Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 02:24 pm BST

PDB ID	:	3KPD
Title	:	Crystal Structure of the CBS domain pair of protein MJ0100 in complex with 5 -methylthioadenosine and S-adenosyl-L-methionine.
Authors	:	Lucas, M.; Oyenarte, I.; Garcia, I.G.; Arribas, E.A.; Encinar, J.A.; Kortazar, D.; Fernandez, J.A.; Mato, J.M.; Martinez-Chantar, M.L.; Martinez-Cruz, L.A.
Deposited on	:	2009-11-16
Resolution	:	2.91 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

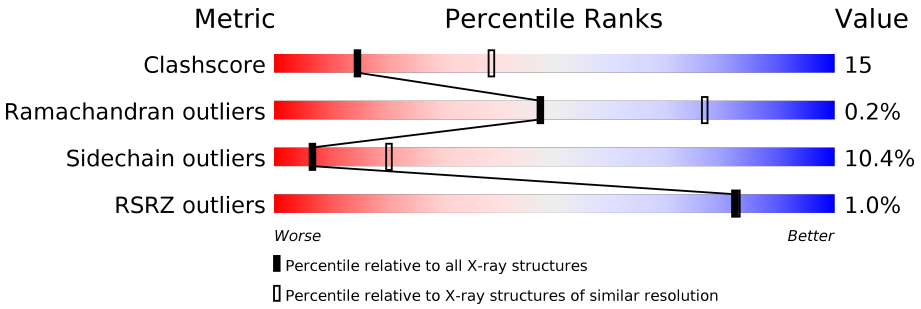
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.91 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))
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	122	2% 68% 27%
1	B	122	% 61% 34% 5%
1	C	122	61% 31% 5%
1	D	122	2% 60% 35%

2 Entry composition

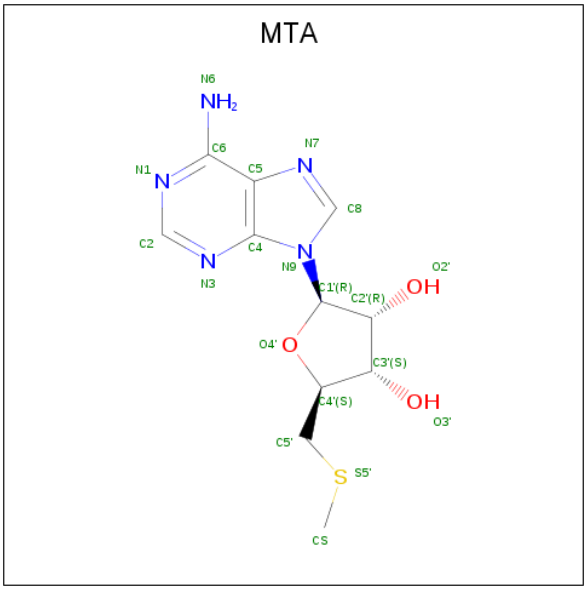
There are 3 unique types of molecules in this entry. The entry contains 3887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein MJ0100.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	1	0
			930	592	161	174	3			
1	B	121	Total	C	N	O	S	0	1	0
			943	600	164	176	3			
1	C	119	Total	C	N	O	S	0	1	0
			930	592	161	174	3			
1	D	119	Total	C	N	O	S	0	1	0
			930	592	161	174	3			

- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

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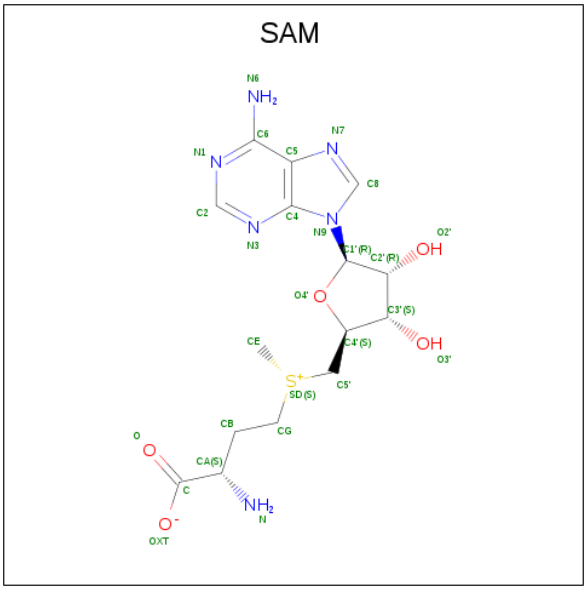
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



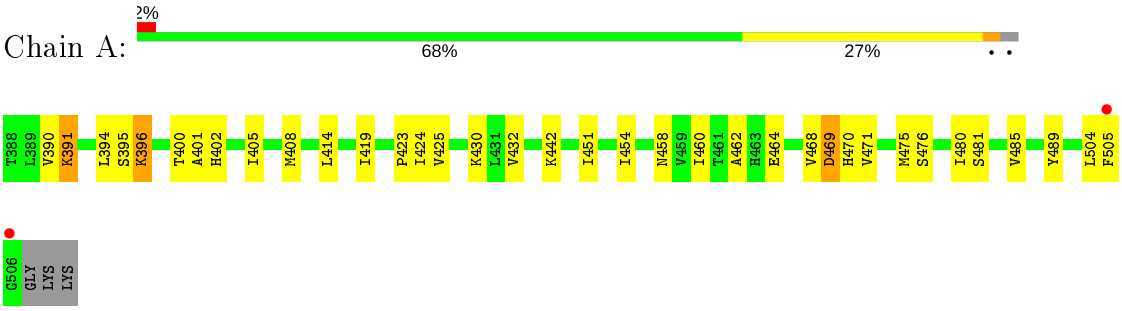
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

3 Residue-property plots (i)

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

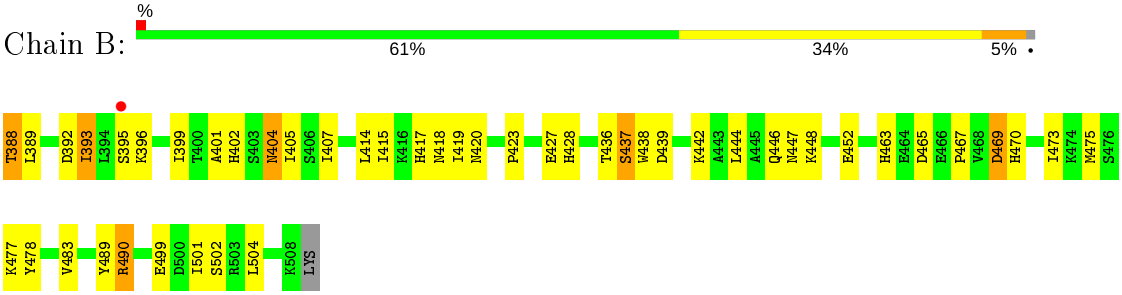
- Molecule 1: Uncharacterized protein MJ0100

Chain A:



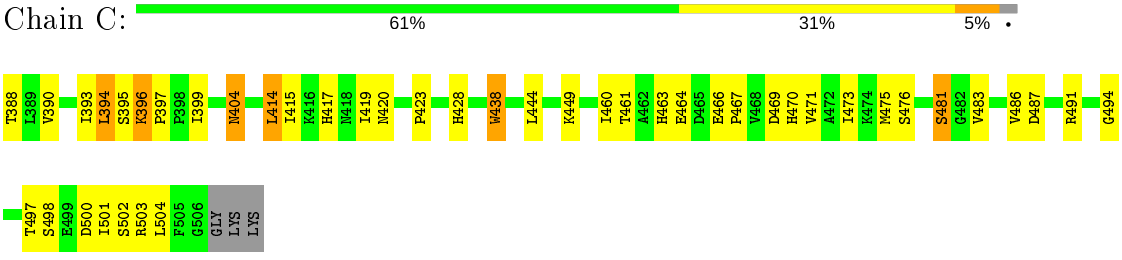
- Molecule 1: Uncharacterized protein MJ0100

Chain B:



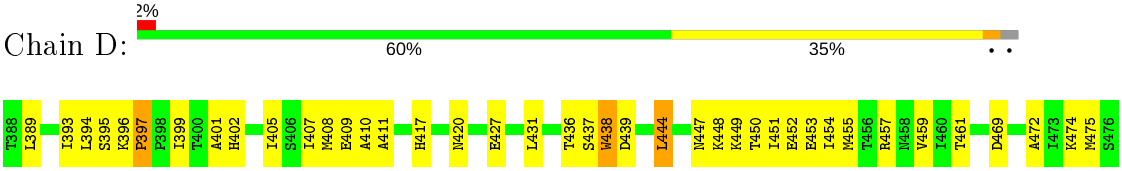
- Molecule 1: Uncharacterized protein MJ0100

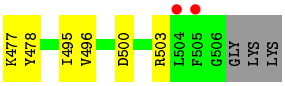
Chain C:



- Molecule 1: Uncharacterized protein MJ0100

Chain D:




K477
V478
I495
V496
D500
R503
L504
F505
G506
GLY
LYS
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	58.67Å 165.79Å 123.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.91 40.23 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.6 ((Not available)-2.91) 99.6 (40.23-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.52 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.234 , 0.334 0.225 , (Not available)	Depositor DCC
R_{free} test set	670 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 20.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3887	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.13% 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, SAM

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	0.54	0/948	0.74	0/1286
1	B	0.58	0/961	0.69	0/1302
1	C	0.58	0/948	0.72	1/1286 (0.1%)
1	D	0.58	0/948	0.76	0/1286
All	All	0.57	0/3805	0.73	1/5160 (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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	414	LEU	CB-CG-CD1	-5.09	102.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	395	SER	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	930	0	972	22	0
1	B	943	0	988	43	0
1	C	930	0	972	41	0
1	D	930	0	972	34	0
2	A	40	0	30	0	0
2	C	20	0	15	6	0
2	D	40	0	30	2	0
3	B	27	0	22	3	0
3	C	27	0	22	1	0
All	All	3887	0	4023	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (120) 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:C:396:LYS:HB2	1:C:397:PRO:HD3	1.45	0.94
1:D:396:LYS:HB3	1:D:397:PRO:HD2	1.55	0.85
1:D:448:LYS:HB2	1:D:454:ILE:HD11	1.60	0.83
1:C:404:ASN:HD22	1:C:404:ASN:H	1.26	0.82
1:B:438:TRP:CH2	1:C:415:ILE:HA	2.15	0.81
1:C:396:LYS:HB2	1:C:397:PRO:CD	2.13	0.79
1:D:452:GLU:HA	1:D:455:MET:HG2	1.66	0.78
1:B:417:HIS:HE1	1:D:427:GLU:OE1	1.67	0.76
1:B:417:HIS:CE1	1:D:427:GLU:OE1	2.41	0.73
1:C:394:LEU:HD11	1:C:494:GLY:HA3	1.73	0.70
1:B:438:TRP:HZ3	1:C:414:LEU:O	1.77	0.68
1:D:401:ALA:HB1	1:D:405:ILE:HD13	1.76	0.68
1:B:393:ILE:HG13	1:B:504:LEU:HD11	1.75	0.67
1:A:400:THR:HG22	1:A:423:PRO:HB2	1.75	0.67
1:A:442:LYS:HG2	1:A:454:ILE:HD11	1.76	0.67
1:B:438:TRP:CZ3	1:C:414:LEU:O	2.48	0.66
1:B:489:TYR:O	1:B:490:ARG:HB2	1.96	0.65
1:D:431:LEU:HD21	1:D:459:VAL:HG11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502[B]:SER:OG	1:C:498:SER:HB2	1.97	0.64
1:D:396:LYS:CB	1:D:397:PRO:HD2	2.26	0.64
1:D:438:TRP:CD1	1:D:438:TRP:C	2.70	0.64
1:A:458:ASN:HD21	1:B:489:TYR:HE1	1.47	0.63
1:A:405:ILE:HG13	1:A:451:ILE:HG13	1.80	0.63
1:C:404:ASN:N	1:C:404:ASN:HD22	1.97	0.62
1:D:393:ILE:HG22	1:D:393:ILE:O	2.00	0.61
1:A:475:MET:HB3	1:A:480:ILE:O	2.00	0.60
1:C:467:PRO:HG2	1:C:470:HIS:CD2	2.37	0.60
1:D:394:LEU:HD12	1:D:395:SER:H	1.66	0.59
1:D:450:THR:OG1	1:D:453:GLU:HG3	2.03	0.58
1:C:469:ASP:O	1:C:473:ILE:HG13	2.04	0.58
1:C:394:LEU:HD13	1:C:395:SER:N	2.19	0.57
1:C:399:ILE:O	1:C:423:PRO:HD2	2.04	0.57
1:B:414:LEU:O	1:C:438:TRP:HZ3	1.87	0.57
1:B:428:HIS:CE1	1:D:399:ILE:HG12	2.41	0.56
1:C:438:TRP:CD1	3:C:1000:SAM:H3'	2.40	0.56
1:B:475:MET:HE1	1:B:501:ILE:HD12	1.86	0.56
1:B:483:VAL:O	1:B:483:VAL:HG23	2.03	0.56
1:B:475:MET:HE1	1:B:501:ILE:CD1	2.36	0.56
1:B:475:MET:CE	1:B:501:ILE:HD12	2.35	0.56
1:D:459:VAL:HG12	1:D:461:THR:HG23	1.88	0.56
1:D:420:ASN:O	1:D:436:THR:HA	2.06	0.55
1:D:394:LEU:HD12	1:D:395:SER:N	2.22	0.55
1:C:396:LYS:CB	1:C:397:PRO:CD	2.86	0.54
1:C:497:THR:HG21	2:C:1:MTA:HCS2	1.90	0.53
1:A:414:LEU:HA	1:A:419:ILE:HG13	1.91	0.53
1:C:420:ASN:H	2:C:1:MTA:HCS1	1.73	0.53
1:B:427:GLU:HG3	1:D:417:HIS:CE1	2.44	0.53
1:B:446:GLN:HB3	1:B:448:LYS:HE3	1.91	0.53
1:C:463:HIS:O	1:C:466:GLU:HB2	2.09	0.53
1:C:471:VAL:O	1:C:475:MET:HG3	2.08	0.53
1:A:394:LEU:O	1:A:396:LYS:HG3	2.09	0.53
3:B:1000:SAM:HA	1:C:420:ASN:HD21	1.73	0.53
1:B:414:LEU:O	1:C:438:TRP:CZ3	2.62	0.52
1:D:405:ILE:HG13	1:D:451:ILE:HG13	1.92	0.52
1:C:438:TRP:CD1	1:C:438:TRP:C	2.82	0.52
1:A:462:ALA:O	1:A:485:VAL:HA	2.10	0.51
1:A:402:HIS:HA	1:A:425:VAL:O	2.11	0.51
1:C:404:ASN:ND2	1:C:404:ASN:H	2.04	0.51
3:B:1000:SAM:HA	1:C:420:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LYS:HB3	1:A:464:GLU:O	2.10	0.50
1:A:469:ASP:OD2	1:A:469:ASP:N	2.42	0.50
1:A:458:ASN:ND2	1:D:397:PRO:HG2	2.27	0.49
1:D:448:LYS:CB	1:D:454:ILE:HD11	2.35	0.49
2:C:1:MTA:H8	2:C:1:MTA:CS	2.42	0.49
1:C:460:ILE:HD12	1:C:460:ILE:N	2.28	0.49
1:A:401:ALA:O	1:A:424:ILE:HA	2.13	0.48
1:C:486:VAL:HA	1:C:491:ARG:O	2.12	0.48
1:D:500:ASP:HA	1:D:503:ARG:HH12	1.77	0.48
1:B:388:THR:HB	1:B:389:LEU:H	1.44	0.48
1:A:458:ASN:ND2	1:D:397:PRO:CG	2.77	0.48
1:B:436:THR:O	1:B:439:ASP:N	2.45	0.48
1:C:461:THR:HB	1:C:486:VAL:HG22	1.95	0.48
1:D:407:ILE:O	1:D:410:ALA:HB3	2.15	0.47
1:A:470:HIS:NE2	1:B:463:HIS:CE1	2.82	0.47
1:B:415:ILE:HA	1:C:438:TRP:CH2	2.50	0.47
1:B:463:HIS:CE1	1:B:465:ASP:OD2	2.68	0.47
1:A:458:ASN:ND2	1:B:489:TYR:HE1	2.14	0.46
1:B:399:ILE:O	1:B:423:PRO:HD2	2.16	0.46
1:B:402:HIS:HB2	1:B:404:ASN:HD22	1.80	0.46
1:D:474:LYS:O	1:D:478:TYR:HD2	2.00	0.45
1:D:438:TRP:CD1	1:D:439:ASP:N	2.85	0.45
1:A:390:VAL:HG21	1:A:471:VAL:HG21	1.97	0.45
1:C:388:THR:HG21	1:C:393:ILE:HD11	1.98	0.45
1:B:446:GLN:O	1:B:447:ASN:C	2.54	0.45
1:C:503:ARG:CZ	1:C:503:ARG:HB2	2.46	0.45
1:D:477:LYS:HD3	1:D:478:TYR:CE2	2.52	0.44
1:B:467:PRO:HG2	1:B:470:HIS:CE1	2.53	0.44
1:D:393:ILE:CG2	1:D:393:ILE:O	2.65	0.44
1:A:489:TYR:N	1:A:489:TYR:CD2	2.86	0.44
1:B:439:ASP:OD1	1:B:442:LYS:NZ	2.48	0.43
1:A:460:ILE:HD11	1:B:489:TYR:OH	2.17	0.43
1:B:418:ASN:HA	1:C:438:TRP:CZ3	2.53	0.43
1:B:467:PRO:HG2	1:B:470:HIS:ND1	2.33	0.43
1:C:467:PRO:CG	1:C:470:HIS:CD2	3.02	0.43
1:B:393:ILE:HA	1:B:393:ILE:HD13	1.74	0.43
1:A:470:HIS:CE1	1:B:463:HIS:CG	3.06	0.43
1:C:483:VAL:O	1:C:483:VAL:HG23	2.19	0.43
1:C:419:ILE:HG22	2:C:1:MTA:H5'1	2.00	0.42
1:D:439:ASP:HB3	1:D:454:ILE:HG23	2.01	0.42
1:B:499:GLU:CD	1:C:481:SER:HB3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:MET:O	1:D:411:ALA:N	2.53	0.42
1:B:417:HIS:O	1:B:419:ILE:HG23	2.19	0.42
1:D:495:ILE:HG21	2:D:1:MTA:C5	2.49	0.42
1:B:401:ALA:HA	1:D:402:HIS:CD2	2.55	0.42
1:B:420:ASN:OD1	1:B:437:SER:OG	2.35	0.42
1:A:470:HIS:CE1	1:B:463:HIS:CD2	3.07	0.42
2:C:1:MTA:HCS2	2:C:1:MTA:H8	2.02	0.42
1:C:390:VAL:HB	1:C:464:GLU:HA	2.02	0.41
1:C:404:ASN:ND2	1:C:404:ASN:N	2.66	0.41
1:B:438:TRP:CD1	3:B:1000:SAM:H3'	2.55	0.41
1:A:468:VAL:HG11	1:A:504:LEU:HD12	2.01	0.41
1:C:417:HIS:O	1:C:419:ILE:HG23	2.21	0.41
1:D:444:LEU:HA	1:D:444:LEU:HD23	1.74	0.41
1:C:500:ASP:OD2	2:C:1:MTA:O2'	2.34	0.41
1:B:477:LYS:HD3	1:B:478:TYR:CE2	2.56	0.40
1:D:495:ILE:HG21	2:D:1:MTA:C4	2.50	0.40
1:D:472:ALA:HA	1:D:475:MET:HE2	2.03	0.40
1:B:463:HIS:HE1	1:B:465:ASP:OD2	2.03	0.40
1:B:469:ASP:O	1:B:473:ILE:HG13	2.21	0.40
1:C:487:ASP:C	1:C:487:ASP:OD1	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	118/122 (97%)	104 (88%)	14 (12%)	0	100	100
1	B	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	C	118/122 (97%)	105 (89%)	13 (11%)	0	100	100
1	D	118/122 (97%)	106 (90%)	11 (9%)	1 (1%)	19	49
All	All	474/488 (97%)	429 (90%)	44 (9%)	1 (0%)	47	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	397	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	107/108 (99%)	98 (92%)	9 (8%)	11 30
1	B	108/108 (100%)	95 (88%)	13 (12%)	5 14
1	C	107/108 (99%)	94 (88%)	13 (12%)	5 14
1	D	107/108 (99%)	97 (91%)	10 (9%)	9 25
All	All	429/432 (99%)	384 (90%)	45 (10%)	7 20

