Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:02 am BST

PDB ID	:	5GM2
Title	:	Crystal structure of methyltransferase TleD complexed with SAH and teleocidin A1
Authors	:	Yu, F.; Li, M.J.; Xu, C.Y.; Zhou, H.; Sun, B.; Wang, Z.J.; Xu, Q.; Xie, M.Y.; Zuo, G.; Huang, P.; Wang, Q.S.; He, J.H.
Deposited on	:	2016-07-12
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

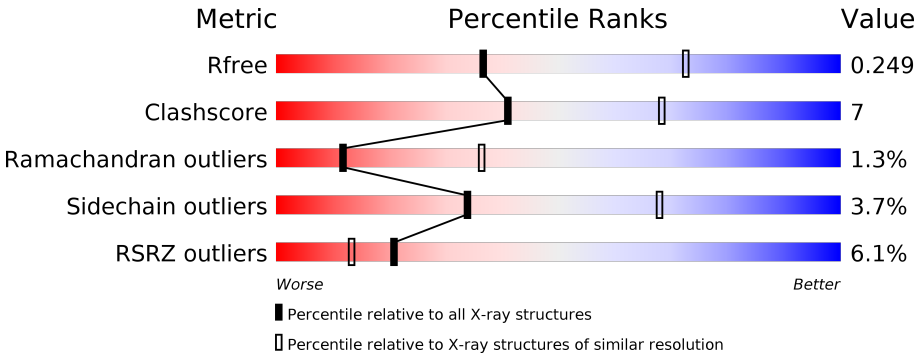
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	297	79% 14% • 5%
1	B	297	% 79% 13% • 5%
1	C	297	4% 71% 21% • 6%
1	D	297	% 80% 12% • 5%
1	E	297	81% 11% • 6%
1	F	297	76% 16% • 6%

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Mol	Chain	Length	Quality of chain
1	G	297	6% 75% 13% • 10%
1	H	297	21% 73% 20% • 5%
1	I	297	72% 14% • 10%
1	J	297	15% 75% 14% • 8%
1	K	297	8% 75% 14% • 10%
1	L	297	4% 75% 13% • 11%
1	M	297	% 72% 15% • 11%
1	N	297	13% 72% 19% • 8%
1	O	297	% 81% 12% • 6%
1	P	297	4% 78% 14% • 6%
1	Q	297	4% 76% 12% • 10%
1	R	297	17% 63% 26% • 8%

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	SAH	H	301	-	-	-	X
2	SAH	J	301	-	-	-	X
2	SAH	K	301	-	-	-	X
2	SAH	N	301	-	-	-	X
2	SAH	R	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39205 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 O-methylransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2166	1375	367	413	11			
1	B	282	Total	C	N	O	S	0	0	0
			2175	1380	369	415	11			
1	C	279	Total	C	N	O	S	11	1	0
			2160	1370	368	411	11			
1	D	281	Total	C	N	O	S	0	0	0
			2166	1375	367	413	11			
1	E	279	Total	C	N	O	S	0	0	0
			2149	1364	364	410	11			
1	F	279	Total	C	N	O	S	0	0	0
			2149	1364	364	410	11			
1	G	266	Total	C	N	O	S	0	0	0
			2042	1297	348	386	11			
1	H	281	Total	C	N	O	S	0	0	0
			2166	1375	367	413	11			
1	I	266	Total	C	N	O	S	9	1	0
			2051	1302	349	389	11			
1	J	272	Total	C	N	O	S	0	0	0
			2094	1330	354	399	11			
1	K	267	Total	C	N	O	S	0	0	0
			2060	1300	355	394	11			
1	L	263	Total	C	N	O	S	0	0	0
			2021	1284	345	381	11			
1	M	264	Total	C	N	O	S	0	0	0
			2027	1286	346	384	11			
1	N	274	Total	C	N	O	S	0	0	0
			2113	1340	359	403	11			
1	O	279	Total	C	N	O	S	0	0	0
			2149	1364	364	410	11			
1	P	279	Total	C	N	O	S	0	0	0
			2149	1364	364	410	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	266	Total	C	N	O	S	0	0	0
			2042	1297	348	386	11			
1	R	273	Total	C	N	O	S	0	0	0
			2116	1345	359	402	10			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	LEU	-	expression tag	UNP A0A077K7L1
A	291	GLU	-	expression tag	UNP A0A077K7L1
A	292	HIS	-	expression tag	UNP A0A077K7L1
A	293	HIS	-	expression tag	UNP A0A077K7L1
A	294	HIS	-	expression tag	UNP A0A077K7L1
A	295	HIS	-	expression tag	UNP A0A077K7L1
A	296	HIS	-	expression tag	UNP A0A077K7L1
A	297	HIS	-	expression tag	UNP A0A077K7L1
B	290	LEU	-	expression tag	UNP A0A077K7L1
B	291	GLU	-	expression tag	UNP A0A077K7L1
B	292	HIS	-	expression tag	UNP A0A077K7L1
B	293	HIS	-	expression tag	UNP A0A077K7L1
B	294	HIS	-	expression tag	UNP A0A077K7L1
B	295	HIS	-	expression tag	UNP A0A077K7L1
B	296	HIS	-	expression tag	UNP A0A077K7L1
B	297	HIS	-	expression tag	UNP A0A077K7L1
C	290	LEU	-	expression tag	UNP A0A077K7L1
C	291	GLU	-	expression tag	UNP A0A077K7L1
C	292	HIS	-	expression tag	UNP A0A077K7L1
C	293	HIS	-	expression tag	UNP A0A077K7L1
C	294	HIS	-	expression tag	UNP A0A077K7L1
C	295	HIS	-	expression tag	UNP A0A077K7L1
C	296	HIS	-	expression tag	UNP A0A077K7L1
C	297	HIS	-	expression tag	UNP A0A077K7L1
D	290	LEU	-	expression tag	UNP A0A077K7L1
D	291	GLU	-	expression tag	UNP A0A077K7L1
D	292	HIS	-	expression tag	UNP A0A077K7L1
D	293	HIS	-	expression tag	UNP A0A077K7L1
D	294	HIS	-	expression tag	UNP A0A077K7L1
D	295	HIS	-	expression tag	UNP A0A077K7L1
D	296	HIS	-	expression tag	UNP A0A077K7L1
D	297	HIS	-	expression tag	UNP A0A077K7L1
E	290	LEU	-	expression tag	UNP A0A077K7L1
E	291	GLU	-	expression tag	UNP A0A077K7L1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	292	HIS	-	expression tag	UNP A0A077K7L1
E	293	HIS	-	expression tag	UNP A0A077K7L1
E	294	HIS	-	expression tag	UNP A0A077K7L1
E	295	HIS	-	expression tag	UNP A0A077K7L1
E	296	HIS	-	expression tag	UNP A0A077K7L1
E	297	HIS	-	expression tag	UNP A0A077K7L1
F	290	LEU	-	expression tag	UNP A0A077K7L1
F	291	GLU	-	expression tag	UNP A0A077K7L1
F	292	HIS	-	expression tag	UNP A0A077K7L1
F	293	HIS	-	expression tag	UNP A0A077K7L1
F	294	HIS	-	expression tag	UNP A0A077K7L1
F	295	HIS	-	expression tag	UNP A0A077K7L1
F	296	HIS	-	expression tag	UNP A0A077K7L1
F	297	HIS	-	expression tag	UNP A0A077K7L1
G	290	LEU	-	expression tag	UNP A0A077K7L1
G	291	GLU	-	expression tag	UNP A0A077K7L1
G	292	HIS	-	expression tag	UNP A0A077K7L1
G	293	HIS	-	expression tag	UNP A0A077K7L1
G	294	HIS	-	expression tag	UNP A0A077K7L1
G	295	HIS	-	expression tag	UNP A0A077K7L1
G	296	HIS	-	expression tag	UNP A0A077K7L1
G	297	HIS	-	expression tag	UNP A0A077K7L1
H	290	LEU	-	expression tag	UNP A0A077K7L1
H	291	GLU	-	expression tag	UNP A0A077K7L1
H	292	HIS	-	expression tag	UNP A0A077K7L1
H	293	HIS	-	expression tag	UNP A0A077K7L1
H	294	HIS	-	expression tag	UNP A0A077K7L1
H	295	HIS	-	expression tag	UNP A0A077K7L1
H	296	HIS	-	expression tag	UNP A0A077K7L1
H	297	HIS	-	expression tag	UNP A0A077K7L1
I	290	LEU	-	expression tag	UNP A0A077K7L1
I	291	GLU	-	expression tag	UNP A0A077K7L1
I	292	HIS	-	expression tag	UNP A0A077K7L1
I	293	HIS	-	expression tag	UNP A0A077K7L1
I	294	HIS	-	expression tag	UNP A0A077K7L1
I	295	HIS	-	expression tag	UNP A0A077K7L1
I	296	HIS	-	expression tag	UNP A0A077K7L1
I	297	HIS	-	expression tag	UNP A0A077K7L1
J	290	LEU	-	expression tag	UNP A0A077K7L1
J	291	GLU	-	expression tag	UNP A0A077K7L1
J	292	HIS	-	expression tag	UNP A0A077K7L1
J	293	HIS	-	expression tag	UNP A0A077K7L1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	294	HIS	-	expression tag	UNP A0A077K7L1
J	295	HIS	-	expression tag	UNP A0A077K7L1
J	296	HIS	-	expression tag	UNP A0A077K7L1
J	297	HIS	-	expression tag	UNP A0A077K7L1
K	290	LEU	-	expression tag	UNP A0A077K7L1
K	291	GLU	-	expression tag	UNP A0A077K7L1
K	292	HIS	-	expression tag	UNP A0A077K7L1
K	293	HIS	-	expression tag	UNP A0A077K7L1
K	294	HIS	-	expression tag	UNP A0A077K7L1
K	295	HIS	-	expression tag	UNP A0A077K7L1
K	296	HIS	-	expression tag	UNP A0A077K7L1
K	297	HIS	-	expression tag	UNP A0A077K7L1
L	290	LEU	-	expression tag	UNP A0A077K7L1
L	291	GLU	-	expression tag	UNP A0A077K7L1
L	292	HIS	-	expression tag	UNP A0A077K7L1
L	293	HIS	-	expression tag	UNP A0A077K7L1
L	294	HIS	-	expression tag	UNP A0A077K7L1
L	295	HIS	-	expression tag	UNP A0A077K7L1
L	296	HIS	-	expression tag	UNP A0A077K7L1
L	297	HIS	-	expression tag	UNP A0A077K7L1
M	290	LEU	-	expression tag	UNP A0A077K7L1
M	291	GLU	-	expression tag	UNP A0A077K7L1
M	292	HIS	-	expression tag	UNP A0A077K7L1
M	293	HIS	-	expression tag	UNP A0A077K7L1
M	294	HIS	-	expression tag	UNP A0A077K7L1
M	295	HIS	-	expression tag	UNP A0A077K7L1
M	296	HIS	-	expression tag	UNP A0A077K7L1
M	297	HIS	-	expression tag	UNP A0A077K7L1
N	290	LEU	-	expression tag	UNP A0A077K7L1
N	291	GLU	-	expression tag	UNP A0A077K7L1
N	292	HIS	-	expression tag	UNP A0A077K7L1
N	293	HIS	-	expression tag	UNP A0A077K7L1
N	294	HIS	-	expression tag	UNP A0A077K7L1
N	295	HIS	-	expression tag	UNP A0A077K7L1
N	296	HIS	-	expression tag	UNP A0A077K7L1
N	297	HIS	-	expression tag	UNP A0A077K7L1
O	290	LEU	-	expression tag	UNP A0A077K7L1
O	291	GLU	-	expression tag	UNP A0A077K7L1
O	292	HIS	-	expression tag	UNP A0A077K7L1
O	293	HIS	-	expression tag	UNP A0A077K7L1
O	294	HIS	-	expression tag	UNP A0A077K7L1
O	295	HIS	-	expression tag	UNP A0A077K7L1

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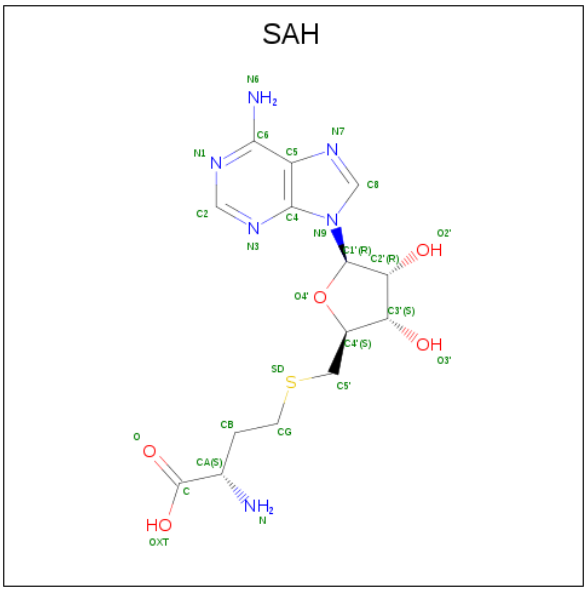
Chain	Residue	Modelled	Actual	Comment	Reference
O	296	HIS	-	expression tag	UNP A0A077K7L1
O	297	HIS	-	expression tag	UNP A0A077K7L1
P	290	LEU	-	expression tag	UNP A0A077K7L1
P	291	GLU	-	expression tag	UNP A0A077K7L1
P	292	HIS	-	expression tag	UNP A0A077K7L1
P	293	HIS	-	expression tag	UNP A0A077K7L1
P	294	HIS	-	expression tag	UNP A0A077K7L1
P	295	HIS	-	expression tag	UNP A0A077K7L1
P	296	HIS	-	expression tag	UNP A0A077K7L1
P	297	HIS	-	expression tag	UNP A0A077K7L1
Q	290	LEU	-	expression tag	UNP A0A077K7L1
Q	291	GLU	-	expression tag	UNP A0A077K7L1
Q	292	HIS	-	expression tag	UNP A0A077K7L1
Q	293	HIS	-	expression tag	UNP A0A077K7L1
Q	294	HIS	-	expression tag	UNP A0A077K7L1
Q	295	HIS	-	expression tag	UNP A0A077K7L1
Q	296	HIS	-	expression tag	UNP A0A077K7L1
Q	297	HIS	-	expression tag	UNP A0A077K7L1
R	290	LEU	-	expression tag	UNP A0A077K7L1
R	291	GLU	-	expression tag	UNP A0A077K7L1
R	292	HIS	-	expression tag	UNP A0A077K7L1
R	293	HIS	-	expression tag	UNP A0A077K7L1
R	294	HIS	-	expression tag	UNP A0A077K7L1
R	295	HIS	-	expression tag	UNP A0A077K7L1
R	296	HIS	-	expression tag	UNP A0A077K7L1
R	297	HIS	-	expression tag	UNP A0A077K7L1

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	I	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	J	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	K	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	L	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	M	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	N	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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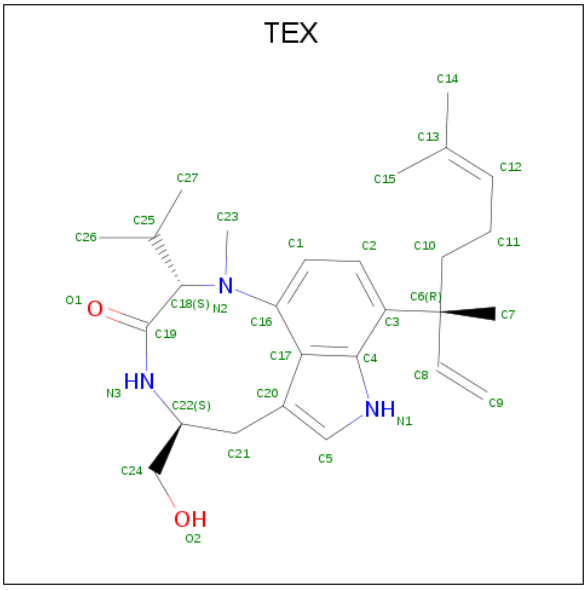
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	P	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	Q	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	R	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is (2S,5S)-9-[(3R)-3,7-dimethylocta-1,6-dien-3-yl]-5-(hydroxymethyl)-1-methyl-2-(propan-2-yl)-1,2,4,5,6,8-hexahydro-3H-[1,4]diazonino[7,6,5-cd]indol-3-one (three-letter code: TEX) (formula: $C_{27}H_{39}N_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			32	27	3	2			
3	B	1	Total	C	N	O		0	0
			32	27	3	2			
3	C	1	Total	C	N	O		0	0
			32	27	3	2			
3	D	1	Total	C	N	O		0	0
			32	27	3	2			
3	E	1	Total	C	N	O		0	0
			32	27	3	2			
3	F	1	Total	C	N	O		0	0
			32	27	3	2			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			32	27	3	2		
3	H	1	Total	C	N	O	0	0
			32	27	3	2		
3	I	1	Total	C	N	O	0	0
			32	27	3	2		
3	J	1	Total	C	N	O	0	0
			32	27	3	2		
3	K	1	Total	C	N	O	0	0
			32	27	3	2		
3	L	1	Total	C	N	O	0	0
			32	27	3	2		
3	M	1	Total	C	N	O	0	0
			32	27	3	2		
3	N	1	Total	C	N	O	0	0
			32	27	3	2		
3	O	1	Total	C	N	O	0	0
			32	27	3	2		
3	P	1	Total	C	N	O	0	0
			32	27	3	2		
3	Q	1	Total	C	N	O	0	0
			32	27	3	2		
3	R	1	Total	C	N	O	0	0
			32	27	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	19	Total	O	0	0
			19	19		
4	C	9	Total	O	0	0
			9	9		
4	D	11	Total	O	0	0
			11	11		
4	E	12	Total	O	0	0
			12	12		
4	F	28	Total	O	0	0
			28	28		
4	G	7	Total	O	0	0
			7	7		

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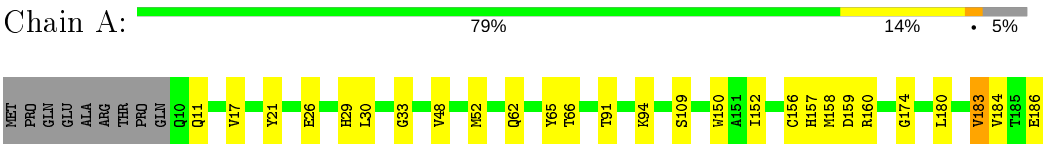
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	4	Total O 4 4	0	0
4	I	14	Total O 14 14	0	0
4	J	2	Total O 2 2	0	0
4	K	3	Total O 3 3	0	0
4	L	3	Total O 3 3	0	0
4	M	5	Total O 5 5	0	0
4	N	5	Total O 5 5	0	0
4	O	8	Total O 8 8	0	0
4	P	2	Total O 2 2	0	0
4	Q	2	Total O 2 2	0	0
4	R	11	Total O 11 11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

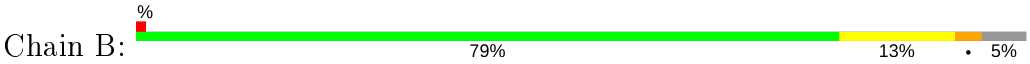
- Molecule 1: O-methylransferase

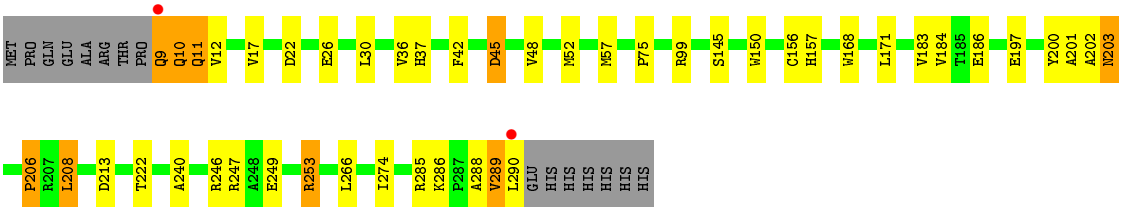
Chain A:



- Molecule 1: O-methylransferase

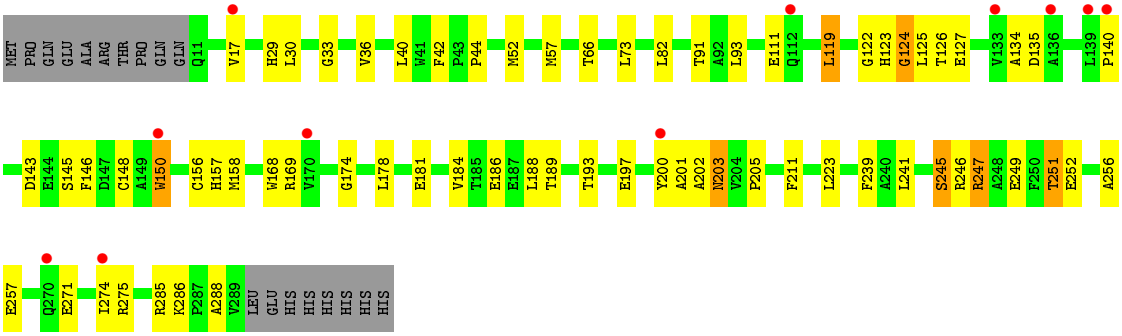
Chain B:





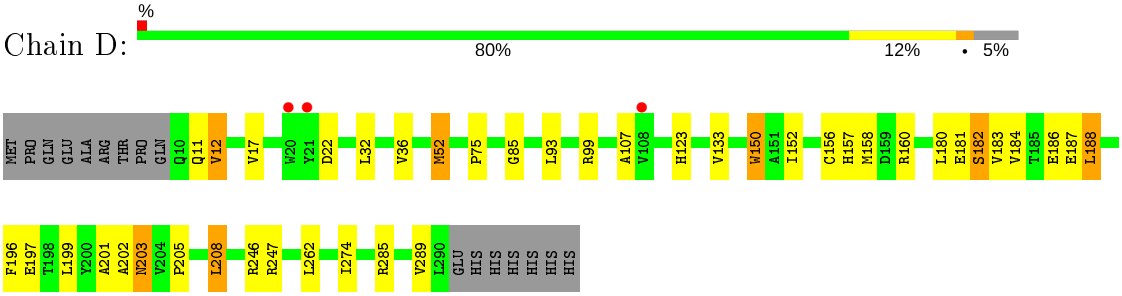
- Molecule 1: O-methylransferase

Chain C:



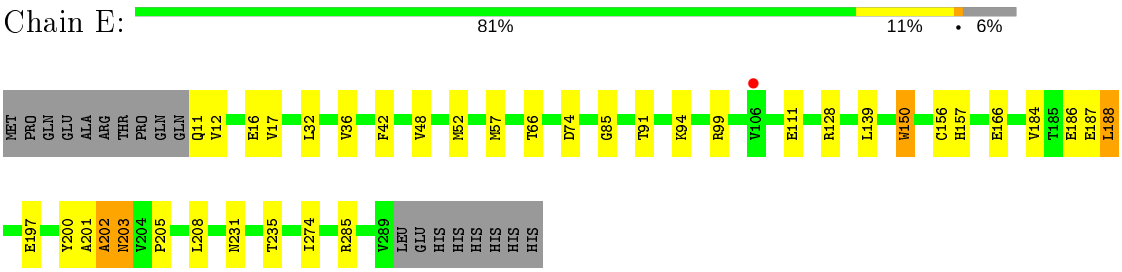
- Molecule 1: O-methylransferase

Chain D:



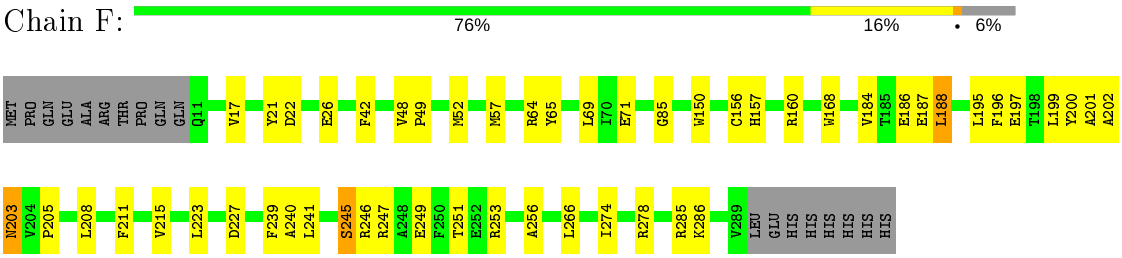
• Molecule 1: O-methylransferase

Chain E:



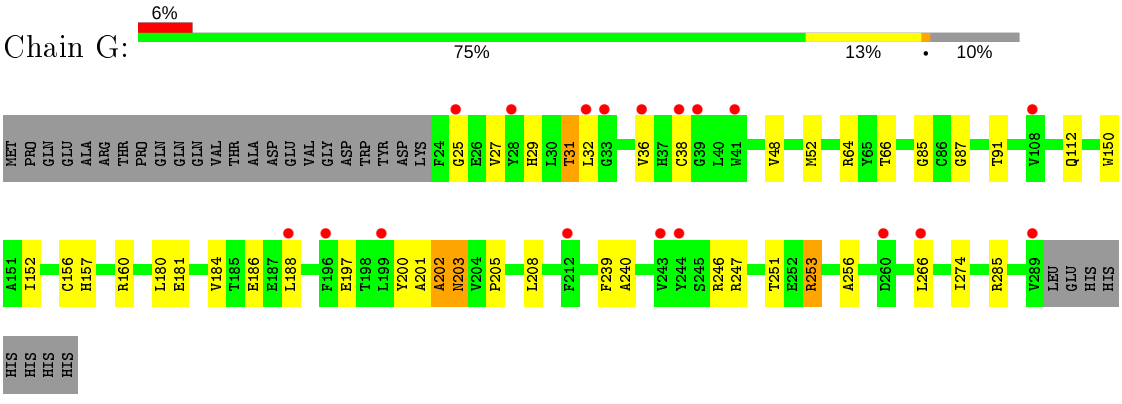
• Molecule 1: O-methylransferase

Chain F:



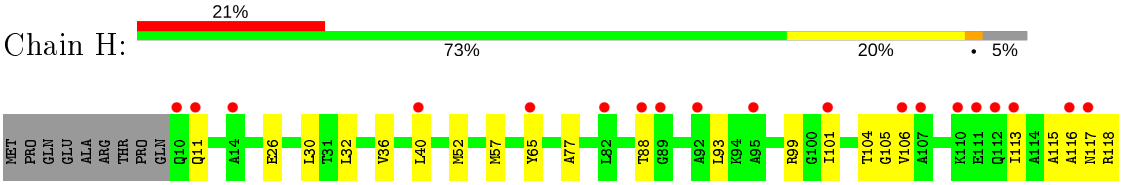
• Molecule 1: O-methylransferase

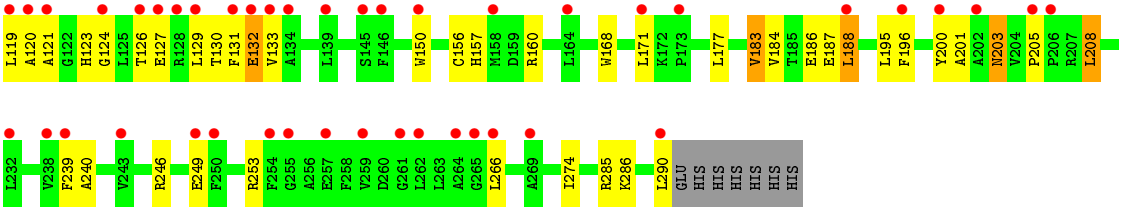
Chain G:



• Molecule 1: O-methylransferase

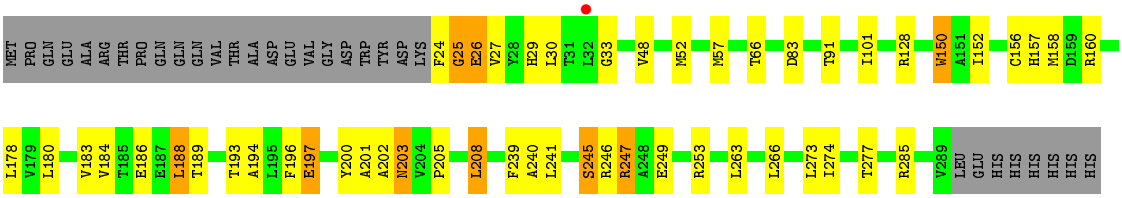
Chain H:





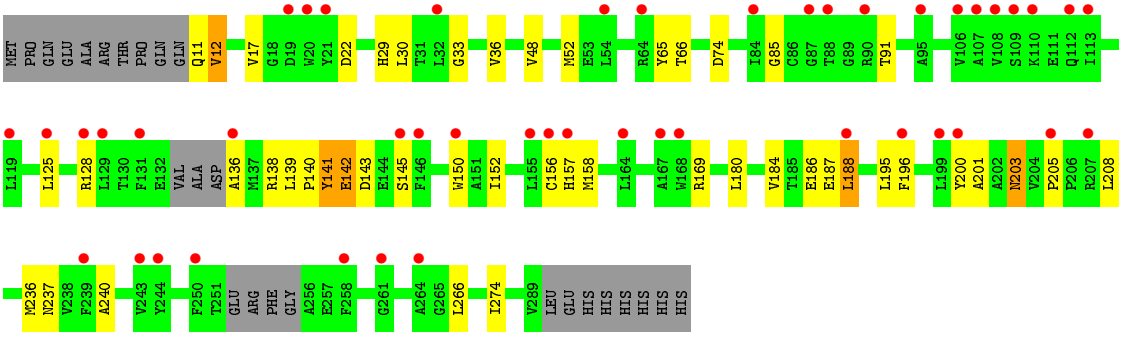
• Molecule 1: O-methylransferase

Chain I:



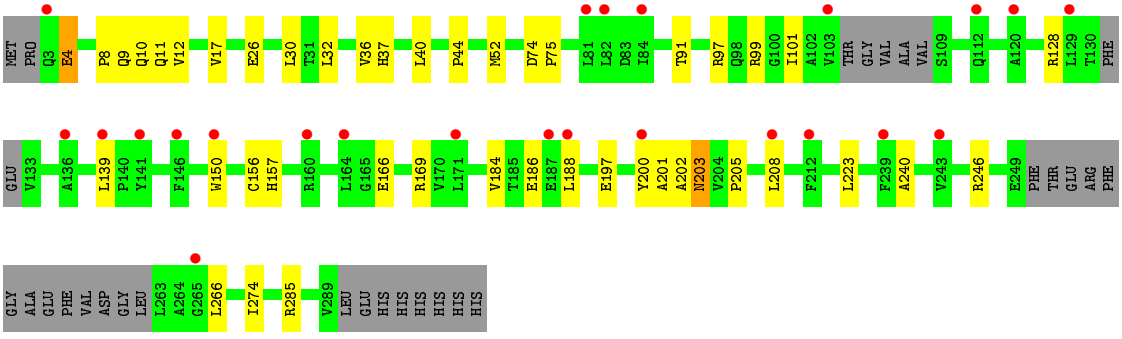
• Molecule 1: O-methylransferase

Chain J:



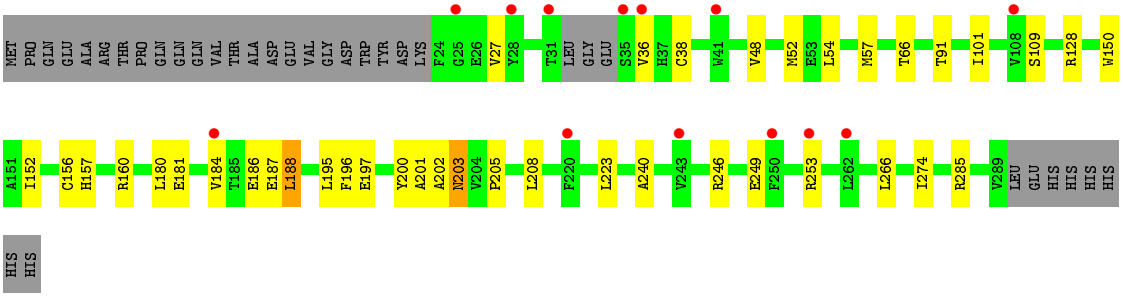
• Molecule 1: O-methylransferase

Chain K:



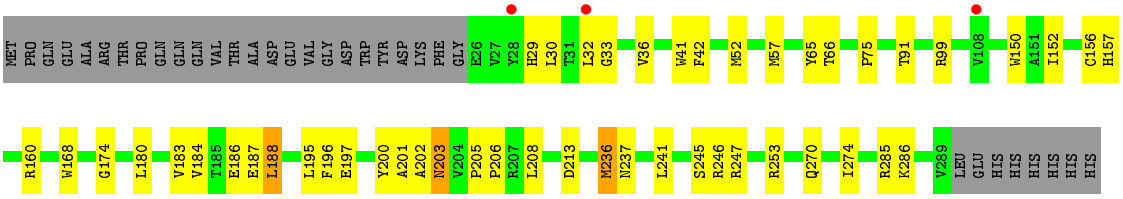
• Molecule 1: O-methylransferase

Chain L:



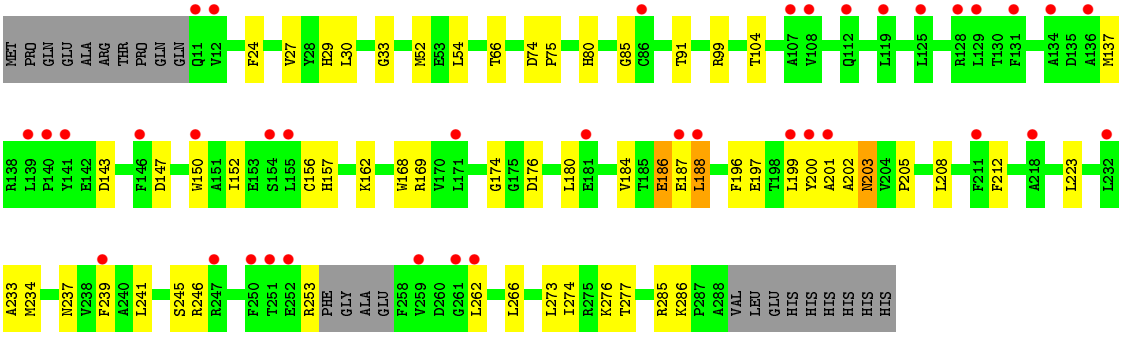
• Molecule 1: O-methylransferase

Chain M:



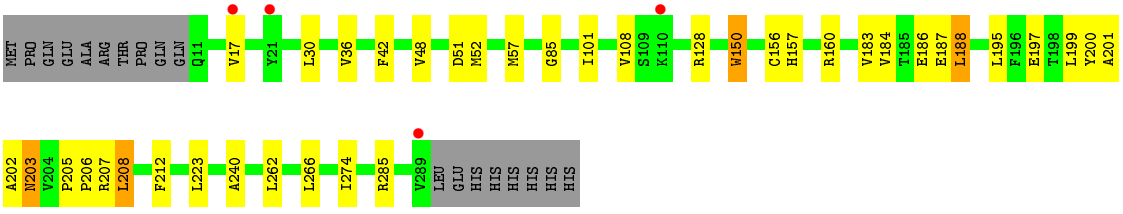
• Molecule 1: O-methylransferase

Chain N:



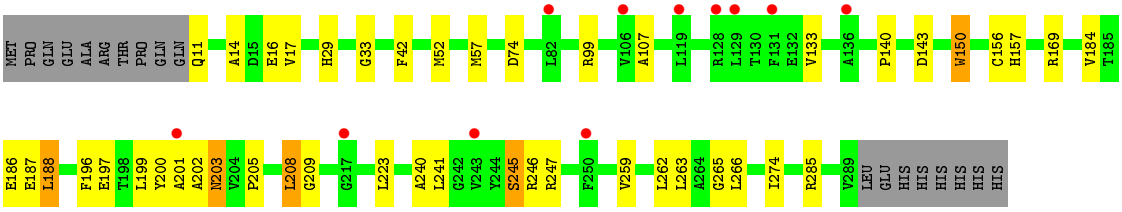
• Molecule 1: O-methylransferase

Chain O:



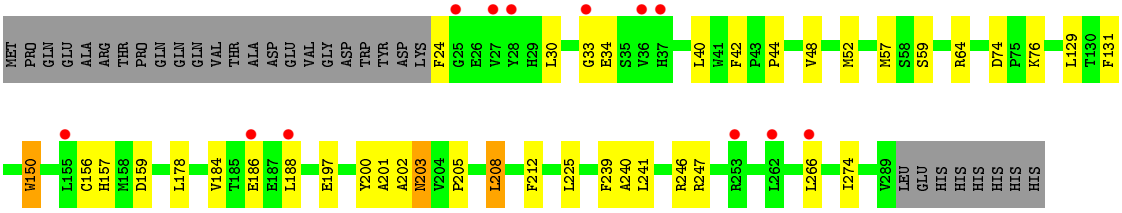
• Molecule 1: O-methylransferase

Chain P:



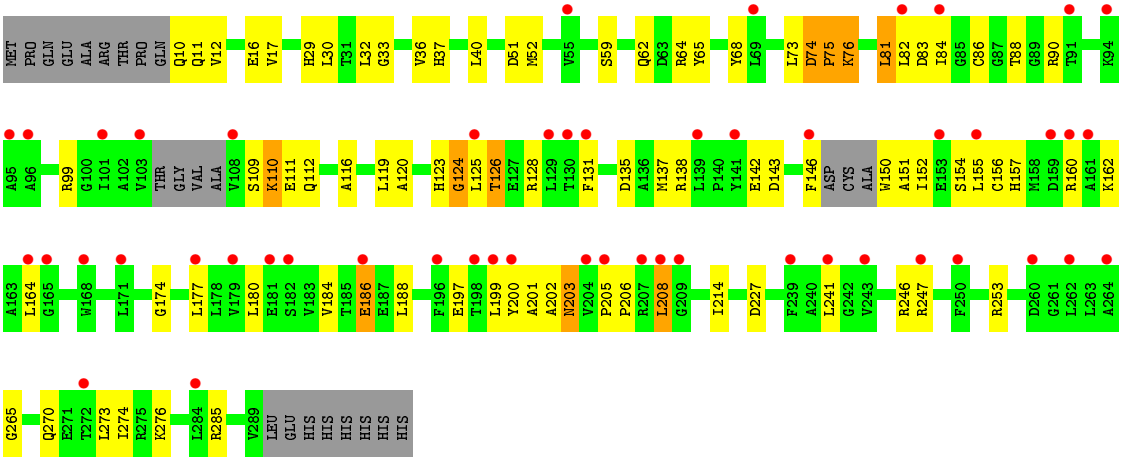
- Molecule 1: O-methylransferase

Chain Q:



- Molecule 1: O-methylransferase

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	257.46Å 152.76Å 154.17Å 90.00° 93.06° 90.00°	Depositor
Resolution (Å)	153.95 – 2.80 153.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.95-2.80) 99.8 (153.95-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.207 , 0.249 0.207 , 0.249	Depositor DCC
R_{free} test set	7113 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.010 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	39205	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TEX, SAH

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	0.26	0/2211	0.48	0/3001
1	B	0.26	0/2220	0.47	0/3013
1	C	0.25	0/2205	0.47	0/2992
1	D	0.25	0/2211	0.46	0/3001
1	E	0.26	0/2194	0.47	0/2978
1	F	0.26	0/2194	0.47	0/2978
1	G	0.25	0/2084	0.45	0/2827
1	H	0.28	0/2211	0.47	0/3001
1	I	0.26	0/2093	0.47	0/2839
1	J	0.25	0/2136	0.44	0/2897
1	K	0.25	0/2099	0.46	0/2845
1	L	0.25	0/2062	0.45	0/2796
1	M	0.25	0/2068	0.45	0/2806
1	N	0.25	0/2156	0.46	0/2925
1	O	0.25	0/2194	0.46	0/2978
1	P	0.25	0/2194	0.44	0/2978
1	Q	0.26	0/2084	0.45	0/2827
1	R	0.25	0/2159	0.48	0/2926
All	All	0.26	0/38775	0.46	0/52608

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2166	0	2127	36	0
1	B	2175	0	2135	36	0
1	C	2160	0	2120	43	0
1	D	2166	0	2127	29	0
1	E	2149	0	2108	28	0
1	F	2149	0	2108	36	0
1	G	2042	0	2017	29	0
1	H	2166	0	2127	42	1
1	I	2051	0	2022	33	0
1	J	2094	0	2057	32	0
1	K	2060	0	2025	26	0
1	L	2021	0	1996	27	0
1	M	2027	0	2005	34	0
1	N	2113	0	2075	40	0
1	O	2149	0	2108	32	0
1	P	2149	0	2108	33	0
1	Q	2042	0	2017	33	0
1	R	2116	0	2076	64	1
2	A	26	0	19	2	0
2	B	26	0	19	0	0
2	C	26	0	19	1	0
2	D	26	0	19	3	0
2	E	26	0	19	1	0
2	F	26	0	19	2	0
2	G	26	0	19	2	0
2	H	26	0	19	1	0
2	I	26	0	19	2	0
2	J	26	0	19	2	0
2	K	26	0	19	1	0
2	L	26	0	19	1	0
2	M	26	0	19	0	0
2	N	26	0	19	2	0
2	O	26	0	19	2	0
2	P	26	0	19	2	0
2	Q	26	0	19	2	0
2	R	26	0	19	1	0
3	A	32	0	0	2	0
3	B	32	0	0	1	0
3	C	32	0	0	1	0
3	D	32	0	0	2	0
3	E	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	32	0	0	2	0
3	G	32	0	0	1	0
3	H	32	0	0	2	0
3	I	32	0	0	1	0
3	J	32	0	0	1	0
3	K	32	0	0	2	0
3	L	32	0	0	1	0
3	M	32	0	0	2	0
3	N	32	0	0	2	0
3	O	32	0	0	2	0
3	P	32	0	0	2	0
3	Q	32	0	0	1	0
3	R	32	0	0	1	0
4	A	21	0	0	2	0
4	B	19	0	0	2	0
4	C	9	0	0	3	0
4	D	11	0	0	0	0
4	E	12	0	0	2	0
4	F	28	0	0	3	0
4	G	7	0	0	2	0
4	H	4	0	0	3	0
4	I	14	0	0	1	0
4	J	2	0	0	1	0
4	K	3	0	0	1	0
4	L	3	0	0	0	0
4	M	5	0	0	1	0
4	N	5	0	0	1	0
4	O	8	0	0	1	0
4	P	2	0	0	0	0
4	Q	2	0	0	0	0
4	R	11	0	0	6	0
All	All	39205	0	37700	548	2

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 7.

