



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 10:04 pm GMT

PDB ID : 2C7V  
Title : Structure of Trypanosoma brucei pteridine reductase (PTR1) in ternary complex with cofactor and the antifolate methotrexate  
Authors : Dawson, A.; Gibellini, F.; Sienkiewicz, N.; Fyfe, P.K.; McLuskey, K.; Fairlamb, A.H.; Hunter, W.N.  
Deposited on : 2005-11-29  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**  
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

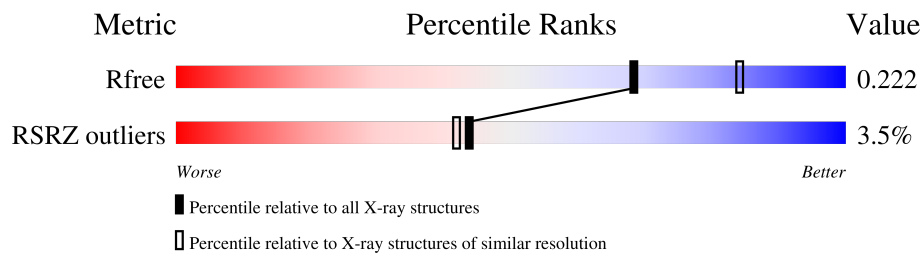
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

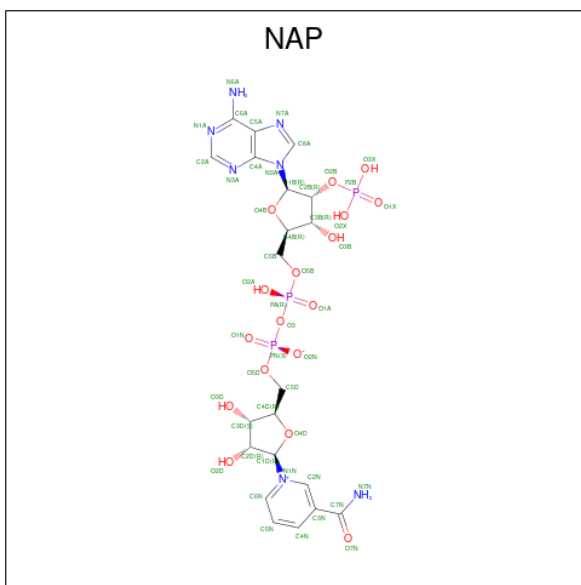
There are 6 unique types of molecules in this entry. The entry contains 8945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PTERIDINE REDUCTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
1	A	253	Total 1933	As 2	C 1215	N 341	O 364	S 11	0	7	0
1	B	254	Total 1945	As 2	C 1220	N 342	O 370	S 11	0	7	0
1	C	260	Total 1984	As 2	C 1242	N 352	O 376	S 12	0	7	0
1	D	257	Total 1950	As 2	C 1225	N 342	O 370	S 11	0	6	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



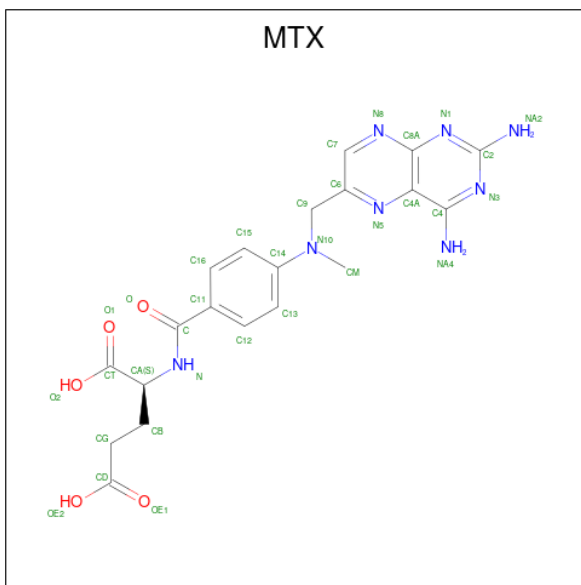
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
3	A	1	Total	C	N	O	0	0
			33	20	8	5		
3	B	1	Total	C	N	O	0	0
			33	20	8	5		
3	C	1	Total	C	N	O	0	0
			33	20	8	5		
3	D	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	B	1	Total	Ni	0	0
			1	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	203	Total O 203 203	0	0
6	B	217	Total O 217 217	0	0
6	C	192	Total O 192 192	0	0
6	D	187	Total O 187 187	0	0

