wwPDB X-ray Structure Validation Summary Report (i)

Jan 16, 2024 – 01:07 am GMT

PDB ID	:	6RKC
Title	:	Inter-dimeric interface controls function and stability of S-methionine adenosyltransferase from U. urealiticum
Authors	:	Shahar, A.; Zarivach, R.; Bershtein, S.; Kleiner, D.; Shmulevich, F.
Deposited on	:	2019-04-30
Resolution	:	2.56 Å(reported)

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

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

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

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

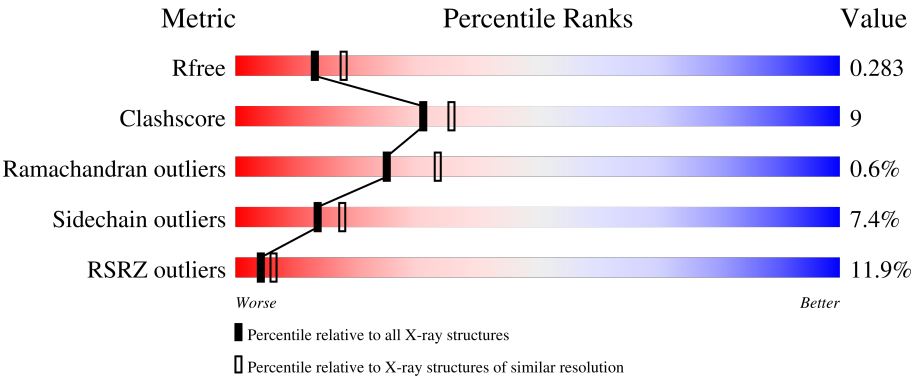
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	382	4% 81% 14%
1	B	382	3% 80% 16%
1	C	382	5% 80% 15%
1	D	382	5% 79% 16%
1	E	382	16% 71% 21%

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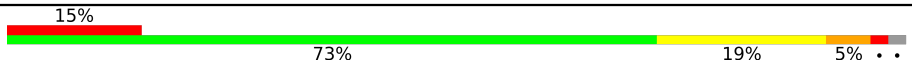
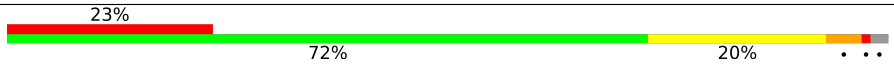
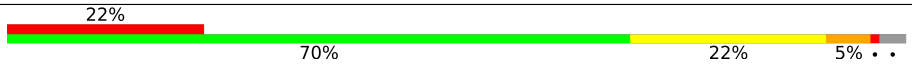
Mol	Chain	Length	Quality of chain
1	F	382	
1	G	382	
1	H	382	

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
3	MG	E	403	-	-	-	X
3	MG	G	402	-	-	-	X
5	PPK	A	405	-	-	X	-
5	PPK	C	405	-	X	-	-
5	PPK	C	408	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 24088 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 Methionine adenosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2917	1851	490	565	11			
1	B	374	Total	C	N	O	S	0	1	0
			2944	1871	495	567	11			
1	C	373	Total	C	N	O	S	0	0	0
			2929	1860	491	567	11			
1	D	372	Total	C	N	O	S	0	0	0
			2917	1851	490	565	11			
1	E	372	Total	C	N	O	S	0	0	0
			2917	1851	490	565	11			
1	F	374	Total	C	N	O	S	0	0	0
			2936	1863	495	567	11			
1	G	373	Total	C	N	O	S	0	0	0
			2929	1860	491	567	11			
1	H	372	Total	C	N	O	S	0	0	0
			2917	1851	490	565	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	HIS	-	expression tag	UNP B2NE58
A	378	HIS	-	expression tag	UNP B2NE58
A	379	HIS	-	expression tag	UNP B2NE58
A	380	HIS	-	expression tag	UNP B2NE58
A	381	HIS	-	expression tag	UNP B2NE58
A	382	HIS	-	expression tag	UNP B2NE58
B	377	HIS	-	expression tag	UNP B2NE58
B	378	HIS	-	expression tag	UNP B2NE58
B	379	HIS	-	expression tag	UNP B2NE58
B	380	HIS	-	expression tag	UNP B2NE58
B	381	HIS	-	expression tag	UNP B2NE58
B	382	HIS	-	expression tag	UNP B2NE58
C	377	HIS	-	expression tag	UNP B2NE58

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Chain	Residue	Modelled	Actual	Comment	Reference
C	378	HIS	-	expression tag	UNP B2NE58
C	379	HIS	-	expression tag	UNP B2NE58
C	380	HIS	-	expression tag	UNP B2NE58
C	381	HIS	-	expression tag	UNP B2NE58
C	382	HIS	-	expression tag	UNP B2NE58
D	377	HIS	-	expression tag	UNP B2NE58
D	378	HIS	-	expression tag	UNP B2NE58
D	379	HIS	-	expression tag	UNP B2NE58
D	380	HIS	-	expression tag	UNP B2NE58
D	381	HIS	-	expression tag	UNP B2NE58
D	382	HIS	-	expression tag	UNP B2NE58
E	377	HIS	-	expression tag	UNP B2NE58
E	378	HIS	-	expression tag	UNP B2NE58
E	379	HIS	-	expression tag	UNP B2NE58
E	380	HIS	-	expression tag	UNP B2NE58
E	381	HIS	-	expression tag	UNP B2NE58
E	382	HIS	-	expression tag	UNP B2NE58
F	377	HIS	-	expression tag	UNP B2NE58
F	378	HIS	-	expression tag	UNP B2NE58
F	379	HIS	-	expression tag	UNP B2NE58
F	380	HIS	-	expression tag	UNP B2NE58
F	381	HIS	-	expression tag	UNP B2NE58
F	382	HIS	-	expression tag	UNP B2NE58
G	377	HIS	-	expression tag	UNP B2NE58
G	378	HIS	-	expression tag	UNP B2NE58
G	379	HIS	-	expression tag	UNP B2NE58
G	380	HIS	-	expression tag	UNP B2NE58
G	381	HIS	-	expression tag	UNP B2NE58
G	382	HIS	-	expression tag	UNP B2NE58
H	377	HIS	-	expression tag	UNP B2NE58
H	378	HIS	-	expression tag	UNP B2NE58
H	379	HIS	-	expression tag	UNP B2NE58
H	380	HIS	-	expression tag	UNP B2NE58
H	381	HIS	-	expression tag	UNP B2NE58
H	382	HIS	-	expression tag	UNP B2NE58

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total K 2 2	0	0
2	C	1	Total K 1 1	0	0

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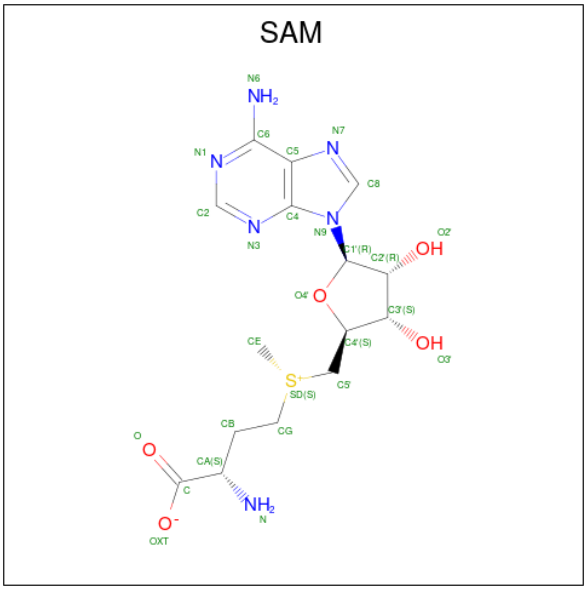
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total K 2 2	0	0
2	G	2	Total K 2 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

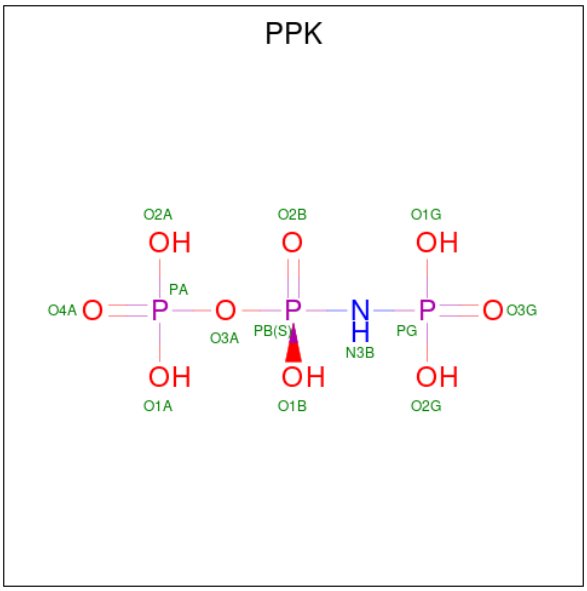
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0
3	B	1	Total Mg 1 1	0	0
3	C	3	Total Mg 3 3	0	0
3	D	1	Total Mg 1 1	0	0
3	E	3	Total Mg 3 3	0	0
3	F	1	Total Mg 1 1	0	0
3	G	3	Total Mg 3 3	0	0
3	H	1	Total Mg 1 1	0	0

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	E	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	E	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	G	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	G	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	H	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	H	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is (DIPHOSPHONO)AMINOPHOSPHONIC ACID (three-letter code: PPK) (formula: $H_6NO_9P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N O P 13 1 9 3	0	0
5	A	1	Total N O P 13 1 9 3	0	0
5	C	1	Total N O P 13 1 9 3	0	0
5	C	1	Total N O P 13 1 9 3	0	0
5	E	1	Total N O P 13 1 9 3	0	0
5	E	1	Total N O P 13 1 9 3	0	0
5	G	1	Total N O P 13 1 9 3	0	0
5	G	1	Total N O P 13 1 9 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	B	21	Total O 21 21	0	0
6	C	16	Total O 16 16	0	0
6	D	18	Total O 18 18	0	0

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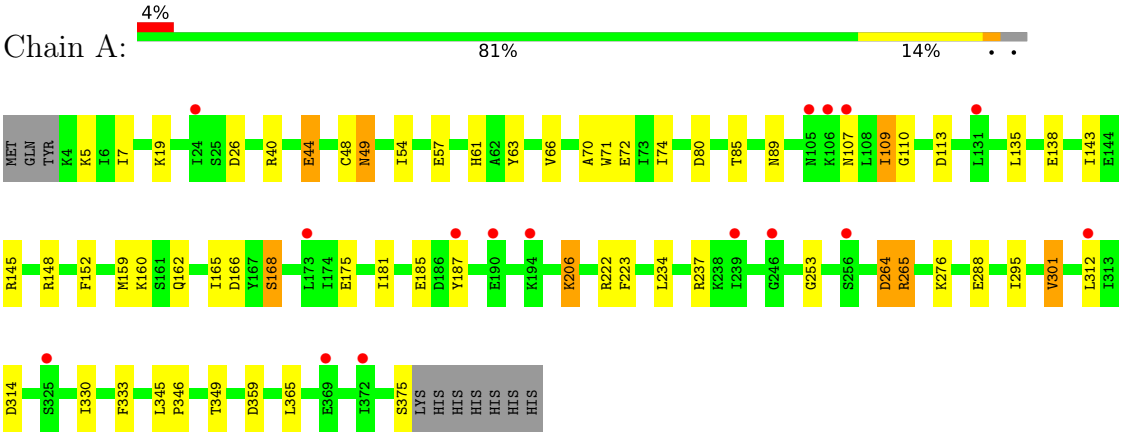
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	15	Total O 15 15	0	0
6	F	12	Total O 12 12	0	0
6	G	10	Total O 10 10	0	0
6	H	6	Total O 6 6	0	0

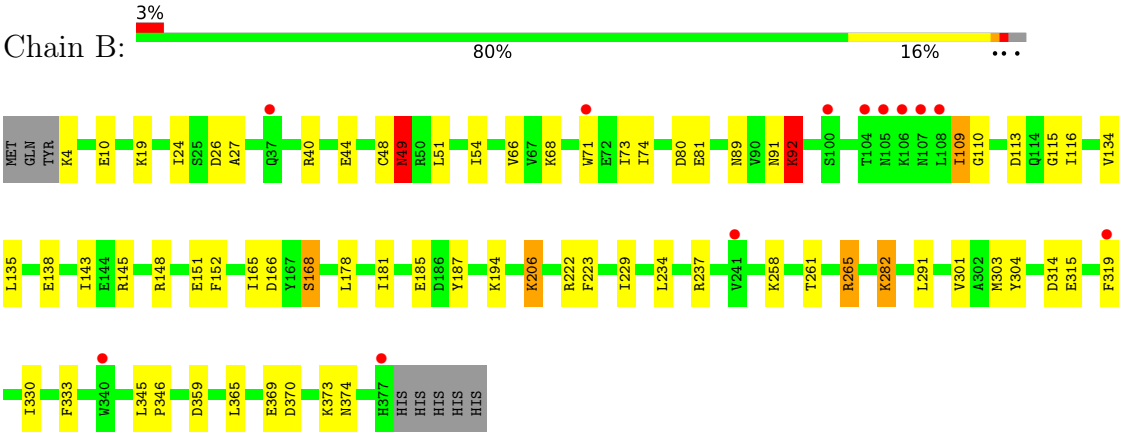
3 Residue-property plots (i)

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.

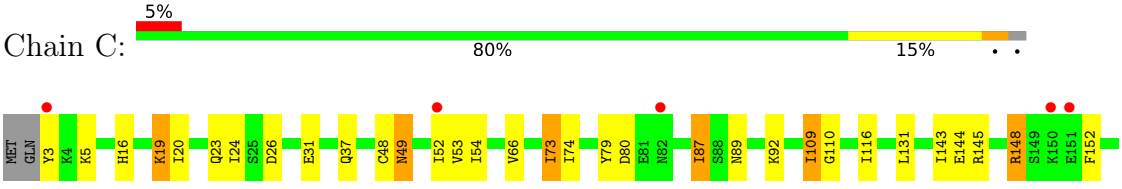
• Molecule 1: Methionine adenosyltransferase

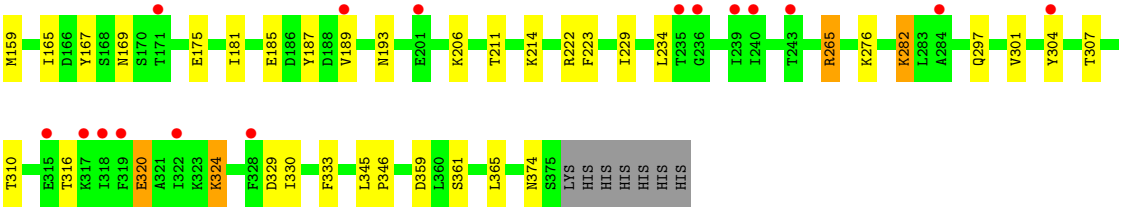


• Molecule 1: Methionine adenosyltransferase



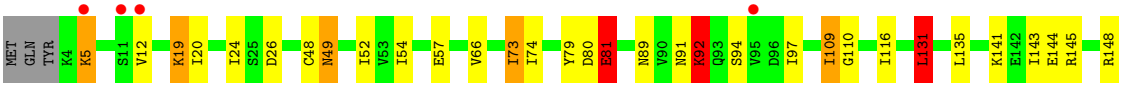
• Molecule 1: Methionine adenosyltransferase

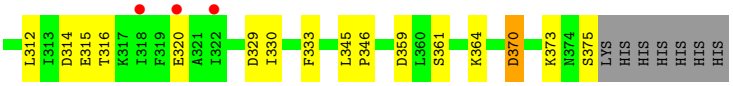




• Molecule 1: Methionine adenosyltransferase

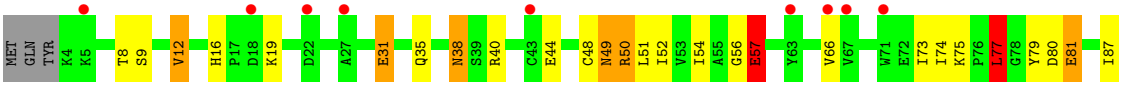
Chain D:

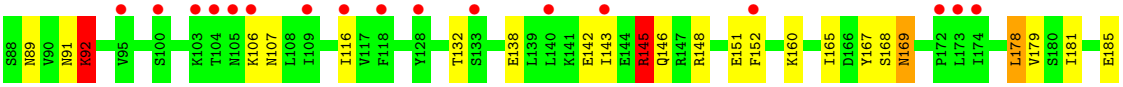


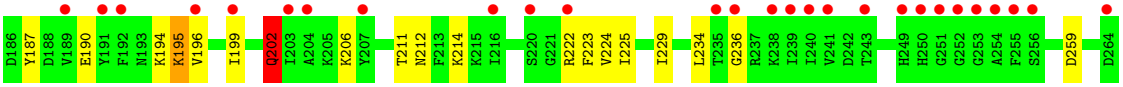


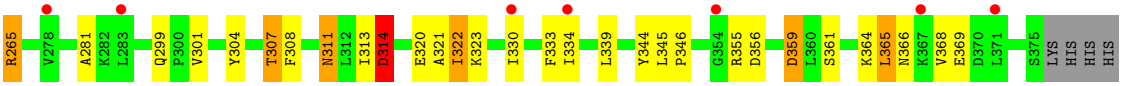
• Molecule 1: Methionine adenosyltransferase

Chain E:



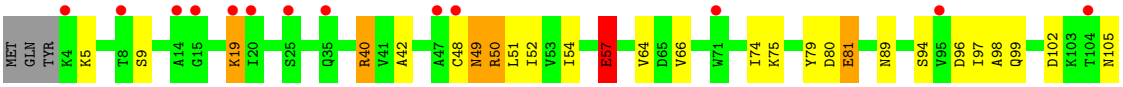


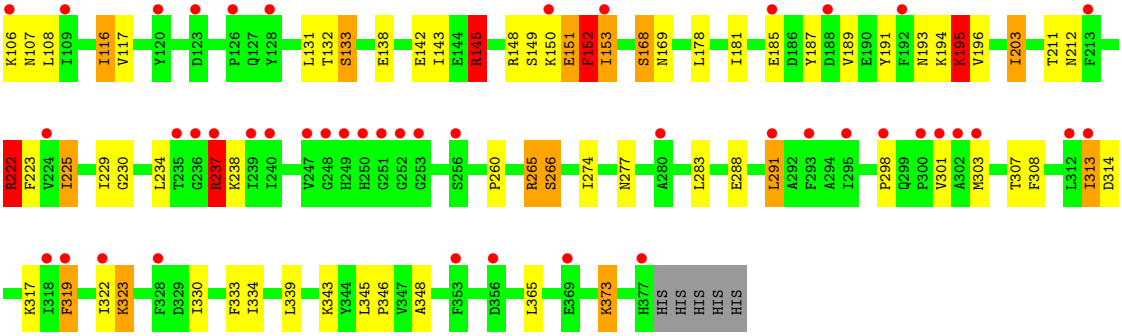




• Molecule 1: Methionine adenosyltransferase

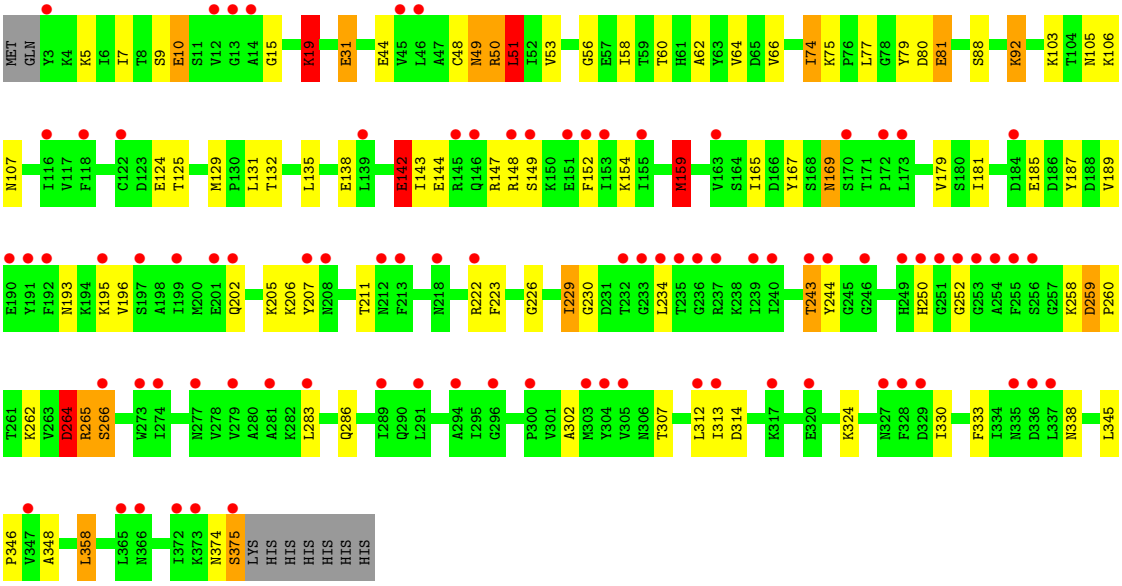
Chain F:





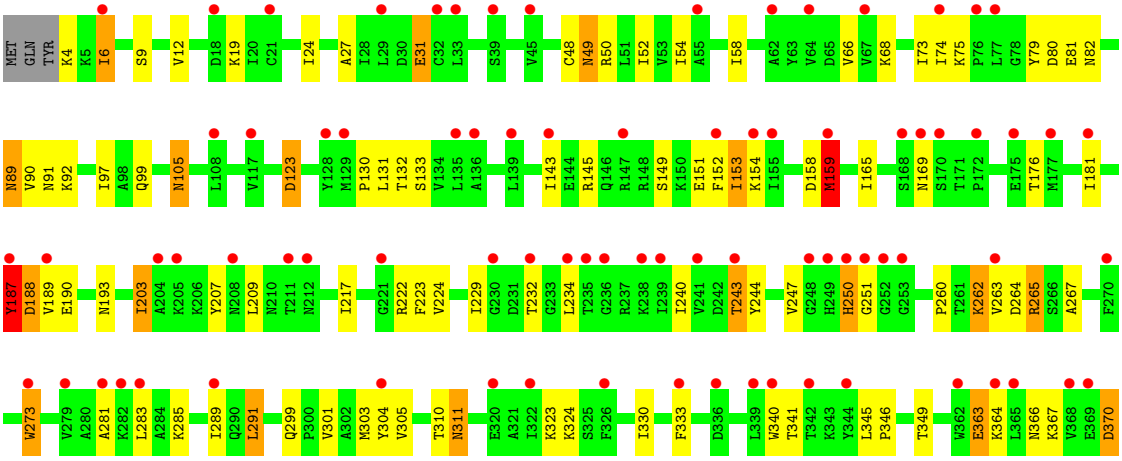
• Molecule 1: Methionine adenosyltransferase

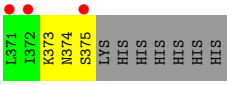
Chain G:



• Molecule 1: Methionine adenosyltransferase

Chain H:




L371
I372
K373
N374
S375
LYS
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	142.37Å 79.47Å 143.79Å 90.00° 105.11° 90.00°	Depositor
Resolution (Å)	47.78 – 2.56 47.78 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.78-2.56) 99.3 (47.78-2.56)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.260 , 0.284 0.260 , 0.283	Depositor DCC
R_{free} test set	4982 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 23.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24088	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6706e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: K, PPK, SAM, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.92	3/2969 (0.1%)	1.06	13/4016 (0.3%)
1	B	0.92	5/3001 (0.2%)	0.99	12/4058 (0.3%)
1	C	0.86	4/2982 (0.1%)	0.98	11/4034 (0.3%)
1	D	0.94	5/2969 (0.2%)	1.03	16/4016 (0.4%)
1	E	0.83	3/2969 (0.1%)	1.12	34/4016 (0.8%)
1	F	0.83	4/2989 (0.1%)	1.11	24/4042 (0.6%)
1	G	0.78	1/2982 (0.0%)	1.07	26/4034 (0.6%)
1	H	0.82	3/2969 (0.1%)	1.11	26/4016 (0.6%)
All	All	0.86	28/23830 (0.1%)	1.06	162/32232 (0.5%)

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	E	0	2
1	F	0	1
1	G	0	1
All	All	0	4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	123	ASP	CB-CG	-8.35	1.34	1.51
1	F	138	GLU	CD-OE2	-7.63	1.17	1.25
1	F	138	GLU	CG-CD	7.04	1.62	1.51
1	D	81	GLU	CG-CD	6.88	1.62	1.51
1	D	320	GLU	CD-OE2	6.65	1.32	1.25

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	ASP	CB-CG-OD1	-18.40	101.74	118.30
1	E	178	LEU	CB-CG-CD1	11.88	131.19	111.00
1	E	57	GLU	OE1-CD-OE2	-11.47	109.54	123.30
1	G	142	GLU	OE1-CD-OE2	-11.29	109.75	123.30
1	F	102	ASP	CB-CG-OD1	-10.98	108.42	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	344	TYR	Peptide
1	E	359	ASP	Mainchain
1	F	212	ASN	Sidechain
1	G	50	ARG	Peptide

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	2917	0	2915	32	0
1	B	2944	0	2944	39	1
1	C	2929	0	2924	36	0
1	D	2917	0	2915	38	0
1	E	2917	0	2915	73	1
1	F	2936	0	2935	78	0
1	G	2929	0	2924	67	0
1	H	2917	0	2915	93	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
2	E	2	0	0	0	0
2	G	2	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
3	G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
4	A	54	0	44	8	0
4	B	54	0	44	0	0
4	C	54	0	44	2	0
4	D	54	0	44	2	0
4	E	54	0	44	1	0
4	F	54	0	44	4	0
4	G	54	0	44	8	0
4	H	54	0	44	7	0
5	A	26	0	2	9	0
5	C	26	0	2	7	0
5	E	26	0	2	3	0
5	G	26	0	2	2	0
6	A	25	0	0	2	0
6	B	21	0	0	0	0
6	C	16	0	0	0	0
6	D	18	0	0	1	0
6	E	15	0	0	1	0
6	F	12	0	0	1	0
6	G	10	0	0	1	0
6	H	6	0	0	0	0
All	All	24088	0	23747	436	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 9.

The worst 5 of 436 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:146:GLN:OE1	1:E:195:LYS:NZ	1.76	1.17
1:E:57:GLU:OE2	4:F:402:SAM:N	1.86	1.08
1:F:145:ARG:NH1	1:F:151:GLU:OE1	1.93	1.00
1:H:130:PRO:HG3	1:H:247:VAL:HG11	1.44	0.99
1:H:74:ILE:HG23	1:H:79:TYR:HB2	1.43	0.98

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)
1:B:373:LYS:NZ	1:E:35:GLN:O[1_556]	2.16	0.04

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	370/382 (97%)	358 (97%)	11 (3%)	1 (0%)	41	50
1	B	373/382 (98%)	362 (97%)	9 (2%)	2 (0%)	29	39
1	C	371/382 (97%)	361 (97%)	9 (2%)	1 (0%)	41	50
1	D	370/382 (97%)	357 (96%)	11 (3%)	2 (0%)	29	39
1	E	370/382 (97%)	353 (95%)	13 (4%)	4 (1%)	14	19
1	F	372/382 (97%)	357 (96%)	12 (3%)	3 (1%)	19	27
1	G	371/382 (97%)	358 (96%)	11 (3%)	2 (0%)	29	39
1	H	370/382 (97%)	352 (95%)	15 (4%)	3 (1%)	19	27
All	All	2967/3056 (97%)	2858 (96%)	91 (3%)	18 (1%)	25	33

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	49	ASN
1	G	313	ILE
1	H	188	ASP
1	A	49	ASN
1	B	49	ASN

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	322/332 (97%)	307 (95%)	15 (5%)	26	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	325/332 (98%)	308 (95%)	17 (5%)	23 31
1	C	323/332 (97%)	302 (94%)	21 (6%)	17 22
1	D	322/332 (97%)	302 (94%)	20 (6%)	18 23
1	E	322/332 (97%)	293 (91%)	29 (9%)	9 11
1	F	324/332 (98%)	295 (91%)	29 (9%)	9 11
1	G	323/332 (97%)	294 (91%)	29 (9%)	9 11
1	H	322/332 (97%)	290 (90%)	32 (10%)	8 9
All	All	2583/2656 (97%)	2391 (93%)	192 (7%)	13 18

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	169	ASN
1	G	169	ASN
1	F	203	ILE
1	F	373	LYS
1	G	264	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	311	ASN
1	G	137	HIS
1	F	82	ASN
1	F	277	ASN
1	G	250	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 23 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SAM	E	406	-	24,29,29	1.46	5 (20%)	23,42,42	2.34	9 (39%)
5	PPK	G	409	2,3	11,12,12	3.52	6 (54%)	15,20,20	2.64	6 (40%)
4	SAM	E	404	-	24,29,29	1.37	2 (8%)	23,42,42	1.82	6 (26%)
5	PPK	E	409	2,3	11,12,12	3.29	6 (54%)	15,20,20	3.05	6 (40%)
4	SAM	C	406	-	24,29,29	1.53	4 (16%)	23,42,42	2.35	9 (39%)
5	PPK	C	405	2,3	11,12,12	4.69	7 (63%)	15,20,20	3.19	9 (60%)
4	SAM	D	403	-	24,29,29	1.79	4 (16%)	23,42,42	3.00	8 (34%)
4	SAM	B	402	-	24,29,29	1.66	5 (20%)	23,42,42	1.97	6 (26%)
4	SAM	A	406	-	24,29,29	1.12	2 (8%)	23,42,42	2.09	7 (30%)
5	PPK	C	408	3	11,12,12	4.60	5 (45%)	15,20,20	5.06	7 (46%)
4	SAM	F	403	-	24,29,29	1.16	2 (8%)	23,42,42	2.07	7 (30%)
4	SAM	H	403	-	24,29,29	1.26	4 (16%)	23,42,42	1.96	7 (30%)
4	SAM	A	404	-	24,29,29	1.32	3 (12%)	23,42,42	1.93	7 (30%)
5	PPK	A	405	2,3	11,12,12	5.68	5 (45%)	15,20,20	3.80	9 (60%)
5	PPK	A	409	2,3	11,12,12	5.94	7 (63%)	15,20,20	3.04	7 (46%)
4	SAM	F	402	-	24,29,29	1.11	1 (4%)	23,42,42	2.01	8 (34%)
5	PPK	E	405	2,3	11,12,12	5.07	7 (63%)	15,20,20	2.42	7 (46%)
4	SAM	D	402	-	24,29,29	1.06	1 (4%)	23,42,42	2.42	9 (39%)
4	SAM	G	405	-	24,29,29	1.28	1 (4%)	23,42,42	2.40	8 (34%)
4	SAM	H	402	-	24,29,29	1.12	0	23,42,42	2.06	8 (34%)
4	SAM	G	403	-	24,29,29	1.12	3 (12%)	23,42,42	2.30	9 (39%)
4	SAM	B	403	-	24,29,29	1.27	3 (12%)	23,42,42	1.84	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PPK	G	404	2,3	11,12,12	4.96	7 (63%)	15,20,20	3.83	4 (26%)
4	SAM	C	404	-	24,29,29	1.41	4 (16%)	23,42,42	2.07	9 (39%)

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
4	SAM	E	406	-	-	9/12/33/33	0/3/3/3
5	PPK	G	409	2,3	-	1/8/12/12	-
4	SAM	E	404	-	-	6/12/33/33	0/3/3/3
5	PPK	E	409	2,3	-	3/8/12/12	-
4	SAM	C	406	-	-	7/12/33/33	0/3/3/3
5	PPK	C	405	2,3	-	2/8/12/12	-
4	SAM	D	403	-	-	4/12/33/33	0/3/3/3
4	SAM	B	402	-	-	7/12/33/33	0/3/3/3
4	SAM	A	406	-	-	4/12/33/33	0/3/3/3
5	PPK	C	408	3	-	2/8/12/12	-
4	SAM	F	403	-	-	3/12/33/33	0/3/3/3
4	SAM	H	403	-	-	4/12/33/33	0/3/3/3
4	SAM	A	404	-	-	4/12/33/33	0/3/3/3
5	PPK	A	405	2,3	-	2/8/12/12	-
5	PPK	A	409	2,3	-	2/8/12/12	-
4	SAM	F	402	-	-	7/12/33/33	0/3/3/3
5	PPK	E	405	2,3	-	1/8/12/12	-
4	SAM	D	402	-	-	4/12/33/33	0/3/3/3
4	SAM	G	405	-	-	5/12/33/33	0/3/3/3
4	SAM	H	402	-	-	5/12/33/33	0/3/3/3
4	SAM	G	403	-	-	6/12/33/33	0/3/3/3
4	SAM	B	403	-	-	3/12/33/33	0/3/3/3
5	PPK	G	404	2,3	-	2/8/12/12	-
4	SAM	C	404	-	-	11/12/33/33	0/3/3/3

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	PPK	PG-O3G	17.47	1.73	1.46
5	A	409	PPK	PG-O3G	15.35	1.70	1.46
5	E	405	PPK	PG-O3G	13.30	1.67	1.46
5	C	405	PPK	PB-O2B	12.98	1.66	1.46
5	C	408	PPK	PG-O3G	12.73	1.66	1.46

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	408	PPK	O3G-PG-N3B	-15.17	89.43	111.77
5	G	404	PPK	O3G-PG-N3B	-12.61	93.20	111.77
5	A	405	PPK	O1B-PB-O2B	10.05	131.00	109.92
5	C	408	PPK	O2B-PB-N3B	-9.59	97.65	111.77
4	D	403	SAM	CB-CA-C	8.65	130.89	110.30

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406	SAM	CB-CG-SD-CE
4	B	402	SAM	N-CA-CB-CG
4	B	402	SAM	C-CA-CB-CG
4	B	402	SAM	CA-CB-CG-SD
4	B	402	SAM	CB-CG-SD-CE

There are no ring outliers.

19 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	409	PPK	1	0
4	E	404	SAM	1	0
5	E	409	PPK	3	0
4	C	406	SAM	1	0
5	C	405	PPK	3	0
4	D	403	SAM	2	0
4	A	406	SAM	7	0
5	C	408	PPK	4	0
4	F	403	SAM	1	0
4	H	403	SAM	6	0
4	A	404	SAM	1	0
5	A	405	PPK	7	0
5	A	409	PPK	2	0

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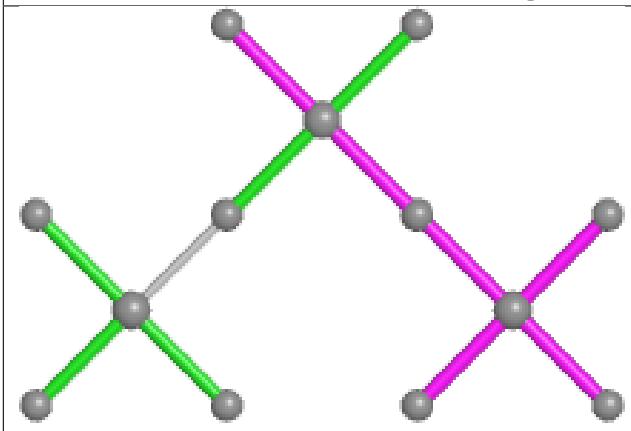
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	402	SAM	3	0
4	G	405	SAM	4	0
4	H	402	SAM	1	0
4	G	403	SAM	4	0
5	G	404	PPK	1	0
4	C	404	SAM	1	0

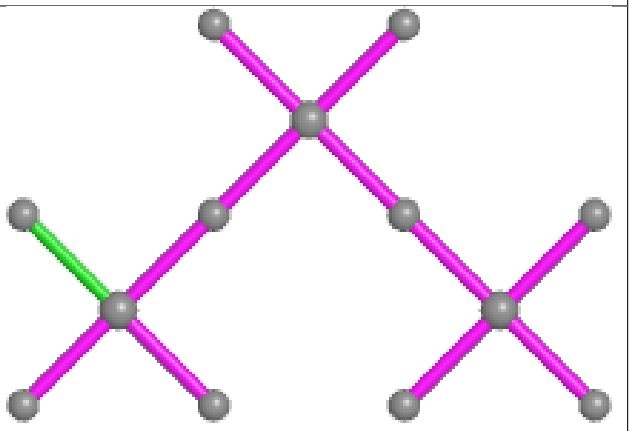
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 SAM E 406

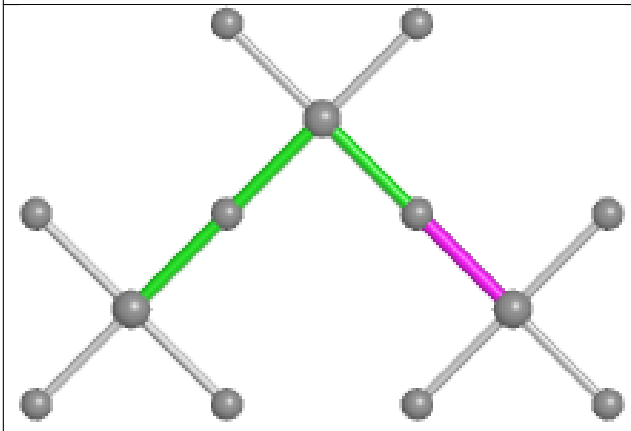
Ligand PPK G 409



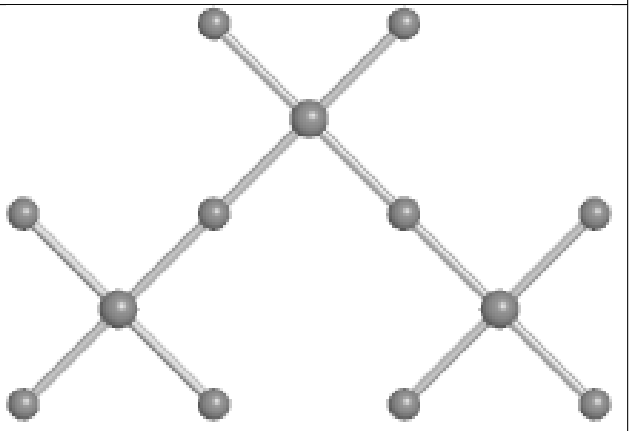
Bond lengths



Bond angles

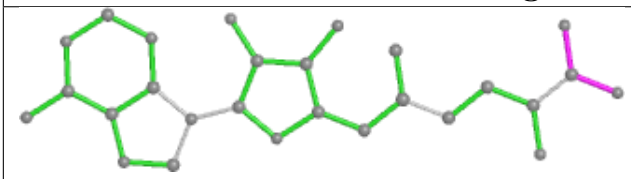


Torsions



Rings

Ligand SAM E 404



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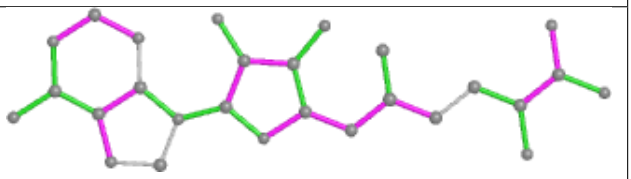
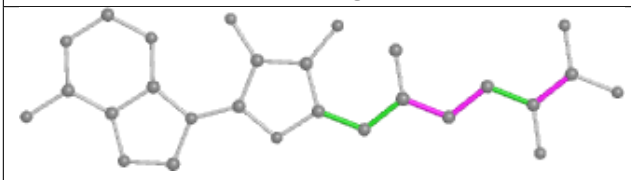