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	LYS
1	A	396	LYS
1	A	408	MET
1	A	430	LYS
1	A	432	VAL
1	A	469	ASP
1	A	476	SER
1	A	481	SER
1	A	505	PHE
1	B	388	THR
1	B	392	ASP
1	B	393	ILE
1	B	395	SER
1	B	396	LYS
1	B	404	ASN
1	B	405	ILE
1	B	407	ILE
1	B	437	SER
1	B	444	LEU

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Mol	Chain	Res	Type
1	B	452	GLU
1	B	469	ASP
1	B	490	ARG
1	C	394	LEU
1	C	396	LYS
1	C	404	ASN
1	C	428	HIS
1	C	438	TRP
1	C	444	LEU
1	C	449	LYS
1	C	476	SER
1	C	481	SER
1	C	501	ILE
1	C	502[A]	SER
1	C	502[B]	SER
1	C	504	LEU
1	D	389	LEU
1	D	409	GLU
1	D	437	SER
1	D	438	TRP
1	D	444	LEU
1	D	447	ASN
1	D	449	LYS
1	D	457	ARG
1	D	469	ASP
1	D	496	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	ASN
1	B	404	ASN
1	B	417	HIS
1	B	428	HIS
1	B	446	GLN
1	B	463	HIS
1	C	404	ASN
1	C	470	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MTA	D	1	-	19,22,22	1.25	2 (10%)	19,32,32	1.90	4 (21%)
2	MTA	C	1	-	19,22,22	1.17	2 (10%)	19,32,32	2.14	3 (15%)
3	SAM	B	1000	-	21,29,29	1.30	2 (9%)	18,42,42	1.41	1 (5%)
3	SAM	C	1000	-	21,29,29	1.34	2 (9%)	18,42,42	1.61	2 (11%)
2	MTA	A	1	-	19,22,22	1.18	2 (10%)	19,32,32	1.71	6 (31%)
2	MTA	A	2	-	19,22,22	1.21	2 (10%)	19,32,32	1.73	4 (21%)
2	MTA	D	2	-	19,22,22	0.99	2 (10%)	19,32,32	2.01	5 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MTA	D	1	-	-	2/3/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MTA	C	1	-	-	3/3/23/23	0/3/3/3
3	SAM	B	1000	-	-	5/8/33/33	0/3/3/3
3	SAM	C	1000	-	-	2/8/33/33	0/3/3/3
2	MTA	A	1	-	-	1/3/23/23	0/3/3/3
2	MTA	A	2	-	-	1/3/23/23	0/3/3/3
2	MTA	D	2	-	-	2/3/23/23	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	SAM	C2-N3	4.56	1.39	1.32
3	C	1000	SAM	C2-N3	4.30	1.39	1.32
2	A	2	MTA	C5'-S5'	-3.21	1.76	1.80
3	C	1000	SAM	C2-N1	3.09	1.39	1.33
2	C	1	MTA	O4'-C1'	2.81	1.45	1.41
2	D	1	MTA	C5-C4	2.76	1.48	1.40
2	A	1	MTA	C5-C4	2.55	1.47	1.40
2	D	1	MTA	C5'-S5'	-2.53	1.77	1.80
2	D	2	MTA	C5-C4	2.42	1.47	1.40
2	A	2	MTA	C5-C4	2.38	1.47	1.40
3	B	1000	SAM	C2-N1	2.37	1.38	1.33
2	C	1	MTA	C5-C4	2.37	1.47	1.40
2	A	1	MTA	C5'-S5'	-2.22	1.77	1.80
2	D	2	MTA	C2'-C1'	-2.06	1.50	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	MTA	CS-S5'-C5'	6.91	114.00	101.30
2	D	1	MTA	CS-S5'-C5'	5.09	110.65	101.30
2	D	2	MTA	CS-S5'-C5'	5.08	110.65	101.30
3	C	1000	SAM	N3-C2-N1	-5.06	120.77	128.68
3	B	1000	SAM	N3-C2-N1	-4.76	121.24	128.68
2	A	2	MTA	CS-S5'-C5'	3.95	108.56	101.30
2	A	1	MTA	CS-S5'-C5'	3.85	108.39	101.30
2	D	1	MTA	N3-C2-N1	-3.75	122.82	128.68
2	D	2	MTA	N3-C2-N1	-3.72	122.86	128.68
2	C	1	MTA	N3-C2-N1	-3.43	123.31	128.68
2	A	2	MTA	C4-C5-N7	-3.38	105.88	109.40
2	C	1	MTA	C4-C5-N7	-3.27	106.00	109.40
2	A	1	MTA	N3-C2-N1	-3.17	123.72	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	MTA	N3-C2-N1	-3.14	123.78	128.68
2	D	2	MTA	C1'-N9-C4	-2.90	121.55	126.64
2	D	2	MTA	C2-N1-C6	2.82	123.58	118.75
2	D	1	MTA	C4-C5-N7	-2.71	106.57	109.40
3	C	1000	SAM	O4'-C1'-C2'	-2.61	103.11	106.93
2	A	1	MTA	O4'-C1'-C2'	-2.46	103.33	106.93
2	A	1	MTA	O3'-C3'-C4'	-2.45	103.97	111.05
2	D	1	MTA	C2-N1-C6	2.23	122.57	118.75
2	D	2	MTA	C4-C5-N7	-2.16	107.14	109.40
2	A	2	MTA	C1'-N9-C4	-2.11	122.94	126.64
2	A	1	MTA	C4-C5-N7	-2.05	107.27	109.40
2	A	1	MTA	O4'-C4'-C5'	2.00	113.98	108.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	MTA	O4'-C4'-C5'-S5'
3	B	1000	SAM	C-CA-CB-CG
3	B	1000	SAM	CA-CB-CG-SD
3	B	1000	SAM	O4'-C4'-C5'-SD
3	B	1000	SAM	C3'-C4'-C5'-SD
2	C	1	MTA	O4'-C4'-C5'-S5'
2	C	1	MTA	C3'-C4'-C5'-S5'
3	C	1000	SAM	N-CA-CB-CG
3	C	1000	SAM	C-CA-CB-CG
2	A	2	MTA	O4'-C4'-C5'-S5'
2	D	2	MTA	O4'-C4'-C5'-S5'
2	D	2	MTA	C3'-C4'-C5'-S5'
2	D	1	MTA	C4'-C5'-S5'-CS
2	A	1	MTA	O4'-C4'-C5'-S5'
3	B	1000	SAM	N-CA-CB-CG
2	C	1	MTA	C4'-C5'-S5'-CS