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### 3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.66Å 90.24Å 82.84Å 90.00° 115.76° 90.00°	Depositor
Resolution (Å)	74.54 – 2.20 28.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (74.54-2.20) 99.2 (28.76-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.153 , 0.223 0.154 , 0.222	Depositor DCC
$R_{free}$ test set	2534 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtrriage
Anisotropy	0.849	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8945	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

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#### 4.3.3 RNA [i](#)

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### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CAF	B	168	1	3,9,10	1.10	0	1,12,14	0.12	0
1	CAF	B	59	1	3,9,10	0.94	0	1,12,14	0.45	0
1	CAF	D	59	1	3,9,10	0.88	0	1,12,14	0.79	0
1	CAF	D	168	1	3,9,10	1.04	0	1,12,14	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CAF	C	168	1	3,9,10	0.90	0	1,12,14	0.12	0
1	CAF	C	59	1	3,9,10	1.04	0	1,12,14	0.62	0
1	CAF	A	59	1	3,9,10	0.77	0	1,12,14	0.26	0
1	CAF	A	168	1	3,9,10	1.02	0	1,12,14	0.08	0

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
1	CAF	B	168	1	-	0/0/8/10	-
1	CAF	B	59	1	-	0/0/8/10	-
1	CAF	D	59	1	-	0/0/8/10	-
1	CAF	D	168	1	-	0/0/8/10	-
1	CAF	C	168	1	-	0/0/8/10	-
1	CAF	C	59	1	-	0/0/8/10	-
1	CAF	A	59	1	-	0/0/8/10	-
1	CAF	A	168	1	-	0/0/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 4.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
3	MTX	B	1272	-	35,35,35	1.97	5 (14%)	46,49,49	1.75	11 (23%)
2	NAP	C	1271	-	45,52,52	1.75	4 (8%)	56,80,80	1.22	5 (8%)
3	MTX	C	1272	-	35,35,35	1.97	5 (14%)	46,49,49	1.93	14 (30%)
2	NAP	B	1271	-	45,52,52	1.62	4 (8%)	56,80,80	1.18	2 (3%)
3	MTX	D	1272	-	35,35,35	2.05	4 (11%)	46,49,49	1.96	13 (28%)