Bond angles



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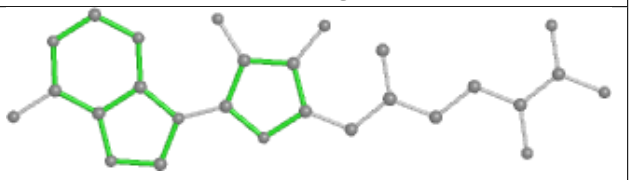
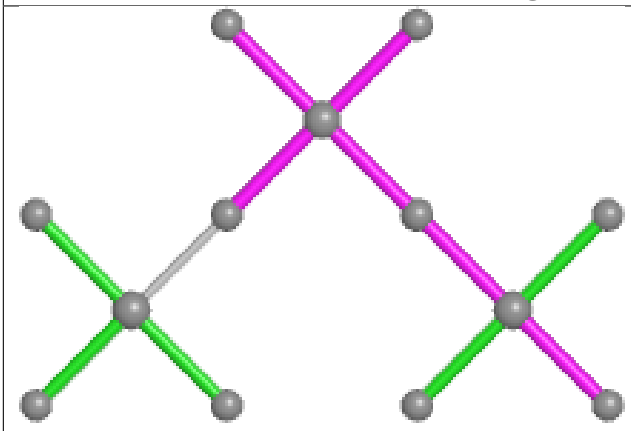


Rings

Ligand PPK E 409



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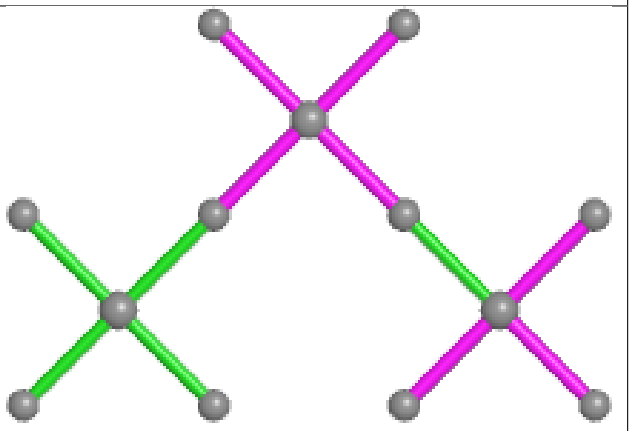
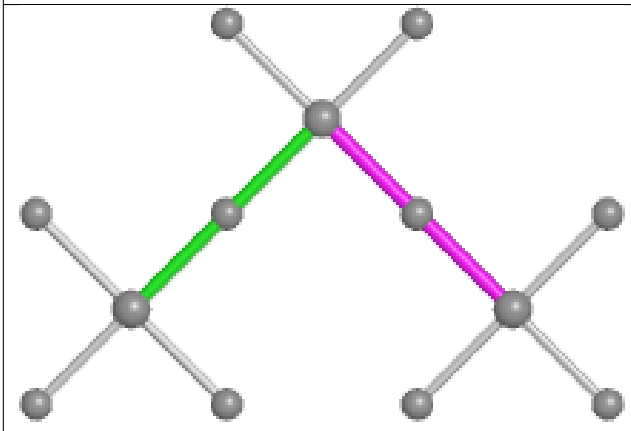
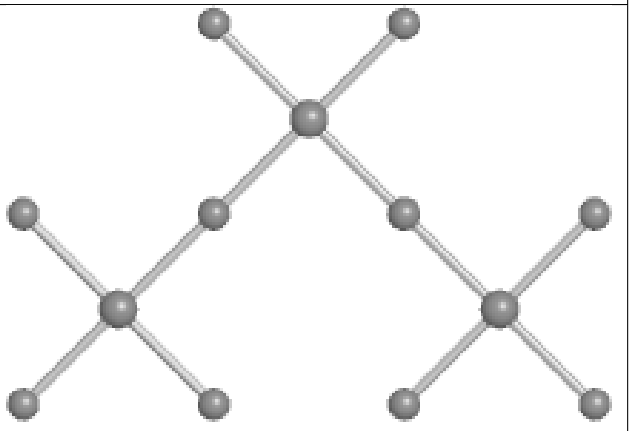


Bond angles

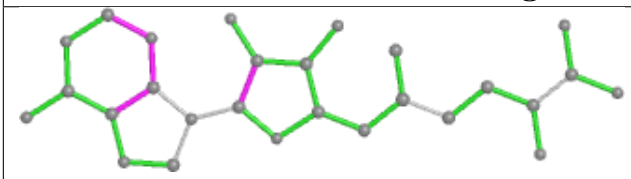


Torsions

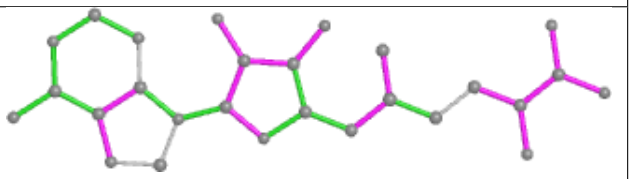


Rings

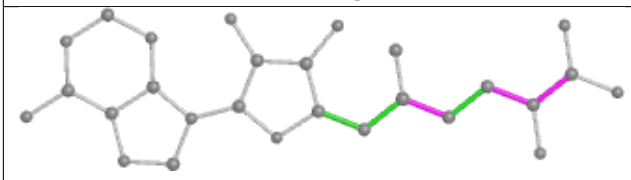
Ligand SAM C 406



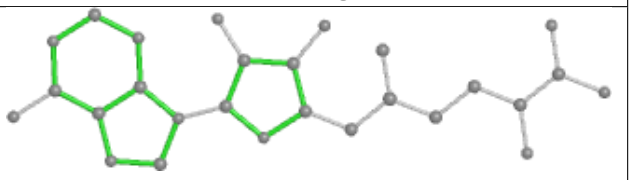
Bond lengths



Bond angles

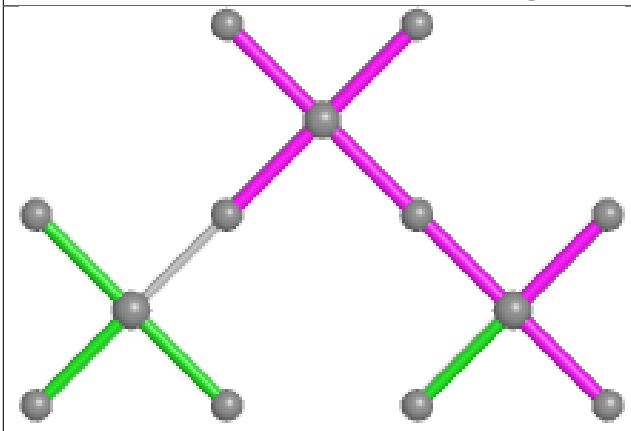


Torsions

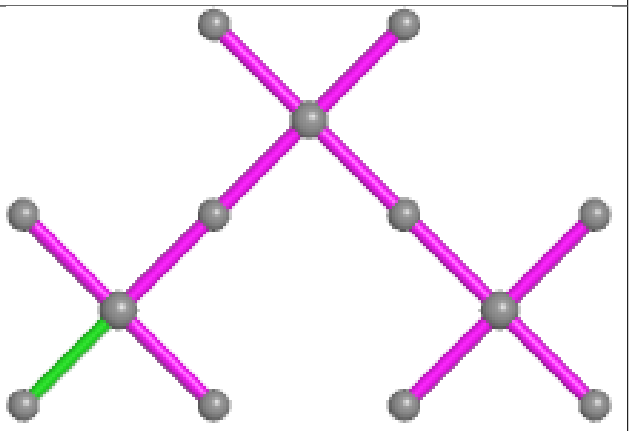


Rings

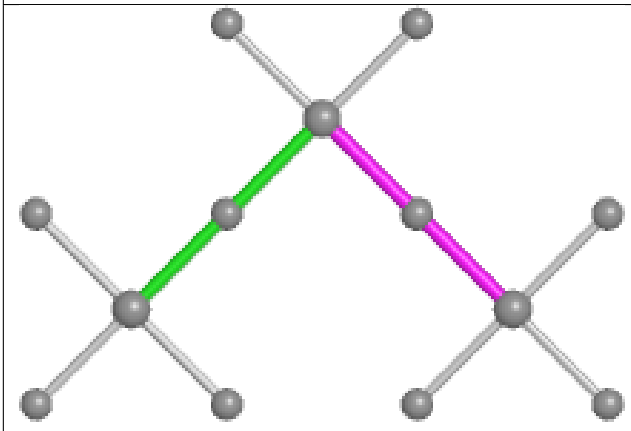
Ligand PPK C 405



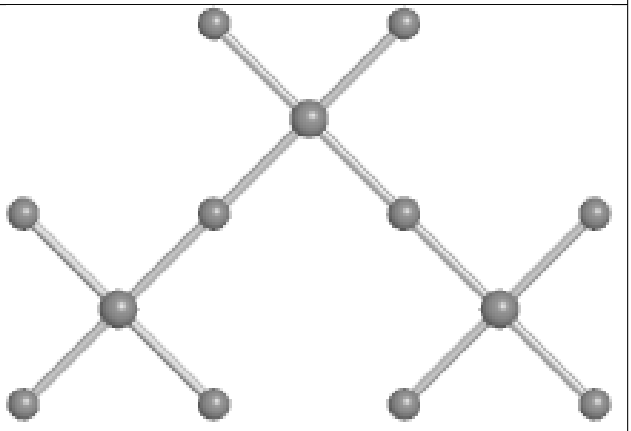
Bond lengths



Bond angles

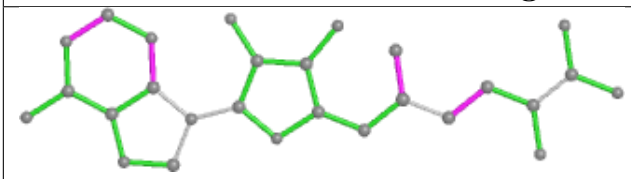


Torsions

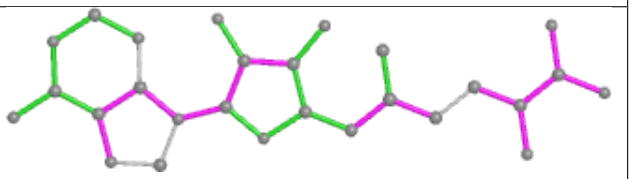


Rings

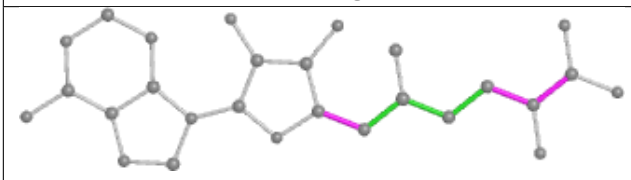
Ligand SAM D 403



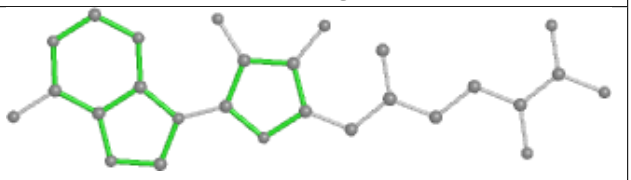
Bond lengths



Bond angles

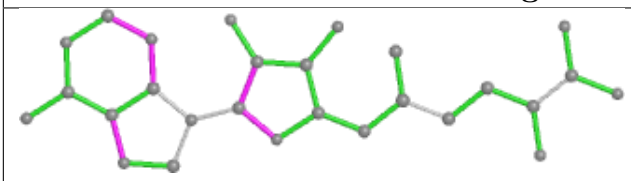


Torsions

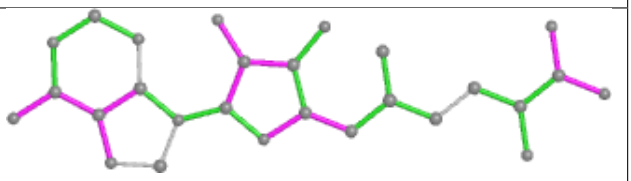


Rings

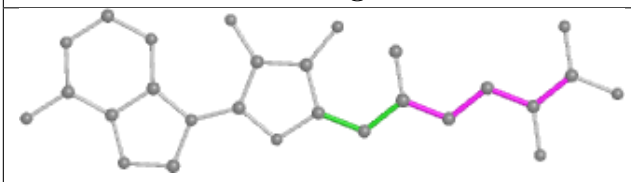
Ligand SAM B 402



Bond lengths



Bond angles



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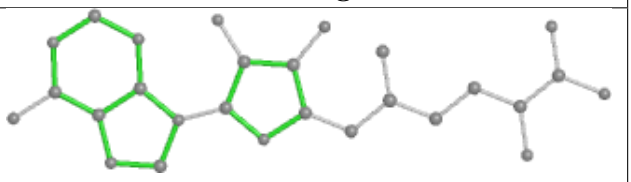
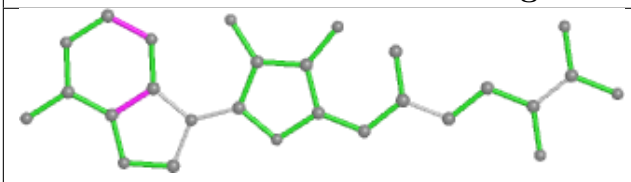


Rings

Ligand SAM A 406



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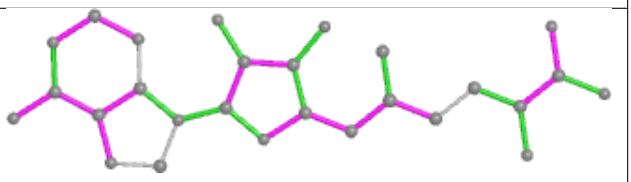
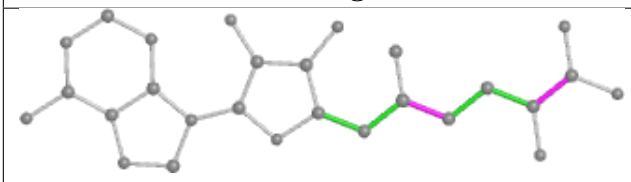


Bond angles



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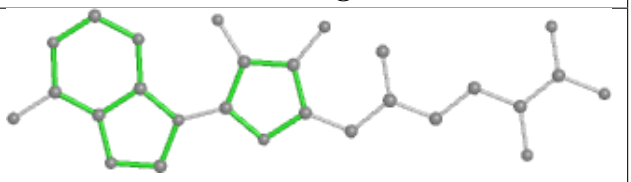
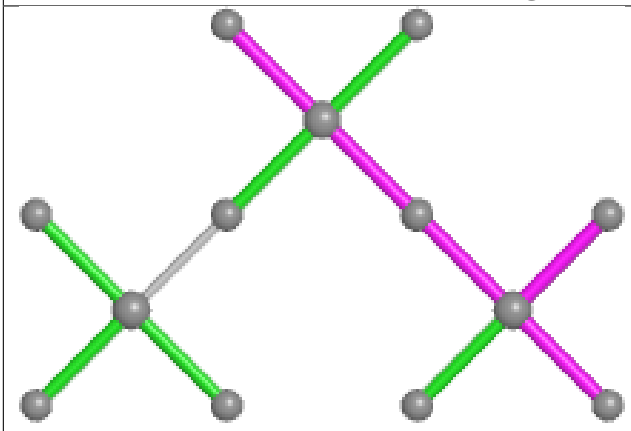


Rings

Ligand PPK C 408



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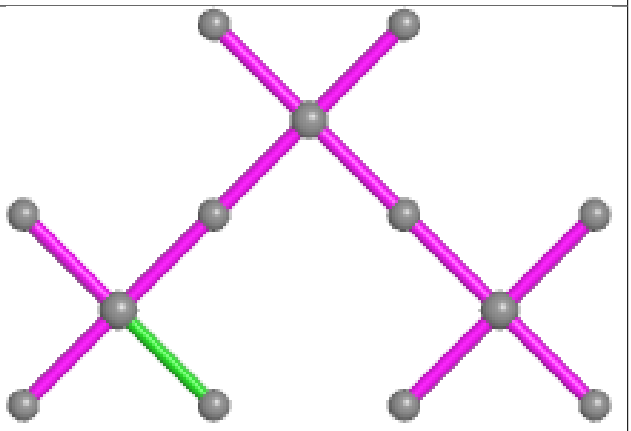
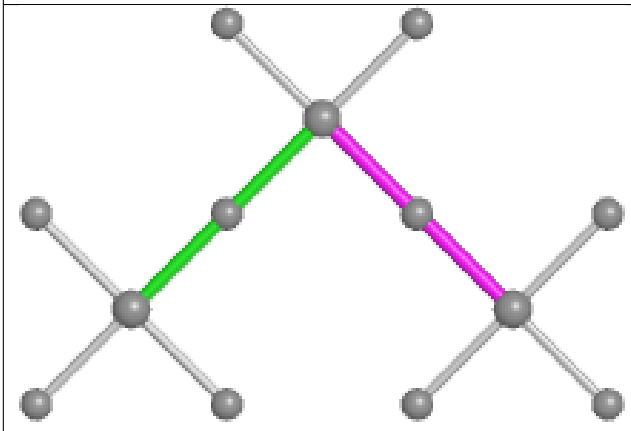


Bond angles



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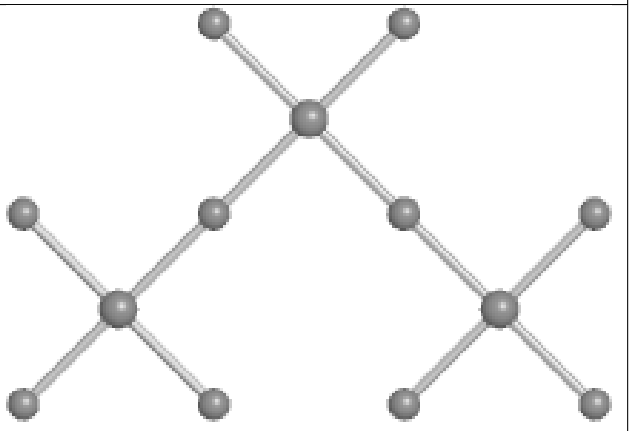
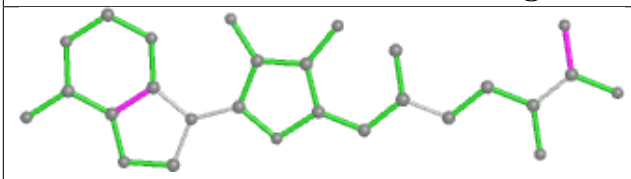


Rings

Ligand SAM F 403



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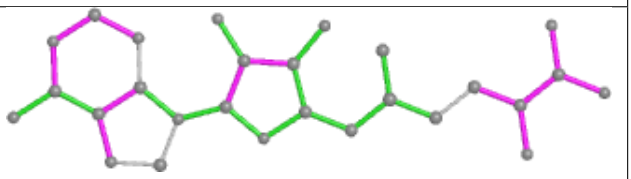
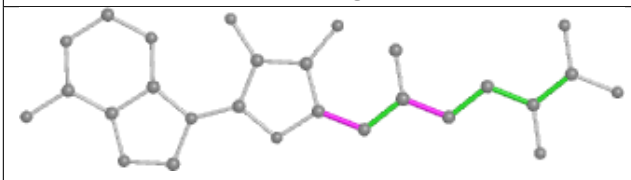


Bond angles



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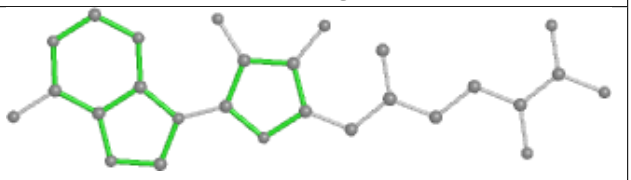
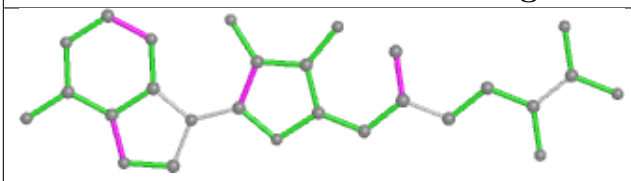


Rings

Ligand SAM H 403



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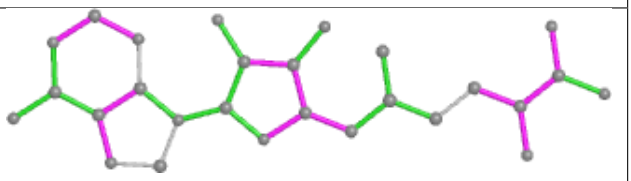
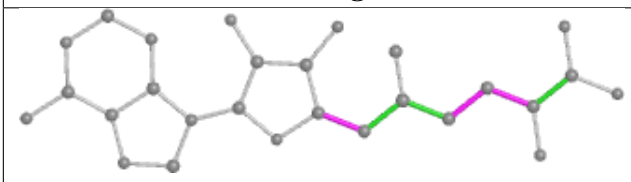