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	MTA	2	0
2	C	1	MTA	6	0
3	B	1000	SAM	3	0

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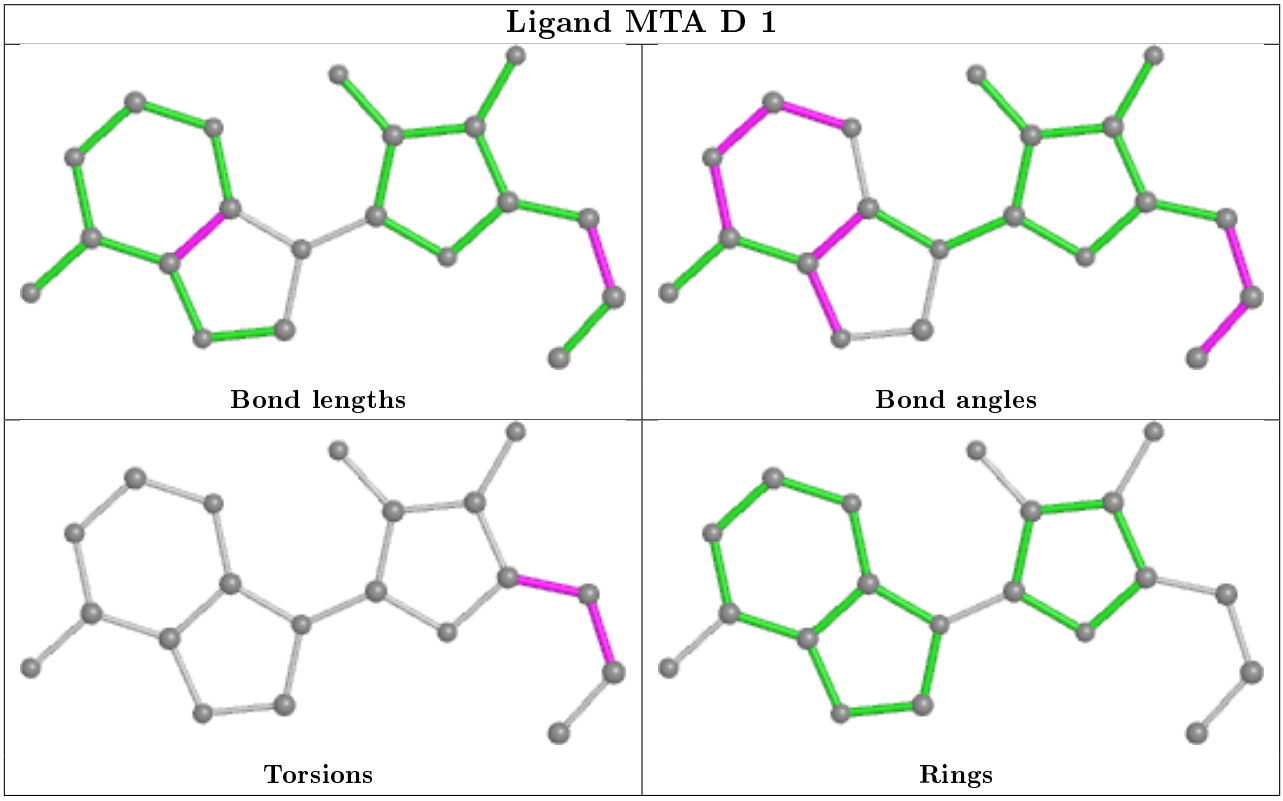
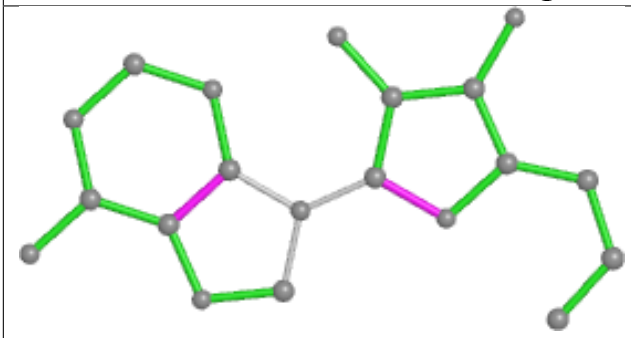
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1000	SAM	1	0

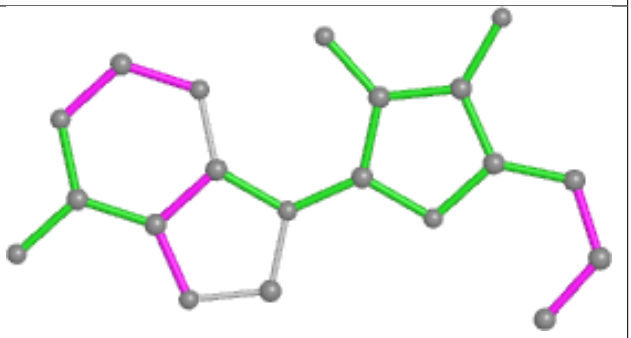
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