3	MTX	A	1272	-	35,35,35	1.87	4 (11%)	46,49,49	1.82	10 (21%)
2	NAP	D	1271	-	45,52,52	1.85	4 (8%)	56,80,80	1.06	2 (3%)
5	ACT	B	1274	-	3,3,3	0.67	0	3,3,3	1.22	0
2	NAP	A	1271	-	45,52,52	1.66	4 (8%)	56,80,80	1.14	3 (5%)
5	ACT	A	1274	-	3,3,3	0.81	0	3,3,3	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MTX	B	1272	-	-	1/25/25/25	0/3/3/3
2	NAP	C	1271	-	-	1/31/67/67	0/5/5/5
3	MTX	C	1272	-	-	5/25/25/25	0/3/3/3
2	NAP	B	1271	-	-	0/31/67/67	0/5/5/5
3	MTX	D	1272	-	-	0/25/25/25	0/3/3/3
3	MTX	A	1272	-	-	2/25/25/25	0/3/3/3
2	NAP	D	1271	-	-	0/31/67/67	0/5/5/5
2	NAP	A	1271	-	-	0/31/67/67	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1271	NAP	O7N-C7N	9.81	1.42	1.24
3	D	1272	MTX	O-C	9.12	1.41	1.23
3	C	1272	MTX	O-C	8.84	1.41	1.23
2	C	1271	NAP	O7N-C7N	8.80	1.41	1.24
2	A	1271	NAP	O7N-C7N	8.68	1.40	1.24
3	B	1272	MTX	O-C	8.65	1.40	1.23
3	A	1272	MTX	O-C	8.49	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1271	NAP	O7N-C7N	8.15	1.39	1.24
2	B	1271	NAP	C2A-N3A	4.28	1.39	1.32
3	D	1272	MTX	C6-N5	4.09	1.39	1.32
2	A	1271	NAP	C2A-N3A	4.05	1.38	1.32
3	B	1272	MTX	C7-N8	4.03	1.38	1.31
2	D	1271	NAP	C2A-N3A	4.00	1.38	1.32
3	D	1272	MTX	C7-N8	3.99	1.38	1.31
3	C	1272	MTX	C6-N5	3.96	1.39	1.32
2	C	1271	NAP	C2A-N3A	3.93	1.38	1.32
3	B	1272	MTX	C6-N5	3.87	1.39	1.32
3	A	1272	MTX	C7-N8	3.85	1.38	1.31
3	C	1272	MTX	C7-N8	3.54	1.37	1.31
2	C	1271	NAP	C2N-N1N	3.53	1.39	1.35
3	A	1272	MTX	C6-N5	3.34	1.38	1.32
3	C	1272	MTX	C4-N3	2.86	1.39	1.33
2	B	1271	NAP	C2A-N1A	2.84	1.39	1.33
2	D	1271	NAP	C2N-N1N	2.72	1.38	1.35
3	B	1272	MTX	C4-N3	2.60	1.38	1.33
2	D	1271	NAP	C2A-N1A	2.60	1.38	1.33
3	A	1272	MTX	C4-N3	2.46	1.38	1.33
3	D	1272	MTX	C4-N3	2.45	1.38	1.33
2	A	1271	NAP	C2N-N1N	2.38	1.37	1.35
2	A	1271	NAP	C2A-N1A	2.33	1.38	1.33
3	B	1272	MTX	C2-N3	2.18	1.39	1.35
2	C	1271	NAP	C2A-N1A	2.17	1.37	1.33
2	B	1271	NAP	C2N-N1N	2.12	1.37	1.35
3	C	1272	MTX	C2-N3	2.02	1.39	1.35