Bond angles



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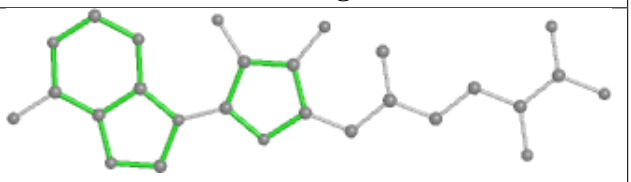
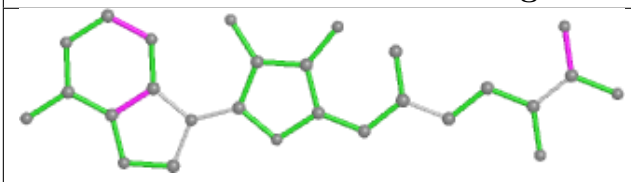
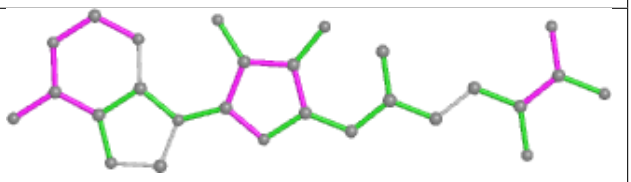


Rings

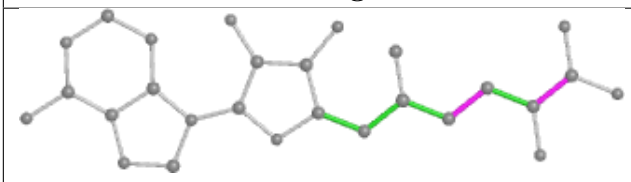
Ligand SAM A 404



Bond lengths



Bond angles



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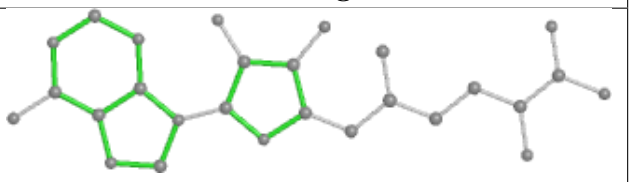
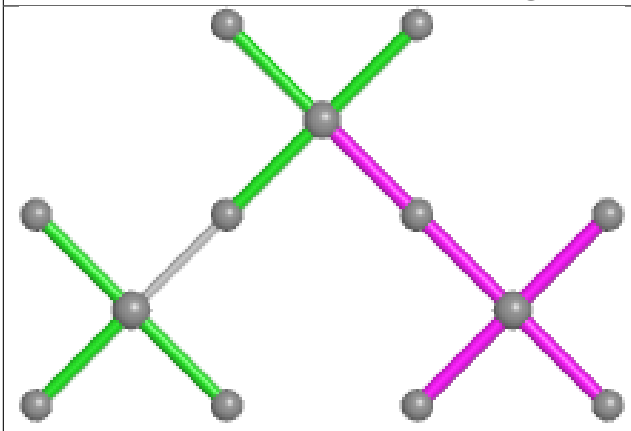


Rings

Ligand PPK A 405



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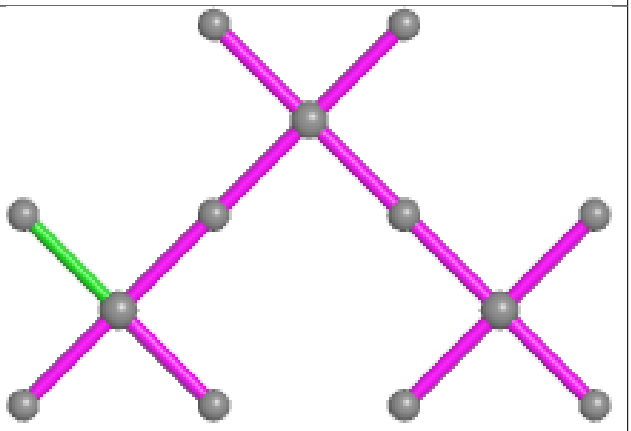
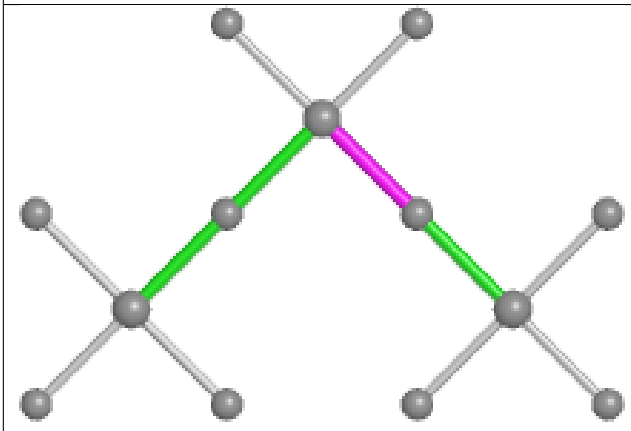
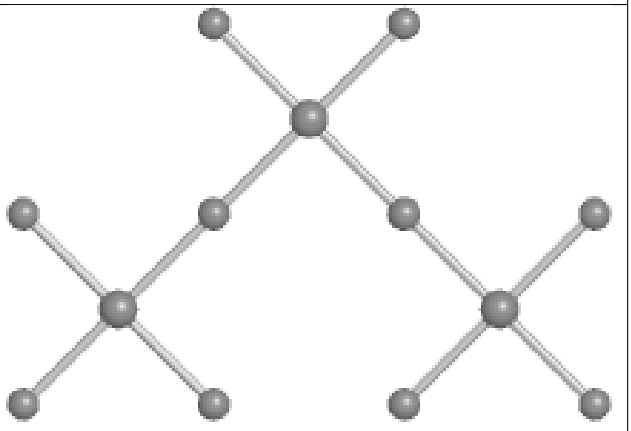


Bond angles

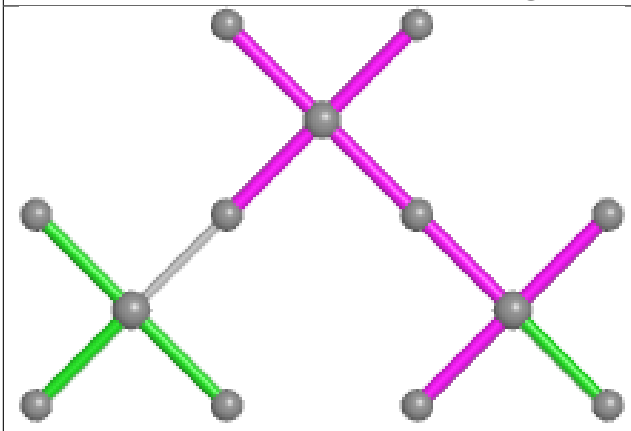


Torsions

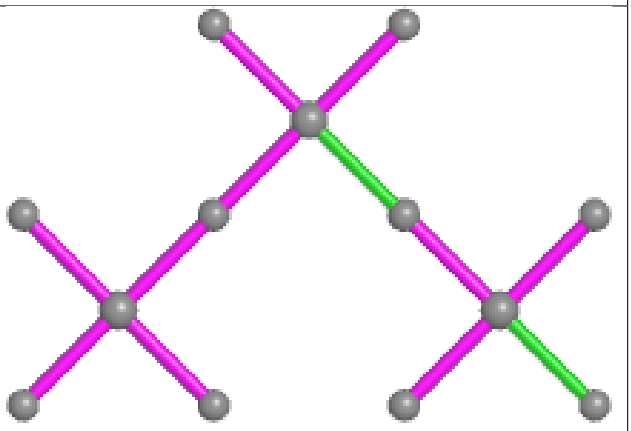


Rings

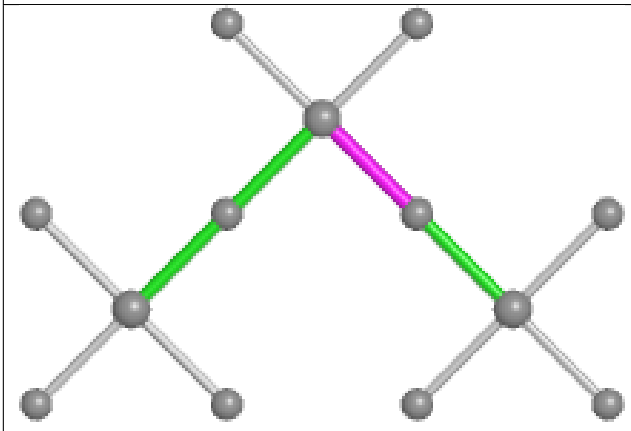
Ligand PPK A 409



Bond lengths



Bond angles



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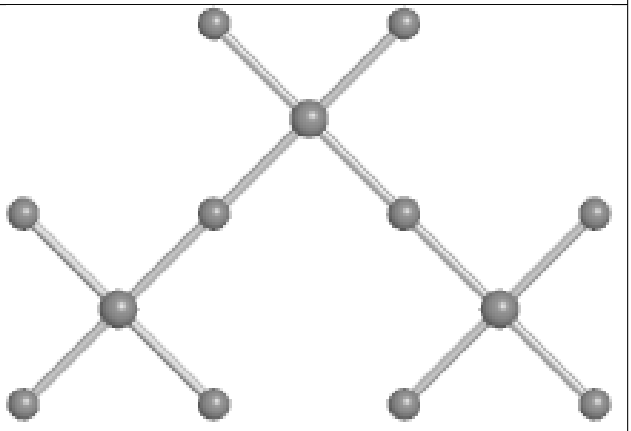
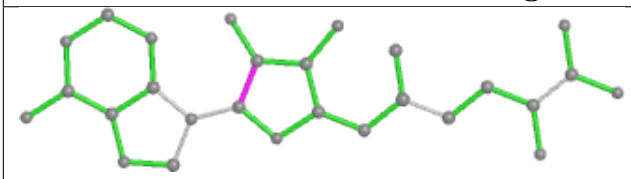


Rings

Ligand SAM F 402



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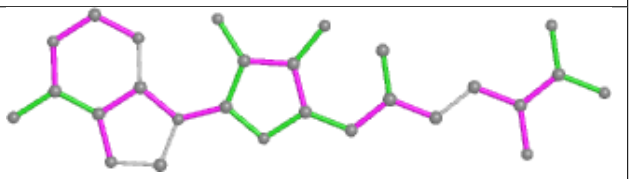
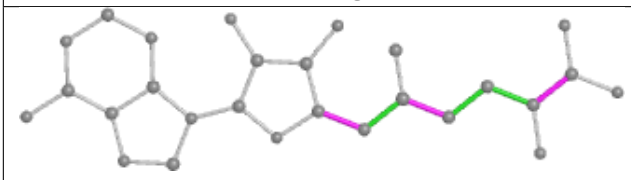


Bond angles



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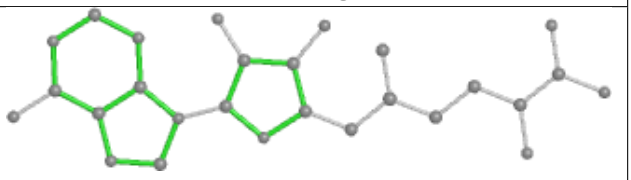
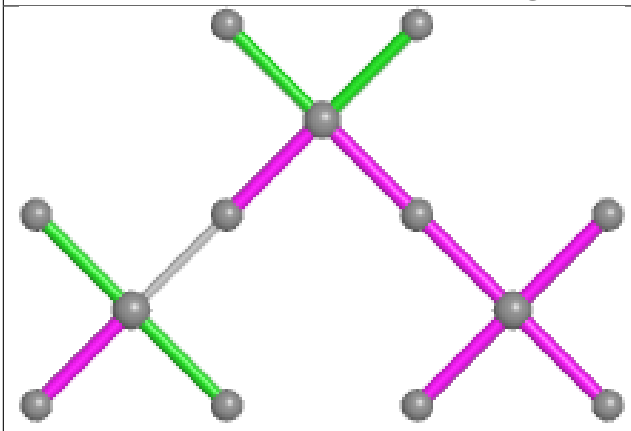
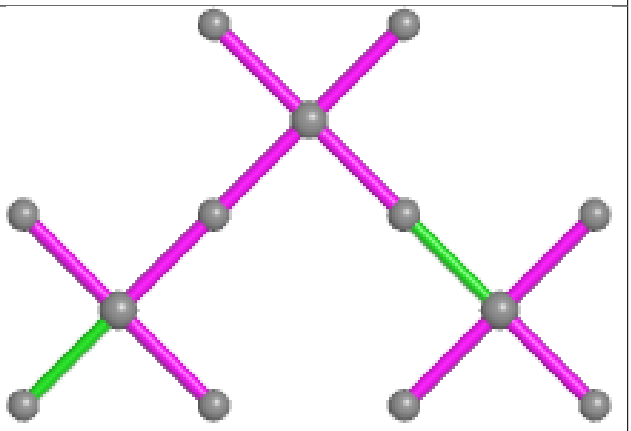


Rings

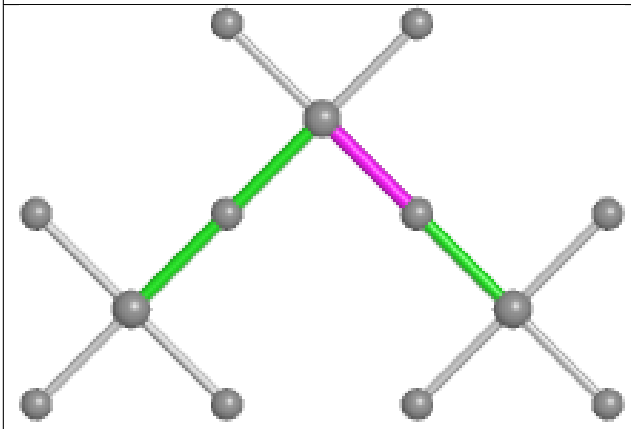
Ligand PPK E 405



Bond lengths



Bond angles



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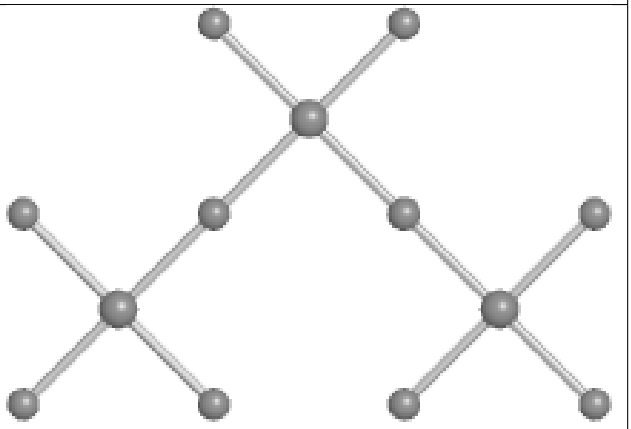
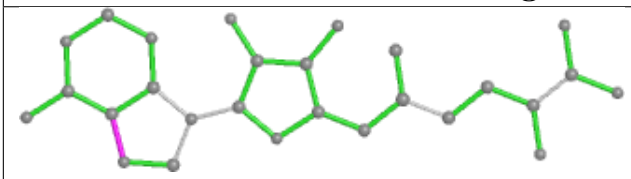


Rings

Ligand SAM D 402



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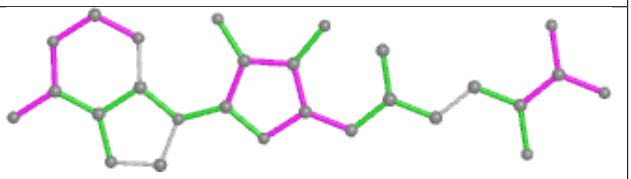
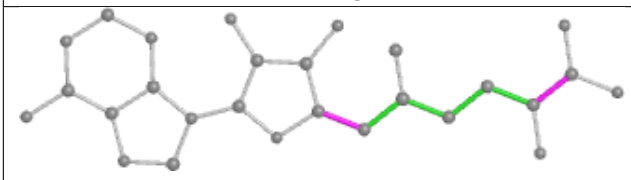


Bond angles



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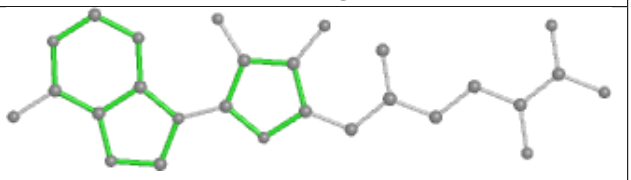
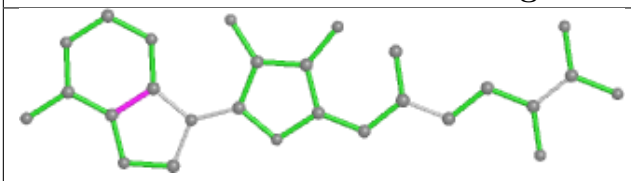
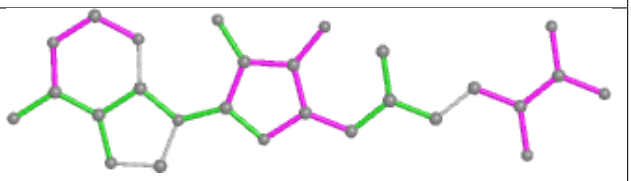