All (548) 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:E:11:GLN:N	4:E:401:HOH:O	1.97	0.97
1:Q:159:ASP:HA	1:R:10:GLN:HE22	1.33	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:197:GLU:HA	1:L:202:ALA:HB2	1.59	0.85
1:D:184:VAL:HG13	1:D:205:PRO:HG2	1.58	0.84
1:F:184:VAL:HG13	1:F:205:PRO:HG2	1.59	0.84
1:N:80:HIS:HE2	1:N:104:THR:HG1	1.25	0.83
1:F:197:GLU:HA	1:F:202:ALA:HB2	1.61	0.81
1:J:184:VAL:HG13	1:J:205:PRO:HG2	1.63	0.81
1:C:184:VAL:HG13	1:C:205:PRO:HG2	1.63	0.81
1:C:125:LEU:O	1:C:127:GLU:N	2.14	0.80
1:M:184:VAL:HG13	1:M:205:PRO:HG2	1.64	0.80
1:M:174:GLY:O	4:M:401:HOH:O	1.98	0.79
1:Q:184:VAL:HG13	1:Q:205:PRO:HG2	1.64	0.79
1:I:52:MET:HB2	1:K:274:ILE:HG23	1.65	0.79
1:I:184:VAL:HG13	1:I:205:PRO:HG2	1.65	0.79
1:L:184:VAL:HG13	1:L:205:PRO:HG2	1.63	0.78
1:E:184:VAL:HG13	1:E:205:PRO:HG2	1.63	0.78
1:A:184:VAL:HG13	1:A:205:PRO:HG2	1.65	0.78
1:C:134:ALA:HB1	4:C:406:HOH:O	1.85	0.77
1:N:184:VAL:HG13	1:N:205:PRO:HG2	1.65	0.77
1:E:197:GLU:HA	1:E:202:ALA:HB2	1.67	0.76
1:J:143:ASP:OD1	1:J:169:ARG:NH1	2.19	0.76
1:H:184:VAL:HG13	1:H:205:PRO:HG2	1.67	0.75
1:R:199:LEU:HD21	1:R:265:GLY:HA3	1.69	0.75
1:R:184:VAL:HG13	1:R:205:PRO:HG2	1.69	0.74
1:K:184:VAL:HG13	1:K:205:PRO:HG2	1.69	0.74
1:G:31:THR:OG1	4:G:401:HOH:O	2.05	0.74
1:I:274:ILE:HG23	1:K:52:MET:HB2	1.67	0.74
1:G:184:VAL:HG13	1:G:205:PRO:HG2	1.70	0.73
1:O:184:VAL:HG13	1:O:205:PRO:HG2	1.68	0.73
1:G:52:MET:HB2	1:H:274:ILE:HG23	1.70	0.73
1:M:152:ILE:HG23	1:M:180:LEU:HD12	1.70	0.72
1:J:74:ASP:O	4:J:401:HOH:O	2.06	0.72
1:H:121:ALA:O	1:H:124:GLY:N	2.19	0.71
1:B:222:THR:O	4:B:401:HOH:O	2.08	0.71
1:G:274:ILE:HG23	1:H:52:MET:HB2	1.71	0.71
1:I:83:ASP:OD1	4:I:401:HOH:O	2.07	0.71
1:R:109:SER:HB3	1:R:112:GLN:HB2	1.72	0.71
1:J:274:ILE:HG23	1:L:52:MET:HB2	1.72	0.71
1:G:202:ALA:HB1	1:H:11:GLN:HB3	1.74	0.70
1:A:30:LEU:O	1:B:246:ARG:NH2	2.24	0.70
1:N:233:ALA:O	1:N:237:ASN:ND2	2.25	0.69
1:E:128:ARG:NH2	4:E:402:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:197:GLU:HA	1:I:202:ALA:HB2	1.75	0.68
1:P:184:VAL:HG13	1:P:205:PRO:HG2	1.75	0.68
1:G:36:VAL:HB	2:H:301:SAH:HB2	1.76	0.68
1:A:156:CYS:O	1:A:203:ASN:HB2	1.94	0.67
1:C:202:ALA:HB1	1:D:11:GLN:HG3	1.75	0.67
1:E:201:ALA:HB1	1:F:17:VAL:HG22	1.76	0.67
1:C:274:ILE:HG23	1:D:52:MET:HB2	1.76	0.67
1:F:157:HIS:CE1	1:F:201:ALA:HB3	2.29	0.67
1:C:251:THR:HG22	1:C:256:ALA:HA	1.75	0.67
1:M:32:LEU:HD21	1:N:239:PHE:HB2	1.77	0.67
1:D:85:GLY:O	2:D:301:SAH:N	2.27	0.67
1:I:25:GLY:O	1:I:27:VAL:N	2.26	0.66
1:J:52:MET:HB2	1:L:274:ILE:HG23	1.77	0.66
1:G:246:ARG:NH2	1:H:30:LEU:O	2.27	0.66
1:O:42:PHE:HZ	1:O:57:MET:HB3	1.62	0.65
1:O:197:GLU:HA	1:O:202:ALA:HB2	1.77	0.65
1:C:52:MET:HB2	1:D:274:ILE:HG23	1.77	0.65
1:A:11:GLN:HB3	1:B:202:ALA:HB1	1.79	0.65
1:B:42:PHE:HZ	1:B:57:MET:HB3	1.60	0.65
1:J:142:GLU:O	1:J:145:SER:OG	2.10	0.65
1:E:42:PHE:HZ	1:E:57:MET:HB3	1.63	0.64
1:Q:33:GLY:HA3	1:R:59:SER:HB2	1.80	0.64
1:A:183:VAL:HG11	1:A:208:LEU:HD23	1.80	0.64
1:F:156:CYS:O	1:F:203:ASN:HB2	1.97	0.63
1:D:197:GLU:HA	1:D:202:ALA:HB2	1.79	0.63
1:Q:197:GLU:HA	1:Q:202:ALA:HB2	1.81	0.63
1:P:157:HIS:CE1	1:P:201:ALA:HB3	2.33	0.63
1:P:42:PHE:HZ	1:P:57:MET:HB3	1.63	0.63
1:R:123:HIS:O	1:R:125:LEU:N	2.32	0.63
1:C:93:LEU:HD22	1:C:119:LEU:HG	1.81	0.63
1:J:141:TYR:HD2	1:J:142:GLU:HG3	1.64	0.63
1:N:143:ASP:OD1	1:N:169:ARG:NH1	2.29	0.63
1:I:201:ALA:HB1	1:K:17:VAL:HG22	1.81	0.62
1:M:274:ILE:HG23	1:N:52:MET:HB2	1.81	0.62
1:D:157:HIS:CE1	1:D:201:ALA:HB3	2.35	0.62
1:C:111:GLU:HG3	1:D:22:ASP:HA	1.81	0.62
1:Q:246:ARG:NH2	1:R:30:LEU:O	2.33	0.62
1:B:157:HIS:CE1	1:B:201:ALA:HB3	2.35	0.62
1:Q:202:ALA:HB1	1:R:11:GLN:HG3	1.81	0.62
1:E:157:HIS:CE1	1:E:201:ALA:HB3	2.35	0.61
1:G:85:GLY:O	2:G:301:SAH:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:CYS:O	1:B:203:ASN:HB2	2.00	0.61
1:M:241:LEU:HB2	1:N:241:LEU:HD13	1.82	0.61
1:L:223:LEU:HD11	1:L:285:ARG:HE	1.65	0.61
1:F:241:LEU:O	1:F:245:SER:OG	2.17	0.61
1:O:30:LEU:O	1:P:246:ARG:NH2	2.33	0.61
1:A:197:GLU:HA	1:A:202:ALA:HB2	1.81	0.61
1:R:156:CYS:SG	4:R:409:HOH:O	2.57	0.61
1:M:157:HIS:CE1	1:M:201:ALA:HB3	2.36	0.60
1:E:156:CYS:O	1:E:203:ASN:HB2	2.01	0.60
1:R:154:SER:OG	4:R:402:HOH:O	2.15	0.60
1:C:157:HIS:CE1	1:C:201:ALA:HB3	2.36	0.60
1:I:157:HIS:CE1	1:I:201:ALA:HB3	2.37	0.60
1:F:64:ARG:NH1	4:F:406:HOH:O	2.33	0.60
1:G:156:CYS:O	1:G:203:ASN:HB2	2.02	0.60
1:R:157:HIS:CE1	1:R:201:ALA:HB3	2.37	0.60
1:G:29:HIS:CE1	1:H:88:THR:HG1	2.19	0.60
1:I:285:ARG:HH21	1:L:48:VAL:HB	1.67	0.60
1:L:101:ILE:O	1:L:128:ARG:NH1	2.33	0.60
1:A:157:HIS:CE1	1:A:201:ALA:HB3	2.38	0.59
1:E:52:MET:HB2	1:F:274:ILE:HG23	1.83	0.59
1:J:17:VAL:HG22	1:L:201:ALA:HB1	1.84	0.59
1:M:197:GLU:HA	1:M:202:ALA:HB2	1.83	0.59
1:P:199:LEU:HD21	1:P:265:GLY:HA3	1.84	0.59
1:B:183:VAL:HG11	1:B:208:LEU:HD23	1.85	0.59
1:J:30:LEU:O	1:L:246:ARG:NH2	2.36	0.59
1:E:17:VAL:HG22	1:F:201:ALA:HB1	1.84	0.59
1:H:157:HIS:CE1	1:H:201:ALA:HB3	2.38	0.59
1:F:42:PHE:HZ	1:F:57:MET:HB3	1.68	0.59
1:O:156:CYS:O	1:O:203:ASN:HB2	2.00	0.59
1:G:27:VAL:HG22	4:G:401:HOH:O	2.02	0.59
1:H:99:ARG:O	4:H:401:HOH:O	2.17	0.58
1:O:285:ARG:HH21	1:Q:48:VAL:HB	1.68	0.58
1:M:156:CYS:O	1:M:203:ASN:HB2	2.03	0.58
1:Q:157:HIS:CE1	1:Q:201:ALA:HB3	2.38	0.58
1:I:27:VAL:HG23	1:I:30:LEU:HD12	1.86	0.58
1:H:106:VAL:HA	1:H:132:GLU:O	2.04	0.58
1:M:246:ARG:NH2	1:N:30:LEU:O	2.37	0.58
1:A:253:ARG:HH12	1:B:26:GLU:HG2	1.67	0.57
1:O:52:MET:HB2	1:P:274:ILE:HG23	1.84	0.57
1:O:36:VAL:HB	2:P:301:SAH:HB2	1.86	0.57
1:R:137:MET:HE3	1:R:162:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:274:ILE:HG23	1:R:52:MET:HB2	1.87	0.57
1:M:52:MET:HB2	1:N:274:ILE:HG23	1.86	0.57
1:F:223:LEU:HD11	1:F:285:ARG:HE	1.70	0.57
1:D:156:CYS:O	1:D:203:ASN:HB2	2.05	0.57
1:A:52:MET:HB2	1:B:274:ILE:HG23	1.86	0.56
1:B:10:GLN:O	1:B:12:VAL:N	2.37	0.56
1:C:285[A]:ARG:HH21	1:E:48:VAL:HB	1.68	0.56
1:H:156:CYS:O	1:H:203:ASN:HB2	2.05	0.56
1:L:157:HIS:CE1	1:L:201:ALA:HB3	2.40	0.56
1:O:157:HIS:CE1	1:O:201:ALA:HB3	2.40	0.56
1:H:104:THR:HA	1:H:130:THR:O	2.06	0.56
1:N:80:HIS:NE2	1:N:104:THR:OG1	2.30	0.56
1:R:151:ALA:HB1	4:R:402:HOH:O	2.04	0.56
2:C:301:SAH:HB2	1:D:36:VAL:HB	1.88	0.56
1:J:125:LEU:HD22	1:J:128:ARG:HH21	1.70	0.56
1:P:240:ALA:HA	1:P:266:LEU:HD13	1.87	0.56
1:R:174:GLY:O	1:R:285:ARG:NH1	2.38	0.56
1:F:49:PRO:O	4:F:401:HOH:O	2.18	0.56
1:H:115:ALA:HA	1:H:118:ARG:HB2	1.88	0.56
1:B:75:PRO:HG2	1:B:99:ARG:HG3	1.86	0.56
1:F:71:GLU:OE1	4:F:402:HOH:O	2.18	0.56
1:A:21:TYR:OH	1:B:157:HIS:NE2	2.32	0.56
1:C:30:LEU:O	1:D:246:ARG:NH2	2.38	0.56
1:H:77:ALA:HA	4:H:401:HOH:O	2.05	0.56
1:K:26:GLU:OE2	4:K:401:HOH:O	2.17	0.56
1:R:51:ASP:OD1	1:R:51:ASP:N	2.39	0.55
1:O:274:ILE:HG23	1:P:52:MET:HB2	1.87	0.55
2:J:301:SAH:HB2	1:L:36:VAL:HB	1.88	0.55
1:M:65:TYR:OH	1:M:180:LEU:HD13	2.07	0.55
1:R:125:LEU:HB3	1:R:128:ARG:HH12	1.71	0.55
1:F:85:GLY:O	2:F:301:SAH:N	2.40	0.55
1:I:246:ARG:NH2	1:K:30:LEU:O	2.40	0.55
1:K:157:HIS:CE1	1:K:201:ALA:HB3	2.42	0.55
1:G:157:HIS:CE1	1:G:201:ALA:HB3	2.42	0.55
1:I:246:ARG:HD2	1:I:249:GLU:OE1	2.07	0.55
1:Q:201:ALA:HB1	1:R:17:VAL:HG22	1.87	0.55
1:M:196:PHE:CE2	1:M:205:PRO:HD3	2.42	0.55
1:R:120:ALA:HB2	1:R:131:PHE:HE2	1.73	0.54
1:E:42:PHE:CZ	1:E:57:MET:HB3	2.41	0.54
1:H:183:VAL:HG11	1:H:208:LEU:HD23	1.89	0.54
1:I:156:CYS:O	1:I:203:ASN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:29:HIS:HA	1:R:33:GLY:O	2.07	0.54
1:C:143:ASP:OD1	1:C:169:ARG:NH1	2.32	0.54
1:J:237:ASN:HD22	1:L:54:LEU:HD13	1.72	0.54
1:E:36:VAL:HB	2:F:301:SAH:HB2	1.87	0.54
1:E:66:THR:HG23	1:E:91:THR:HG23	1.88	0.54
1:F:195:LEU:HD22	1:F:199:LEU:HG	1.90	0.54
1:A:251:THR:HG22	1:A:256:ALA:HA	1.90	0.54
1:L:157:HIS:ND1	1:L:201:ALA:HB3	2.23	0.54
1:R:73:LEU:HD21	1:R:81:LEU:HD21	1.90	0.54
1:B:157:HIS:ND1	1:B:201:ALA:HB3	2.23	0.54
1:J:157:HIS:CE1	1:J:201:ALA:HB3	2.43	0.54
1:E:32:LEU:HD21	1:F:239:PHE:HB2	1.90	0.53
1:O:183:VAL:HG11	1:O:208:LEU:HD23	1.90	0.53
1:R:142:GLU:HG2	1:R:143:ASP:H	1.73	0.53
1:C:239:PHE:HB2	1:D:32:LEU:HD21	1.90	0.53
1:G:66:THR:HG23	1:G:91:THR:HG23	1.90	0.53
1:J:85:GLY:O	2:J:301:SAH:N	2.42	0.53
1:L:156:CYS:O	1:L:203:ASN:HB2	2.08	0.53
1:C:42:PHE:HZ	1:C:57:MET:HB3	1.73	0.53
1:I:66:THR:HG23	1:I:91:THR:HG23	1.90	0.53
1:J:22:ASP:OD1	1:L:109:SER:OG	2.23	0.53
1:A:66:THR:HG23	1:A:91:THR:HG23	1.90	0.53
1:A:26:GLU:OE1	1:B:253:ARG:NH1	2.42	0.53
1:I:101:ILE:O	1:I:128:ARG:NH1	2.42	0.53
1:P:156:CYS:O	1:P:203:ASN:HB2	2.08	0.53
1:L:187:GLU:O	1:L:188:LEU:HB2	2.09	0.53
1:H:105:GLY:O	1:H:132:GLU:N	2.40	0.53
1:N:197:GLU:HG2	1:N:202:ALA:HB2	1.91	0.53
1:O:101:ILE:O	1:O:128:ARG:NH1	2.41	0.53
1:P:241:LEU:O	1:P:245:SER:OG	2.26	0.53
1:R:164:LEU:HD12	1:R:214:ILE:HG22	1.91	0.53
1:R:75:PRO:HG3	1:R:99:ARG:HD2	1.92	0.52
1:H:285:ARG:HH21	1:J:48:VAL:HB	1.75	0.52
1:D:152:ILE:HG23	1:D:180:LEU:HD22	1.91	0.52
1:K:223:LEU:HD11	1:K:285:ARG:HE	1.74	0.52
1:M:157:HIS:ND1	1:M:201:ALA:HB3	2.24	0.52
1:J:141:TYR:CD2	1:J:142:GLU:HG3	2.45	0.52
1:J:240:ALA:HA	1:J:266:LEU:HD13	1.92	0.52
1:I:30:LEU:O	1:K:246:ARG:NH2	2.42	0.52
1:O:17:VAL:HG22	1:P:201:ALA:HB1	1.92	0.52
1:C:271:GLU:HG3	1:C:275:ARG:HE	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:156:CYS:O	1:J:203:ASN:HB2	2.09	0.52
1:K:75:PRO:HG2	1:K:99:ARG:HG3	1.91	0.52
1:R:155:LEU:N	4:R:402:HOH:O	2.42	0.52
1:A:152:ILE:HG23	1:A:180:LEU:HD22	1.92	0.51
1:N:85:GLY:O	2:N:301:SAH:N	2.43	0.51
1:Q:157:HIS:ND1	1:Q:201:ALA:HB3	2.26	0.51
1:E:274:ILE:HG23	1:F:52:MET:HB2	1.91	0.51
1:H:157:HIS:ND1	1:H:201:ALA:HB3	2.25	0.51
1:M:237:ASN:HD22	1:N:54:LEU:HD13	1.74	0.51
1:R:157:HIS:CD2	2:R:301:SAH:H8	2.45	0.51
1:C:36:VAL:HB	2:D:301:SAH:HB2	1.93	0.51
1:G:285:ARG:HH21	1:I:48:VAL:HB	1.76	0.51
1:J:152:ILE:HG23	1:J:180:LEU:HD22	1.93	0.51
1:M:241:LEU:HD22	1:N:241:LEU:HB2	1.91	0.51
1:M:41:TRP:CD1	1:N:234:MET:HB3	2.46	0.51
1:R:84:ILE:O	4:R:403:HOH:O	2.19	0.51
1:C:201:ALA:HB1	1:D:17:VAL:HG22	1.93	0.51
1:G:157:HIS:ND1	1:G:201:ALA:HB3	2.26	0.51
1:I:152:ILE:HG23	1:I:180:LEU:HD22	1.93	0.51
1:A:157:HIS:ND1	1:A:201:ALA:HB3	2.26	0.51
1:D:183:VAL:HG11	1:D:208:LEU:HD23	1.92	0.51
1:K:156:CYS:O	1:K:203:ASN:HB2	2.11	0.50
1:K:240:ALA:HA	1:K:266:LEU:HD13	1.93	0.50
1:A:246:ARG:NH2	1:B:30:LEU:O	2.43	0.50
1:N:152:ILE:HG23	1:N:180:LEU:HD22	1.92	0.50
1:R:156:CYS:O	1:R:203:ASN:HB2	2.11	0.50
1:N:176:ASP:N	4:N:402:HOH:O	2.45	0.50
1:N:156:CYS:O	1:N:203:ASN:HB2	2.12	0.50
1:M:66:THR:HG23	1:M:91:THR:HG23	1.94	0.50
1:N:137:MET:HE3	1:N:162:LYS:HD2	1.94	0.50
1:D:157:HIS:ND1	1:D:201:ALA:HB3	2.27	0.49
1:H:113:ILE:HG21	1:H:133:VAL:HG23	1.94	0.49
1:C:197:GLU:HA	1:C:202:ALA:HB2	1.94	0.49
1:G:240:ALA:HA	1:G:266:LEU:HD13	1.93	0.49
1:L:246:ARG:HD2	1:L:249:GLU:OE1	2.13	0.49
1:H:88:THR:HA	1:H:116:ALA:HB2	1.94	0.49
1:I:240:ALA:HA	1:I:266:LEU:HD13	1.95	0.49
1:Q:30:LEU:O	1:R:246:ARG:NH2	2.45	0.49
1:H:101:ILE:HG23	4:H:401:HOH:O	2.13	0.49
1:A:156:CYS:HB3	3:A:302:TEX:O2	2.13	0.49
1:Q:156:CYS:O	1:Q:203:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:LEU:HD21	1:H:239:PHE:HB2	1.94	0.49
1:I:157:HIS:ND1	1:I:201:ALA:HB3	2.27	0.49
1:C:156:CYS:O	1:C:203:ASN:HB2	2.13	0.49
1:Q:34:GLU:OE1	1:R:90:ARG:NH1	2.46	0.49
1:R:125:LEU:HB3	1:R:128:ARG:NH1	2.27	0.48
1:B:213:ASP:OD1	4:B:402:HOH:O	2.20	0.48
1:D:196:PHE:CE2	1:D:205:PRO:HD3	2.48	0.48
2:I:301:SAH:HB2	1:K:36:VAL:HB	1.95	0.48
1:N:157:HIS:CE1	1:N:201:ALA:HB3	2.48	0.48
4:O:402:HOH:O	1:P:197:GLU:HB2	2.13	0.48
1:I:196:PHE:CE2	1:I:205:PRO:HD3	2.49	0.48
1:M:156:CYS:HB3	3:M:302:TEX:O2	2.13	0.48
1:O:212:PHE:HB3	1:R:208:LEU:HD12	1.96	0.48
1:D:199:LEU:HD22	1:D:262:LEU:HD23	1.96	0.47
1:P:143:ASP:OD1	1:P:169:ARG:NH1	2.41	0.47
2:A:301:SAH:HB2	1:B:36:VAL:HB	1.95	0.47
1:B:48:VAL:HB	1:D:285:ARG:HH21	1.80	0.47
1:F:156:CYS:HB3	3:F:302:TEX:O2	2.14	0.47
1:B:171:LEU:O	1:B:286:LYS:NZ	2.37	0.47
1:J:29:HIS:HA	1:J:33:GLY:O	2.14	0.47
1:N:223:LEU:HD11	1:N:285:ARG:HE	1.79	0.47
1:A:201:ALA:HB1	1:B:17:VAL:HG22	1.97	0.47
1:A:247:ARG:NH1	4:A:408:HOH:O	2.46	0.47
1:N:156:CYS:HB3	3:N:302:TEX:O2	2.14	0.47
1:O:201:ALA:HB1	1:P:17:VAL:HG22	1.96	0.47
1:C:157:HIS:ND1	1:C:201:ALA:HB3	2.29	0.47
1:E:74:ASP:OD1	1:E:99:ARG:NH1	2.38	0.47
1:F:42:PHE:CZ	1:F:57:MET:HB3	2.49	0.47
1:H:196:PHE:CE2	1:H:205:PRO:HD3	2.49	0.47
1:J:138:ARG:CZ	1:J:138:ARG:HB3	2.44	0.47
1:J:157:HIS:ND1	1:J:201:ALA:HB3	2.28	0.47
1:Q:40:LEU:HD23	1:R:64:ARG:HG2	1.95	0.47
1:C:66:THR:HG23	1:C:91:THR:HG23	1.96	0.47
1:E:157:HIS:ND1	1:E:201:ALA:HB3	2.30	0.47
1:K:166:GLU:OE2	1:K:169:ARG:NH2	2.38	0.47
1:I:239:PHE:HB2	1:K:32:LEU:HD21	1.96	0.47
1:M:236:MET:HB3	1:M:270:GLN:OE1	2.15	0.47
1:R:160:ARG:NE	1:R:206:PRO:HD3	2.29	0.47
1:R:186:GLU:HB2	1:R:276:LYS:HG2	1.97	0.47
1:K:40:LEU:HD21	1:K:44:PRO:HD3	1.96	0.47
1:M:29:HIS:HA	1:M:33:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:259:VAL:O	1:P:263:LEU:HG	2.15	0.47
1:A:253:ARG:NH1	1:B:26:GLU:HG2	2.30	0.47
1:B:288:ALA:O	1:B:289:VAL:HG22	2.15	0.47
1:O:195:LEU:HD22	1:O:199:LEU:HG	1.96	0.47
1:E:139:LEU:H	1:E:166:GLU:HG2	1.80	0.47
1:P:157:HIS:ND1	1:P:201:ALA:HB3	2.30	0.47
1:G:48:VAL:HB	1:L:285:ARG:HH21	1.80	0.46
1:R:160:ARG:CZ	1:R:206:PRO:HD3	2.45	0.46
1:A:48:VAL:HB	1:E:285:ARG:HH21	1.80	0.46
1:A:158:MET:O	1:A:203:ASN:ND2	2.48	0.46
1:C:17:VAL:HG11	2:D:301:SAH:H8	1.97	0.46
2:G:301:SAH:HB2	1:H:36:VAL:HB	1.96	0.46
1:N:75:PRO:HG2	1:N:99:ARG:HG3	1.98	0.46
1:P:157:HIS:CD2	2:P:301:SAH:H8	2.50	0.46
1:A:62:GLN:O	1:A:65:TYR:HB3	2.15	0.46
1:C:40:LEU:HD21	1:C:44:PRO:HD3	1.97	0.46
1:O:285:ARG:NH2	1:Q:48:VAL:O	2.47	0.46
1:P:29:HIS:HA	1:P:33:GLY:O	2.16	0.46
1:R:135:ASP:HB3	1:R:138:ARG:HB2	1.98	0.46
1:D:107:ALA:O	1:D:133:VAL:HA	2.15	0.46
1:C:203:ASN:H	1:D:11:GLN:HG3	1.80	0.46
1:N:66:THR:HG23	1:N:91:THR:HG23	1.98	0.46
1:D:75:PRO:HG2	1:D:99:ARG:HG3	1.98	0.46
1:L:223:LEU:HD11	1:L:285:ARG:NE	2.30	0.46
1:N:174:GLY:O	1:N:285:ARG:NH1	2.49	0.46
2:I:301:SAH:O	1:K:37:HIS:HD2	1.98	0.46
1:C:241:LEU:O	1:C:245:SER:OG	2.32	0.45
1:K:139:LEU:H	1:K:166:GLU:HG2	1.80	0.45
1:R:197:GLU:HG3	1:R:202:ALA:HB2	1.99	0.45
1:Q:241:LEU:HD22	1:R:241:LEU:HB2	1.98	0.45
1:F:195:LEU:HD23	1:F:195:LEU:HA	1.85	0.45
1:O:223:LEU:HA	1:R:227:ASP:HB2	1.97	0.45
1:E:12:VAL:HG21	1:F:201:ALA:O	2.16	0.45
1:H:246:ARG:HD2	1:H:249:GLU:OE1	2.16	0.45
1:G:197:GLU:OE1	1:H:11:GLN:NE2	2.49	0.45
1:M:42:PHE:HZ	1:M:57:MET:HB3	1.81	0.45
1:N:196:PHE:CE2	1:N:205:PRO:HD3	2.51	0.45
1:C:201:ALA:O	1:D:12:VAL:HG21	2.17	0.45
1:H:240:ALA:HA	1:H:266:LEU:HD13	1.98	0.45
1:I:247:ARG:HG3	1:I:263:LEU:HD11	1.99	0.45
1:I:183:VAL:HG11	1:I:208:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:152:ILE:HG23	1:L:180:LEU:HD22	1.98	0.45
1:O:157:HIS:ND1	1:O:201:ALA:HB3	2.30	0.45
1:O:160:ARG:CZ	1:O:206:PRO:HD3	2.47	0.45
1:P:197:GLU:HA	1:P:202:ALA:HB2	1.98	0.45
1:Q:74:ASP:OD2	1:Q:76:LYS:HE2	2.17	0.45
1:L:195:LEU:HA	1:L:195:LEU:HD23	1.81	0.45
1:L:196:PHE:CE2	1:L:205:PRO:HD3	2.52	0.45
1:M:156:CYS:HA	1:M:160:ARG:NH2	2.32	0.45
1:M:213:ASP:OD1	1:P:209:GLY:HA3	2.17	0.45
3:P:302:TEX:C18	3:P:302:TEX:C21	2.95	0.45
1:O:199:LEU:HD22	1:O:262:LEU:HD23	1.98	0.44
1:C:29:HIS:HA	1:C:33:GLY:O	2.17	0.44
3:G:302:TEX:C21	3:G:302:TEX:C18	2.95	0.44
1:H:171:LEU:HD11	1:H:177:LEU:HB2	2.00	0.44
3:H:302:TEX:C18	3:H:302:TEX:C21	2.95	0.44
1:L:160:ARG:NE	1:L:181:GLU:OE1	2.40	0.44
1:F:196:PHE:CE2	1:F:205:PRO:HD3	2.52	0.44
1:F:240:ALA:HA	1:F:266:LEU:HD13	1.99	0.44
1:P:208:LEU:HA	1:P:208:LEU:HD22	1.86	0.44
2:A:301:SAH:O	1:B:37:HIS:HD2	2.00	0.44
1:B:42:PHE:CZ	1:B:57:MET:HB3	2.46	0.44
1:H:129:LEU:HB3	1:H:131:PHE:CE2	2.53	0.44
1:J:141:TYR:HD2	1:J:142:GLU:H	1.65	0.44
3:J:302:TEX:C18	3:J:302:TEX:C21	2.95	0.44
1:I:189:THR:O	1:I:193:THR:HG23	2.18	0.44
3:L:302:TEX:C21	3:L:302:TEX:C18	2.96	0.44
3:F:302:TEX:C21	3:F:302:TEX:C18	2.96	0.44
1:J:136:ALA:HA	1:J:139:LEU:HD21	2.00	0.44
1:J:66:THR:HG23	1:J:91:THR:HG23	1.98	0.44
3:M:302:TEX:C18	3:M:302:TEX:C21	2.95	0.44
1:A:156:CYS:HA	1:A:160:ARG:NH2	2.33	0.44
3:I:302:TEX:C18	3:I:302:TEX:C21	2.96	0.44
1:F:187:GLU:O	1:F:188:LEU:HB2	2.17	0.44
1:G:239:PHE:HB2	1:H:32:LEU:HD21	1.99	0.44
1:Q:239:PHE:HB2	1:R:32:LEU:HD21	1.98	0.44
1:B:45:ASP:OD1	1:B:45:ASP:N	2.44	0.43
1:K:10:GLN:O	1:K:12:VAL:N	2.46	0.43
1:J:36:VAL:HB	2:L:301:SAH:HB2	2.00	0.43
1:M:160:ARG:CZ	1:M:206:PRO:HD3	2.48	0.43
1:R:75:PRO:CD	1:R:76:LYS:H	2.31	0.43
1:B:197:GLU:HA	1:B:202:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ILE:HG23	1:G:180:LEU:HD22	2.00	0.43
1:N:74:ASP:OD1	1:N:99:ARG:NH1	2.40	0.43
1:Q:129:LEU:HB3	1:Q:131:PHE:CE2	2.54	0.43
3:Q:302:TEX:C18	3:Q:302:TEX:C21	2.97	0.43
1:E:111:GLU:HG3	1:F:22:ASP:HA	1.99	0.43
1:N:199:LEU:HD22	1:N:262:LEU:HD23	1.99	0.43
1:P:150:TRP:O	1:P:150:TRP:HD1	2.01	0.43
1:A:29:HIS:HA	1:A:33:GLY:O	2.19	0.43
1:E:150:TRP:O	1:E:150:TRP:HD1	2.00	0.43
1:I:194:ALA:O	1:I:197:GLU:N	2.51	0.43
1:A:109:SER:OG	1:B:22:ASP:OD1	2.25	0.43
1:P:197:GLU:HG2	1:P:202:ALA:HB2	2.00	0.43
1:Q:150:TRP:HA	1:Q:178:LEU:O	2.19	0.43
3:R:302:TEX:C21	3:R:302:TEX:C18	2.96	0.43
1:R:75:PRO:HD3	1:R:99:ARG:NH1	2.33	0.43
1:B:184:VAL:HG22	1:B:206:PRO:O	2.18	0.43
1:H:156:CYS:HB3	3:H:302:TEX:O2	2.17	0.43
1:M:30:LEU:O	1:N:246:ARG:NH2	2.51	0.43
1:A:246:ARG:HD2	1:A:249:GLU:OE1	2.19	0.43
1:B:240:ALA:HA	1:B:266:LEU:HD13	2.00	0.43
3:E:302:TEX:C18	3:E:302:TEX:C21	2.96	0.43
1:G:251:THR:HG22	1:G:256:ALA:HA	2.00	0.43
1:J:158:MET:O	1:J:203:ASN:ND2	2.52	0.43
1:R:73:LEU:O	1:R:73:LEU:HD12	2.18	0.43
1:A:159:ASP:HB2	1:B:9:GLN:N	2.33	0.43
1:K:197:GLU:HG3	1:K:202:ALA:HB2	2.01	0.43
3:N:302:TEX:C21	3:N:302:TEX:C18	2.97	0.43
1:O:108:VAL:HG11	1:P:14:ALA:HB1	2.01	0.43
1:Q:52:MET:HB2	1:R:274:ILE:HG23	2.00	0.43
1:G:197:GLU:HA	1:G:202:ALA:HB2	2.01	0.43
1:O:85:GLY:O	2:O:301:SAH:N	2.52	0.43
1:P:187:GLU:O	1:P:188:LEU:HB2	2.18	0.43
1:R:62:GLN:O	1:R:65:TYR:HB3	2.18	0.43
1:F:157:HIS:ND1	1:F:201:ALA:HB3	2.34	0.43
1:F:227:ASP:OD1	1:F:278:ARG:HD3	2.19	0.43
3:K:302:TEX:C21	3:K:302:TEX:C18	2.97	0.43
1:M:42:PHE:CZ	1:M:57:MET:HB3	2.53	0.43
1:N:80:HIS:N	1:N:147:ASP:OD2	2.41	0.43
1:O:150:TRP:HD1	1:O:150:TRP:O	2.01	0.43
1:O:156:CYS:HB3	3:O:302:TEX:O2	2.19	0.43
3:O:302:TEX:C21	3:O:302:TEX:C18	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:TRP:NE1	1:B:286:LYS:HG3	2.34	0.42
1:D:187:GLU:O	1:D:188:LEU:HB2	2.18	0.42
3:D:302:TEX:C21	3:D:302:TEX:C18	2.97	0.42
1:F:246:ARG:HD2	1:F:249:GLU:OE1	2.19	0.42
1:N:223:LEU:HD11	1:N:285:ARG:NE	2.33	0.42
1:P:223:LEU:HD11	1:P:285:ARG:HE	1.84	0.42
1:Q:240:ALA:HA	1:Q:266:LEU:HD13	2.01	0.42
1:R:177:LEU:HA	4:R:408:HOH:O	2.18	0.42
1:A:94:LYS:NZ	4:A:407:HOH:O	2.41	0.42
3:C:302:TEX:C18	3:C:302:TEX:C21	2.96	0.42
1:J:196:PHE:CE2	1:J:205:PRO:HD3	2.54	0.42
1:J:12:VAL:HG21	1:L:201:ALA:O	2.20	0.42
1:A:187:GLU:O	1:A:188:LEU:HB2	2.18	0.42
1:C:246:ARG:HD2	1:C:249:GLU:OE1	2.18	0.42
1:C:82:LEU:HD22	1:C:146:PHE:HE2	1.84	0.42
1:E:187:GLU:O	1:E:188:LEU:HB2	2.19	0.42
1:N:157:HIS:ND1	1:N:201:ALA:HB3	2.34	0.42
3:A:302:TEX:C21	3:A:302:TEX:C18	2.97	0.42
1:C:223:LEU:HD11	1:C:285[A]:ARG:NE	2.34	0.42
1:F:223:LEU:HD11	1:F:285:ARG:NE	2.34	0.42
1:M:195:LEU:HD23	1:M:195:LEU:HA	1.84	0.42
2:O:301:SAH:H8	1:P:17:VAL:HG11	2.00	0.42
1:R:143:ASP:OD1	1:R:143:ASP:N	2.53	0.42
1:Q:64:ARG:HG2	1:R:40:LEU:HD23	2.02	0.42
1:D:93:LEU:HD21	1:D:123:HIS:CD2	2.54	0.42
1:F:156:CYS:HA	1:F:160:ARG:NH2	2.35	0.42
1:H:156:CYS:HA	1:H:160:ARG:NH2	2.34	0.42
1:Q:212:PHE:HZ	1:Q:225:LEU:HD12	1.84	0.42
1:R:75:PRO:HD2	1:R:76:LYS:H	1.84	0.42
3:B:302:TEX:C18	3:B:302:TEX:C21	2.98	0.42
1:E:157:HIS:NE2	1:F:21:TYR:OH	2.34	0.42
1:O:240:ALA:HA	1:O:266:LEU:HD13	2.00	0.42
1:Q:59:SER:HB2	1:R:33:GLY:HA3	2.01	0.42
2:Q:301:SAH:HB2	1:R:36:VAL:HB	2.02	0.42
2:Q:301:SAH:O	1:R:37:HIS:HD2	2.02	0.42
1:C:119:LEU:HA	1:C:119:LEU:HD12	1.85	0.42
1:C:181:GLU:HG2	1:C:211:PHE:CE1	2.55	0.42
1:C:247:ARG:O	1:C:251:THR:OG1	2.29	0.42
1:I:158:MET:O	1:I:203:ASN:ND2	2.52	0.42
1:C:150:TRP:HA	1:C:178:LEU:O	2.19	0.42
1:J:65:TYR:CE2	1:L:38:CYS:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:157:HIS:CD2	2:K:301:SAH:H8	2.55	0.42
1:M:241:LEU:O	1:M:245:SER:OG	2.31	0.42
1:R:75:PRO:HG3	1:R:99:ARG:CD	2.50	0.42
1:E:85:GLY:O	2:E:301:SAH:N	2.52	0.42
1:I:156:CYS:HA	1:I:160:ARG:NH2	2.35	0.42
1:I:29:HIS:HA	1:I:33:GLY:O	2.19	0.42
1:R:83:ASP:HB3	1:R:86:CYS:HB3	2.02	0.42
1:E:231:ASN:O	1:E:235:THR:OG1	2.23	0.42
1:F:251:THR:HG22	1:F:256:ALA:HA	2.02	0.42
1:K:223:LEU:HD11	1:K:285:ARG:NE	2.35	0.42
1:K:156:CYS:HB3	3:K:302:TEX:O2	2.19	0.42
1:M:75:PRO:HG2	1:M:99:ARG:HG3	2.01	0.42
1:O:156:CYS:HA	1:O:160:ARG:NH2	2.34	0.42
1:P:107:ALA:O	1:P:133:VAL:HA	2.20	0.42
1:C:174:GLY:N	1:C:288:ALA:HB2	2.34	0.41
1:G:64:ARG:HG2	1:H:40:LEU:HD23	2.01	0.41
1:C:122:GLY:O	1:C:124:GLY:N	2.53	0.41
1:C:82:LEU:HD22	1:C:146:PHE:CE2	2.56	0.41
1:F:211:PHE:O	1:F:215:VAL:HG23	2.20	0.41
1:N:187:GLU:O	1:N:188:LEU:HB2	2.20	0.41
1:Q:202:ALA:HB1	1:Q:203:ASN:H	1.64	0.41
1:C:140:PRO:HD3	4:C:406:HOH:O	2.20	0.41
1:D:182:SER:HB2	3:D:302:TEX:N3	2.35	0.41
1:G:87:GLY:O	1:G:112:GLN:HB3	2.20	0.41
1:H:119:LEU:O	1:H:121:ALA:N	2.54	0.41
1:H:187:GLU:O	1:H:188:LEU:HB2	2.20	0.41
1:I:273:LEU:HD12	1:I:277:THR:OG1	2.20	0.41
1:K:74:ASP:OD1	1:K:99:ARG:NH1	2.43	0.41
1:O:187:GLU:O	1:O:188:LEU:HB2	2.19	0.41
1:Q:274:ILE:HG12	1:R:52:MET:HB2	2.01	0.41
1:A:17:VAL:HG22	1:B:201:ALA:HB1	2.02	0.41
1:K:266:LEU:HD23	1:K:266:LEU:HA	1.94	0.41
1:R:88:THR:HA	1:R:116:ALA:HB2	2.02	0.41
1:F:168:TRP:CZ2	1:F:286:LYS:HE3	2.56	0.41
1:F:65:TYR:CE1	1:F:69:LEU:HD11	2.55	0.41
1:H:113:ILE:HA	1:H:113:ILE:HD13	1.86	0.41
1:H:119:LEU:C	1:H:121:ALA:H	2.24	0.41
1:O:187:GLU:HA	1:O:207:ARG:HH22	1.85	0.41
1:Q:42:PHE:HZ	1:Q:57:MET:HB3	1.85	0.41
1:Q:52:MET:HB2	1:R:274:ILE:HG12	2.03	0.41
1:C:168:TRP:CZ2	1:C:286:LYS:HE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:187:GLU:O	1:M:188:LEU:HB2	2.21	0.41
1:R:124:GLY:O	1:R:125:LEU:HD23	2.21	0.41
1:G:157:HIS:HD1	1:G:201:ALA:HB3	1.86	0.41
1:O:51:ASP:OD1	1:O:51:ASP:N	2.54	0.41
1:P:262:LEU:HD23	1:P:262:LEU:HA	1.94	0.41
1:A:195:LEU:HD22	1:A:199:LEU:HG	2.03	0.41
1:A:174:GLY:O	1:A:285:ARG:NH1	2.54	0.41
1:B:285:ARG:HH21	1:F:48:VAL:HB	1.85	0.41
1:B:48:VAL:O	1:D:285:ARG:NH2	2.54	0.41
1:L:240:ALA:HA	1:L:266:LEU:HD13	2.02	0.41
1:M:36:VAL:HB	2:N:301:SAH:HB2	2.02	0.41
1:B:246:ARG:HD2	1:B:249:GLU:OE1	2.21	0.41
1:H:93:LEU:HD21	1:H:123:HIS:CD2	2.56	0.41
1:I:150:TRP:HA	1:I:178:LEU:O	2.21	0.41
1:M:285:ARG:HH21	1:O:48:VAL:HB	1.85	0.41
1:L:66:THR:HG23	1:L:91:THR:HG23	2.01	0.41
1:O:195:LEU:HA	1:O:195:LEU:HD23	1.85	0.41
1:N:212:PHE:HB3	1:Q:208:LEU:HD12	2.03	0.41
1:R:110:LYS:HG3	1:R:110:LYS:H	1.47	0.41
1:G:160:ARG:NE	1:G:181:GLU:OE1	2.50	0.41
1:N:266:LEU:HA	1:N:266:LEU:HD23	1.93	0.41
1:N:273:LEU:HD12	1:N:277:THR:OG1	2.21	0.41
1:R:82:LEU:HB2	1:R:146:PHE:CD1	2.56	0.41
1:B:208:LEU:HD22	1:B:208:LEU:HA	1.92	0.40
1:C:73:LEU:HD21	1:C:148:CYS:HB2	2.03	0.40
1:G:253:ARG:NH1	1:H:26:GLU:OE1	2.54	0.40
1:J:187:GLU:O	1:J:188:LEU:HB2	2.20	0.40
1:J:195:LEU:HD23	1:J:195:LEU:HA	1.87	0.40
1:N:186:GLU:HB2	1:N:276:LYS:HG2	2.03	0.40
1:A:271:GLU:OE2	1:A:275:ARG:NE	2.54	0.40
1:C:135:ASP:N	4:C:406:HOH:O	2.43	0.40
1:C:189:THR:O	1:C:193:THR:HG23	2.21	0.40
1:H:195:LEU:HA	1:H:195:LEU:HD23	1.91	0.40
1:N:24:PHE:O	1:N:27:VAL:HG12	2.21	0.40
1:P:184:VAL:CG1	1:P:205:PRO:HG2	2.50	0.40
1:A:196:PHE:CE2	1:A:205:PRO:HD3	2.56	0.40
1:I:241:LEU:O	1:I:245:SER:OG	2.24	0.40
1:N:29:HIS:HA	1:N:33:GLY:O	2.21	0.40
1:P:196:PHE:CE2	1:P:205:PRO:HD3	2.57	0.40
1:Q:44:PRO:HB3	1:R:68:TYR:CZ	2.56	0.40
1:A:196:PHE:HB3	1:A:202:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:TRP:HD1	1:D:150:TRP:O	2.03	0.40
1:D:160:ARG:NE	1:D:181:GLU:OE1	2.37	0.40
1:E:66:THR:HB	1:E:94:LYS:HE2	2.03	0.40
1:G:38:CYS:HB2	1:H:65:TYR:CE2	2.56	0.40
1:I:188:LEU:HD13	1:I:193:THR:HG22	2.04	0.40
1:M:168:TRP:CZ2	1:M:286:LYS:HE3	2.56	0.40
1:Q:159:ASP:HA	1:R:10:GLN:NE2	2.17	0.40
1:R:152:ILE:HG23	1:R:180:LEU:HD22	2.03	0.40
1:H:168:TRP:CZ2	1:H:286:LYS:HE3	2.57	0.40
1:K:101:ILE:O	1:K:128:ARG:NH1	2.53	0.40
1:N:168:TRP:CZ2	1:N:286:LYS:HE3	2.56	0.40
1:P:156:CYS:HB3	3:P:302:TEX:O2	2.22	0.40
1:P:74:ASP:HA	1:P:99:ARG:HH12	1.86	0.40

All (2) 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:R:126:THR:OG1	1:R:126:THR:OG1[2_455]	2.09	0.11
1:H:117:ASN:OD1	1:H:126:THR:OG1[2_555]	2.12	0.08