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1272	MTX	N1-C2-N3	-5.38	120.05	127.22
2	A	1271	NAP	N3A-C2A-N1A	-5.37	120.29	128.68
2	D	1271	NAP	N3A-C2A-N1A	-5.36	120.31	128.68
2	B	1271	NAP	N3A-C2A-N1A	-5.28	120.43	128.68
3	D	1272	MTX	N1-C2-N3	-5.27	120.19	127.22
3	B	1272	MTX	N1-C2-N3	-5.27	120.19	127.22
3	C	1272	MTX	N1-C2-N3	-5.25	120.21	127.22
2	C	1271	NAP	N3A-C2A-N1A	-5.18	120.58	128.68
3	B	1272	MTX	C2-N1-C8A	4.55	120.56	115.36
3	C	1272	MTX	C9-C6-N5	4.44	124.08	116.96
3	D	1272	MTX	C7-N8-C8A	4.17	120.89	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1272	MTX	C2-N1-C8A	4.13	120.07	115.36
3	A	1272	MTX	C7-N8-C8A	4.08	120.79	116.69
3	A	1272	MTX	C2-N1-C8A	3.95	119.87	115.36
3	A	1272	MTX	N8-C8A-N1	3.81	120.17	115.82
3	D	1272	MTX	C6-C7-N8	-3.77	119.44	123.13
3	C	1272	MTX	C7-N8-C8A	3.71	120.42	116.69
2	C	1271	NAP	C3N-C7N-N7N	3.71	122.20	117.75
2	B	1271	NAP	C3N-C7N-N7N	3.62	122.09	117.75
3	D	1272	MTX	C9-C6-N5	3.53	122.62	116.96
3	C	1272	MTX	C2-N1-C8A	3.48	119.33	115.36
3	D	1272	MTX	N8-C8A-N1	3.40	119.70	115.82
3	B	1272	MTX	N8-C8A-N1	3.29	119.58	115.82
3	C	1272	MTX	C9-C6-C7	-3.08	116.22	121.60
3	A	1272	MTX	C6-C7-N8	-3.07	120.12	123.13
3	B	1272	MTX	C6-C7-N8	-2.98	120.20	123.13
3	D	1272	MTX	C8A-C4A-N5	-2.87	118.94	122.41
3	B	1272	MTX	C9-C6-N5	2.86	121.54	116.96
3	C	1272	MTX	C4A-C4-N3	-2.84	119.14	121.01
3	C	1272	MTX	C6-C7-N8	-2.82	120.36	123.13
3	B	1272	MTX	C7-N8-C8A	2.81	119.52	116.69
3	A	1272	MTX	C9-C6-N5	2.81	121.46	116.96
3	C	1272	MTX	C8A-C4A-N5	-2.62	119.24	122.41
2	A	1271	NAP	C3N-C7N-N7N	2.58	120.85	117.75
3	D	1272	MTX	C9-C6-C7	-2.47	117.29	121.60
3	B	1272	MTX	O2-CT-CA	2.44	121.50	113.40
3	C	1272	MTX	OE2-CD-CG	2.40	121.74	114.03
3	D	1272	MTX	O2-CT-O1	-2.40	118.65	124.09
3	D	1272	MTX	C4-C4A-N5	2.38	122.16	120.33
3	A	1272	MTX	C8A-C4A-N5	-2.30	119.63	122.41
3	B	1272	MTX	C8A-C4A-N5	-2.29	119.64	122.41
3	B	1272	MTX	OE2-CD-CG	2.27	121.32	114.03
3	D	1272	MTX	C4A-C4-N3	-2.26	119.53	121.01
2	D	1271	NAP	PN-O3-PA	-2.24	125.14	132.83
3	A	1272	MTX	O2-CT-O1	-2.23	119.03	124.09
3	C	1272	MTX	C4-C4A-N5	2.22	122.04	120.33
3	A	1272	MTX	O2-CT-CA	2.19	120.68	113.40
3	B	1272	MTX	NA2-C2-N3	2.18	120.65	117.25
3	C	1272	MTX	CB-CA-N	2.18	115.29	110.88
2	C	1271	NAP	O7N-C7N-N7N	-2.17	119.50	122.58
3	C	1272	MTX	CA-N-C	2.14	126.83	121.60
3	D	1272	MTX	OE2-CD-OE1	-2.13	118.00	123.30
2	C	1271	NAP	C4A-C5A-N7A	-2.12	107.19	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1272	MTX	N8-C8A-N1	2.12	118.24	115.82
3	D	1272	MTX	O2-CT-CA	2.11	120.42	113.40
2	C	1271	NAP	C1B-N9A-C4A	-2.10	122.95	126.64
3	A	1272	MTX	NA2-C2-N1	2.09	121.20	117.79
3	B	1272	MTX	C9-C6-C7	-2.09	117.95	121.60
2	A	1271	NAP	C4A-C5A-N7A	-2.04	107.27	109.40
3	C	1272	MTX	O2-CT-CA	2.04	120.19	113.40

There are no chirality outliers.