Rings

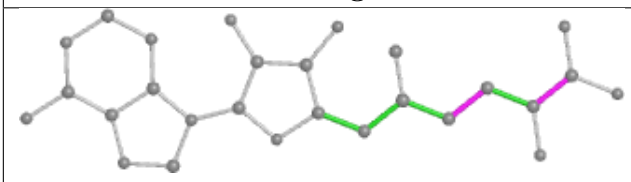
Ligand SAM G 405



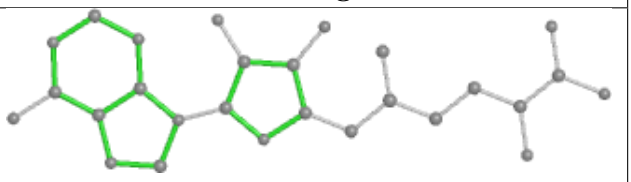
Bond lengths



Bond angles

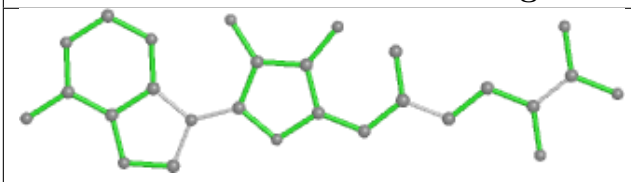


Torsions

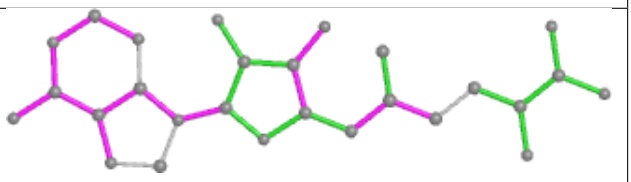


Rings

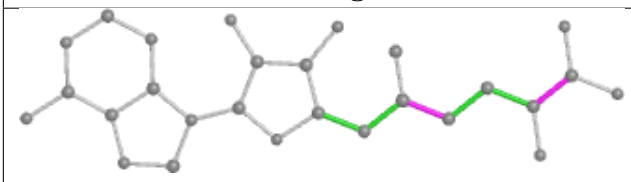
Ligand SAM H 402



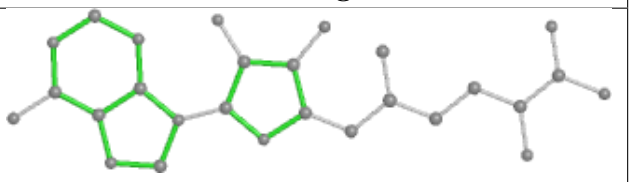
Bond lengths



Bond angles

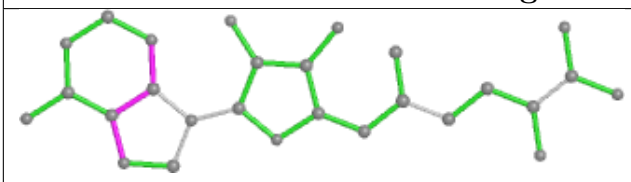


Torsions

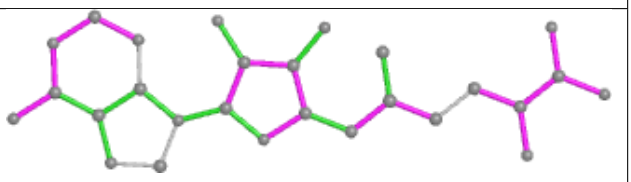


Rings

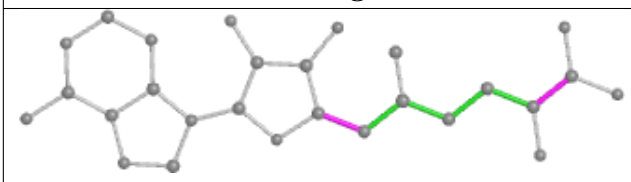
Ligand SAM G 403



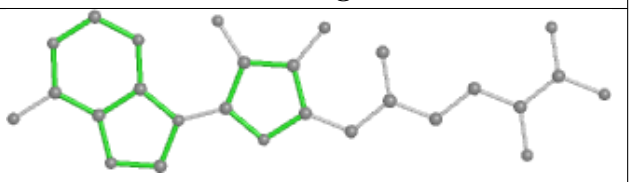
Bond lengths



Bond angles

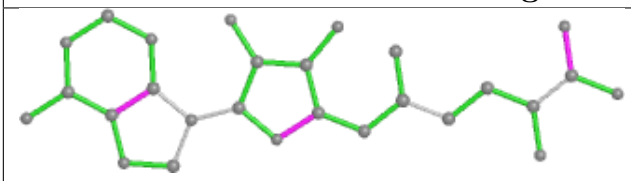


Torsions

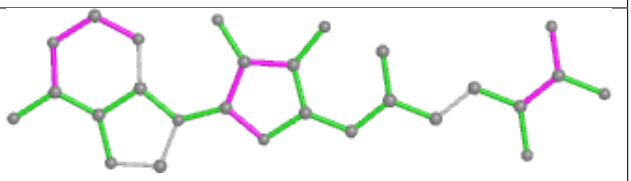


Rings

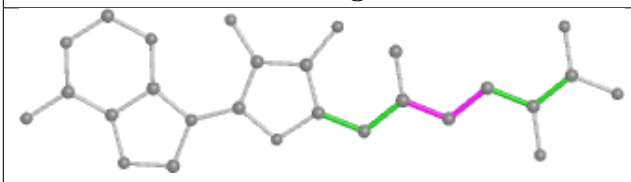
Ligand SAM B 403



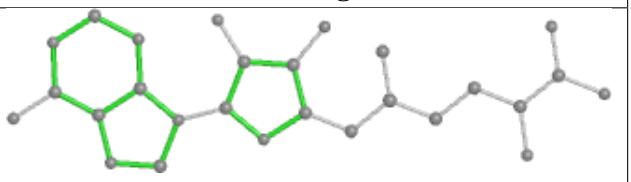
Bond lengths



Bond angles

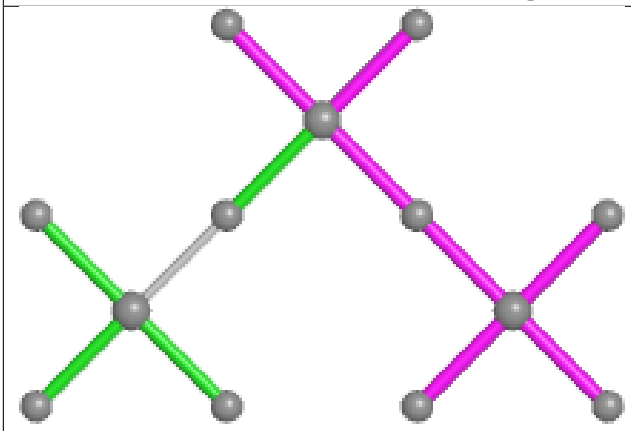


Torsions

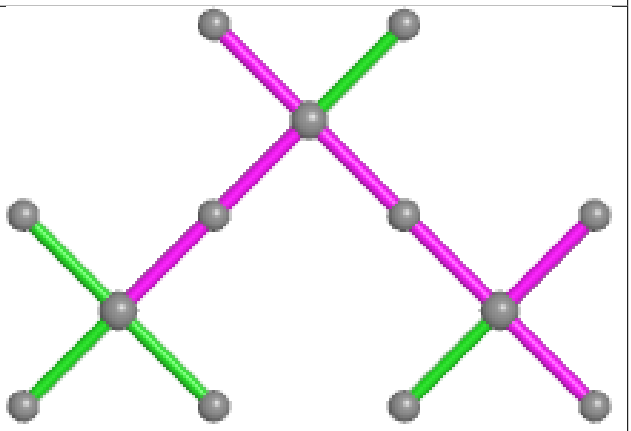


Rings

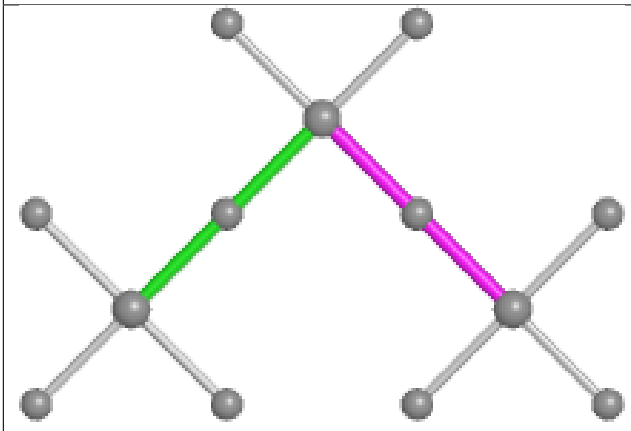
Ligand PPK G 404



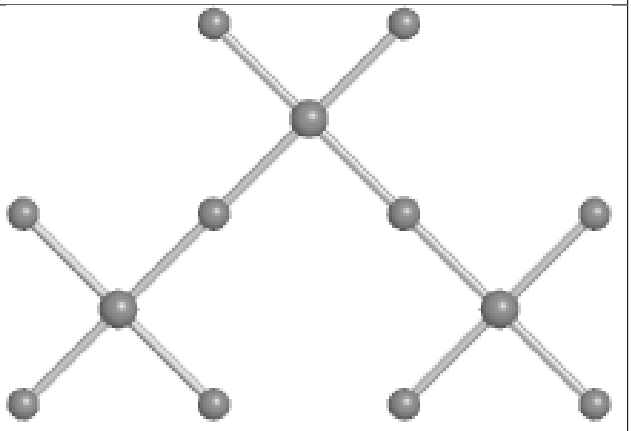
Bond lengths



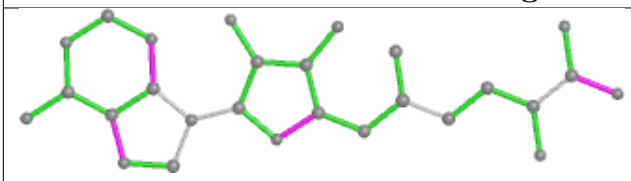
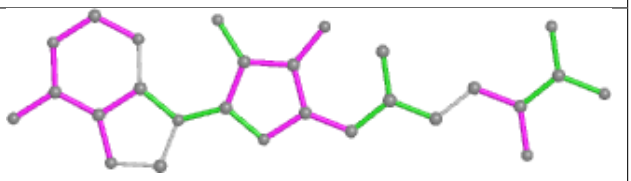
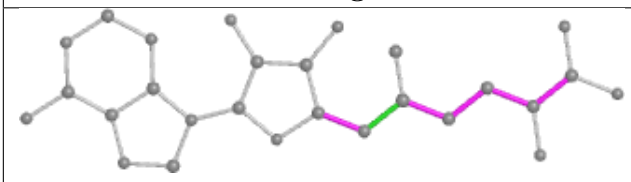
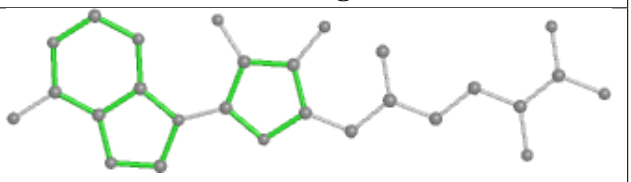
Bond angles



Torsions



Rings

Ligand SAM C 404	
 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	372/382 (97%)	0.57	16 (4%)	35	44	36, 47, 66, 89	0
1	B	374/382 (97%)	0.52	12 (3%)	47	57	34, 46, 65, 96	0
1	C	373/382 (97%)	0.62	21 (5%)	24	31	44, 57, 84, 106	0
1	D	372/382 (97%)	0.54	18 (4%)	30	39	44, 58, 81, 94	0
1	E	372/382 (97%)	1.11	60 (16%)	1	2	58, 75, 89, 109	0
1	F	374/382 (97%)	1.05	58 (15%)	2	3	60, 74, 95, 131	0
1	G	373/382 (97%)	1.35	87 (23%)	0	0	62, 80, 98, 125	0
1	H	372/382 (97%)	1.26	84 (22%)	0	0	63, 80, 99, 120	0
All	All	2982/3056 (97%)	0.88	356 (11%)	4	6	34, 68, 92, 131	0

The worst 5 of 356 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	322	ILE	7.1
1	G	149	SER	7.1
1	H	108	LEU	6.1
1	G	313	ILE	5.9
1	G	14	ALA	5.8

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	G	402	1/1	0.76	0.54	72,72,72,72	0
3	MG	E	403	1/1	0.77	0.45	68,68,68,68	0
2	K	G	408	1/1	0.77	0.27	121,121,121,121	0
4	SAM	G	403	27/27	0.81	0.22	78,81,86,86	0
4	SAM	F	403	27/27	0.83	0.22	76,78,96,97	0
4	SAM	G	405	27/27	0.86	0.27	77,87,94,95	0
2	K	E	408	1/1	0.88	0.29	75,75,75,75	0
4	SAM	H	403	27/27	0.88	0.23	76,81,85,87	0
4	SAM	H	402	27/27	0.89	0.26	76,81,97,101	0
3	MG	A	407	1/1	0.90	0.48	39,39,39,39	0
4	SAM	A	406	27/27	0.90	0.22	60,62,101,104	0
4	SAM	E	406	27/27	0.90	0.18	71,75,81,83	0
3	MG	A	403	1/1	0.90	0.52	37,37,37,37	0
4	SAM	E	404	27/27	0.92	0.18	69,71,81,82	0
4	SAM	A	404	27/27	0.92	0.19	44,45,54,54	0
4	SAM	F	402	27/27	0.92	0.17	61,63,70,71	0
4	SAM	C	404	27/27	0.92	0.19	54,56,58,58	0
3	MG	C	402	1/1	0.93	0.34	40,40,40,40	0
3	MG	C	403	1/1	0.93	0.51	60,60,60,60	0
4	SAM	B	403	27/27	0.93	0.14	48,52,67,69	0
3	MG	A	402	1/1	0.93	0.47	66,66,66,66	0
3	MG	B	401	1/1	0.93	0.54	60,60,60,60	0
3	MG	G	406	1/1	0.93	0.50	67,67,67,67	0
3	MG	E	407	1/1	0.94	0.34	49,49,49,49	0
4	SAM	C	406	27/27	0.94	0.19	53,55,68,71	0
4	SAM	D	402	27/27	0.94	0.18	53,55,59,60	0
4	SAM	D	403	27/27	0.94	0.16	49,52,61,61	0
3	MG	F	401	1/1	0.94	0.31	77,77,77,77	0
3	MG	G	407	1/1	0.94	0.62	60,60,60,60	0
5	PPK	E	409	13/13	0.94	0.22	60,63,69,71	0
2	K	C	401	1/1	0.95	0.19	67,67,67,67	0
2	K	A	401	1/1	0.95	0.12	50,50,50,50	0
2	K	A	408	1/1	0.95	0.16	57,57,57,57	0
4	SAM	B	402	27/27	0.95	0.17	37,39,46,46	0
3	MG	C	407	1/1	0.95	0.56	53,53,53,53	0
5	PPK	E	405	13/13	0.95	0.19	59,60,61,62	0
3	MG	D	401	1/1	0.95	0.30	39,39,39,39	0

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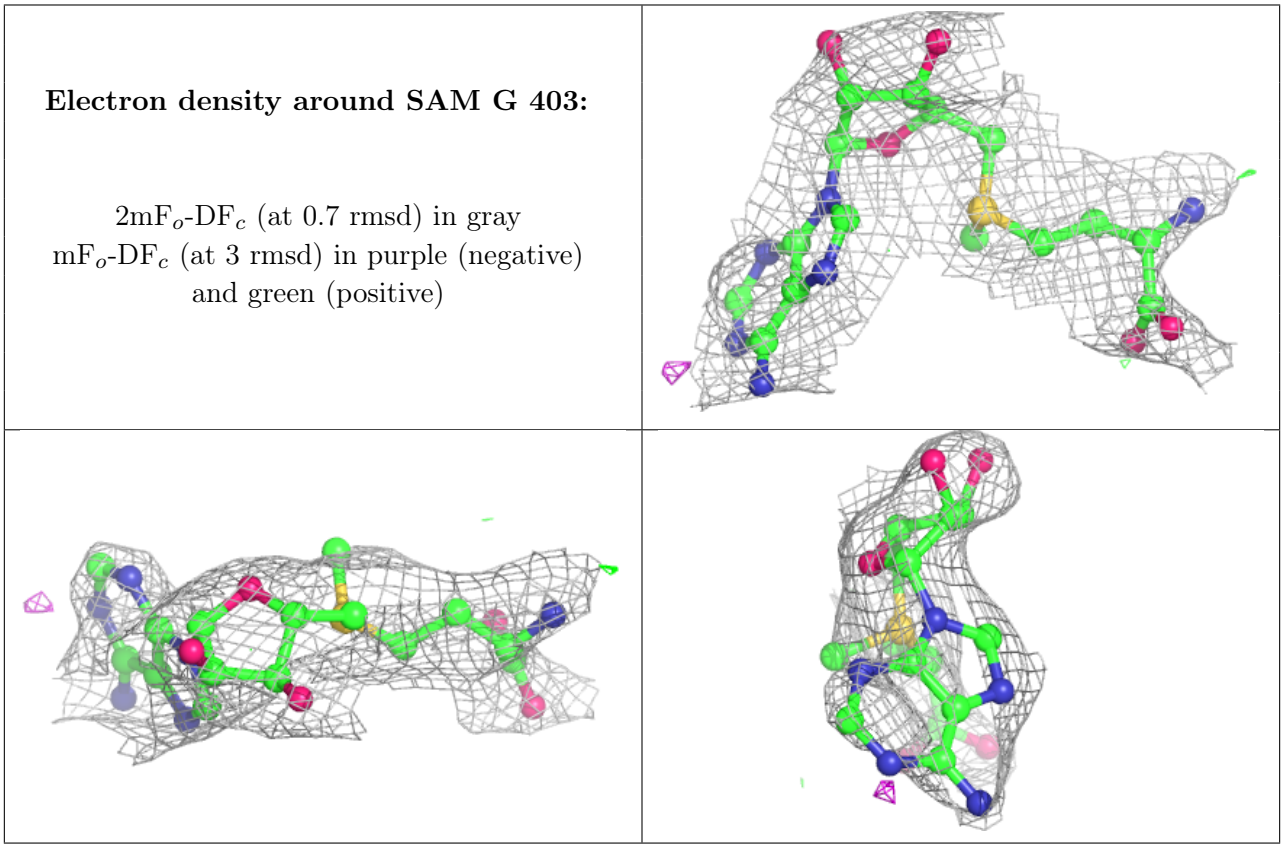
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PPK	G	409	13/13	0.95	0.17	70,72,73,74	0
2	K	E	401	1/1	0.96	0.18	73,73,73,73	0
5	PPK	A	405	13/13	0.96	0.24	41,42,43,43	0
5	PPK	C	405	13/13	0.96	0.21	41,42,43,43	0
5	PPK	C	408	13/13	0.97	0.20	42,42,43,43	0
5	PPK	G	404	13/13	0.97	0.26	61,62,64,66	0
2	K	G	401	1/1	0.97	0.21	67,67,67,67	0
3	MG	H	401	1/1	0.98	0.29	60,60,60,60	0
5	PPK	A	409	13/13	0.98	0.21	36,36,38,38	0
3	MG	E	402	1/1	0.99	0.35	73,73,73,73	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.

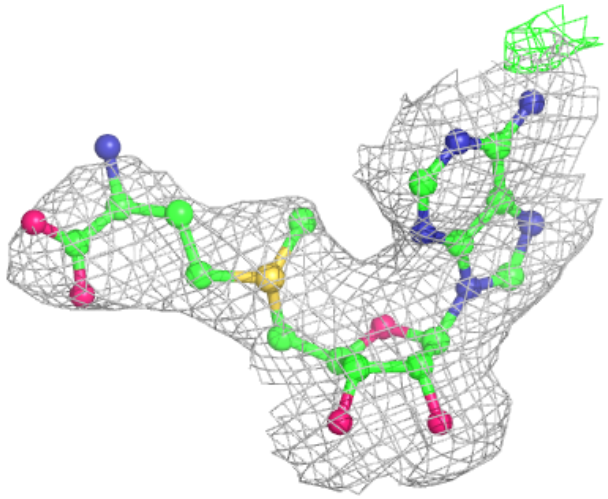
Electron density around SAM G 403:

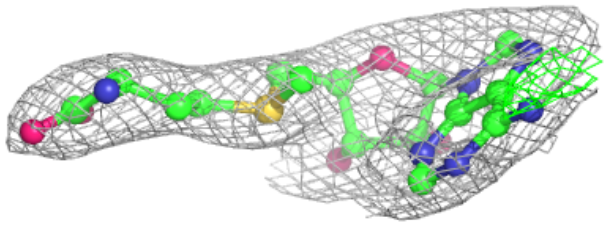
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

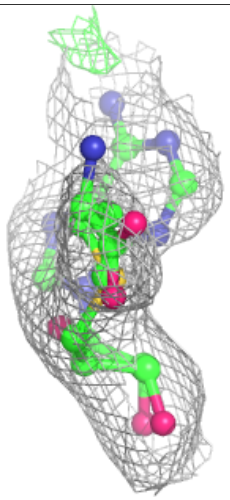


Electron density around SAM F 403:

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

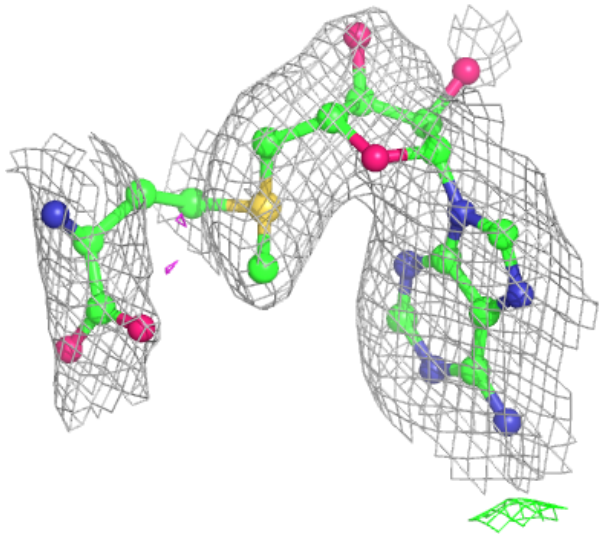


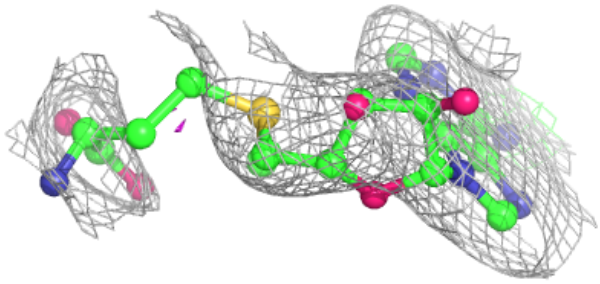


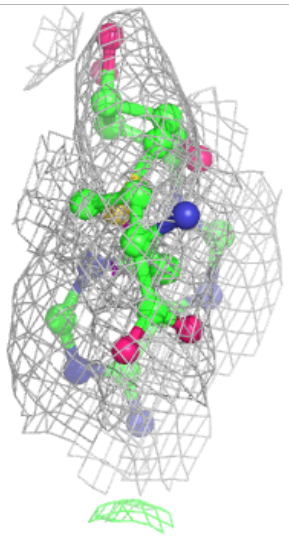


Electron density around SAM G 405:

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

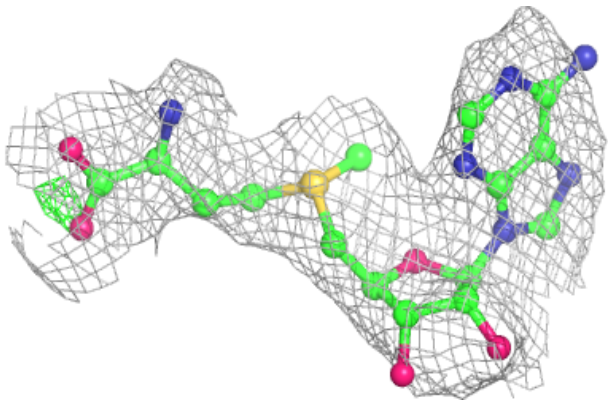


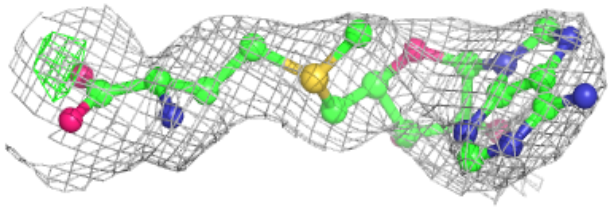


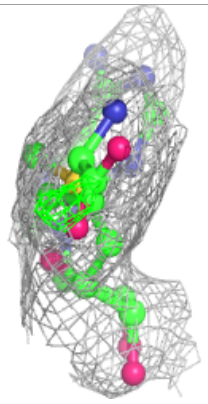


Electron density around SAM H 403:

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

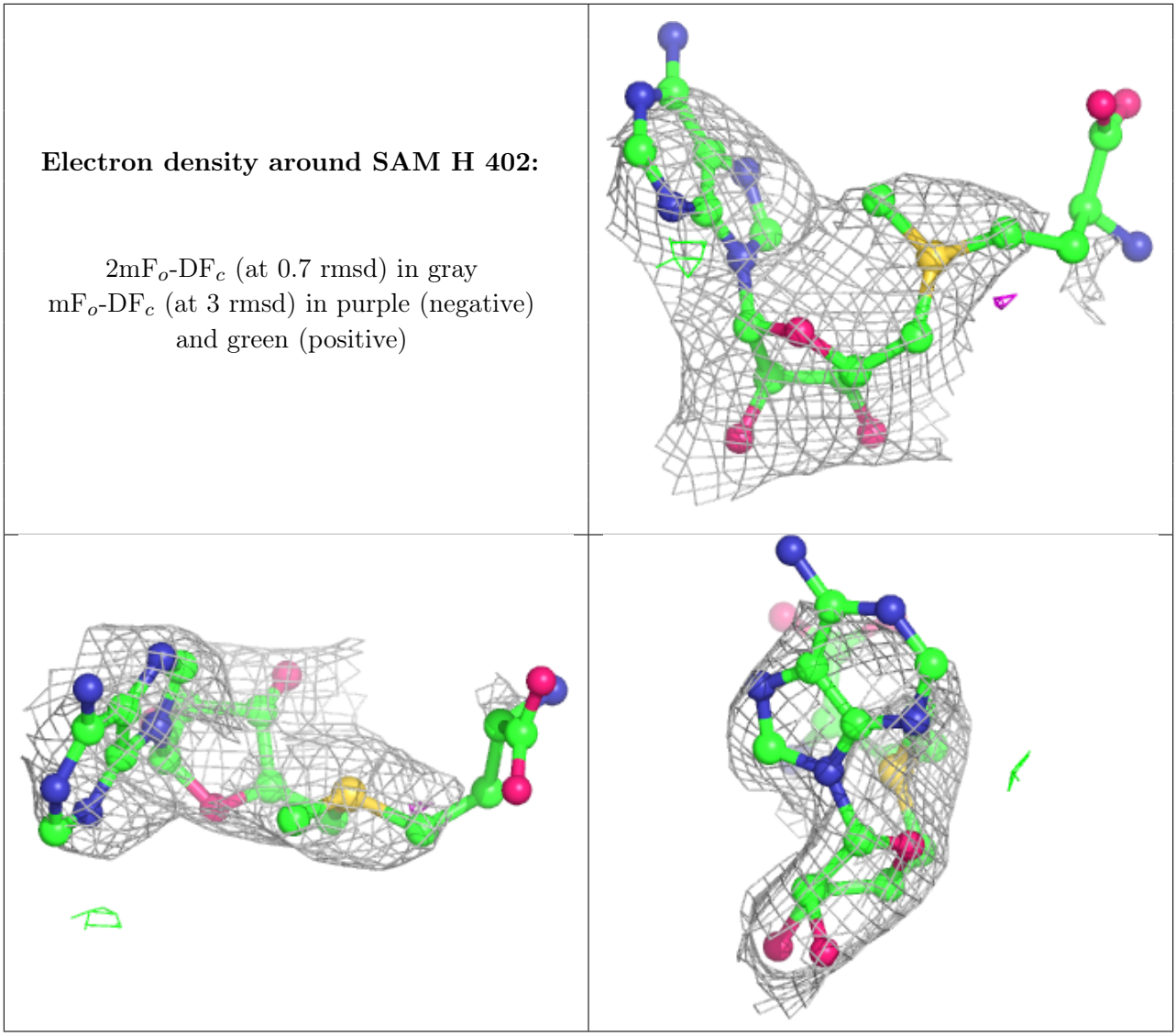






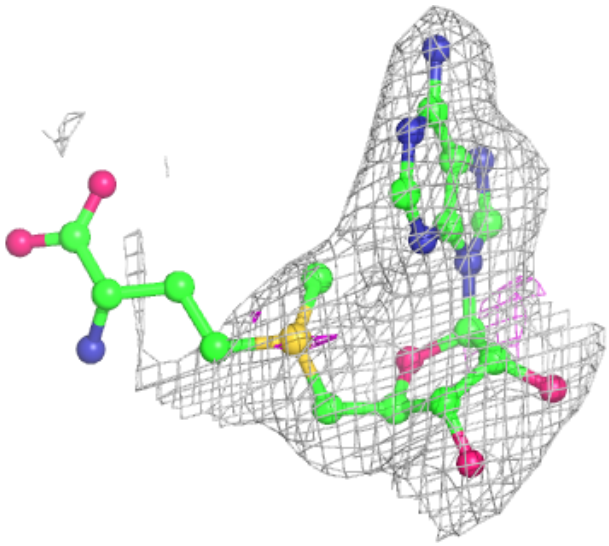
Electron density around SAM H 402:

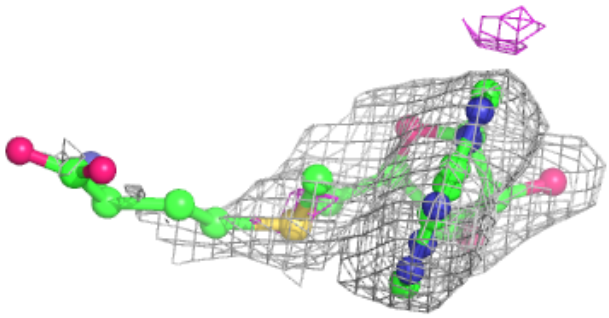
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

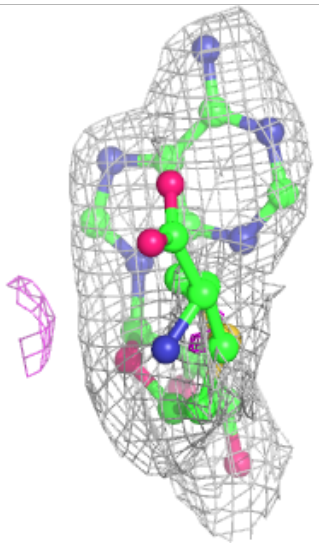


Electron density around SAM A 406:

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

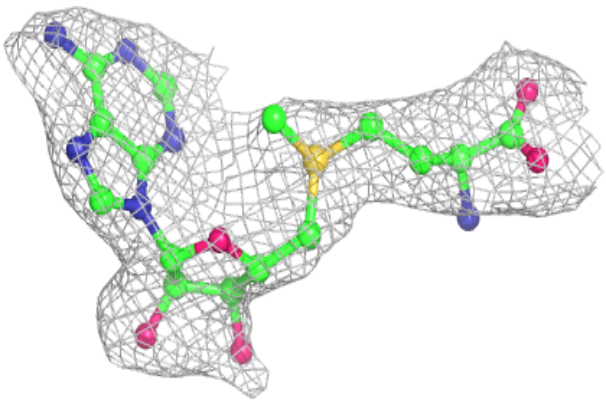


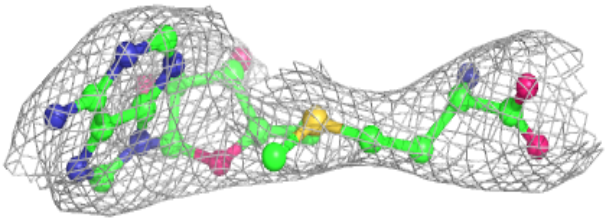


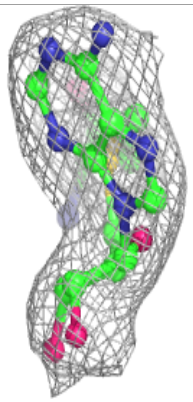


Electron density around SAM E 406:

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

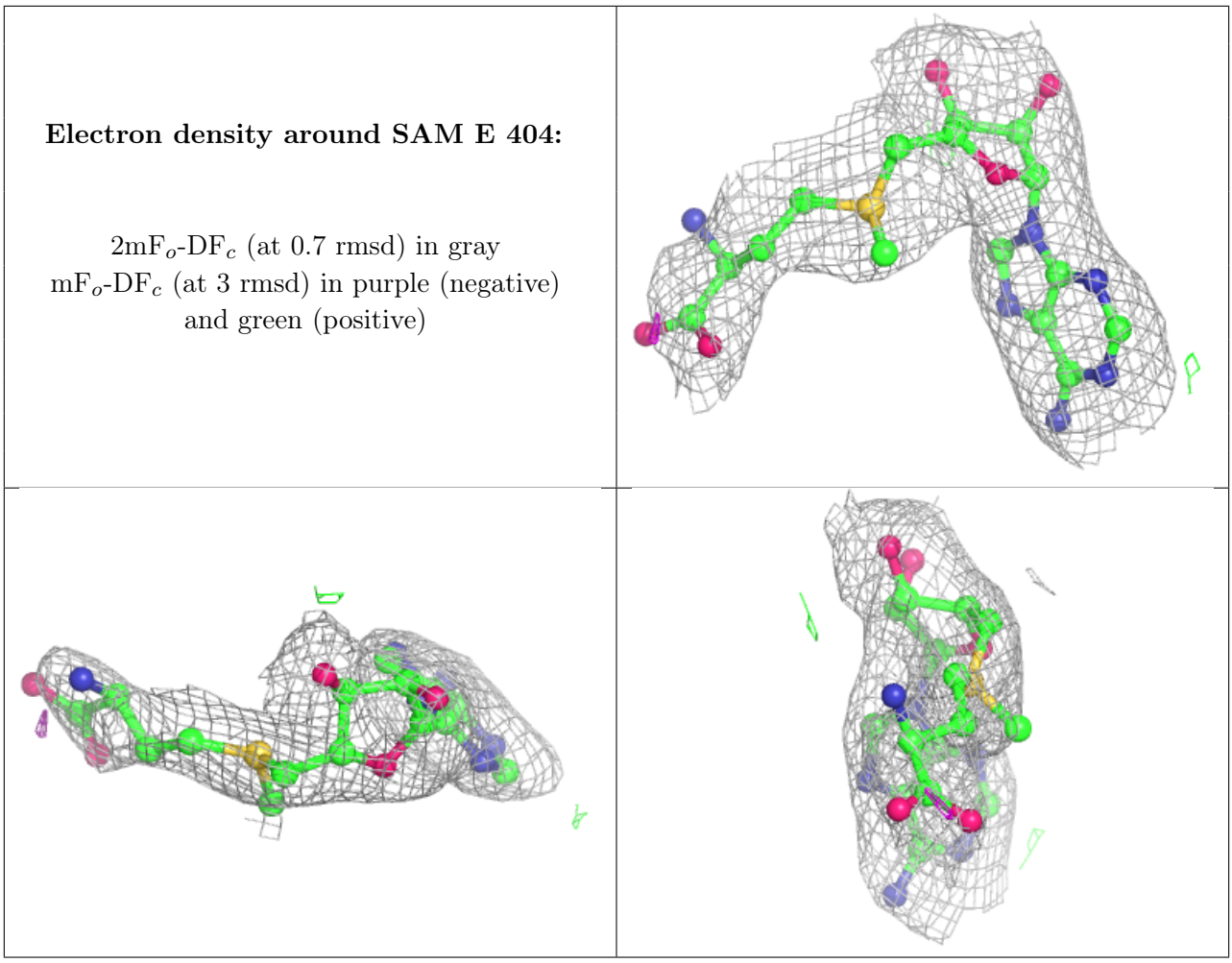






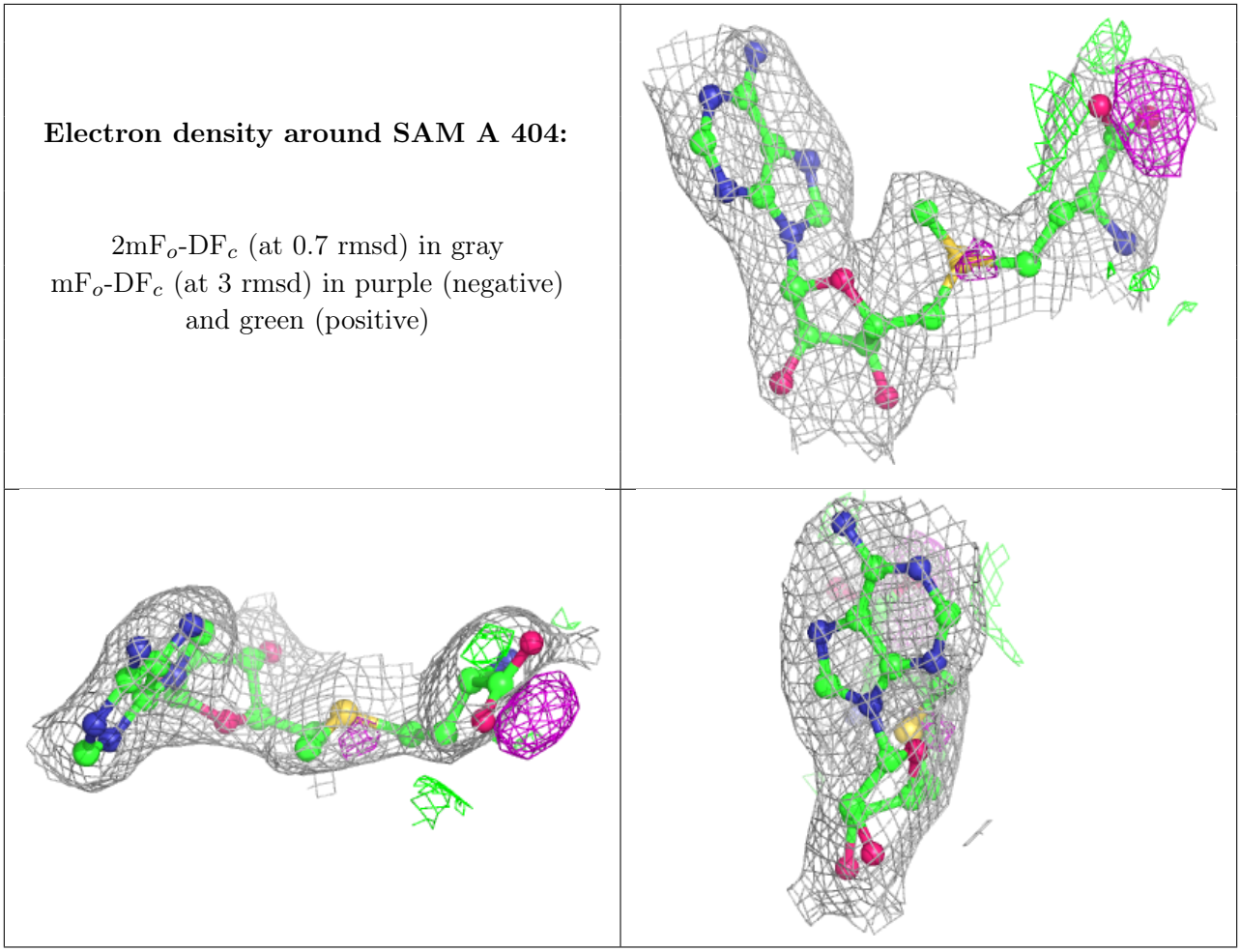
Electron density around SAM E 404:

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



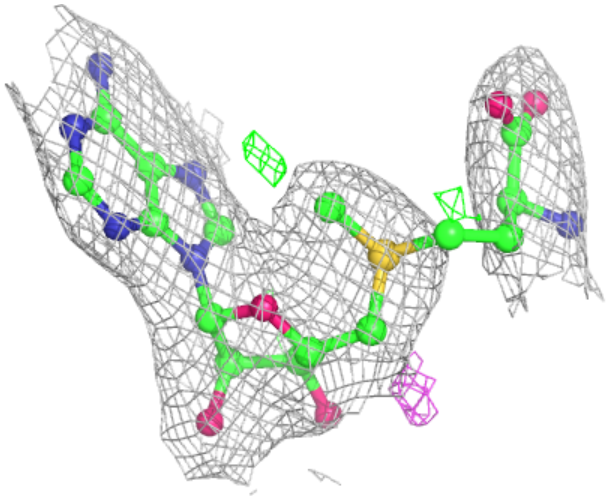
Electron density around SAM A 404:

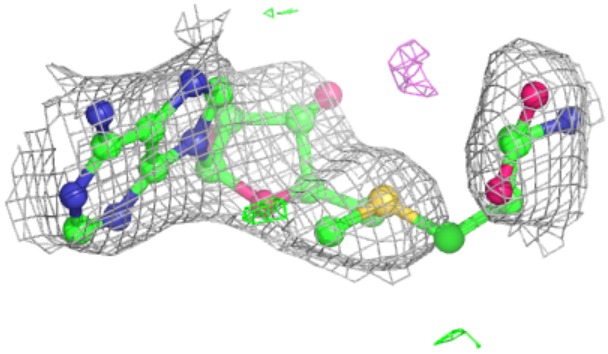
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

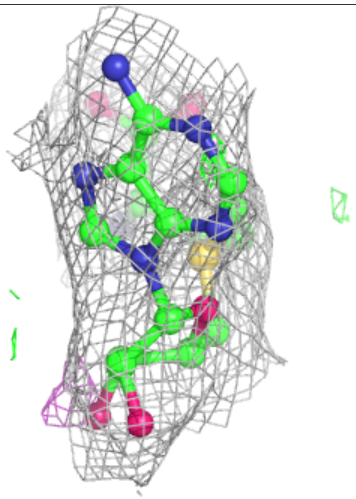


Electron density around SAM F 402:

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

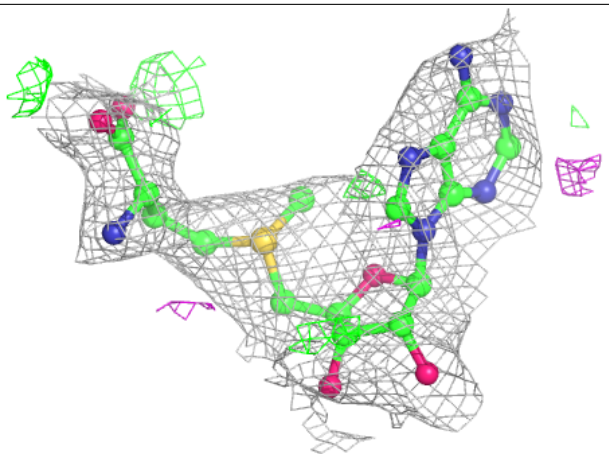


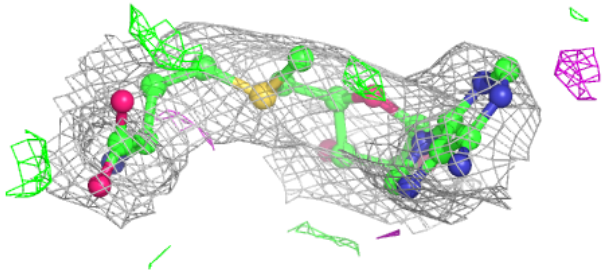


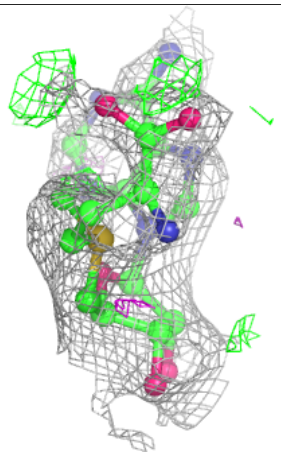


Electron density around SAM C 404:

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

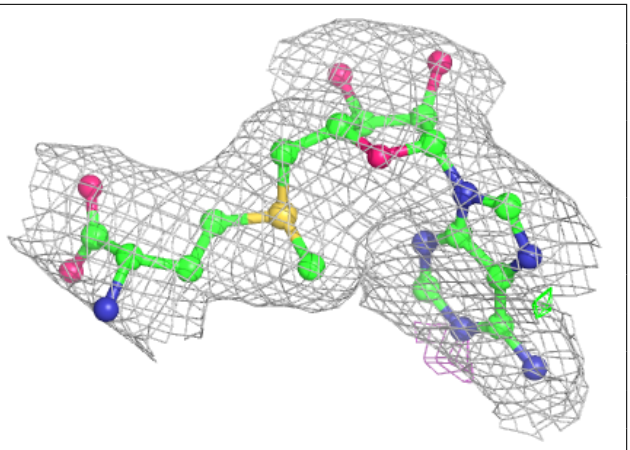


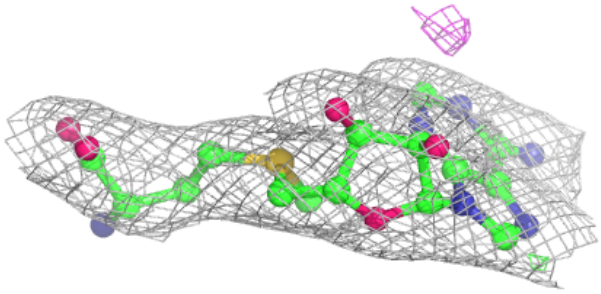


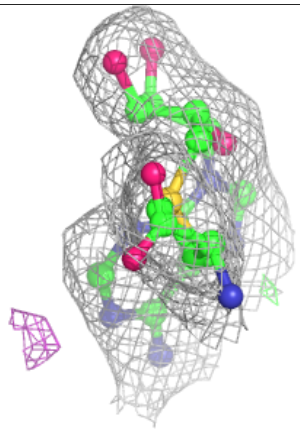


Electron density around SAM B 403:

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

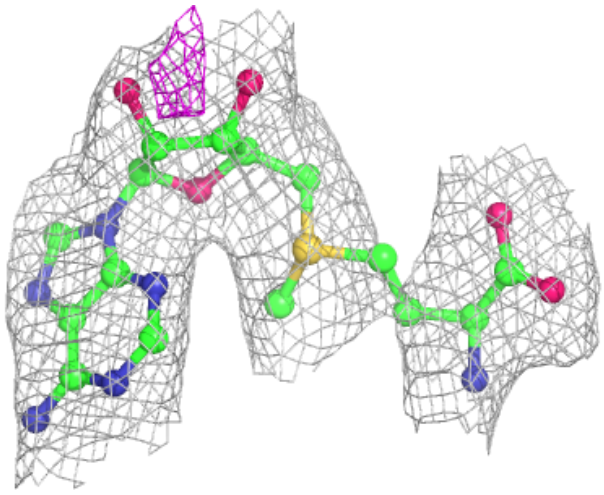


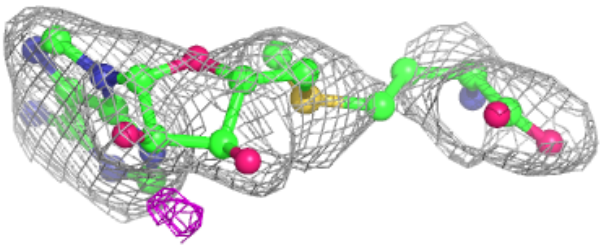


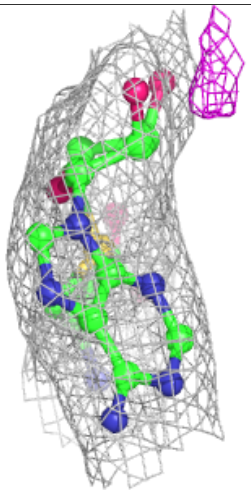


Electron density around SAM C 406:

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

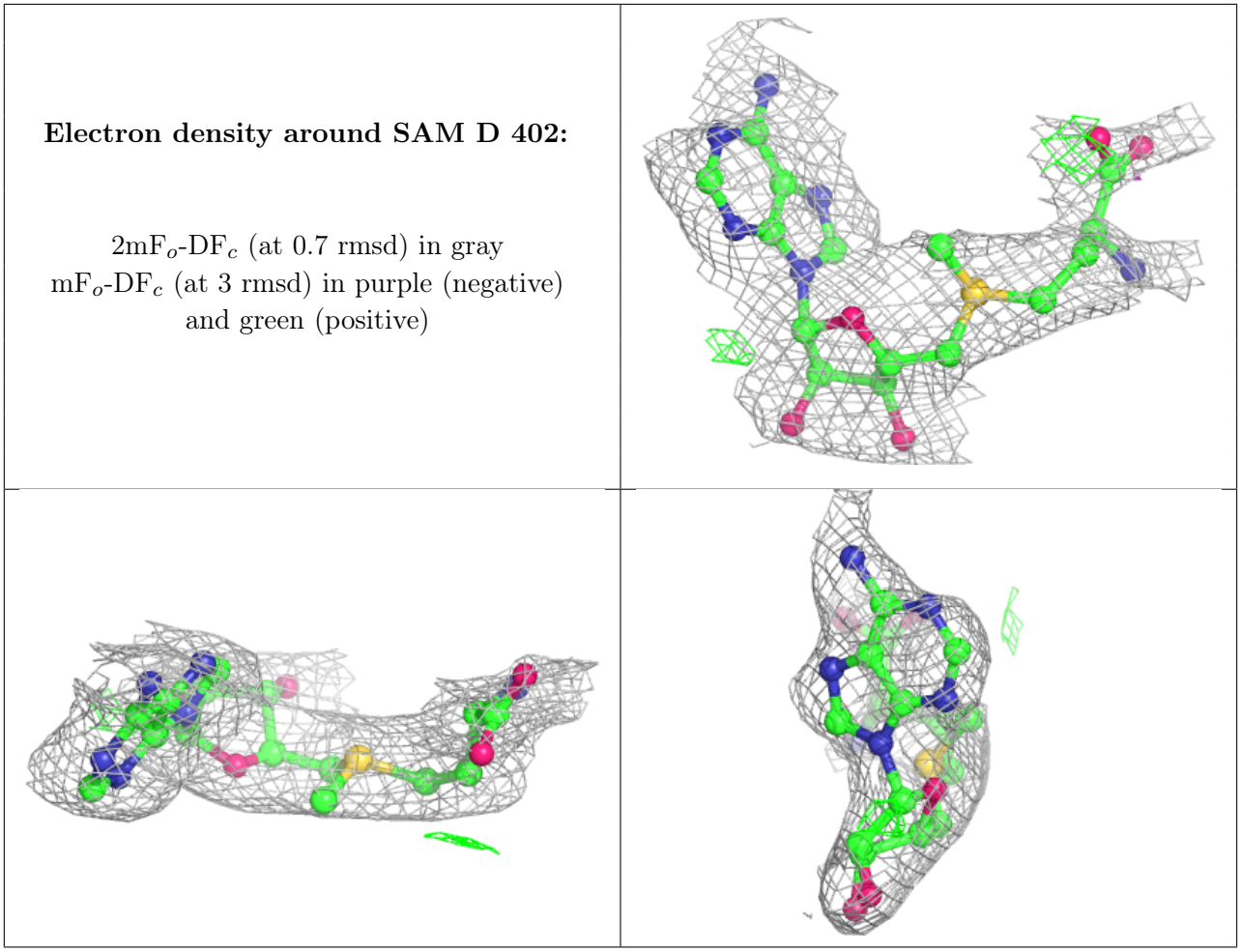






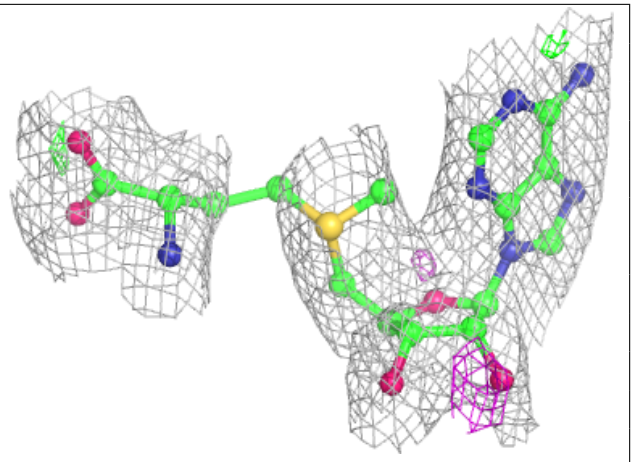
Electron density around SAM D 402:

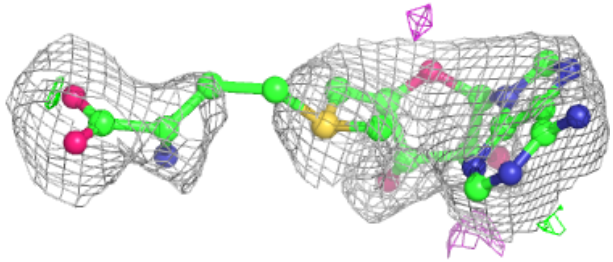
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

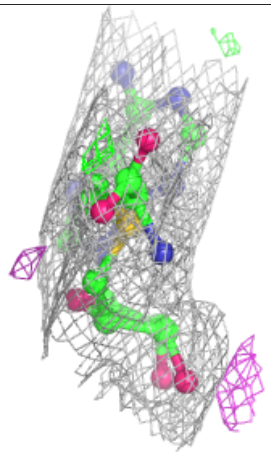


Electron density around SAM D 403:

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

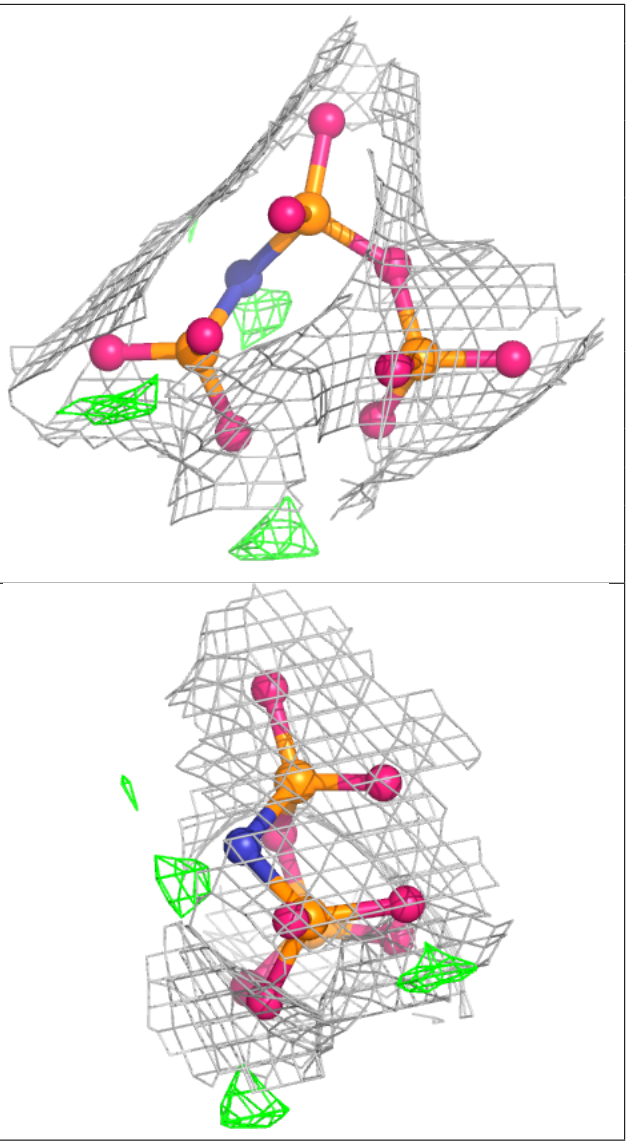


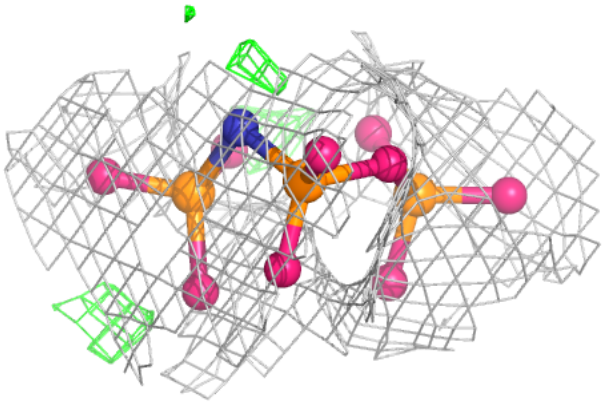




Electron density around PPK E 409:

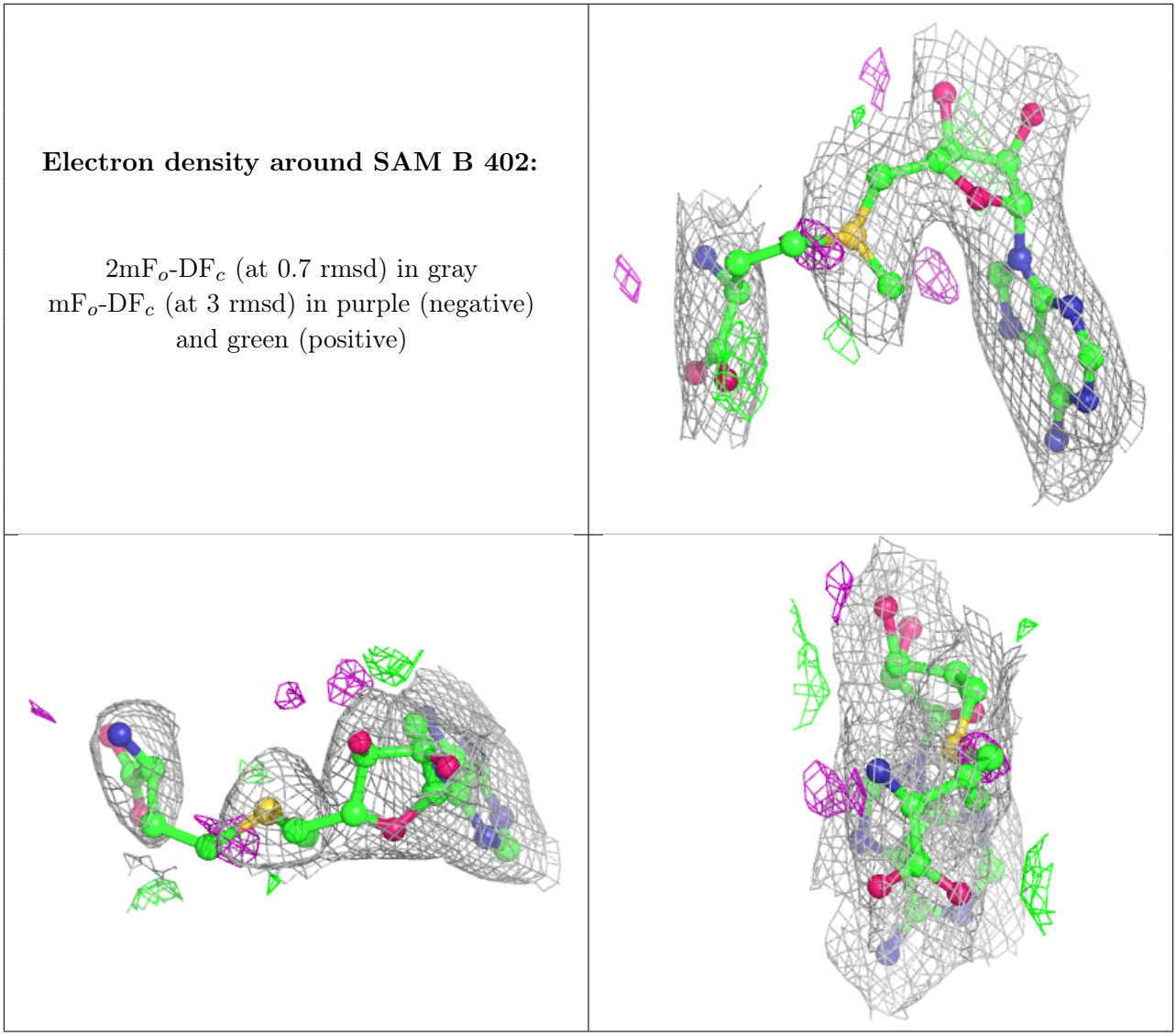
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





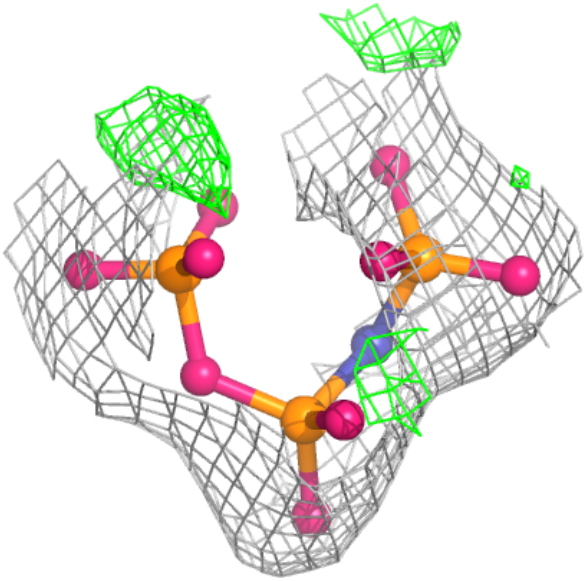
Electron density around SAM B 402:

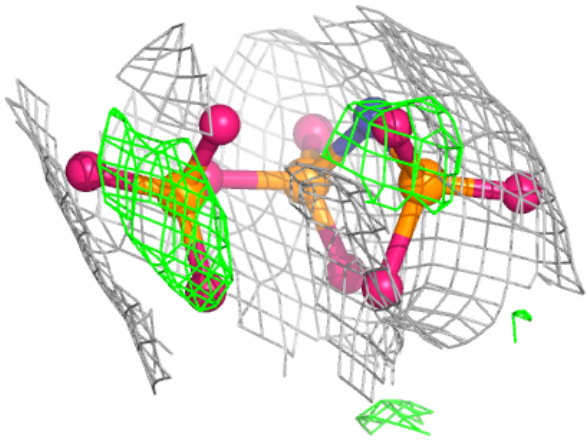
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