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	279/297 (94%)	268 (96%)	9 (3%)	2 (1%)	22 53
1	B	280/297 (94%)	269 (96%)	6 (2%)	5 (2%)	8 28
1	C	278/297 (94%)	261 (94%)	12 (4%)	5 (2%)	8 28
1	D	279/297 (94%)	268 (96%)	8 (3%)	3 (1%)	14 41
1	E	277/297 (93%)	265 (96%)	8 (3%)	4 (1%)	11 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	277/297 (93%)	269 (97%)	6 (2%)	2 (1%)	22	53
1	G	264/297 (89%)	252 (96%)	8 (3%)	4 (2%)	10	33
1	H	279/297 (94%)	260 (93%)	15 (5%)	4 (1%)	11	34
1	I	265/297 (89%)	253 (96%)	8 (3%)	4 (2%)	10	33
1	J	266/297 (90%)	254 (96%)	9 (3%)	3 (1%)	14	41
1	K	259/297 (87%)	240 (93%)	15 (6%)	4 (2%)	10	33
1	L	259/297 (87%)	249 (96%)	8 (3%)	2 (1%)	19	49
1	M	262/297 (88%)	250 (95%)	10 (4%)	2 (1%)	19	49
1	N	270/297 (91%)	256 (95%)	12 (4%)	2 (1%)	22	53
1	O	277/297 (93%)	267 (96%)	8 (3%)	2 (1%)	22	53
1	P	277/297 (93%)	264 (95%)	9 (3%)	4 (1%)	11	34
1	Q	264/297 (89%)	251 (95%)	11 (4%)	2 (1%)	19	49
1	R	267/297 (90%)	249 (93%)	11 (4%)	7 (3%)	5	18
All	All	4879/5346 (91%)	4645 (95%)	173 (4%)	61 (1%)	12	36

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	C	126	THR
1	E	203	ASN
1	I	203	ASN
1	R	75	PRO
1	R	124	GLY
1	B	10	GLN
1	B	11	GLN
1	B	203	ASN
1	B	289	VAL
1	C	123	HIS
1	C	203	ASN
1	D	203	ASN
1	F	203	ASN
1	G	203	ASN
1	H	203	ASN
1	I	25	GLY
1	I	26	GLU
1	L	203	ASN

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Mol	Chain	Res	Type
1	M	203	ASN
1	O	203	ASN
1	P	16	GLU
1	P	203	ASN
1	Q	203	ASN
1	C	188	LEU
1	E	16	GLU
1	G	188	LEU
1	H	120	ALA
1	J	140	PRO
1	J	203	ASN
1	K	203	ASN
1	N	203	ASN
1	R	16	GLU
1	R	203	ASN
1	C	124	GLY
1	D	188	LEU
1	E	188	LEU
1	H	188	LEU
1	I	188	LEU
1	J	188	LEU
1	K	4	GLU
1	K	188	LEU
1	M	188	LEU
1	N	188	LEU
1	O	188	LEU
1	P	188	LEU
1	Q	188	LEU
1	R	76	LYS
1	R	188	LEU
1	E	202	ALA
1	F	188	LEU
1	G	25	GLY
1	G	202	ALA
1	H	127	GLU
1	K	8	PRO
1	A	188	LEU
1	L	188	LEU
1	D	289	VAL
1	P	140	PRO
1	R	74	ASP
1	B	206	PRO

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	224/239 (94%)	218 (97%)	6 (3%)	44	78
1	B	225/239 (94%)	213 (95%)	12 (5%)	22	54
1	C	223/239 (93%)	212 (95%)	11 (5%)	25	57
1	D	224/239 (94%)	216 (96%)	8 (4%)	35	69
1	E	222/239 (93%)	218 (98%)	4 (2%)	59	86
1	F	222/239 (93%)	214 (96%)	8 (4%)	35	69
1	G	211/239 (88%)	204 (97%)	7 (3%)	38	72
1	H	224/239 (94%)	215 (96%)	9 (4%)	31	65
1	I	212/239 (89%)	201 (95%)	11 (5%)	23	55
1	J	217/239 (91%)	208 (96%)	9 (4%)	30	64
1	K	214/239 (90%)	205 (96%)	9 (4%)	30	63
1	L	209/239 (87%)	202 (97%)	7 (3%)	38	72
1	M	210/239 (88%)	202 (96%)	8 (4%)	33	67
1	N	219/239 (92%)	213 (97%)	6 (3%)	44	78
1	O	222/239 (93%)	218 (98%)	4 (2%)	59	86
1	P	222/239 (93%)	215 (97%)	7 (3%)	39	73
1	Q	211/239 (88%)	205 (97%)	6 (3%)	43	77
1	R	219/239 (92%)	204 (93%)	15 (7%)	16	42
All	All	3930/4302 (91%)	3783 (96%)	147 (4%)	34	68

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	TRP
1	A	183	VAL
1	A	186	GLU
1	A	208	LEU
1	A	247	ARG
1	A	253	ARG

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Mol	Chain	Res	Type
1	B	9	GLN
1	B	11	GLN
1	B	45	ASP
1	B	52	MET
1	B	145	SER
1	B	150	TRP
1	B	186	GLU
1	B	200	TYR
1	B	208	LEU
1	B	247	ARG
1	B	253	ARG
1	B	290	LEU
1	C	119	LEU
1	C	145	SER
1	C	150	TRP
1	C	158	MET
1	C	186	GLU
1	C	200	TYR
1	C	245	SER
1	C	247	ARG
1	C	251	THR
1	C	252	GLU
1	C	257	GLU
1	D	12	VAL
1	D	52	MET
1	D	150	TRP
1	D	158	MET
1	D	182	SER
1	D	186	GLU
1	D	208	LEU
1	D	247	ARG
1	E	150	TRP
1	E	186	GLU
1	E	200	TYR
1	E	208	LEU
1	F	26	GLU
1	F	150	TRP
1	F	186	GLU
1	F	200	TYR
1	F	208	LEU
1	F	245	SER
1	F	247	ARG

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Mol	Chain	Res	Type
1	F	253	ARG
1	G	31	THR
1	G	150	TRP
1	G	186	GLU
1	G	200	TYR
1	G	208	LEU
1	G	247	ARG
1	G	253	ARG
1	H	57	MET
1	H	132	GLU
1	H	150	TRP
1	H	183	VAL
1	H	186	GLU
1	H	200	TYR
1	H	208	LEU
1	H	253	ARG
1	H	290	LEU
1	I	24	PHE
1	I	26	GLU
1	I	57	MET
1	I	150	TRP
1	I	186	GLU
1	I	197	GLU
1	I	200	TYR
1	I	208	LEU
1	I	245	SER
1	I	247	ARG
1	I	253	ARG
1	J	11	GLN
1	J	12	VAL
1	J	141	TYR
1	J	142	GLU
1	J	150	TRP
1	J	186	GLU
1	J	200	TYR
1	J	208	LEU
1	J	236	MET
1	K	4	GLU
1	K	9	GLN
1	K	11	GLN
1	K	91	THR
1	K	97	ARG

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Mol	Chain	Res	Type
1	K	150	TRP
1	K	186	GLU
1	K	200	TYR
1	K	208	LEU
1	L	27	VAL
1	L	57	MET
1	L	150	TRP
1	L	186	GLU
1	L	200	TYR
1	L	208	LEU
1	L	253	ARG
1	M	150	TRP
1	M	183	VAL
1	M	186	GLU
1	M	200	TYR
1	M	208	LEU
1	M	236	MET
1	M	247	ARG
1	M	253	ARG
1	N	150	TRP
1	N	186	GLU
1	N	200	TYR
1	N	208	LEU
1	N	245	SER
1	N	253	ARG
1	O	150	TRP
1	O	186	GLU
1	O	200	TYR
1	O	208	LEU
1	P	11	GLN
1	P	150	TRP
1	P	186	GLU
1	P	200	TYR
1	P	208	LEU
1	P	245	SER
1	P	247	ARG
1	Q	24	PHE
1	Q	150	TRP
1	Q	186	GLU
1	Q	200	TYR
1	Q	208	LEU
1	Q	247	ARG

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Mol	Chain	Res	Type
1	R	12	VAL
1	R	74	ASP
1	R	81	LEU
1	R	110	LYS
1	R	111	GLU
1	R	119	LEU
1	R	126	THR
1	R	150	TRP
1	R	186	GLU
1	R	200	TYR
1	R	208	LEU
1	R	247	ARG
1	R	253	ARG
1	R	270	GLN
1	R	273	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	10	GLN
1	R	157	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

36 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	SAH	L	301	-	21,28,28	1.18	2 (9%)	20,40,40	1.81	2 (10%)
2	SAH	F	301	-	21,28,28	1.19	2 (9%)	20,40,40	1.74	2 (10%)
2	SAH	E	301	-	21,28,28	1.16	2 (9%)	20,40,40	1.80	2 (10%)
2	SAH	A	301	-	21,28,28	1.17	2 (9%)	20,40,40	1.75	2 (10%)
2	SAH	G	301	-	21,28,28	1.21	2 (9%)	20,40,40	1.74	3 (15%)
3	TEX	N	302	-	31,34,34	0.75	1 (3%)	26,50,50	1.43	3 (11%)
3	TEX	L	302	-	31,34,34	0.77	1 (3%)	26,50,50	1.48	4 (15%)
3	TEX	E	302	-	31,34,34	0.78	2 (6%)	26,50,50	1.34	3 (11%)
3	TEX	D	302	-	31,34,34	0.79	1 (3%)	26,50,50	1.38	3 (11%)
3	TEX	B	302	-	31,34,34	0.77	1 (3%)	26,50,50	1.32	2 (7%)
2	SAH	N	301	-	21,28,28	1.18	2 (9%)	20,40,40	1.77	3 (15%)
2	SAH	J	301	-	21,28,28	1.19	2 (9%)	20,40,40	1.78	3 (15%)
2	SAH	H	301	-	21,28,28	1.19	2 (9%)	20,40,40	1.77	2 (10%)
2	SAH	O	301	-	21,28,28	1.16	2 (9%)	20,40,40	1.82	2 (10%)
3	TEX	M	302	-	31,34,34	0.76	1 (3%)	26,50,50	1.44	3 (11%)
2	SAH	D	301	-	21,28,28	1.16	2 (9%)	20,40,40	1.79	2 (10%)
2	SAH	B	301	-	21,28,28	1.17	2 (9%)	20,40,40	1.73	2 (10%)
3	TEX	O	302	-	31,34,34	0.75	1 (3%)	26,50,50	1.48	4 (15%)
3	TEX	H	302	-	31,34,34	0.78	1 (3%)	26,50,50	1.33	3 (11%)
2	SAH	Q	301	-	21,28,28	1.16	2 (9%)	20,40,40	1.80	2 (10%)
2	SAH	P	301	-	21,28,28	1.17	2 (9%)	20,40,40	1.78	3 (15%)
2	SAH	I	301	-	21,28,28	1.17	2 (9%)	20,40,40	1.74	2 (10%)
2	SAH	K	301	-	21,28,28	1.19	2 (9%)	20,40,40	1.77	3 (15%)
3	TEX	Q	302	-	31,34,34	0.76	1 (3%)	26,50,50	1.43	3 (11%)
3	TEX	G	302	-	31,34,34	0.75	1 (3%)	26,50,50	1.43	4 (15%)
2	SAH	R	301	-	21,28,28	1.20	2 (9%)	20,40,40	1.76	2 (10%)
3	TEX	C	302	-	31,34,34	0.79	1 (3%)	26,50,50	1.38	3 (11%)
2	SAH	M	301	-	21,28,28	1.15	2 (9%)	20,40,40	1.78	2 (10%)
3	TEX	R	302	-	31,34,34	0.78	1 (3%)	26,50,50	1.28	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	TEX	P	302	-	31,34,34	0.76	1 (3%)	26,50,50	1.34	2 (7%)
2	SAH	C	301	-	21,28,28	1.15	2 (9%)	20,40,40	1.81	2 (10%)
3	TEX	K	302	-	31,34,34	0.77	1 (3%)	26,50,50	1.26	1 (3%)
3	TEX	J	302	-	31,34,34	0.77	1 (3%)	26,50,50	1.26	2 (7%)
3	TEX	I	302	-	31,34,34	0.78	1 (3%)	26,50,50	1.34	3 (11%)
3	TEX	F	302	-	31,34,34	0.78	2 (6%)	26,50,50	1.51	4 (15%)
3	TEX	A	302	-	31,34,34	0.77	1 (3%)	26,50,50	1.35	2 (7%)

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	SAH	L	301	-	-	2/7/31/31	0/3/3/3
2	SAH	F	301	-	-	3/7/31/31	0/3/3/3
2	SAH	E	301	-	-	3/7/31/31	0/3/3/3
2	SAH	A	301	-	-	2/7/31/31	0/3/3/3
2	SAH	G	301	-	-	3/7/31/31	0/3/3/3
3	TEX	N	302	-	-	9/27/42/42	0/2/3/3
3	TEX	L	302	-	-	9/27/42/42	0/2/3/3
3	TEX	E	302	-	-	7/27/42/42	0/2/3/3
3	TEX	D	302	-	-	7/27/42/42	0/2/3/3
3	TEX	B	302	-	-	7/27/42/42	0/2/3/3
2	SAH	N	301	-	-	0/7/31/31	0/3/3/3
2	SAH	J	301	-	-	3/7/31/31	0/3/3/3
2	SAH	H	301	-	-	2/7/31/31	0/3/3/3
2	SAH	O	301	-	-	1/7/31/31	0/3/3/3
3	TEX	M	302	-	-	9/27/42/42	0/2/3/3
2	SAH	D	301	-	-	3/7/31/31	0/3/3/3
2	SAH	B	301	-	-	2/7/31/31	0/3/3/3
3	TEX	O	302	-	-	9/27/42/42	0/2/3/3
3	TEX	H	302	-	-	10/27/42/42	0/2/3/3
2	SAH	Q	301	-	-	3/7/31/31	0/3/3/3
2	SAH	P	301	-	-	3/7/31/31	0/3/3/3
2	SAH	I	301	-	-	2/7/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	K	301	-	-	3/7/31/31	0/3/3/3
3	TEX	Q	302	-	-	9/27/42/42	0/2/3/3
3	TEX	G	302	-	-	12/27/42/42	0/2/3/3
2	SAH	R	301	-	-	3/7/31/31	0/3/3/3
3	TEX	C	302	-	-	9/27/42/42	0/2/3/3
2	SAH	M	301	-	-	3/7/31/31	0/3/3/3
3	TEX	R	302	-	-	9/27/42/42	0/2/3/3
3	TEX	P	302	-	-	9/27/42/42	0/2/3/3
2	SAH	C	301	-	-	1/7/31/31	0/3/3/3
3	TEX	K	302	-	-	7/27/42/42	0/2/3/3
3	TEX	J	302	-	-	10/27/42/42	0/2/3/3
3	TEX	I	302	-	-	9/27/42/42	0/2/3/3
3	TEX	F	302	-	-	11/27/42/42	0/2/3/3
3	TEX	A	302	-	-	9/27/42/42	0/2/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	301	SAH	C2-N3	4.00	1.38	1.32
2	G	301	SAH	C2-N3	3.98	1.38	1.32
2	K	301	SAH	C2-N3	3.97	1.38	1.32
2	H	301	SAH	C2-N3	3.97	1.38	1.32
2	R	301	SAH	C2-N3	3.95	1.38	1.32
2	L	301	SAH	C2-N3	3.91	1.38	1.32
2	N	301	SAH	C2-N3	3.90	1.38	1.32
2	P	301	SAH	C2-N3	3.85	1.38	1.32
2	F	301	SAH	C2-N3	3.81	1.38	1.32
2	Q	301	SAH	C2-N3	3.81	1.38	1.32
2	B	301	SAH	C2-N3	3.80	1.38	1.32
2	D	301	SAH	C2-N3	3.80	1.38	1.32
2	A	301	SAH	C2-N3	3.79	1.38	1.32
2	C	301	SAH	C2-N3	3.79	1.38	1.32
2	O	301	SAH	C2-N3	3.79	1.38	1.32
2	E	301	SAH	C2-N3	3.78	1.38	1.32
2	M	301	SAH	C2-N3	3.78	1.38	1.32
2	I	301	SAH	C2-N3	3.75	1.38	1.32
3	J	302	TEX	C3-C4	-2.89	1.40	1.43
3	K	302	TEX	C3-C4	-2.88	1.40	1.43
3	R	302	TEX	C3-C4	-2.87	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	TEX	C3-C4	-2.85	1.40	1.43
3	C	302	TEX	C3-C4	-2.83	1.40	1.43
3	D	302	TEX	C3-C4	-2.81	1.40	1.43
3	H	302	TEX	C3-C4	-2.79	1.40	1.43
3	I	302	TEX	C3-C4	-2.76	1.40	1.43
3	N	302	TEX	C3-C4	-2.76	1.40	1.43
3	A	302	TEX	C3-C4	-2.72	1.40	1.43
3	P	302	TEX	C3-C4	-2.69	1.40	1.43
3	L	302	TEX	C3-C4	-2.68	1.40	1.43
3	O	302	TEX	C3-C4	-2.67	1.40	1.43
3	M	302	TEX	C3-C4	-2.65	1.40	1.43
3	Q	302	TEX	C3-C4	-2.65	1.40	1.43
3	F	302	TEX	C3-C4	-2.65	1.40	1.43
3	E	302	TEX	C3-C4	-2.62	1.40	1.43
3	G	302	TEX	C3-C4	-2.58	1.40	1.43
2	R	301	SAH	C2-N1	2.51	1.38	1.33
2	E	301	SAH	C2-N1	2.48	1.38	1.33
2	H	301	SAH	C2-N1	2.48	1.38	1.33
2	G	301	SAH	C2-N1	2.48	1.38	1.33
2	I	301	SAH	C2-N1	2.48	1.38	1.33
2	L	301	SAH	C2-N1	2.47	1.38	1.33
2	B	301	SAH	C2-N1	2.46	1.38	1.33
2	K	301	SAH	C2-N1	2.46	1.38	1.33
2	F	301	SAH	C2-N1	2.43	1.38	1.33
2	D	301	SAH	C2-N1	2.42	1.38	1.33
2	Q	301	SAH	C2-N1	2.41	1.38	1.33
2	N	301	SAH	C2-N1	2.40	1.38	1.33
2	P	301	SAH	C2-N1	2.40	1.38	1.33
2	J	301	SAH	C2-N1	2.39	1.38	1.33
2	C	301	SAH	C2-N1	2.38	1.38	1.33
2	M	301	SAH	C2-N1	2.37	1.38	1.33
2	O	301	SAH	C2-N1	2.37	1.38	1.33
2	A	301	SAH	C2-N1	2.36	1.38	1.33
3	E	302	TEX	C20-C17	2.06	1.44	1.41
3	F	302	TEX	C20-C17	2.01	1.44	1.41

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	SAH	N3-C2-N1	-5.89	119.47	128.68
2	O	301	SAH	N3-C2-N1	-5.89	119.48	128.68
2	M	301	SAH	N3-C2-N1	-5.88	119.49	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	301	SAH	N3-C2-N1	-5.84	119.55	128.68
2	E	301	SAH	N3-C2-N1	-5.77	119.66	128.68
2	L	301	SAH	N3-C2-N1	-5.75	119.69	128.68
2	P	301	SAH	N3-C2-N1	-5.75	119.70	128.68
2	H	301	SAH	N3-C2-N1	-5.72	119.73	128.68
2	I	301	SAH	N3-C2-N1	-5.71	119.75	128.68
2	D	301	SAH	N3-C2-N1	-5.69	119.78	128.68
2	A	301	SAH	N3-C2-N1	-5.65	119.85	128.68
2	F	301	SAH	N3-C2-N1	-5.65	119.86	128.68
2	K	301	SAH	N3-C2-N1	-5.60	119.93	128.68
2	J	301	SAH	N3-C2-N1	-5.59	119.95	128.68
2	R	301	SAH	N3-C2-N1	-5.55	120.01	128.68
2	B	301	SAH	N3-C2-N1	-5.50	120.08	128.68
2	N	301	SAH	N3-C2-N1	-5.49	120.10	128.68
2	G	301	SAH	N3-C2-N1	-5.45	120.16	128.68
3	O	302	TEX	C2-C3-C4	-5.00	116.76	120.28
3	N	302	TEX	C2-C3-C4	-4.97	116.78	120.28
3	F	302	TEX	C2-C3-C4	-4.97	116.78	120.28
3	M	302	TEX	C2-C3-C4	-4.96	116.79	120.28
3	G	302	TEX	C2-C3-C4	-4.94	116.80	120.28
3	L	302	TEX	C2-C3-C4	-4.94	116.80	120.28
3	R	302	TEX	C2-C3-C4	-4.90	116.83	120.28
3	Q	302	TEX	C2-C3-C4	-4.89	116.83	120.28
3	A	302	TEX	C2-C3-C4	-4.82	116.88	120.28
3	J	302	TEX	C2-C3-C4	-4.80	116.89	120.28
3	I	302	TEX	C2-C3-C4	-4.80	116.90	120.28
3	P	302	TEX	C2-C3-C4	-4.79	116.90	120.28
3	D	302	TEX	C2-C3-C4	-4.79	116.90	120.28
3	C	302	TEX	C2-C3-C4	-4.79	116.90	120.28
3	H	302	TEX	C2-C3-C4	-4.75	116.93	120.28
3	E	302	TEX	C2-C3-C4	-4.75	116.93	120.28
3	K	302	TEX	C2-C3-C4	-4.71	116.96	120.28
3	B	302	TEX	C2-C3-C4	-4.69	116.97	120.28
2	B	301	SAH	C5'-SD-CG	-4.07	90.06	102.27
2	N	301	SAH	C5'-SD-CG	-4.06	90.09	102.27
2	L	301	SAH	C5'-SD-CG	-4.03	90.18	102.27
2	Q	301	SAH	C5'-SD-CG	-3.98	90.33	102.27
2	O	301	SAH	C5'-SD-CG	-3.95	90.42	102.27
2	F	301	SAH	C5'-SD-CG	-3.95	90.42	102.27
2	R	301	SAH	C5'-SD-CG	-3.94	90.46	102.27
2	J	301	SAH	C5'-SD-CG	-3.93	90.47	102.27
2	C	301	SAH	C5'-SD-CG	-3.92	90.50	102.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	SAH	C5'-SD-CG	-3.91	90.54	102.27
2	D	301	SAH	C5'-SD-CG	-3.89	90.58	102.27
2	K	301	SAH	C5'-SD-CG	-3.89	90.58	102.27
2	P	301	SAH	C5'-SD-CG	-3.87	90.64	102.27
2	H	301	SAH	C5'-SD-CG	-3.87	90.67	102.27
2	G	301	SAH	C5'-SD-CG	-3.85	90.72	102.27
2	E	301	SAH	C5'-SD-CG	-3.70	91.17	102.27
2	I	301	SAH	C5'-SD-CG	-3.63	91.36	102.27
2	M	301	SAH	C5'-SD-CG	-3.62	91.42	102.27
3	C	302	TEX	C10-C11-C12	3.01	119.65	112.41
3	N	302	TEX	C3-C6-C8	2.99	116.49	110.28
3	F	302	TEX	C3-C6-C8	2.96	116.42	110.28
3	O	302	TEX	C3-C6-C8	2.95	116.41	110.28
3	L	302	TEX	C3-C6-C8	2.88	116.25	110.28
3	D	302	TEX	C10-C11-C12	2.84	119.25	112.41
3	M	302	TEX	C3-C6-C8	2.77	116.04	110.28
3	G	302	TEX	C3-C6-C8	2.77	116.03	110.28
3	B	302	TEX	C10-C11-C12	2.68	118.85	112.41
3	F	302	TEX	C10-C11-C12	2.64	118.77	112.41
3	Q	302	TEX	C3-C6-C8	2.60	115.67	110.28
3	E	302	TEX	C10-C11-C12	2.55	118.55	112.41
3	L	302	TEX	C10-C11-C12	2.53	118.50	112.41
3	H	302	TEX	C10-C11-C12	2.52	118.47	112.41
3	O	302	TEX	C10-C11-C12	2.42	118.24	112.41
3	I	302	TEX	C10-C11-C12	2.38	118.15	112.41
3	A	302	TEX	C10-C11-C12	2.38	118.15	112.41
2	G	301	SAH	C3'-C2'-C1'	2.36	104.52	100.98
3	Q	302	TEX	C10-C11-C12	2.33	118.02	112.41
3	M	302	TEX	C10-C11-C12	2.31	117.96	112.41
3	P	302	TEX	C10-C11-C12	2.30	117.95	112.41
3	C	302	TEX	C11-C10-C6	2.29	119.18	115.72
3	D	302	TEX	C11-C10-C6	2.24	119.10	115.72
2	J	301	SAH	C3'-C2'-C1'	2.23	104.33	100.98
3	F	302	TEX	C11-C10-C6	2.21	119.06	115.72
2	K	301	SAH	C3'-C2'-C1'	2.21	104.31	100.98
3	E	302	TEX	C11-C10-C6	2.12	118.92	115.72
3	L	302	TEX	C11-C10-C6	2.09	118.88	115.72
3	I	302	TEX	C11-C10-C6	2.09	118.87	115.72
3	G	302	TEX	C10-C11-C12	2.08	117.42	112.41
3	N	302	TEX	C10-C11-C12	2.07	117.39	112.41
3	H	302	TEX	C11-C10-C6	2.05	118.82	115.72
3	G	302	TEX	C11-C10-C6	2.04	118.80	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	301	SAH	C3'-C2'-C1'	2.03	104.04	100.98
3	J	302	TEX	C10-C11-C12	2.01	117.25	112.41
2	P	301	SAH	C3'-C2'-C1'	2.01	104.00	100.98
3	O	302	TEX	C11-C10-C6	2.00	118.74	115.72

There are no chirality outliers.

All (203) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	301	SAH	C-CA-CB-CG
2	F	301	SAH	C-CA-CB-CG
2	E	301	SAH	N-CA-CB-CG
2	E	301	SAH	C-CA-CB-CG
2	A	301	SAH	C-CA-CB-CG
2	G	301	SAH	C-CA-CB-CG
3	N	302	TEX	C2-C3-C6-C7
3	N	302	TEX	C4-C3-C6-C7
3	N	302	TEX	C4-C3-C6-C10
3	N	302	TEX	C10-C6-C8-C9
3	N	302	TEX	C17-C16-N2-C23
3	L	302	TEX	C2-C3-C6-C7
3	L	302	TEX	C4-C3-C6-C7
3	L	302	TEX	C4-C3-C6-C10
3	L	302	TEX	C10-C6-C8-C9
3	Q	302	TEX	C2-C3-C6-C7
3	Q	302	TEX	C4-C3-C6-C7
3	Q	302	TEX	C4-C3-C6-C10
3	Q	302	TEX	C10-C6-C8-C9
3	Q	302	TEX	C17-C16-N2-C23
3	E	302	TEX	C2-C3-C6-C7
3	E	302	TEX	C4-C3-C6-C7
3	E	302	TEX	C4-C3-C6-C10
3	D	302	TEX	C2-C3-C6-C7
3	D	302	TEX	C4-C3-C6-C7
3	D	302	TEX	C4-C3-C6-C10
3	B	302	TEX	C2-C3-C6-C7
3	B	302	TEX	C4-C3-C6-C7
3	B	302	TEX	C4-C3-C6-C10
3	B	302	TEX	C17-C16-N2-C23
2	J	301	SAH	N-CA-CB-CG
2	J	301	SAH	C-CA-CB-CG
2	H	301	SAH	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	M	302	TEX	C2-C3-C6-C7
3	M	302	TEX	C4-C3-C6-C7
3	M	302	TEX	C4-C3-C6-C10
3	M	302	TEX	C10-C6-C8-C9
2	B	301	SAH	C-CA-CB-CG
3	H	302	TEX	C2-C3-C6-C7
3	H	302	TEX	C4-C3-C6-C7
3	H	302	TEX	C4-C3-C6-C10
2	Q	301	SAH	N-CA-CB-CG
2	Q	301	SAH	C-CA-CB-CG
2	P	301	SAH	N-CA-CB-CG
2	P	301	SAH	C-CA-CB-CG
2	I	301	SAH	C-CA-CB-CG
2	K	301	SAH	C-CA-CB-CG
3	O	302	TEX	C2-C3-C6-C7
3	O	302	TEX	C4-C3-C6-C7
3	O	302	TEX	C4-C3-C6-C10
3	O	302	TEX	C10-C6-C8-C9
3	O	302	TEX	C17-C16-N2-C23
3	G	302	TEX	C2-C3-C6-C7
3	G	302	TEX	C4-C3-C6-C7
3	G	302	TEX	C4-C3-C6-C10
3	G	302	TEX	C10-C6-C8-C9
2	R	301	SAH	C-CA-CB-CG
3	C	302	TEX	C2-C3-C6-C7
3	C	302	TEX	C4-C3-C6-C7
3	C	302	TEX	C4-C3-C6-C10
2	M	301	SAH	C-CA-CB-CG
3	R	302	TEX	C2-C3-C6-C7
3	R	302	TEX	C4-C3-C6-C7
3	R	302	TEX	C4-C3-C6-C10
3	P	302	TEX	C2-C3-C6-C7
3	P	302	TEX	C4-C3-C6-C7
3	P	302	TEX	C4-C3-C6-C10
3	K	302	TEX	C2-C3-C6-C7
3	K	302	TEX	C4-C3-C6-C7
3	K	302	TEX	C4-C3-C6-C10
3	K	302	TEX	C17-C16-N2-C23
3	J	302	TEX	C2-C3-C6-C7
3	J	302	TEX	C4-C3-C6-C7
3	J	302	TEX	C4-C3-C6-C10
3	I	302	TEX	C2-C3-C6-C7

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Mol	Chain	Res	Type	Atoms
3	I	302	TEX	C4-C3-C6-C7
3	I	302	TEX	C4-C3-C6-C10
3	I	302	TEX	C19-C18-C25-C26
3	F	302	TEX	C2-C3-C6-C7
3	F	302	TEX	C4-C3-C6-C7
3	F	302	TEX	C4-C3-C6-C10
3	F	302	TEX	C10-C6-C8-C9
3	A	302	TEX	C2-C3-C6-C7
3	A	302	TEX	C4-C3-C6-C7
3	A	302	TEX	C4-C3-C6-C10
3	A	302	TEX	C17-C16-N2-C23
3	D	302	TEX	C10-C11-C12-C13
3	C	302	TEX	C10-C11-C12-C13
3	F	302	TEX	C10-C11-C12-C13
3	L	302	TEX	C10-C11-C12-C13
3	I	302	TEX	C10-C11-C12-C13
3	E	302	TEX	C10-C11-C12-C13
3	M	302	TEX	C10-C11-C12-C13
3	O	302	TEX	C10-C11-C12-C13
3	A	302	TEX	C10-C11-C12-C13
3	B	302	TEX	C10-C11-C12-C13
3	Q	302	TEX	C10-C11-C12-C13
3	P	302	TEX	C10-C11-C12-C13
3	G	302	TEX	C10-C11-C12-C13
3	N	302	TEX	C3-C6-C8-C9
3	L	302	TEX	C3-C6-C8-C9
3	Q	302	TEX	C3-C6-C8-C9
3	M	302	TEX	C3-C6-C8-C9
3	O	302	TEX	C3-C6-C8-C9
3	G	302	TEX	C3-C6-C8-C9
3	F	302	TEX	C3-C6-C8-C9
2	L	301	SAH	N-CA-CB-CG
2	A	301	SAH	N-CA-CB-CG
2	G	301	SAH	N-CA-CB-CG
3	L	302	TEX	C2-C3-C6-C10
3	Q	302	TEX	C2-C3-C6-C10
2	H	301	SAH	N-CA-CB-CG
3	M	302	TEX	C2-C3-C6-C10
3	H	302	TEX	C2-C3-C6-C10
2	I	301	SAH	N-CA-CB-CG
2	K	301	SAH	N-CA-CB-CG
2	R	301	SAH	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	M	301	SAH	N-CA-CB-CG
3	P	302	TEX	C2-C3-C6-C10
3	K	302	TEX	C2-C3-C6-C10
3	J	302	TEX	C2-C3-C6-C10
3	F	302	TEX	C2-C3-C6-C10
3	A	302	TEX	C2-C3-C6-C10
3	R	302	TEX	C10-C11-C12-C13
3	J	302	TEX	C10-C11-C12-C13
3	N	302	TEX	C10-C11-C12-C13
3	G	302	TEX	C19-C18-C25-C26
3	C	302	TEX	C19-C18-C25-C26
3	C	302	TEX	C19-C18-C25-C27
3	J	302	TEX	C19-C18-C25-C26
3	I	302	TEX	C19-C18-C25-C27
3	N	302	TEX	C1-C16-N2-C23
3	L	302	TEX	C1-C16-N2-C23
3	Q	302	TEX	C1-C16-N2-C23
3	E	302	TEX	C1-C16-N2-C23
3	D	302	TEX	C1-C16-N2-C23
3	B	302	TEX	C1-C16-N2-C23
3	M	302	TEX	C1-C16-N2-C23
3	H	302	TEX	C1-C16-N2-C23
3	O	302	TEX	C1-C16-N2-C23
3	G	302	TEX	C1-C16-N2-C23
3	C	302	TEX	C1-C16-N2-C23
3	R	302	TEX	C1-C16-N2-C23
3	P	302	TEX	C1-C16-N2-C23
3	K	302	TEX	C1-C16-N2-C23
3	J	302	TEX	C1-C16-N2-C23
3	I	302	TEX	C1-C16-N2-C23
3	F	302	TEX	C1-C16-N2-C23
3	A	302	TEX	C1-C16-N2-C23
3	L	302	TEX	C17-C16-N2-C23
3	E	302	TEX	C17-C16-N2-C23
3	D	302	TEX	C17-C16-N2-C23
3	M	302	TEX	C17-C16-N2-C23
3	H	302	TEX	C1-C16-N2-C18
3	H	302	TEX	C17-C16-N2-C23
3	G	302	TEX	C1-C16-N2-C18
3	G	302	TEX	C17-C16-N2-C23
3	C	302	TEX	C17-C16-N2-C23
3	R	302	TEX	C1-C16-N2-C18

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Mol	Chain	Res	Type	Atoms
3	R	302	TEX	C17-C16-N2-C23
3	P	302	TEX	C17-C16-N2-C23
3	J	302	TEX	C1-C16-N2-C18
3	J	302	TEX	C17-C16-N2-C23
3	I	302	TEX	C17-C16-N2-C23
3	F	302	TEX	C17-C16-N2-C23
2	G	301	SAH	CB-CG-SD-C5'
3	H	302	TEX	C10-C11-C12-C13
3	K	302	TEX	C10-C11-C12-C13
2	F	301	SAH	CB-CG-SD-C5'
2	K	301	SAH	CB-CG-SD-C5'
2	M	301	SAH	CB-CG-SD-C5'
2	D	301	SAH	CB-CG-SD-C5'
2	P	301	SAH	CB-CG-SD-C5'
2	F	301	SAH	N-CA-CB-CG
3	N	302	TEX	C2-C3-C6-C10
3	E	302	TEX	C2-C3-C6-C10
3	D	302	TEX	C2-C3-C6-C10
3	B	302	TEX	C2-C3-C6-C10
2	O	301	SAH	N-CA-CB-CG
2	D	301	SAH	N-CA-CB-CG
2	B	301	SAH	N-CA-CB-CG
3	O	302	TEX	C2-C3-C6-C10
3	G	302	TEX	C2-C3-C6-C10
3	C	302	TEX	C2-C3-C6-C10
3	R	302	TEX	C2-C3-C6-C10
2	C	301	SAH	N-CA-CB-CG
3	I	302	TEX	C2-C3-C6-C10
2	E	301	SAH	CB-CG-SD-C5'
2	J	301	SAH	CB-CG-SD-C5'
2	Q	301	SAH	CB-CG-SD-C5'
2	R	301	SAH	CB-CG-SD-C5'
2	D	301	SAH	C-CA-CB-CG
3	H	302	TEX	C19-C18-C25-C26
3	H	302	TEX	C19-C18-C25-C27
3	G	302	TEX	C19-C18-C25-C27
3	R	302	TEX	C19-C18-C25-C27
3	P	302	TEX	C19-C18-C25-C26
3	P	302	TEX	C19-C18-C25-C27
3	J	302	TEX	C19-C18-C25-C27
3	F	302	TEX	C19-C18-C25-C26
3	F	302	TEX	C19-C18-C25-C27

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Mol	Chain	Res	Type	Atoms
3	A	302	TEX	C19-C18-C25-C26
3	A	302	TEX	C19-C18-C25-C27

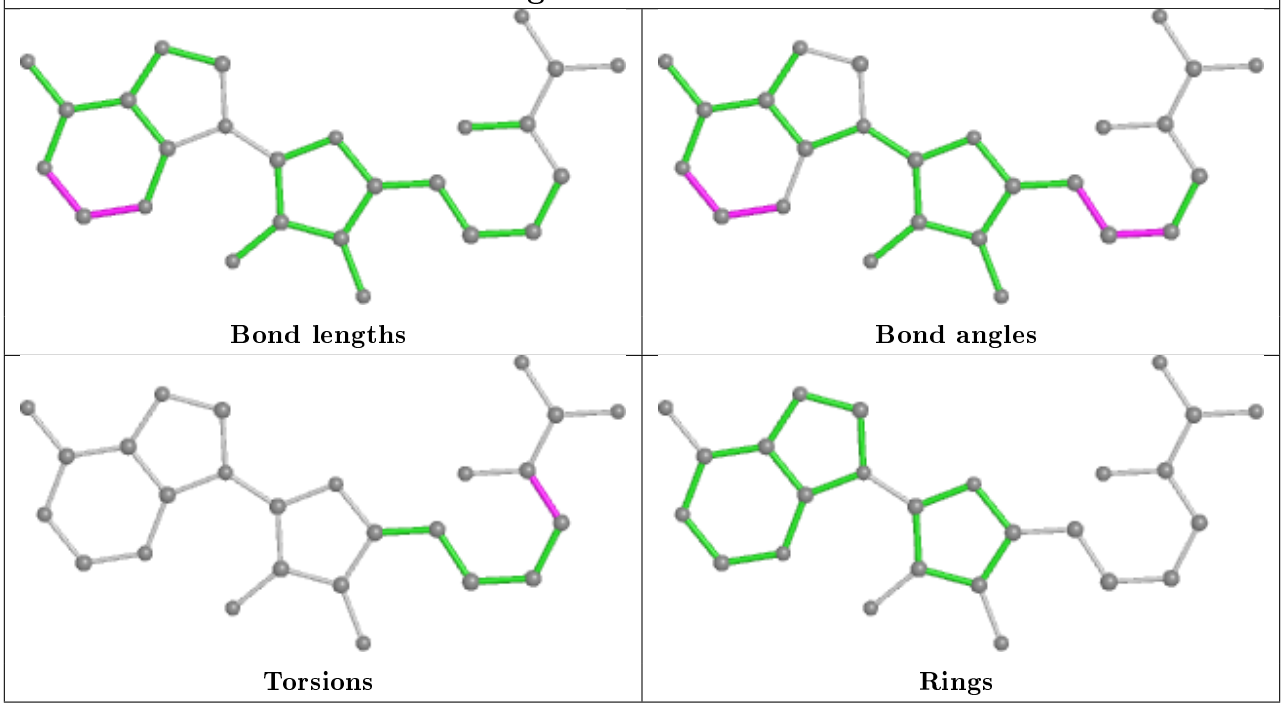
There are no ring outliers.