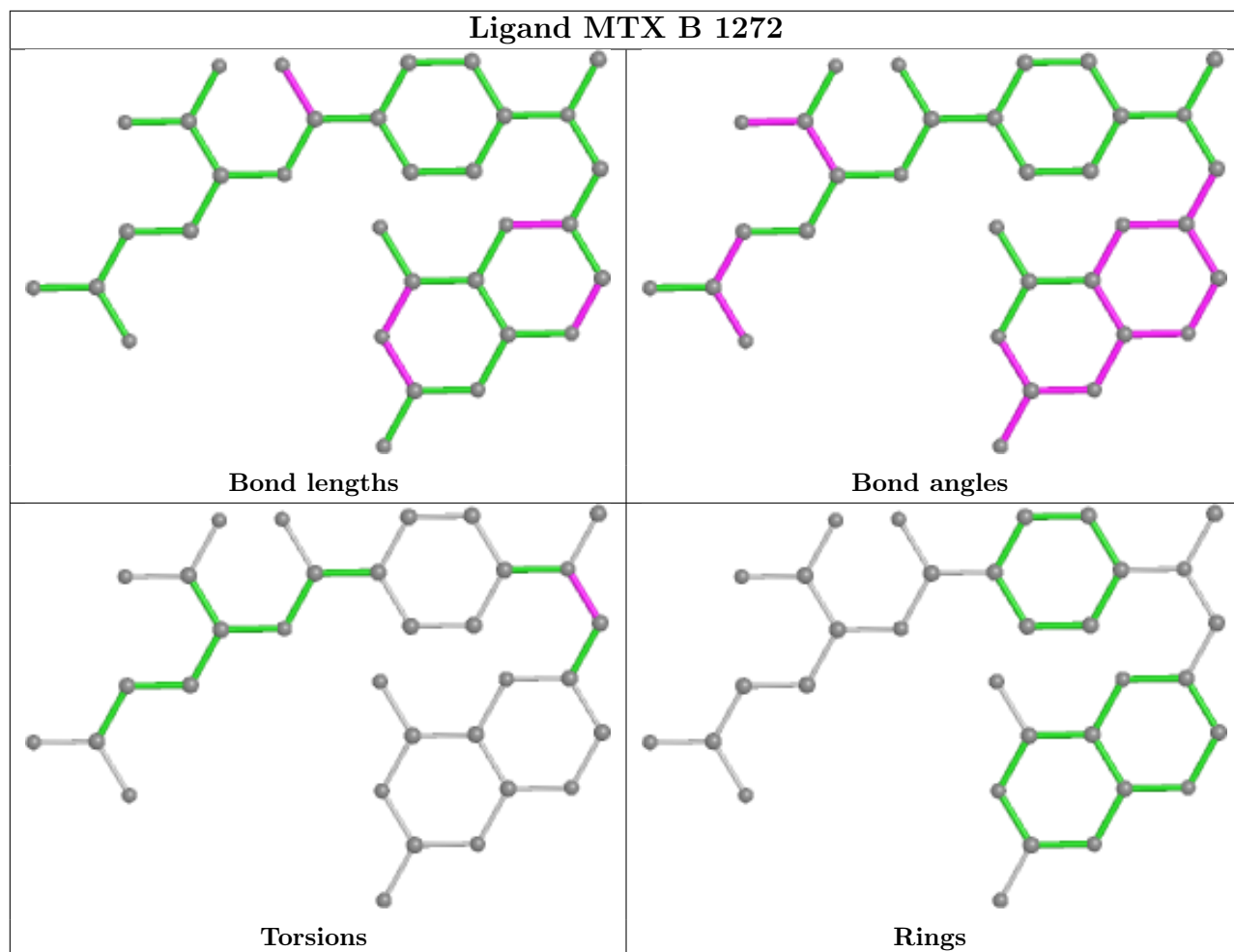
All (9) torsion outliers are listed below:

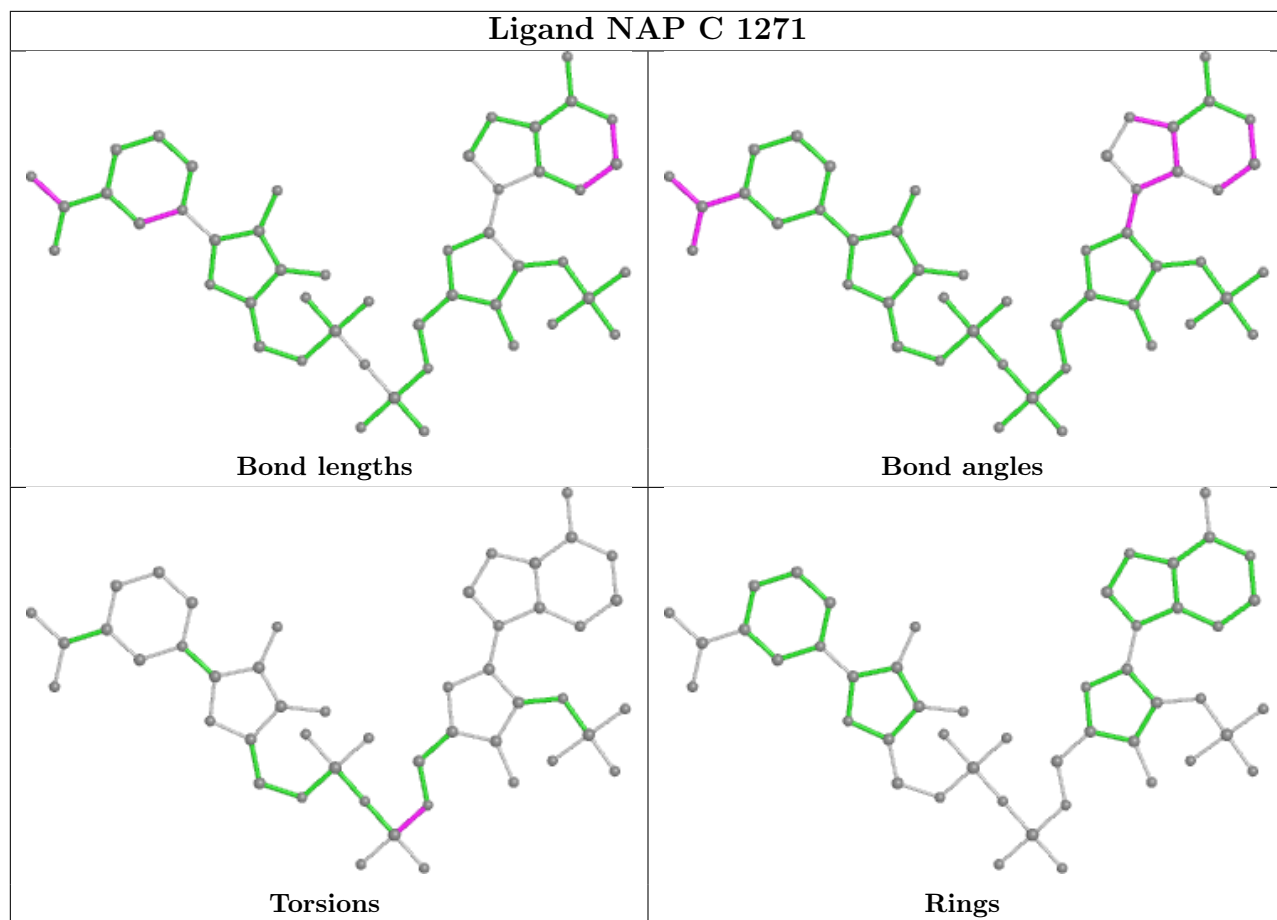
Mol	Chain	Res	Type	Atoms
3	C	1272	MTX	N-CA-CB-CG
3	C	1272	MTX	CT-CA-CB-CG
3	A	1272	MTX	C6-C9-N10-CM
3	B	1272	MTX	C6-C9-N10-CM
3	C	1272	MTX	OE1-CD-CG-CB
3	C	1272	MTX	OE2-CD-CG-CB
3	C	1272	MTX	CA-CB-CG-CD
3	A	1272	MTX	CT-CA-CB-CG
2	C	1271	NAP	C5B-O5B-PA-O1A

