Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 10:29 PM JST

PDB ID	:	7XIF
Title	:	Crystal structure of the aminopropyltransferase, SpeE from hyperthermophilic crenarchaeon, Pyrobaculum calidifontis in complex with 5'-methylthioadenosine (MTA) alone or together with spermidine or thermospermine
Authors	:	Mizohata, E.; Yasuda, Y.
Deposited on	:	2022-04-13
Resolution	:	2.14 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

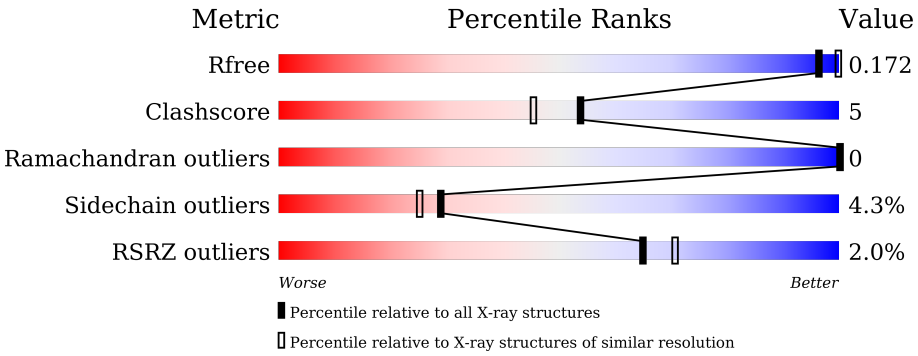
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	84% 7% • 7%
1	B	309	78% 13% • 7%
1	C	309	83% 8% • 7%
1	D	309	81% 11% • 7%
1	E	309	80% 12% • 7%

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Mol	Chain	Length	Quality of chain
1	F	309	81% 10% 7%
1	G	309	83% 8% 7%
1	H	309	81% 11% 7%
1	I	309	80% 11% 7%
1	J	309	83% 8% 7%
1	K	309	8% 81% 11% 7%
1	L	309	81% 10% 7%

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
4	TER	G	302	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 28933 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 Polyamine aminopropyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	1	0
			2282	1464	385	426	7			
1	B	286	Total	C	N	O	S	0	1	0
			2284	1465	388	424	7			
1	C	286	Total	C	N	O	S	0	0	0
			2276	1460	385	424	7			
1	D	288	Total	C	N	O	S	0	1	0
			2302	1475	392	428	7			
1	E	286	Total	C	N	O	S	0	1	0
			2284	1465	388	424	7			
1	F	286	Total	C	N	O	S	0	1	0
			2284	1465	388	424	7			
1	G	286	Total	C	N	O	S	0	2	0
			2291	1469	386	429	7			
1	H	286	Total	C	N	O	S	0	1	0
			2282	1463	386	426	7			
1	I	286	Total	C	N	O	S	0	0	0
			2276	1460	385	424	7			
1	J	286	Total	C	N	O	S	0	0	0
			2276	1460	385	424	7			
1	K	286	Total	C	N	O	S	0	0	0
			2276	1460	385	424	7			
1	L	286	Total	C	N	O	S	0	1	0
			2282	1464	385	426	7			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A3MU81
A	-18	GLY	-	expression tag	UNP A3MU81
A	-17	SER	-	expression tag	UNP A3MU81
A	-16	SER	-	expression tag	UNP A3MU81
A	-15	HIS	-	expression tag	UNP A3MU81

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP A3MU81
A	-13	HIS	-	expression tag	UNP A3MU81
A	-12	HIS	-	expression tag	UNP A3MU81
A	-11	HIS	-	expression tag	UNP A3MU81
A	-10	HIS	-	expression tag	UNP A3MU81
A	-9	SER	-	expression tag	UNP A3MU81
A	-8	SER	-	expression tag	UNP A3MU81
A	-7	GLY	-	expression tag	UNP A3MU81
A	-6	LEU	-	expression tag	UNP A3MU81
A	-5	VAL	-	expression tag	UNP A3MU81
A	-4	PRO	-	expression tag	UNP A3MU81
A	-3	ARG	-	expression tag	UNP A3MU81
A	-2	GLY	-	expression tag	UNP A3MU81
A	-1	SER	-	expression tag	UNP A3MU81
A	0	HIS	-	expression tag	UNP A3MU81
B	-19	MET	-	initiating methionine	UNP A3MU81
B	-18	GLY	-	expression tag	UNP A3MU81
B	-17	SER	-	expression tag	UNP A3MU81
B	-16	SER	-	expression tag	UNP A3MU81
B	-15	HIS	-	expression tag	UNP A3MU81
B	-14	HIS	-	expression tag	UNP A3MU81
B	-13	HIS	-	expression tag	UNP A3MU81
B	-12	HIS	-	expression tag	UNP A3MU81
B	-11	HIS	-	expression tag	UNP A3MU81
B	-10	HIS	-	expression tag	UNP A3MU81
B	-9	SER	-	expression tag	UNP A3MU81
B	-8	SER	-	expression tag	UNP A3MU81
B	-7	GLY	-	expression tag	UNP A3MU81
B	-6	LEU	-	expression tag	UNP A3MU81
B	-5	VAL	-	expression tag	UNP A3MU81
B	-4	PRO	-	expression tag	UNP A3MU81
B	-3	ARG	-	expression tag	UNP A3MU81
B	-2	GLY	-	expression tag	UNP A3MU81
B	-1	SER	-	expression tag	UNP A3MU81
B	0	HIS	-	expression tag	UNP A3MU81
C	-19	MET	-	initiating methionine	UNP A3MU81
C	-18	GLY	-	expression tag	UNP A3MU81
C	-17	SER	-	expression tag	UNP A3MU81
C	-16	SER	-	expression tag	UNP A3MU81
C	-15	HIS	-	expression tag	UNP A3MU81
C	-14	HIS	-	expression tag	UNP A3MU81
C	-13	HIS	-	expression tag	UNP A3MU81

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP A3MU81
C	-11	HIS	-	expression tag	UNP A3MU81
C	-10	HIS	-	expression tag	UNP A3MU81
C	-9	SER	-	expression tag	UNP A3MU81
C	-8	SER	-	expression tag	UNP A3MU81
C	-7	GLY	-	expression tag	UNP A3MU81
C	-6	LEU	-	expression tag	UNP A3MU81
C	-5	VAL	-	expression tag	UNP A3MU81
C	-4	PRO	-	expression tag	UNP A3MU81
C	-3	ARG	-	expression tag	UNP A3MU81
C	-2	GLY	-	expression tag	UNP A3MU81
C	-1	SER	-	expression tag	UNP A3MU81
C	0	HIS	-	expression tag	UNP A3MU81
D	-19	MET	-	initiating methionine	UNP A3MU81
D	-18	GLY	-	expression tag	UNP A3MU81
D	-17	SER	-	expression tag	UNP A3MU81
D	-16	SER	-	expression tag	UNP A3MU81
D	-15	HIS	-	expression tag	UNP A3MU81
D	-14	HIS	-	expression tag	UNP A3MU81
D	-13	HIS	-	expression tag	UNP A3MU81
D	-12	HIS	-	expression tag	UNP A3MU81
D	-11	HIS	-	expression tag	UNP A3MU81
D	-10	HIS	-	expression tag	UNP A3MU81
D	-9	SER	-	expression tag	UNP A3MU81
D	-8	SER	-	expression tag	UNP A3MU81
D	-7	GLY	-	expression tag	UNP A3MU81
D	-6	LEU	-	expression tag	UNP A3MU81
D	-5	VAL	-	expression tag	UNP A3MU81
D	-4	PRO	-	expression tag	UNP A3MU81
D	-3	ARG	-	expression tag	UNP A3MU81
D	-2	GLY	-	expression tag	UNP A3MU81
D	-1	SER	-	expression tag	UNP A3MU81
D	0	HIS	-	expression tag	UNP A3MU81
E	-19	MET	-	initiating methionine	UNP A3MU81
E	-18	GLY	-	expression tag	UNP A3MU81
E	-17	SER	-	expression tag	UNP A3MU81
E	-16	SER	-	expression tag	UNP A3MU81
E	-15	HIS	-	expression tag	UNP A3MU81
E	-14	HIS	-	expression tag	UNP A3MU81
E	-13	HIS	-	expression tag	UNP A3MU81
E	-12	HIS	-	expression tag	UNP A3MU81
E	-11	HIS	-	expression tag	UNP A3MU81

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP A3MU81
E	-9	SER	-	expression tag	UNP A3MU81
E	-8	SER	-	expression tag	UNP A3MU81
E	-7	GLY	-	expression tag	UNP A3MU81
E	-6	LEU	-	expression tag	UNP A3MU81
E	-5	VAL	-	expression tag	UNP A3MU81
E	-4	PRO	-	expression tag	UNP A3MU81
E	-3	ARG	-	expression tag	UNP A3MU81
E	-2	GLY	-	expression tag	UNP A3MU81
E	-1	SER	-	expression tag	UNP A3MU81
E	0	HIS	-	expression tag	UNP A3MU81
F	-19	MET	-	initiating methionine	UNP A3MU81
F	-18	GLY	-	expression tag	UNP A3MU81
F	-17	SER	-	expression tag	UNP A3MU81
F	-16	SER	-	expression tag	UNP A3MU81
F	-15	HIS	-	expression tag	UNP A3MU81
F	-14	HIS	-	expression tag	UNP A3MU81
F	-13	HIS	-	expression tag	UNP A3MU81
F	-12	HIS	-	expression tag	UNP A3MU81
F	-11	HIS	-	expression tag	UNP A3MU81
F	-10	HIS	-	expression tag	UNP A3MU81
F	-9	SER	-	expression tag	UNP A3MU81
F	-8	SER	-	expression tag	UNP A3MU81
F	-7	GLY	-	expression tag	UNP A3MU81
F	-6	LEU	-	expression tag	UNP A3MU81
F	-5	VAL	-	expression tag	UNP A3MU81
F	-4	PRO	-	expression tag	UNP A3MU81
F	-3	ARG	-	expression tag	UNP A3MU81
F	-2	GLY	-	expression tag	UNP A3MU81
F	-1	SER	-	expression tag	UNP A3MU81
F	0	HIS	-	expression tag	UNP A3MU81
G	-19	MET	-	initiating methionine	UNP A3MU81
G	-18	GLY	-	expression tag	UNP A3MU81
G	-17	SER	-	expression tag	UNP A3MU81
G	-16	SER	-	expression tag	UNP A3MU81
G	-15	HIS	-	expression tag	UNP A3MU81
G	-14	HIS	-	expression tag	UNP A3MU81
G	-13	HIS	-	expression tag	UNP A3MU81
G	-12	HIS	-	expression tag	UNP A3MU81
G	-11	HIS	-	expression tag	UNP A3MU81
G	-10	HIS	-	expression tag	UNP A3MU81
G	-9	SER	-	expression tag	UNP A3MU81

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	expression tag	UNP A3MU81
G	-7	GLY	-	expression tag	UNP A3MU81
G	-6	LEU	-	expression tag	UNP A3MU81
G	-5	VAL	-	expression tag	UNP A3MU81
G	-4	PRO	-	expression tag	UNP A3MU81
G	-3	ARG	-	expression tag	UNP A3MU81
G	-2	GLY	-	expression tag	UNP A3MU81
G	-1	SER	-	expression tag	UNP A3MU81
G	0	HIS	-	expression tag	UNP A3MU81
H	-19	MET	-	initiating methionine	UNP A3MU81
H	-18	GLY	-	expression tag	UNP A3MU81
H	-17	SER	-	expression tag	UNP A3MU81
H	-16	SER	-	expression tag	UNP A3MU81
H	-15	HIS	-	expression tag	UNP A3MU81
H	-14	HIS	-	expression tag	UNP A3MU81
H	-13	HIS	-	expression tag	UNP A3MU81
H	-12	HIS	-	expression tag	UNP A3MU81
H	-11	HIS	-	expression tag	UNP A3MU81
H	-10	HIS	-	expression tag	UNP A3MU81
H	-9	SER	-	expression tag	UNP A3MU81
H	-8	SER	-	expression tag	UNP A3MU81
H	-7	GLY	-	expression tag	UNP A3MU81
H	-6	LEU	-	expression tag	UNP A3MU81
H	-5	VAL	-	expression tag	UNP A3MU81
H	-4	PRO	-	expression tag	UNP A3MU81
H	-3	ARG	-	expression tag	UNP A3MU81
H	-2	GLY	-	expression tag	UNP A3MU81
H	-1	SER	-	expression tag	UNP A3MU81
H	0	HIS	-	expression tag	UNP A3MU81
I	-19	MET	-	initiating methionine	UNP A3MU81
I	-18	GLY	-	expression tag	UNP A3MU81
I	-17	SER	-	expression tag	UNP A3MU81
I	-16	SER	-	expression tag	UNP A3MU81
I	-15	HIS	-	expression tag	UNP A3MU81
I	-14	HIS	-	expression tag	UNP A3MU81
I	-13	HIS	-	expression tag	UNP A3MU81
I	-12	HIS	-	expression tag	UNP A3MU81
I	-11	HIS	-	expression tag	UNP A3MU81
I	-10	HIS	-	expression tag	UNP A3MU81
I	-9	SER	-	expression tag	UNP A3MU81
I	-8	SER	-	expression tag	UNP A3MU81
I	-7	GLY	-	expression tag	UNP A3MU81

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP A3MU81
I	-5	VAL	-	expression tag	UNP A3MU81
I	-4	PRO	-	expression tag	UNP A3MU81
I	-3	ARG	-	expression tag	UNP A3MU81
I	-2	GLY	-	expression tag	UNP A3MU81
I	-1	SER	-	expression tag	UNP A3MU81
I	0	HIS	-	expression tag	UNP A3MU81
J	-19	MET	-	initiating methionine	UNP A3MU81
J	-18	GLY	-	expression tag	UNP A3MU81
J	-17	SER	-	expression tag	UNP A3MU81
J	-16	SER	-	expression tag	UNP A3MU81
J	-15	HIS	-	expression tag	UNP A3MU81
J	-14	HIS	-	expression tag	UNP A3MU81
J	-13	HIS	-	expression tag	UNP A3MU81
J	-12	HIS	-	expression tag	UNP A3MU81
J	-11	HIS	-	expression tag	UNP A3MU81
J	-10	HIS	-	expression tag	UNP A3MU81
J	-9	SER	-	expression tag	UNP A3MU81
J	-8	SER	-	expression tag	UNP A3MU81
J	-7	GLY	-	expression tag	UNP A3MU81
J	-6	LEU	-	expression tag	UNP A3MU81
J	-5	VAL	-	expression tag	UNP A3MU81
J	-4	PRO	-	expression tag	UNP A3MU81
J	-3	ARG	-	expression tag	UNP A3MU81
J	-2	GLY	-	expression tag	UNP A3MU81
J	-1	SER	-	expression tag	UNP A3MU81
J	0	HIS	-	expression tag	UNP A3MU81
K	-19	MET	-	initiating methionine	UNP A3MU81
K	-18	GLY	-	expression tag	UNP A3MU81
K	-17	SER	-	expression tag	UNP A3MU81
K	-16	SER	-	expression tag	UNP A3MU81
K	-15	HIS	-	expression tag	UNP A3MU81
K	-14	HIS	-	expression tag	UNP A3MU81
K	-13	HIS	-	expression tag	UNP A3MU81
K	-12	HIS	-	expression tag	UNP A3MU81
K	-11	HIS	-	expression tag	UNP A3MU81
K	-10	HIS	-	expression tag	UNP A3MU81
K	-9	SER	-	expression tag	UNP A3MU81
K	-8	SER	-	expression tag	UNP A3MU81
K	-7	GLY	-	expression tag	UNP A3MU81
K	-6	LEU	-	expression tag	UNP A3MU81
K	-5	VAL	-	expression tag	UNP A3MU81

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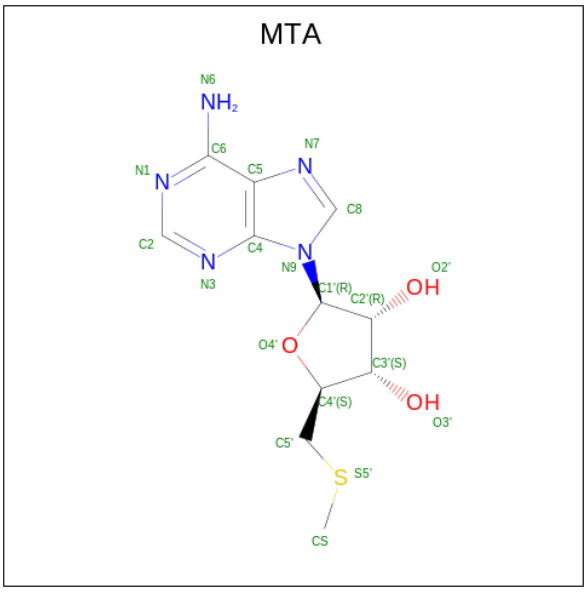
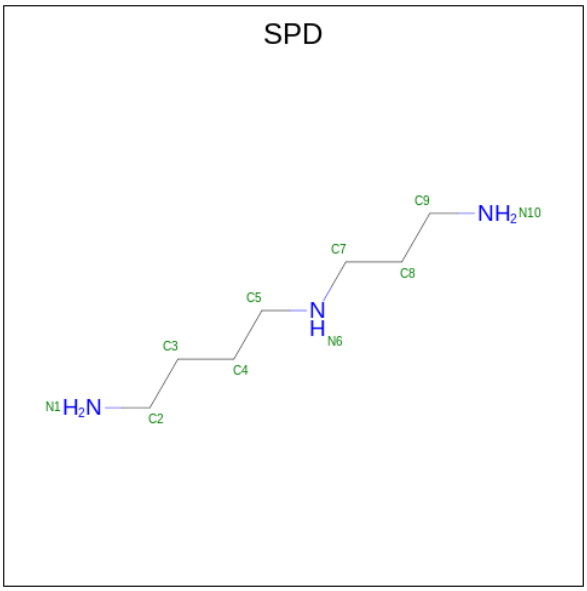
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP A3MU81
K	-3	ARG	-	expression tag	UNP A3MU81
K	-2	GLY	-	expression tag	UNP A3MU81
K	-1	SER	-	expression tag	UNP A3MU81
K	0	HIS	-	expression tag	UNP A3MU81
L	-19	MET	-	initiating methionine	UNP A3MU81
L	-18	GLY	-	expression tag	UNP A3MU81
L	-17	SER	-	expression tag	UNP A3MU81
L	-16	SER	-	expression tag	UNP A3MU81
L	-15	HIS	-	expression tag	UNP A3MU81
L	-14	HIS	-	expression tag	UNP A3MU81
L	-13	HIS	-	expression tag	UNP A3MU81
L	-12	HIS	-	expression tag	UNP A3MU81
L	-11	HIS	-	expression tag	UNP A3MU81
L	-10	HIS	-	expression tag	UNP A3MU81
L	-9	SER	-	expression tag	UNP A3MU81
L	-8	SER	-	expression tag	UNP A3MU81
L	-7	GLY	-	expression tag	UNP A3MU81
L	-6	LEU	-	expression tag	UNP A3MU81
L	-5	VAL	-	expression tag	UNP A3MU81
L	-4	PRO	-	expression tag	UNP A3MU81
L	-3	ARG	-	expression tag	UNP A3MU81
L	-2	GLY	-	expression tag	UNP A3MU81
L	-1	SER	-	expression tag	UNP A3MU81
L	0	HIS	-	expression tag	UNP A3MU81

- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: $C_{11}H_{15}N_5O_3S$) (labeled as "Ligand of Interest" by depositor).



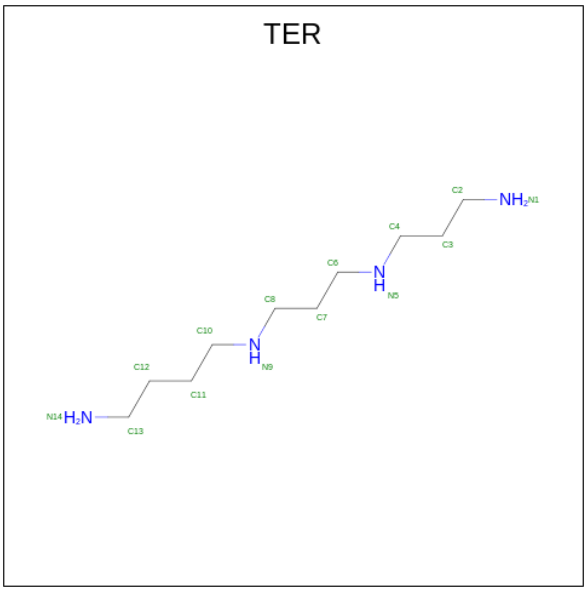
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	E	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	F	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	G	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	H	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	I	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	J	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	K	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	L	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 3 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 7 3	0	0
3	B	1	Total C N 10 7 3	0	0
3	C	1	Total C N 10 7 3	0	0
3	D	1	Total C N 10 7 3	0	0
3	H	1	Total C N 10 7 3	0	0

- Molecule 4 is N-(3-AMINO-PROPYL)-N-(5-AMINOPROPYL)-1,4-DIAMINOBUTANE (three-letter code: TER) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N 14 10 4	0	0
4	F	1	Total C N 14 10 4	0	0
4	G	1	Total C N 14 10 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	89	Total O 89 89	0	0
5	B	146	Total O 146 146	0	0
5	C	109	Total O 109 109	0	0
5	D	120	Total O 120 120	0	0
5	E	131	Total O 131 131	0	0
5	F	125	Total O 125 125	0	0
5	G	110	Total O 110 110	0	0
5	H	120	Total O 120 120	0	0
5	I	83	Total O 83 83	0	0

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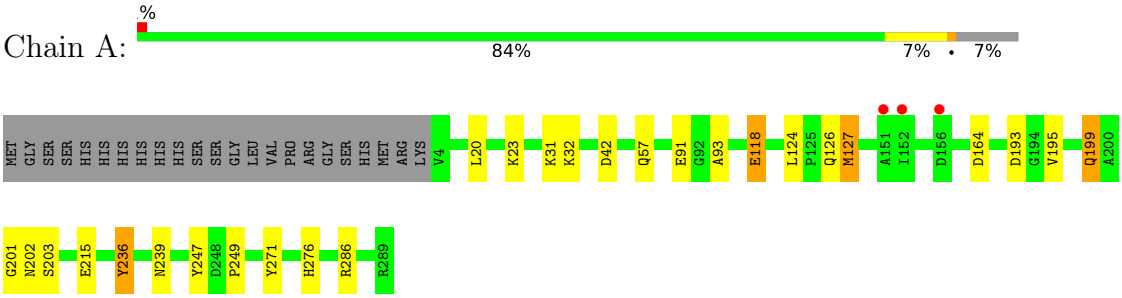
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	41	Total O 41 41	0	0
5	K	55	Total O 55 55	0	0
5	L	77	Total O 77 77	0	0