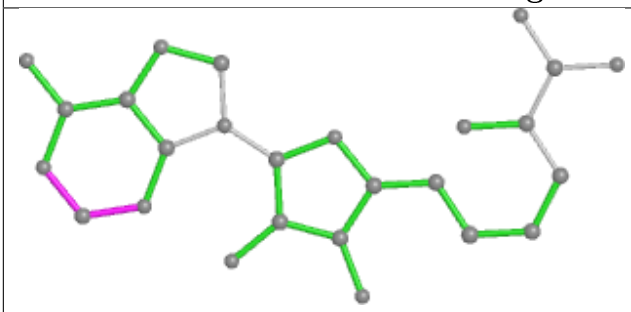
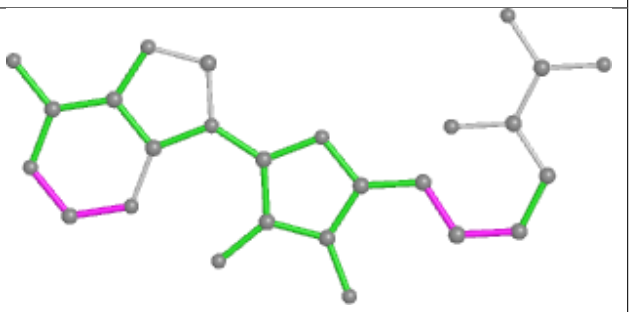
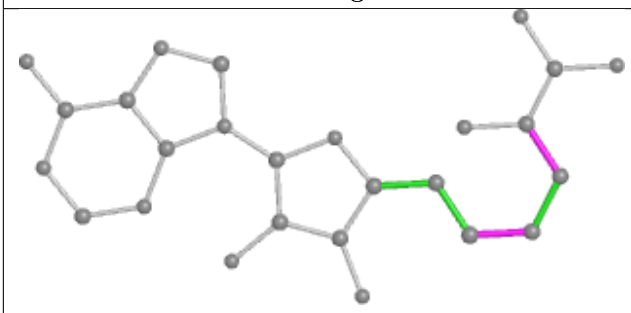
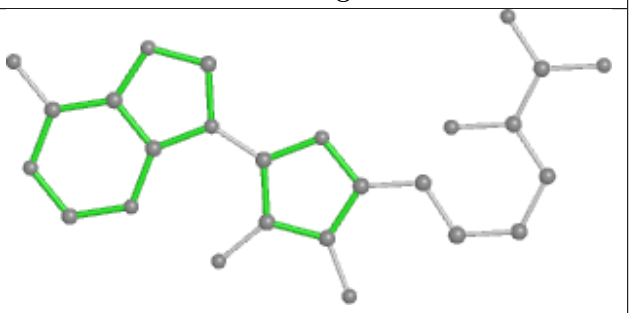
34 monomers are involved in 54 short contacts:

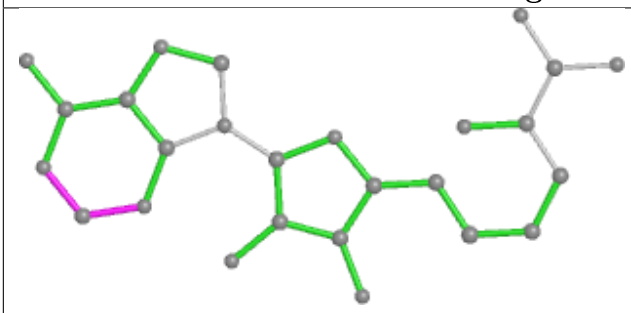
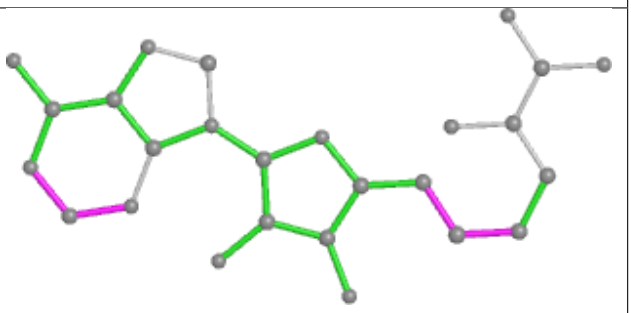
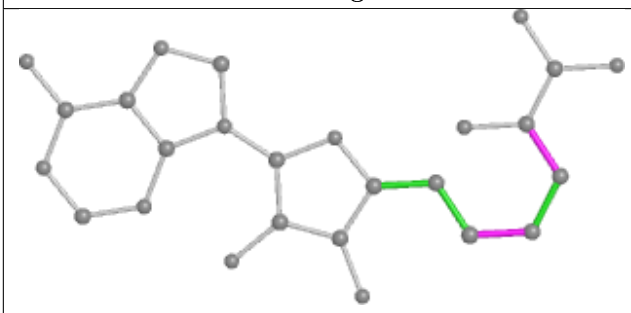
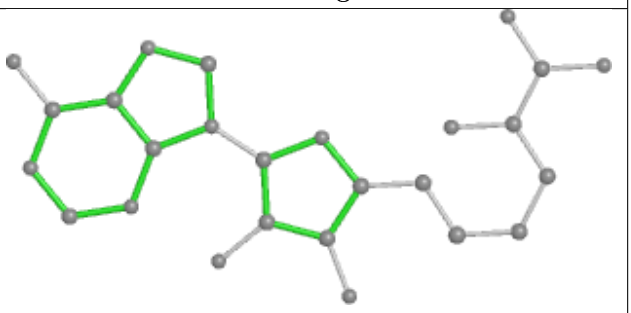
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301	SAH	1	0
2	F	301	SAH	2	0
2	E	301	SAH	1	0
2	A	301	SAH	2	0
2	G	301	SAH	2	0
3	N	302	TEX	2	0
3	L	302	TEX	1	0
3	E	302	TEX	1	0
3	D	302	TEX	2	0
3	B	302	TEX	1	0
2	N	301	SAH	2	0
2	J	301	SAH	2	0
2	H	301	SAH	1	0
2	O	301	SAH	2	0
3	M	302	TEX	2	0
2	D	301	SAH	3	0
3	O	302	TEX	2	0
3	H	302	TEX	2	0
2	Q	301	SAH	2	0
2	P	301	SAH	2	0
2	I	301	SAH	2	0
2	K	301	SAH	1	0
3	Q	302	TEX	1	0
3	G	302	TEX	1	0
2	R	301	SAH	1	0
3	C	302	TEX	1	0
3	R	302	TEX	1	0
3	P	302	TEX	2	0
2	C	301	SAH	1	0
3	K	302	TEX	2	0
3	J	302	TEX	1	0
3	I	302	TEX	1	0
3	F	302	TEX	2	0
3	A	302	TEX	2	0

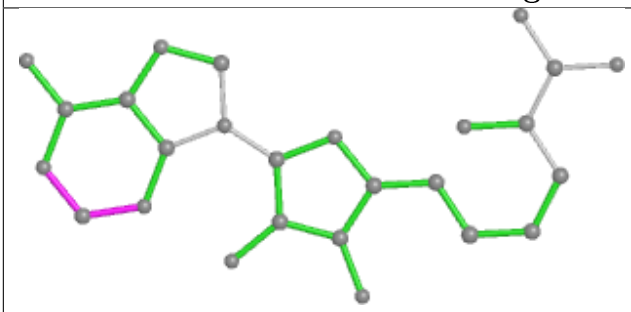
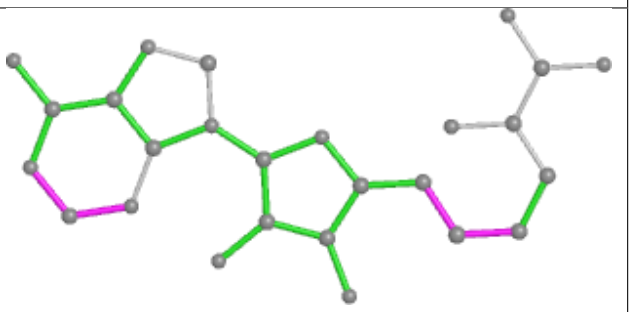
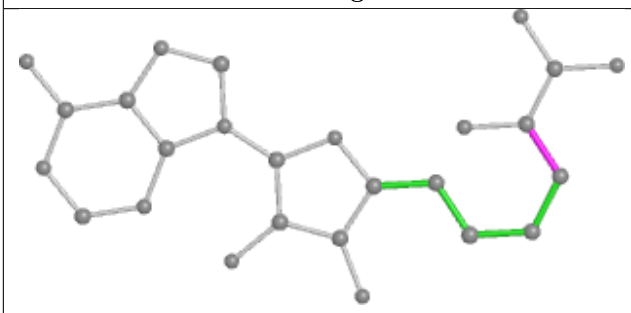
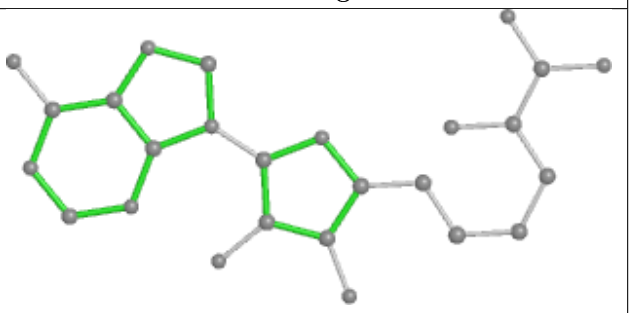
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 SAH L 301



Ligand SAH F 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH E 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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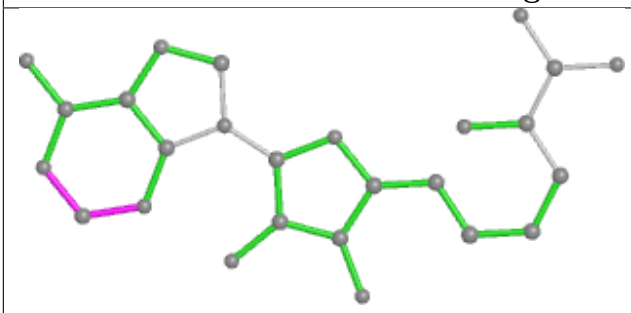
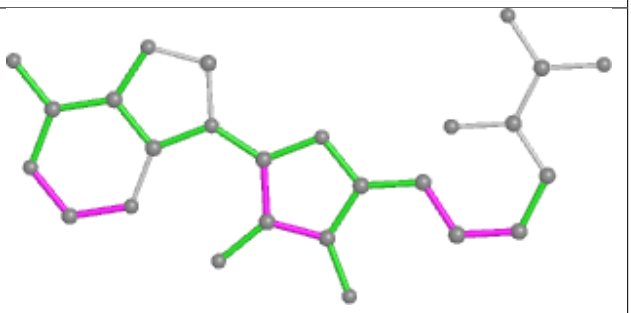
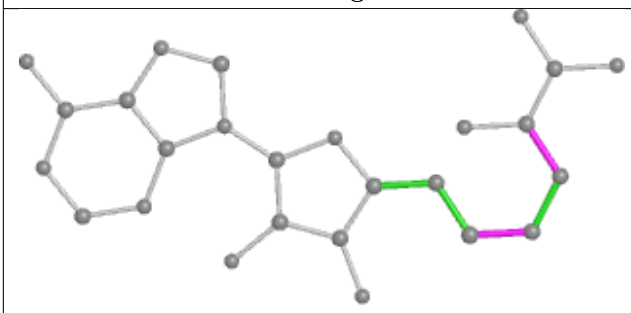
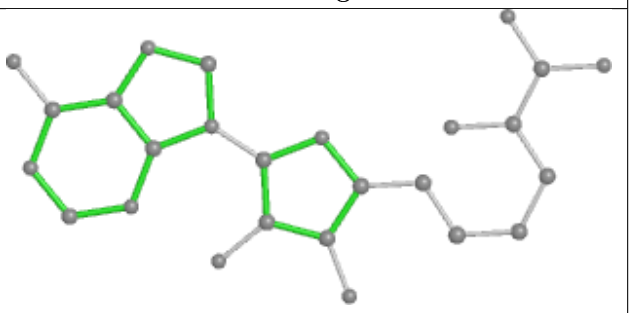
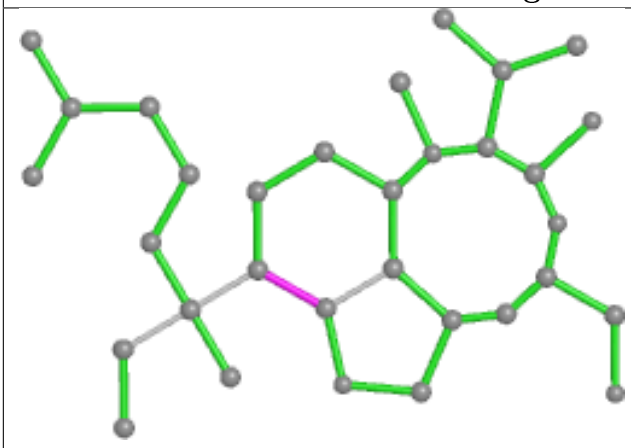
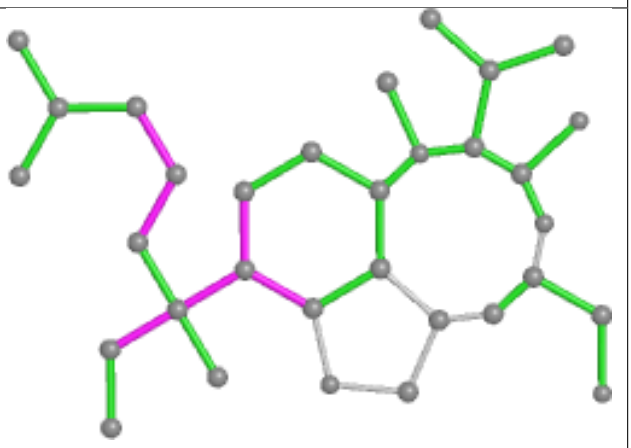
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TEX N 302



Bond lengths



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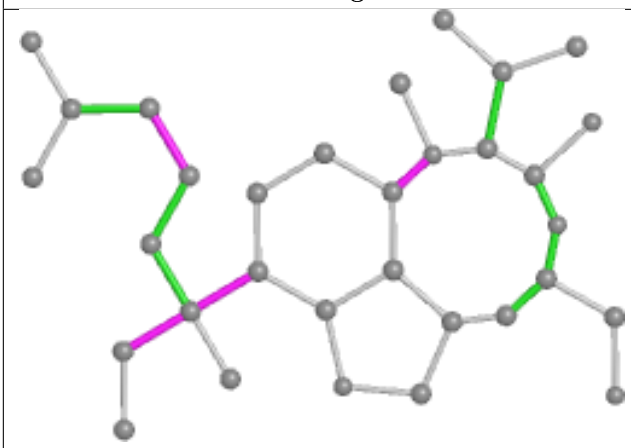

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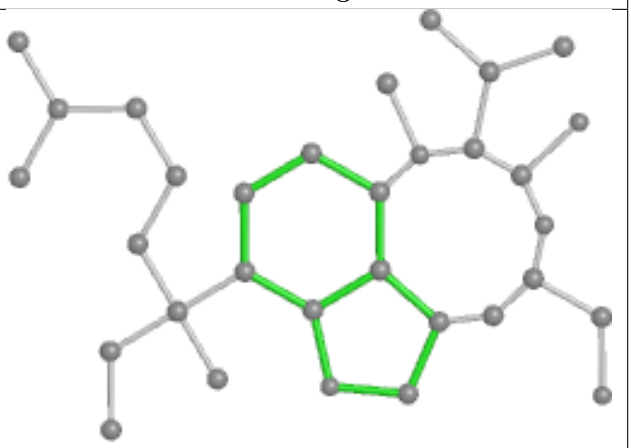
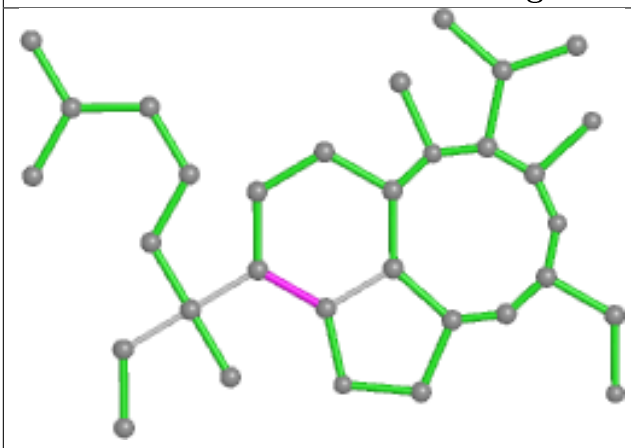


Rings

Ligand TEX L 302



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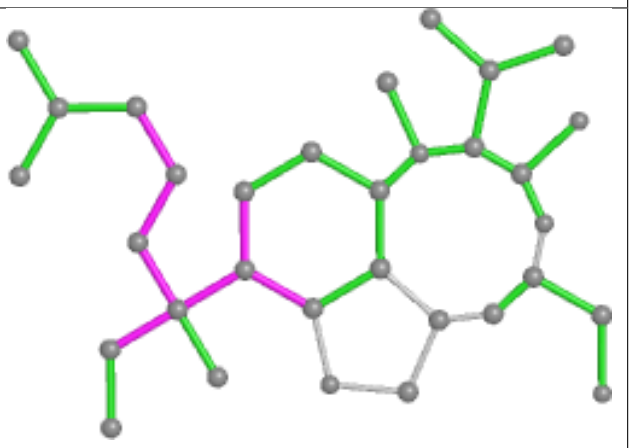

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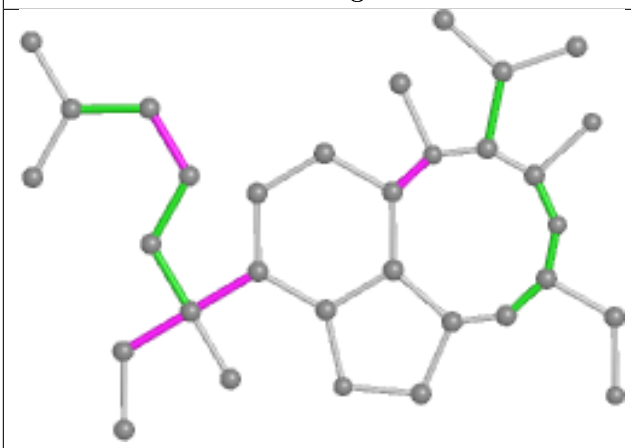

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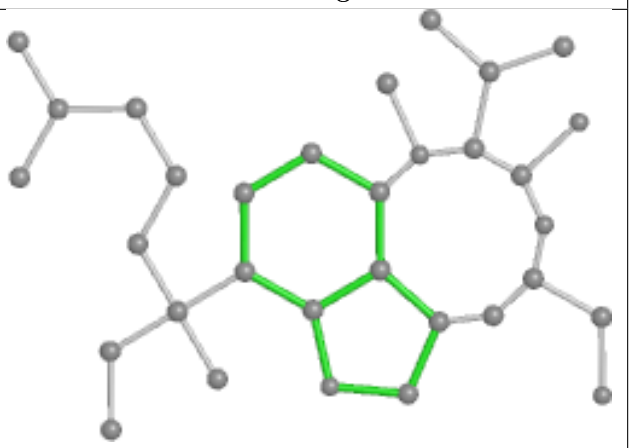
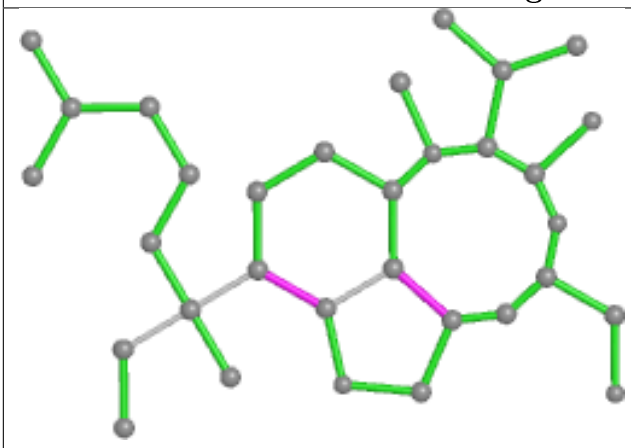


Rings

Ligand TEX E 302



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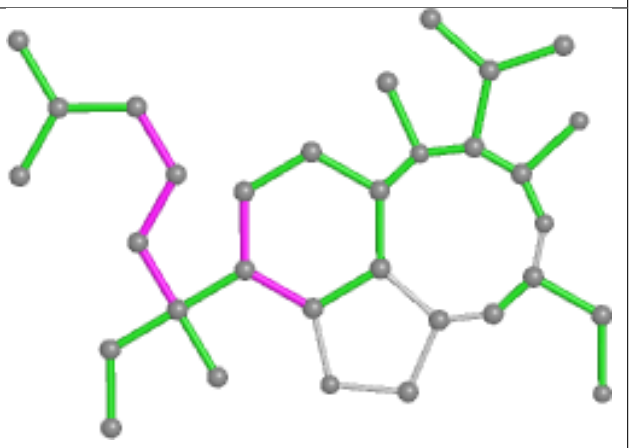

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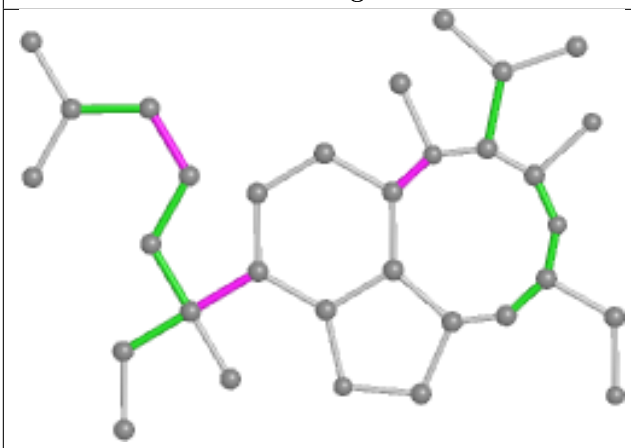

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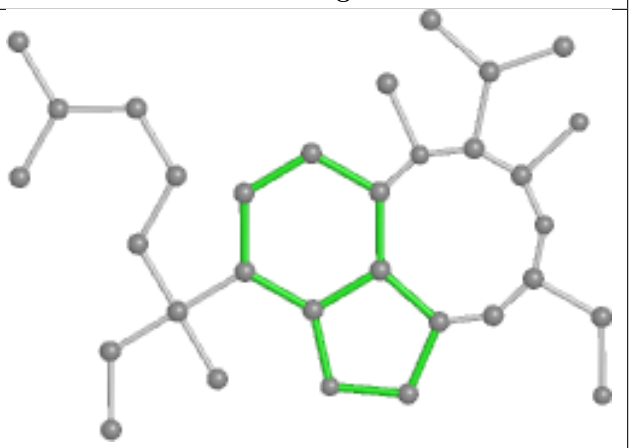
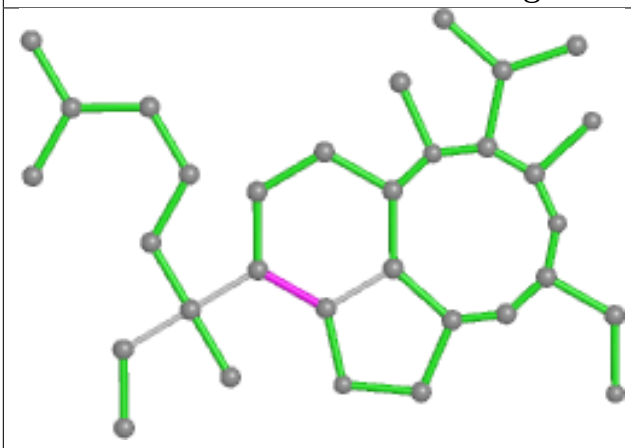


Rings

Ligand TEX D 302



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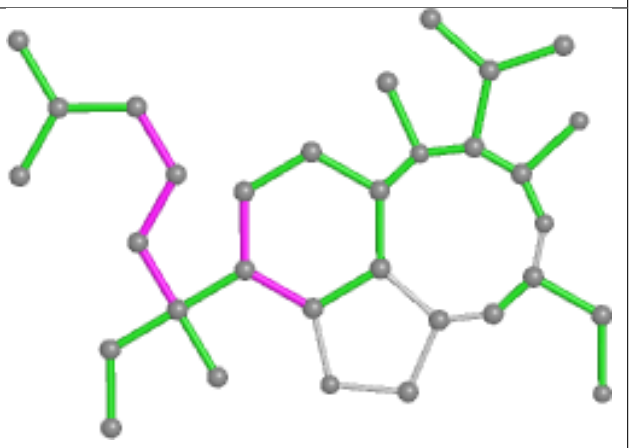

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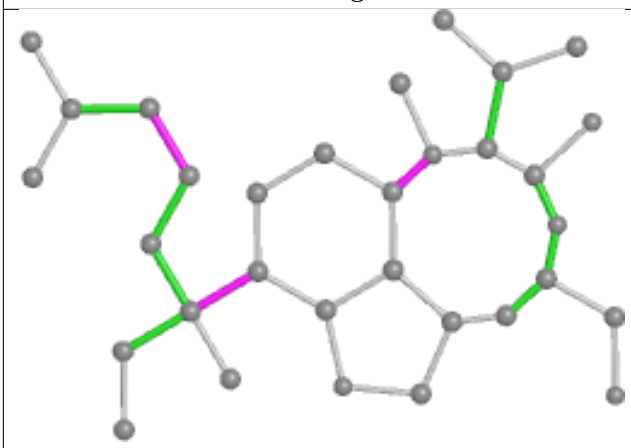

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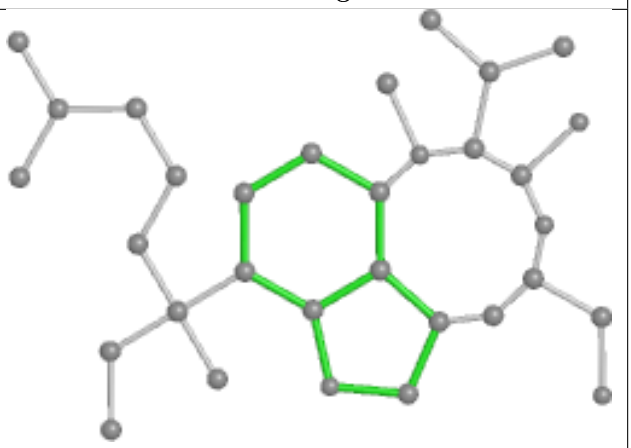
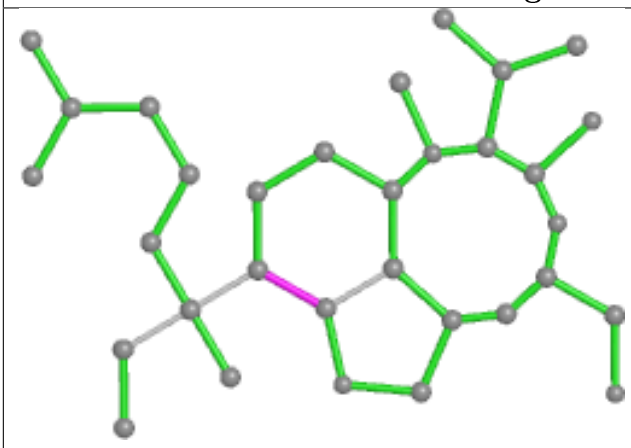


Rings

Ligand TEX B 302



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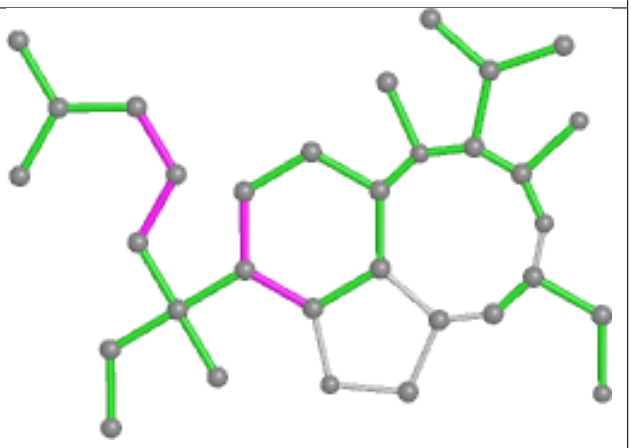

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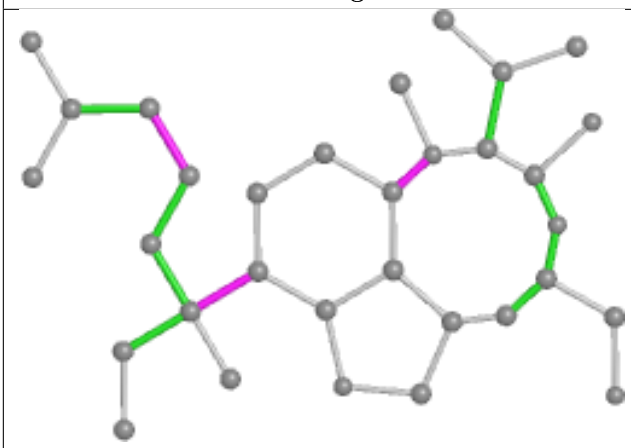

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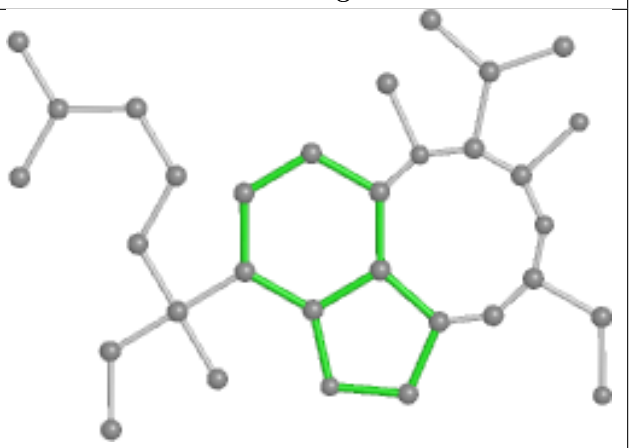
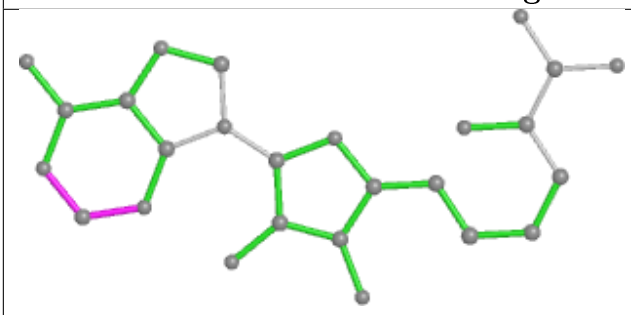


Rings

Ligand SAH N 301



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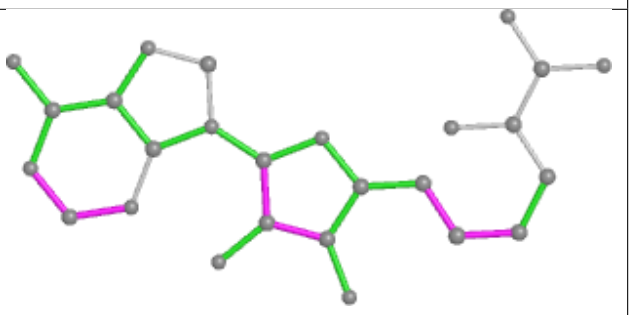

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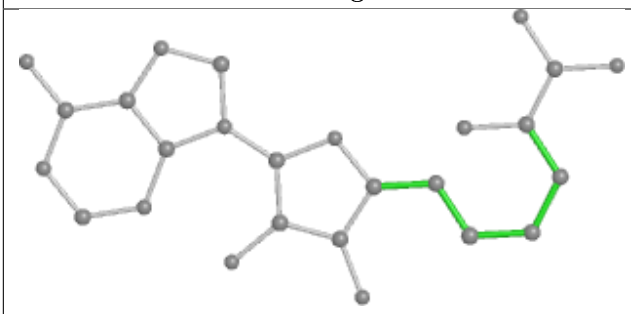

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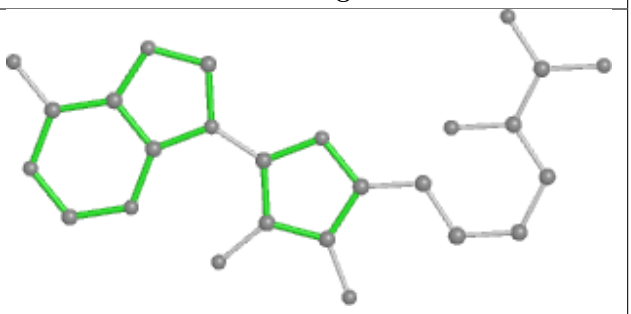
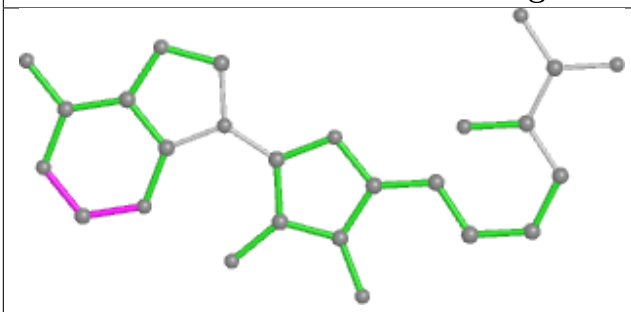
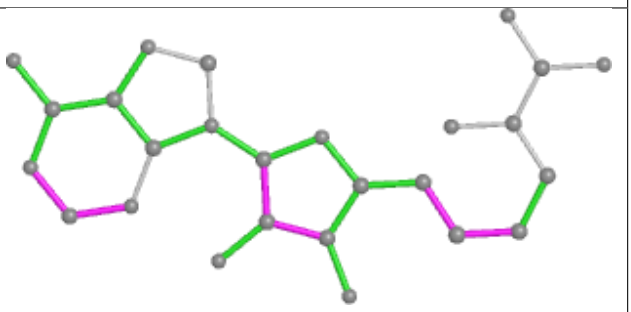
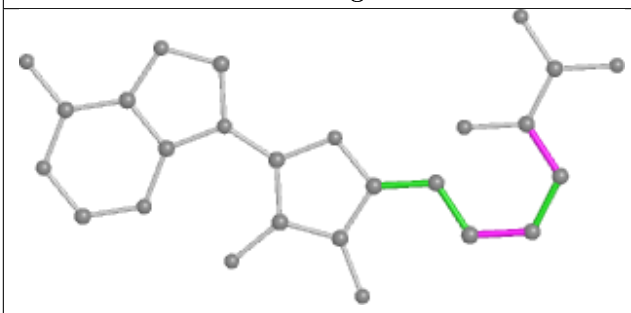
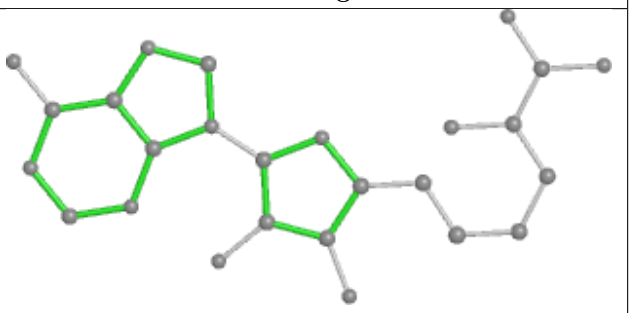
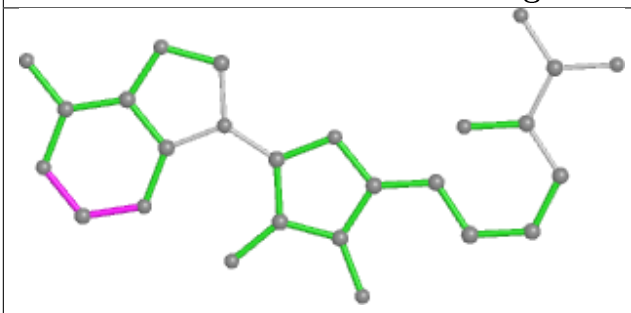
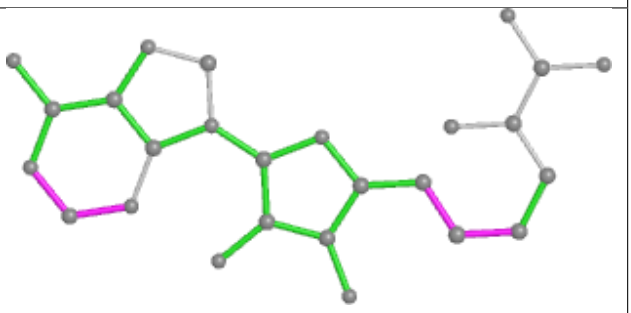
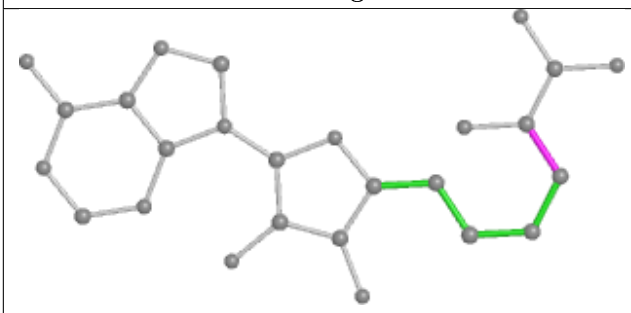
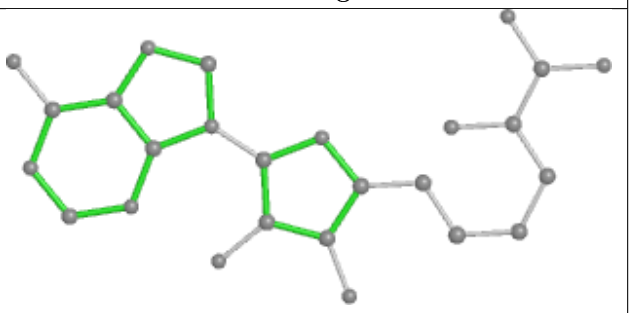
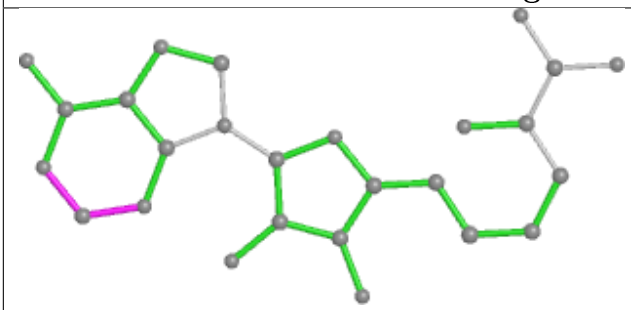


Rings

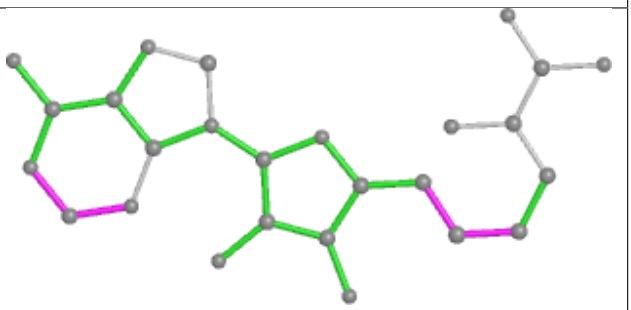
Ligand SAH J 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH H 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

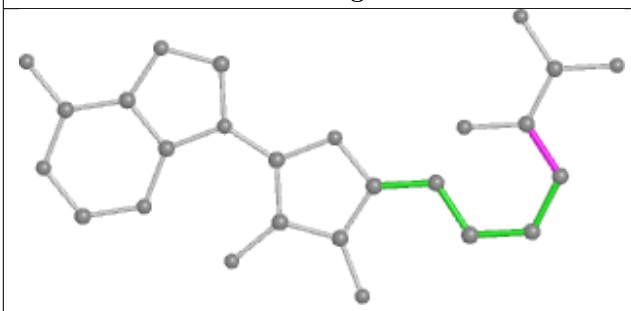
Ligand SAH O 301



Bond lengths



Bond angles



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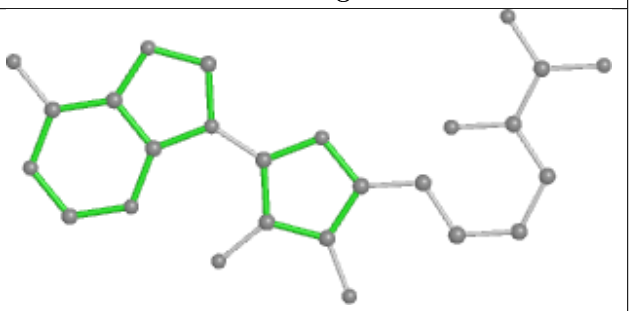
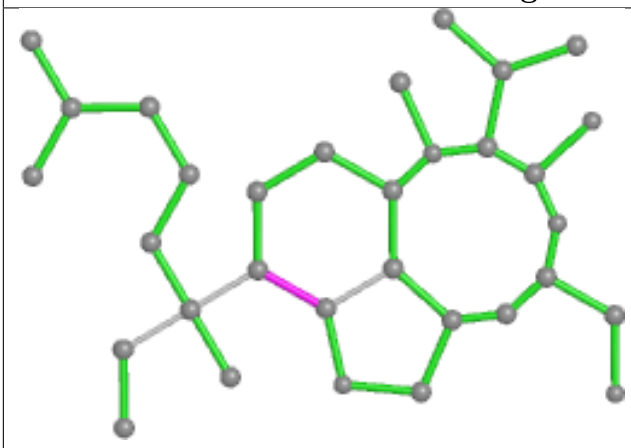


Rings

Ligand TEX M 302



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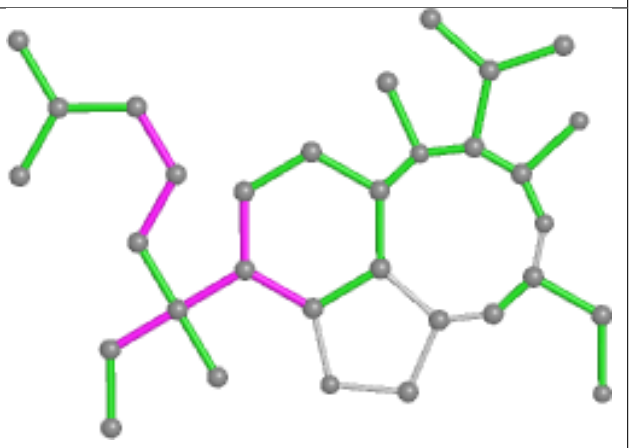

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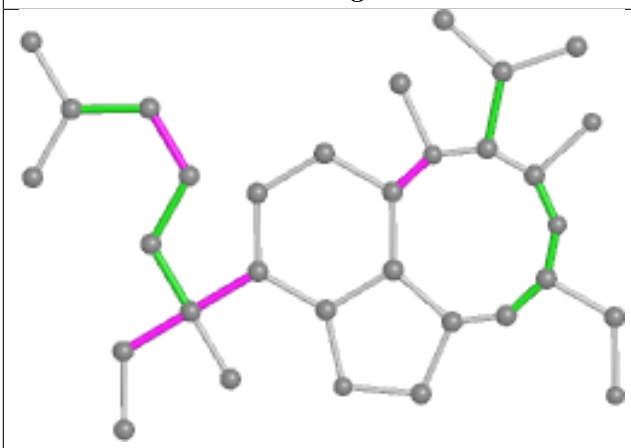

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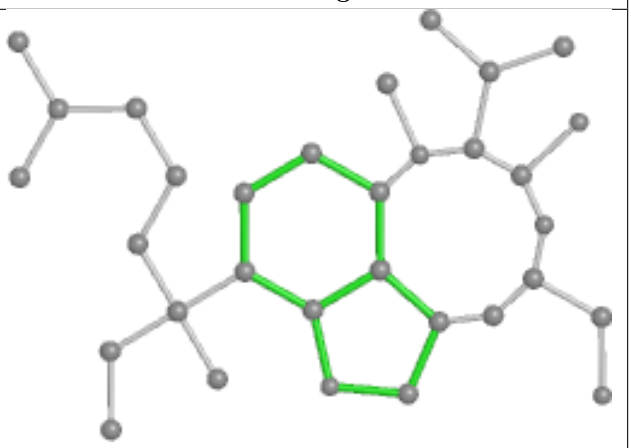
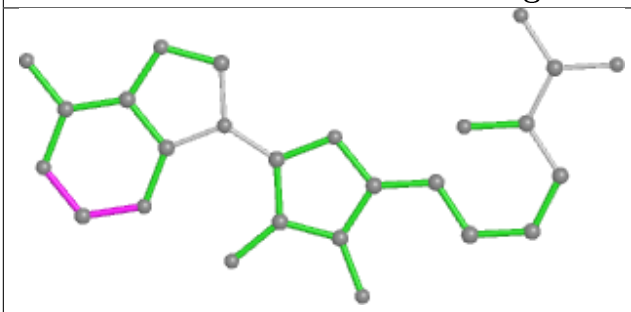
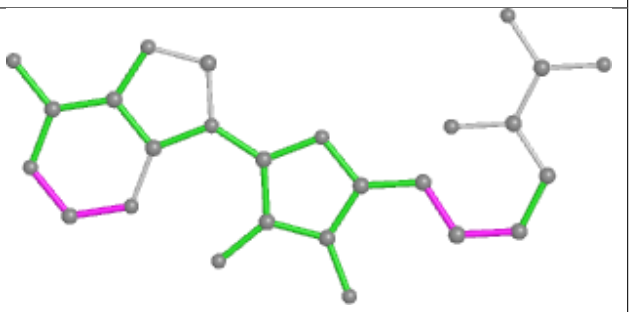
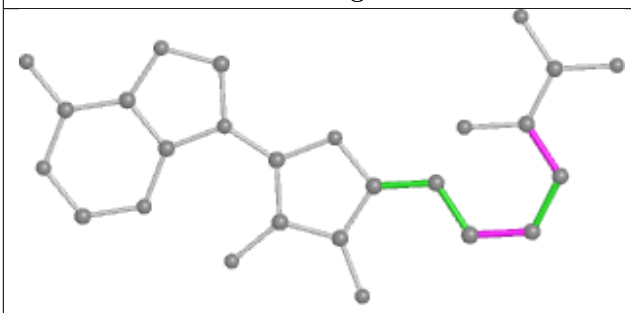
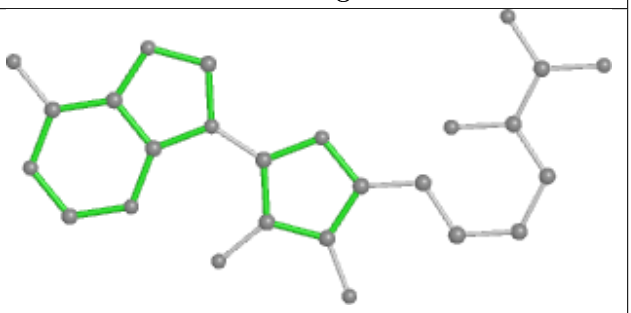
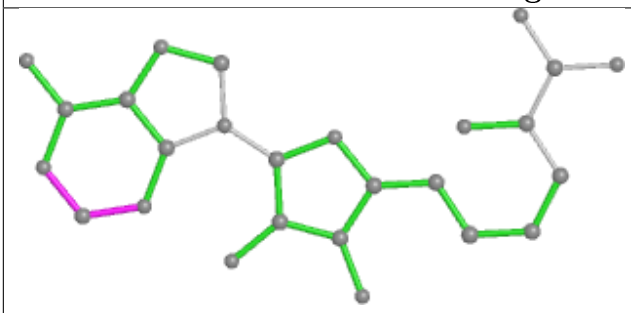
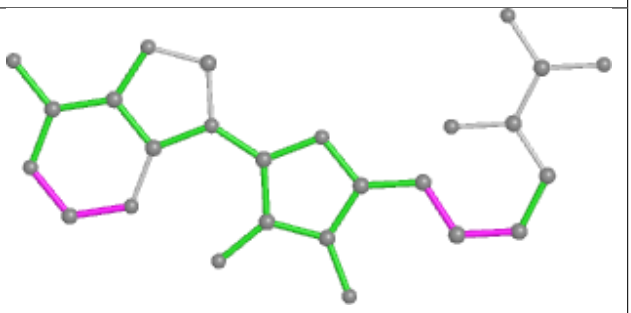
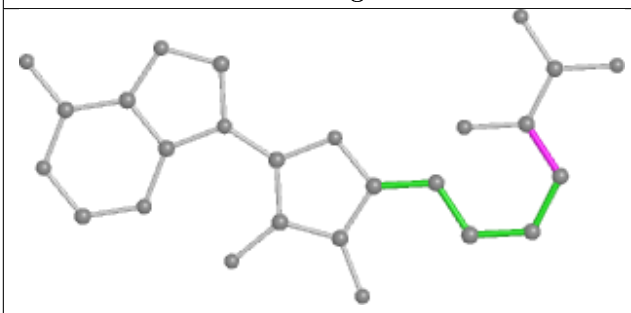
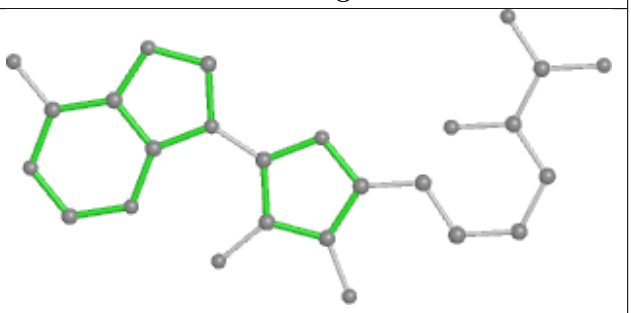
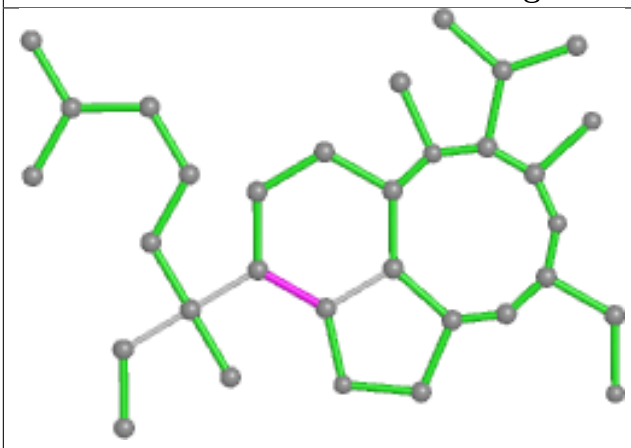