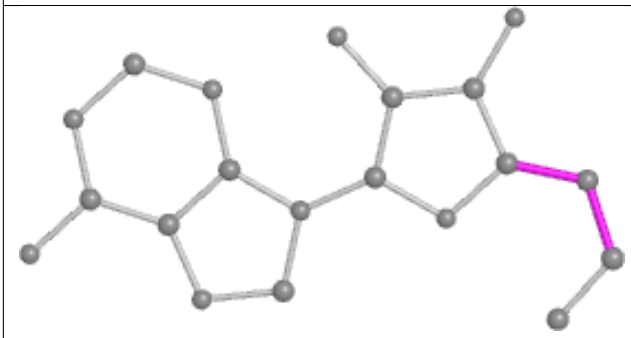
Ligand MTA C 1



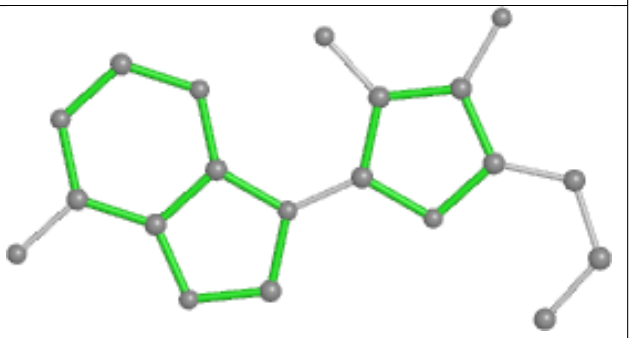
Bond lengths



Bond angles

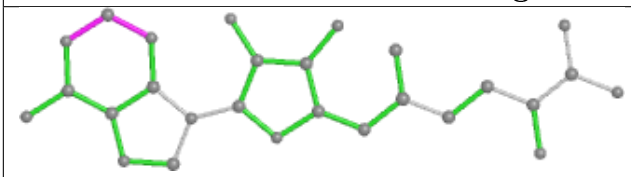


Torsions

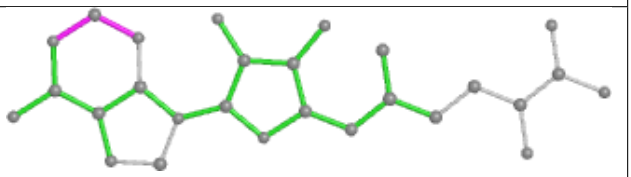


Rings

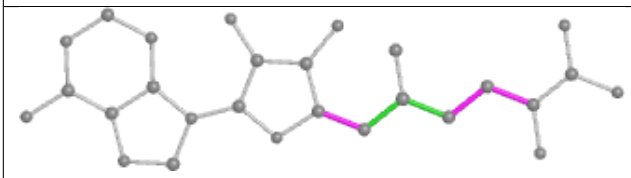
Ligand SAM B 1000



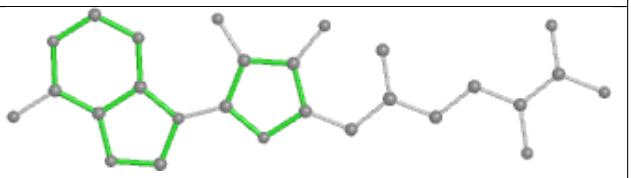
Bond lengths



Bond angles

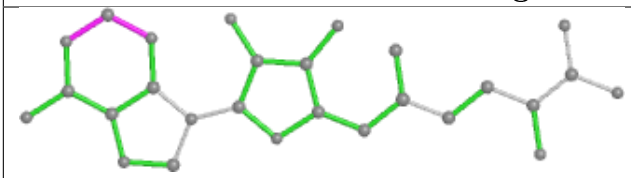


Torsions

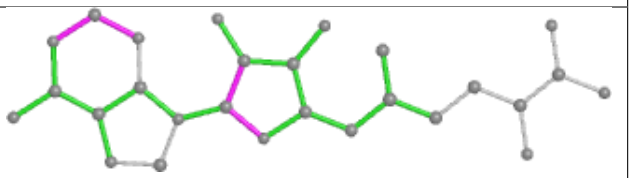


Rings

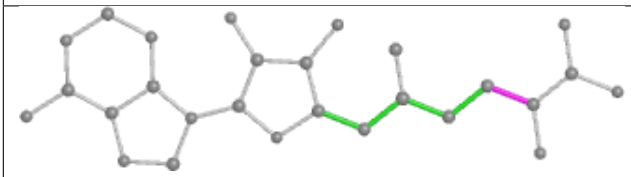
Ligand SAM C 1000



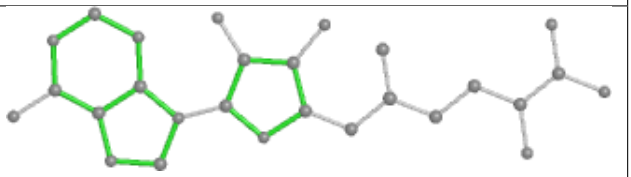
Bond lengths



Bond angles

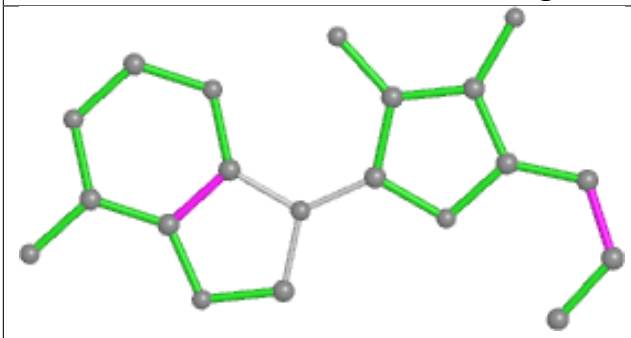


Torsions

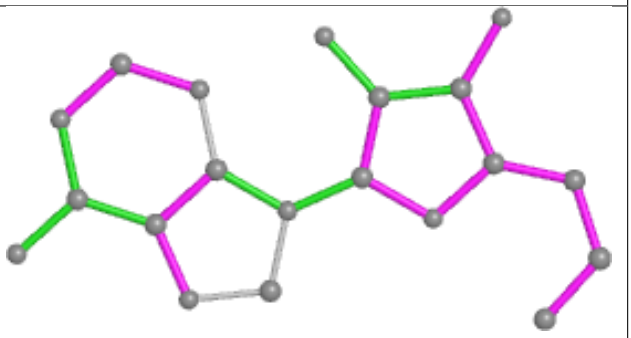


Rings

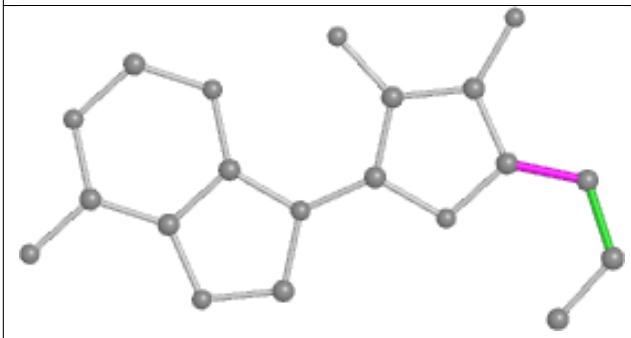
Ligand MTA A 1



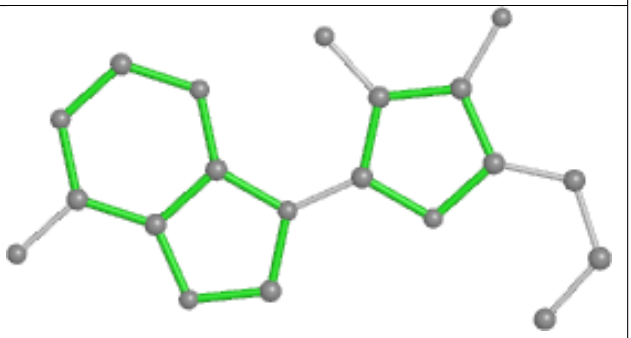
Bond lengths



Bond angles

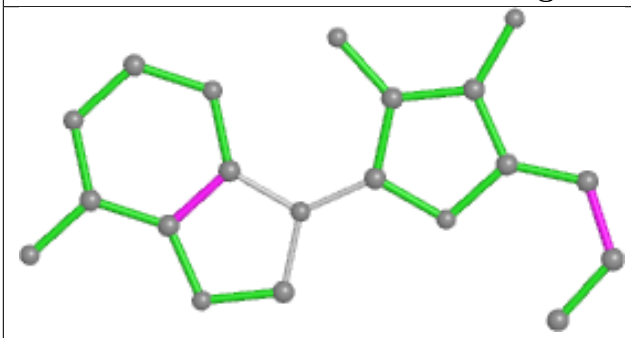


Torsions

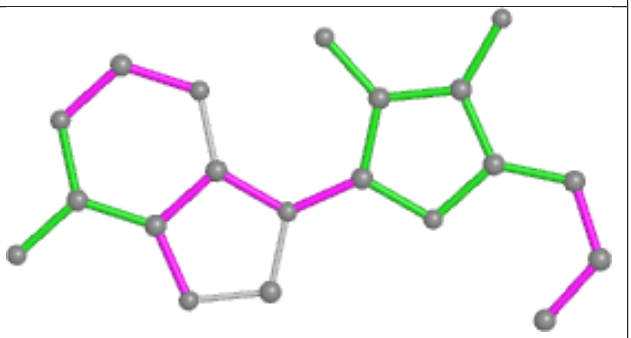


Rings

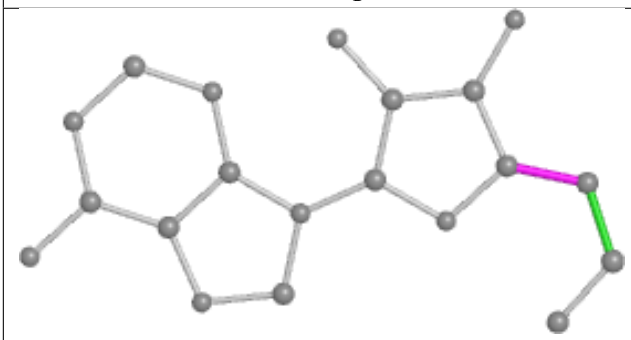
Ligand MTA A 2



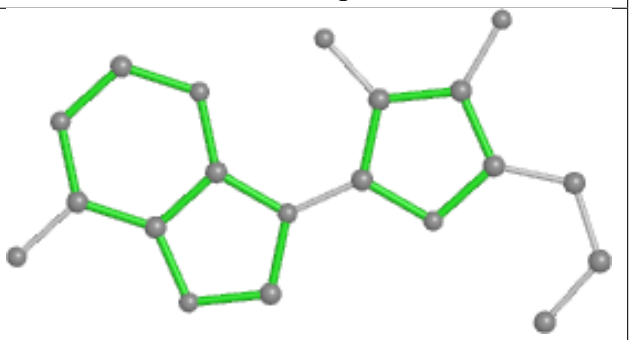
Bond lengths



Bond angles

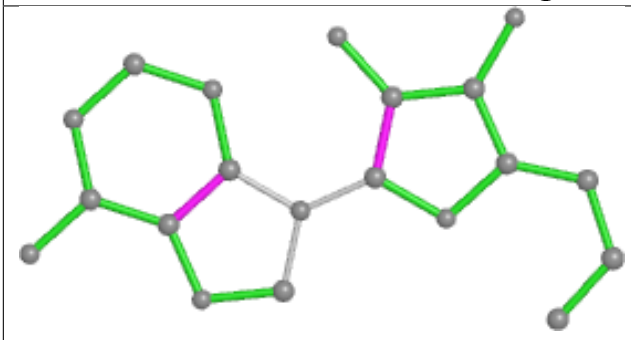


Torsions

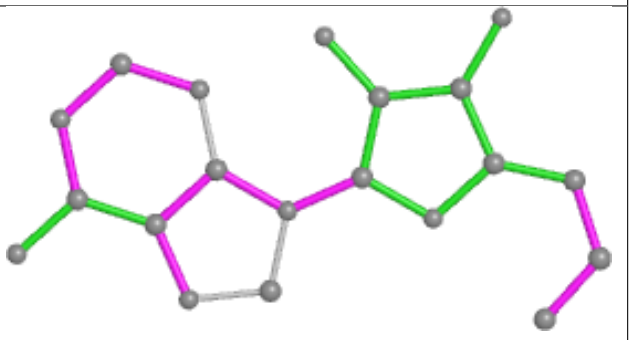


Rings

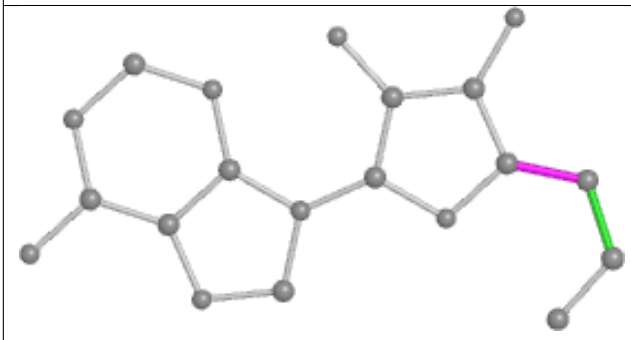
Ligand MTA D 2



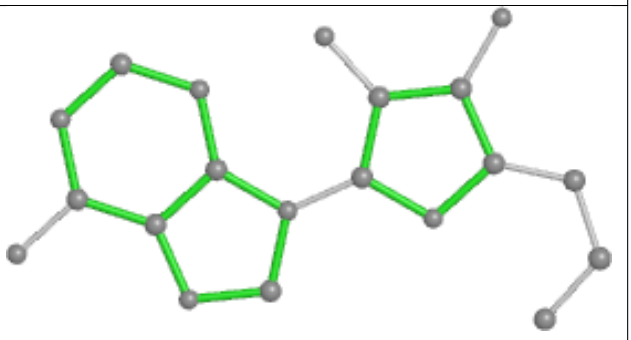