3 Residue-property plots (i)

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

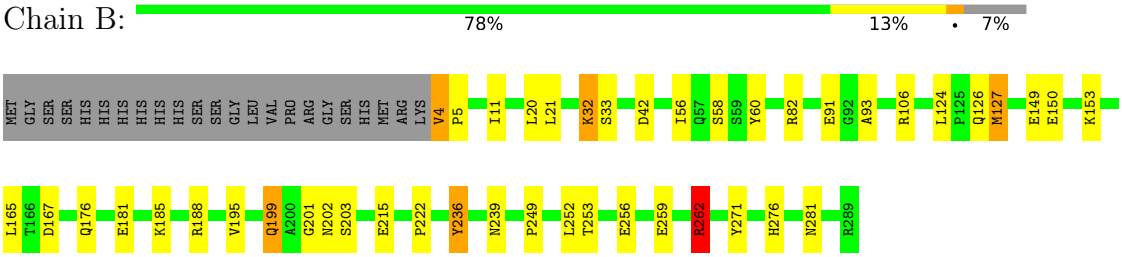
• Molecule 1: Polyamine aminopropyltransferase

Chain A:



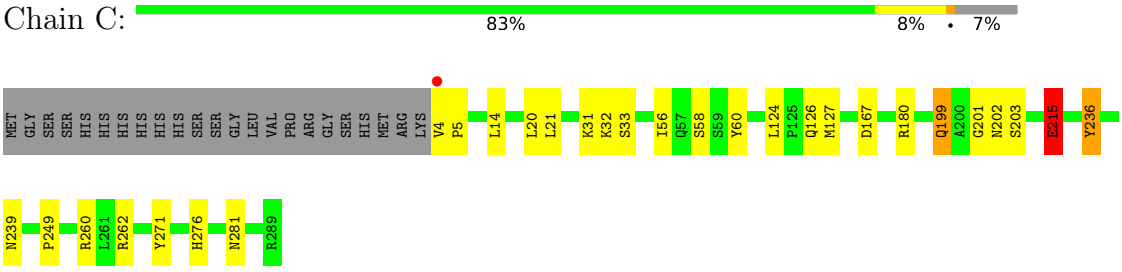
• Molecule 1: Polyamine aminopropyltransferase

Chain B:



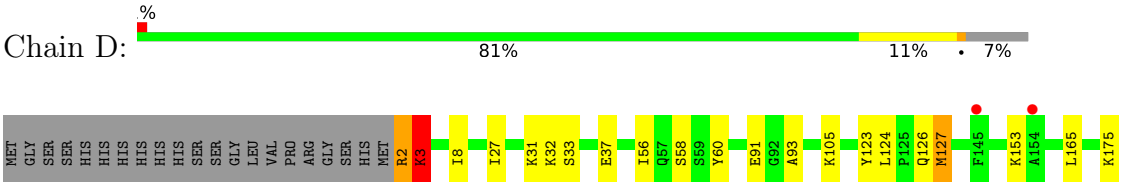
• Molecule 1: Polyamine aminopropyltransferase

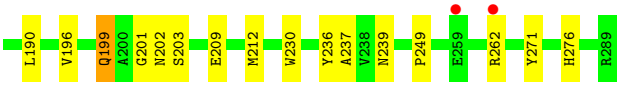
Chain C:



• Molecule 1: Polyamine aminopropyltransferase

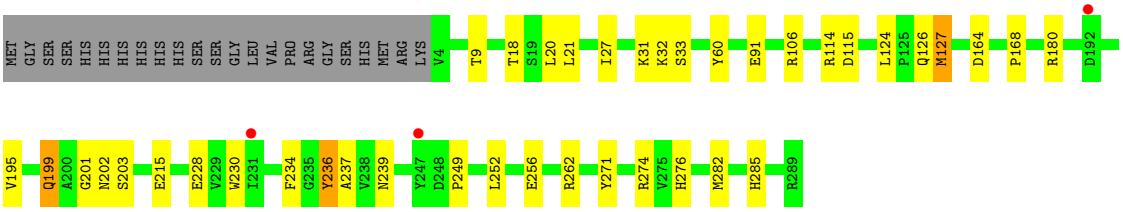
Chain D:





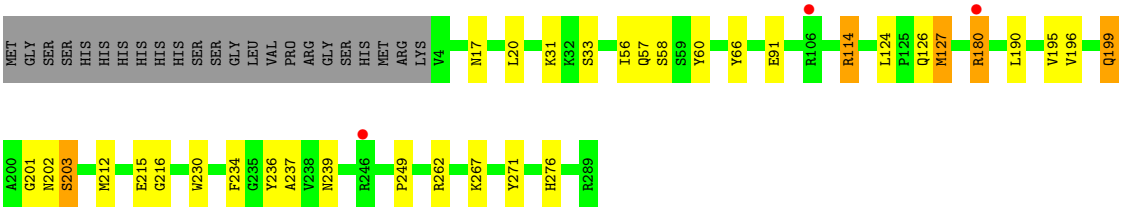
• Molecule 1: Polyamine aminopropyltransferase

Chain E:



• Molecule 1: Polyamine aminopropyltransferase

Chain F:

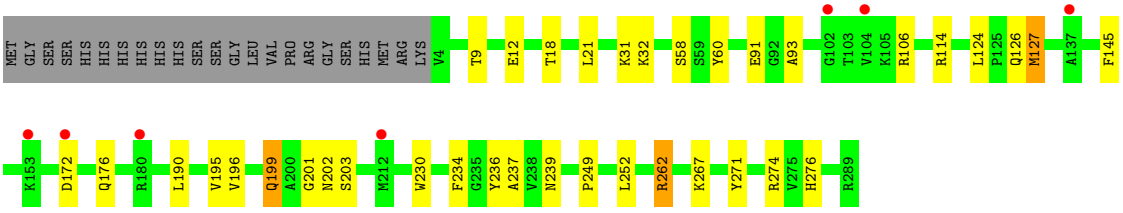


• Molecule 1: Polyamine aminopropyltransferase

Chain G:

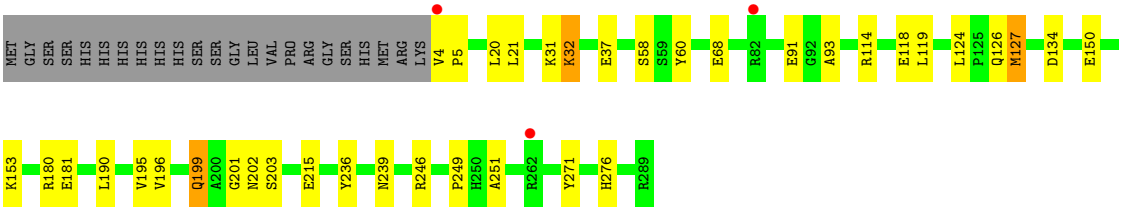
• Molecule 1: Polyamine aminopropyltransferase

Chain H:



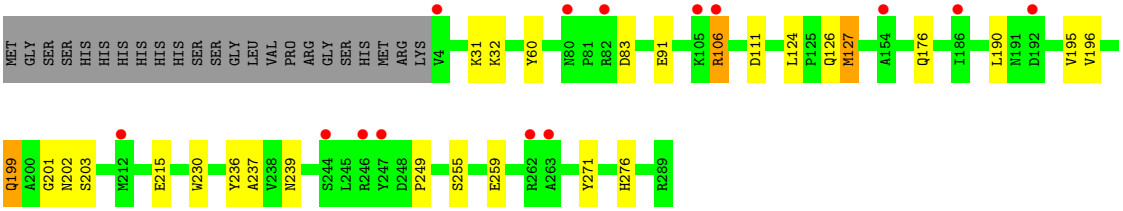
• Molecule 1: Polyamine aminopropyltransferase

Chain I:



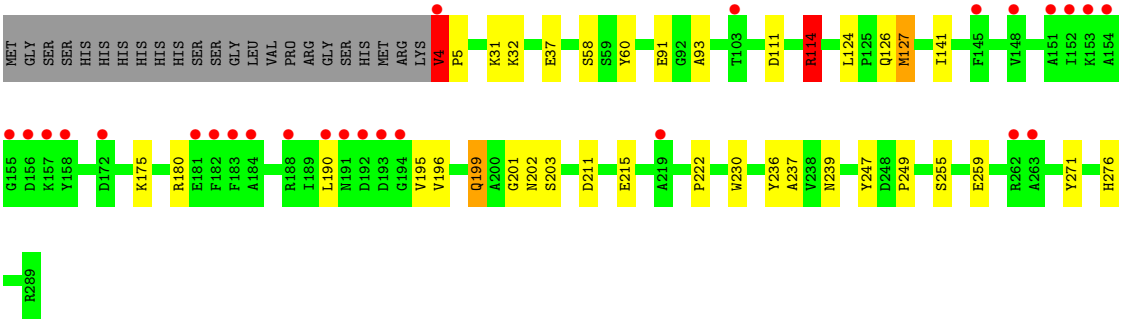
• Molecule 1: Polyamine aminopropyltransferase

Chain J:



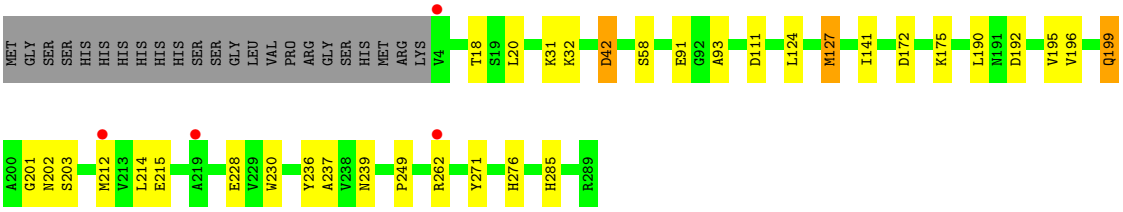
• Molecule 1: Polyamine aminopropyltransferase

Chain K:



• Molecule 1: Polyamine aminopropyltransferase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	166.16Å 166.16Å 149.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.11 – 2.14 47.11 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.11-2.14) 100.0 (47.11-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.160 , 0.190 0.147 , 0.172	Depositor DCC
R_{free} test set	12887 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.140 for h,-h-k,-l 0.013 for -k,-h,-l	Xtriage
Reported twinning fraction	0.498 for H, K, L 0.502 for K, H, -L	Depositor
Outliers	0 of 254668 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	28933	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.32% 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: MTA, TER, SPD

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	0.71	0/2338	0.88	1/3176 (0.0%)
1	B	0.77	1/2340 (0.0%)	0.93	4/3178 (0.1%)
1	C	0.72	1/2329 (0.0%)	0.86	1/3164 (0.0%)
1	D	0.74	1/2355 (0.0%)	0.86	0/3197
1	E	0.72	0/2340	0.84	1/3178 (0.0%)
1	F	0.69	0/2340	0.86	0/3178
1	G	0.72	0/2347	0.85	0/3189
1	H	0.72	0/2335	0.83	0/3172
1	I	0.71	1/2329 (0.0%)	0.85	0/3164
1	J	0.67	0/2329	0.85	1/3164 (0.0%)
1	K	0.68	0/2329	0.86	3/3164 (0.1%)
1	L	0.69	0/2338	0.86	1/3176 (0.0%)
All	All	0.71	4/28049 (0.0%)	0.86	12/38100 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	181	GLU	CD-OE1	6.22	1.32	1.25
1	D	3	LYS	C-O	6.09	1.34	1.23
1	C	215	GLU	CD-OE2	5.21	1.31	1.25
1	B	150	GLU	CD-OE1	5.06	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	4	VAL	CA-CB-CG1	7.21	121.72	110.90
1	B	4	VAL	CB-CA-C	7.05	124.80	111.40
1	L	42	ASP	CB-CG-OD1	-6.83	112.16	118.30
1	B	262[A]	ARG	CG-CD-NE	-6.41	98.33	111.80
1	B	262[B]	ARG	CG-CD-NE	-6.41	98.33	111.80
1	K	4	VAL	CB-CA-C	6.22	123.22	111.40
1	J	176	GLN	CB-CA-C	6.14	122.69	110.40
1	B	4	VAL	CA-CB-CG2	5.78	119.57	110.90
1	K	114	ARG	CB-CG-CD	5.51	125.92	111.60
1	A	118	GLU	CB-CG-CD	5.36	128.66	114.20
1	E	282	MET	CG-SD-CE	5.14	108.43	100.20
1	C	260	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	4	VAL	Peptide
1	C	5	PRO	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2282	0	2271	20	0
1	B	2284	0	2278	39	0
1	C	2276	0	2265	16	0
1	D	2302	0	2295	28	0
1	E	2284	0	2278	34	0
1	F	2284	0	2278	28	0
1	G	2291	0	2277	23	0
1	H	2282	0	2269	26	0
1	I	2276	0	2265	35	0
1	J	2276	0	2265	18	0
1	K	2276	0	2265	22	0
1	L	2282	0	2271	24	0
2	A	20	0	15	1	0
2	B	20	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	15	0	0
2	D	20	0	15	0	0
2	E	20	0	15	2	0
2	F	20	0	15	2	0
2	G	20	0	15	3	0
2	H	20	0	15	0	0
2	I	20	0	15	0	0
2	J	20	0	15	1	0
2	K	20	0	15	1	0
2	L	20	0	15	1	0
3	A	10	0	19	1	0
3	B	10	0	19	3	0
3	C	10	0	19	2	0
3	D	10	0	19	3	0
3	H	10	0	19	2	0
4	E	14	0	26	6	0
4	F	14	0	26	8	0
4	G	14	0	26	9	0
5	A	89	0	0	2	0
5	B	146	0	0	4	0
5	C	109	0	0	1	0
5	D	120	0	0	4	0
5	E	131	0	0	6	0
5	F	125	0	0	3	0
5	G	110	0	0	2	0
5	H	120	0	0	3	0
5	I	83	0	0	8	0
5	J	41	0	0	0	1
5	K	55	0	0	1	0
5	L	77	0	0	5	1
All	All	28933	0	27630	294	1

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 5.

