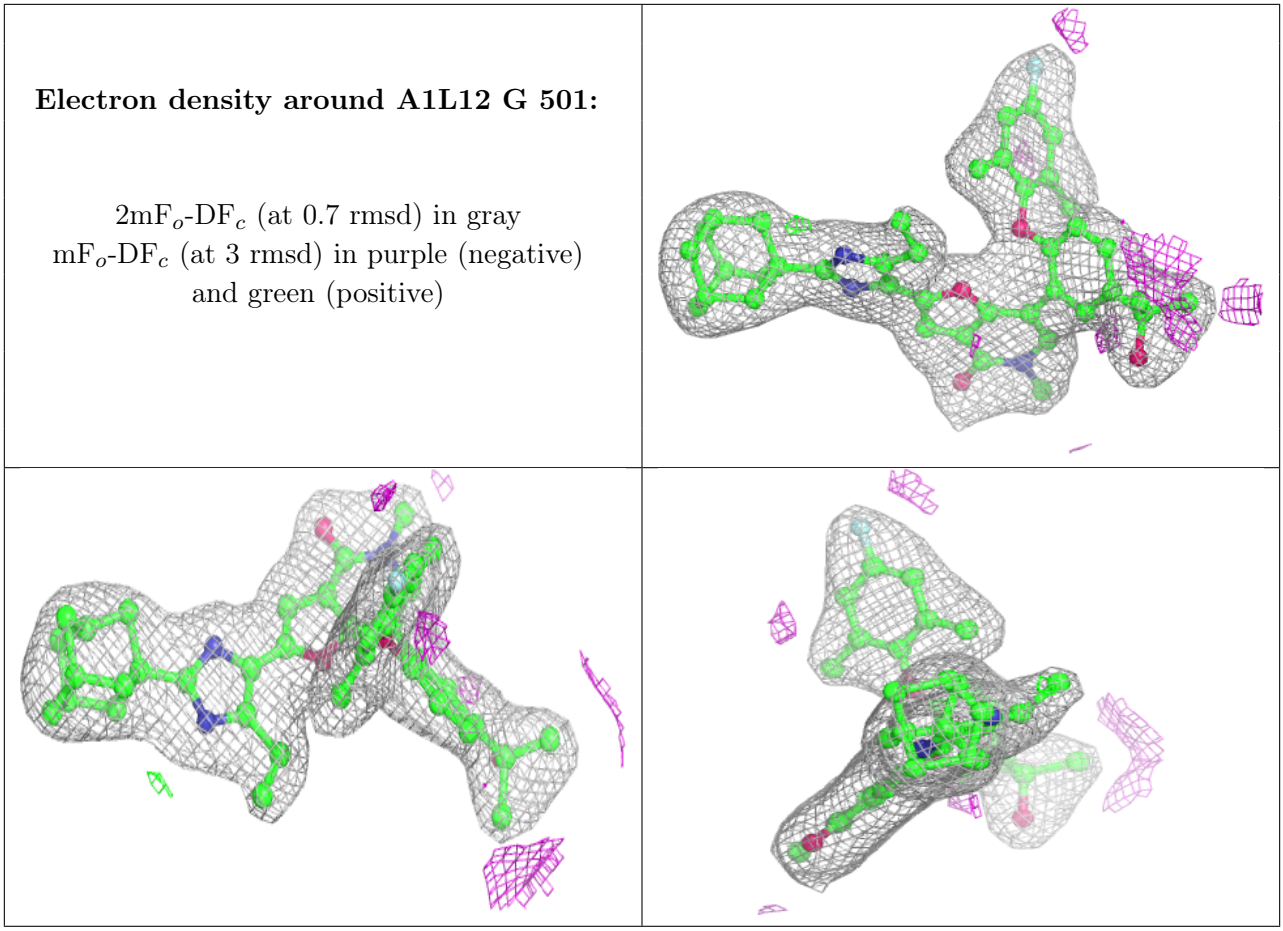






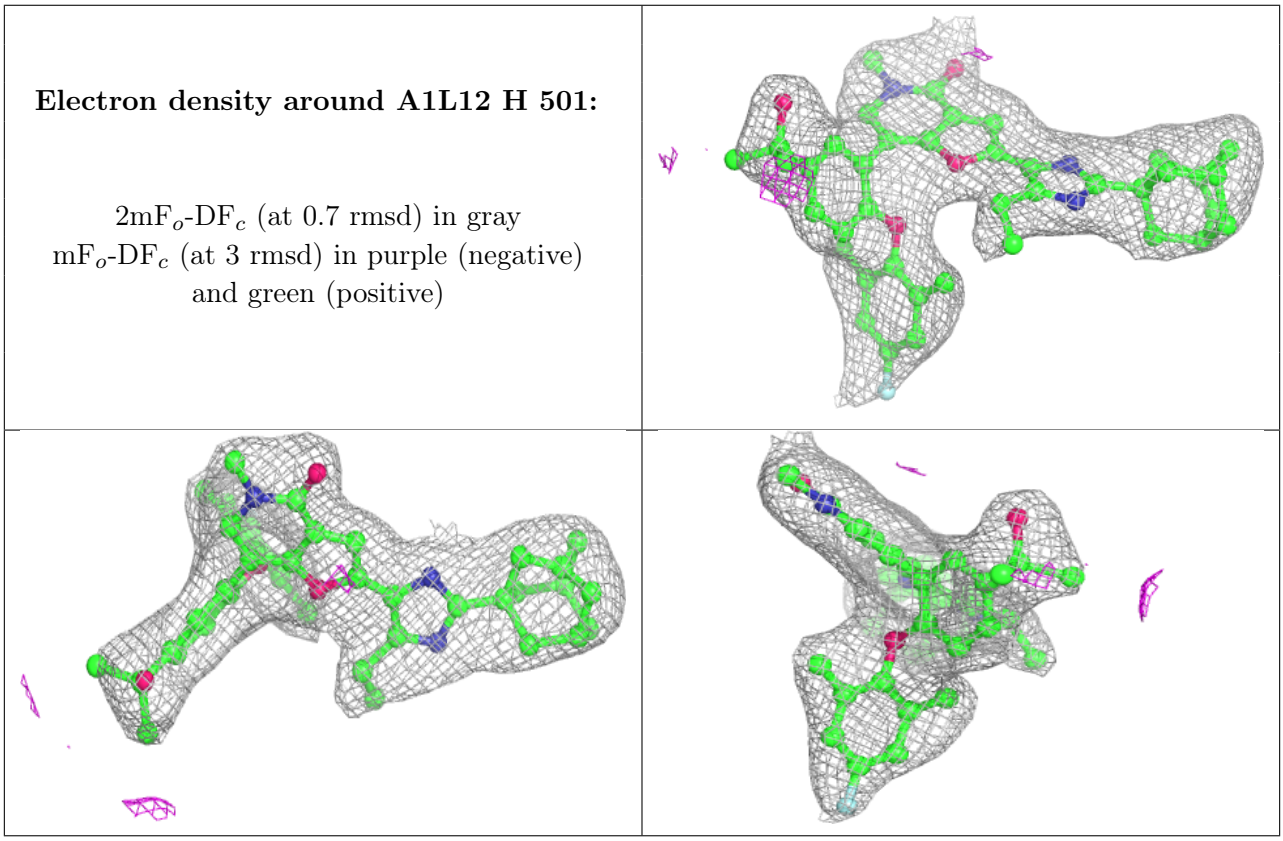
Electron density around A1L12 G 501:

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



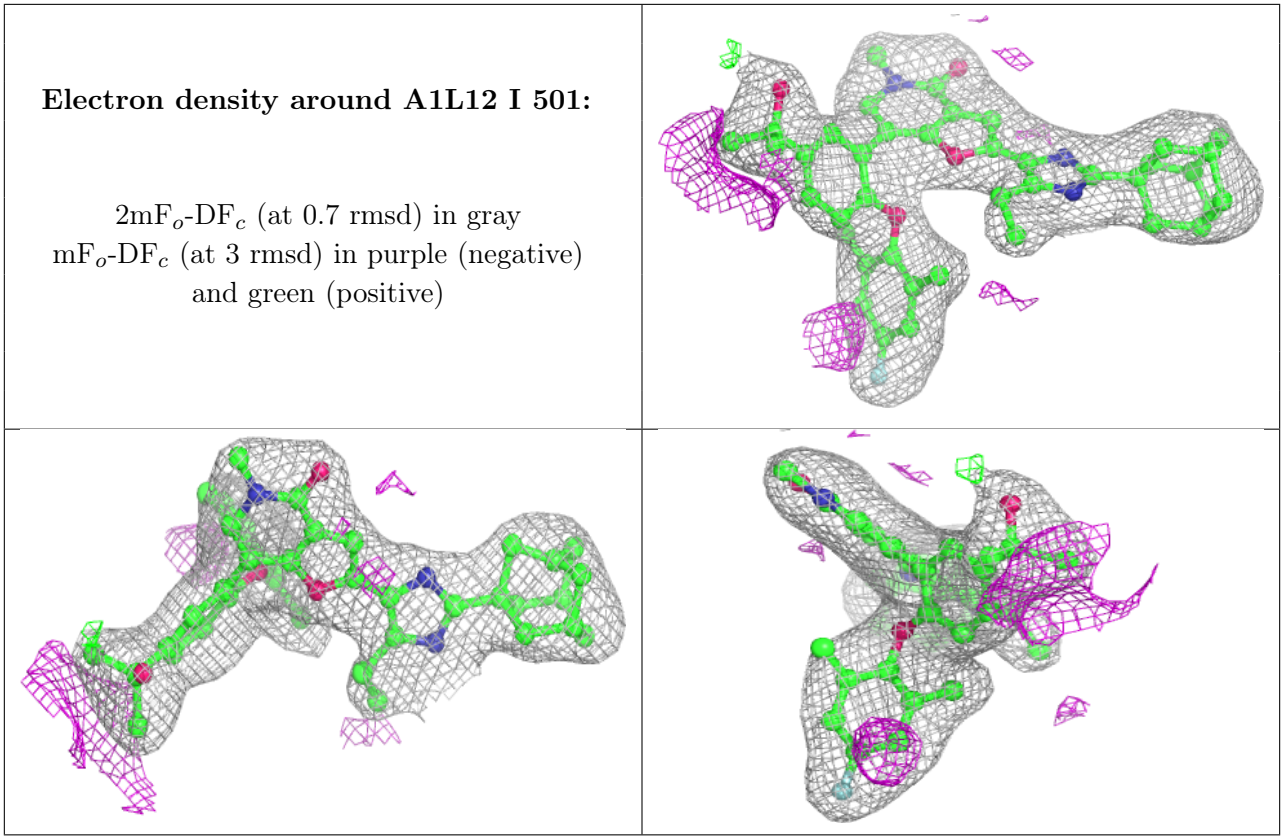
Electron density around A1L12 H 501:

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



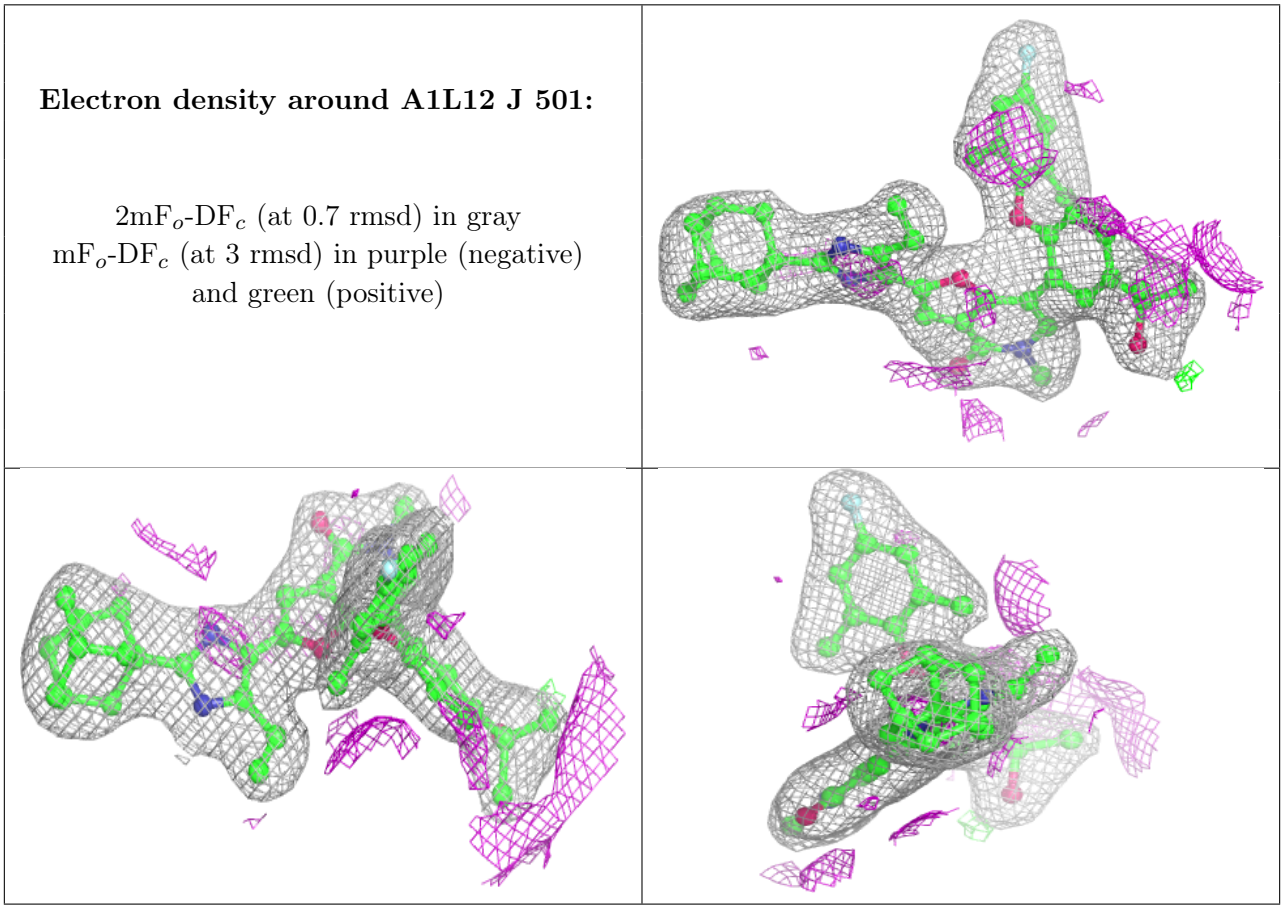
Electron density around A1L12 I 501:

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



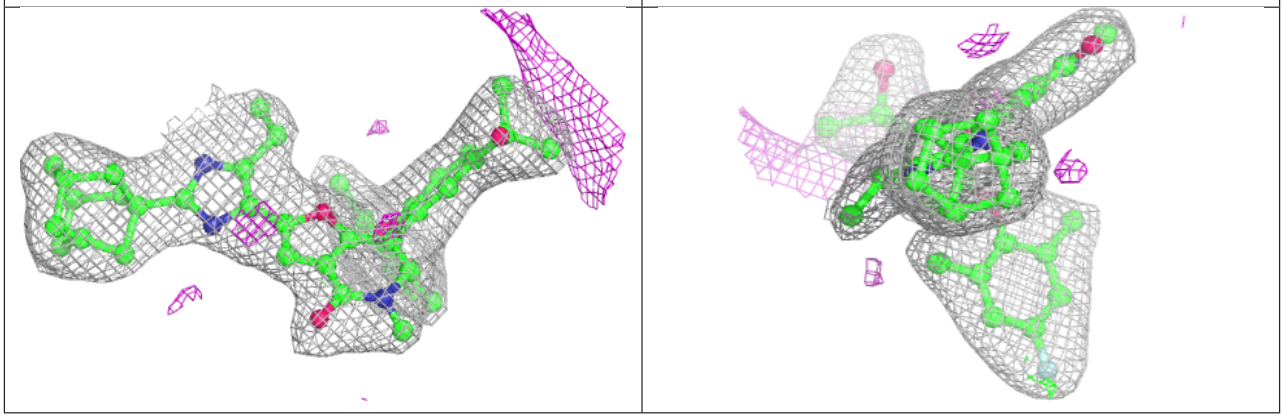
Electron density around A1L12 J 501:

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



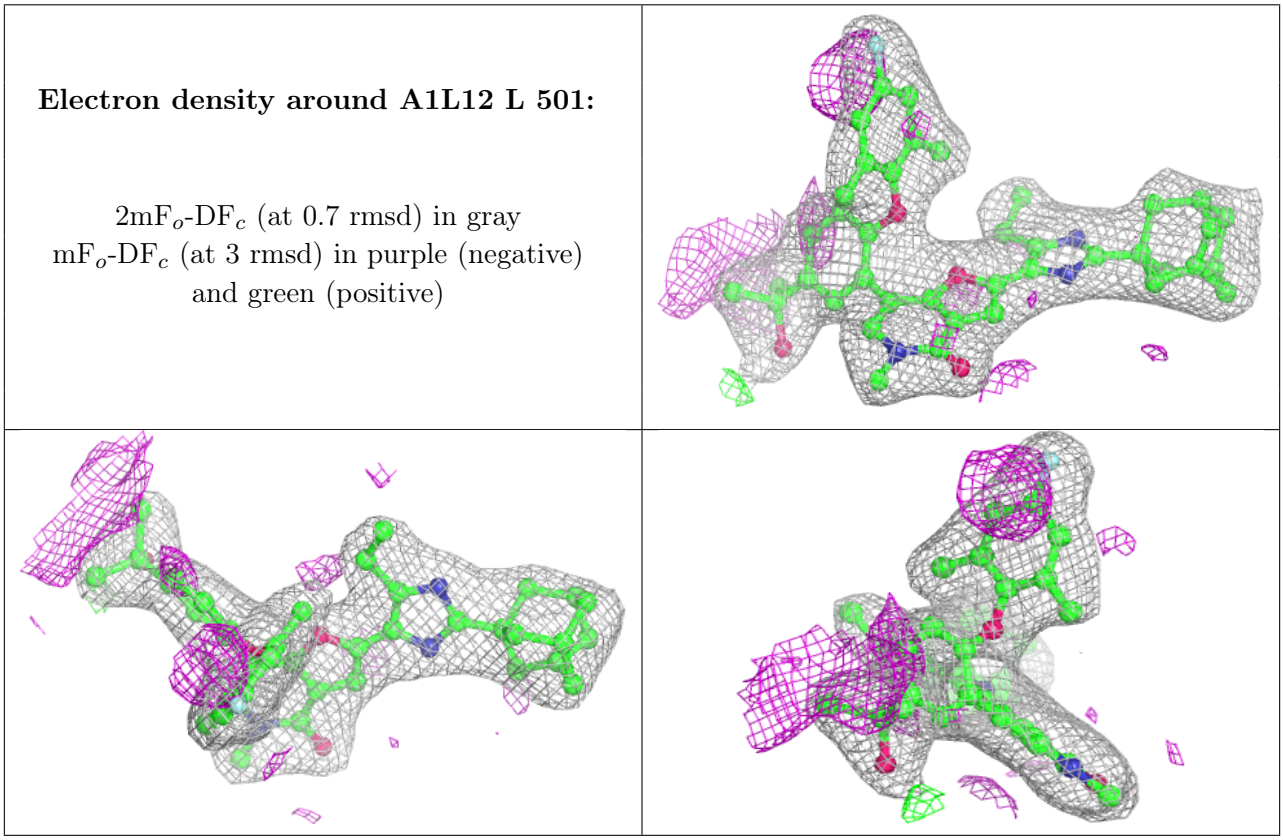
Electron density around A1L12 K 501:

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



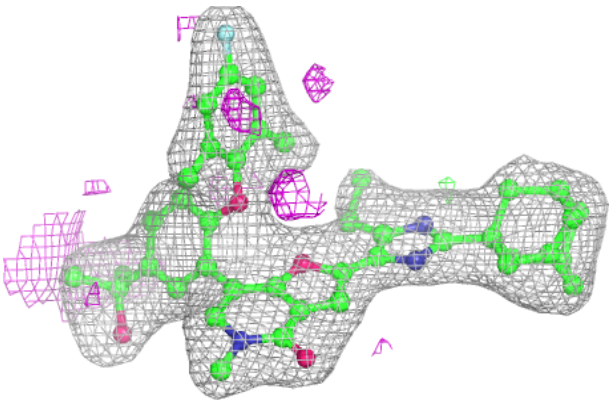
Electron density around A1L12 L 501:

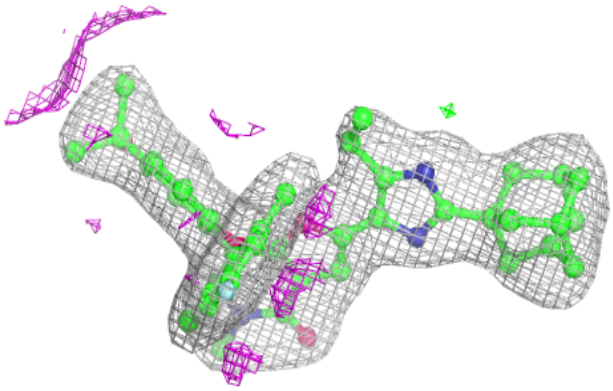
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

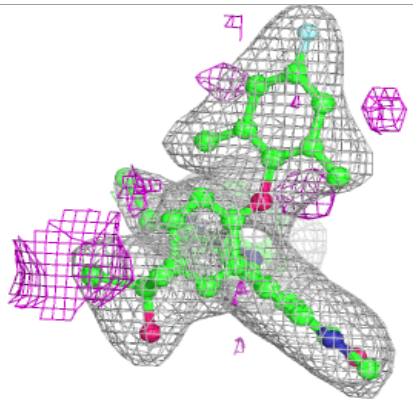


Electron density around A1L12 M 501:

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

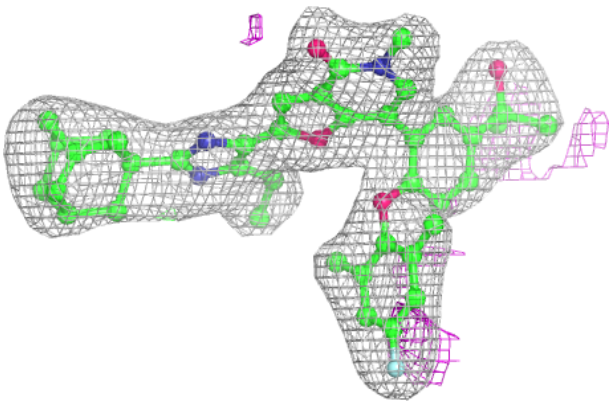


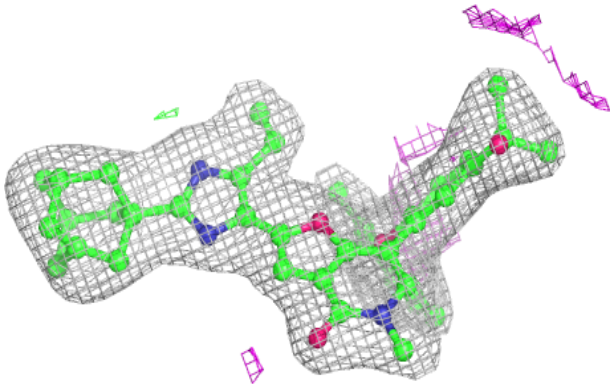


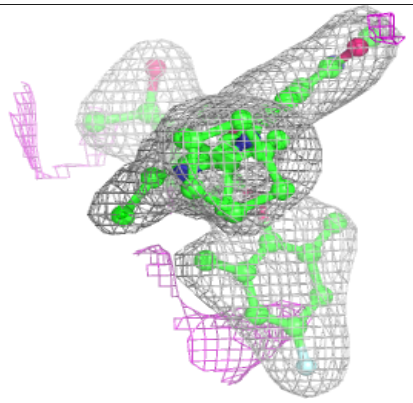


Electron density around A1L12 N 501:

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

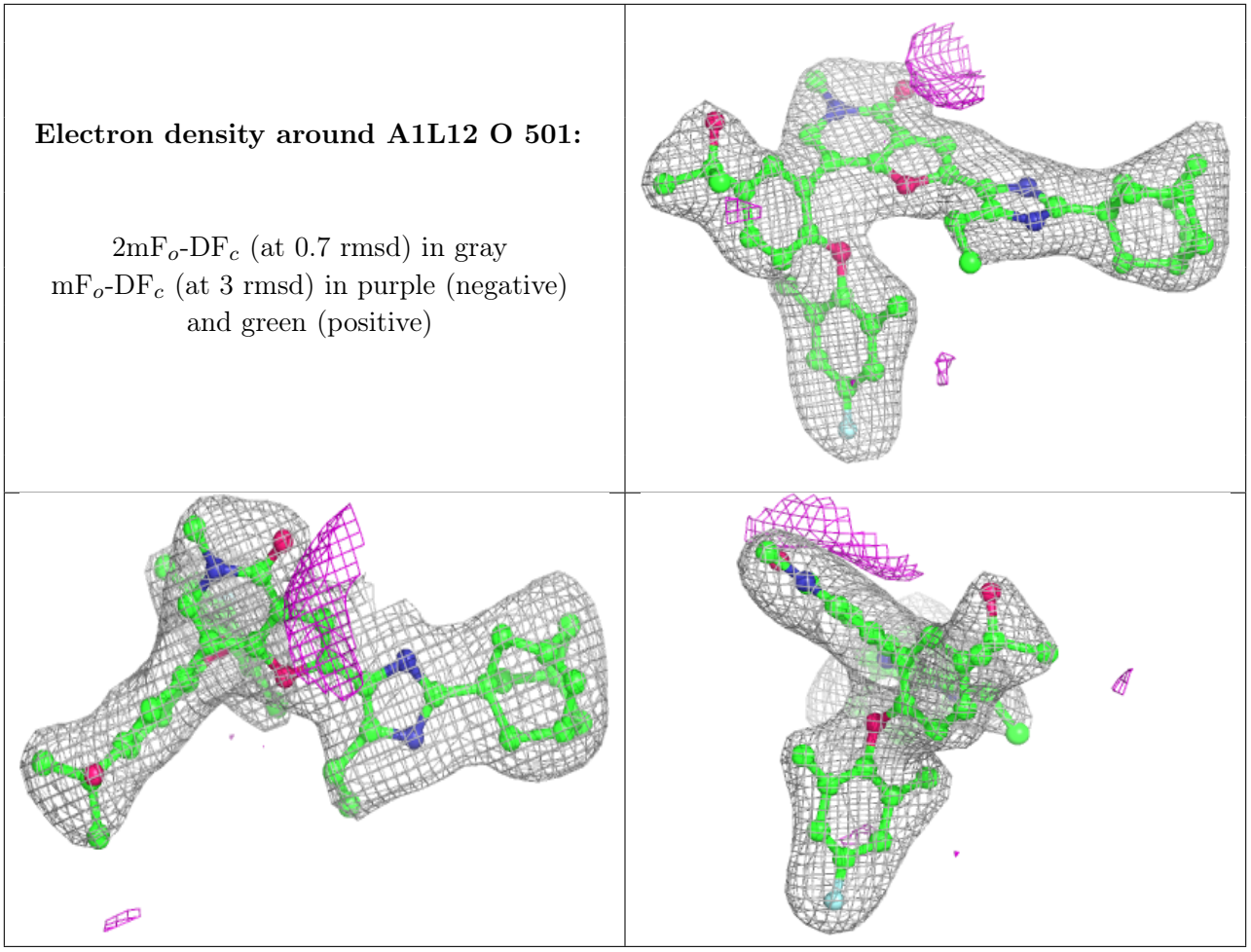






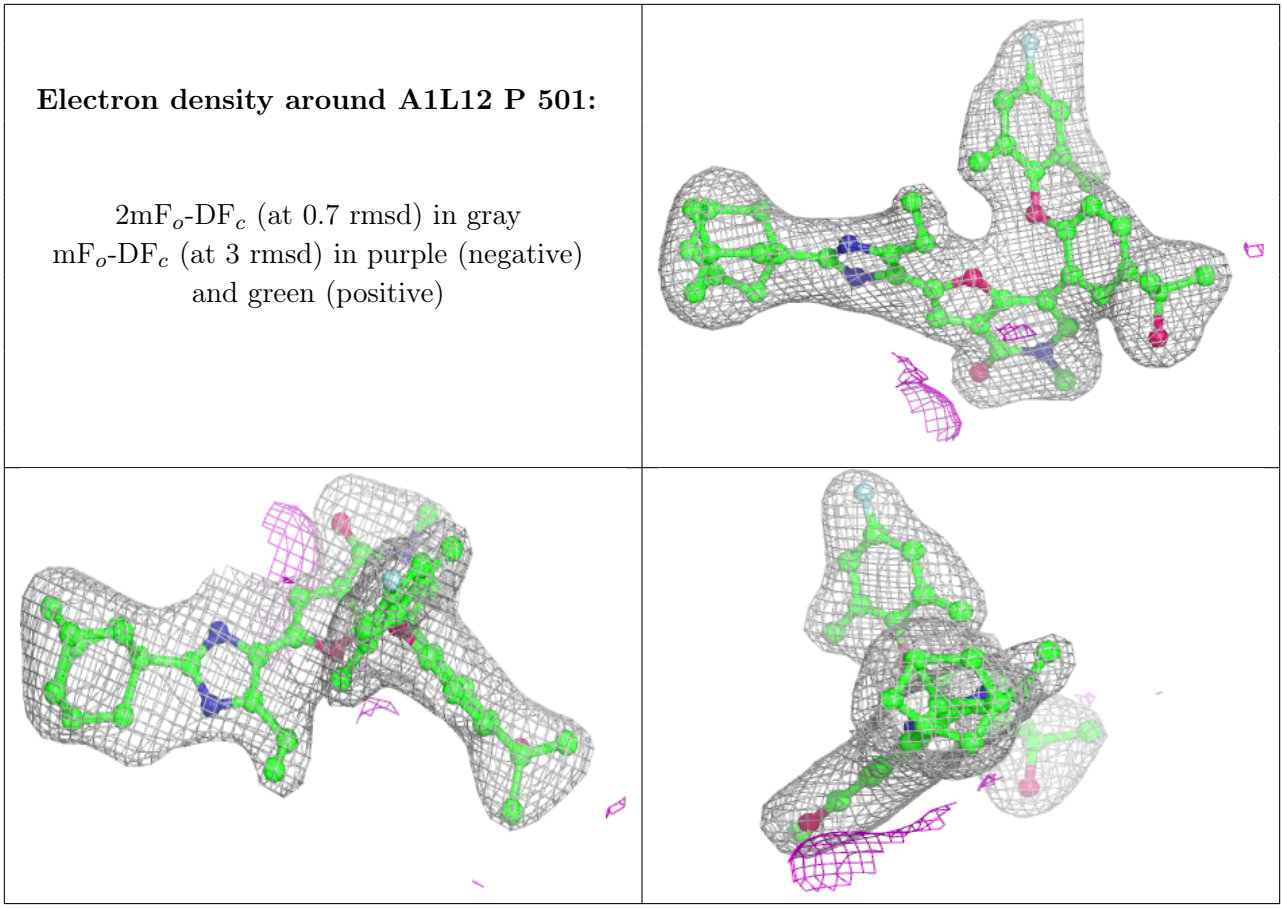
Electron density around A1L12 O 501:

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



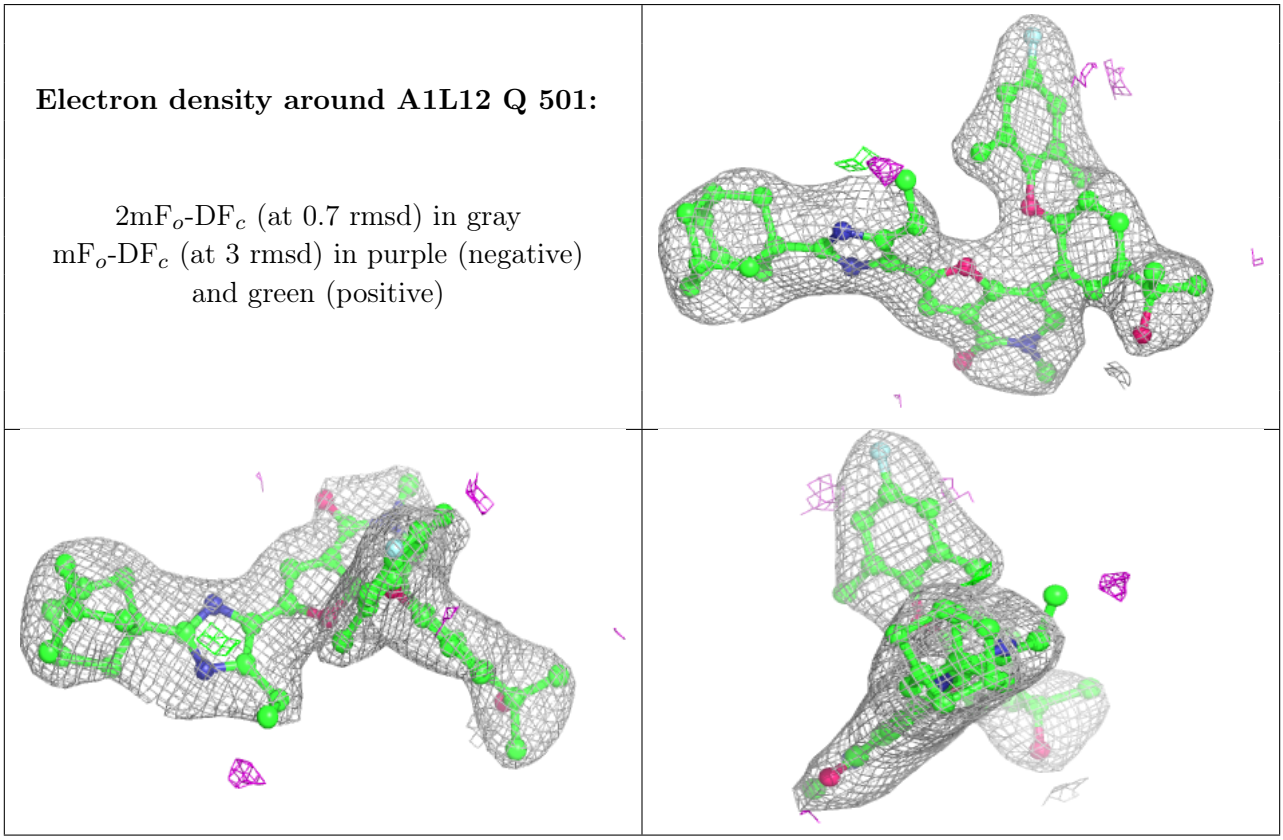
Electron density around A1L12 P 501:

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



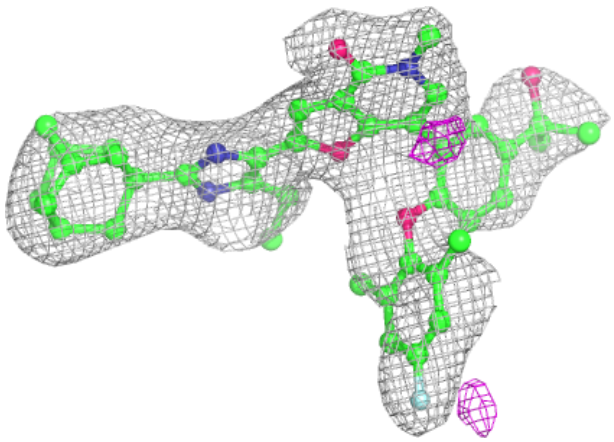
Electron density around A1L12 Q 501:

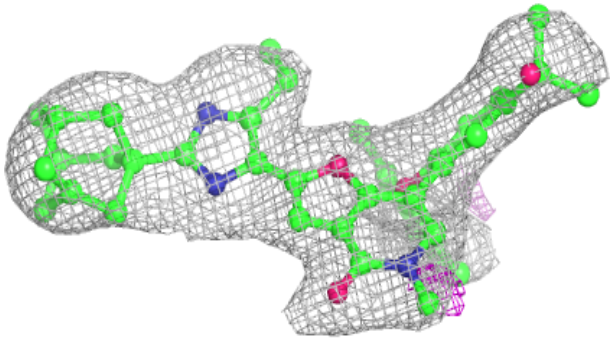
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

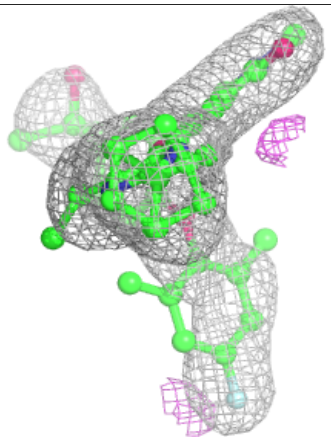


Electron density around A1L12 R 501:

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

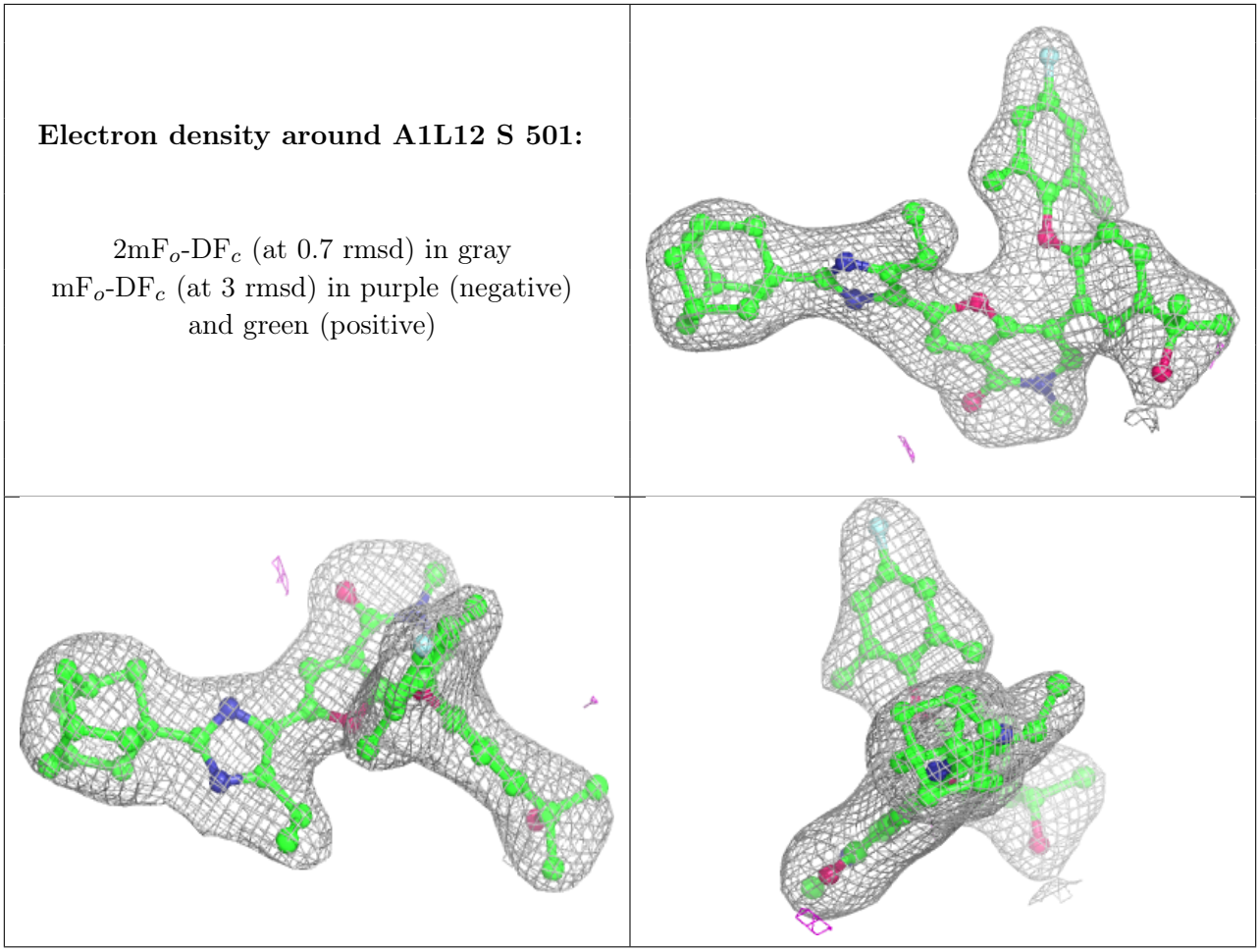






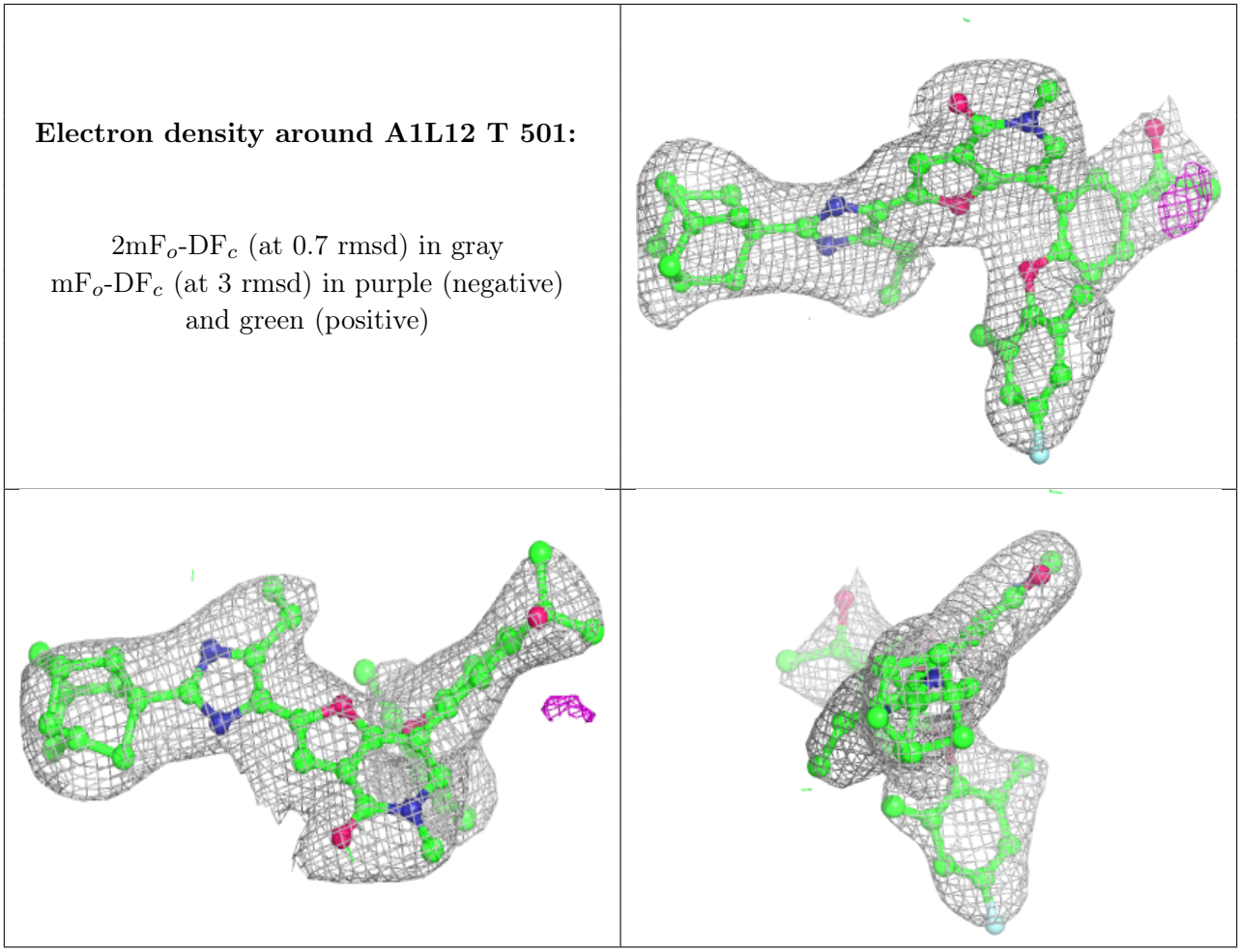
Electron density around A1L12 S 501:

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



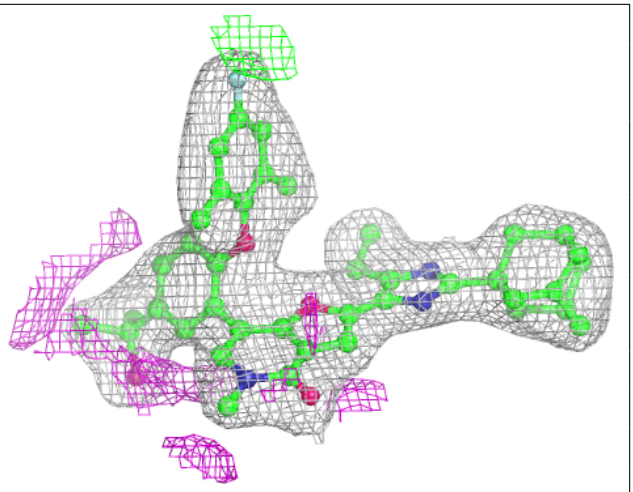
Electron density around A1L12 T 501:

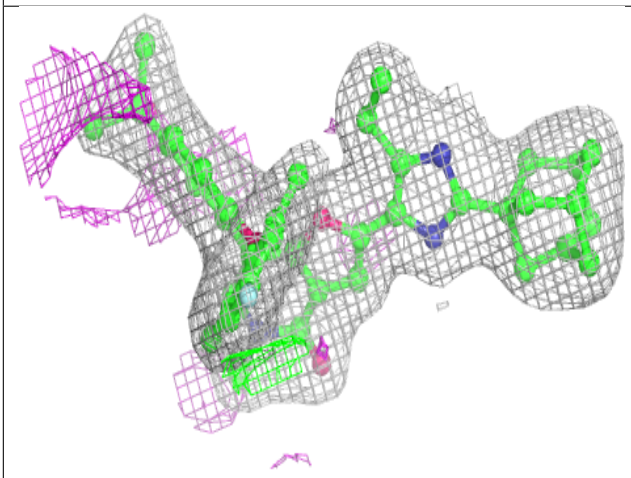
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