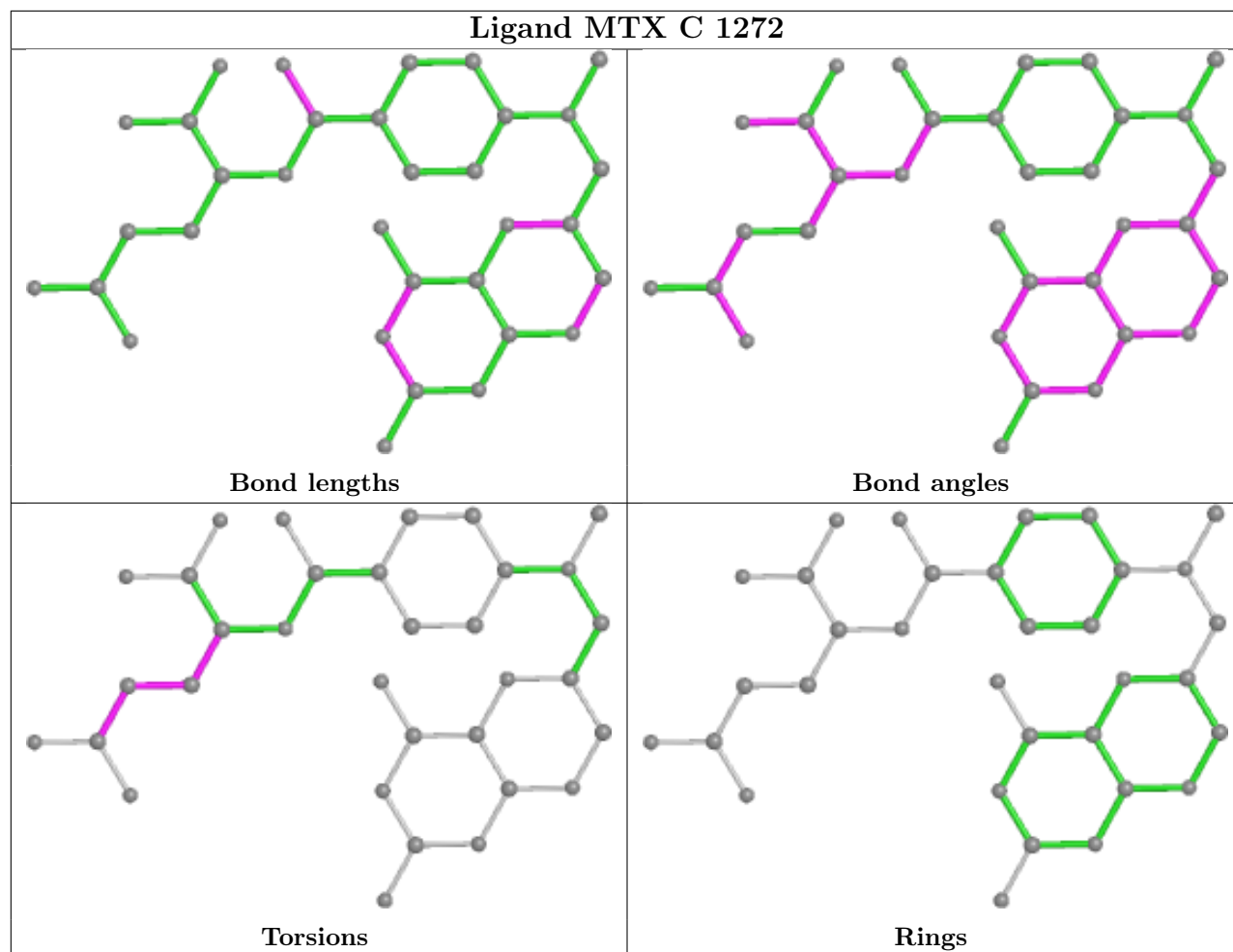
There are no ring outliers.