All (294) 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:G:176:GLN:OE1	5:G:401:HOH:O	1.62	1.14
1:D:105:LYS:NZ	5:D:401:HOH:O	1.95	1.00
1:B:176:GLN:HG3	1:I:246:ARG:NH1	1.77	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:HD13	1:B:21:LEU:CD2	1.99	0.93
1:L:212:MET:SD	5:L:462:HOH:O	2.26	0.92
1:B:20:LEU:HD23	1:E:20:LEU:HD23	1.52	0.92
1:L:212:MET:CG	5:L:462:HOH:O	2.19	0.90
1:I:180:ARG:HD3	5:I:443:HOH:O	1.72	0.89
1:L:212:MET:HG3	5:L:462:HOH:O	1.73	0.87
2:F:301:MTA:S5'	4:F:302:TER:H41	2.17	0.85
1:B:4:VAL:HG23	1:B:5:PRO:HD3	1.57	0.84
1:B:32:LYS:NZ	5:B:401:HOH:O	2.11	0.83
1:L:214:LEU:HD23	5:L:409:HOH:O	1.77	0.83
1:B:167:ASP:OD2	3:B:302:SPD:H52	1.80	0.82
2:G:301:MTA:S5'	4:G:302:TER:H42	2.18	0.82
1:C:180:ARG:HB2	1:C:180:ARG:CZ	2.09	0.81
1:I:20:LEU:HD23	1:L:20:LEU:HD23	1.60	0.81
1:I:31:LYS:HD2	1:I:119:LEU:HD11	1.63	0.80
1:D:212:MET:HE2	5:D:455:HOH:O	1.81	0.79
1:F:114[A]:ARG:NH2	5:F:402:HOH:O	2.14	0.79
1:D:209:GLU:OE2	5:D:402:HOH:O	2.02	0.77
1:I:150:GLU:OE2	5:I:401:HOH:O	2.04	0.76
1:A:20:LEU:HD23	1:F:20:LEU:HD23	1.68	0.75
1:J:83:ASP:OD2	1:J:106:ARG:HD3	1.88	0.74
1:H:234:PHE:O	3:H:302:SPD:H22	1.86	0.73
1:H:9:THR:HG21	1:H:21:LEU:HD22	1.69	0.73
1:C:167:ASP:OD2	3:C:302:SPD:H52	1.89	0.72
1:G:164:ASP:OD2	4:G:302:TER:N1	2.24	0.71
1:E:9:THR:HG21	1:E:21:LEU:HD22	1.72	0.71
1:G:9:THR:HG21	1:G:21:LEU:HD22	1.72	0.71
1:G:124:LEU:HD13	1:G:127:MET:HE2	1.74	0.69
1:A:118:GLU:OE1	5:A:401:HOH:O	2.10	0.69
1:E:124:LEU:HD13	1:E:127:MET:HE2	1.75	0.69
2:G:301:MTA:S5'	4:G:302:TER:C4	2.81	0.69
1:H:124:LEU:HD13	1:H:127:MET:HE2	1.75	0.69
1:H:267:LYS:HE3	5:H:484:HOH:O	1.94	0.68
1:J:124:LEU:HD13	1:J:127:MET:HE2	1.77	0.67
1:F:91:GLU:OE2	4:F:302:TER:H21	1.94	0.67
1:C:124:LEU:HB3	1:C:127:MET:HG3	1.76	0.66
1:B:20:LEU:HD23	1:E:20:LEU:CD2	2.26	0.66
1:G:12[B]:GLU:OE2	1:G:13:PRO:O	2.15	0.64
1:B:281:ASN:OD1	1:E:274:ARG:HD2	1.97	0.64
1:D:124:LEU:HD13	1:D:127:MET:HE2	1.79	0.64
1:G:91:GLU:OE2	4:G:302:TER:H21	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD13	1:A:127:MET:HE2	1.81	0.63
1:B:11:ILE:HD13	1:B:21:LEU:HD23	1.80	0.63
1:K:111:ASP:OD2	2:K:301:MTA:O3'	2.15	0.62
1:E:256:GLU:HB2	5:E:491:HOH:O	2.00	0.62
1:G:12[B]:GLU:OE2	4:G:302:TER:N14	2.34	0.61
1:I:31:LYS:CD	1:I:119:LEU:HD11	2.30	0.61
1:E:115:ASP:OD2	5:E:401:HOH:O	2.16	0.60
1:B:91:GLU:HG3	1:B:127:MET:HG2	1.84	0.59
1:F:56:ILE:O	4:F:302:TER:H102	2.02	0.59
1:B:252:LEU:CD1	5:B:481:HOH:O	2.50	0.58
1:K:211:ASP:O	1:K:215:GLU:OE1	2.22	0.58
1:I:190:LEU:HD11	1:I:196:VAL:HG22	1.86	0.57
1:J:91:GLU:HG3	1:J:127:MET:HG2	1.86	0.57
1:K:91:GLU:HG3	1:K:127:MET:HG2	1.86	0.56
1:I:202:ASN:HA	1:I:239:ASN:HD22	1.70	0.56
1:H:202:ASN:HA	1:H:239:ASN:HD22	1.71	0.56
1:L:190:LEU:HD11	1:L:196:VAL:HG22	1.86	0.56
1:I:91:GLU:HG3	1:I:127:MET:HG2	1.88	0.56
1:J:83:ASP:OD2	1:J:106:ARG:CD	2.52	0.56
1:L:202:ASN:HA	1:L:239:ASN:HD22	1.71	0.56
1:A:91:GLU:HG3	1:A:127:MET:HG2	1.87	0.55
1:C:202:ASN:HA	1:C:239:ASN:HD22	1.71	0.55
1:D:91:GLU:HG3	1:D:127:MET:HG2	1.87	0.55
1:F:190:LEU:HD11	1:F:196:VAL:HG22	1.88	0.55
1:A:164:ASP:O	2:A:301:MTA:H5'2	2.05	0.55
1:A:202:ASN:HA	1:A:239:ASN:HD22	1.71	0.55
1:J:202:ASN:HA	1:J:239:ASN:HD22	1.71	0.55
1:K:190:LEU:HD11	1:K:196:VAL:HG22	1.88	0.55
1:D:190:LEU:HD11	1:D:196:VAL:HG22	1.89	0.55
1:F:267:LYS:HE2	5:F:454:HOH:O	2.06	0.55
1:B:202:ASN:HA	1:B:239:ASN:HD22	1.71	0.55
1:D:202:ASN:HA	1:D:239:ASN:HD22	1.72	0.55
1:G:202:ASN:HA	1:G:239:ASN:HD22	1.70	0.55
1:A:271:TYR:OH	1:A:276:HIS:HD2	1.90	0.54
2:F:301:MTA:S5'	4:F:302:TER:C4	2.92	0.54
1:G:12[B]:GLU:OE1	4:G:302:TER:N14	2.41	0.54
1:L:111:ASP:OD1	2:L:301:MTA:H1'	2.07	0.54
1:B:259:GLU:OE1	1:B:262[B]:ARG:HD2	2.07	0.54
1:E:91:GLU:HG3	1:E:127:MET:HG2	1.90	0.54
1:F:91:GLU:HG3	1:F:127:MET:HG2	1.90	0.54
1:E:202:ASN:HA	1:E:239:ASN:HD22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:202:ASN:HA	1:K:239:ASN:HD22	1.72	0.54
1:A:57:GLN:NE2	3:A:302:SPD:H81	2.22	0.54
1:K:124:LEU:HD13	1:K:127:MET:HE2	1.90	0.53
1:F:202:ASN:HA	1:F:239:ASN:HD22	1.73	0.53
1:K:114:ARG:HE	1:K:141:ILE:HG13	1.73	0.53
1:B:11:ILE:HD13	1:B:21:LEU:HD21	1.86	0.53
1:J:111:ASP:OD1	2:J:301:MTA:H1'	2.09	0.53
1:B:176:GLN:HG3	1:I:246:ARG:HH11	1.67	0.53
1:G:91:GLU:HG3	1:G:127:MET:HG2	1.92	0.52
1:J:190:LEU:HD11	1:J:196:VAL:HG22	1.90	0.52
1:C:281:ASN:OD1	1:H:274:ARG:HD2	2.10	0.52
1:D:56:ILE:O	3:D:302:SPD:C5	2.57	0.52
1:E:236:TYR:CE2	4:E:302:TER:H131	2.45	0.52
1:E:271:TYR:OH	1:E:276:HIS:CD2	2.63	0.52
1:H:271:TYR:OH	1:H:276:HIS:HD2	1.92	0.52
1:H:145:PHE:CE2	1:H:176:GLN:HG3	2.45	0.52
1:L:271:TYR:OH	1:L:276:HIS:HD2	1.93	0.52
1:E:271:TYR:OH	1:E:276:HIS:HD2	1.92	0.52
1:H:91:GLU:HG3	1:H:127:MET:HG2	1.92	0.52
1:B:188:ARG:NH2	1:I:251:ALA:O	2.43	0.51
1:E:164:ASP:OD1	4:E:302:TER:H41	2.10	0.51
1:H:190:LEU:HD11	1:H:196:VAL:HG22	1.92	0.51
1:A:271:TYR:OH	1:A:276:HIS:CD2	2.63	0.51
1:G:271:TYR:OH	1:G:276:HIS:CD2	2.63	0.51
1:G:271:TYR:OH	1:G:276:HIS:HD2	1.92	0.51
1:K:190:LEU:HD11	1:K:196:VAL:CG2	2.41	0.51
1:C:271:TYR:OH	1:C:276:HIS:HD2	1.94	0.51
1:C:271:TYR:OH	1:C:276:HIS:CD2	2.64	0.51
1:B:82:ARG:HG2	5:B:444:HOH:O	2.10	0.51
1:B:124:LEU:HD13	1:B:127:MET:HE2	1.91	0.51
1:B:271:TYR:OH	1:B:276:HIS:HD2	1.94	0.51
1:F:190:LEU:HD11	1:F:196:VAL:CG2	2.40	0.51
1:I:124:LEU:HD13	1:I:127:MET:HE2	1.91	0.51
1:I:190:LEU:HD11	1:I:196:VAL:CG2	2.41	0.51
1:L:91:GLU:HG3	1:L:127:MET:HG2	1.93	0.51
1:L:271:TYR:OH	1:L:276:HIS:CD2	2.64	0.51
1:B:106:ARG:HG3	5:B:457:HOH:O	2.10	0.51
1:H:252:LEU:HD11	5:H:444:HOH:O	2.10	0.51
1:J:83:ASP:OD2	1:J:106:ARG:CZ	2.59	0.51
1:F:271:TYR:OH	1:F:276:HIS:CD2	2.65	0.50
1:J:271:TYR:OH	1:J:276:HIS:CD2	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:O	3:B:302:SPD:H51	2.12	0.50
1:F:124:LEU:HD13	1:F:127:MET:HE2	1.93	0.50
1:H:271:TYR:OH	1:H:276:HIS:CD2	2.63	0.50
1:L:124:LEU:HD13	1:L:127:MET:HE2	1.94	0.50
1:B:271:TYR:OH	1:B:276:HIS:CD2	2.64	0.50
1:I:114:ARG:O	1:I:118:GLU:HG2	2.11	0.50
1:D:271:TYR:OH	1:D:276:HIS:CD2	2.65	0.49
1:I:271:TYR:OH	1:I:276:HIS:CD2	2.65	0.49
1:J:190:LEU:HD11	1:J:196:VAL:CG2	2.42	0.49
1:B:222:PRO:O	1:H:262:ARG:NH2	2.46	0.49
1:K:271:TYR:OH	1:K:276:HIS:CD2	2.65	0.49
1:D:8:ILE:HG21	1:E:27:ILE:HD11	1.93	0.49
1:F:271:TYR:OH	1:F:276:HIS:HD2	1.95	0.49
1:K:271:TYR:OH	1:K:276:HIS:HD2	1.96	0.49
1:C:249:PRO:O	1:C:276:HIS:HE1	1.96	0.49
1:F:234:PHE:O	4:F:302:TER:H131	2.13	0.49
1:C:14:LEU:HD22	1:C:20:LEU:HD11	1.94	0.49
1:D:91:GLU:HG3	1:D:127:MET:HE3	1.95	0.49
1:F:66:TYR:CE2	4:F:302:TER:H32	2.48	0.48
1:D:56:ILE:O	3:D:302:SPD:H52	2.12	0.48
1:D:249:PRO:O	1:D:276:HIS:HE1	1.96	0.48
1:E:168:PRO:HA	5:E:428:HOH:O	2.12	0.48
1:J:249:PRO:O	1:J:276:HIS:HE1	1.96	0.48
1:J:91:GLU:HG3	1:J:127:MET:HE3	1.95	0.48
1:B:176:GLN:CG	1:I:246:ARG:NH1	2.65	0.48
1:J:83:ASP:OD2	1:J:106:ARG:NE	2.47	0.48
1:D:271:TYR:OH	1:D:276:HIS:HD2	1.97	0.48
1:H:91:GLU:HG3	1:H:127:MET:HE3	1.96	0.48
1:H:190:LEU:HD11	1:H:196:VAL:CG2	2.43	0.48
1:L:190:LEU:HD11	1:L:196:VAL:CG2	2.43	0.48
1:G:12[B]:GLU:CD	4:G:302:TER:N14	2.68	0.48
1:L:249:PRO:O	1:L:276:HIS:HE1	1.97	0.48
1:D:27:ILE:HG13	1:E:27:ILE:HD12	1.95	0.47
1:B:236:TYR:HA	1:E:230:TRP:CZ2	2.50	0.47
1:G:249:PRO:O	1:G:276:HIS:HE1	1.97	0.47
1:I:68:GLU:OE2	5:I:402:HOH:O	2.20	0.47
1:I:134:ASP:OD1	5:I:403:HOH:O	2.20	0.47
1:C:56:ILE:O	3:C:302:SPD:H51	2.14	0.47
1:A:193:ASP:HB2	1:A:247:TYR:CE2	2.49	0.47
1:G:91:GLU:HG3	1:G:127:MET:HE3	1.97	0.47
1:I:249:PRO:O	1:I:276:HIS:HE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:GLU:HB2	5:K:428:HOH:O	2.14	0.47
1:A:91:GLU:HG3	1:A:127:MET:HE3	1.97	0.47
1:D:190:LEU:HD11	1:D:196:VAL:CG2	2.44	0.47
1:E:249:PRO:O	1:E:276:HIS:HE1	1.98	0.47
1:H:249:PRO:O	1:H:276:HIS:HE1	1.98	0.46
1:K:249:PRO:O	1:K:276:HIS:HE1	1.98	0.46
1:F:249:PRO:O	1:F:276:HIS:HE1	1.98	0.46
1:A:286:ARG:HD2	5:A:463:HOH:O	2.14	0.46
1:J:271:TYR:OH	1:J:276:HIS:HD2	1.97	0.46
1:H:12:GLU:OE2	3:H:302:SPD:H32	2.16	0.46
1:B:20:LEU:CD2	1:E:20:LEU:CD2	2.92	0.46
1:I:20:LEU:CD2	1:L:20:LEU:HD23	2.41	0.46
1:D:165:LEU:HB2	5:D:412:HOH:O	2.15	0.45
1:F:57:GLN:HE21	4:F:302:TER:H42	1.81	0.45
1:A:249:PRO:O	1:A:276:HIS:HE1	1.98	0.45
1:B:4:VAL:CG2	1:B:5:PRO:HD3	2.38	0.45
1:I:93:ALA:HB2	1:I:127:MET:HG3	1.98	0.45
1:F:212:MET:HB3	5:F:459:HOH:O	2.15	0.45
1:E:164:ASP:OD1	4:E:302:TER:C4	2.65	0.45
1:B:249:PRO:O	1:B:276:HIS:HE1	1.99	0.45
1:F:91:GLU:OE1	4:F:302:TER:N1	2.50	0.45
1:A:236:TYR:HA	1:F:230:TRP:CZ2	2.52	0.45
1:C:215:GLU:HB3	5:C:470:HOH:O	2.17	0.44
1:B:20:LEU:CD2	1:E:20:LEU:HD23	2.35	0.44
1:E:9:THR:HG21	1:E:21:LEU:CD2	2.44	0.44
1:C:21:LEU:O	1:H:18:THR:HA	2.17	0.44
1:I:134:ASP:CG	5:I:403:HOH:O	2.55	0.44
1:L:228:GLU:OE2	1:L:285:HIS:ND1	2.48	0.44
1:K:255:SER:O	1:K:259:GLU:OE1	2.35	0.44
1:E:203:SER:H	1:E:239:ASN:ND2	2.16	0.44
1:G:9:THR:HG21	1:G:21:LEU:CD2	2.45	0.44
1:A:20:LEU:HD23	1:F:20:LEU:CD2	2.45	0.44
1:B:93:ALA:HB2	1:B:127:MET:HG3	1.98	0.44
1:I:32:LYS:HD3	5:I:462:HOH:O	2.18	0.44
1:F:180:ARG:HG3	1:F:216:GLY:HA2	2.00	0.43
1:I:271:TYR:OH	1:I:276:HIS:HD2	1.99	0.43
2:G:301:MTA:S5'	4:G:302:TER:H41	2.57	0.43
1:B:60:TYR:CZ	1:B:126:GLN:HB2	2.53	0.43
1:C:60:TYR:CZ	1:C:126:GLN:HB2	2.54	0.43
1:E:91:GLU:HG3	1:E:127:MET:HE3	2.00	0.43
1:H:124:LEU:HD13	1:H:127:MET:CE	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:TYR:CZ	1:D:126:GLN:HB2	2.53	0.43
1:D:93:ALA:HB2	1:D:127:MET:HG3	1.99	0.43
1:I:37:GLU:OE2	5:I:404:HOH:O	2.21	0.43
1:F:124:LEU:HD13	1:F:127:MET:CE	2.49	0.43
1:E:106:ARG:CD	5:E:407:HOH:O	2.66	0.43
1:D:3:LYS:HD2	1:D:3:LYS:N	2.33	0.43
1:G:199:GLN:NE2	1:G:201:GLY:H	2.17	0.43
1:C:236:TYR:HA	1:H:230:TRP:CZ2	2.54	0.43
1:G:124:LEU:HD13	1:G:127:MET:CE	2.47	0.43
1:K:60:TYR:CZ	1:K:126:GLN:HB2	2.54	0.43
1:I:20:LEU:HD23	1:L:20:LEU:CD2	2.41	0.43
1:L:141:ILE:HB	5:L:401:HOH:O	2.19	0.43
1:D:199:GLN:NE2	1:D:201:GLY:H	2.17	0.42
1:J:199:GLN:NE2	1:J:201:GLY:H	2.17	0.42
1:K:4:VAL:N	1:K:5:PRO:HD3	2.34	0.42
1:B:165:LEU:O	3:B:302:SPD:N10	2.46	0.42
1:D:56:ILE:O	3:D:302:SPD:H51	2.19	0.42
1:I:124:LEU:HD13	1:I:127:MET:CE	2.50	0.42
1:L:203:SER:H	1:L:239:ASN:ND2	2.17	0.42
1:A:203:SER:H	1:A:239:ASN:ND2	2.17	0.42
1:C:199:GLN:NE2	1:C:201:GLY:H	2.17	0.42
1:K:199:GLN:NE2	1:K:201:GLY:H	2.17	0.42
1:B:91:GLU:CG	1:B:127:MET:HG2	2.49	0.42
1:B:124:LEU:HD13	1:B:127:MET:CE	2.50	0.42
1:L:124:LEU:HD13	1:L:127:MET:CE	2.49	0.42
1:L:199:GLN:NE2	1:L:201:GLY:H	2.18	0.42
1:D:2:ARG:HD3	1:D:2:ARG:C	2.40	0.42
1:E:124:LEU:HD13	1:E:127:MET:CE	2.46	0.42
1:G:164:ASP:OD1	4:G:302:TER:H41	2.20	0.42
1:H:199:GLN:NE2	1:H:201:GLY:H	2.18	0.42
1:I:153:LYS:HA	1:I:153:LYS:HD3	1.62	0.42
1:B:199:GLN:NE2	1:B:201:GLY:H	2.17	0.42
1:F:199:GLN:NE2	1:F:201:GLY:H	2.18	0.42
1:K:91:GLU:CG	1:K:127:MET:HG2	2.50	0.42
1:L:93:ALA:HB2	1:L:127:MET:HG3	2.01	0.42
1:I:4:VAL:HA	1:I:5:PRO:HD3	1.95	0.42
1:A:93:ALA:HB2	1:A:127:MET:HG3	2.01	0.42
1:B:21:LEU:O	1:E:18:THR:HA	2.20	0.42
2:E:301:MTA:S5'	4:E:302:TER:H31	2.60	0.42
1:F:60:TYR:CZ	1:F:126:GLN:HB2	2.55	0.42
1:B:203:SER:H	1:B:239:ASN:ND2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:ARG:NE	5:E:407:HOH:O	2.46	0.41
1:E:228:GLU:OE2	1:E:285:HIS:ND1	2.49	0.41
1:H:60:TYR:CZ	1:H:126:GLN:HB2	2.55	0.41
1:I:32:LYS:HD3	5:I:467:HOH:O	2.20	0.41
1:A:199:GLN:NE2	1:A:201:GLY:H	2.18	0.41
5:G:505:HOH:O	1:K:222:PRO:HB3	2.19	0.41
1:H:230:TRP:HA	1:H:237:ALA:HA	2.02	0.41
1:I:60:TYR:CZ	1:I:126:GLN:HB2	2.55	0.41
1:D:203:SER:H	1:D:239:ASN:ND2	2.18	0.41
1:D:212:MET:HE3	1:D:212:MET:HB3	1.80	0.41
1:E:60:TYR:CZ	1:E:126:GLN:HB2	2.56	0.41
2:E:301:MTA:S5'	4:E:302:TER:H42	2.60	0.41
1:F:203:SER:H	1:F:239:ASN:ND2	2.17	0.41
1:I:203:SER:H	1:I:239:ASN:ND2	2.17	0.41
1:B:253:THR:OG1	1:B:256:GLU:HG3	2.20	0.41
1:D:91:GLU:CG	1:D:127:MET:HG2	2.49	0.41
1:J:203:SER:H	1:J:239:ASN:ND2	2.18	0.41
1:I:199:GLN:NE2	1:I:201:GLY:H	2.18	0.41
1:K:203:SER:H	1:K:239:ASN:ND2	2.17	0.41
1:G:203:SER:H	1:G:239:ASN:ND2	2.17	0.41
1:K:230:TRP:HA	1:K:237:ALA:HA	2.03	0.41
1:A:91:GLU:CG	1:A:127:MET:HG2	2.51	0.41
1:E:199:GLN:NE2	1:E:201:GLY:H	2.19	0.41
1:J:230:TRP:HA	1:J:237:ALA:HA	2.02	0.41
1:F:230:TRP:HA	1:F:237:ALA:HA	2.03	0.41
1:G:93:ALA:HB2	1:G:127:MET:HG3	2.03	0.41
1:H:106:ARG:HG3	5:H:496:HOH:O	2.21	0.41
1:D:230:TRP:HA	1:D:237:ALA:HA	2.03	0.41
1:E:234:PHE:CE2	4:E:302:TER:H82	2.56	0.41
1:I:91:GLU:CG	1:I:127:MET:HG2	2.51	0.41
1:A:23:LYS:HD2	1:F:17:ASN:HD22	1.86	0.40
1:D:123:TYR:CE1	1:G:34:PRO:HG3	2.56	0.40
1:E:230:TRP:HA	1:E:237:ALA:HA	2.03	0.40
1:G:230:TRP:HA	1:G:237:ALA:HA	2.04	0.40
1:I:21:LEU:O	1:L:18:THR:HA	2.21	0.40
1:C:203:SER:H	1:C:239:ASN:ND2	2.19	0.40
1:E:252:LEU:HD13	5:E:413:HOH:O	2.21	0.40
1:F:203:SER:OG	1:F:239:ASN:OD1	2.39	0.40
1:H:93:ALA:HB2	1:H:127:MET:HG3	2.04	0.40
1:H:203:SER:H	1:H:239:ASN:ND2	2.18	0.40
1:B:149:GLU:OE2	1:B:185:LYS:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:TYR:CZ	1:J:126:GLN:HB2	2.56	0.40
1:K:93:ALA:HB2	1:K:127:MET:HG3	2.03	0.40
1:L:230:TRP:HA	1:L:237:ALA:HA	2.03	0.40
1:K:124:LEU:HD13	1:K:127:MET:CE	2.51	0.40

All (1) 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)
5:J:432:HOH:O	5:L:460:HOH:O[2_445]	2.17	0.03

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	285/309 (92%)	278 (98%)	7 (2%)	0	100	100
1	B	285/309 (92%)	278 (98%)	7 (2%)	0	100	100
1	C	284/309 (92%)	278 (98%)	6 (2%)	0	100	100
1	D	287/309 (93%)	281 (98%)	6 (2%)	0	100	100
1	E	285/309 (92%)	279 (98%)	6 (2%)	0	100	100
1	F	285/309 (92%)	279 (98%)	6 (2%)	0	100	100
1	G	286/309 (93%)	280 (98%)	6 (2%)	0	100	100
1	H	285/309 (92%)	279 (98%)	6 (2%)	0	100	100
1	I	284/309 (92%)	278 (98%)	6 (2%)	0	100	100
1	J	284/309 (92%)	278 (98%)	6 (2%)	0	100	100
1	K	284/309 (92%)	278 (98%)	6 (2%)	0	100	100
1	L	285/309 (92%)	279 (98%)	6 (2%)	0	100	100
All	All	3419/3708 (92%)	3345 (98%)	74 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/265 (93%)	237 (96%)	9 (4%)	34	31
1	B	246/265 (93%)	233 (95%)	13 (5%)	22	18
1	C	245/265 (92%)	237 (97%)	8 (3%)	38	35
1	D	248/265 (94%)	234 (94%)	14 (6%)	21	16
1	E	246/265 (93%)	234 (95%)	12 (5%)	25	20
1	F	246/265 (93%)	233 (95%)	13 (5%)	22	18
1	G	247/265 (93%)	238 (96%)	9 (4%)	35	32
1	H	246/265 (93%)	235 (96%)	11 (4%)	27	23
1	I	245/265 (92%)	238 (97%)	7 (3%)	42	40
1	J	245/265 (92%)	235 (96%)	10 (4%)	30	27
1	K	245/265 (92%)	233 (95%)	12 (5%)	25	20
1	L	246/265 (93%)	233 (95%)	13 (5%)	22	18
All	All	2951/3180 (93%)	2820 (96%)	131 (4%)	29	24

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	32	LYS
1	A	42	ASP
1	A	126	GLN
1	A	127	MET
1	A	195	VAL
1	A	199	GLN
1	A	215	GLU
1	A	236	TYR
1	B	32	LYS
1	B	33	SER

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Mol	Chain	Res	Type
1	B	42	ASP
1	B	58	SER
1	B	127	MET
1	B	153	LYS
1	B	181	GLU
1	B	195	VAL
1	B	199	GLN
1	B	215	GLU
1	B	236	TYR
1	B	262[A]	ARG
1	B	262[B]	ARG
1	C	31	LYS
1	C	32	LYS
1	C	33	SER
1	C	58	SER
1	C	199	GLN
1	C	215	GLU
1	C	236	TYR
1	C	262	ARG
1	D	2	ARG
1	D	3	LYS
1	D	31	LYS
1	D	32	LYS
1	D	33	SER
1	D	37	GLU
1	D	58[A]	SER
1	D	58[B]	SER
1	D	127	MET
1	D	153	LYS
1	D	175	LYS
1	D	199	GLN
1	D	236	TYR
1	D	262	ARG
1	E	31	LYS
1	E	32	LYS
1	E	33	SER
1	E	114[A]	ARG
1	E	114[B]	ARG
1	E	127	MET
1	E	180	ARG
1	E	195	VAL
1	E	199	GLN

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Mol	Chain	Res	Type
1	E	215	GLU
1	E	236	TYR
1	E	262	ARG
1	F	31	LYS
1	F	33	SER
1	F	58	SER
1	F	114[A]	ARG
1	F	114[B]	ARG
1	F	127	MET
1	F	180	ARG
1	F	195	VAL
1	F	199	GLN
1	F	203	SER
1	F	215	GLU
1	F	236	TYR
1	F	262	ARG
1	G	31	LYS
1	G	33	SER
1	G	114	ARG
1	G	127	MET
1	G	195	VAL
1	G	199	GLN
1	G	212	MET
1	G	215	GLU
1	G	236	TYR
1	H	31	LYS
1	H	32	LYS
1	H	58[A]	SER
1	H	58[B]	SER
1	H	114	ARG
1	H	127	MET
1	H	172	ASP
1	H	195	VAL
1	H	199	GLN
1	H	236	TYR
1	H	262	ARG
1	I	32	LYS
1	I	58	SER
1	I	127	MET
1	I	195	VAL
1	I	199	GLN
1	I	215	GLU

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Mol	Chain	Res	Type
1	I	236	TYR
1	J	31	LYS
1	J	32	LYS
1	J	106	ARG
1	J	127	MET
1	J	195	VAL
1	J	199	GLN
1	J	215	GLU
1	J	236	TYR
1	J	255	SER
1	J	259	GLU
1	K	4	VAL
1	K	31	LYS
1	K	32	LYS
1	K	58	SER
1	K	114	ARG
1	K	127	MET
1	K	175	LYS
1	K	180	ARG
1	K	195	VAL
1	K	199	GLN
1	K	236	TYR
1	K	247	TYR
1	L	31	LYS
1	L	32	LYS
1	L	42	ASP
1	L	58	SER
1	L	127	MET
1	L	172	ASP
1	L	175	LYS
1	L	192	ASP
1	L	195	VAL
1	L	199	GLN
1	L	215	GLU
1	L	236	TYR
1	L	262	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	57	GLN

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Mol	Chain	Res	Type
1	A	129	GLN
1	A	191	ASN
1	A	199	GLN
1	A	239	ASN
1	A	276	HIS
1	B	36	GLN
1	B	129	GLN
1	B	191	ASN
1	B	199	GLN
1	B	239	ASN
1	B	276	HIS
1	C	36	GLN
1	C	57	GLN
1	C	129	GLN
1	C	191	ASN
1	C	199	GLN
1	C	239	ASN
1	C	276	HIS
1	D	36	GLN
1	D	191	ASN
1	D	199	GLN
1	D	239	ASN
1	D	276	HIS
1	E	36	GLN
1	E	129	GLN
1	E	191	ASN
1	E	199	GLN
1	E	239	ASN
1	E	276	HIS
1	F	17	ASN
1	F	36	GLN
1	F	57	GLN
1	F	129	GLN
1	F	176	GLN
1	F	191	ASN
1	F	199	GLN
1	F	239	ASN
1	F	276	HIS
1	G	36	GLN
1	G	129	GLN
1	G	191	ASN
1	G	199	GLN