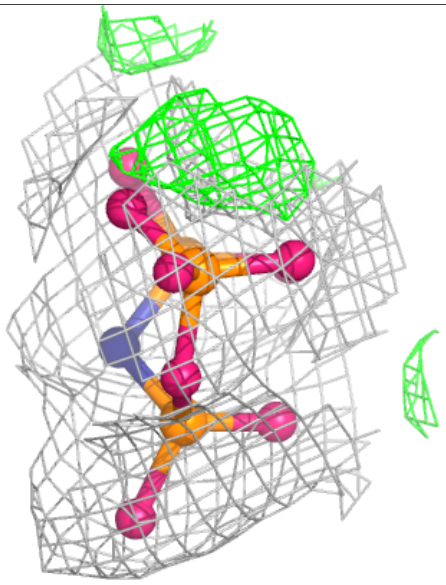


Electron density around PPK E 405:

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

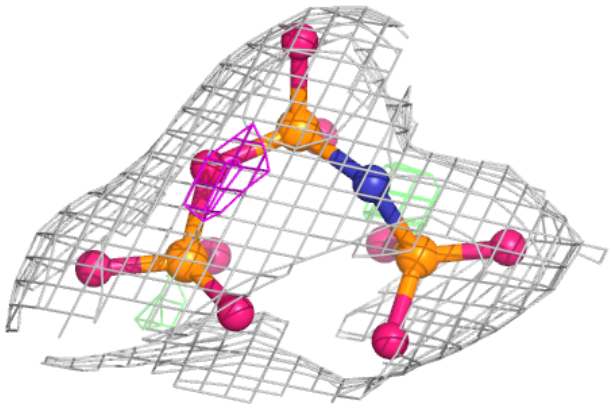


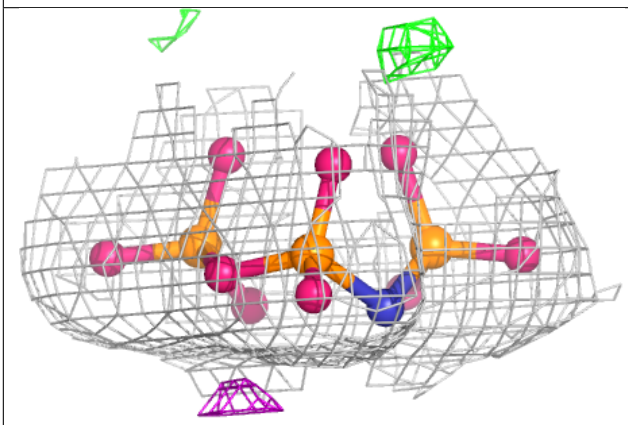


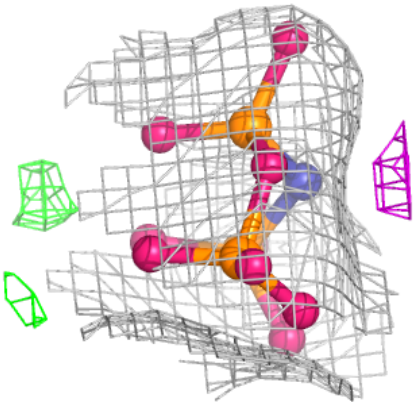


Electron density around PPK G 409:

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

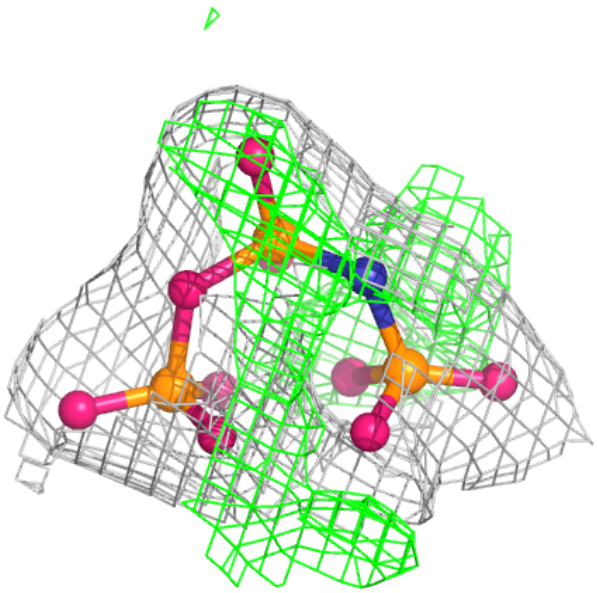


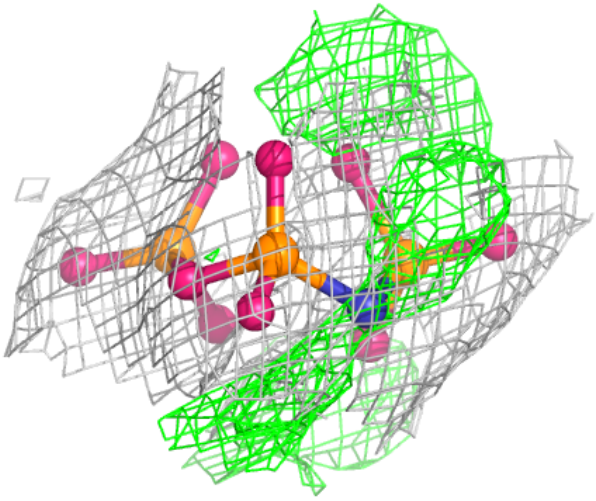


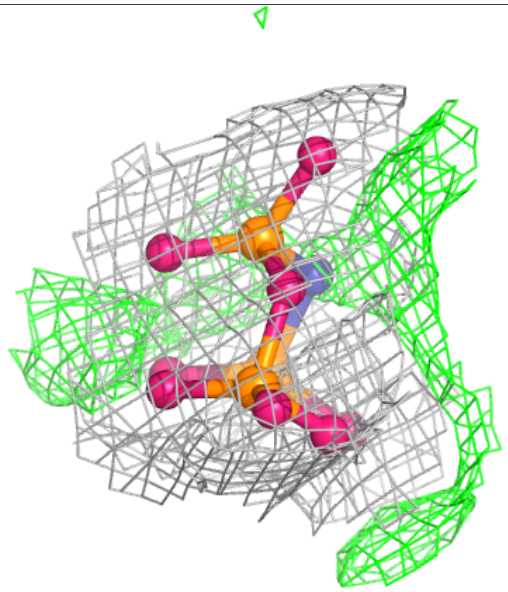


Electron density around PPK A 405:

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

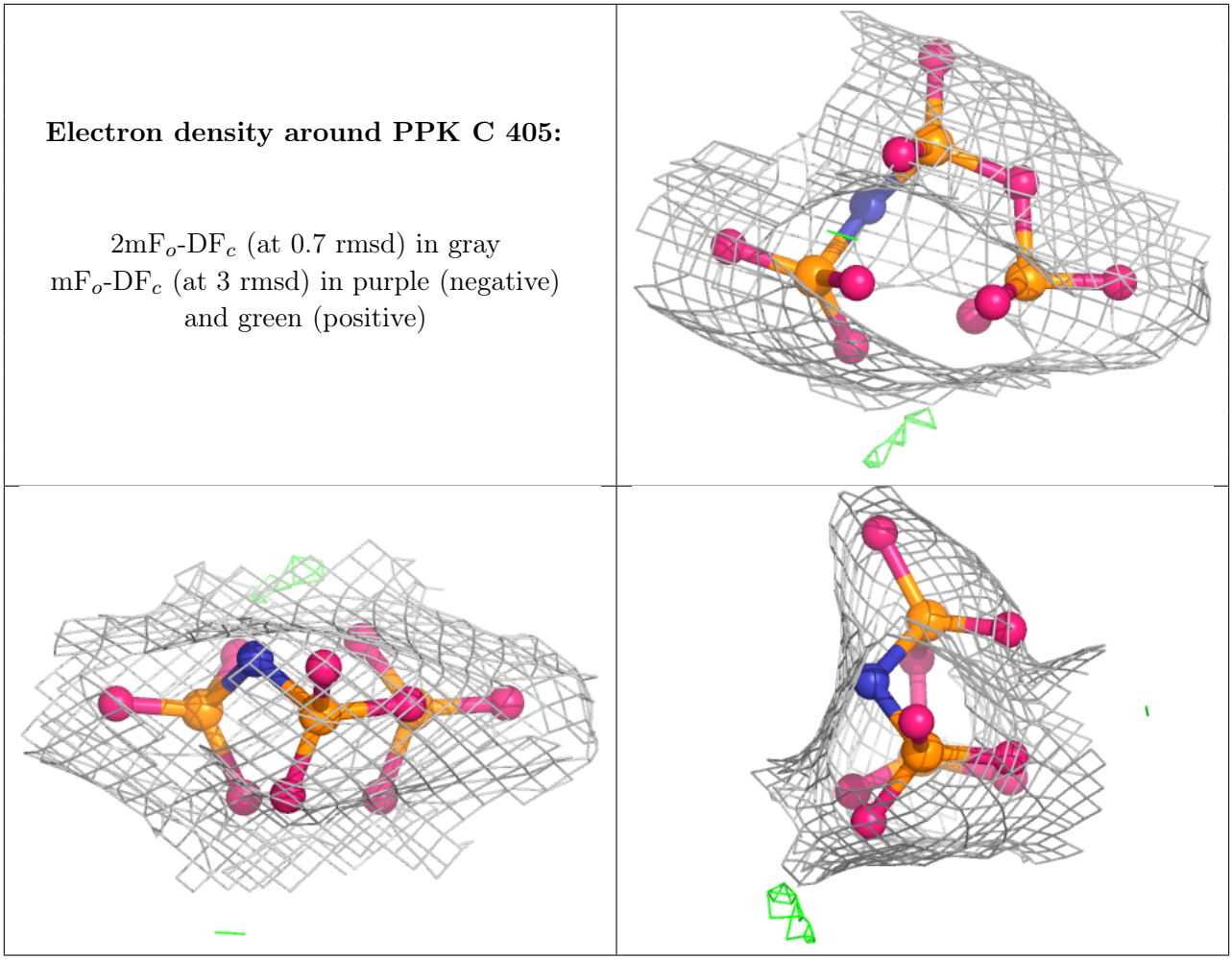






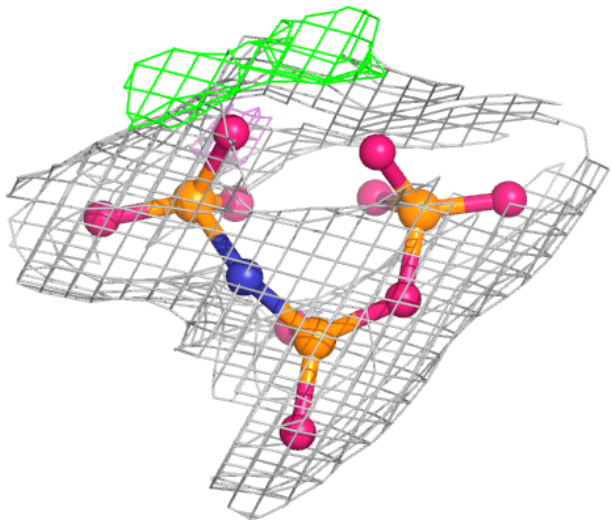
Electron density around PPK C 405:

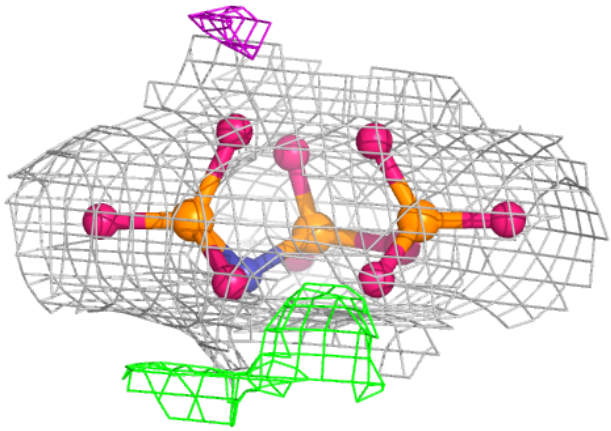
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

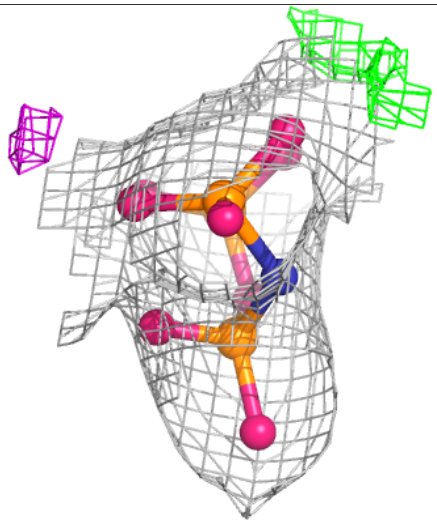


Electron density around PPK C 408:

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

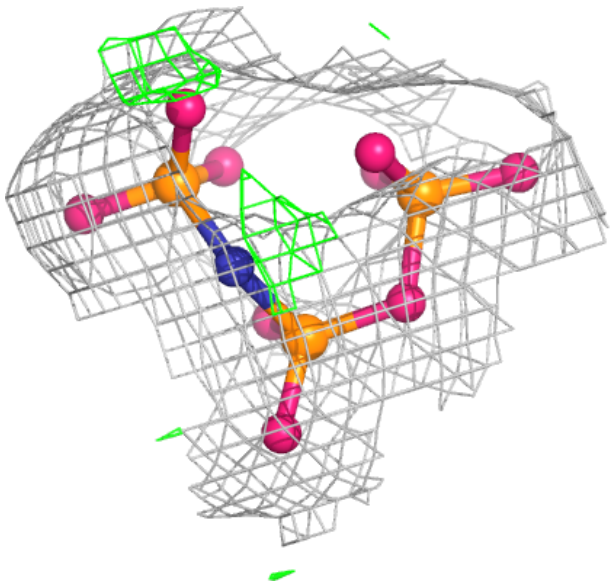


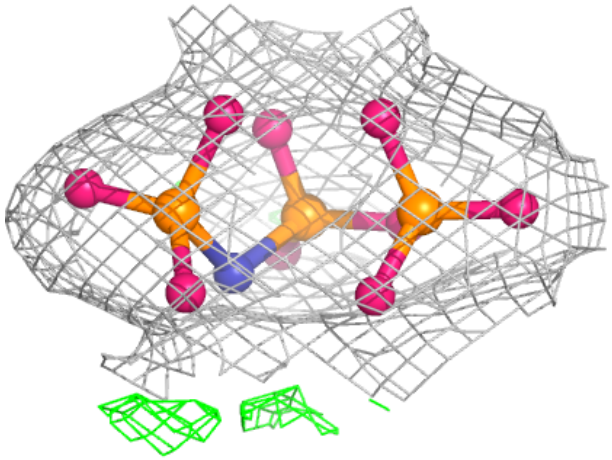


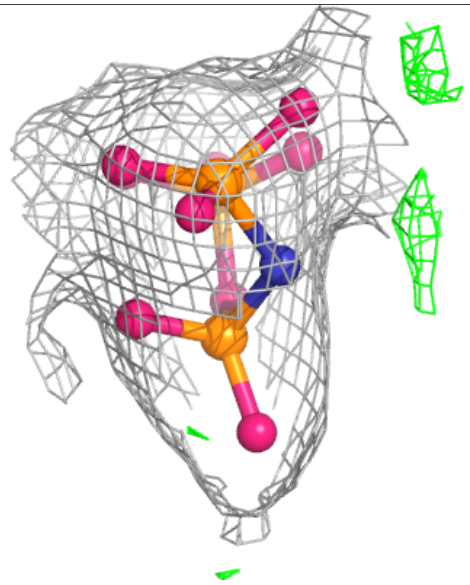


Electron density around PPK G 404:

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

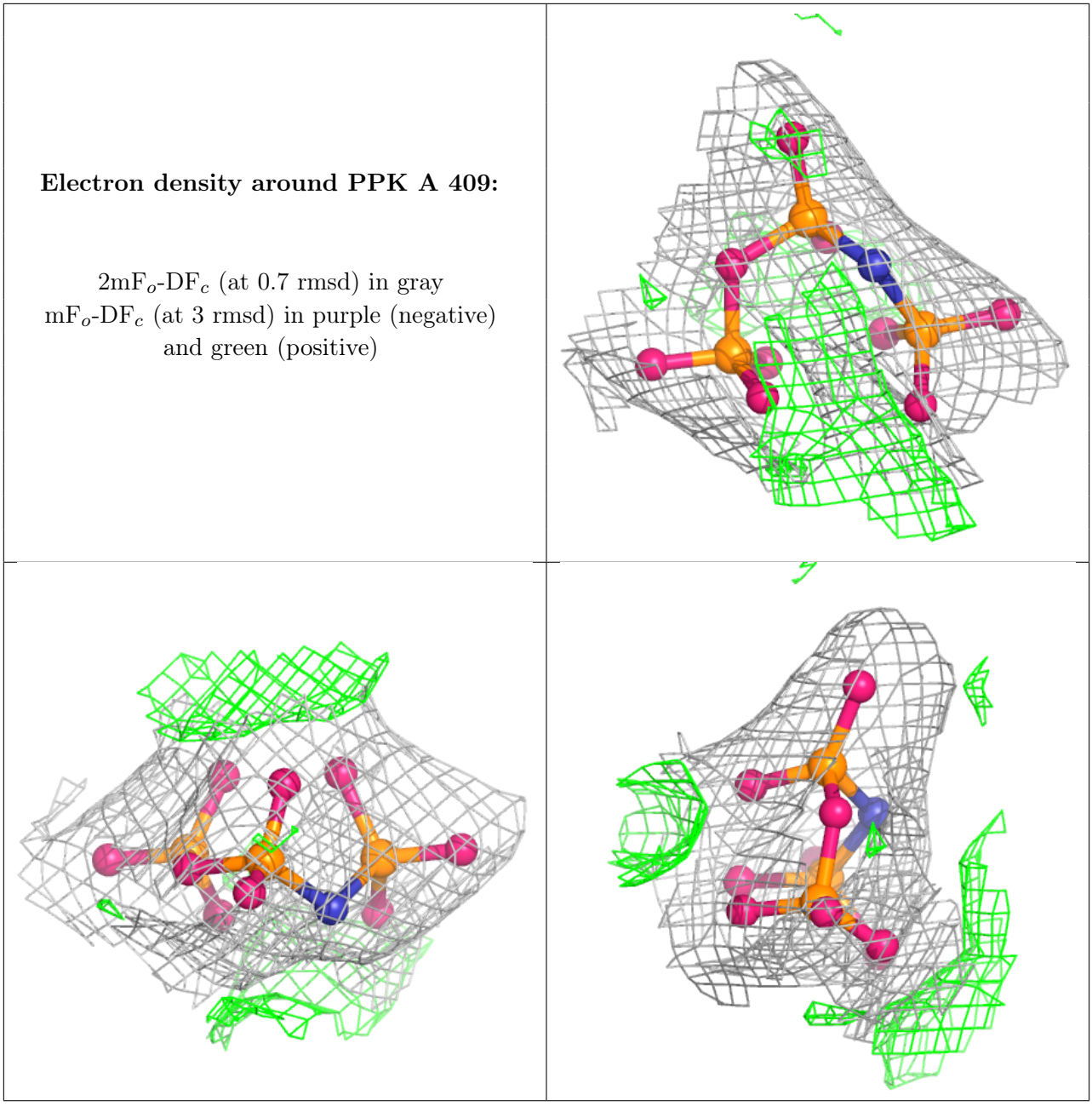






Electron density around PPK A 409:

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



6.5 Other polymers

There are no such residues in this entry.