Rings

Ligand SAH D 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH B 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TEX O 302



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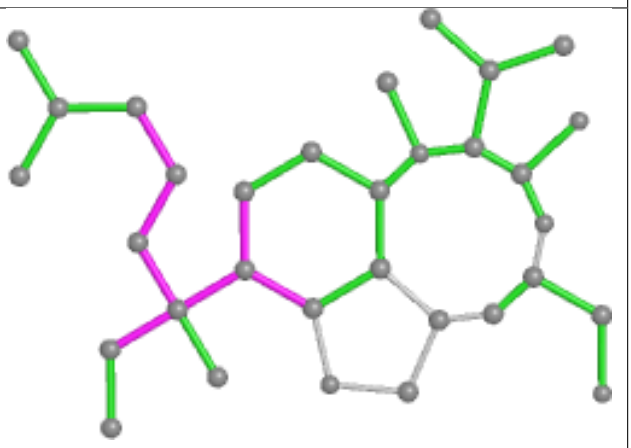

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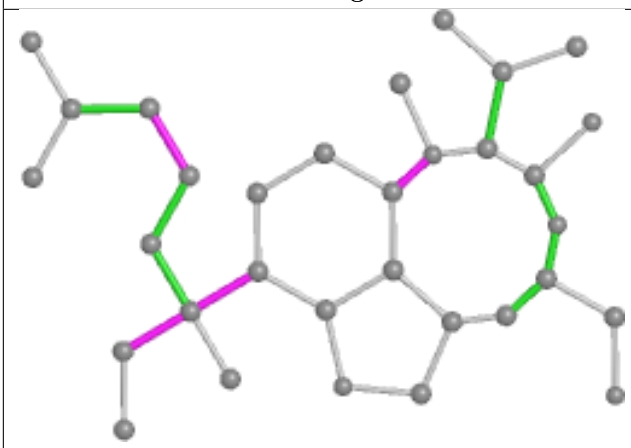

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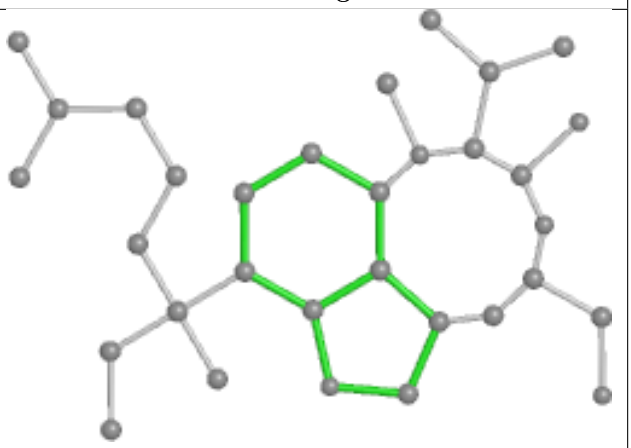

Rings

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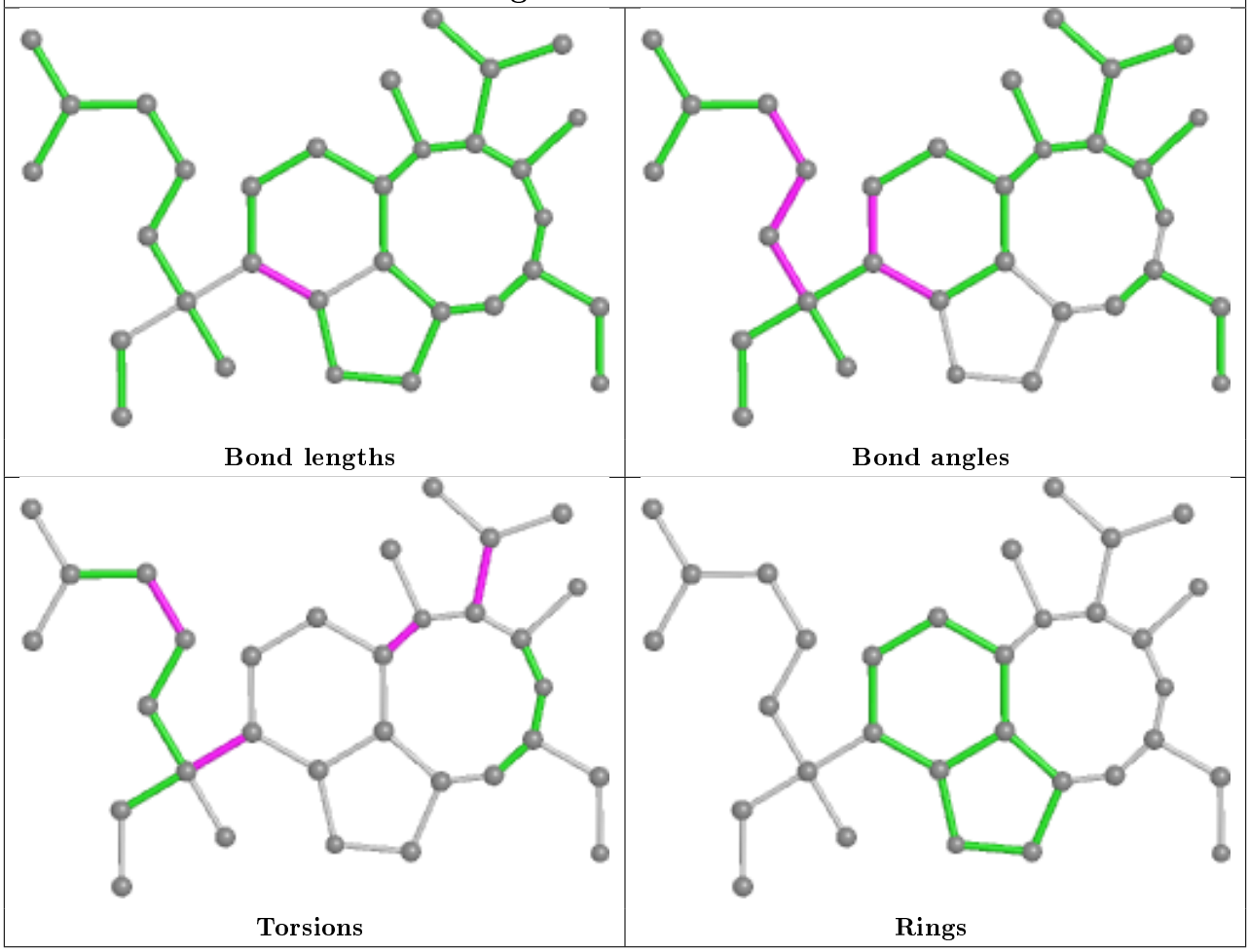

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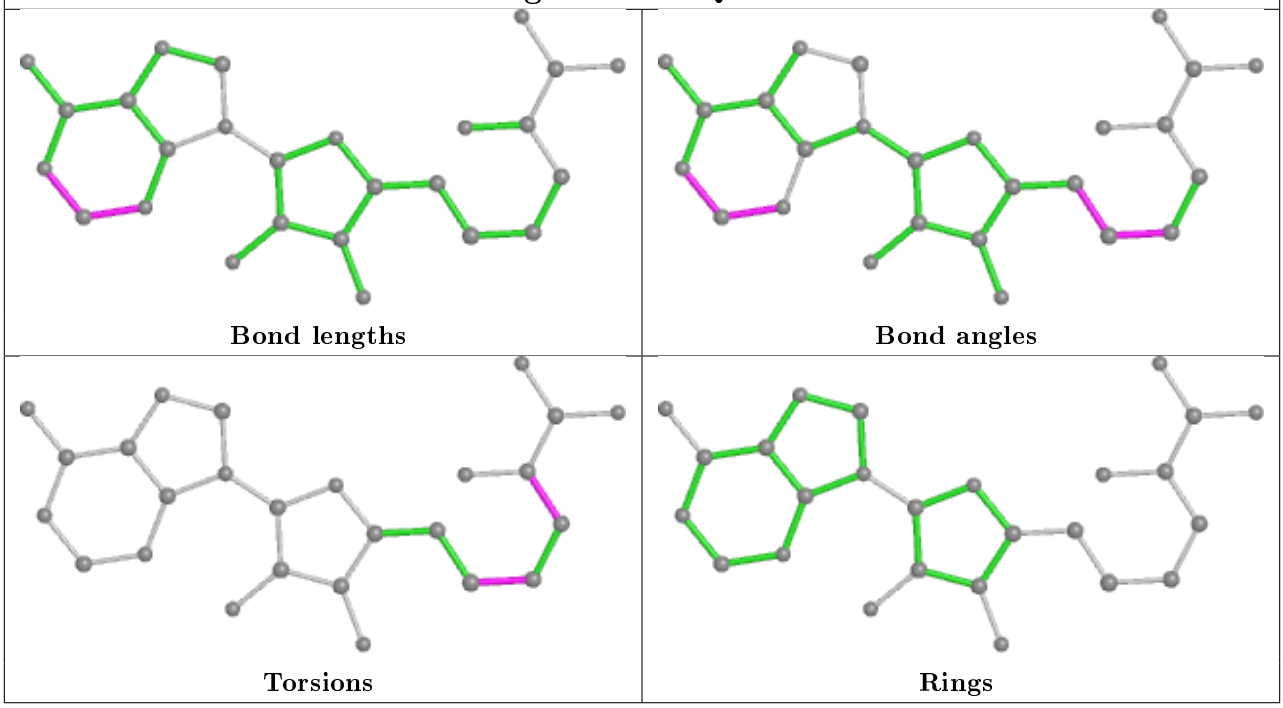

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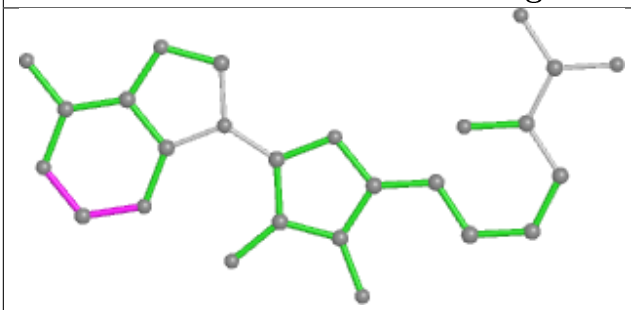

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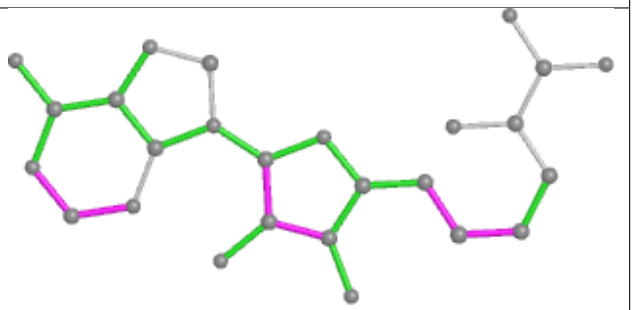

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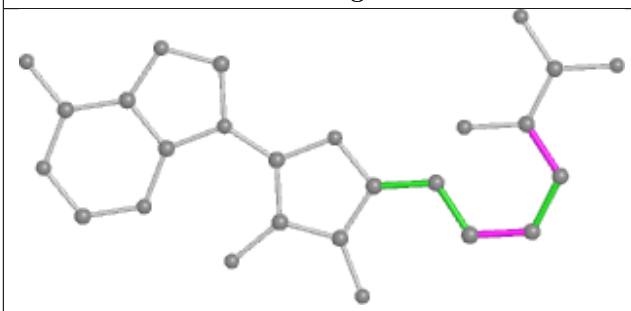

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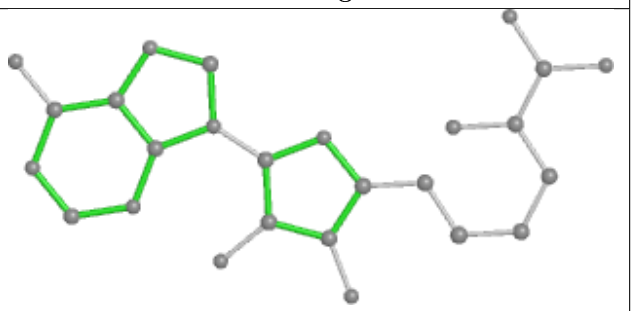
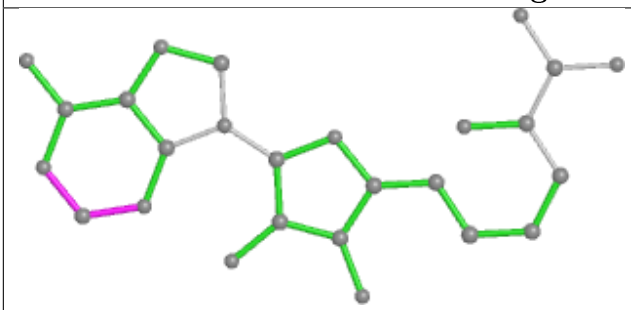


Rings

Ligand SAH I 301



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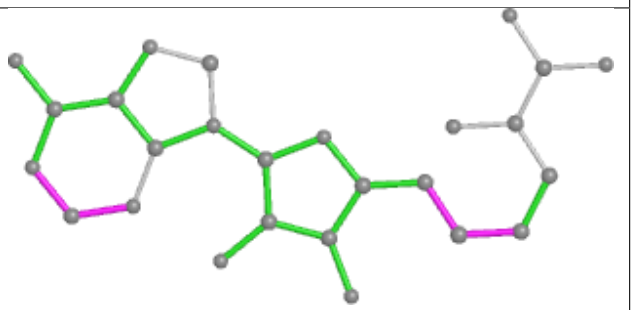

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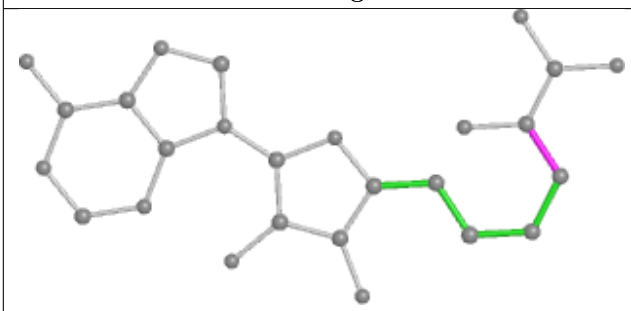

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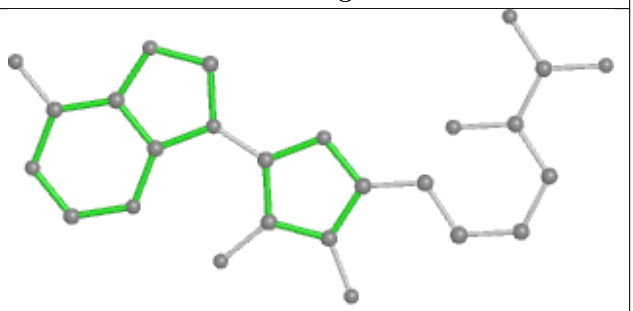

Rings

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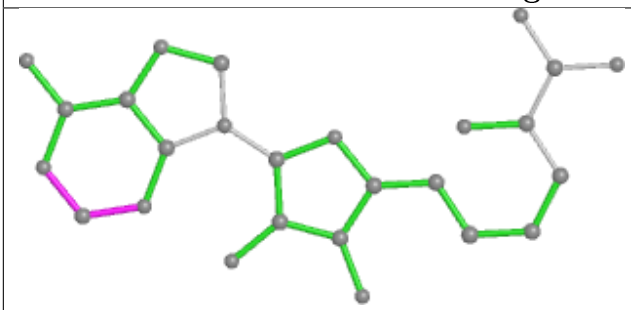

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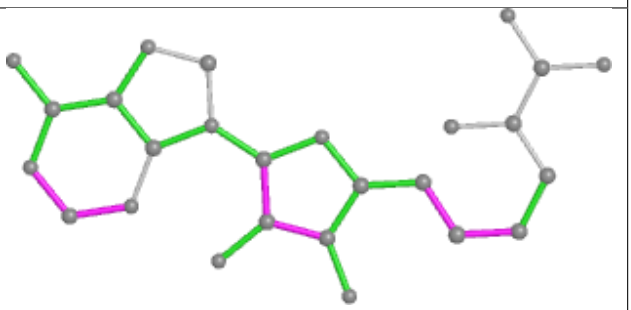

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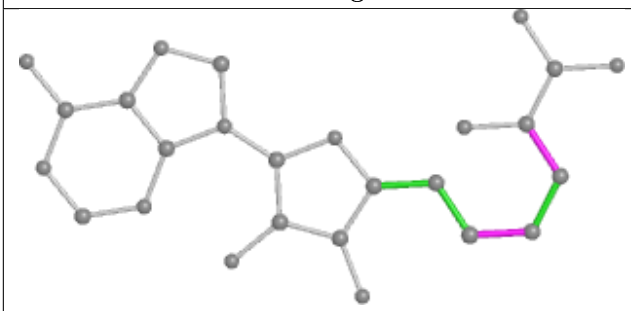

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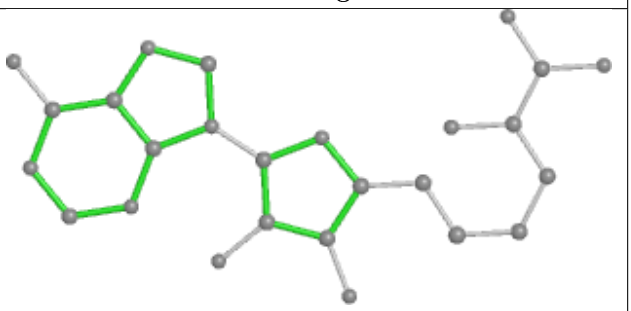

Rings

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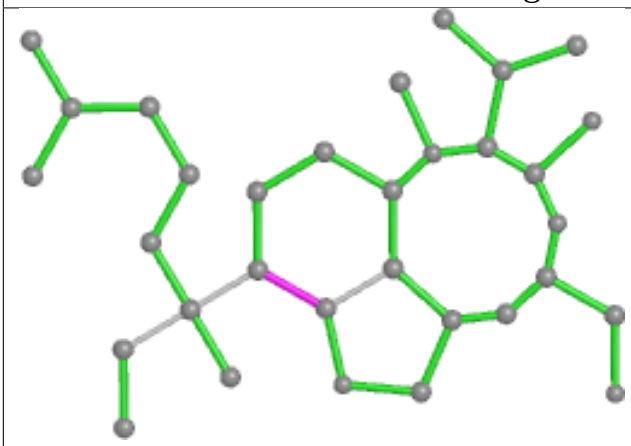

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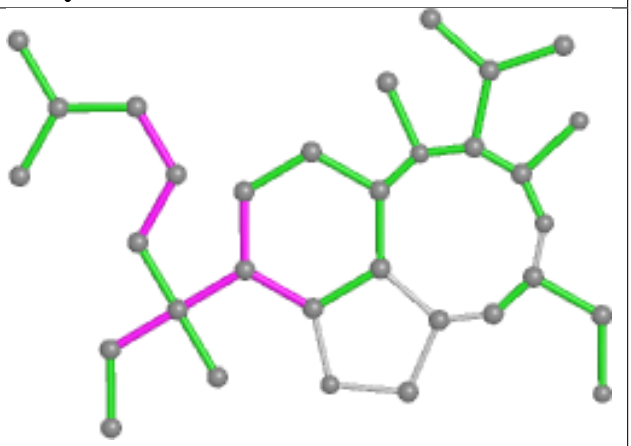

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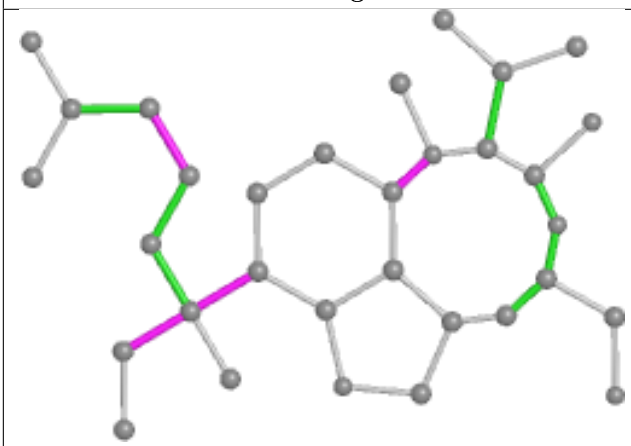

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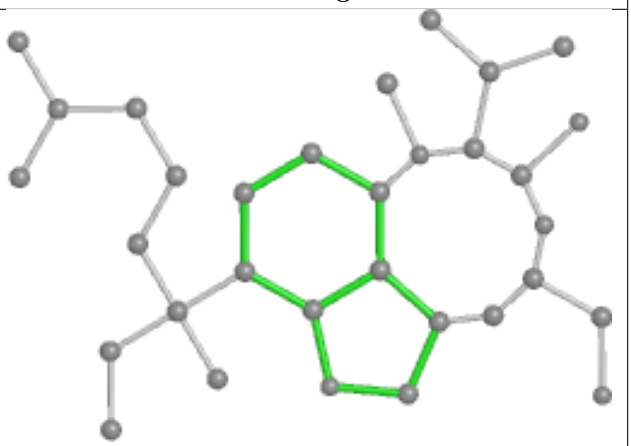

Rings

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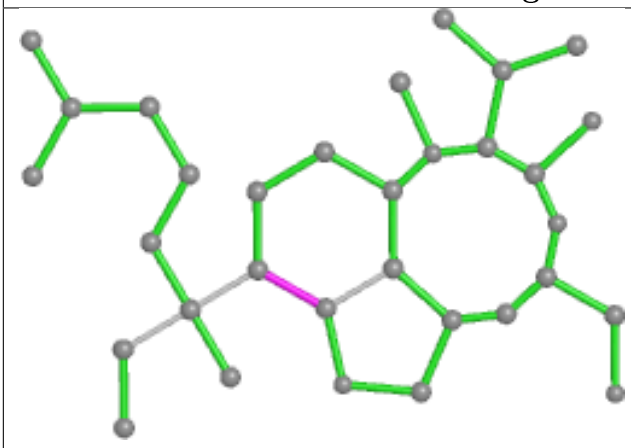

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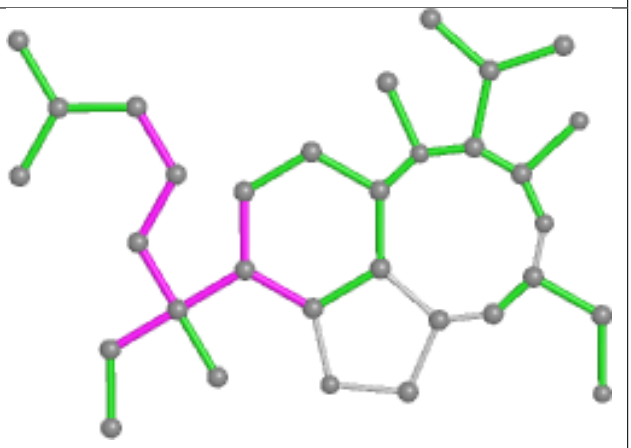

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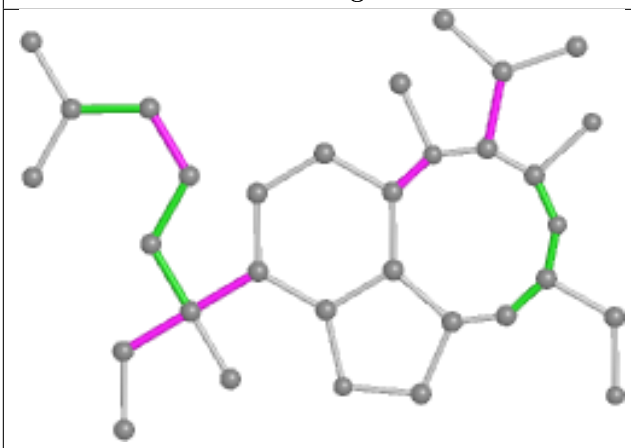

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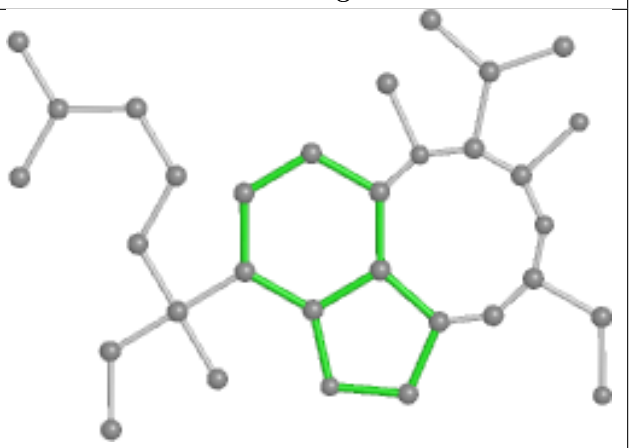
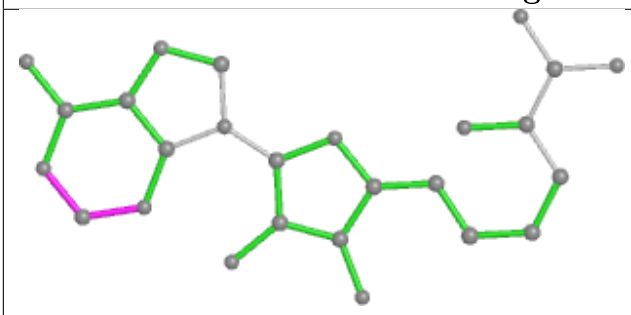


Rings

Ligand SAH R 301



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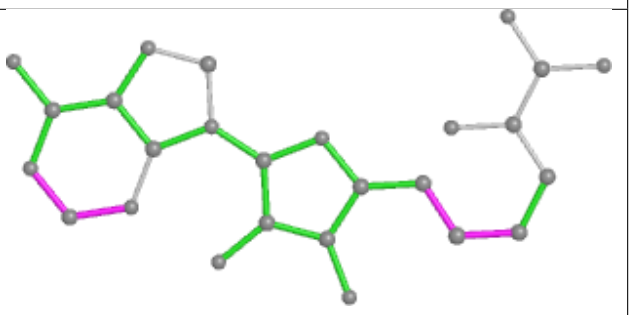

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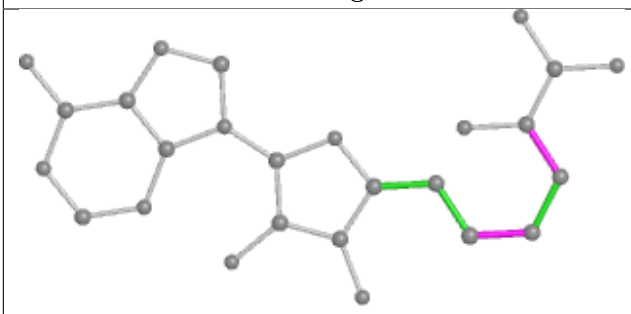

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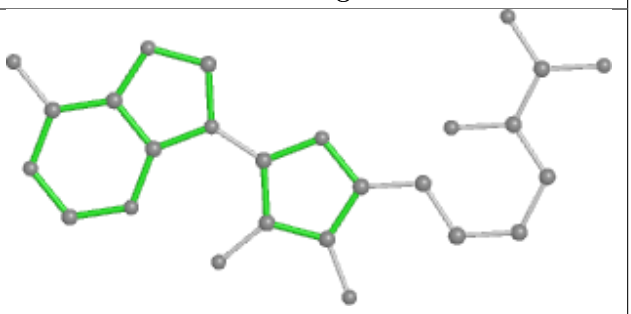

Rings

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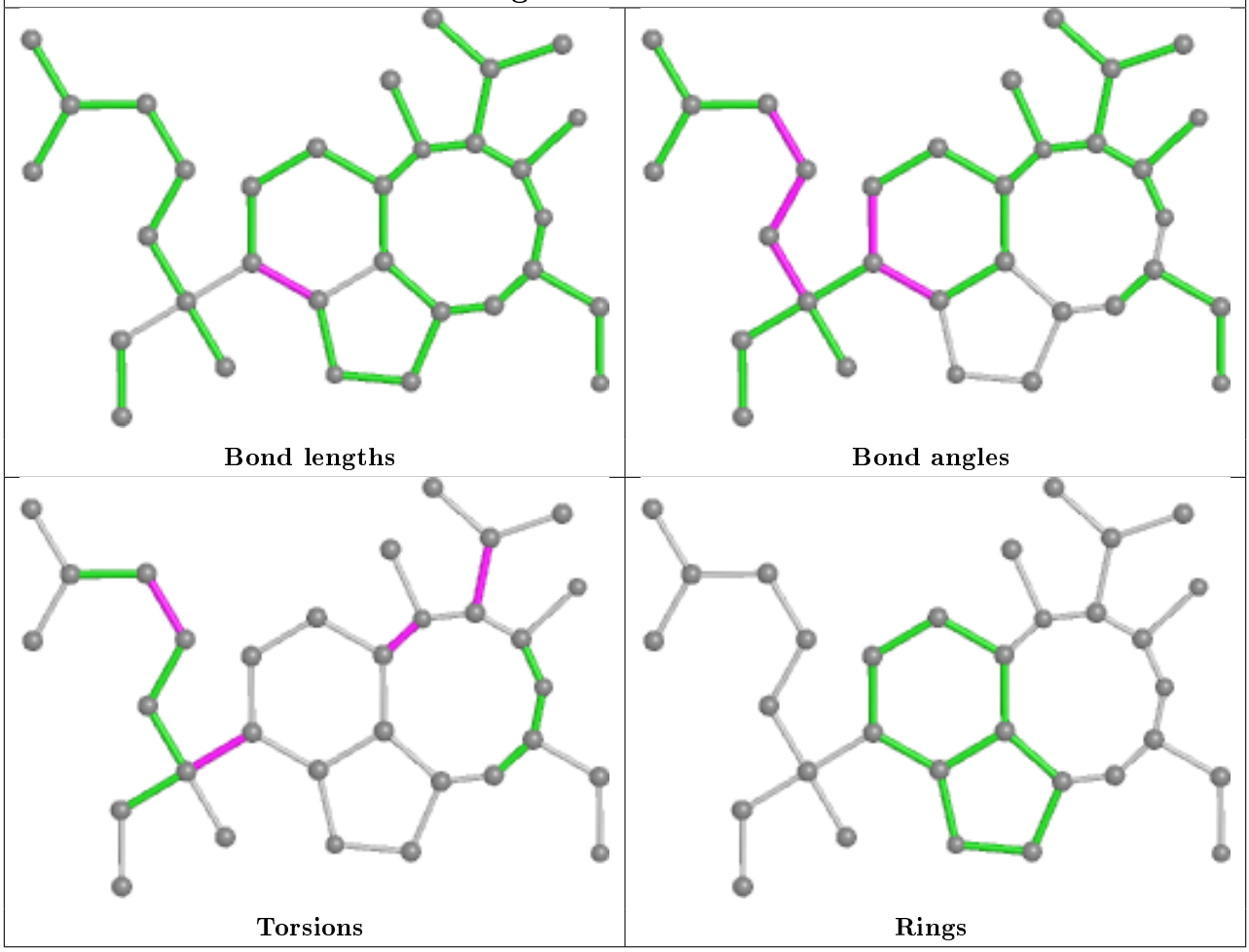

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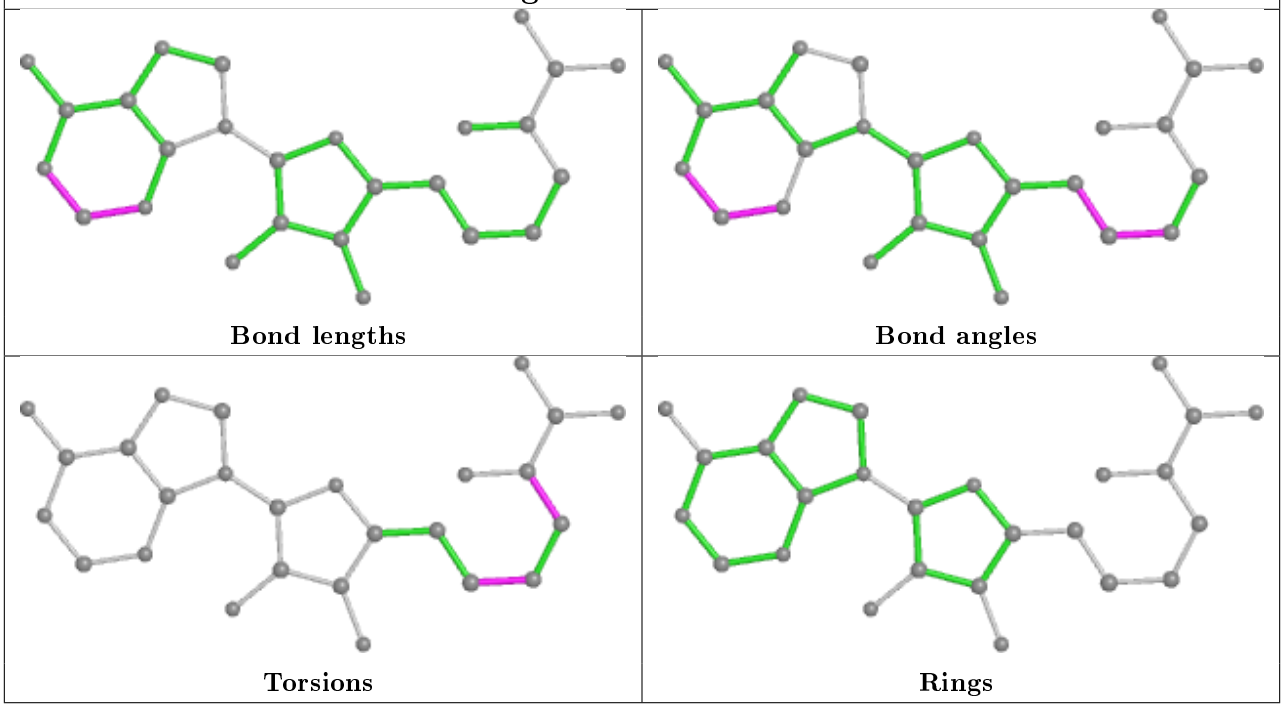

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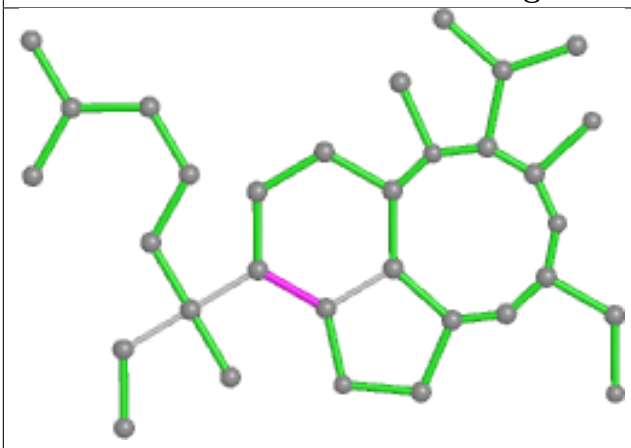

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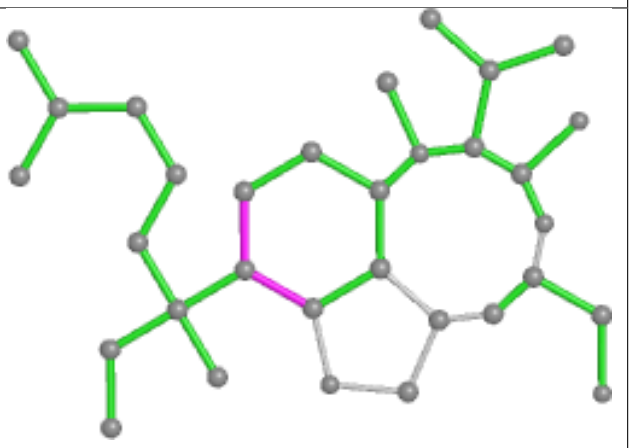

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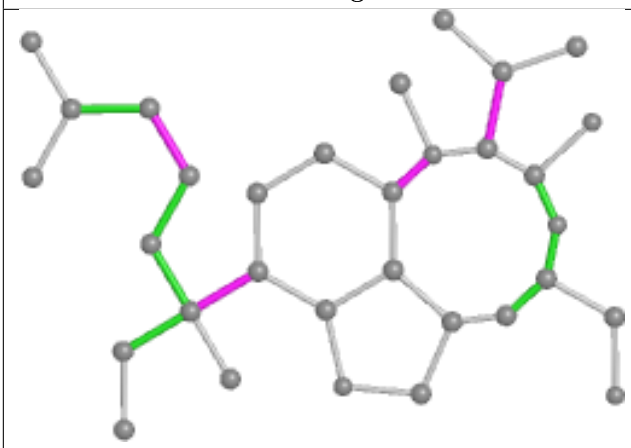

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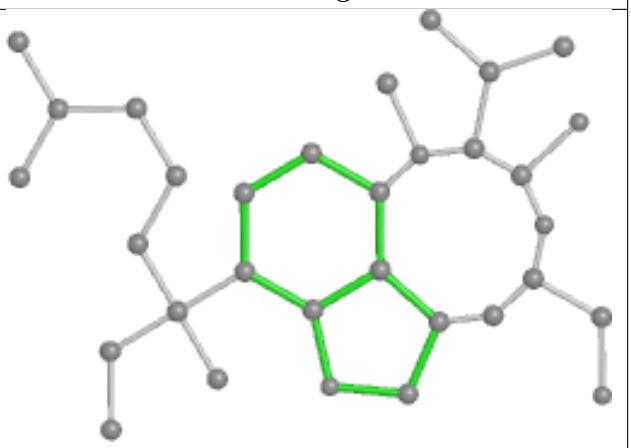
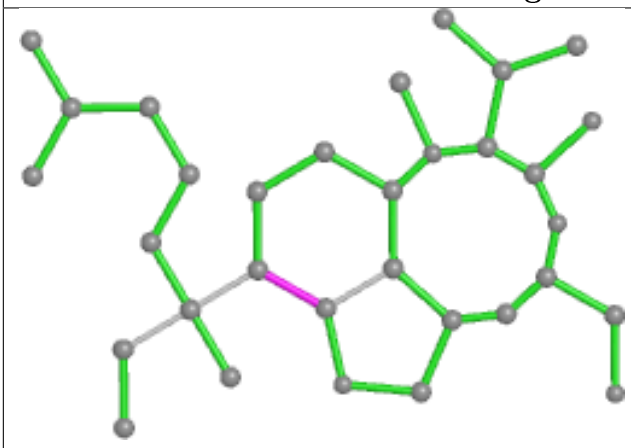


Rings

Ligand TEX P 302



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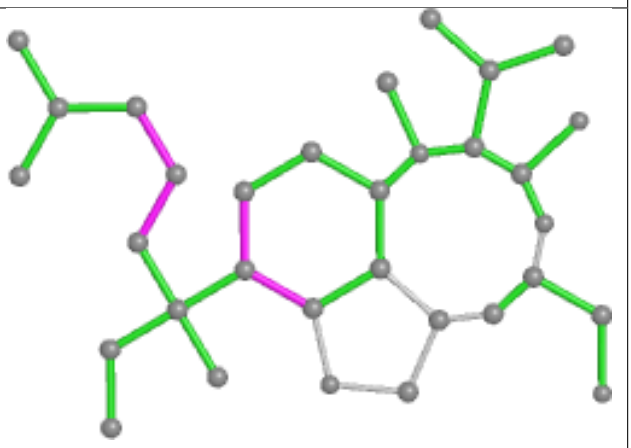

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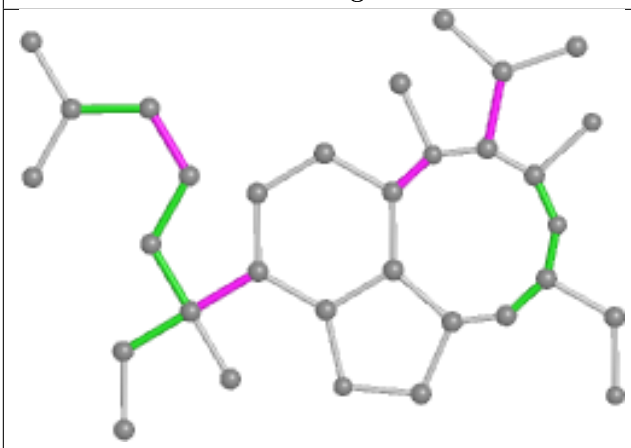

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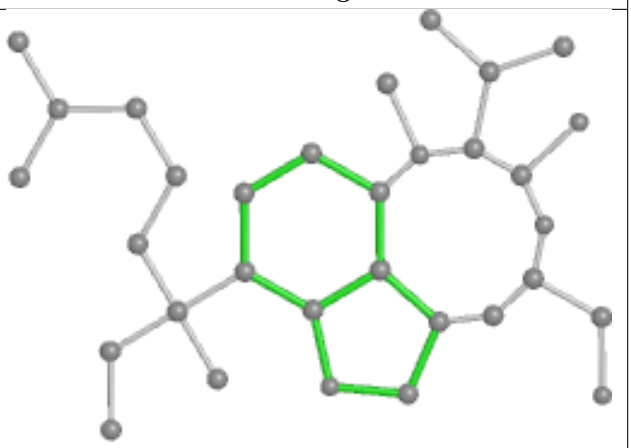
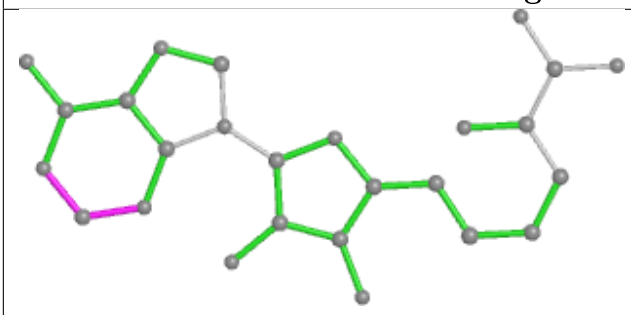


Rings

Ligand SAH C 301



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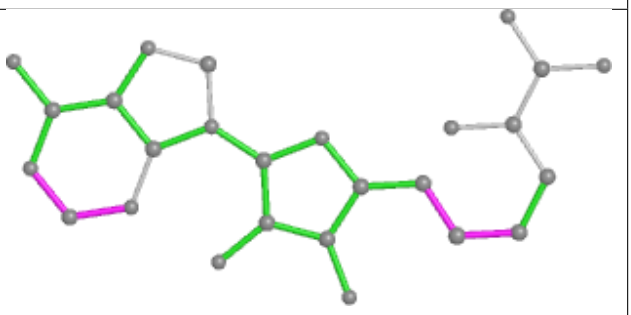

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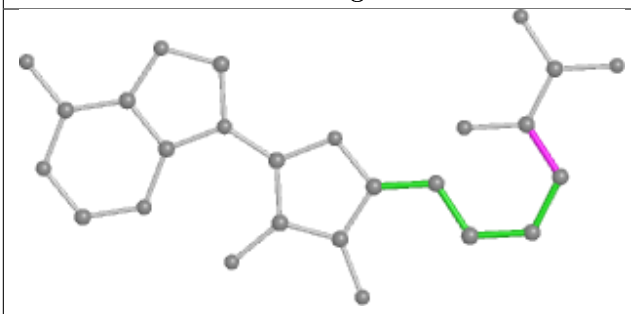