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Mol	Chain	Res	Type
1	G	239	ASN
1	G	276	HIS
1	H	17	ASN
1	H	36	GLN
1	H	126	GLN
1	H	129	GLN
1	H	191	ASN
1	H	199	GLN
1	H	239	ASN
1	H	276	HIS
1	I	36	GLN
1	I	129	GLN
1	I	191	ASN
1	I	199	GLN
1	I	239	ASN
1	I	276	HIS
1	J	36	GLN
1	J	129	GLN
1	J	191	ASN
1	J	199	GLN
1	J	239	ASN
1	J	276	HIS
1	K	36	GLN
1	K	129	GLN
1	K	191	ASN
1	K	199	GLN
1	K	239	ASN
1	K	276	HIS
1	L	36	GLN
1	L	57	GLN
1	L	129	GLN
1	L	176	GLN
1	L	191	ASN
1	L	199	GLN
1	L	239	ASN
1	L	276	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
3	SPD	H	302	-	9,9,9	0.42	0	8,8,8	0.29	0
2	MTA	E	301	-	19,22,22	0.70	0	19,32,32	1.50	3 (15%)
2	MTA	H	301	-	19,22,22	0.87	1 (5%)	19,32,32	1.02	1 (5%)
2	MTA	D	301	-	19,22,22	0.74	1 (5%)	19,32,32	1.22	1 (5%)
2	MTA	J	301	-	19,22,22	0.63	0	19,32,32	1.24	2 (10%)
4	TER	G	302	-	13,13,13	0.37	0	12,12,12	0.88	0
3	SPD	A	302	-	9,9,9	0.54	0	8,8,8	0.34	0
4	TER	E	302	-	13,13,13	0.23	0	12,12,12	0.48	0
2	MTA	K	301	-	19,22,22	0.69	0	19,32,32	1.18	2 (10%)
4	TER	F	302	-	13,13,13	0.26	0	12,12,12	0.75	0
2	MTA	I	301	-	19,22,22	0.72	0	19,32,32	1.14	1 (5%)
3	SPD	B	302	-	9,9,9	0.36	0	8,8,8	0.29	0
3	SPD	D	302	-	9,9,9	0.25	0	8,8,8	0.75	0
2	MTA	F	301	-	19,22,22	1.17	1 (5%)	19,32,32	1.45	4 (21%)
2	MTA	B	301	-	19,22,22	0.80	1 (5%)	19,32,32	1.19	2 (10%)
2	MTA	A	301	-	19,22,22	0.77	1 (5%)	19,32,32	1.28	3 (15%)
2	MTA	G	301	-	19,22,22	0.75	0	19,32,32	0.96	0
3	SPD	C	302	-	9,9,9	0.59	0	8,8,8	0.63	0
2	MTA	C	301	-	19,22,22	0.68	0	19,32,32	1.20	2 (10%)
2	MTA	L	301	-	19,22,22	0.84	2 (10%)	19,32,32	1.19	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SPD	H	302	-	-	4/7/7/7	-
2	MTA	E	301	-	-	2/3/23/23	0/3/3/3
2	MTA	H	301	-	-	2/3/23/23	0/3/3/3
2	MTA	D	301	-	-	0/3/23/23	0/3/3/3
2	MTA	J	301	-	-	2/3/23/23	0/3/3/3
4	TER	G	302	-	-	7/11/11/11	-
3	SPD	A	302	-	-	1/7/7/7	-
4	TER	E	302	-	-	5/11/11/11	-
2	MTA	K	301	-	-	2/3/23/23	0/3/3/3
4	TER	F	302	-	-	5/11/11/11	-
2	MTA	I	301	-	-	2/3/23/23	0/3/3/3
3	SPD	B	302	-	-	2/7/7/7	-
3	SPD	D	302	-	-	4/7/7/7	-
2	MTA	F	301	-	-	0/3/23/23	0/3/3/3
2	MTA	B	301	-	-	2/3/23/23	0/3/3/3
2	MTA	A	301	-	-	0/3/23/23	0/3/3/3
2	MTA	G	301	-	-	2/3/23/23	0/3/3/3
3	SPD	C	302	-	-	3/7/7/7	-
2	MTA	C	301	-	-	2/3/23/23	0/3/3/3
2	MTA	L	301	-	-	2/3/23/23	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	MTA	C5'-S5'	4.16	1.86	1.80
2	H	301	MTA	C8-N7	-2.35	1.30	1.34
2	B	301	MTA	C8-N7	-2.13	1.30	1.34
2	L	301	MTA	C5'-S5'	2.11	1.83	1.80
2	D	301	MTA	C8-N7	-2.06	1.31	1.34
2	L	301	MTA	C8-N7	-2.06	1.31	1.34
2	A	301	MTA	C8-N7	-2.04	1.31	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	301	MTA	C5-C6-N6	3.63	125.86	120.35
2	I	301	MTA	C5-C6-N6	3.31	125.38	120.35
2	F	301	MTA	O3'-C3'-C4'	-3.27	101.59	111.05
2	E	301	MTA	C5-C6-N6	3.11	125.08	120.35
2	J	301	MTA	CS-S5'-C5'	2.97	106.77	101.30
2	E	301	MTA	O4'-C1'-C2'	-2.86	102.74	106.93
2	C	301	MTA	C5-C6-N6	2.86	124.70	120.35
2	E	301	MTA	CS-S5'-C5'	2.79	106.42	101.30
2	D	301	MTA	CS-S5'-C5'	-2.76	96.22	101.30
2	J	301	MTA	C5-C6-N6	2.67	124.41	120.35
2	B	301	MTA	C5-C6-N6	2.55	124.22	120.35
2	A	301	MTA	O4'-C1'-C2'	-2.51	103.26	106.93
2	A	301	MTA	C5-C6-N6	2.47	124.11	120.35
2	H	301	MTA	O4'-C1'-C2'	-2.44	103.36	106.93
2	C	301	MTA	O4'-C1'-C2'	-2.43	103.38	106.93
2	F	301	MTA	C4-C5-N7	2.41	111.91	109.40
2	F	301	MTA	O3'-C3'-C2'	2.41	119.62	111.82
2	A	301	MTA	O3'-C3'-C4'	-2.40	104.11	111.05
2	B	301	MTA	CS-S5'-C5'	-2.18	97.28	101.30
2	F	301	MTA	O4'-C1'-C2'	-2.17	103.76	106.93
2	K	301	MTA	O4'-C1'-C2'	-2.09	103.88	106.93
2	K	301	MTA	C5-C6-N6	2.07	123.49	120.35

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	MTA	O4'-C4'-C5'-S5'
2	B	301	MTA	C3'-C4'-C5'-S5'
2	E	301	MTA	O4'-C4'-C5'-S5'
2	E	301	MTA	C3'-C4'-C5'-S5'
2	I	301	MTA	O4'-C4'-C5'-S5'
2	I	301	MTA	C3'-C4'-C5'-S5'
2	J	301	MTA	O4'-C4'-C5'-S5'
2	J	301	MTA	C3'-C4'-C5'-S5'
2	L	301	MTA	C3'-C4'-C5'-S5'
4	F	302	TER	C3-C4-N5-C6
4	G	302	TER	C3-C4-N5-C6
3	H	302	SPD	C3-C4-C5-N6
4	G	302	TER	N9-C10-C11-C12
4	E	302	TER	C2-C3-C4-N5
4	G	302	TER	C2-C3-C4-N5
4	G	302	TER	C6-C7-C8-N9

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Mol	Chain	Res	Type	Atoms
4	F	302	TER	C11-C10-N9-C8
4	G	302	TER	C7-C6-N5-C4
4	E	302	TER	N5-C6-C7-C8
3	D	302	SPD	C8-C7-N6-C5
4	E	302	TER	C11-C12-C13-N14
3	C	302	SPD	N6-C7-C8-C9
3	H	302	SPD	C2-C3-C4-C5
3	A	302	SPD	C7-C8-C9-N10
3	D	302	SPD	C7-C8-C9-N10
3	H	302	SPD	C7-C8-C9-N10
3	D	302	SPD	C3-C4-C5-N6
4	G	302	TER	C11-C12-C13-N14
4	E	302	TER	C7-C6-N5-C4
4	E	302	TER	C10-C11-C12-C13
3	H	302	SPD	N1-C2-C3-C4
3	B	302	SPD	N6-C7-C8-C9
4	F	302	TER	C6-C7-C8-N9
3	D	302	SPD	C4-C5-N6-C7
3	C	302	SPD	C7-C8-C9-N10
2	C	301	MTA	C3'-C4'-C5'-S5'
2	G	301	MTA	C3'-C4'-C5'-S5'
2	H	301	MTA	C3'-C4'-C5'-S5'
2	K	301	MTA	C3'-C4'-C5'-S5'
4	F	302	TER	C7-C8-N9-C10
2	C	301	MTA	O4'-C4'-C5'-S5'
2	G	301	MTA	O4'-C4'-C5'-S5'
2	H	301	MTA	O4'-C4'-C5'-S5'
2	K	301	MTA	O4'-C4'-C5'-S5'
2	L	301	MTA	O4'-C4'-C5'-S5'
4	G	302	TER	N1-C2-C3-C4
4	F	302	TER	C2-C3-C4-N5
3	B	302	SPD	C7-C8-C9-N10
3	C	302	SPD	C2-C3-C4-C5

There are no ring outliers.

15 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	302	SPD	2	0
2	E	301	MTA	2	0
2	J	301	MTA	1	0
4	G	302	TER	9	0

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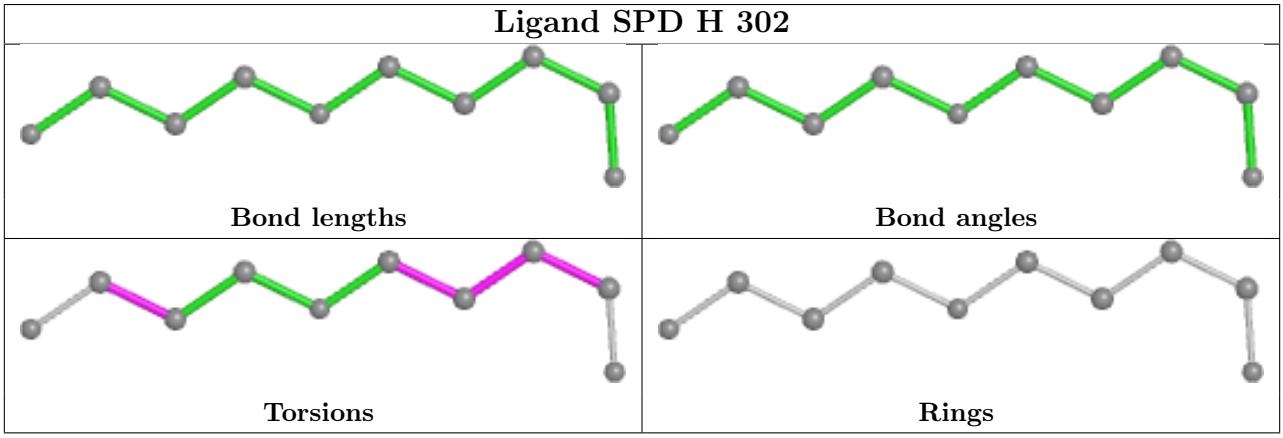
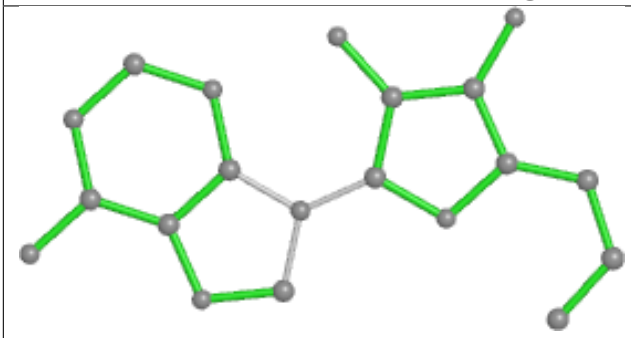
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	SPD	1	0
4	E	302	TER	6	0
2	K	301	MTA	1	0
4	F	302	TER	8	0
3	B	302	SPD	3	0
3	D	302	SPD	3	0
2	F	301	MTA	2	0
2	A	301	MTA	1	0
2	G	301	MTA	3	0
3	C	302	SPD	2	0
2	L	301	MTA	1	0

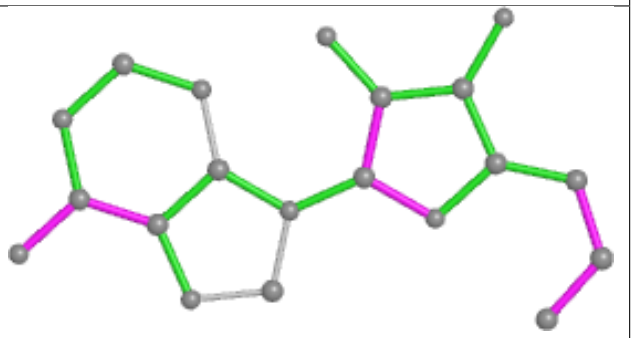
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