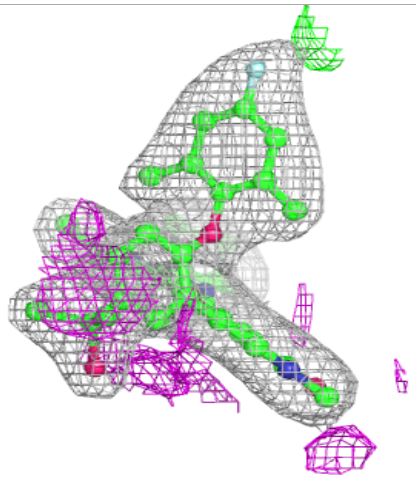


Electron density around A1L12 A 501:

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

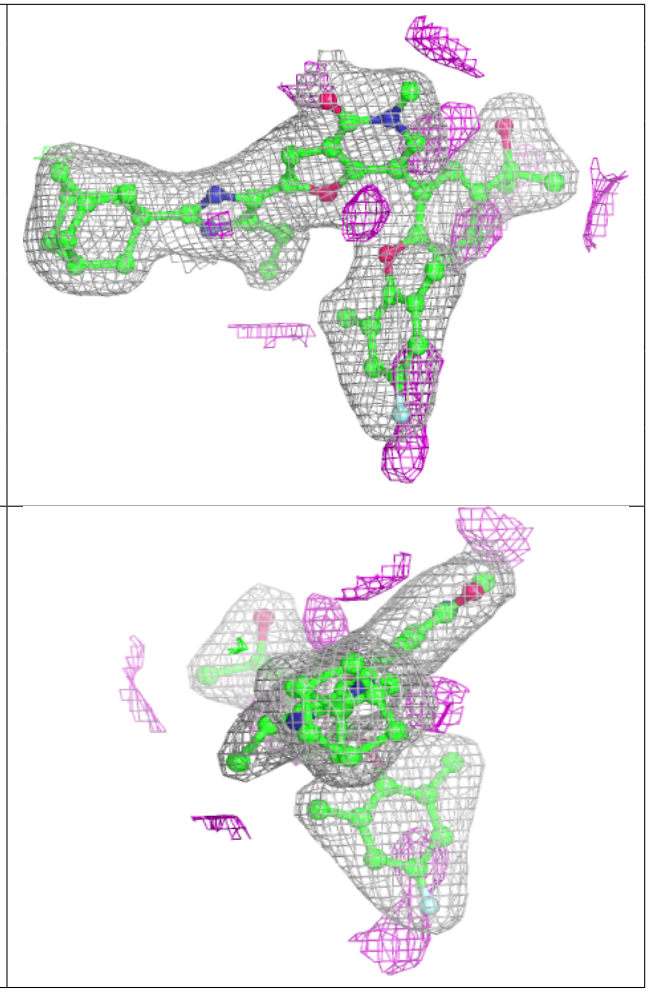






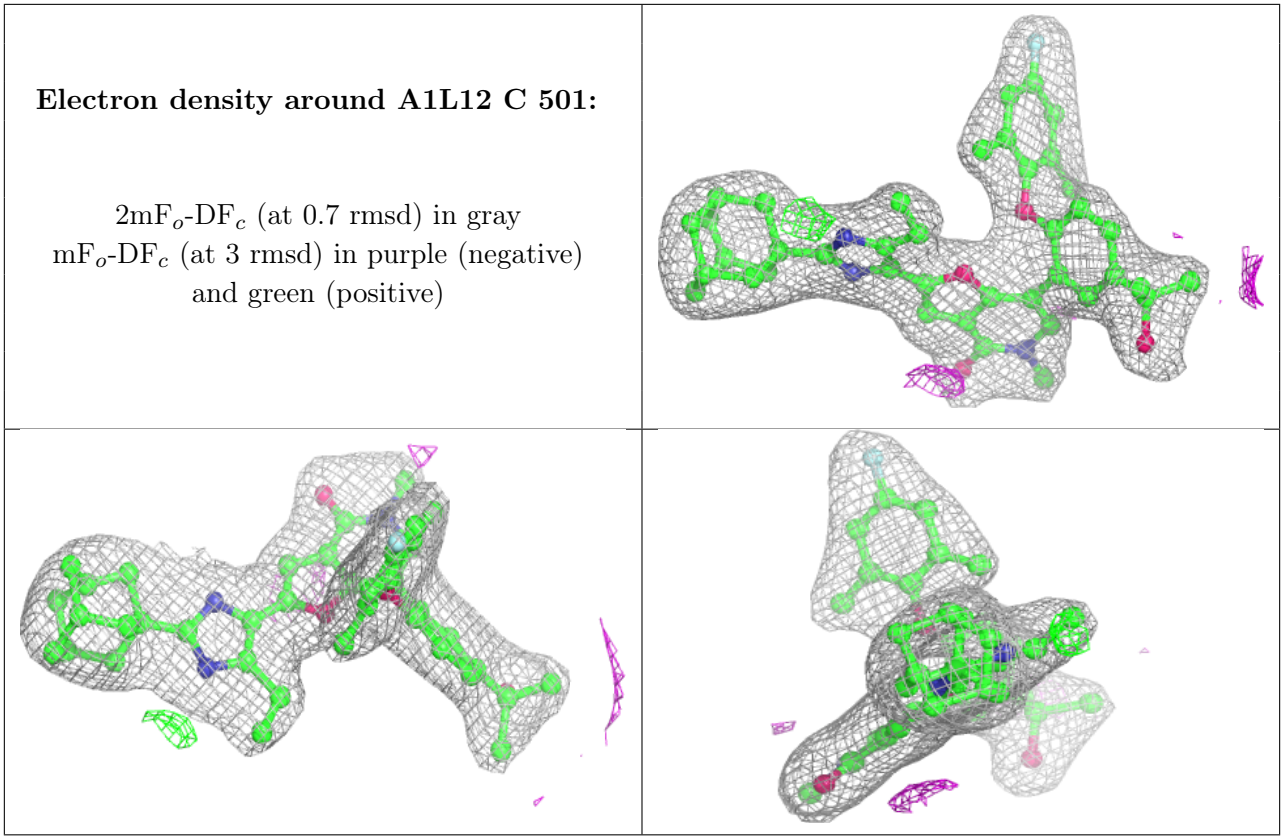
Electron density around A1L12 B 502:

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



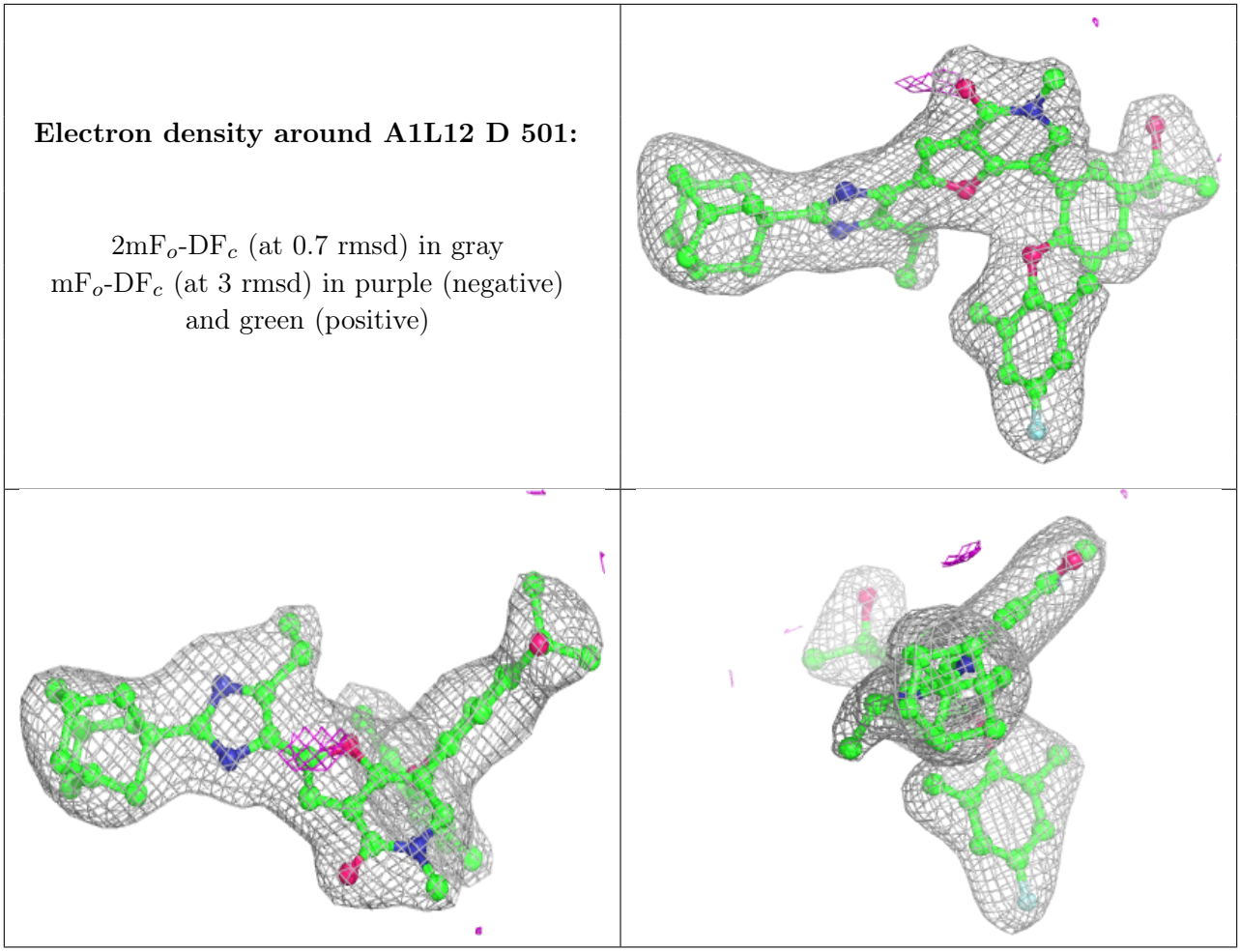
Electron density around A1L12 C 501:

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



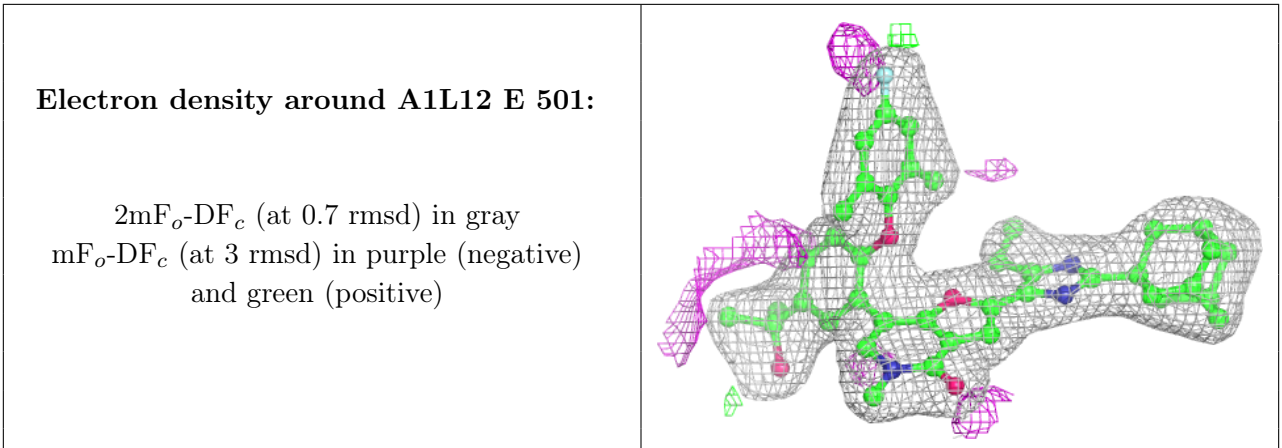
Electron density around A1L12 D 501:

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



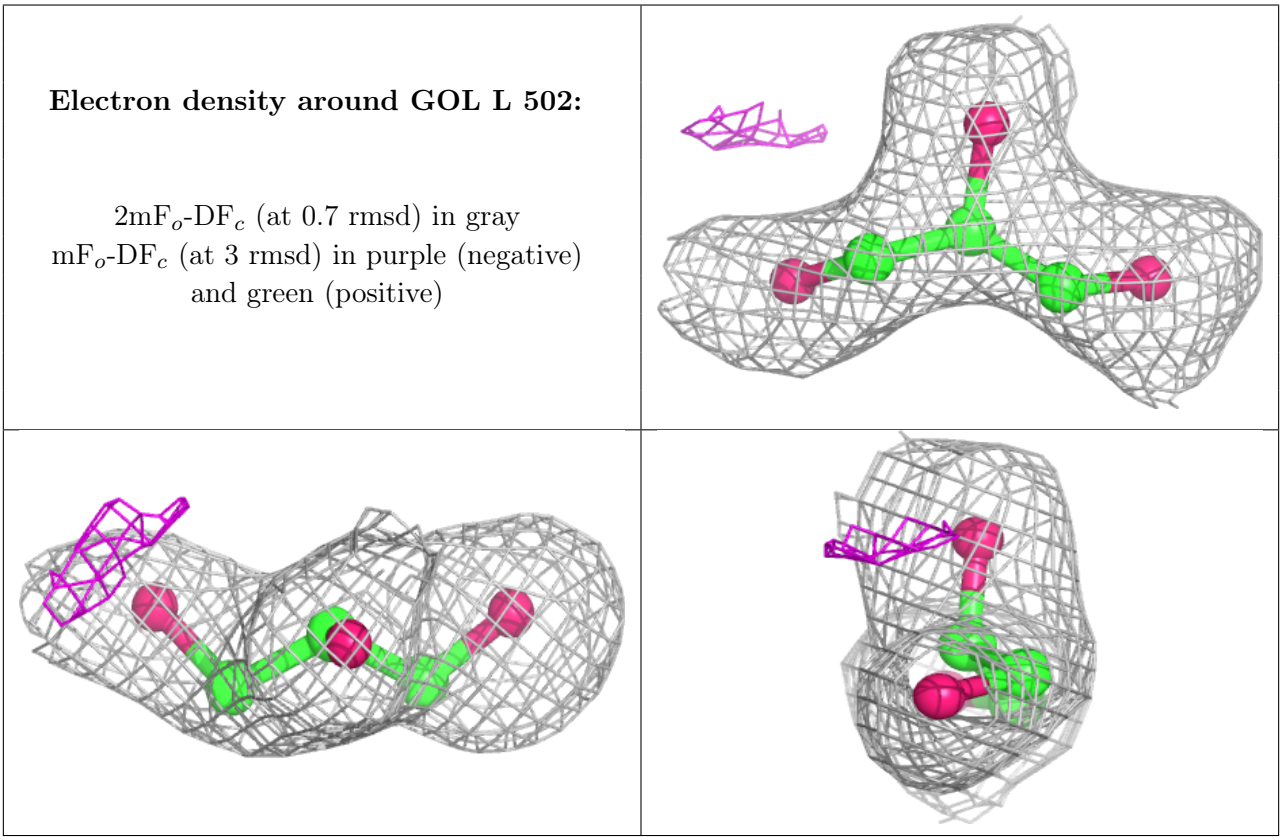
Electron density around A1L12 E 501:

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



Electron density around GOL 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)



6.5 Other polymers (i)

There are no such residues in this entry.