Bond lengths



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	119/122 (97%)	-0.30	2 (1%) 70 70	47, 64, 79, 88	0
1	B	121/122 (99%)	-0.52	1 (0%) 86 86	37, 48, 72, 85	0
1	C	119/122 (97%)	-0.45	0 100 100	40, 55, 74, 78	0
1	D	119/122 (97%)	-0.23	2 (1%) 70 70	40, 57, 89, 106	0
All	All	478/488 (97%)	-0.38	5 (1%) 82 82	37, 57, 82, 106	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	504	LEU	5.0
1	D	505	PHE	4.0
1	A	506	GLY	3.8
1	A	505	PHE	3.2
1	B	395	SER	2.3

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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

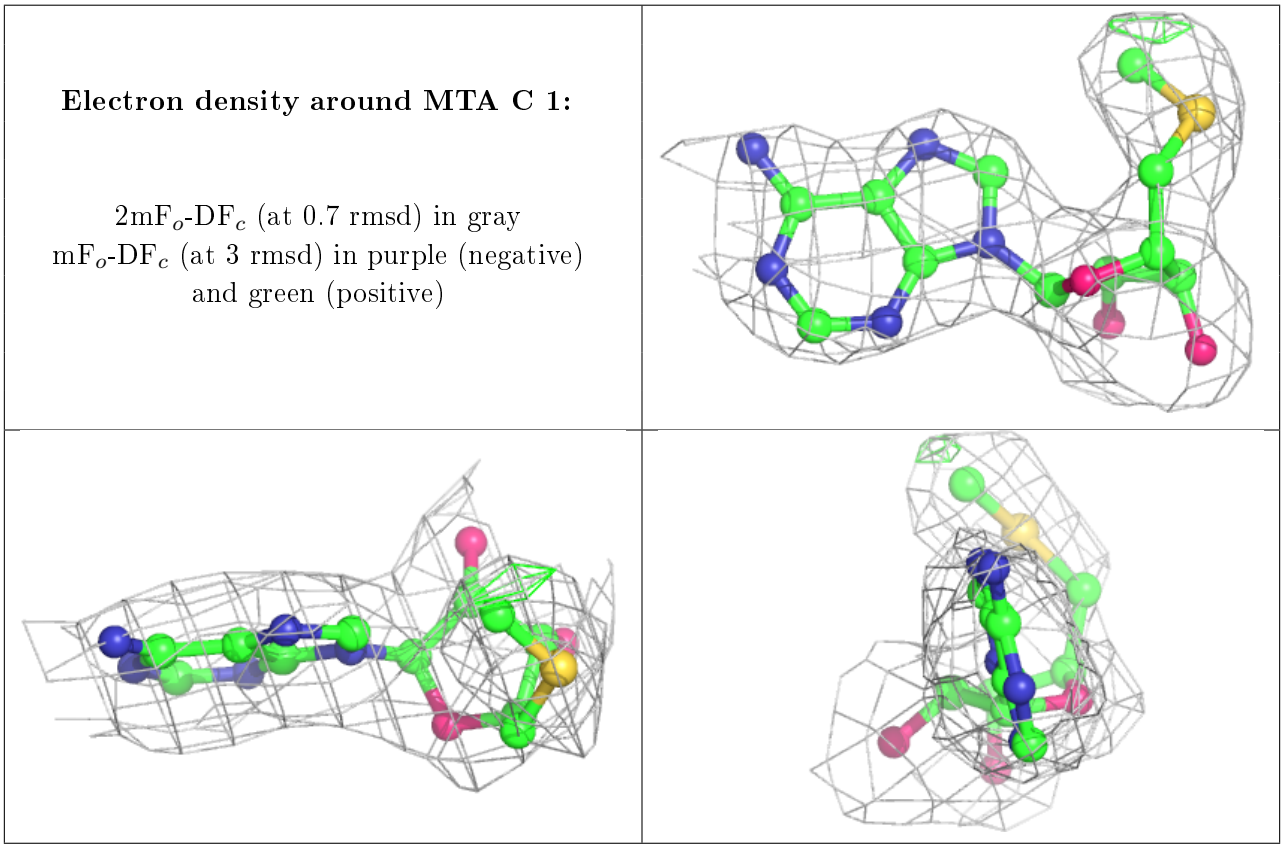
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MTA	C	1	20/20	0.89	0.18	58,63,73,76	0
2	MTA	D	1	20/20	0.90	0.25	75,80,92,94	0
2	MTA	D	2	20/20	0.91	0.17	54,56,70,71	0
3	SAM	B	1000	27/27	0.94	0.20	42,52,75,75	0
2	MTA	A	1	20/20	0.95	0.14	41,45,64,64	0
2	MTA	A	2	20/20	0.96	0.15	58,61,74,76	0
3	SAM	C	1000	27/27	0.96	0.16	42,44,51,51	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.

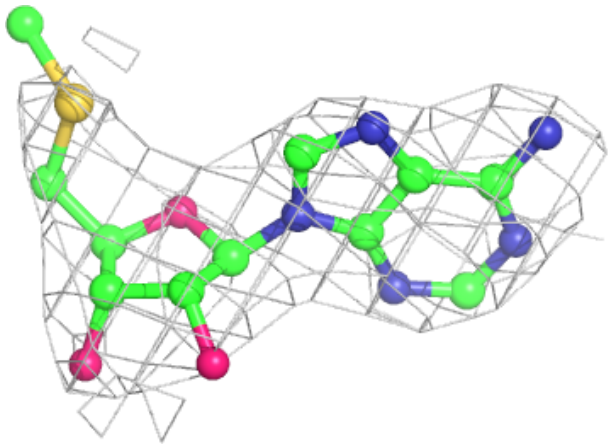
Electron density around MTA C 1:

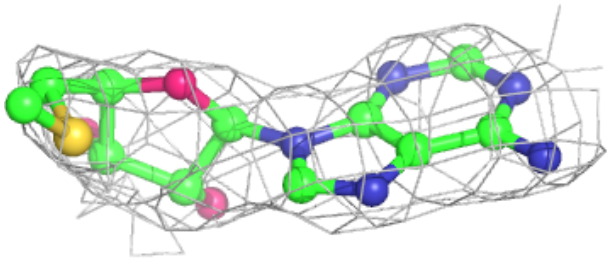
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

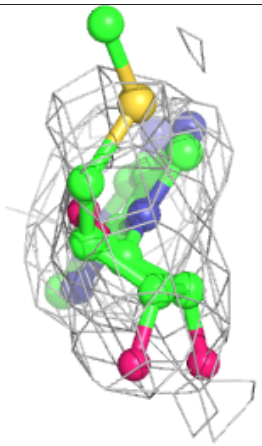


Electron density around MTA D 1:

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

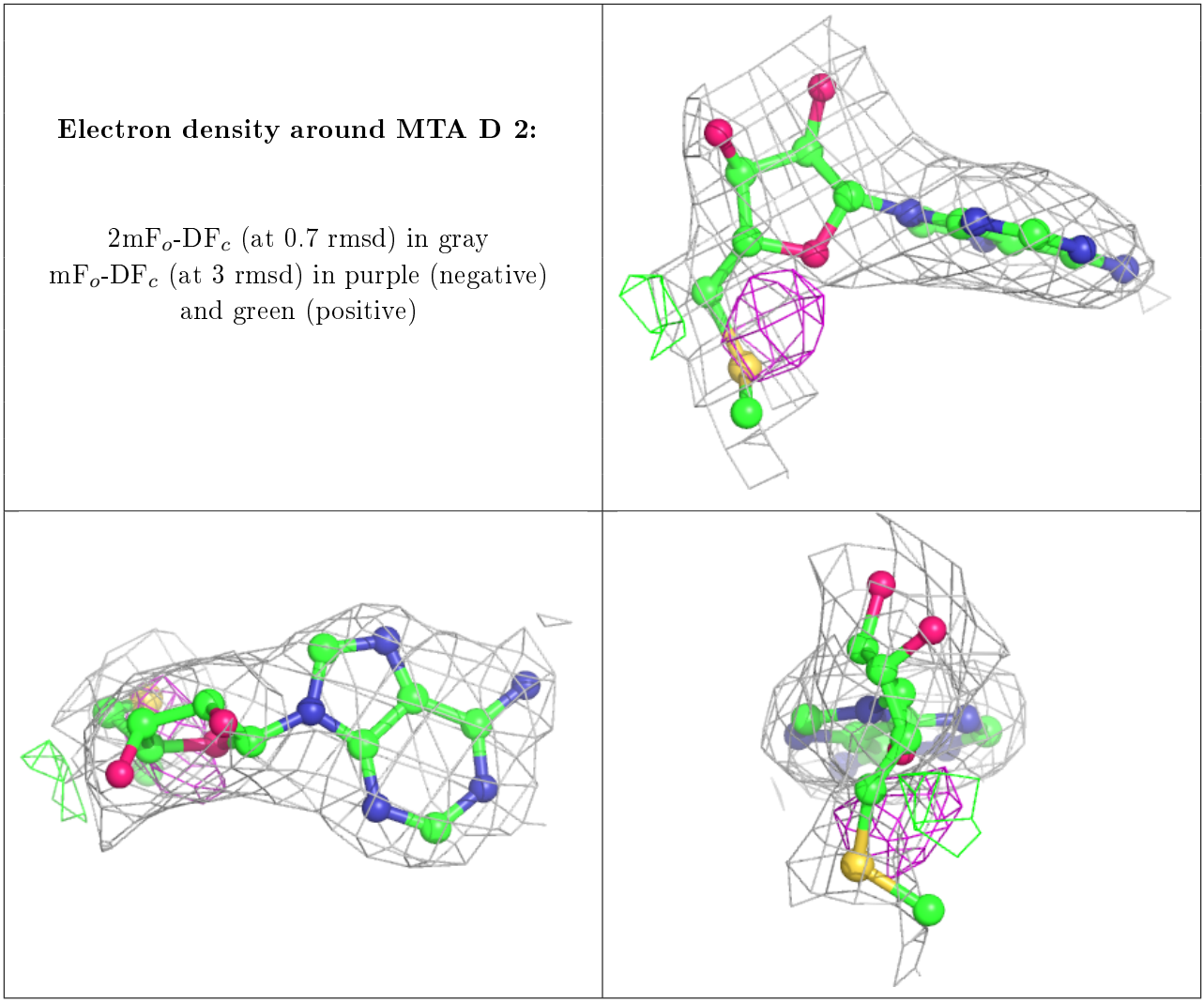






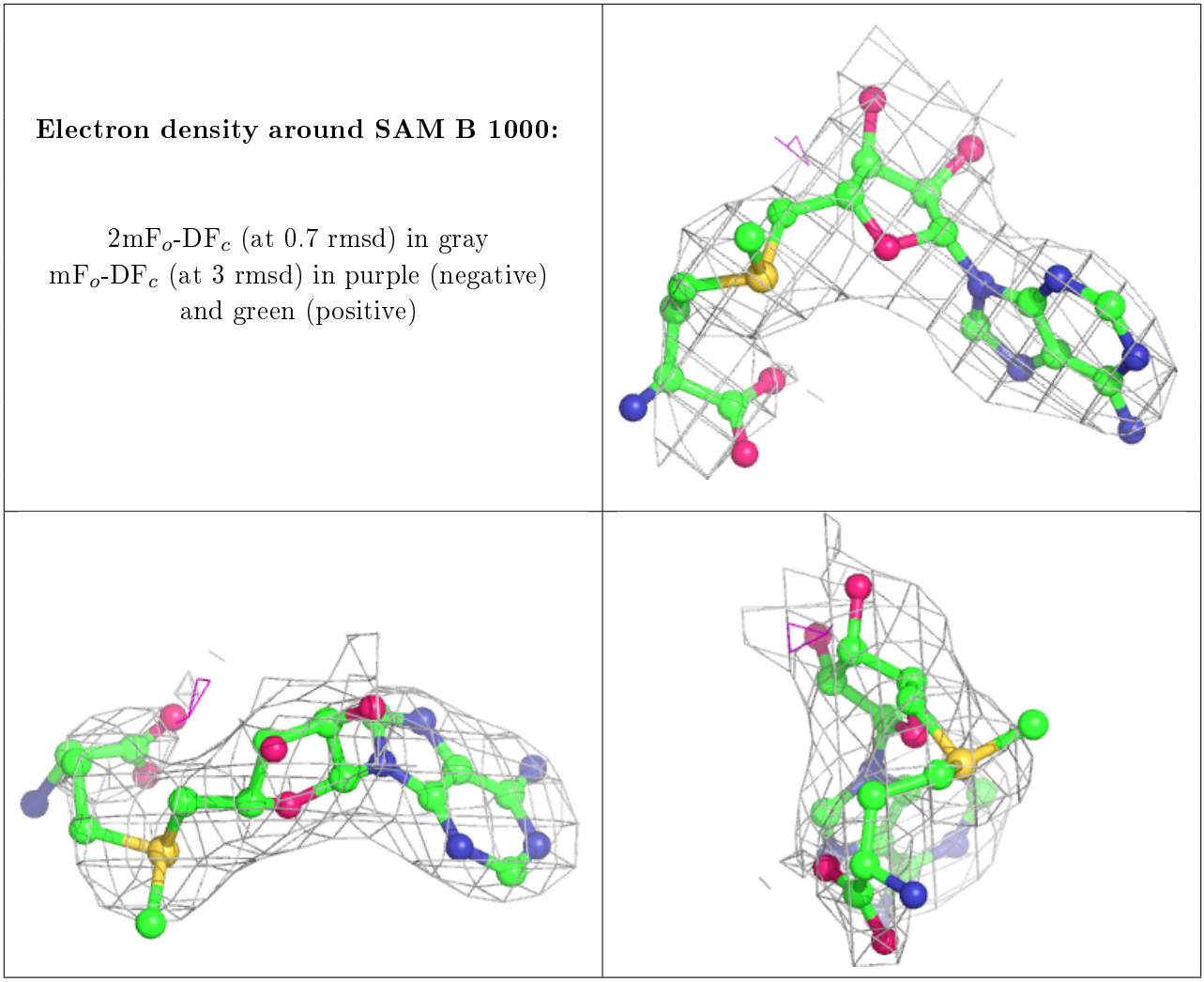
Electron density around MTA D 2:

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



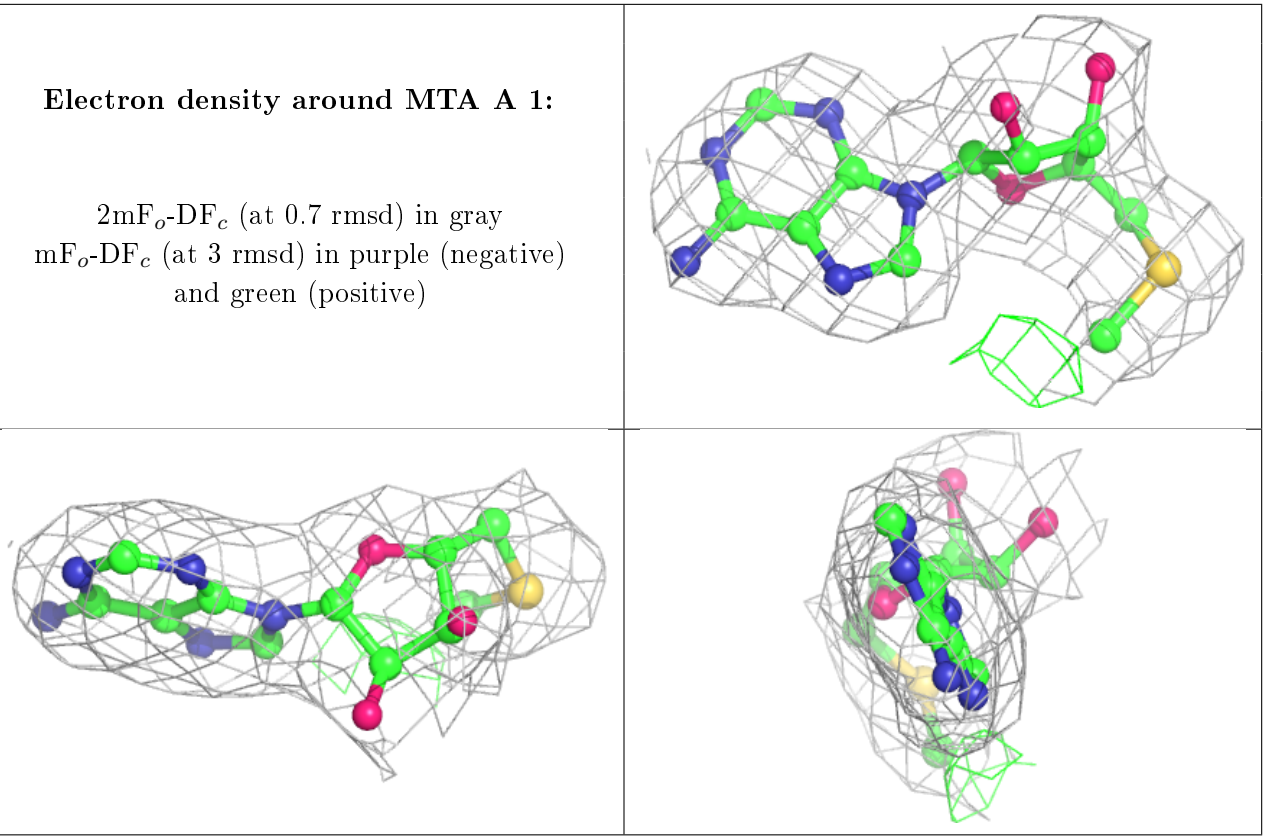
Electron density around SAM B 1000:

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



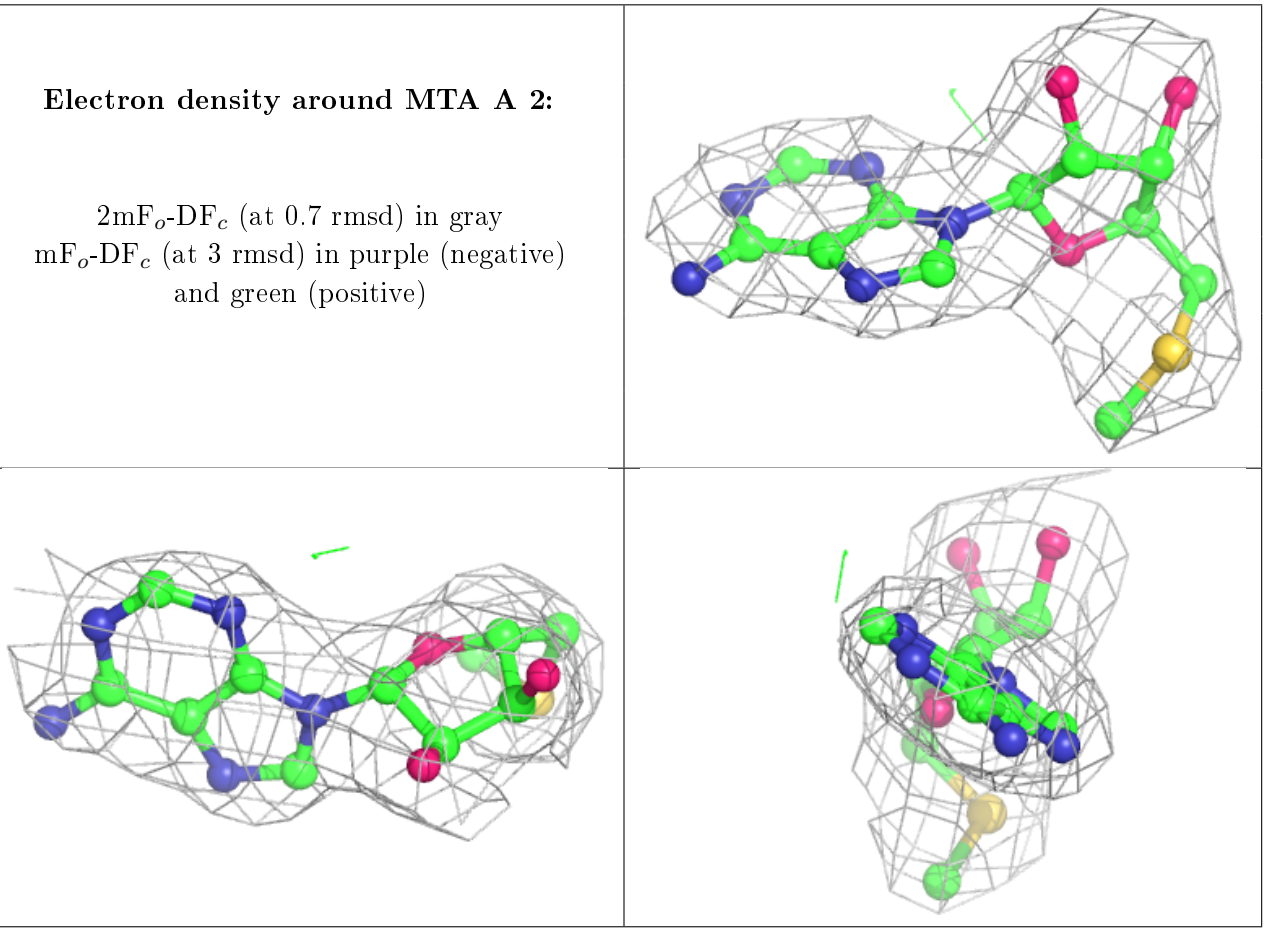
Electron density around MTA A 1:

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



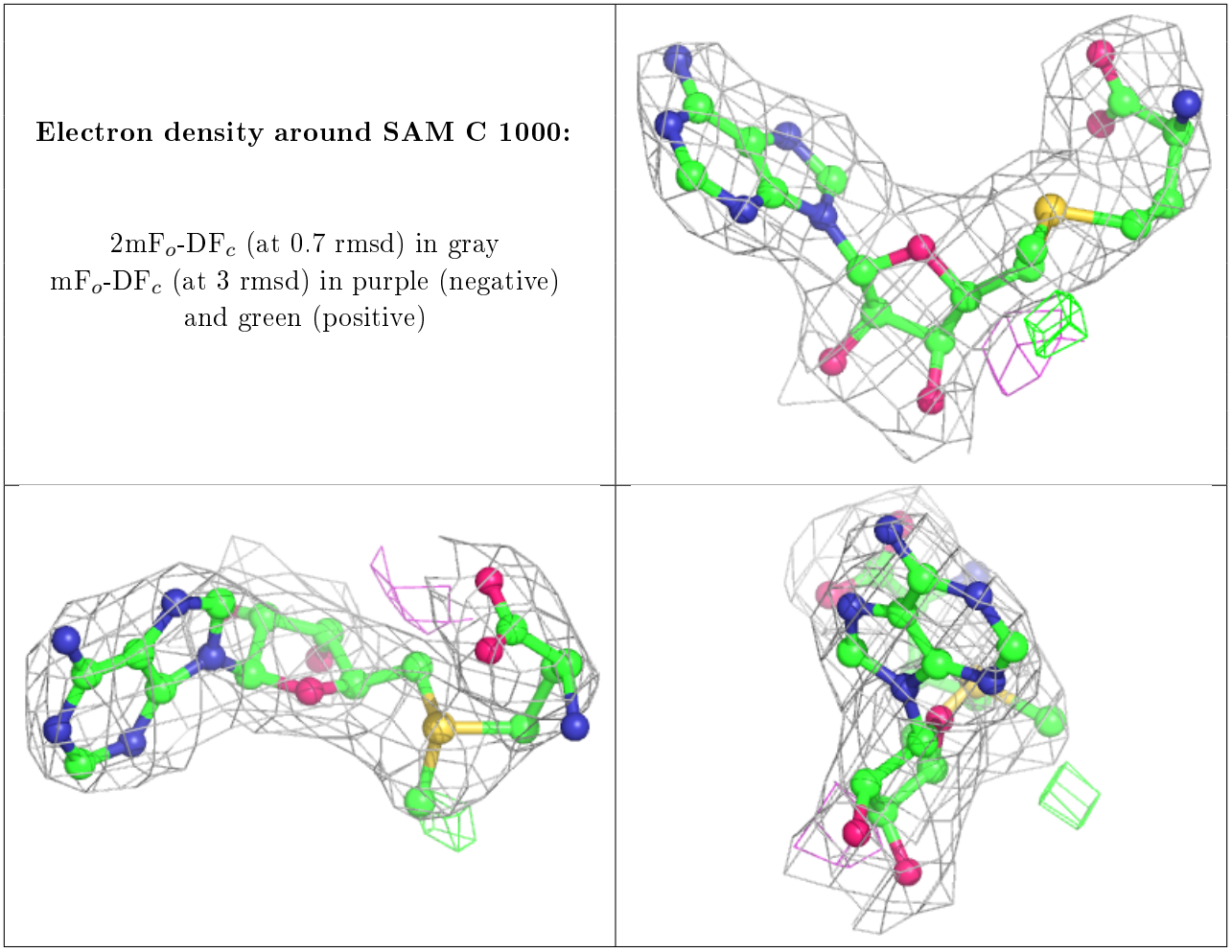
Electron density around MTA A 2:

$2mF_o$-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 1000:

$2mF_o$-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.