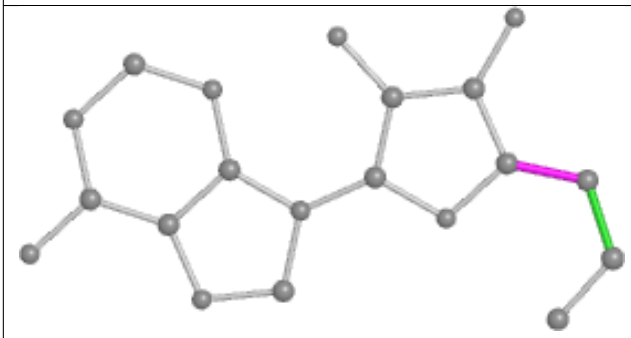
Ligand MTA E 301



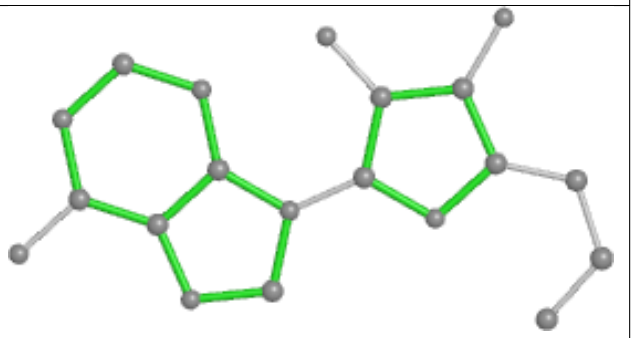
Bond lengths



Bond angles

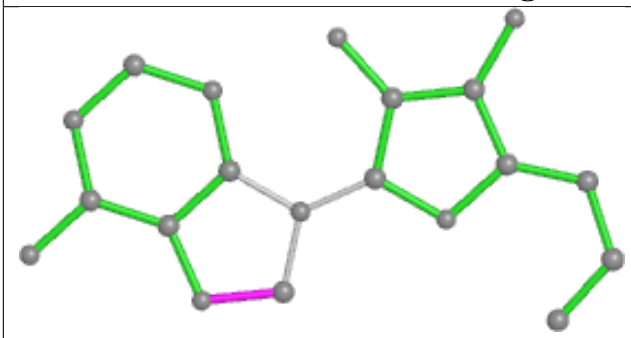


Torsions

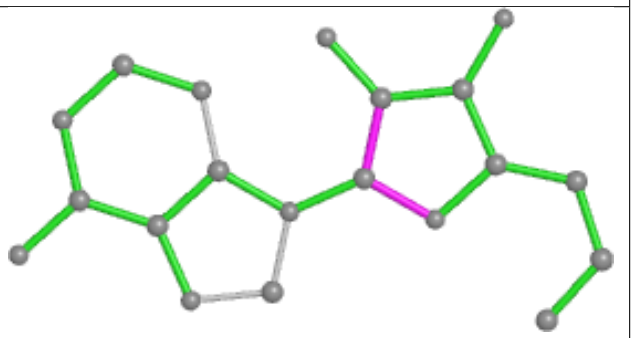


Rings

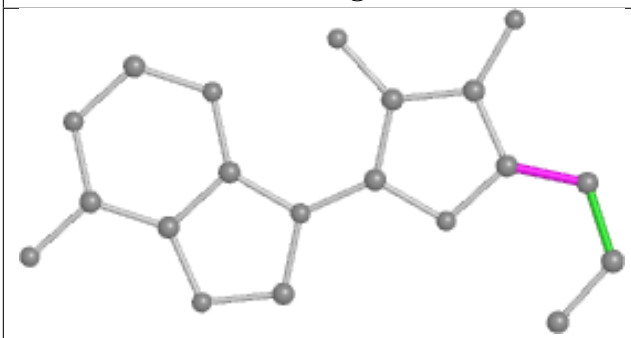
Ligand MTA H 301



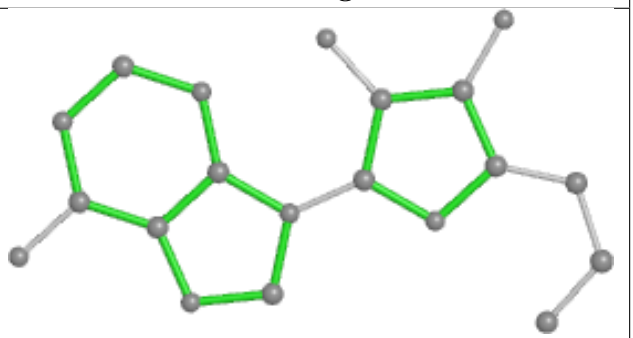
Bond lengths



Bond angles

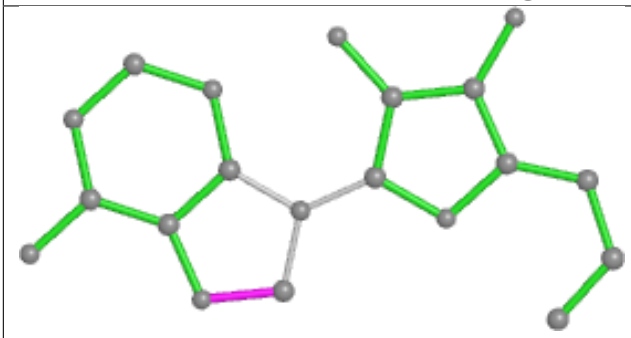


Torsions

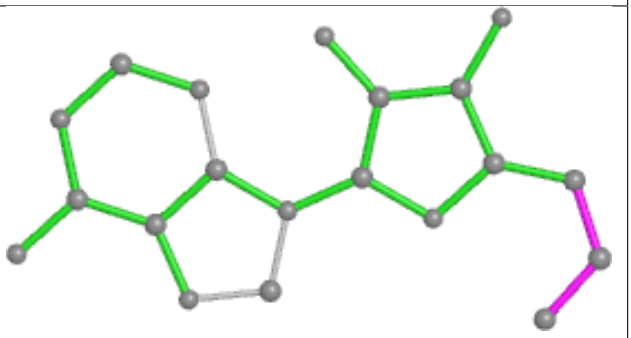


Rings

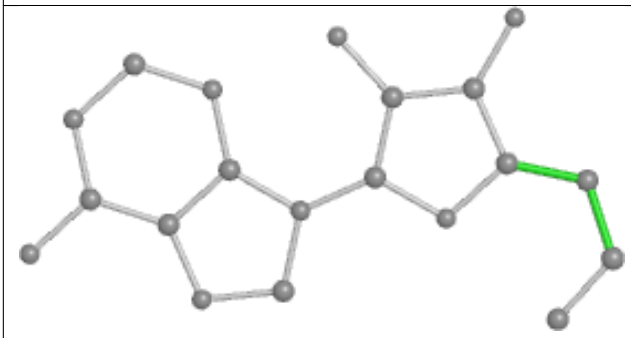
Ligand MTA D 301



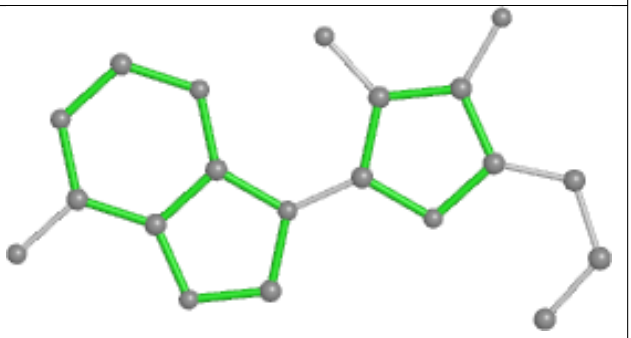
Bond lengths



Bond angles

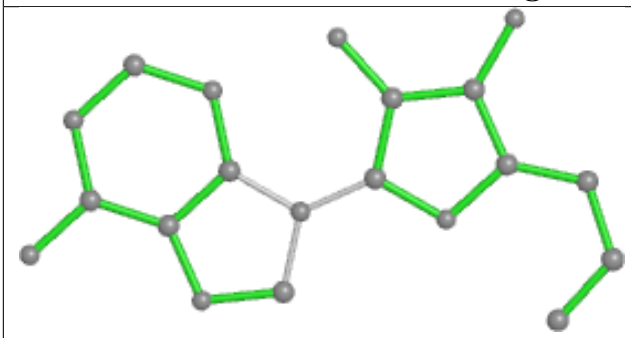


Torsions

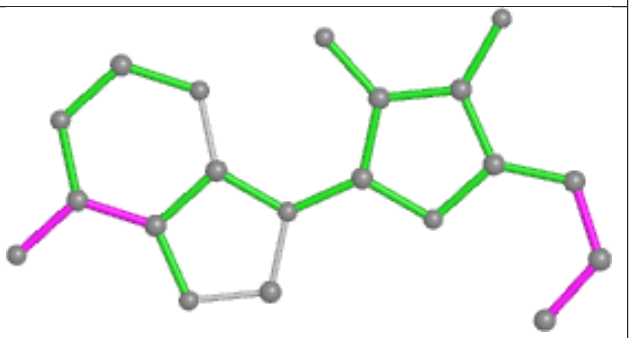


Rings

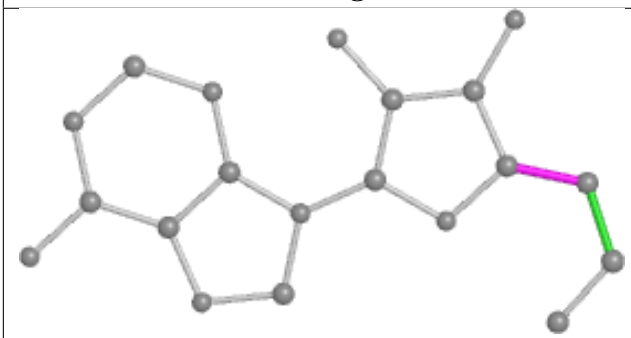
Ligand MTA J 301



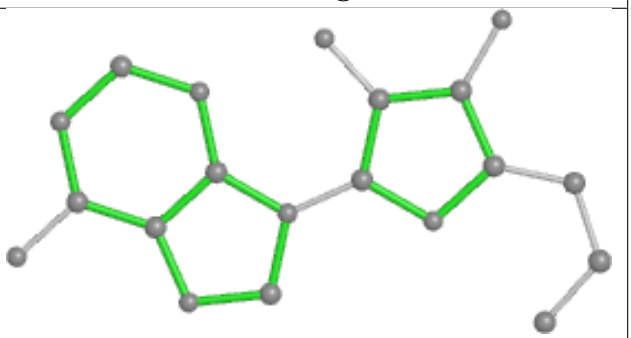
Bond lengths



Bond angles

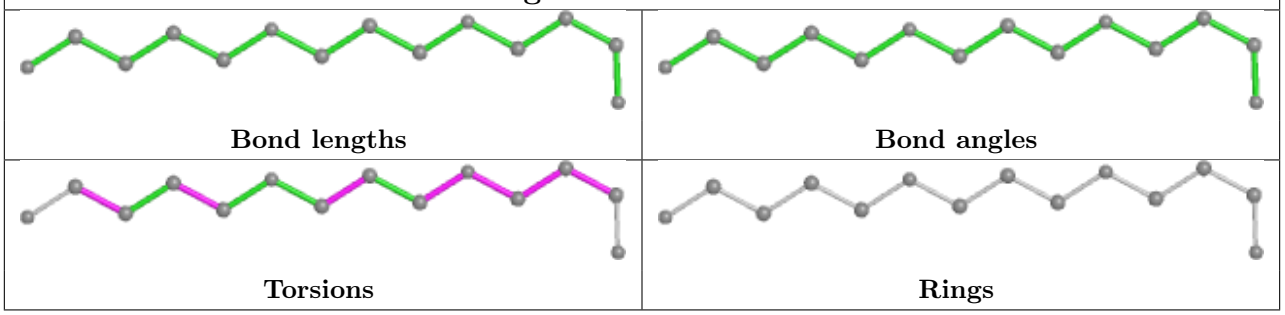


Torsions

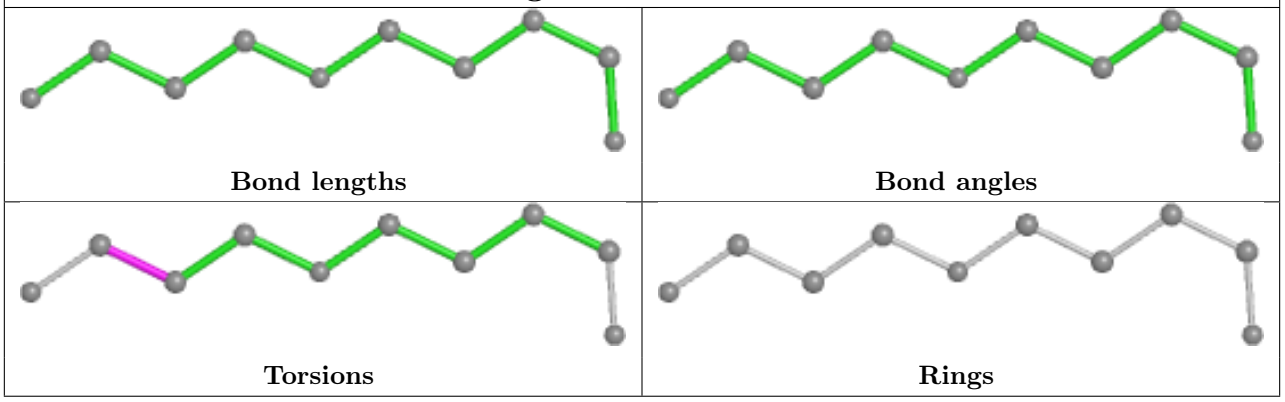


Rings

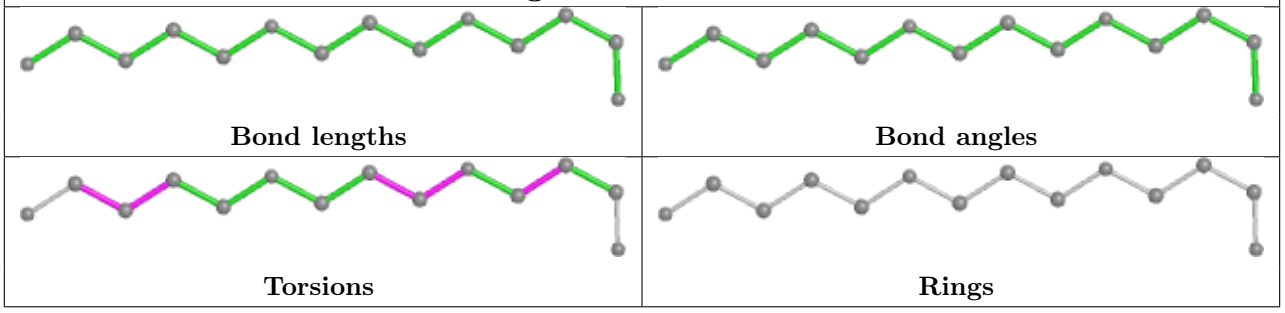
Ligand TER G 302



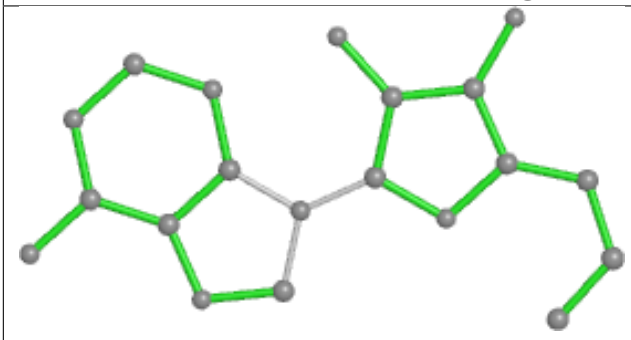
Ligand SPD A 302



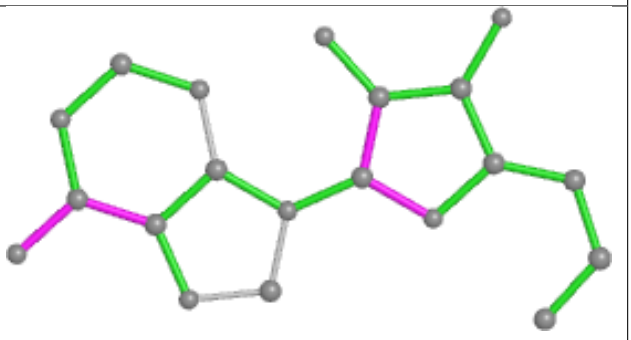
Ligand TER E 302



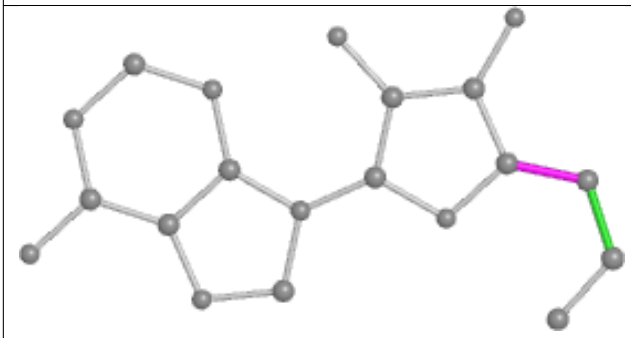
Ligand MTA K 301



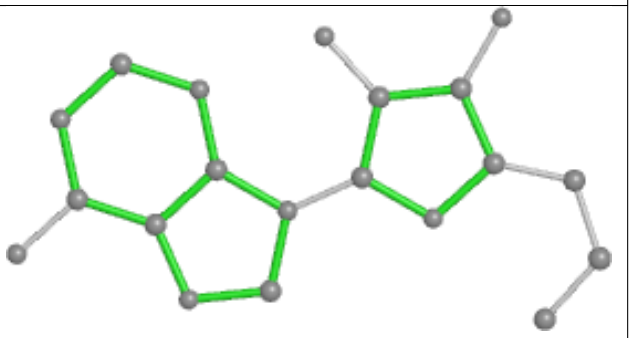
Bond lengths



Bond angles

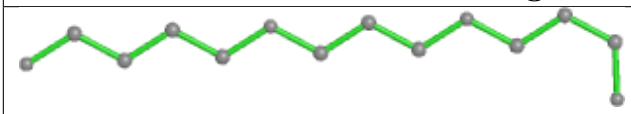


Torsions

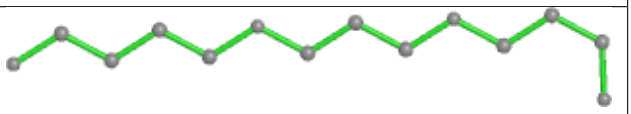


Rings

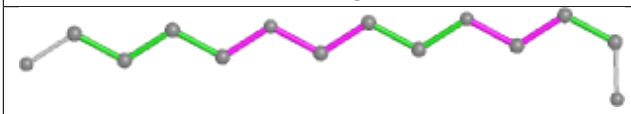
Ligand TER F 302



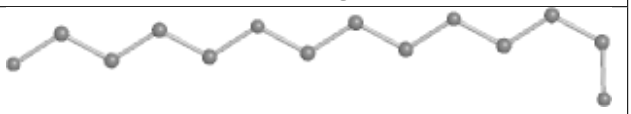
Bond lengths



Bond angles

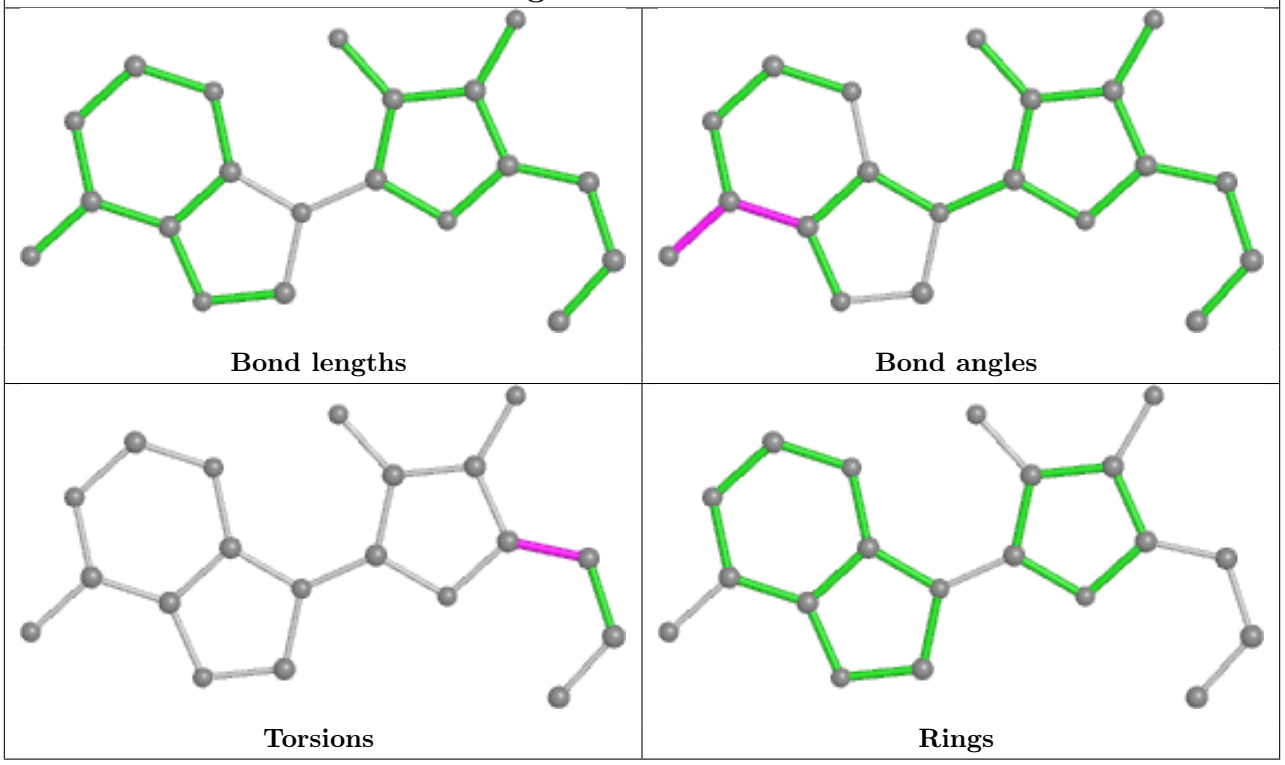


Torsions

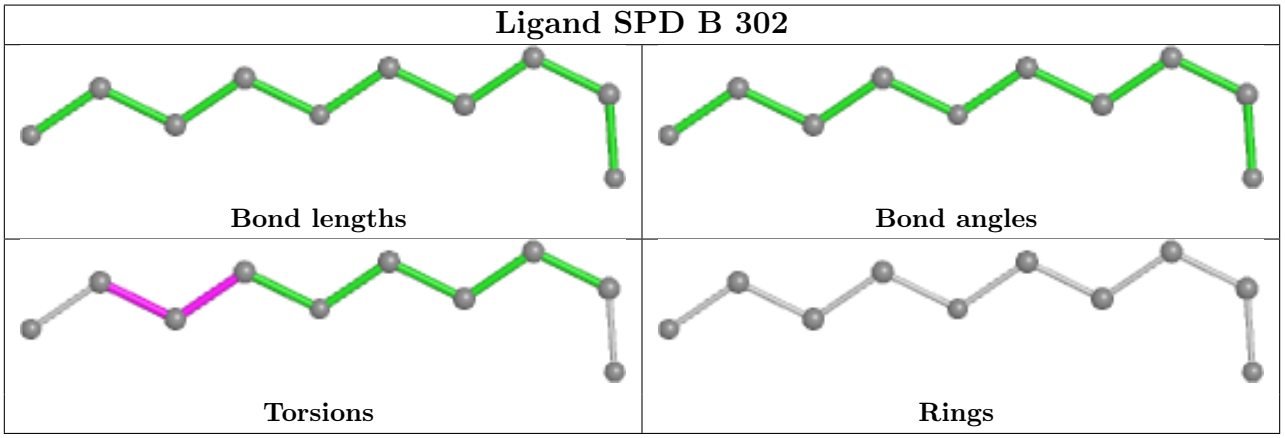


Rings

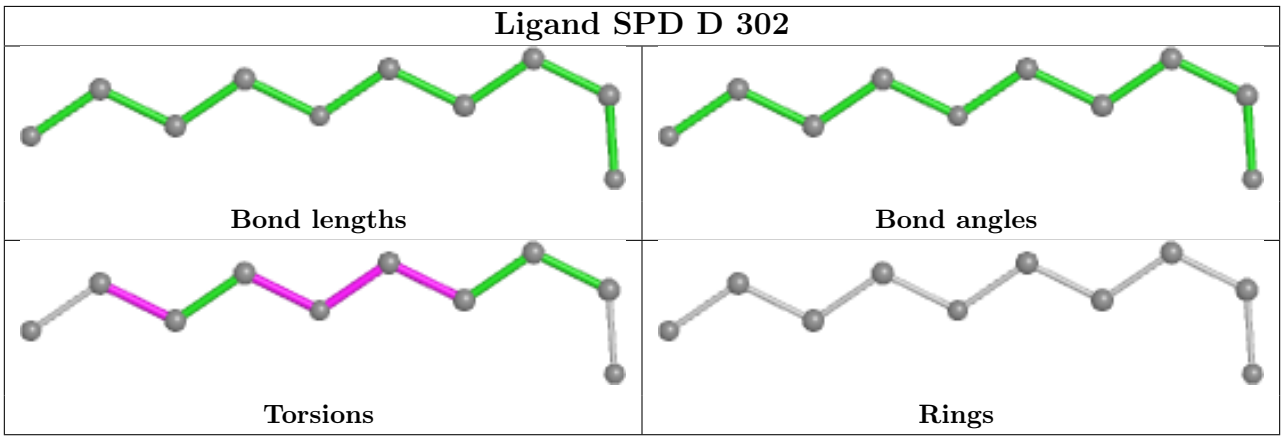
Ligand MTA I 301



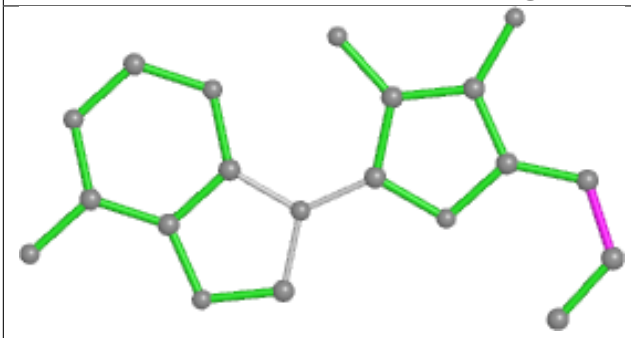
Ligand SPD B 302



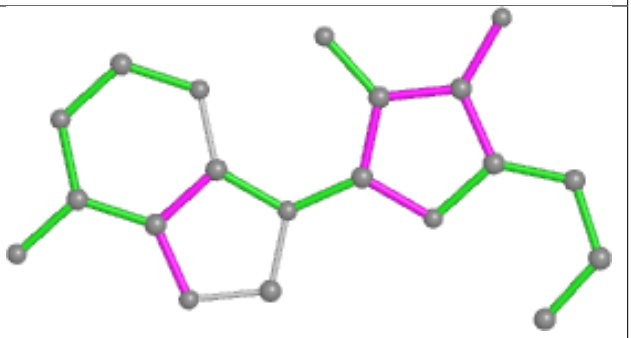
Ligand SPD D 302



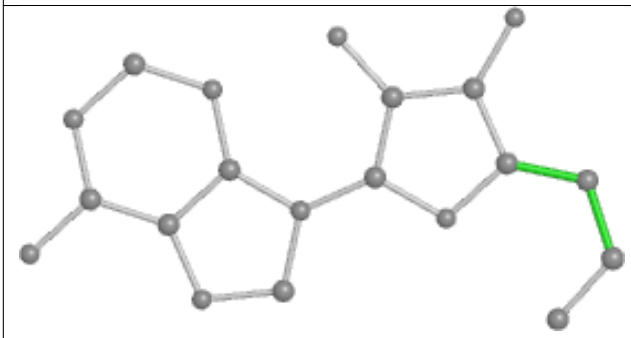
Ligand MTA F 301



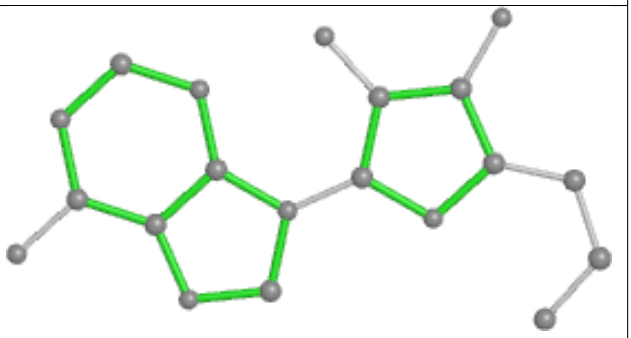
Bond lengths



Bond angles

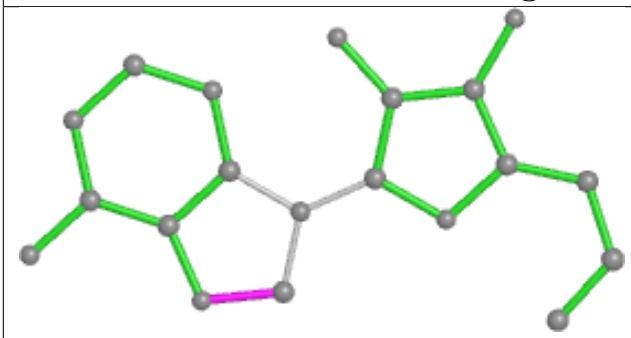


Torsions

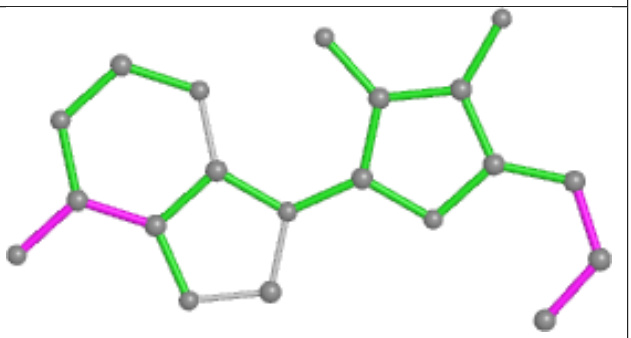


Rings

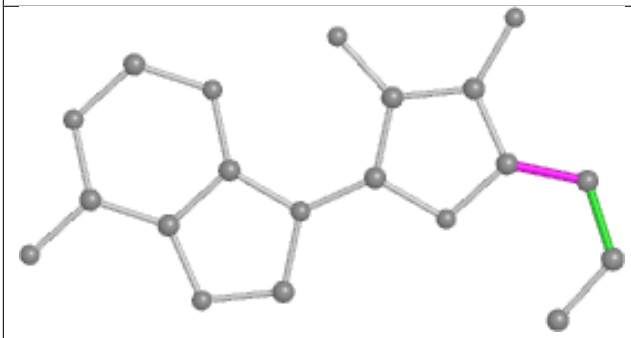
Ligand MTA B 301



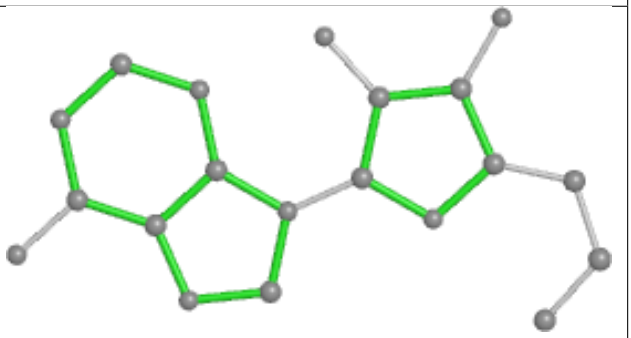
Bond lengths



Bond angles

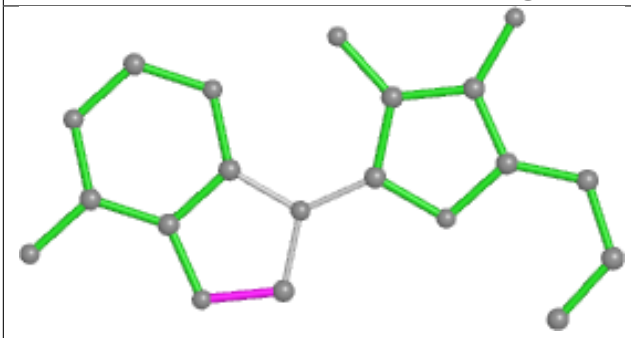


Torsions

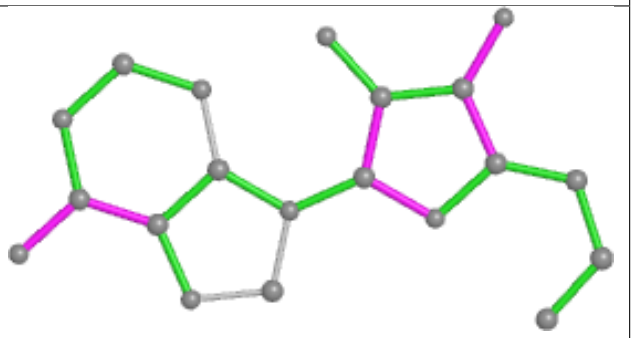


Rings

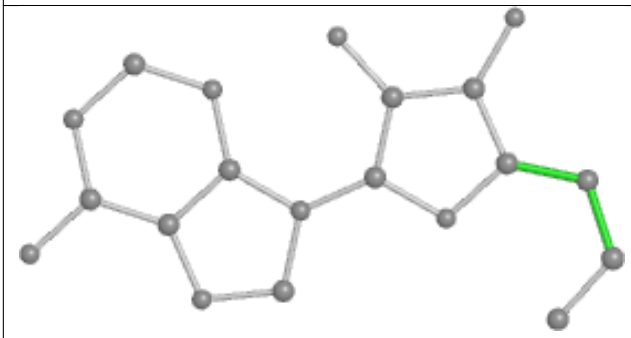
Ligand MTA A 301



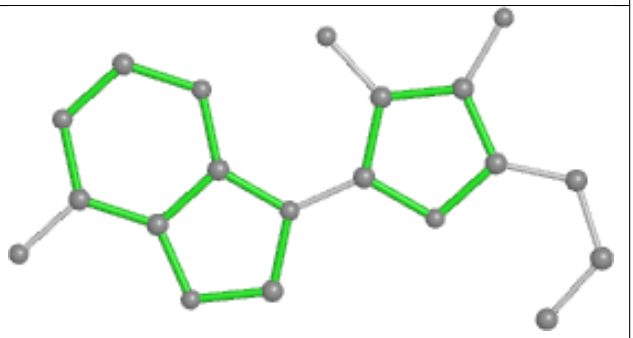
Bond lengths



Bond angles

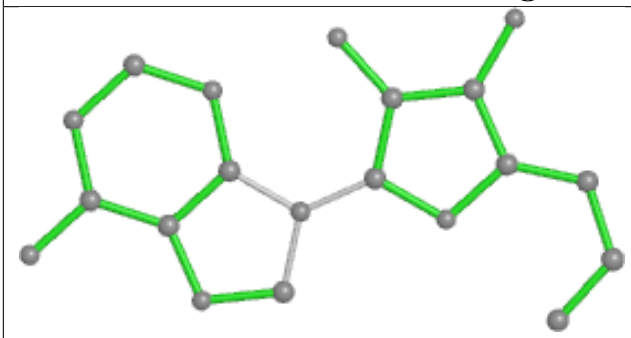


Torsions

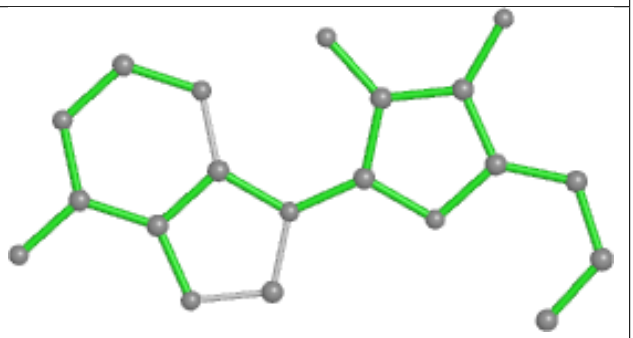


Rings

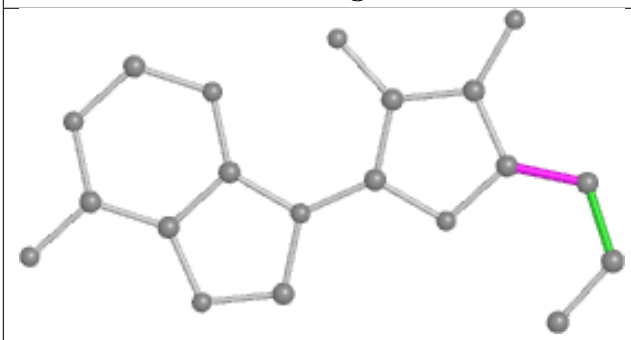
Ligand MTA G 301



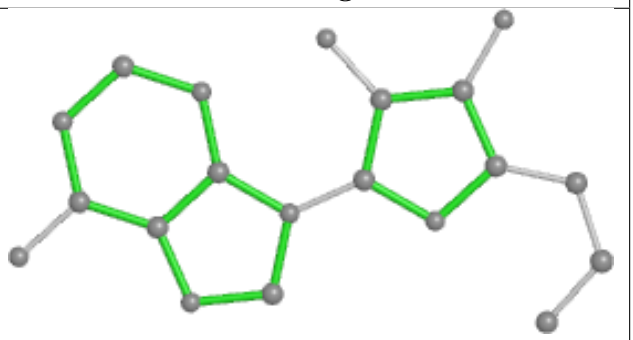
Bond lengths



Bond angles

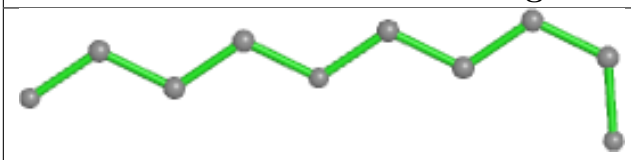


Torsions

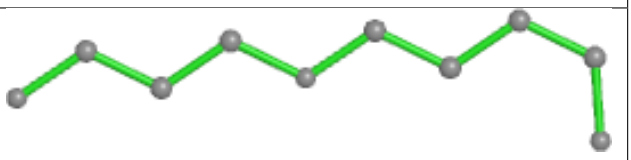


Rings

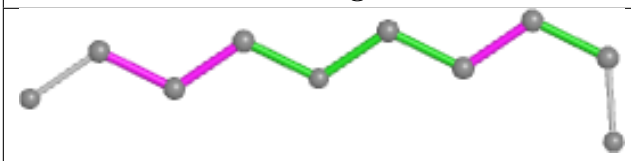
Ligand SPD C 302



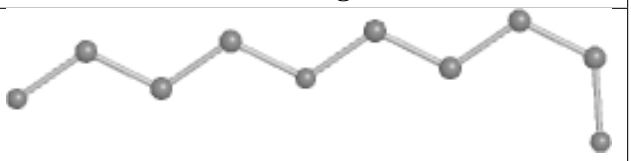
Bond lengths



Bond angles

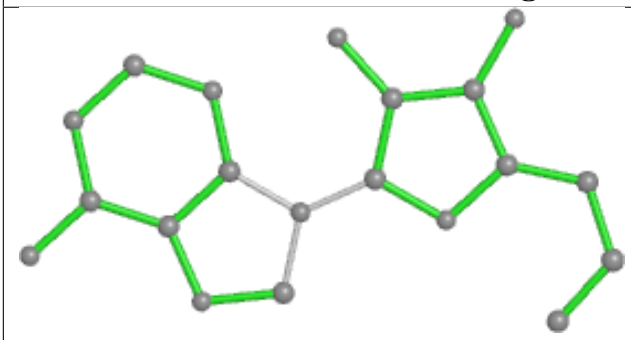


Torsions

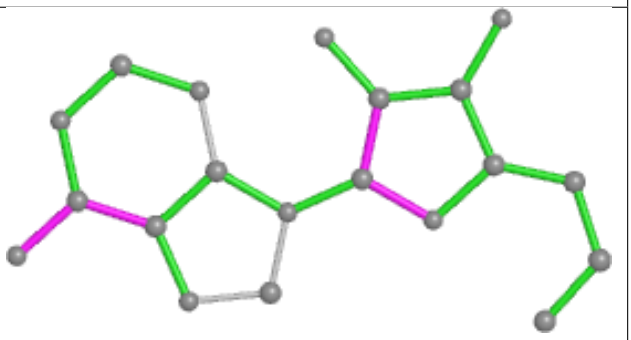


Rings

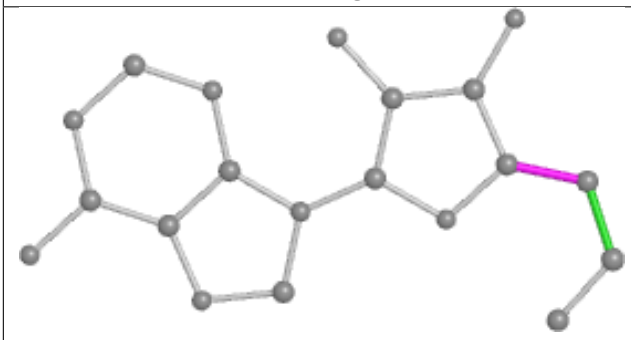
Ligand MTA C 301



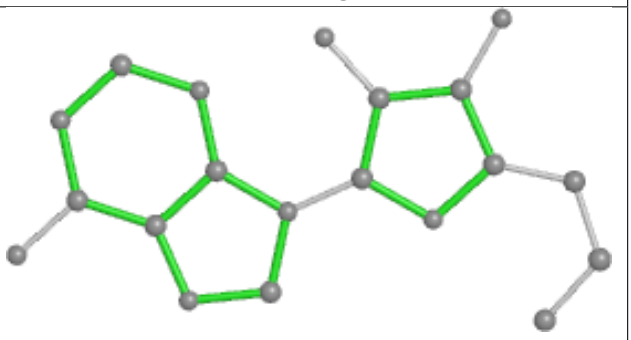
Bond lengths



Bond angles

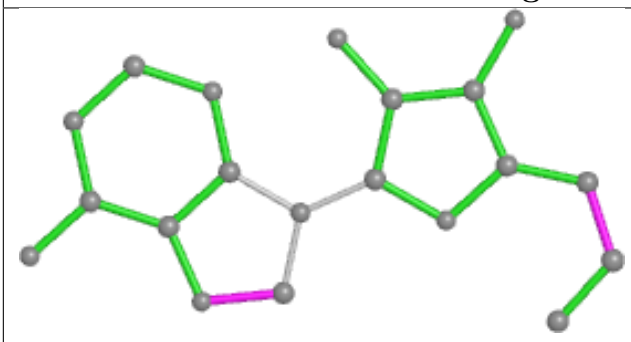


Torsions

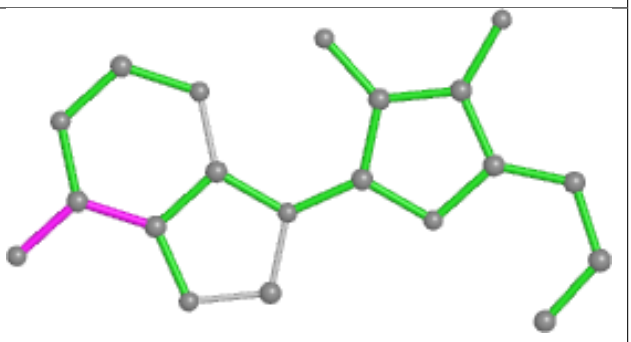


Rings

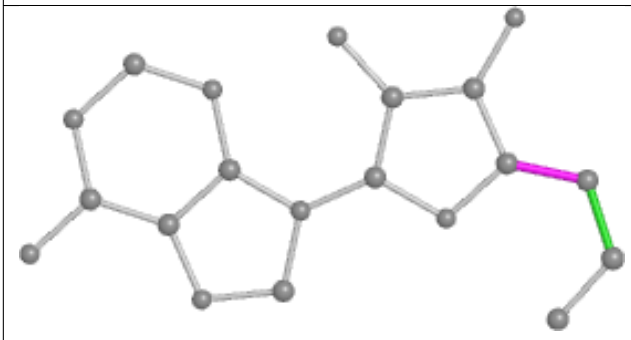
Ligand MTA L 301



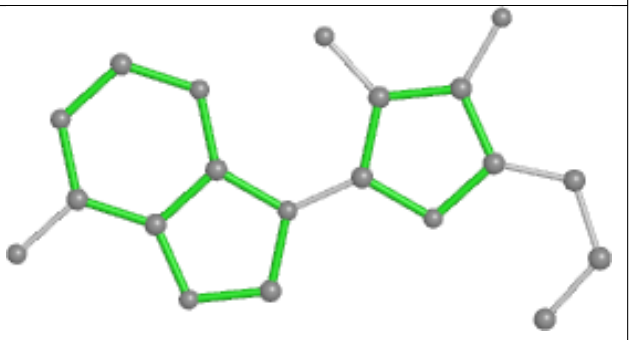
Bond lengths



Bond angles



Torsions