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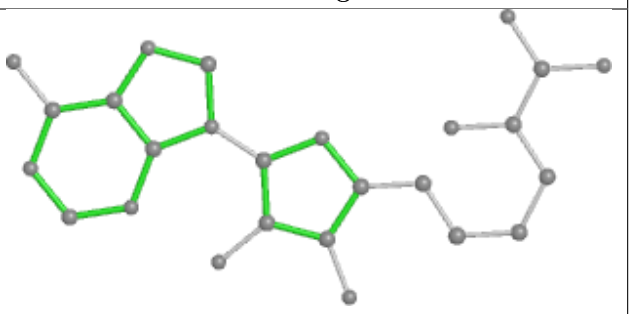
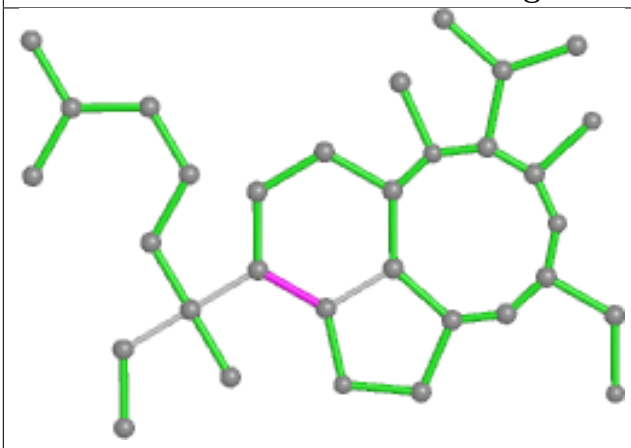


Rings

Ligand TEX K 302



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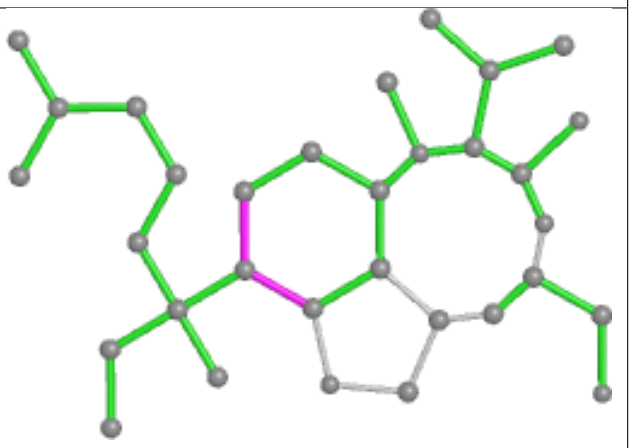

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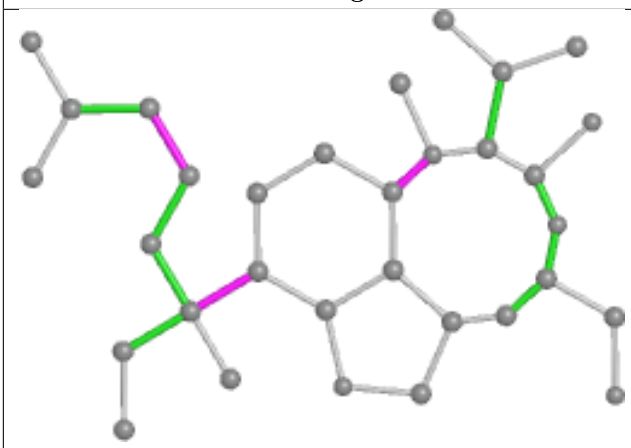

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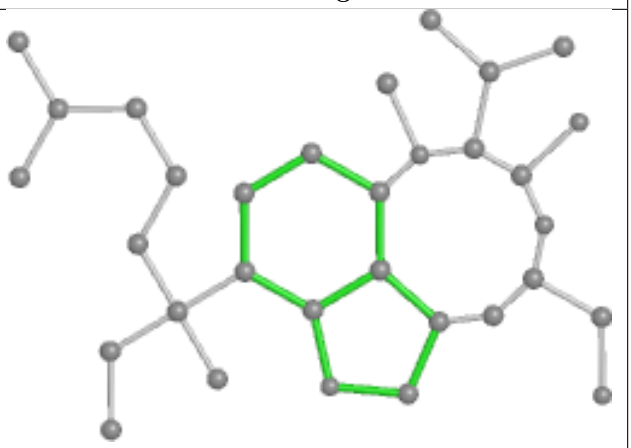

Rings

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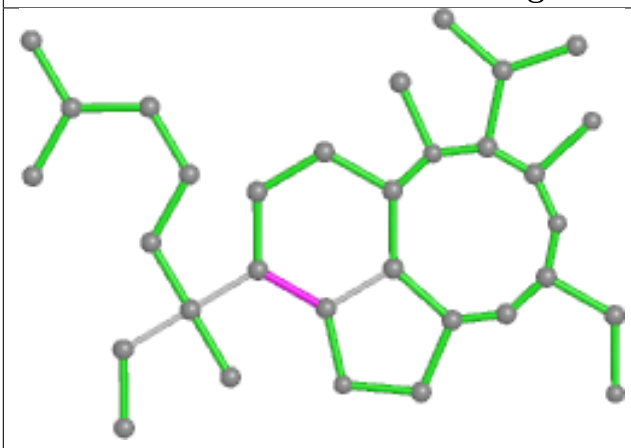

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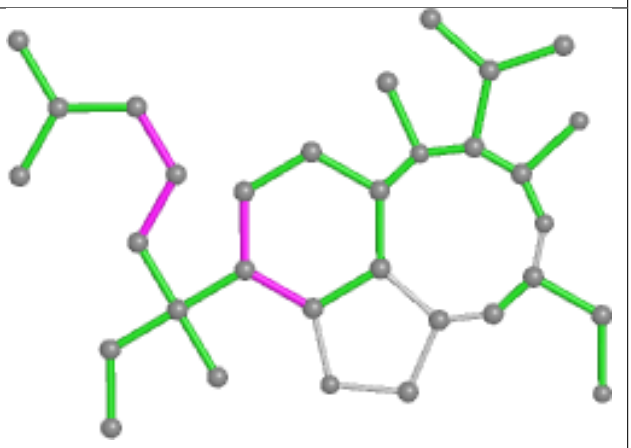
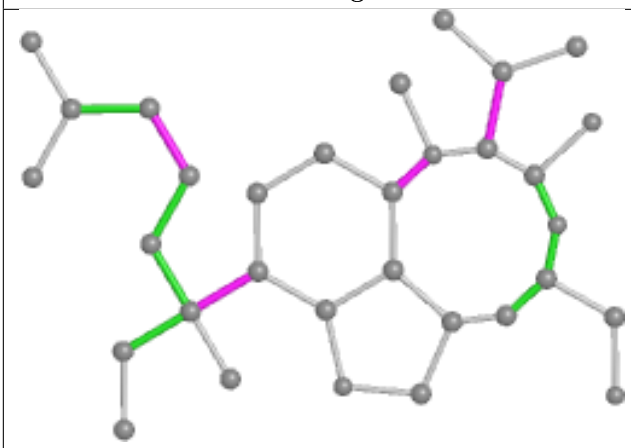
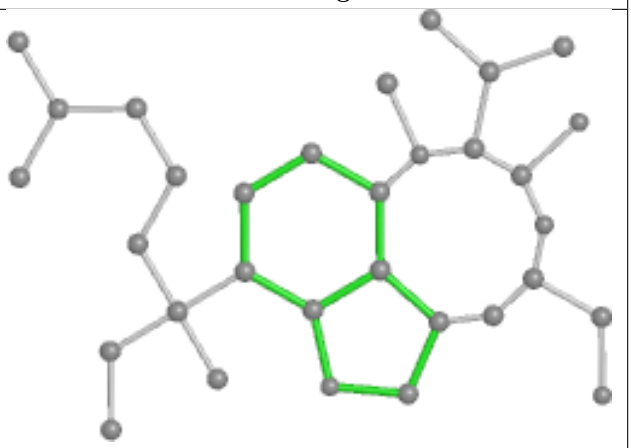


Bond angles

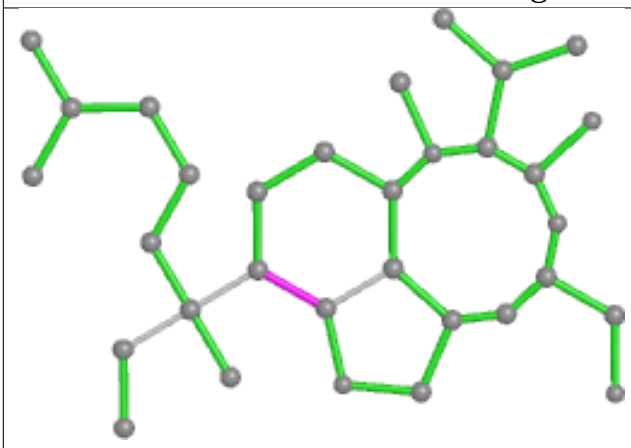


Torsions

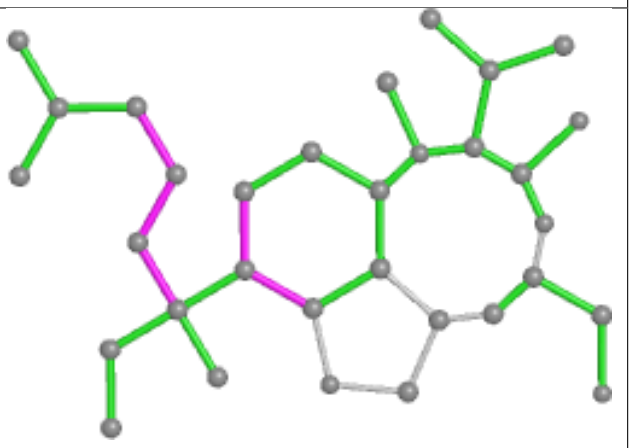


Rings

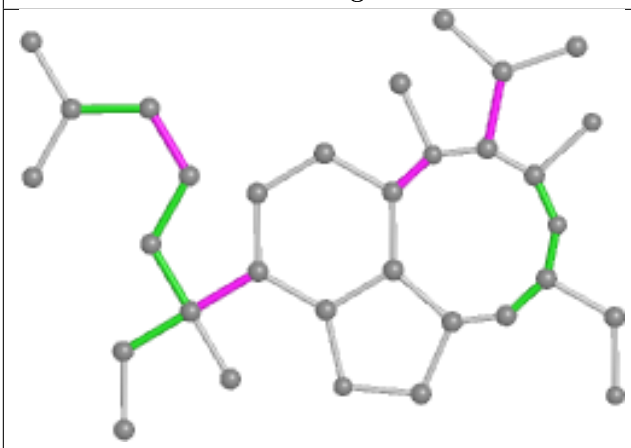
Ligand TEX I 302



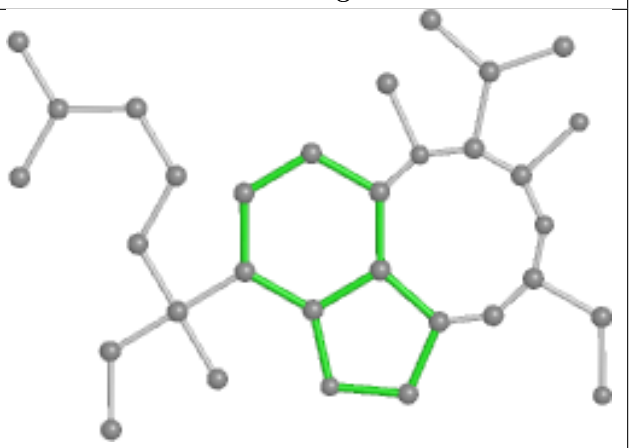
Bond lengths



Bond angles

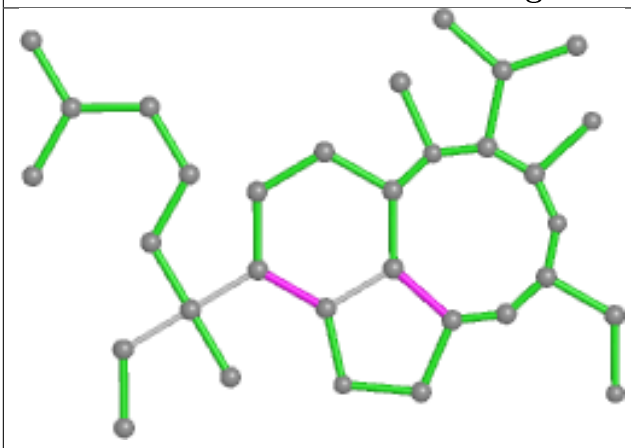


Torsions

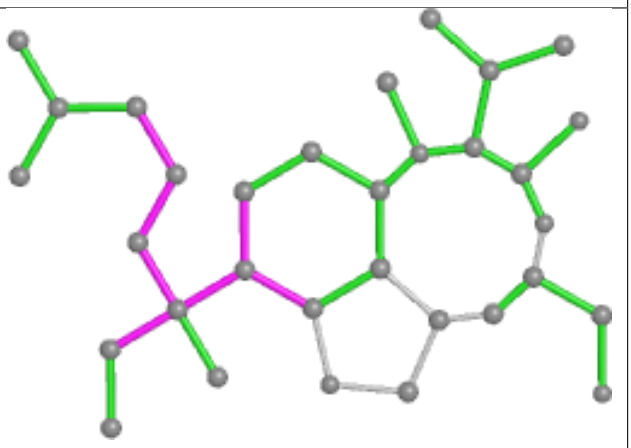


Rings

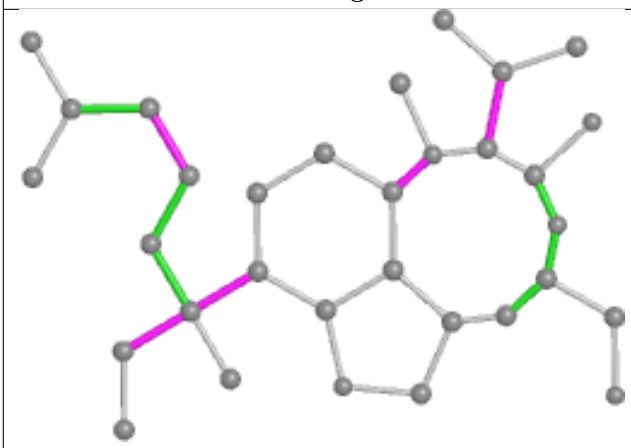
Ligand TEX F 302



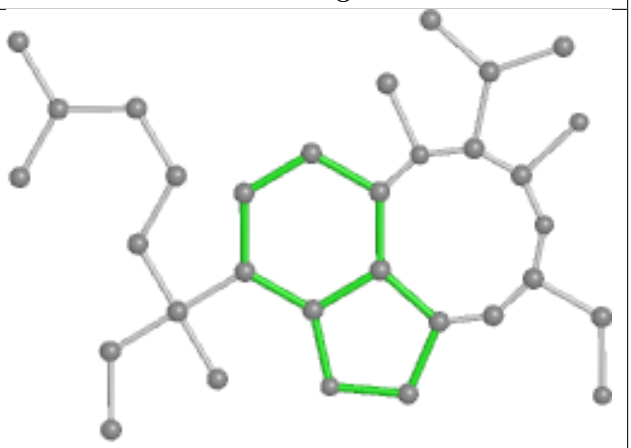
Bond lengths



Bond angles

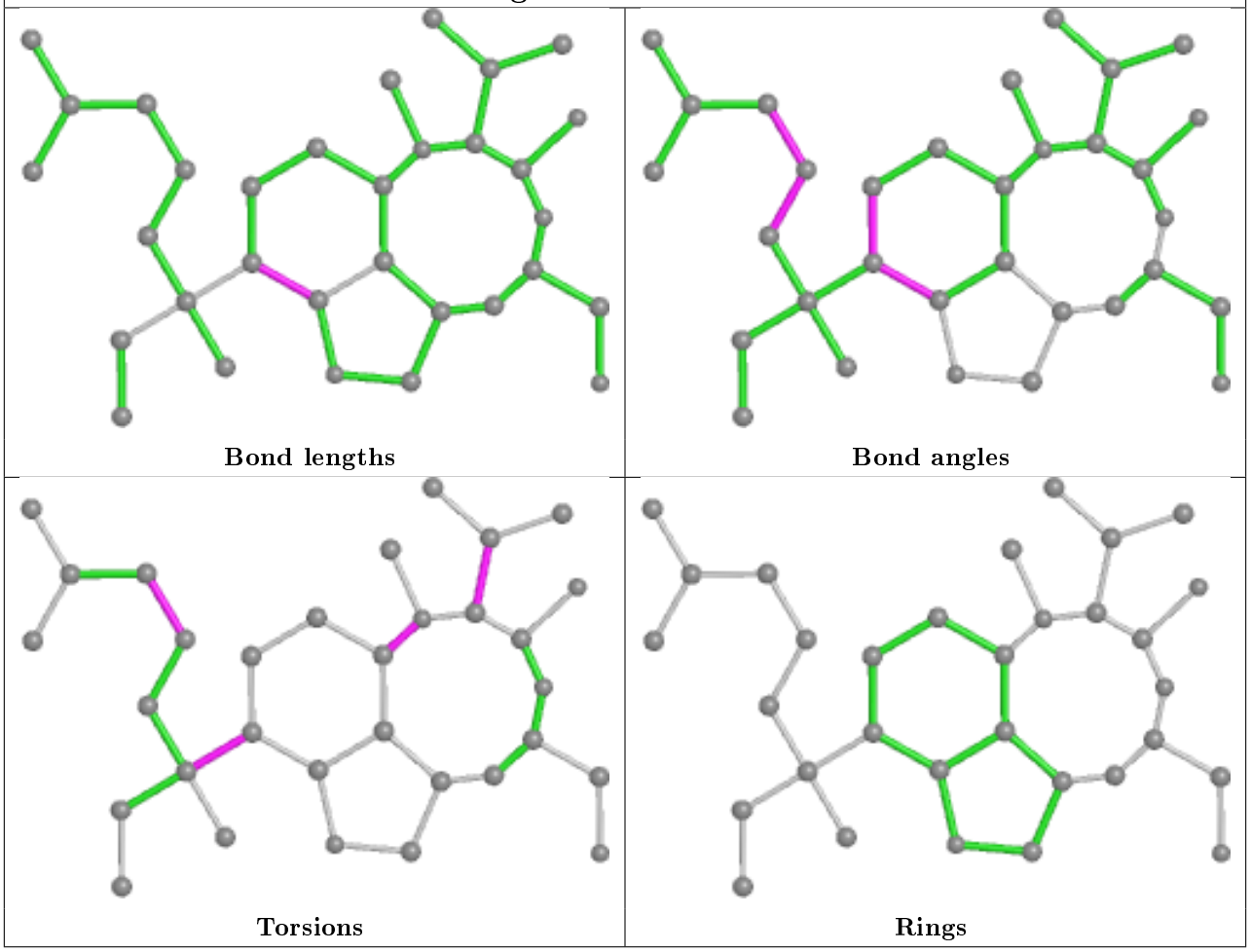


Torsions



Rings

Ligand TEX A 302



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	281/297 (94%)	-0.03	1 (0%) 92 91	34, 53, 80, 130	0
1	B	282/297 (94%)	0.03	2 (0%) 87 84	41, 63, 98, 122	0
1	C	279/297 (93%)	0.39	11 (3%) 39 29	51, 82, 127, 146	0
1	D	281/297 (94%)	0.14	3 (1%) 80 75	48, 76, 116, 156	0
1	E	279/297 (93%)	0.03	1 (0%) 92 91	42, 71, 105, 130	0
1	F	279/297 (93%)	-0.01	0 100 100	36, 55, 94, 126	0
1	G	266/297 (89%)	0.44	18 (6%) 17 10	53, 98, 152, 189	0
1	H	281/297 (94%)	1.31	62 (22%) 0 0	83, 126, 176, 251	0
1	I	266/297 (89%)	-0.03	1 (0%) 92 91	29, 55, 105, 155	0
1	J	272/297 (91%)	0.90	46 (16%) 1 1	68, 120, 169, 209	0
1	K	267/297 (89%)	0.52	24 (8%) 9 5	38, 113, 160, 199	0
1	L	263/297 (88%)	0.34	13 (4%) 29 20	56, 92, 139, 183	0
1	M	264/297 (88%)	0.10	3 (1%) 80 75	45, 73, 126, 188	0
1	N	274/297 (92%)	0.84	38 (13%) 2 1	60, 122, 163, 231	0
1	O	279/297 (93%)	0.17	4 (1%) 75 70	44, 78, 122, 157	0
1	P	279/297 (93%)	0.37	11 (3%) 39 29	58, 99, 127, 159	0
1	Q	266/297 (89%)	0.26	12 (4%) 33 23	42, 74, 144, 193	0
1	R	273/297 (91%)	1.05	51 (18%) 1 1	68, 130, 178, 228	0
All	All	4931/5346 (92%)	0.38	301 (6%) 21 13	29, 85, 152, 251	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	265	GLY	9.8
1	H	134	ALA	9.8
1	J	87	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
1	N	250	PHE	7.2
1	H	127	GLU	7.2
1	R	250	PHE	7.2
1	H	262	LEU	6.5
1	R	164	LEU	6.5
1	L	25	GLY	6.4
1	H	131	PHE	6.3
1	R	82	LEU	6.2
1	H	110	LYS	6.2
1	J	250	PHE	6.0
1	H	132	GLU	6.0
1	G	28	TYR	5.4
1	R	160	ARG	5.4
1	J	88	THR	5.3
1	R	200	TYR	5.2
1	G	32	LEU	5.2
1	K	82	LEU	5.1
1	H	133	VAL	5.0
1	K	136	ALA	5.0
1	J	146	PHE	5.0
1	Q	27	VAL	4.9
1	J	131	PHE	4.9
1	N	199	LEU	4.8
1	H	243	VAL	4.8
1	J	125	LEU	4.7
1	H	124	GLY	4.7
1	H	255	GLY	4.6
1	H	120	ALA	4.6
1	R	196	PHE	4.5
1	H	250	PHE	4.5
1	N	136	ALA	4.4
1	H	261	GLY	4.4
1	H	254	PHE	4.4
1	Q	28	TYR	4.4
1	D	21	TYR	4.3
1	H	290	LEU	4.3
1	H	266	LEU	4.3
1	H	239	PHE	4.3
1	N	200	TYR	4.3
1	R	55	VAL	4.3
1	J	112	GLN	4.3
1	N	112	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	90	ARG	4.2
1	Q	253	ARG	4.2
1	R	181	GLU	4.2
1	J	155	LEU	4.1
1	N	261	GLY	4.1
1	R	131	PHE	4.1
1	K	187	GLU	4.1
1	H	126	THR	4.1
1	R	208	LEU	4.1
1	R	101	ILE	4.0
1	J	243	VAL	4.0
1	O	289	VAL	4.0
1	H	232	LEU	4.0
1	H	119	LEU	4.0
1	H	11	GLN	3.9
1	N	247	ARG	3.9
1	R	125	LEU	3.9
1	K	139	LEU	3.9
1	H	117	ASN	3.9
1	N	131	PHE	3.8
1	H	188	LEU	3.7
1	G	188	LEU	3.7
1	H	10	GLN	3.7
1	R	239	PHE	3.7
1	G	199	LEU	3.7
1	N	129	LEU	3.6
1	K	112	GLN	3.6
1	G	41	TRP	3.5
1	N	119	LEU	3.5
1	J	108	VAL	3.5
1	R	161	ALA	3.5
1	N	155	LEU	3.5
1	R	260	ASP	3.5
1	N	252	GLU	3.5
1	J	157	HIS	3.5
1	H	107	ALA	3.5
1	K	160	ARG	3.4
1	R	243	VAL	3.4
1	L	28	TYR	3.4
1	O	21	TYR	3.4
1	C	170	VAL	3.4
1	G	33	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	145	SER	3.4
1	R	159	ASP	3.4
1	J	128	ARG	3.3
1	R	171	LEU	3.3
1	R	199	LEU	3.3
1	C	136	ALA	3.2
1	H	129	LEU	3.2
1	H	249	GLU	3.2
1	L	35	SER	3.2
1	N	134	ALA	3.2
1	G	266	LEU	3.2
1	K	208	LEU	3.2
1	H	89	GLY	3.2
1	Q	266	LEU	3.2
1	N	146	PHE	3.2
1	N	139	LEU	3.2
1	Q	262	LEU	3.2
1	H	196	PHE	3.2
1	J	129	LEU	3.1
1	M	28	TYR	3.1
1	J	109	SER	3.1
1	H	164	LEU	3.1
1	K	129	LEU	3.1
1	R	108	VAL	3.1
1	R	153	GLU	3.1
1	J	156	CYS	3.1
1	R	205	PRO	3.1
1	K	120	ALA	3.0
1	J	54	LEU	3.0
1	C	139	LEU	3.0
1	J	20	TRP	3.0
1	H	200	TYR	3.0
1	N	232	LEU	3.0
1	N	259	VAL	3.0
1	H	257	GLU	3.0
1	J	200	TYR	3.0
1	Q	33	GLY	2.9
1	Q	188	LEU	2.9
1	H	112	GLN	2.9
1	H	150	TRP	2.9
1	N	125	LEU	2.9
1	K	212	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	92	ALA	2.9
1	J	264	ALA	2.9
1	J	64	ARG	2.9
1	G	108	VAL	2.9
1	J	196	PHE	2.9
1	K	239	PHE	2.9
1	H	14	ALA	2.9
1	H	259	VAL	2.9
1	L	31	THR	2.8
1	J	205	PRO	2.8
1	J	261	GLY	2.8
1	M	32	LEU	2.8
1	K	265	GLY	2.8
1	G	212	PHE	2.8
1	L	36	VAL	2.8
1	H	269	ALA	2.8
1	G	289	VAL	2.7
1	R	103	VAL	2.7
1	N	150	TRP	2.7
1	P	250	PHE	2.7
1	K	171	LEU	2.7
1	J	110	LYS	2.7
1	G	39	GLY	2.7
1	Q	37	HIS	2.7
1	R	165	GLY	2.7
1	G	244	TYR	2.7
1	H	202	ALA	2.7
1	K	200	TYR	2.7
1	H	88	THR	2.7
1	N	140	PRO	2.7
1	C	270	GLN	2.6
1	R	139	LEU	2.6
1	K	81	LEU	2.6
1	J	150	TRP	2.6
1	R	146	PHE	2.6
1	C	274	ILE	2.6
1	J	107	ALA	2.6
1	K	3	GLN	2.5
1	K	84	ILE	2.5
1	G	36	VAL	2.5
1	L	253	ARG	2.5
1	R	96	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	154	SER	2.5
1	N	188	LEU	2.5
1	L	184	VAL	2.5
1	M	108	VAL	2.5
1	R	179	VAL	2.5
1	L	220	PHE	2.5
1	N	171	LEU	2.5
1	R	177	LEU	2.5
1	G	196	PHE	2.5
1	J	258	PHE	2.5
1	R	198	THR	2.5
1	C	200	TYR	2.5
1	J	168	TRP	2.5
1	N	12	VAL	2.5
1	A	290	LEU	2.4
1	L	262	LEU	2.4
1	P	243	VAL	2.4
1	H	128	ARG	2.4
1	N	262	LEU	2.4
1	H	205	PRO	2.4
1	H	264	ALA	2.4
1	R	186	GLU	2.4
1	P	129	LEU	2.4
1	C	17	VAL	2.4
1	H	106	VAL	2.4
1	R	94	LYS	2.4
1	R	84	ILE	2.4
1	R	284	LEU	2.4
1	G	243	VAL	2.4
1	J	95	ALA	2.4
1	H	158	MET	2.4
1	K	188	LEU	2.4
1	B	9	GLN	2.3
1	C	140	PRO	2.3
1	G	38	CYS	2.3
1	E	106	VAL	2.3
1	L	108	VAL	2.3
1	N	141	TYR	2.3
1	P	201	ALA	2.3
1	K	164	LEU	2.3
1	L	41	TRP	2.3
1	N	187	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	171	LEU	2.3
1	I	32	LEU	2.3
1	J	119	LEU	2.3
1	R	129	LEU	2.3
1	J	207	ARG	2.3
1	K	103	VAL	2.3
1	J	164	LEU	2.3
1	J	199	LEU	2.3
1	P	217	GLY	2.3
1	H	111	GLU	2.3
1	B	290	LEU	2.3
1	H	139	LEU	2.3
1	J	167	ALA	2.3
1	J	106	VAL	2.3
1	Q	186	GLU	2.3
1	J	188	LEU	2.3
1	N	201	ALA	2.3
1	P	82	LEU	2.3
1	N	11	GLN	2.3
1	C	133	VAL	2.3
1	J	145	SER	2.3
1	G	260	ASP	2.3
1	P	128	ARG	2.3
1	J	113	ILE	2.3
1	L	250	PHE	2.3
1	N	211	PHE	2.3
1	Q	36	VAL	2.2
1	R	130	THR	2.2
1	R	182	SER	2.2
1	R	207	ARG	2.2
1	J	19	ASP	2.2
1	N	108	VAL	2.2
1	D	20	TRP	2.2
1	J	244	TYR	2.2
1	K	141	TYR	2.2
1	O	17	VAL	2.2
1	Q	25	GLY	2.2
1	N	181	GLU	2.2
1	H	113	ILE	2.2
1	R	247	ARG	2.2
1	Q	155	LEU	2.2
1	H	116	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	136	ALA	2.2
1	R	95	ALA	2.2
1	H	82	LEU	2.2
1	H	146	PHE	2.2
1	N	128	ARG	2.2
1	K	146	PHE	2.2
1	N	86	CYS	2.2
1	H	173	PRO	2.2
1	C	150	TRP	2.2
1	J	32	LEU	2.2
1	R	168	TRP	2.2
1	J	84	ILE	2.2
1	J	21	TYR	2.2
1	R	209	GLY	2.1
1	H	40	LEU	2.1
1	R	69	LEU	2.1
1	P	136	ALA	2.1
1	K	243	VAL	2.1
1	H	206	PRO	2.1
1	L	243	VAL	2.1
1	R	272	THR	2.1
1	J	239	PHE	2.1
1	N	239	PHE	2.1
1	H	121	ALA	2.1
1	N	218	ALA	2.1
1	O	110	LYS	2.1
1	P	119	LEU	2.1
1	P	106	VAL	2.1
1	C	112	GLN	2.1
1	H	95	ALA	2.1
1	N	107	ALA	2.1
1	R	141	TYR	2.1
1	R	262	LEU	2.0
1	K	150	TRP	2.0
1	R	91	THR	2.0
1	R	241	LEU	2.0
1	G	25	GLY	2.0
1	R	264	ALA	2.0
1	H	238	VAL	2.0
1	P	131	PHE	2.0
1	H	101	ILE	2.0
1	H	65	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	108	VAL	2.0
1	N	251	THR	2.0
1	R	204	VAL	2.0
1	R	155	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
2	SAH	N	301	26/26	0.22	0.80	458,483,511,517	0
2	SAH	R	301	26/26	0.32	0.75	355,370,387,399	0
2	SAH	K	301	26/26	0.43	0.67	363,373,393,401	0
2	SAH	J	301	26/26	0.55	0.55	302,313,330,334	0
2	SAH	H	301	26/26	0.72	0.52	118,120,127,128	0
2	SAH	G	301	26/26	0.77	0.37	194,201,205,207	0
3	TEX	C	302	32/32	0.83	0.49	93,101,103,104	0
2	SAH	L	301	26/26	0.84	0.28	94,102,119,125	0
3	TEX	R	302	32/32	0.86	0.52	114,117,123,126	0
3	TEX	I	302	32/32	0.86	0.36	91,95,96,97	0
3	TEX	J	302	32/32	0.87	0.62	134,141,154,154	0
3	TEX	H	302	32/32	0.87	0.54	119,126,130,135	0
3	TEX	L	302	32/32	0.88	0.45	72,75,78,80	0
2	SAH	P	301	26/26	0.88	0.26	107,110,116,117	0
3	TEX	N	302	32/32	0.89	0.50	95,100,105,106	0
3	TEX	B	302	32/32	0.90	0.36	90,93,96,99	0
3	TEX	K	302	32/32	0.90	0.40	113,118,119,120	0
3	TEX	Q	302	32/32	0.91	0.34	110,112,114,115	0
3	TEX	G	302	32/32	0.91	0.38	101,103,108,109	0

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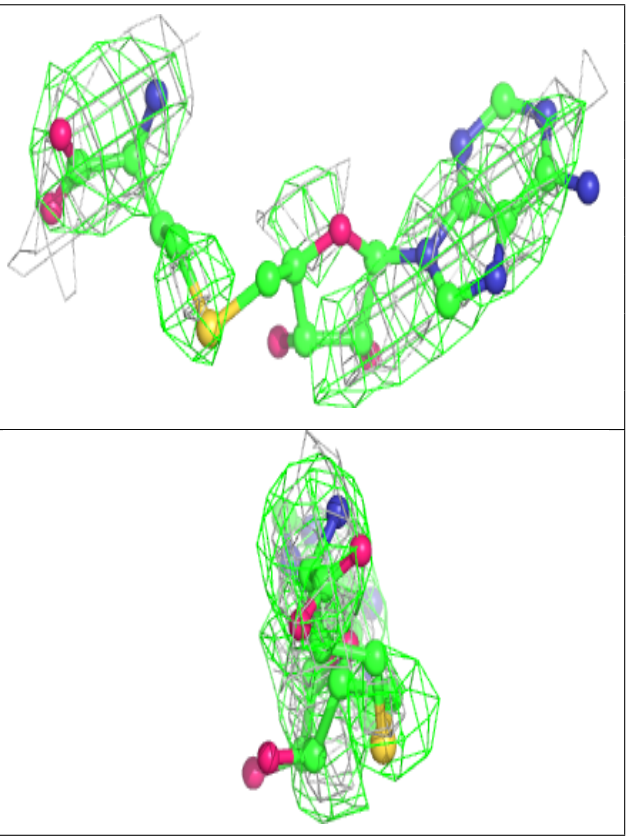
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TEX	D	302	32/32	0.92	0.30	89,92,96,97	0
3	TEX	M	302	32/32	0.92	0.41	72,75,77,81	0
3	TEX	E	302	32/32	0.92	0.33	61,65,69,70	0
2	SAH	Q	301	26/26	0.93	0.29	70,72,74,75	0
3	TEX	P	302	32/32	0.93	0.37	104,109,112,113	0
2	SAH	C	301	26/26	0.93	0.22	69,75,79,81	0
3	TEX	F	302	32/32	0.93	0.32	78,80,82,84	0
2	SAH	E	301	26/26	0.94	0.25	71,74,77,78	0
3	TEX	O	302	32/32	0.95	0.31	96,102,106,107	0
2	SAH	D	301	26/26	0.95	0.25	75,79,82,84	0
2	SAH	B	301	26/26	0.95	0.25	72,75,77,78	0
2	SAH	I	301	26/26	0.95	0.27	66,73,85,87	0
2	SAH	M	301	26/26	0.95	0.25	73,79,84,86	0
2	SAH	O	301	26/26	0.95	0.21	59,62,64,64	0
3	TEX	A	302	32/32	0.95	0.31	87,90,94,95	0
2	SAH	F	301	26/26	0.96	0.27	100,104,113,115	0
2	SAH	A	301	26/26	0.96	0.23	55,62,66,66	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.

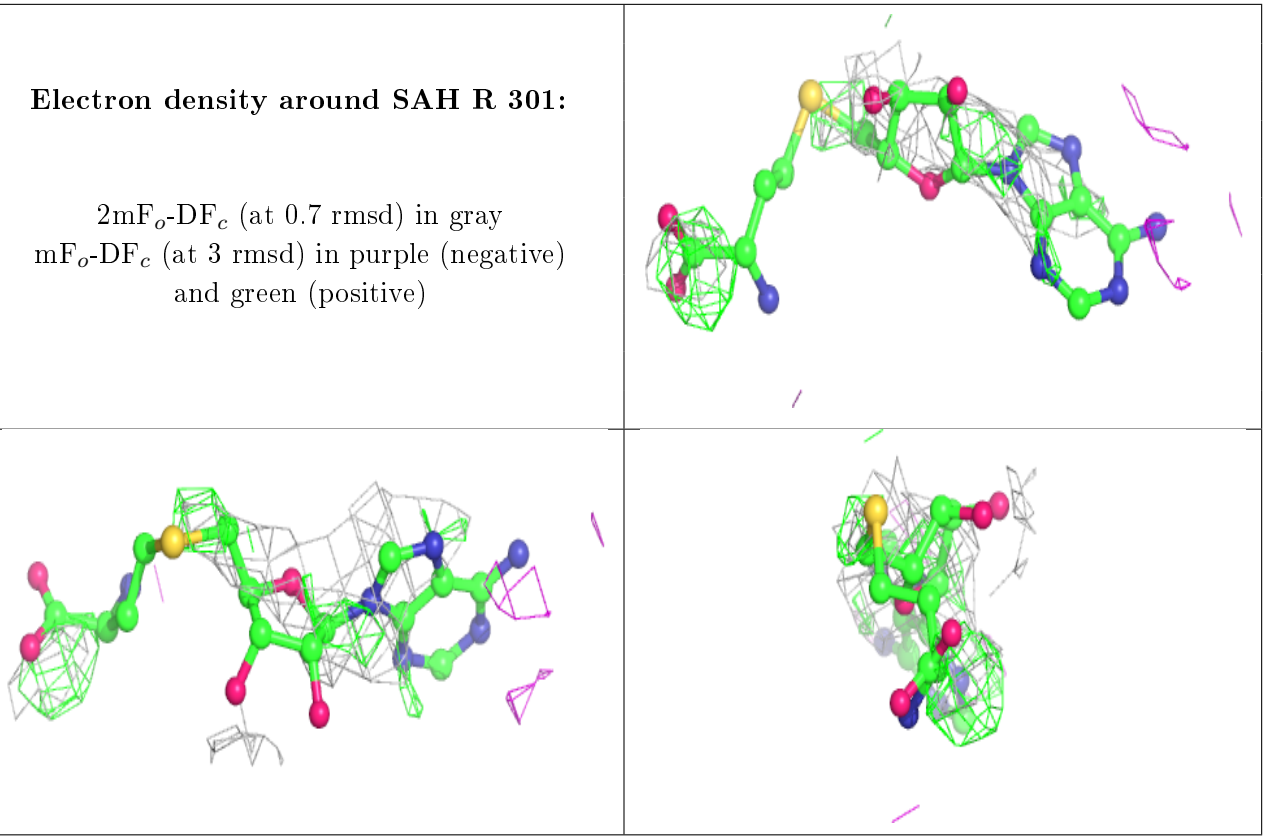
Electron density around SAH N 301:

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



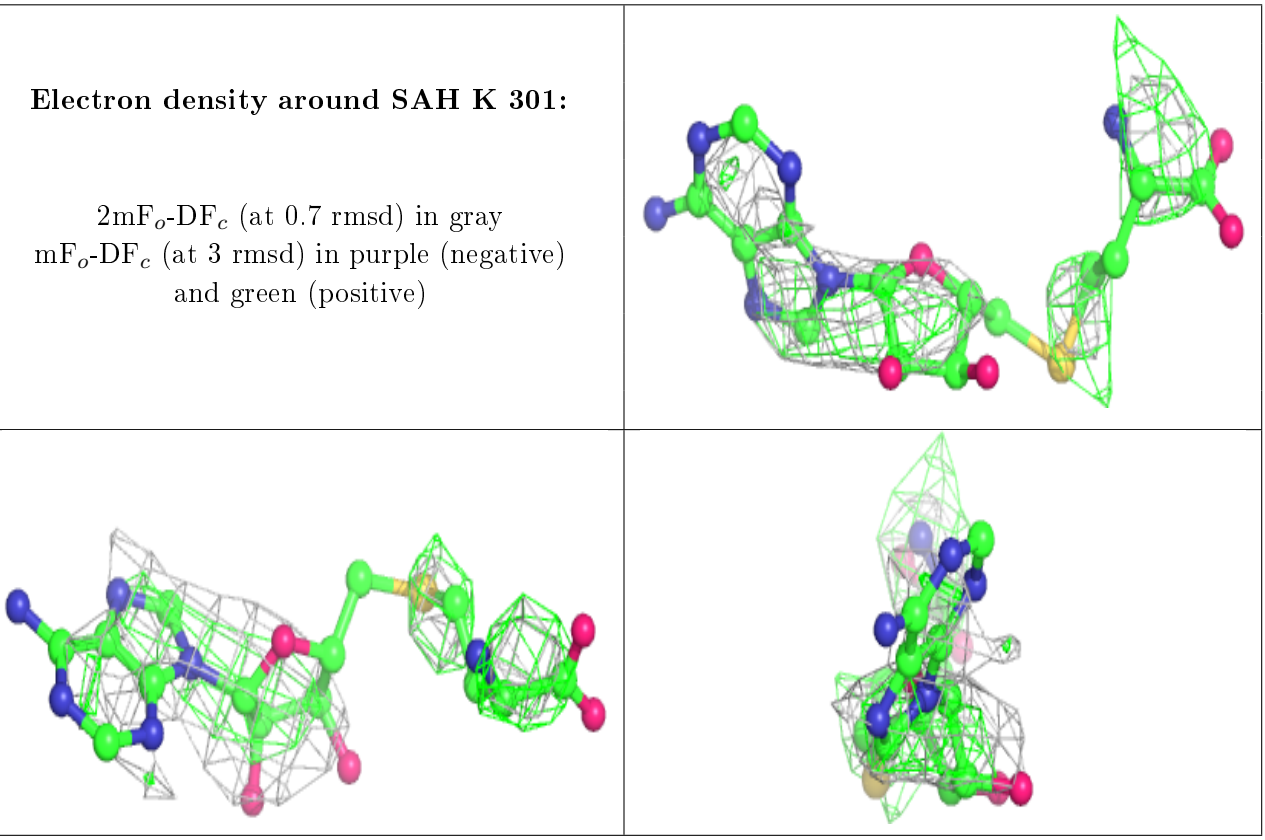
Electron density around SAH R 301:

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



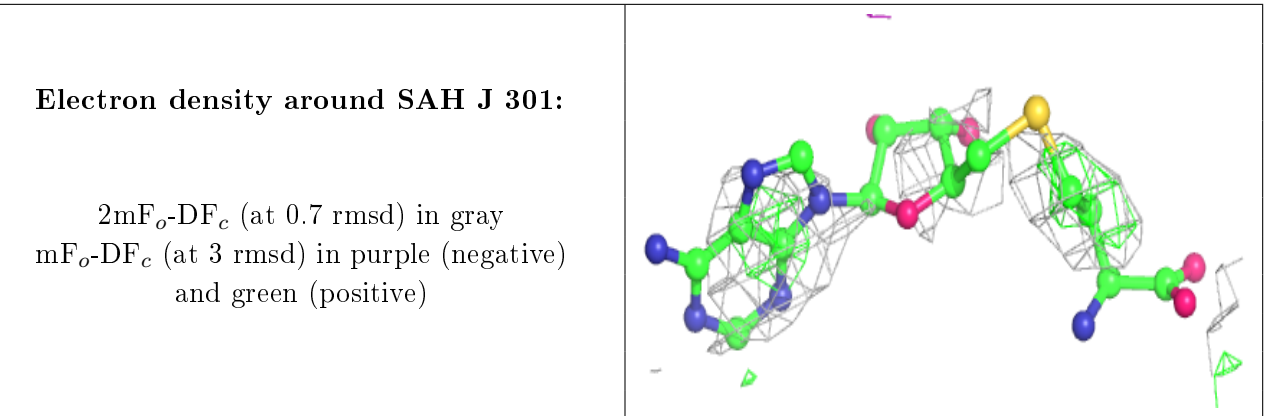
Electron density around SAH K 301:

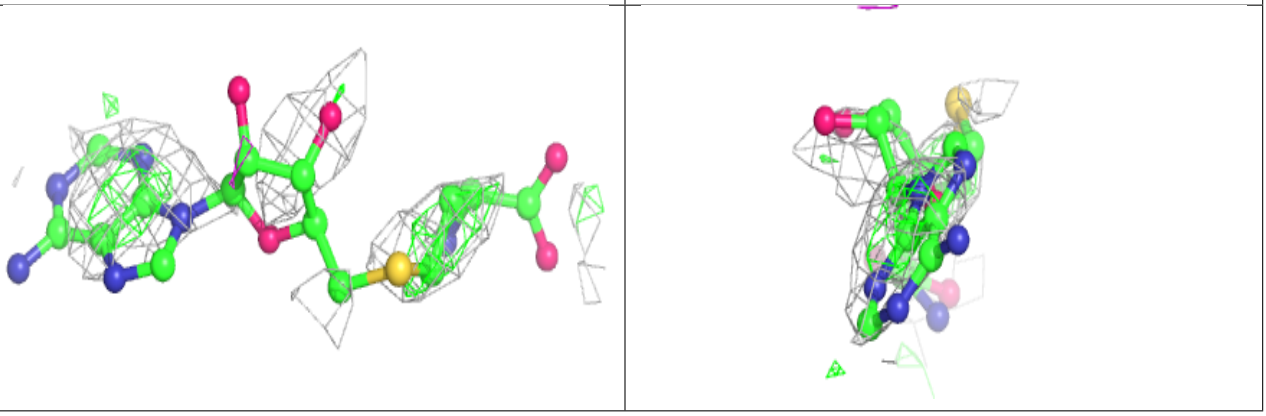
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SAH J 301:

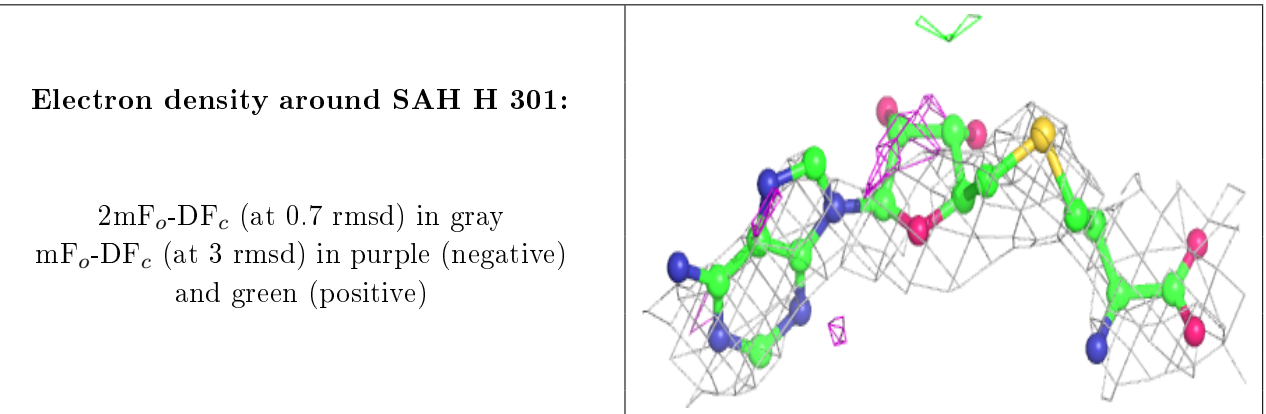
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

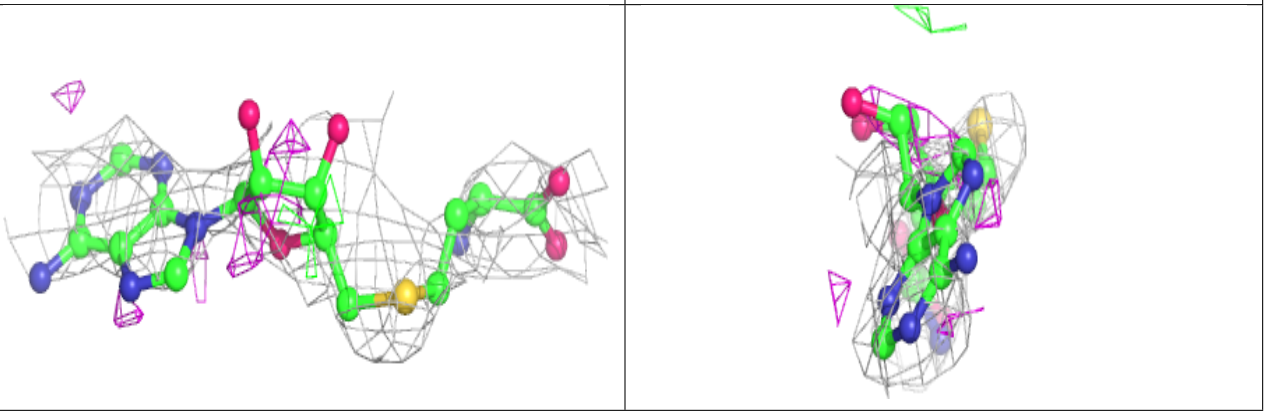




Electron density around SAH H 301:

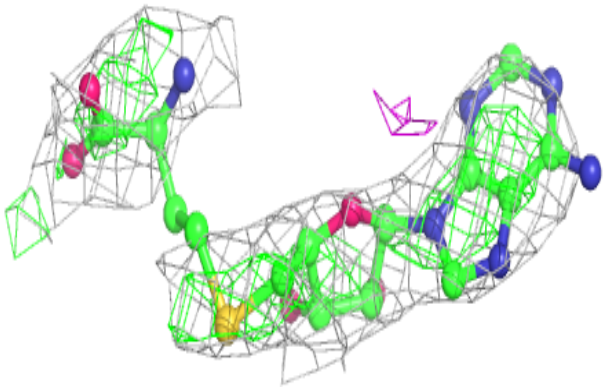
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

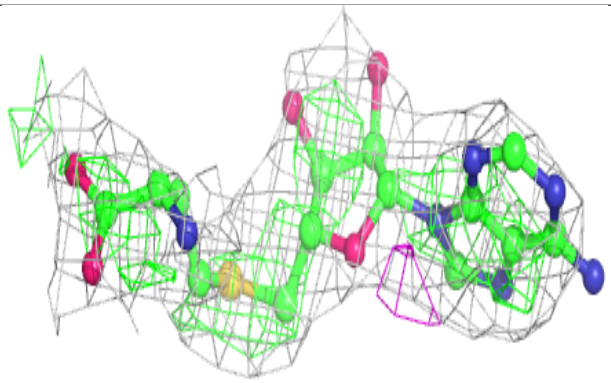


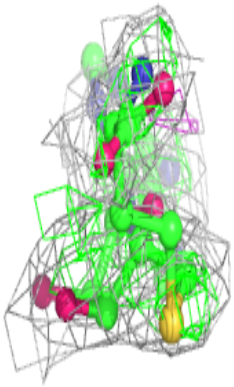


Electron density around SAH G 301:

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

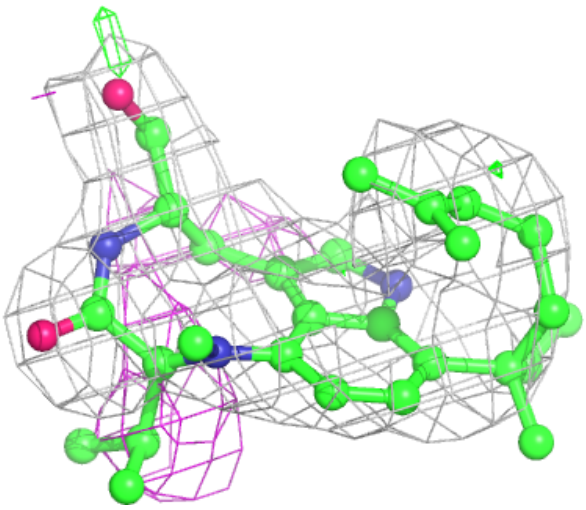


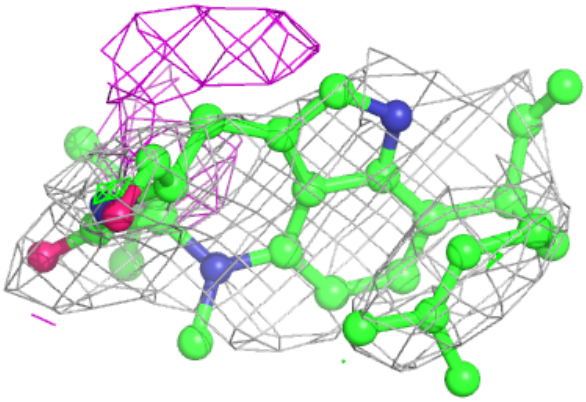


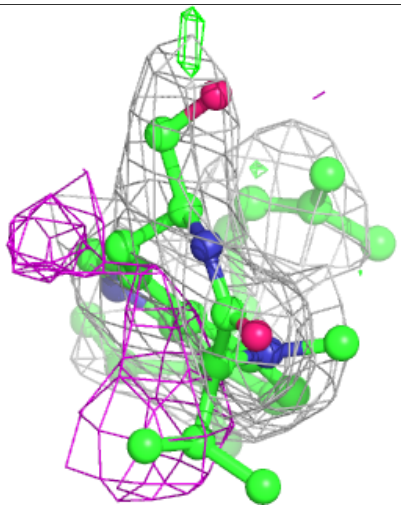


Electron density around TEX C 302:

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

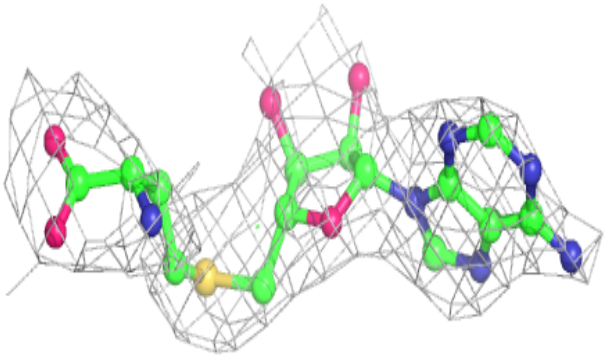


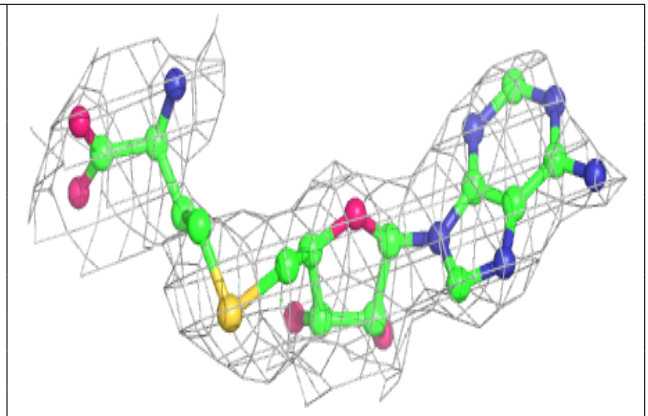


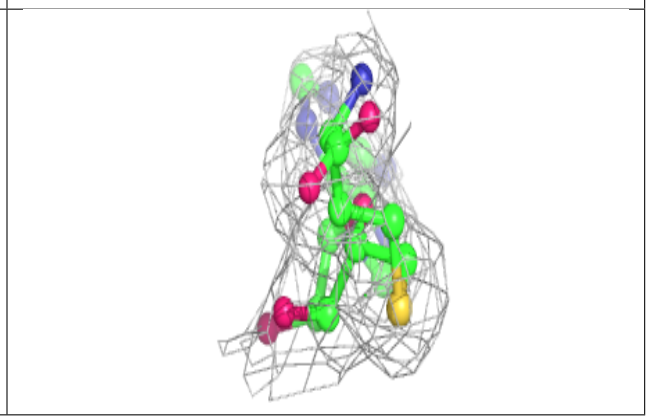


Electron density around SAH L 301:

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

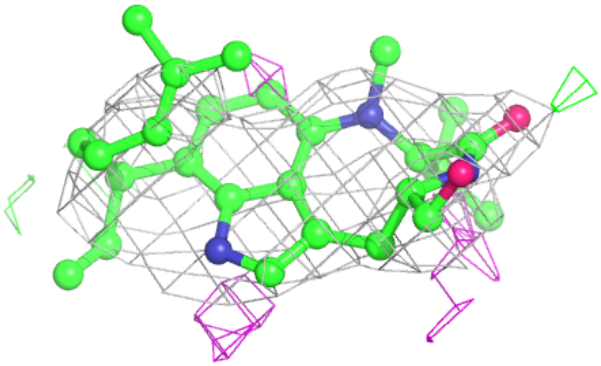


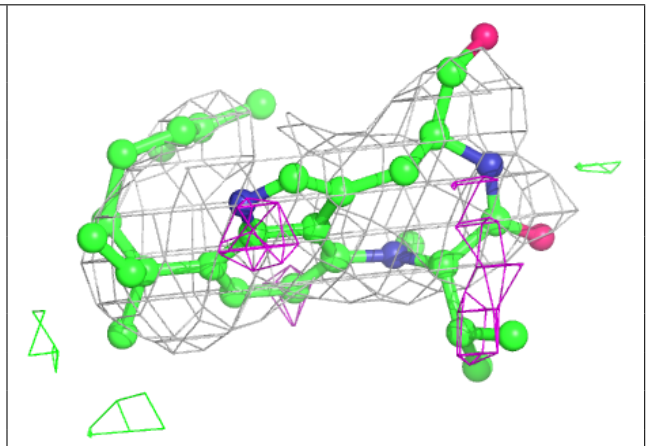


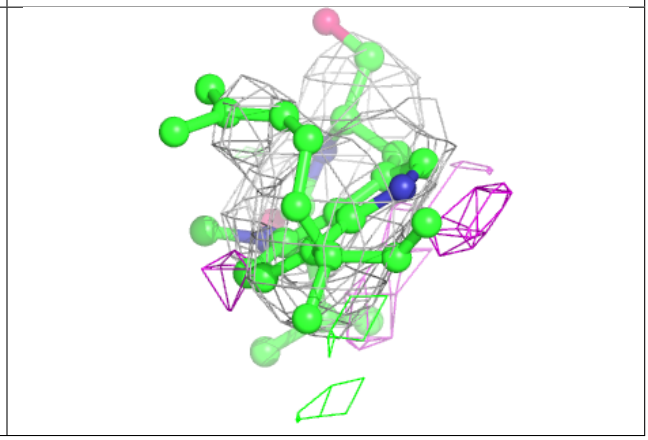


Electron density around TEX R 302:

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

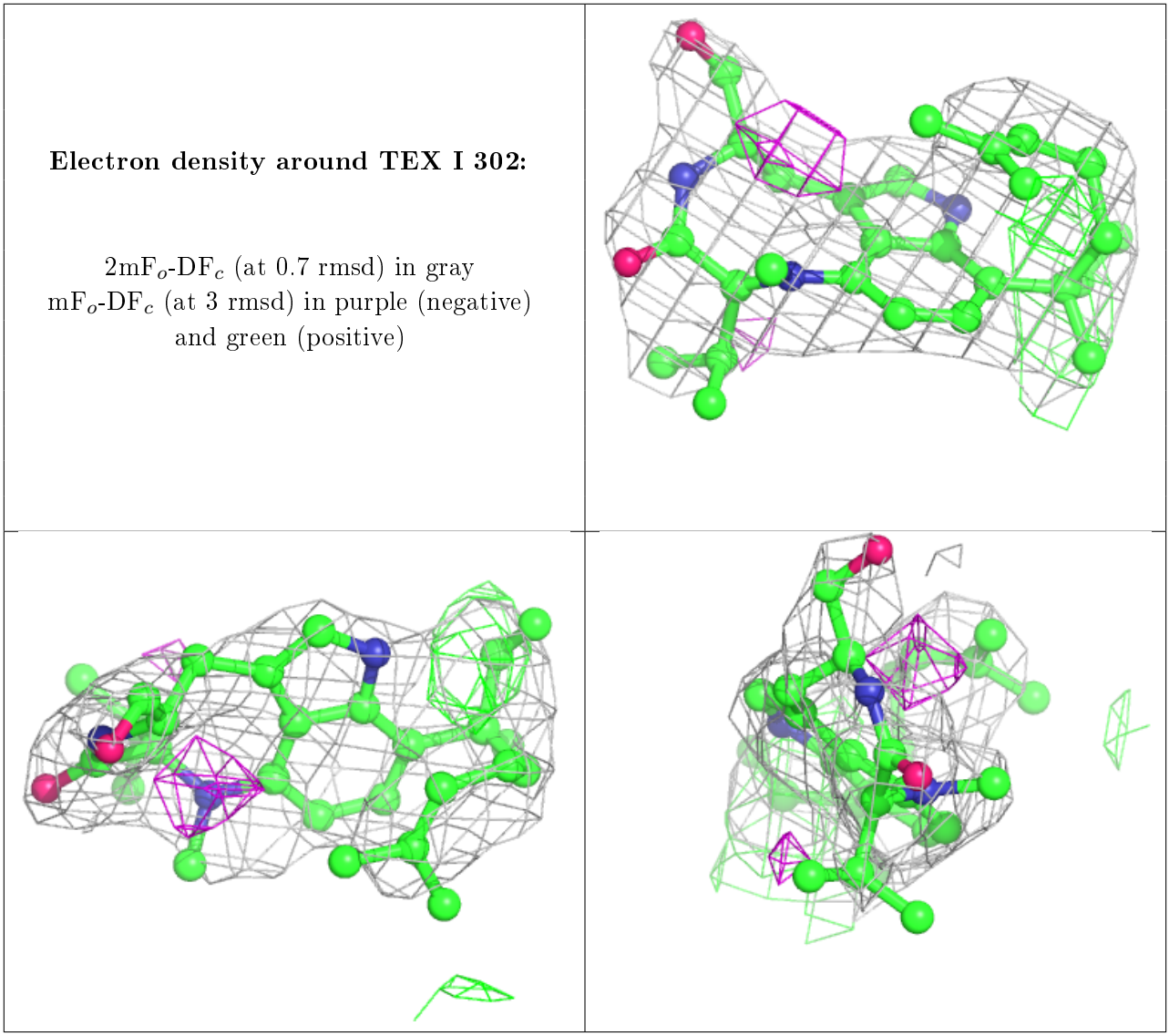






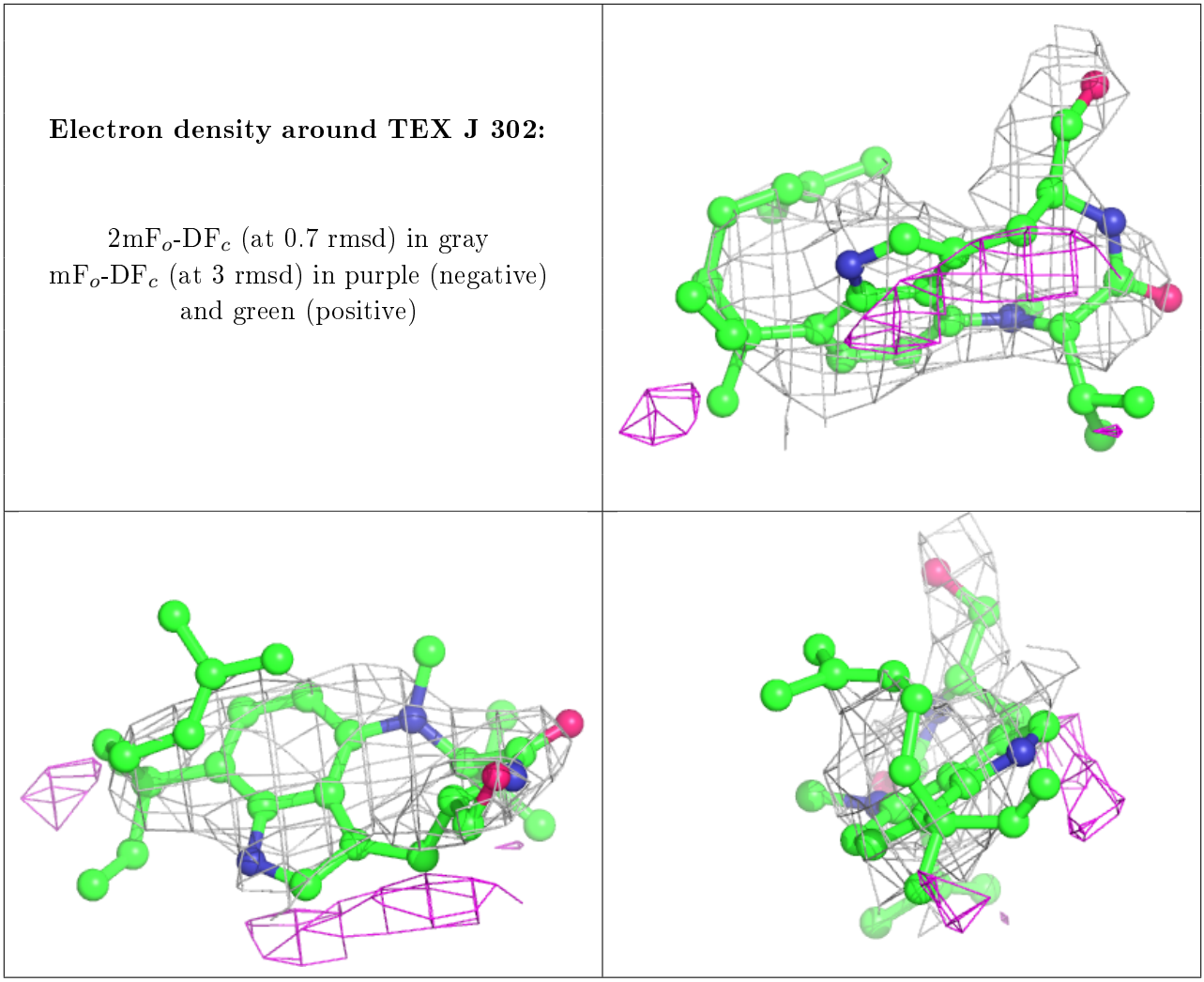
Electron density around TEX I 302:

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



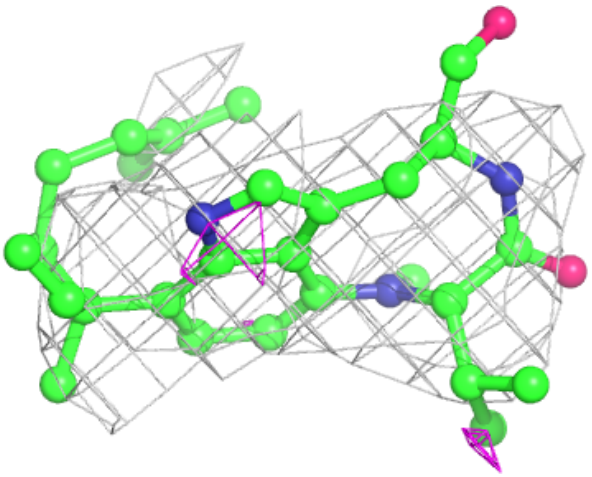
Electron density around TEX J 302:

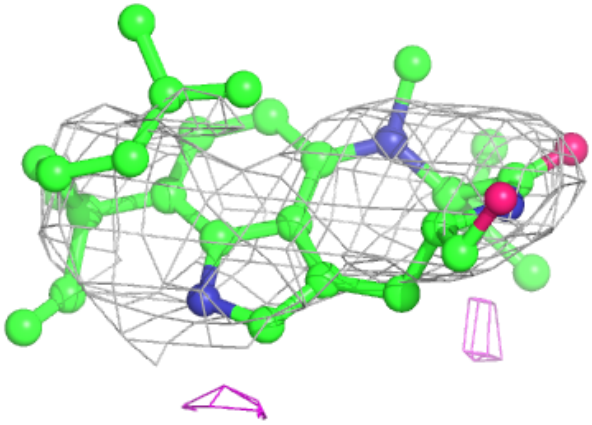
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

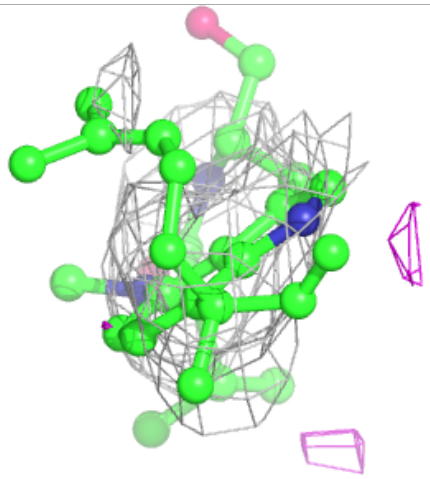


Electron density around TEX H 302:

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

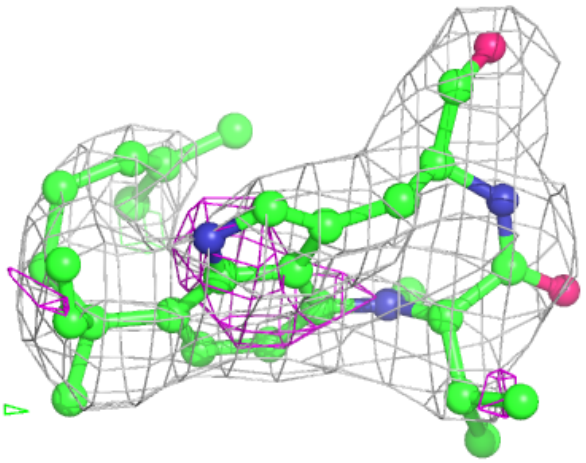


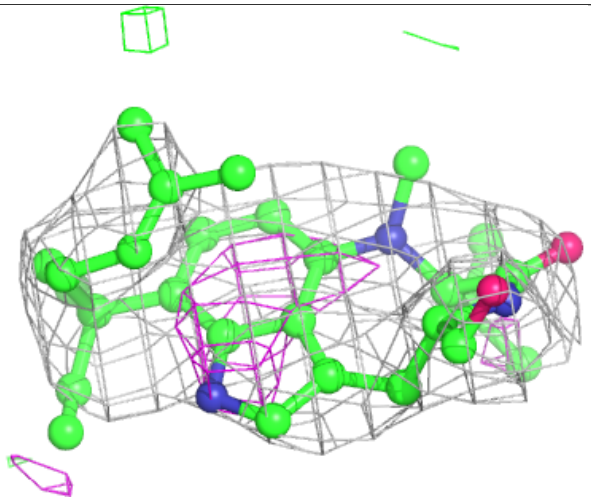


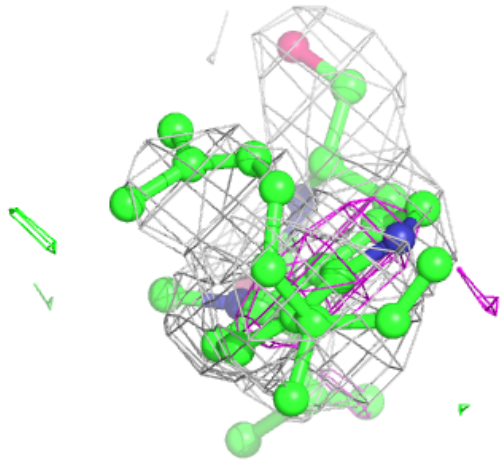


Electron density around TEX L 302:

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

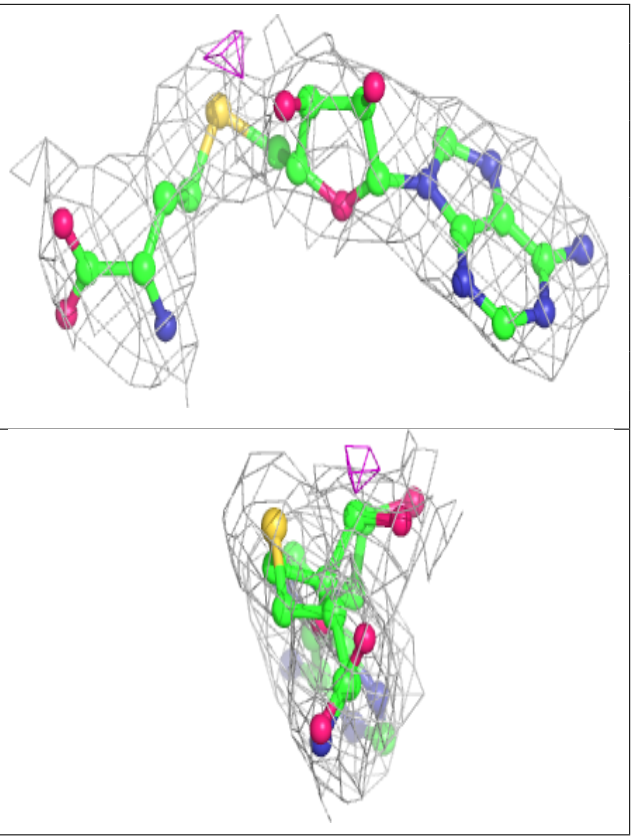


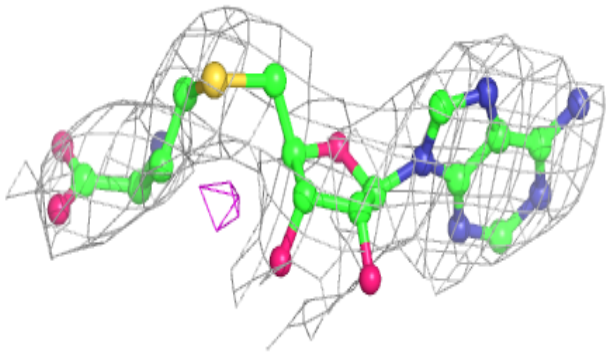




Electron density around SAH P 301:

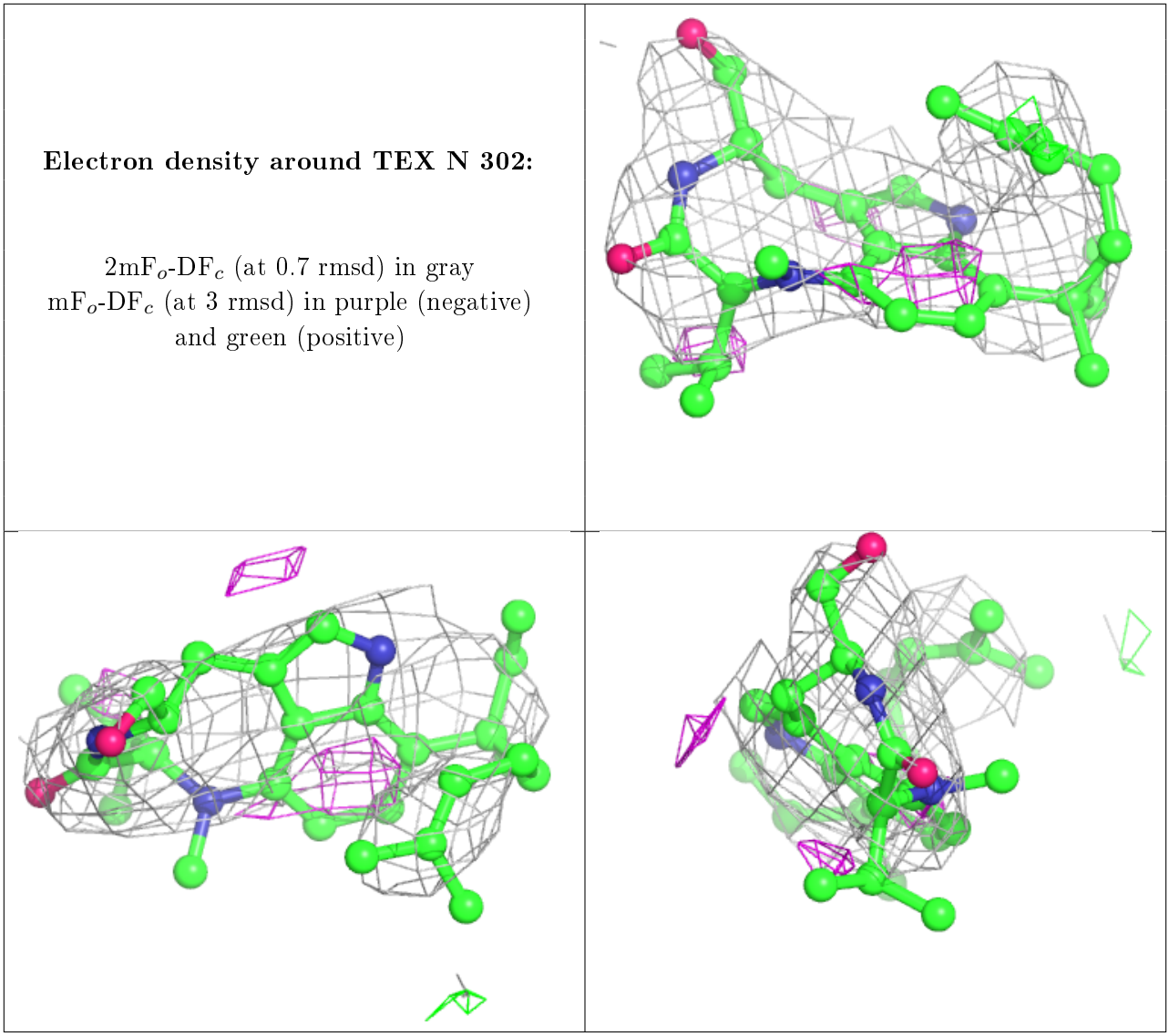
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





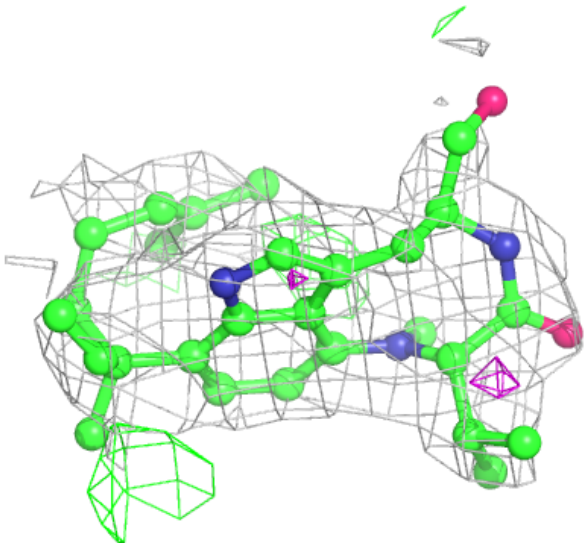
Electron density around TEX N 302:

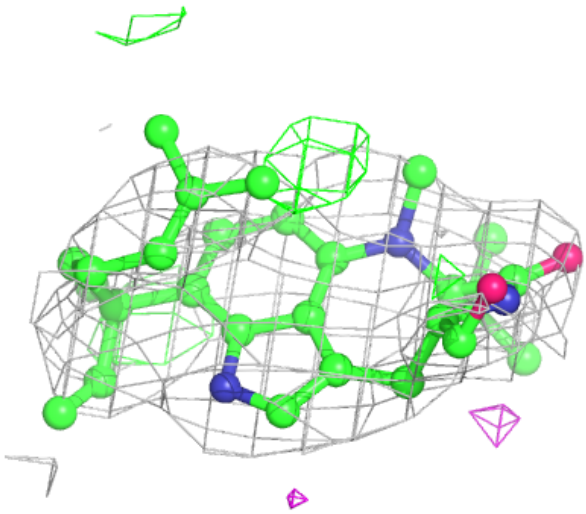
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

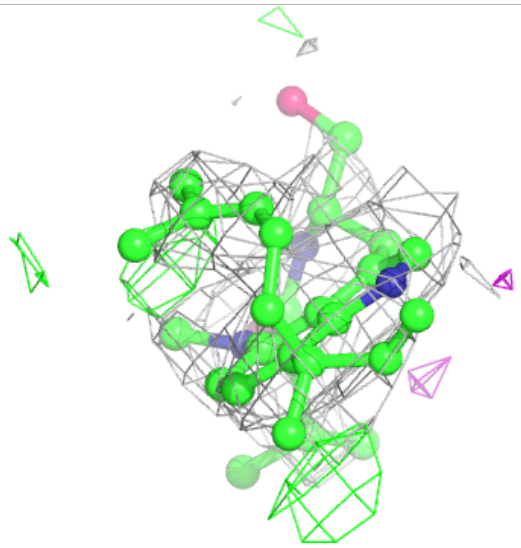


Electron density around TEX B 302:

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

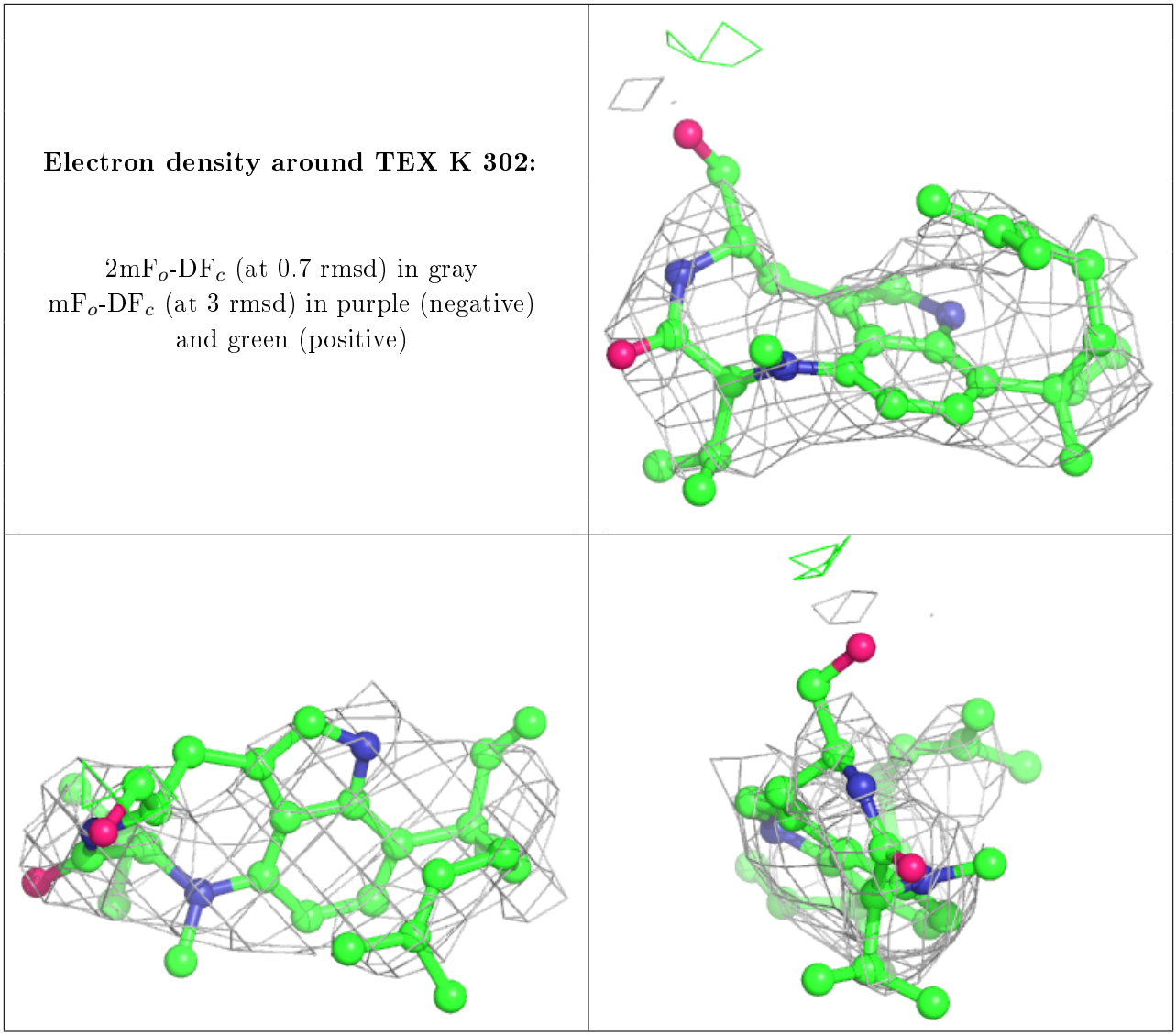






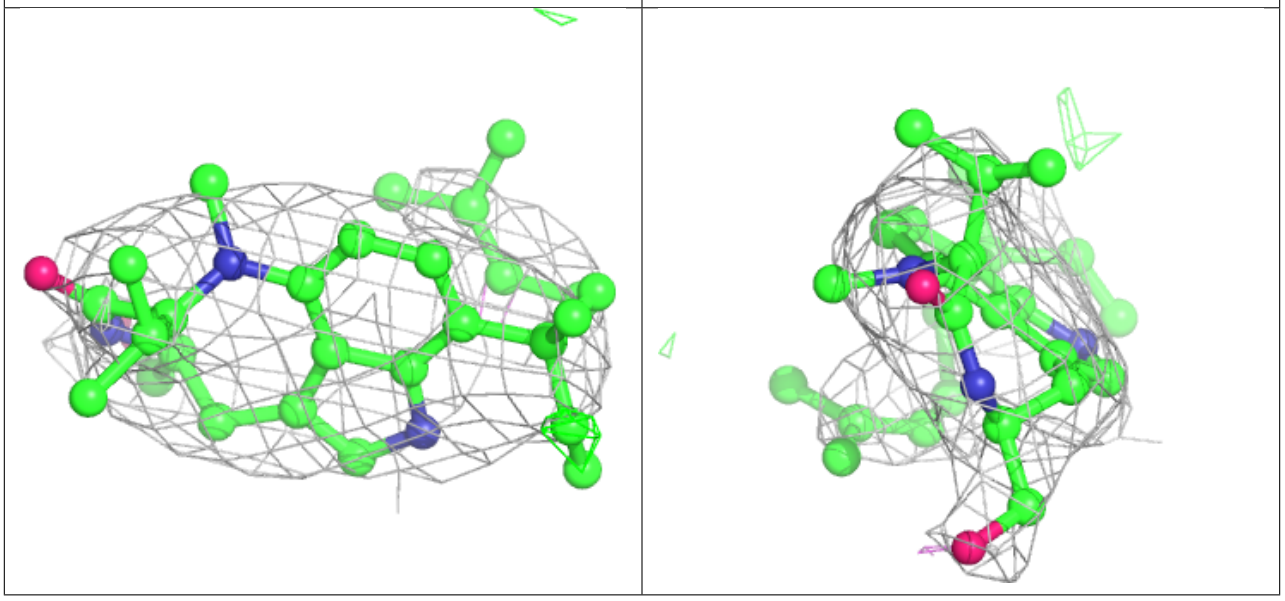
Electron density around TEX K 302:

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



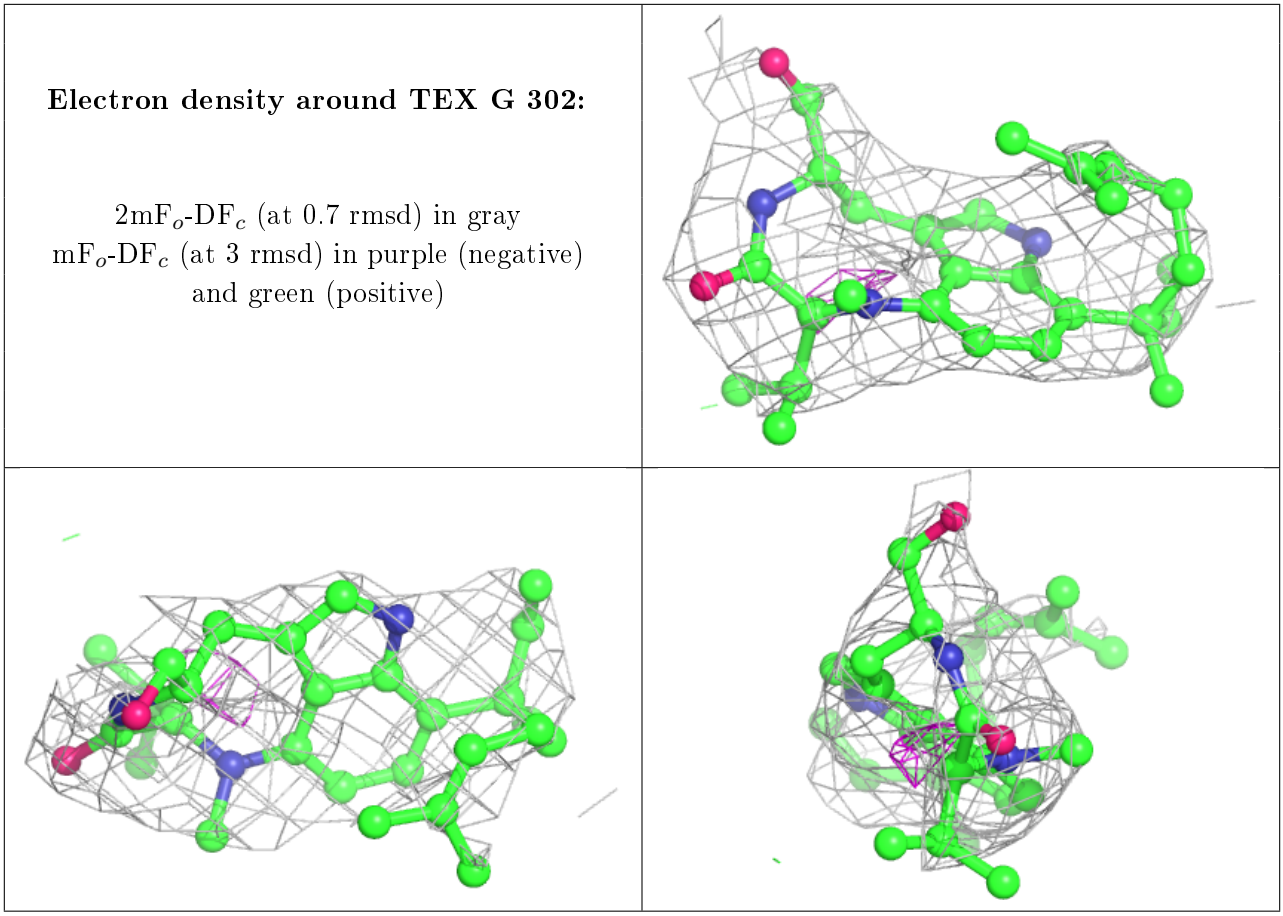
Electron density around TEX Q 302:

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



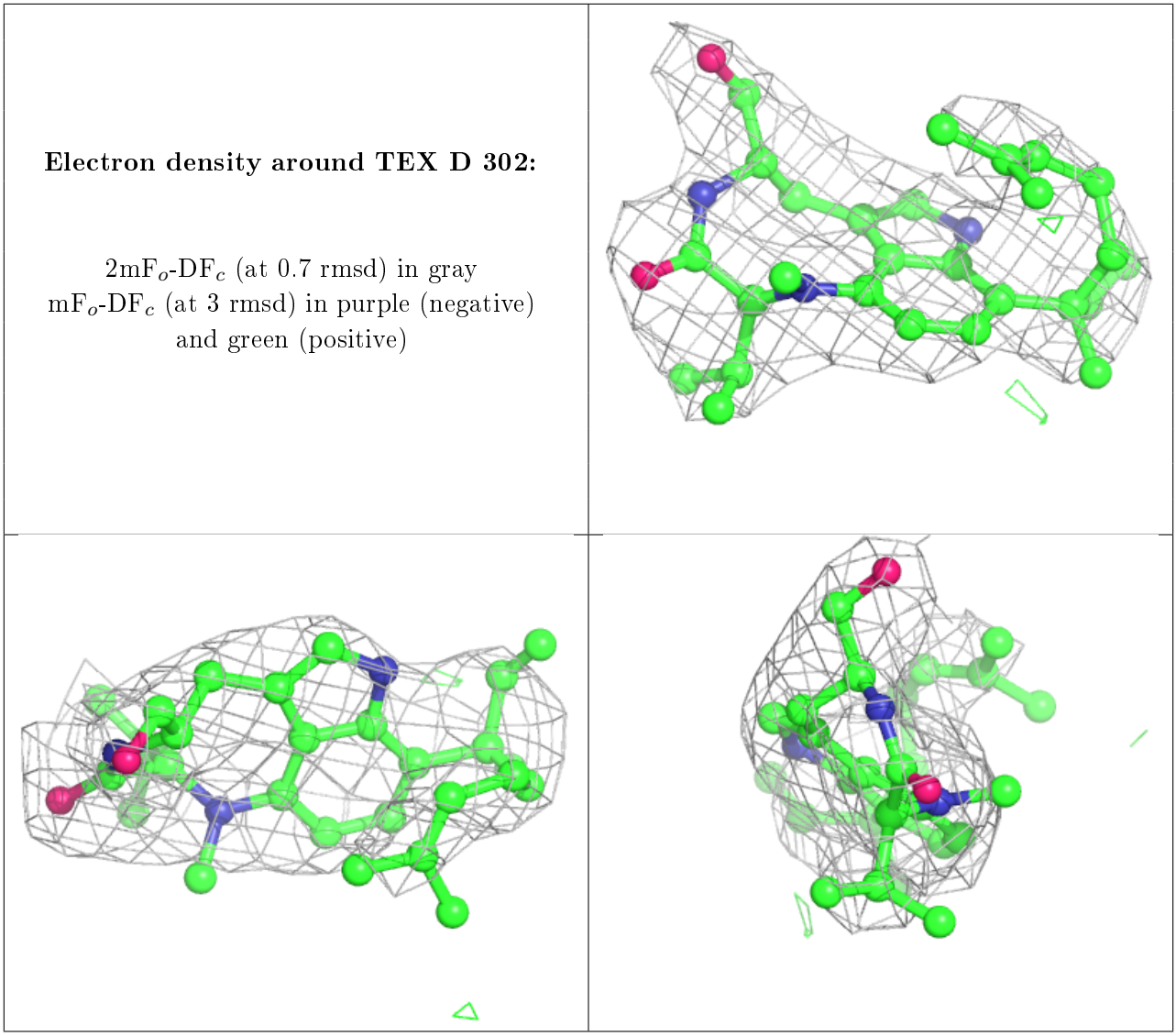
Electron density around TEX G 302:

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



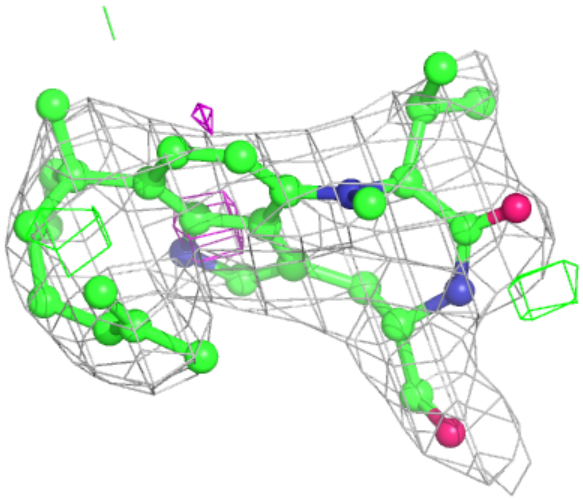
Electron density around TEX D 302:

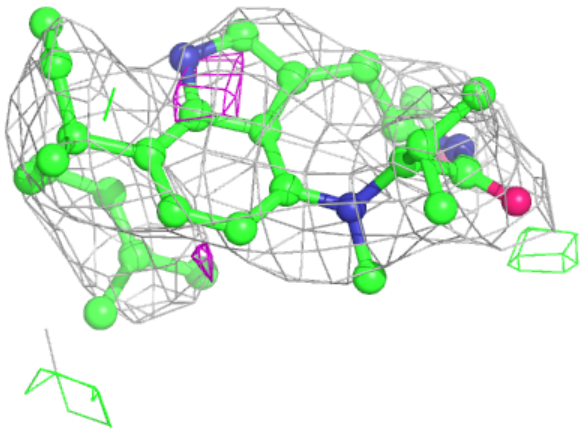
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

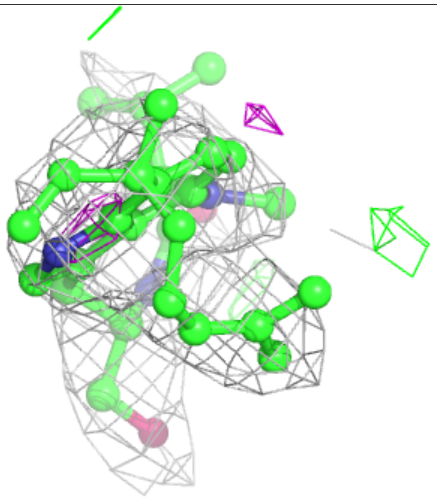


Electron density around TEX M 302:

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

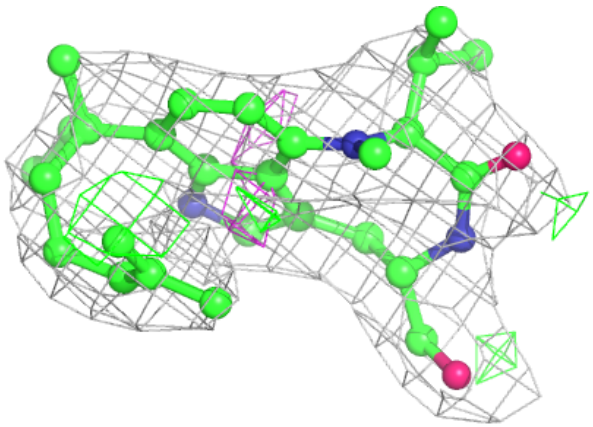


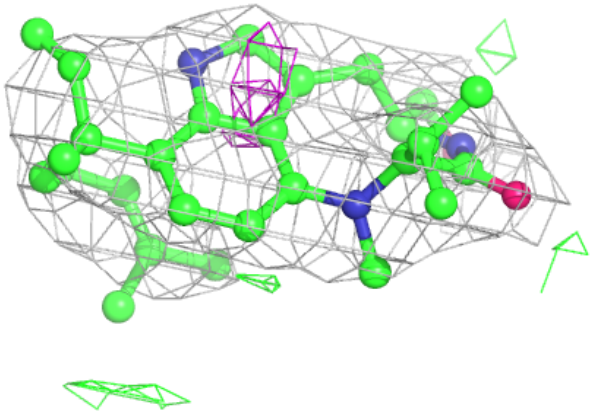


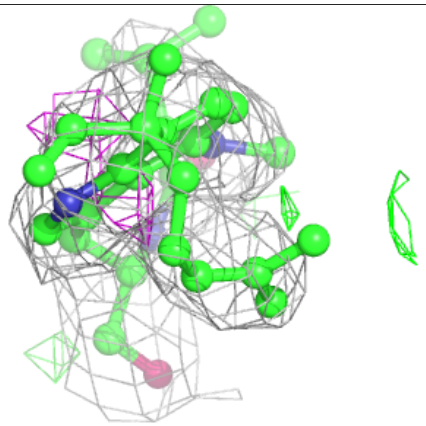


Electron density around TEX E 302:

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

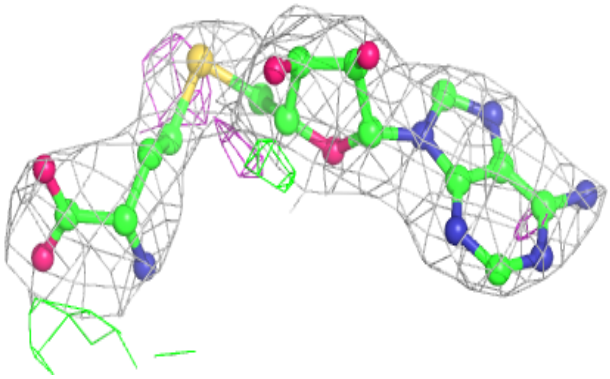


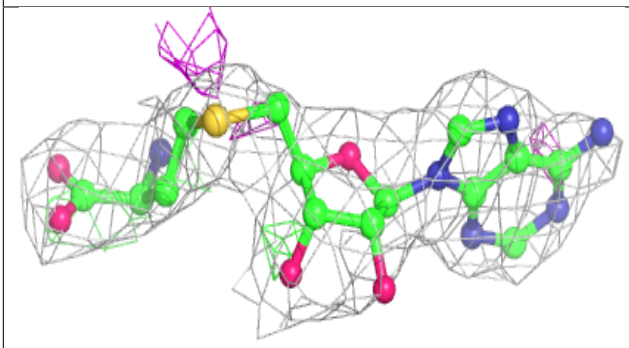


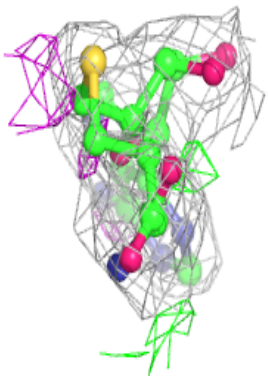


Electron density around SAH Q 301:

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

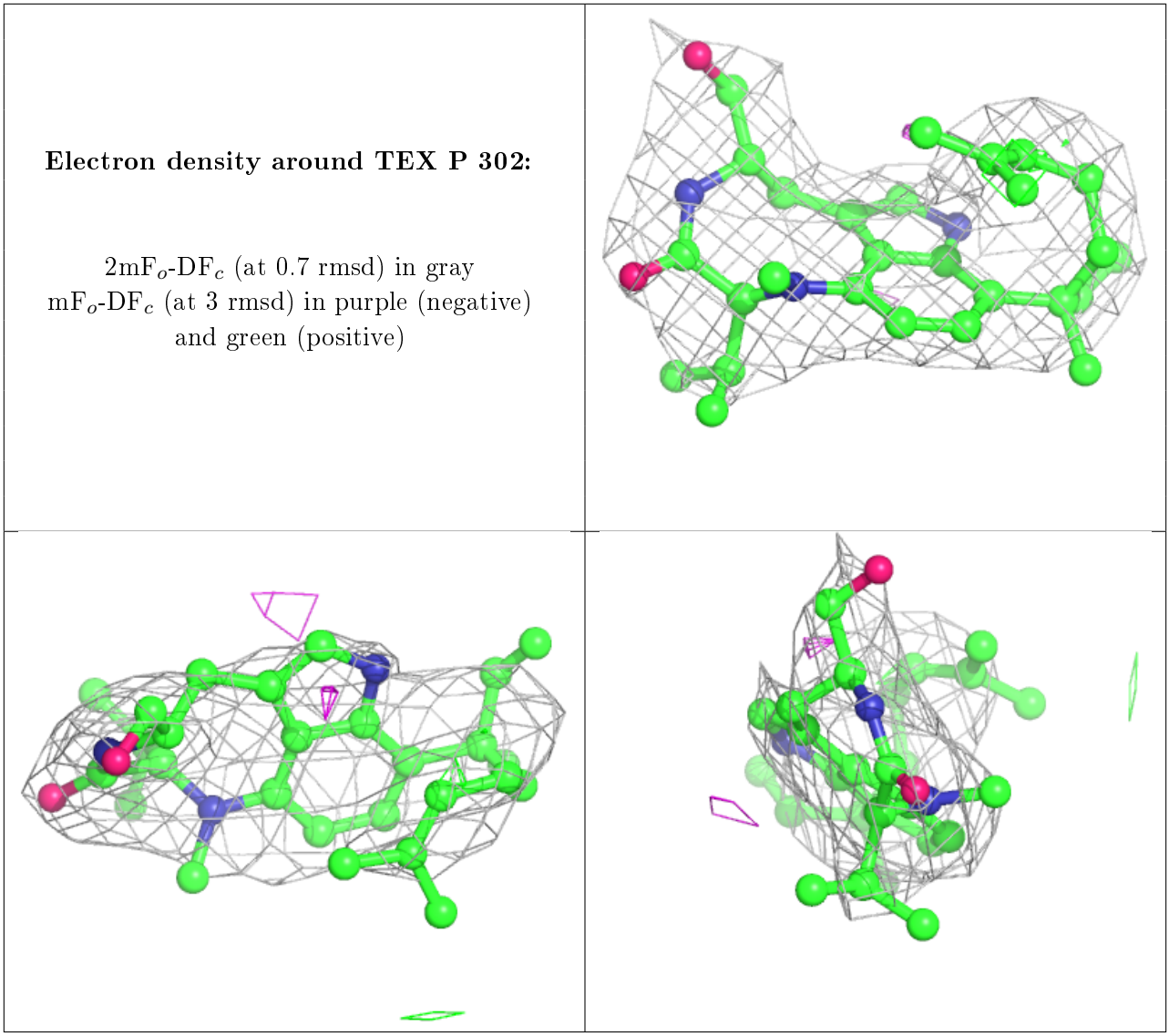






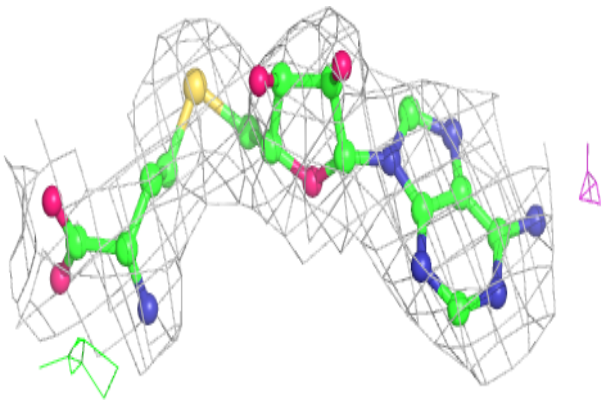
Electron density around TEX P 302:

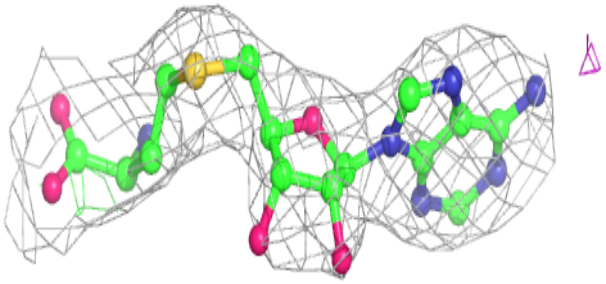
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

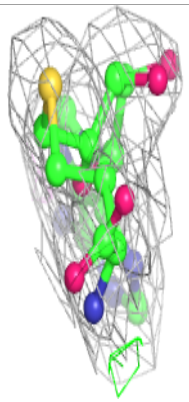


Electron density around SAH C 301:

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

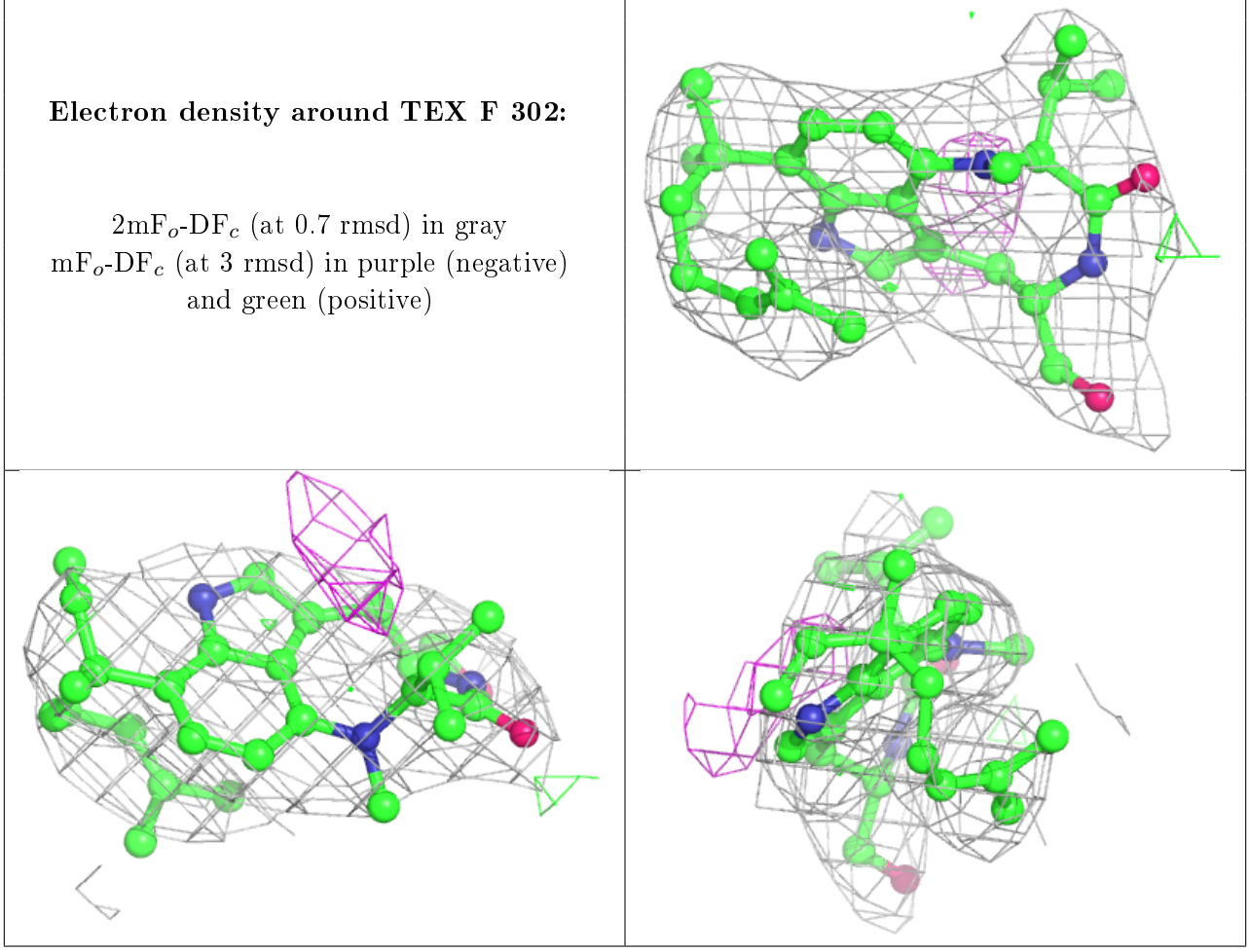






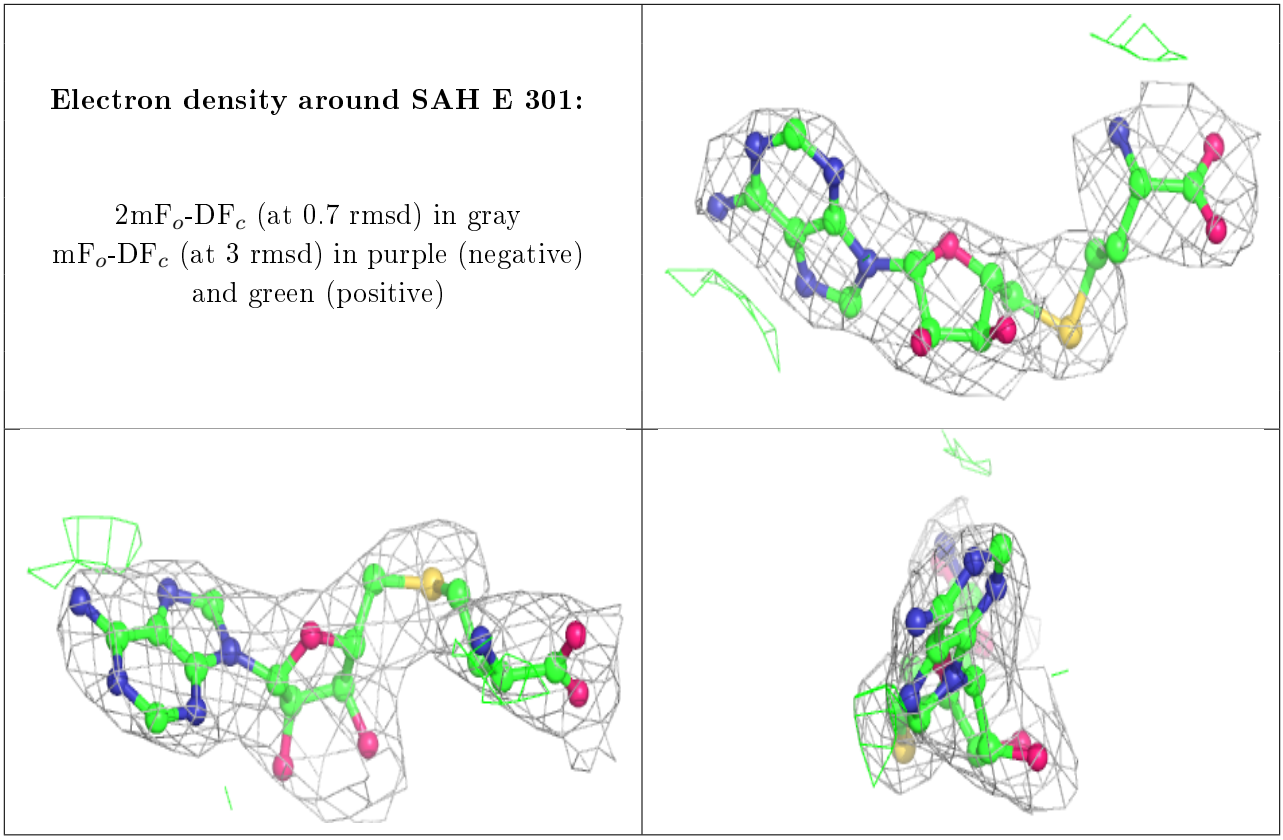
Electron density around TEX F 302:

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



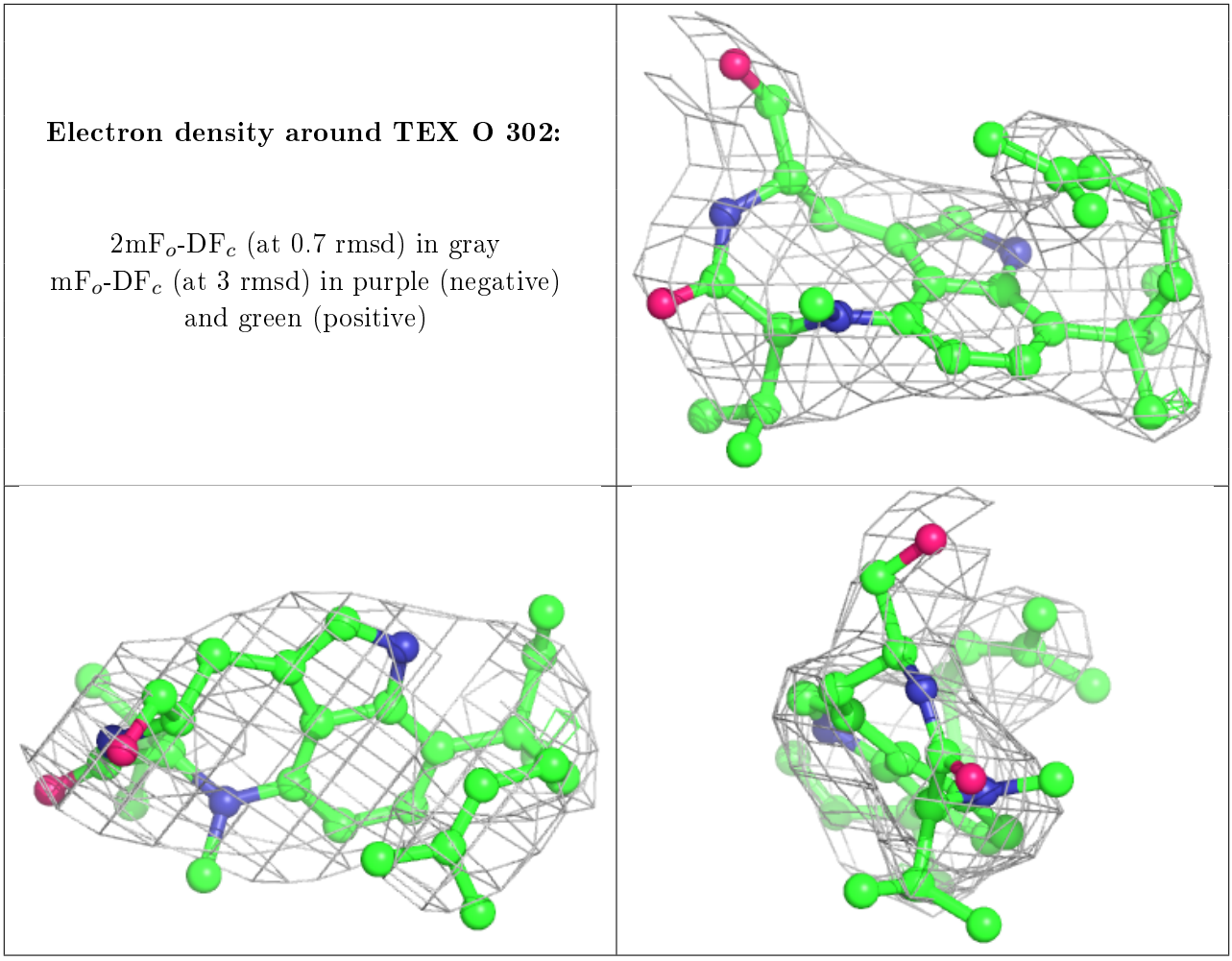
Electron density around SAH E 301:

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



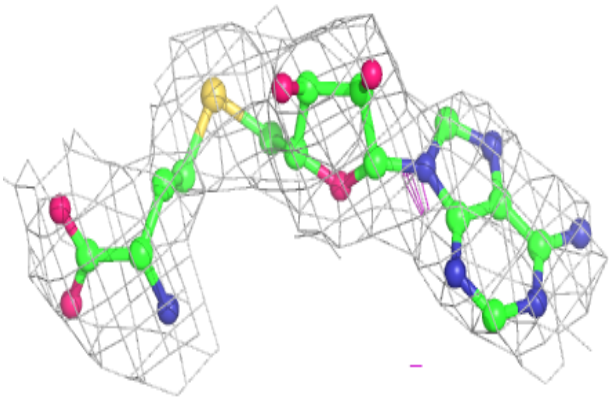
Electron density around TEX O 302:

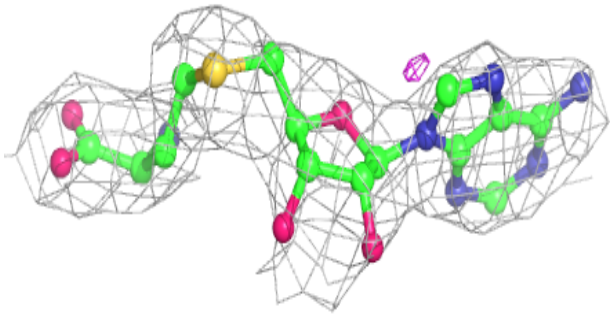
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

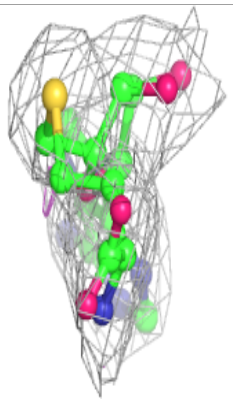


Electron density around SAH D 301:

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

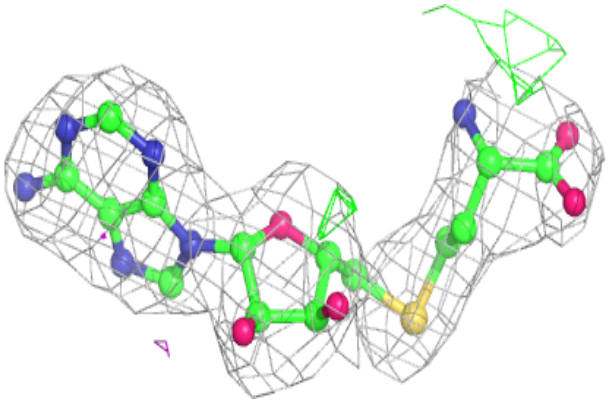


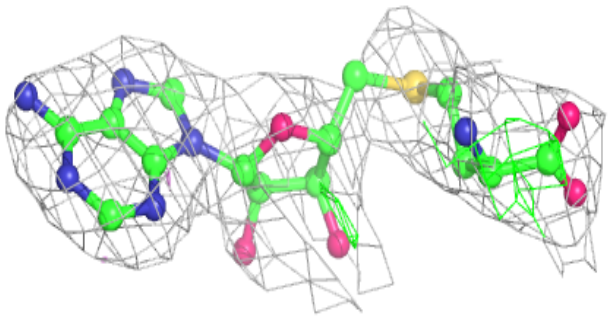


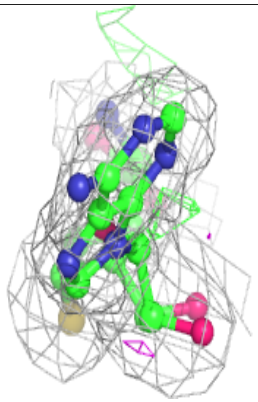


Electron density around SAH B 301:

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

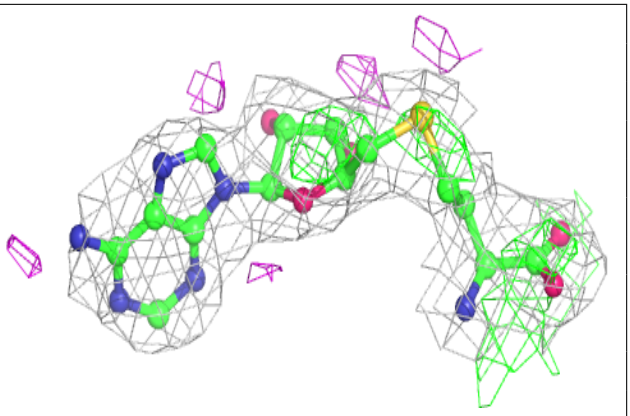


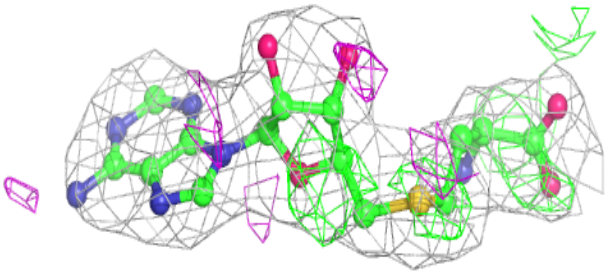


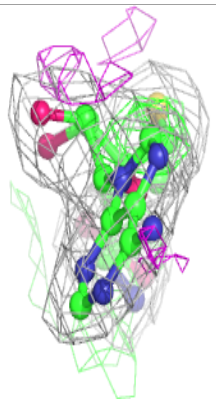


Electron density around SAH I 301:

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

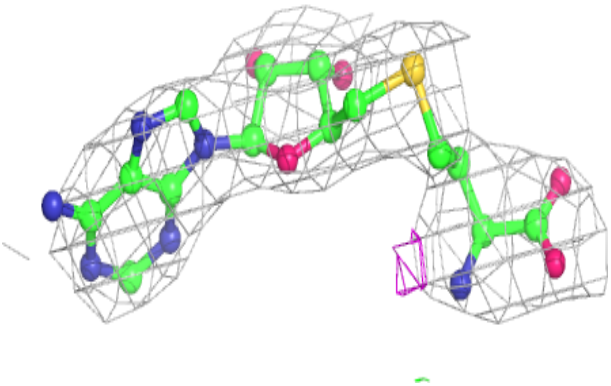


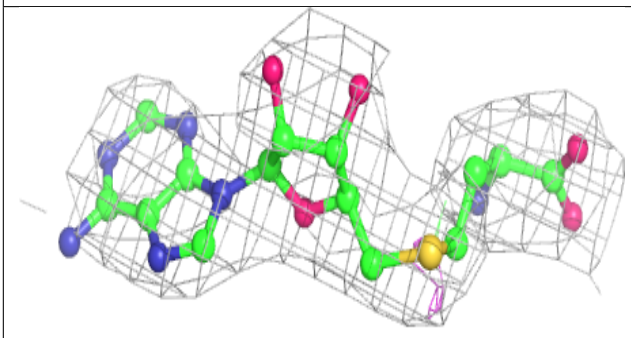


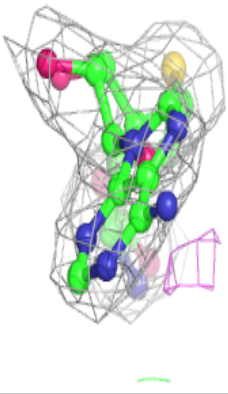


Electron density around SAH M 301:

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

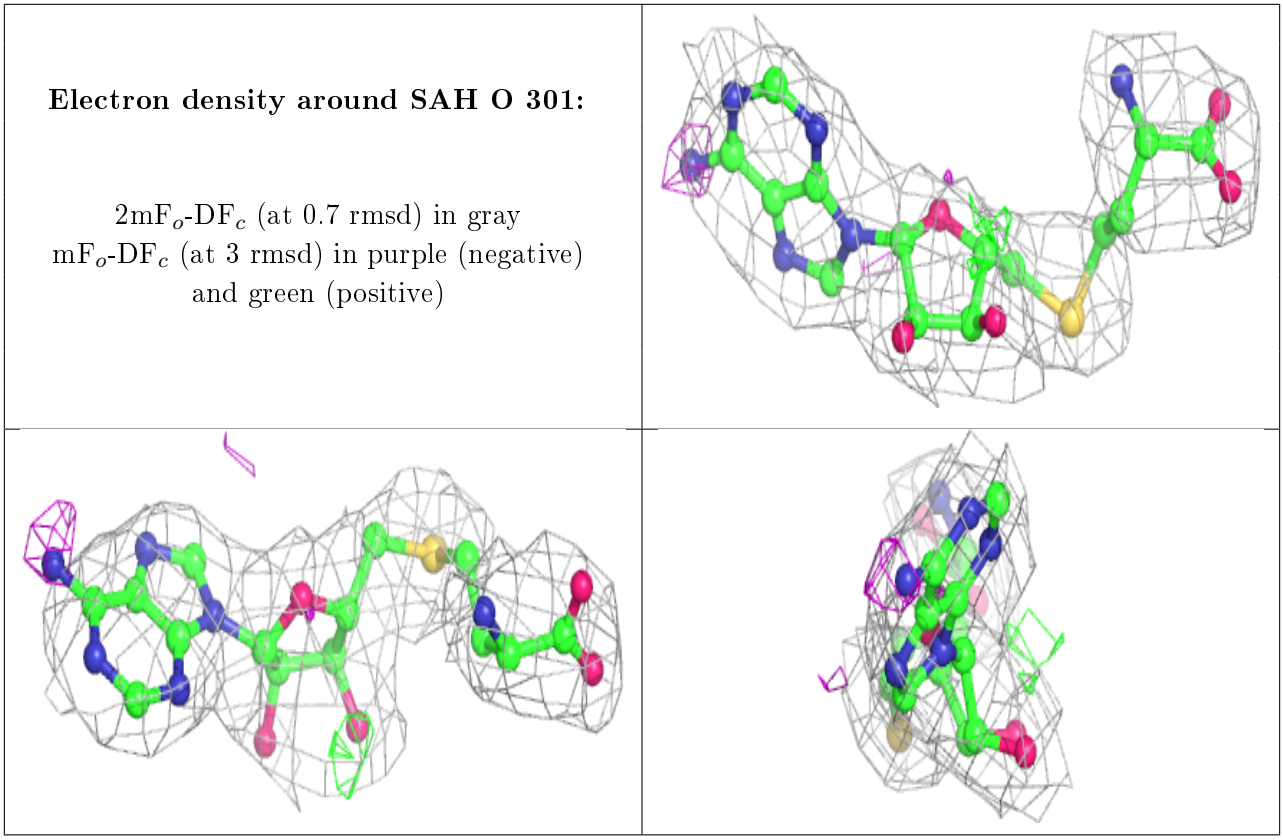






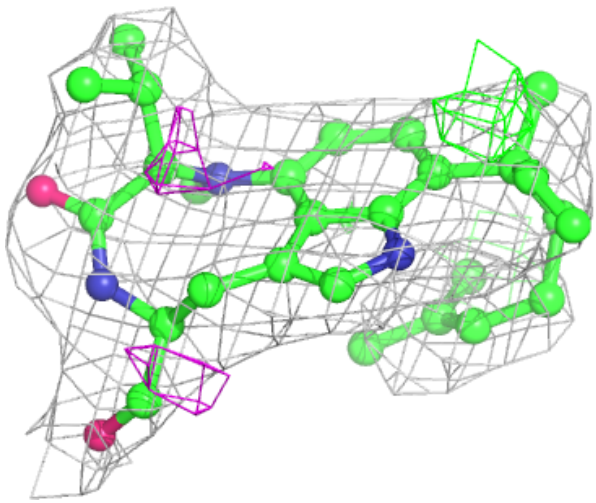
Electron density around SAH O 301:

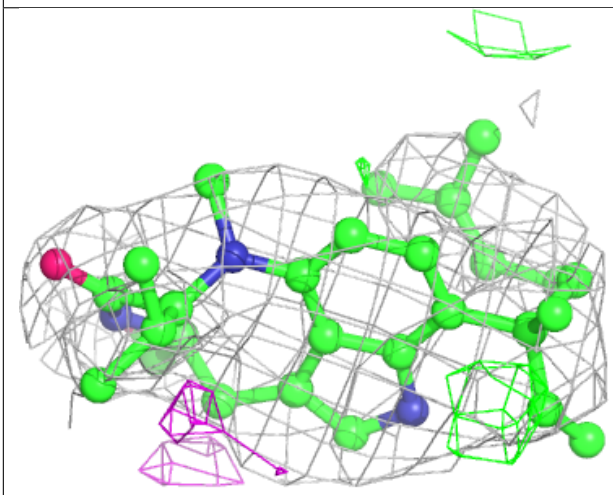
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

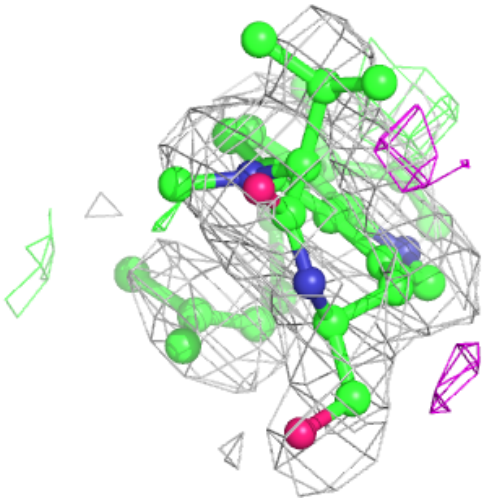


Electron density around TEX A 302:

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

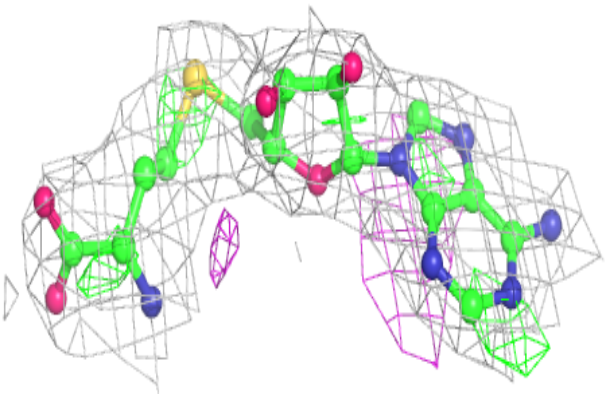


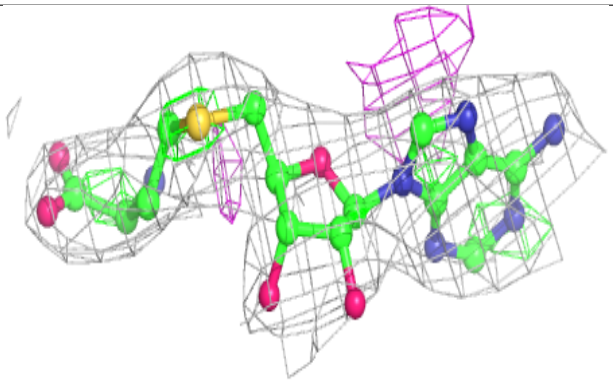


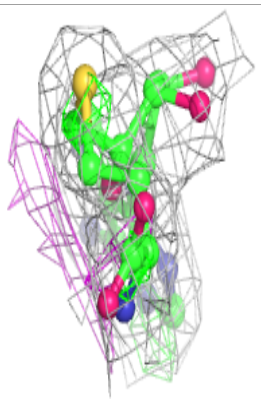


Electron density around SAH F 301:

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

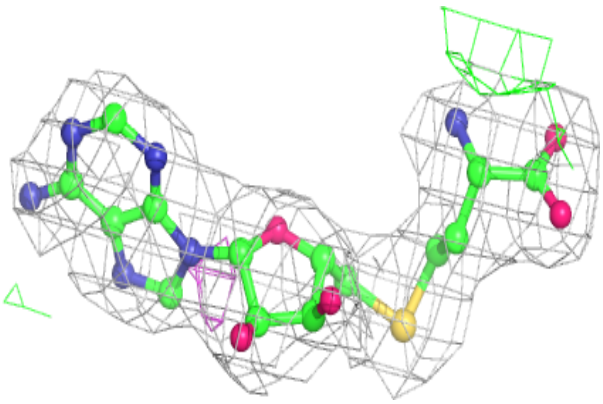


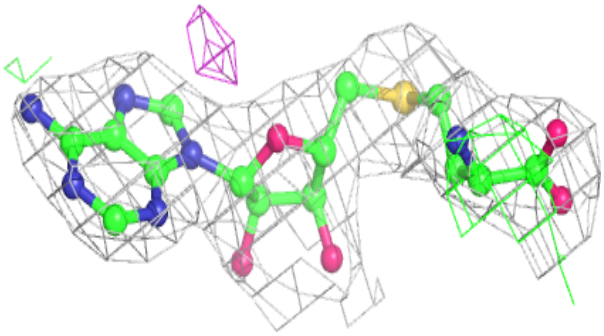


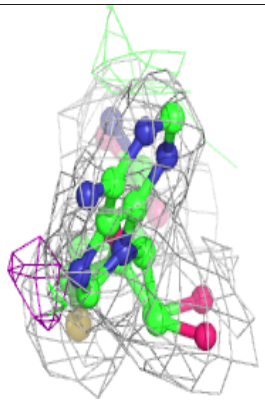


Electron density around SAH A 301:

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







6.5 Other polymers (i)

There are no such residues in this entry.