Rings

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	286/309 (92%)	-0.42	3 (1%) 82 86	32, 46, 67, 97	0
1	B	286/309 (92%)	-0.50	0 100 100	26, 36, 53, 70	0
1	C	286/309 (92%)	-0.45	1 (0%) 94 95	31, 42, 62, 96	0
1	D	288/309 (93%)	-0.21	4 (1%) 75 80	28, 43, 66, 85	0
1	E	286/309 (92%)	-0.22	3 (1%) 82 86	26, 39, 59, 94	0
1	F	286/309 (92%)	-0.23	3 (1%) 82 86	32, 47, 69, 114	0
1	G	286/309 (92%)	-0.53	0 100 100	28, 41, 65, 81	0
1	H	286/309 (92%)	-0.27	7 (2%) 59 65	30, 47, 72, 99	0
1	I	286/309 (92%)	-0.43	3 (1%) 82 86	34, 45, 68, 89	0
1	J	286/309 (92%)	-0.10	14 (4%) 29 36	38, 54, 80, 109	0
1	K	286/309 (92%)	0.26	26 (9%) 9 12	37, 62, 94, 119	0
1	L	286/309 (92%)	-0.23	4 (1%) 75 80	36, 53, 78, 118	0
All	All	3434/3708 (92%)	-0.28	68 (1%) 65 71	26, 46, 75, 119	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	4	VAL	4.5
1	K	194	GLY	4.5
1	K	4	VAL	4.2
1	J	106	ARG	3.9
1	K	152	ILE	3.9
1	K	145	PHE	3.9
1	A	152	ILE	3.8
1	J	4	VAL	3.8
1	K	148	VAL	3.8
1	K	155	GLY	3.7
1	K	192	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	K	103	THR	3.4
1	K	188	ARG	3.3
1	K	190	LEU	3.3
1	K	151	ALA	3.1
1	J	263	ALA	3.1
1	J	186	ILE	3.0
1	J	246	ARG	2.9
1	K	158	TYR	2.9
1	L	262	ARG	2.9
1	K	219	ALA	2.8
1	J	105	LYS	2.8
1	J	247	TYR	2.8
1	K	156	ASP	2.8
1	K	153	LYS	2.8
1	D	262	ARG	2.7
1	L	219	ALA	2.7
1	K	154	ALA	2.7
1	K	191	ASN	2.6
1	C	4	VAL	2.6
1	A	156	ASP	2.6
1	E	247	TYR	2.6
1	H	153	LYS	2.5
1	H	180	ARG	2.5
1	F	106	ARG	2.5
1	K	182	PHE	2.5
1	K	172	ASP	2.4
1	E	231	ILE	2.4
1	I	82	ARG	2.4
1	J	262	ARG	2.4
1	K	263	ALA	2.4
1	K	184	ALA	2.4
1	F	180	ARG	2.4
1	J	212	MET	2.4
1	K	193	ASP	2.4
1	I	4	VAL	2.3
1	J	192	ASP	2.3
1	D	259	GLU	2.3
1	J	82	ARG	2.3
1	E	192	ASP	2.3
1	J	80	ASN	2.3
1	K	157	LYS	2.3
1	H	102	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	183	PHE	2.2
1	H	104	VAL	2.2
1	H	172	ASP	2.2
1	K	181	GLU	2.2
1	I	262	ARG	2.2
1	H	212	MET	2.2
1	K	262	ARG	2.2
1	D	154	ALA	2.1
1	A	151	ALA	2.1
1	J	154	ALA	2.1
1	J	244	SER	2.1
1	D	145	PHE	2.1
1	F	246	ARG	2.0
1	L	212	MET	2.0
1	H	137	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TER	F	302	14/14	0.93	0.20	39,49,68,68	0
3	SPD	H	302	10/10	0.94	0.13	34,37,49,54	0
3	SPD	C	302	10/10	0.95	0.13	31,39,44,50	0
3	SPD	D	302	10/10	0.95	0.24	40,52,72,74	0
2	MTA	K	301	20/20	0.95	0.09	53,58,66,67	0
4	TER	E	302	14/14	0.95	0.24	33,51,59,60	0
3	SPD	A	302	10/10	0.95	0.17	35,40,50,53	0
4	TER	G	302	14/14	0.95	0.09	36,41,48,50	0

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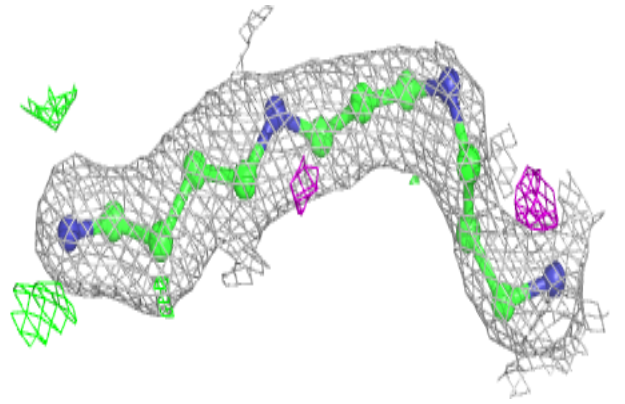
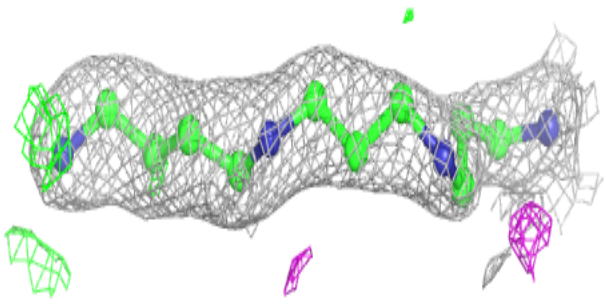
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MTA	D	301	20/20	0.96	0.08	33,38,46,48	0
2	MTA	J	301	20/20	0.96	0.10	44,48,53,56	0
3	SPD	B	302	10/10	0.96	0.15	35,41,47,48	0
2	MTA	E	301	20/20	0.97	0.11	26,31,35,37	0
2	MTA	L	301	20/20	0.97	0.08	38,42,47,51	0
2	MTA	F	301	20/20	0.97	0.10	31,35,43,48	0
2	MTA	I	301	20/20	0.97	0.07	37,42,47,48	0
2	MTA	A	301	20/20	0.97	0.06	33,39,45,46	0
2	MTA	C	301	20/20	0.98	0.07	30,35,40,43	0
2	MTA	B	301	20/20	0.98	0.08	25,30,33,34	0
2	MTA	G	301	20/20	0.98	0.07	25,32,38,39	0
2	MTA	H	301	20/20	0.98	0.07	37,41,49,51	0

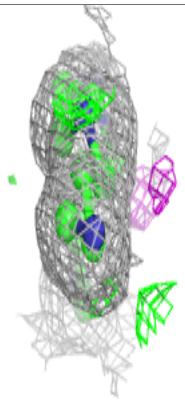
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TER 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)

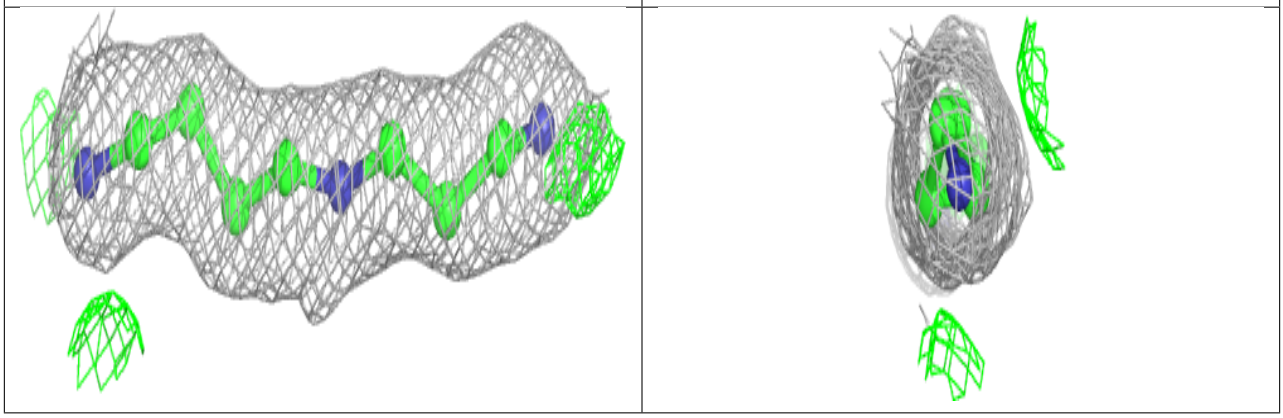






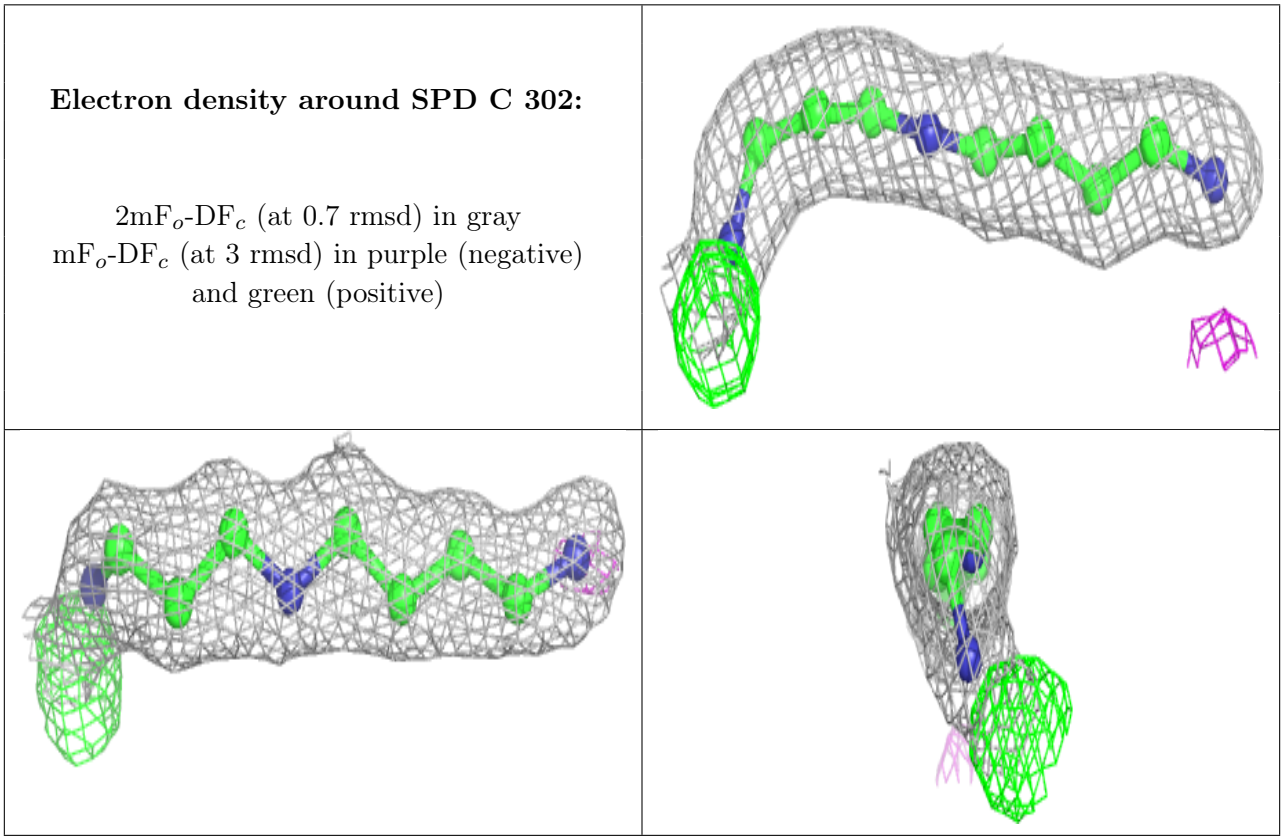
Electron density around SPD H 302:

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



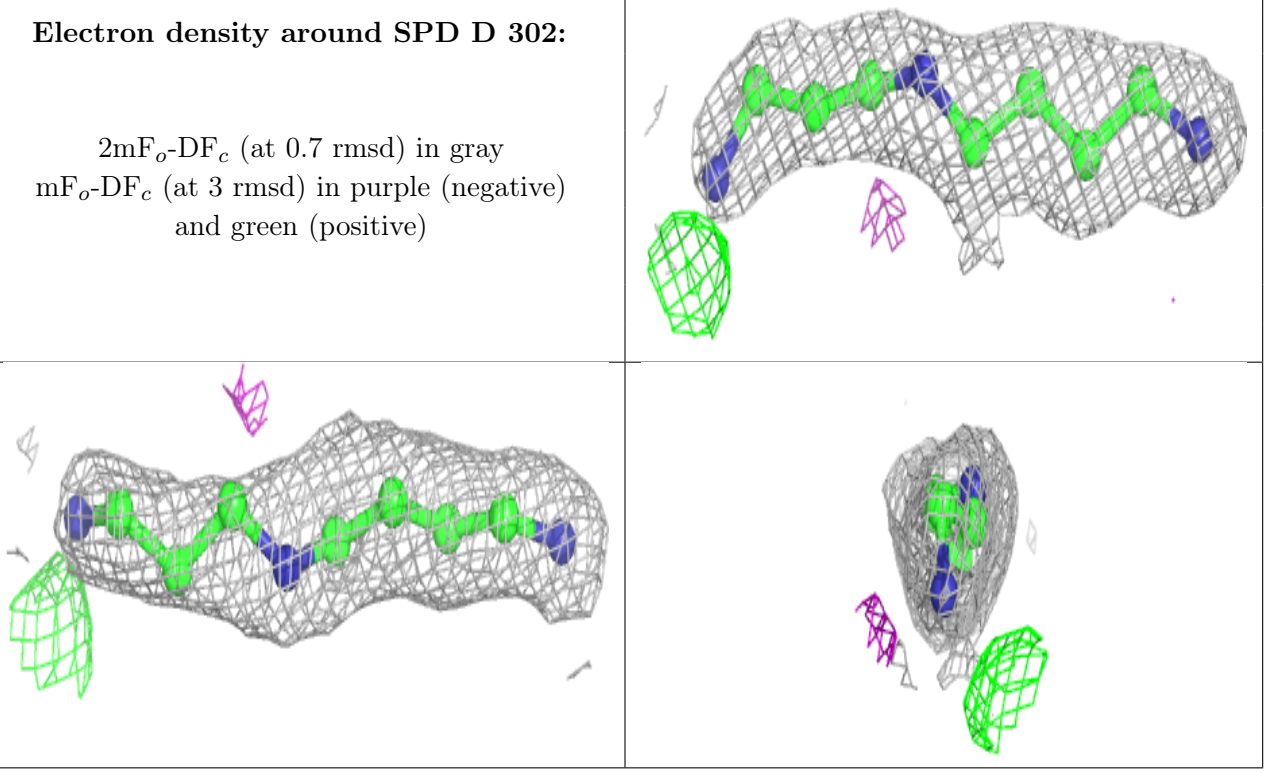
Electron density around SPD C 302:

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



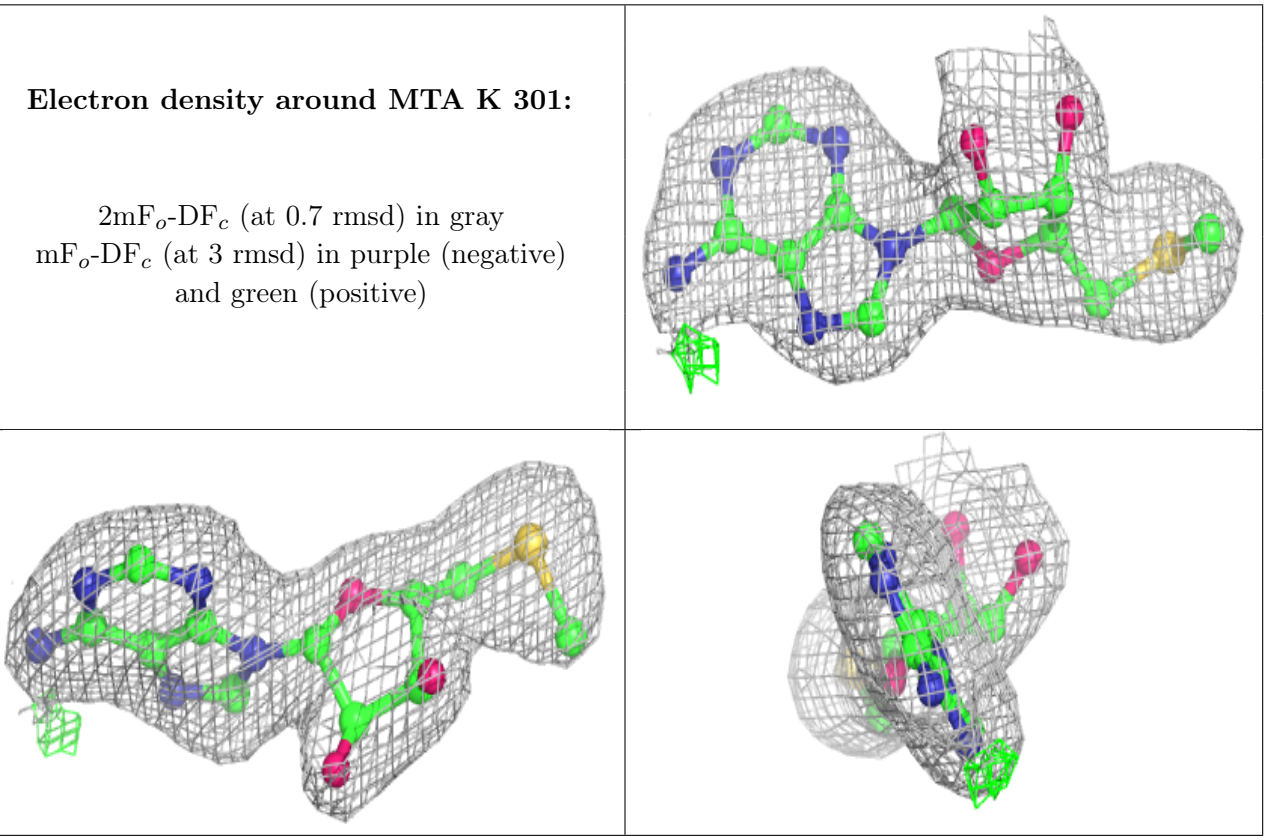
Electron density around SPD D 302:

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



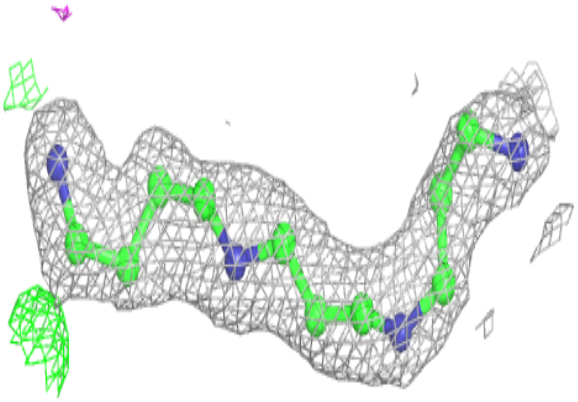
Electron density around MTA K 301:

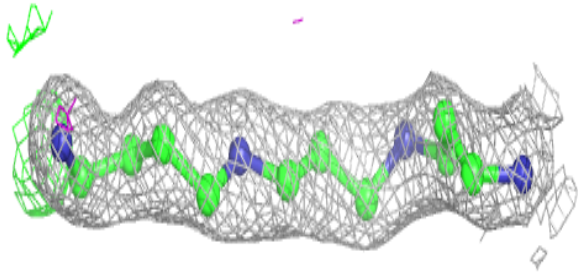
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

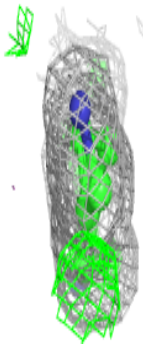


Electron density around TER E 302:

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

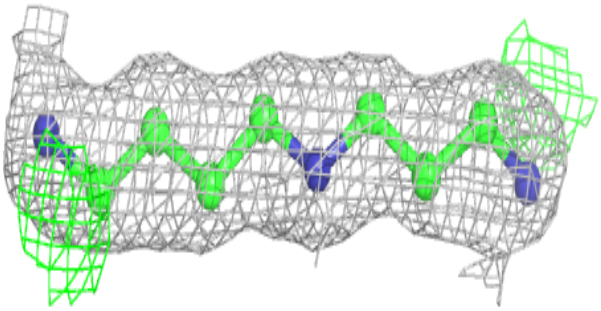


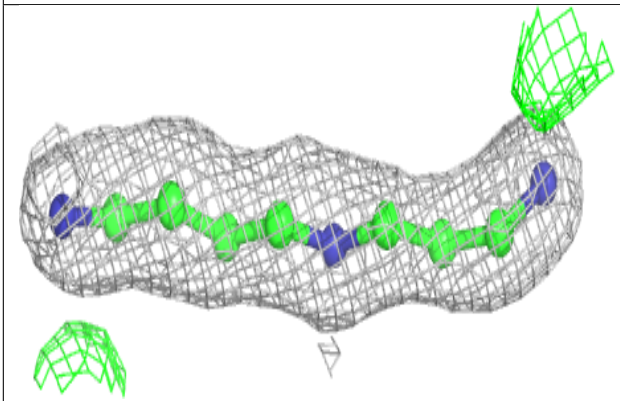


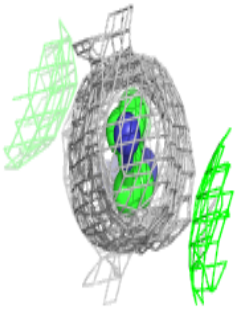


Electron density around SPD A 302:

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

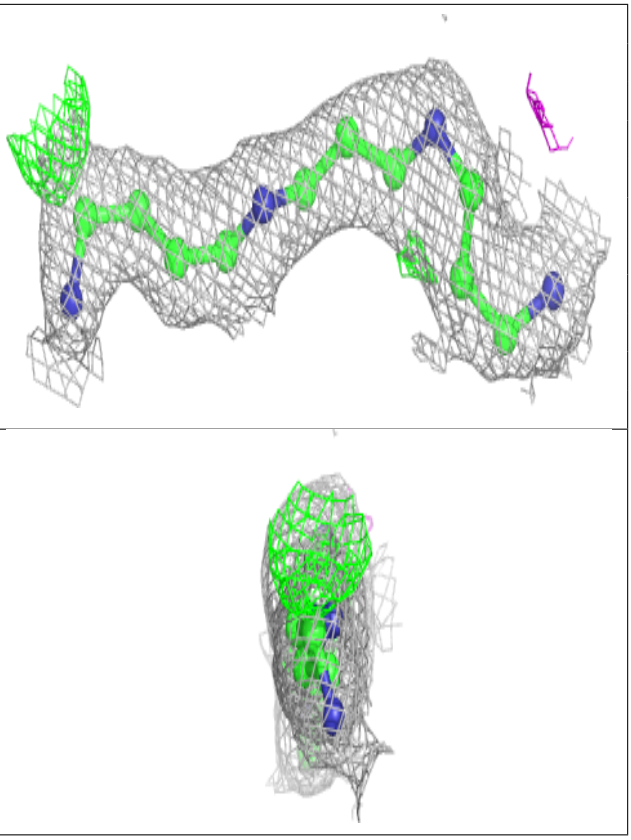






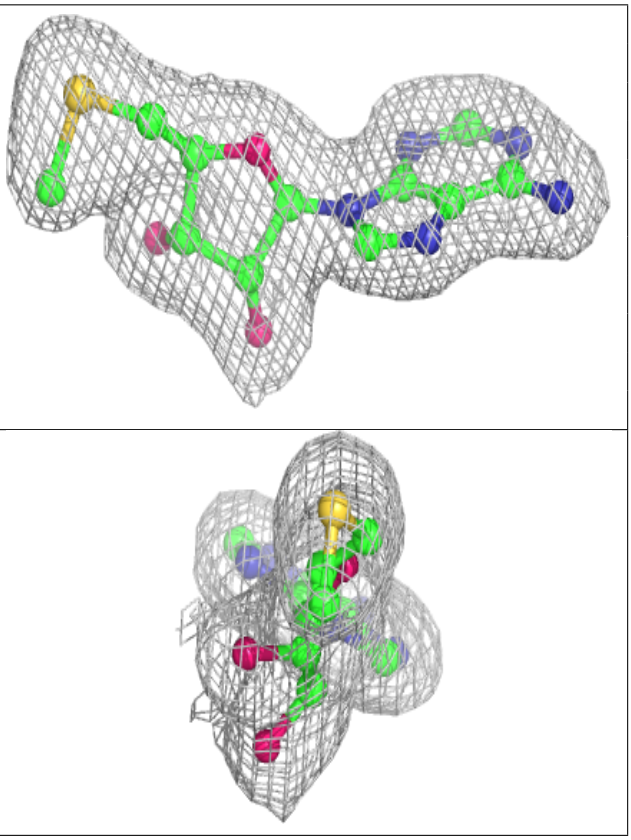
Electron density around TER G 302:

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



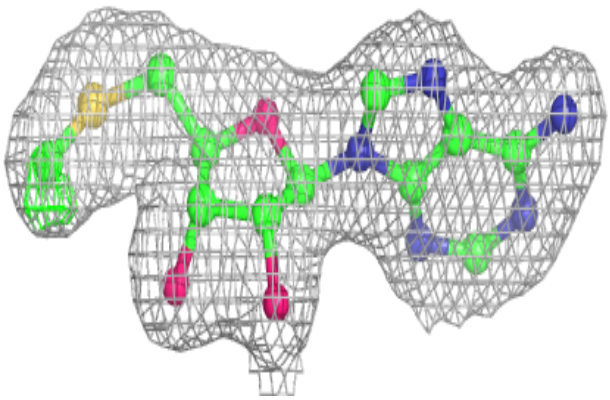
Electron density around MTA D 301:

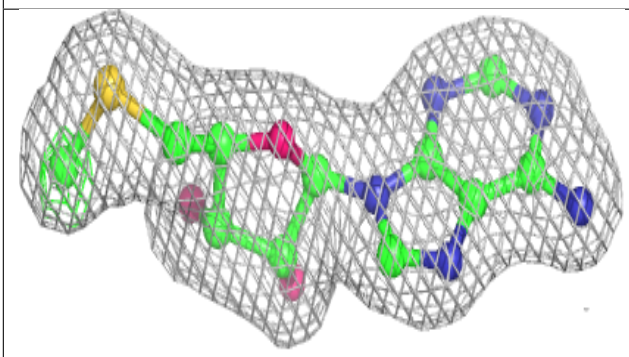
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

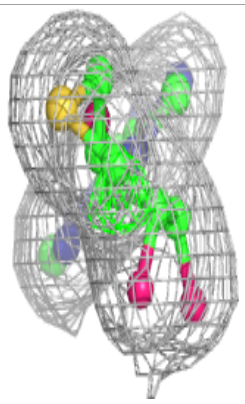


Electron density around MTA J 301:

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

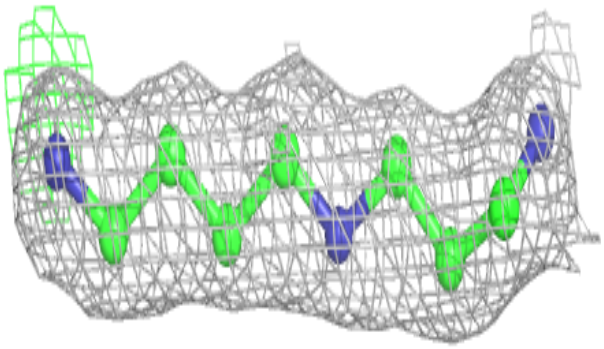


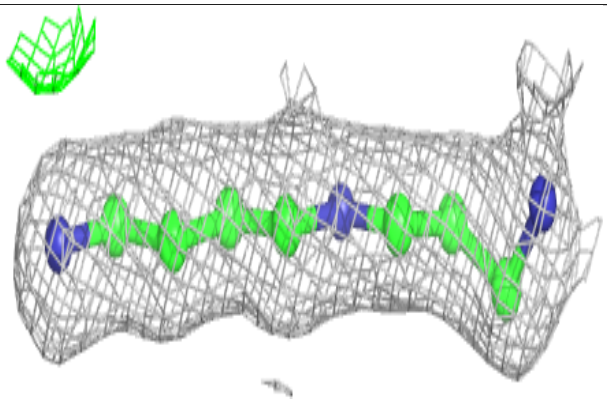


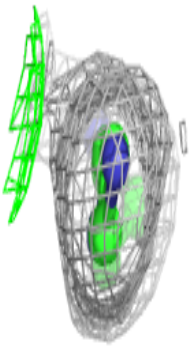


Electron density around SPD B 302:

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

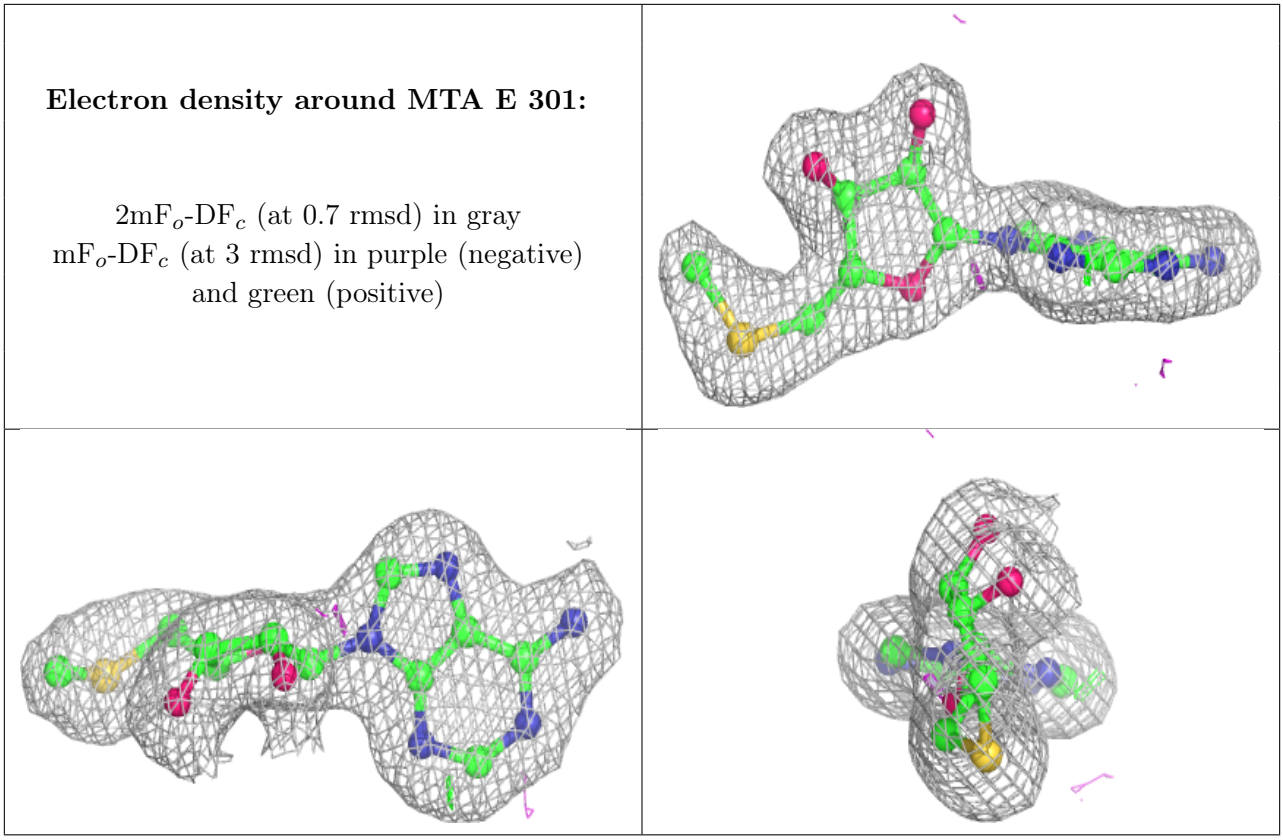






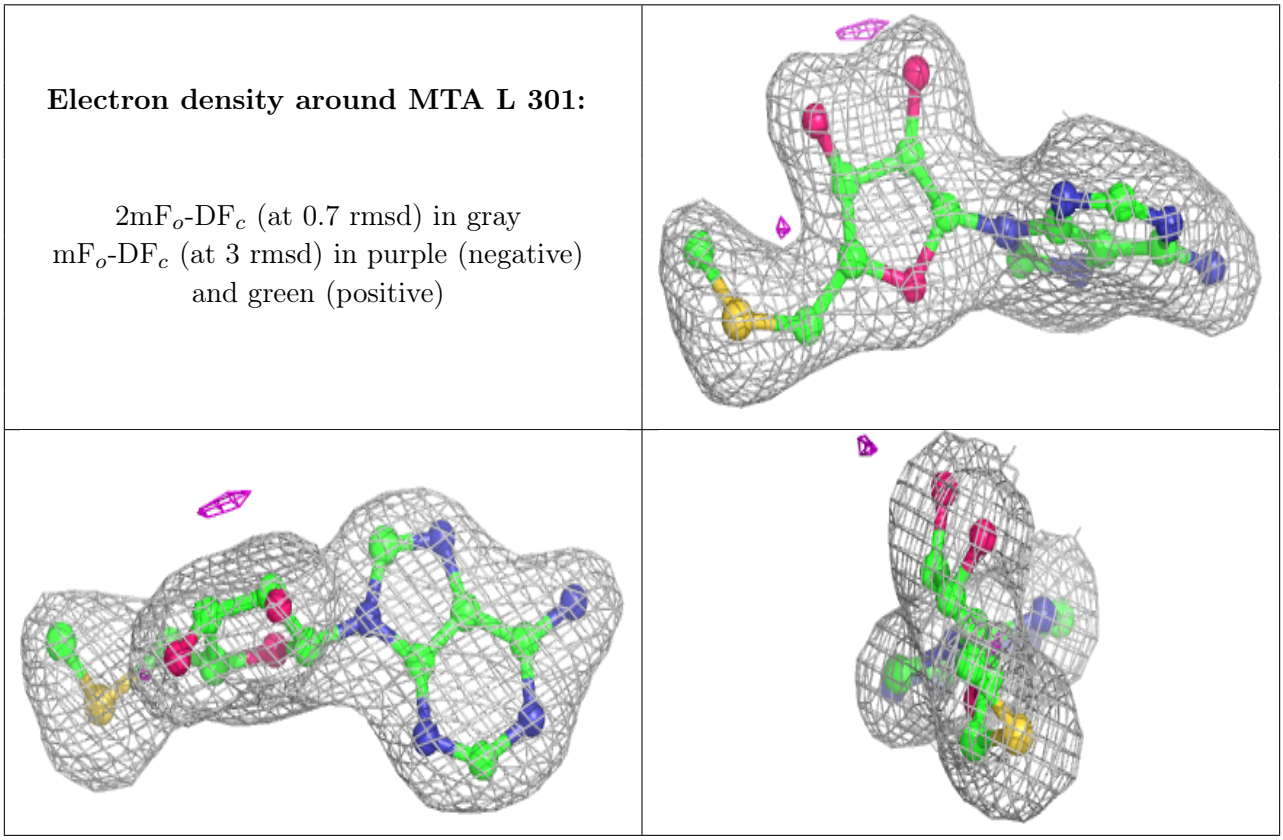
Electron density around MTA E 301:

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



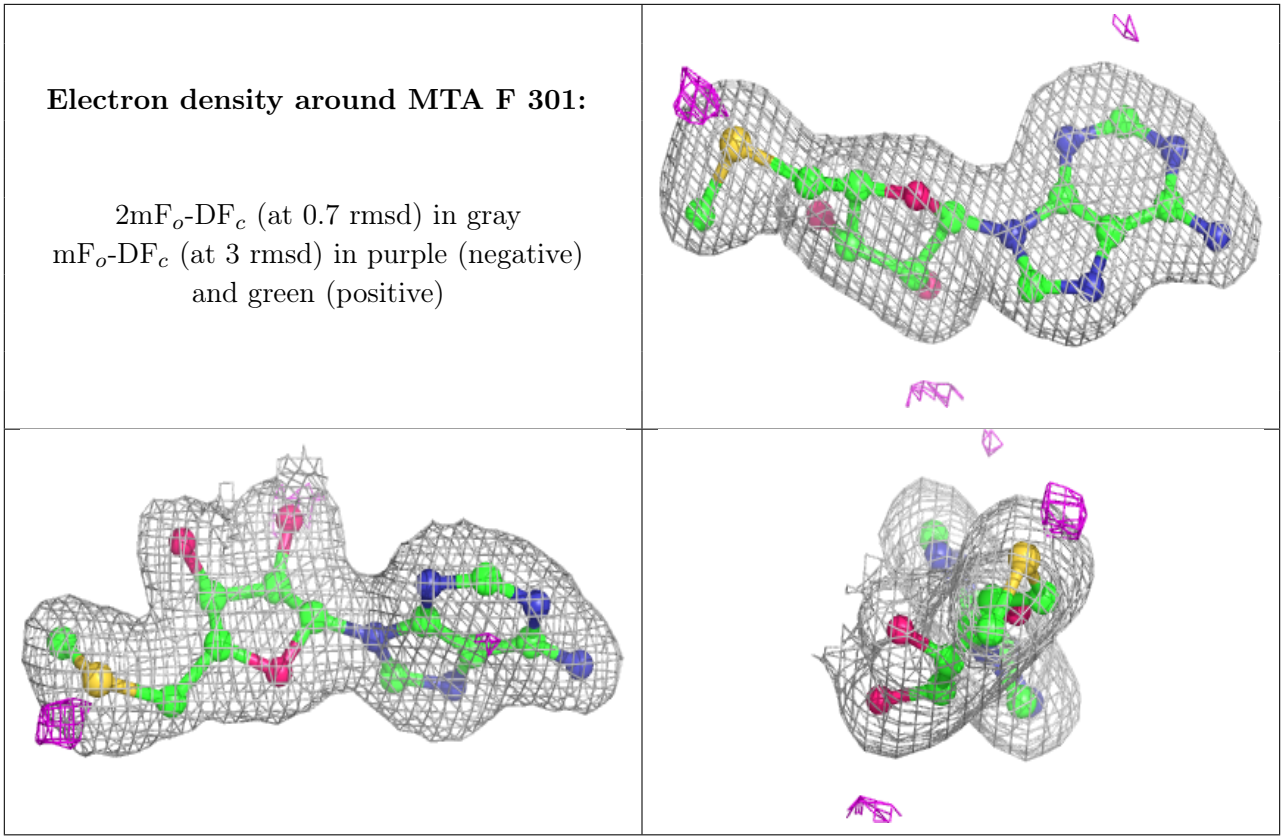
Electron density around MTA L 301:

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



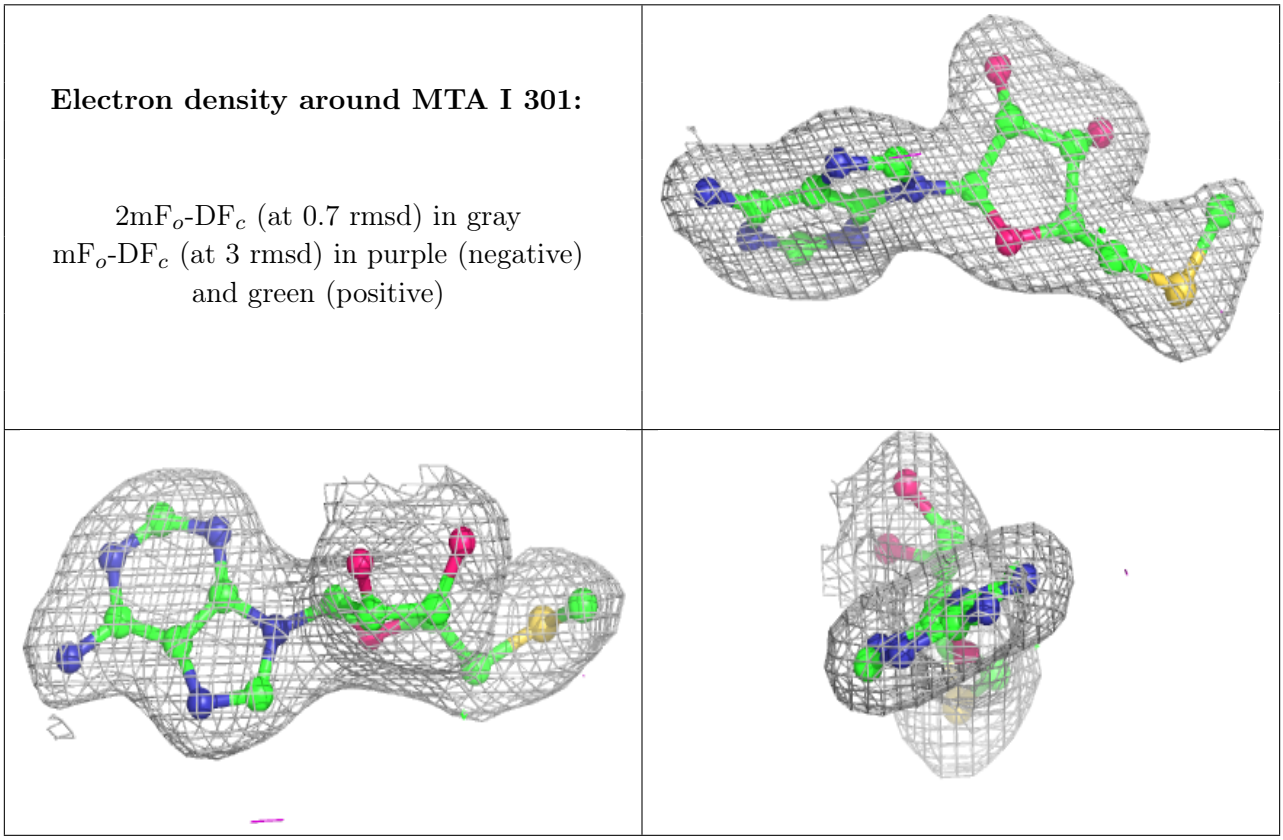
Electron density around MTA F 301:

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



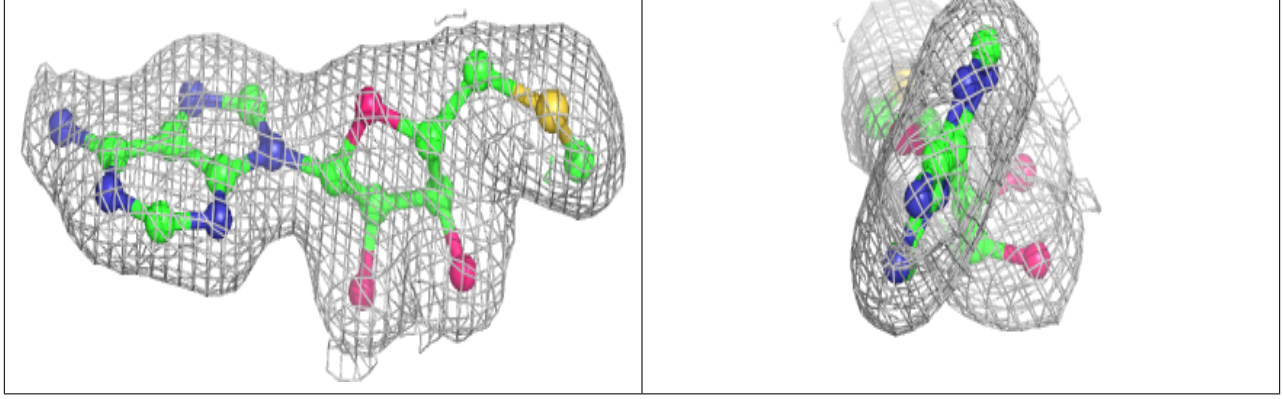
Electron density around MTA I 301:

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



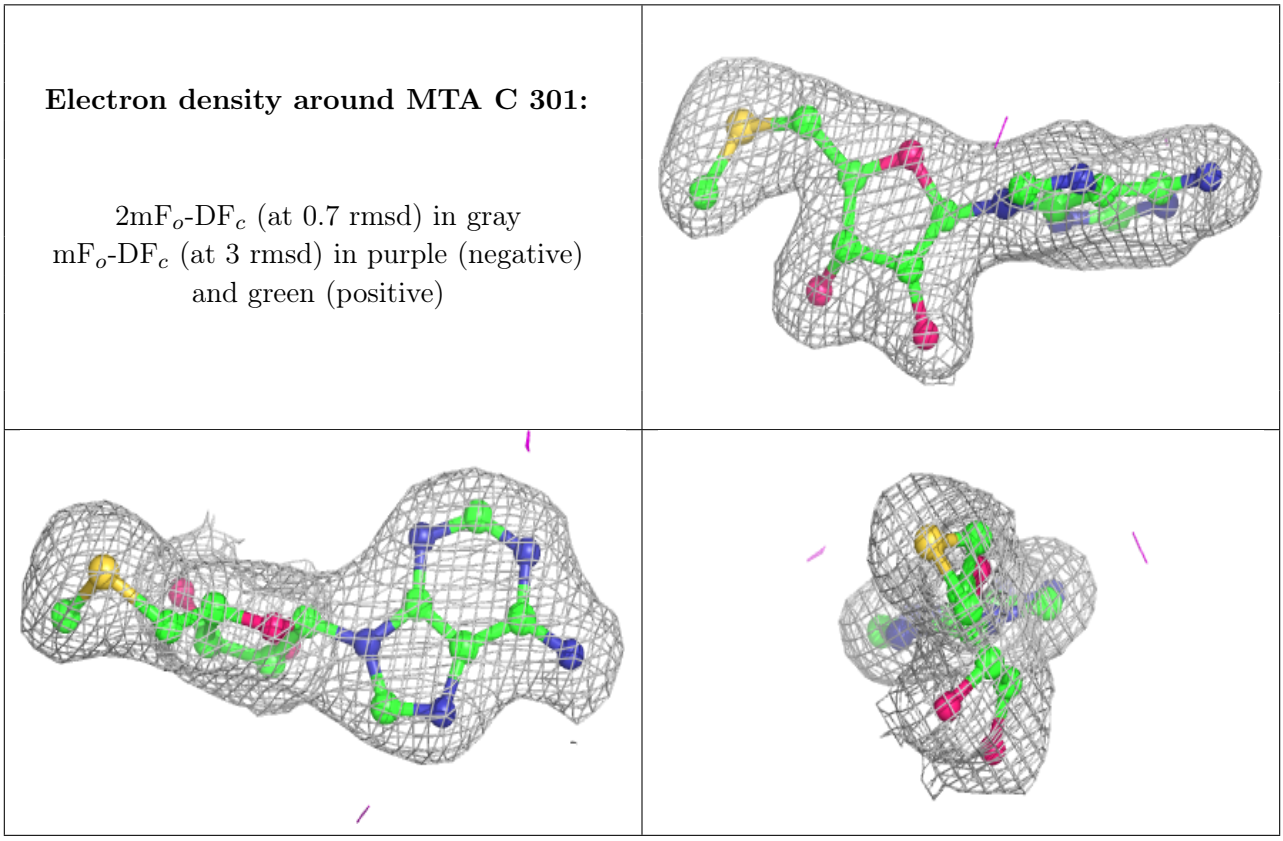
Electron density around MTA A 301:

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



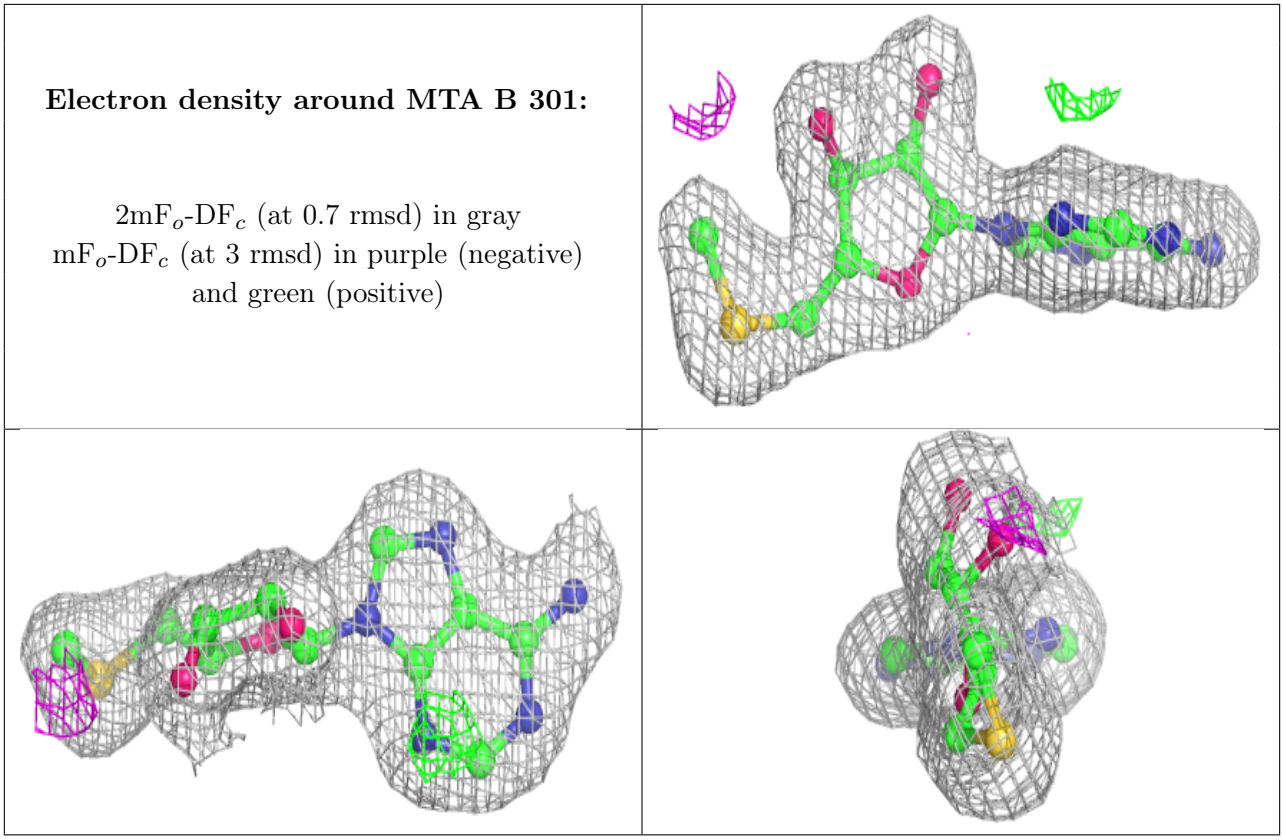
Electron density around MTA C 301:

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



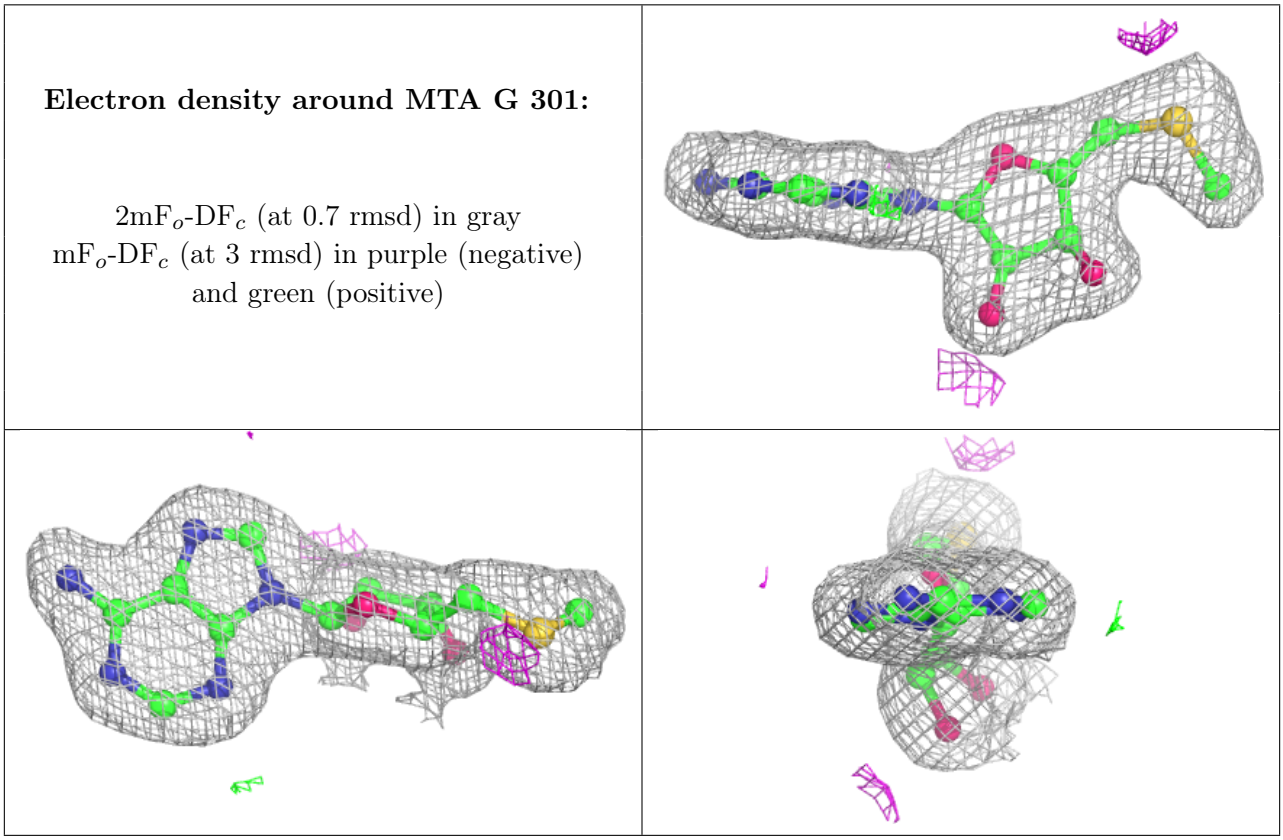
Electron density around MTA B 301:

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



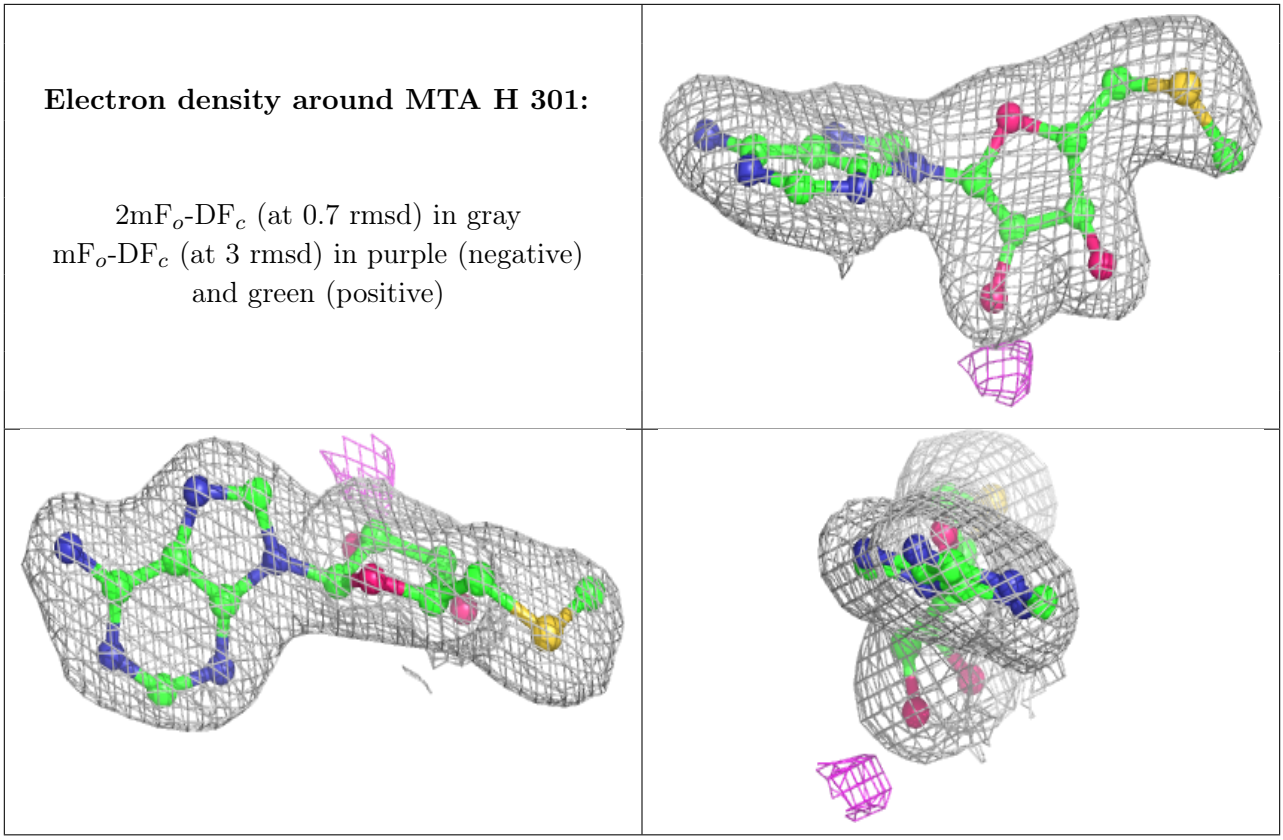
Electron density around MTA G 301:

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



Electron density around MTA 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)



6.5 Other polymers (i)

There are no such residues in this entry.