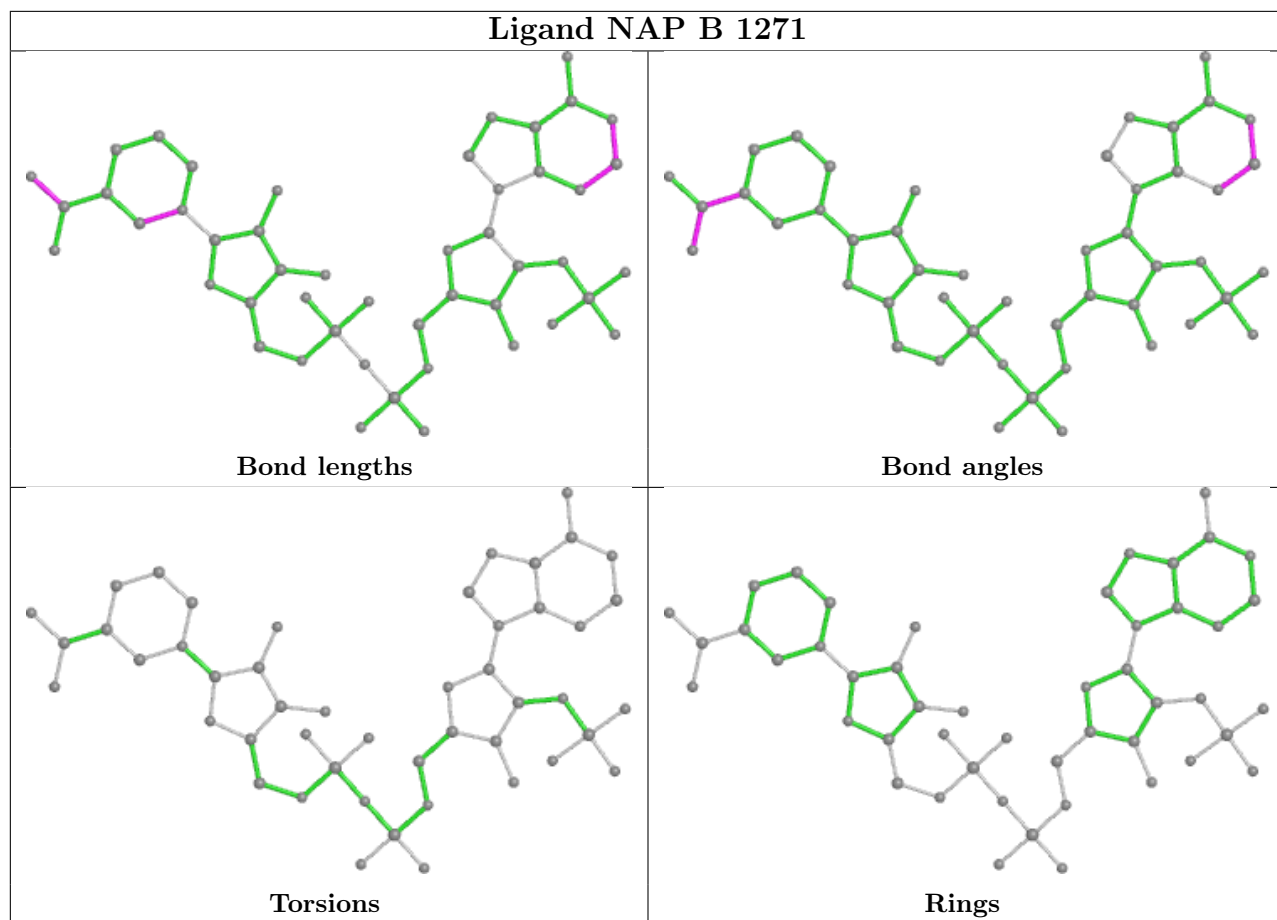
No monomer is involved in short contacts.

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

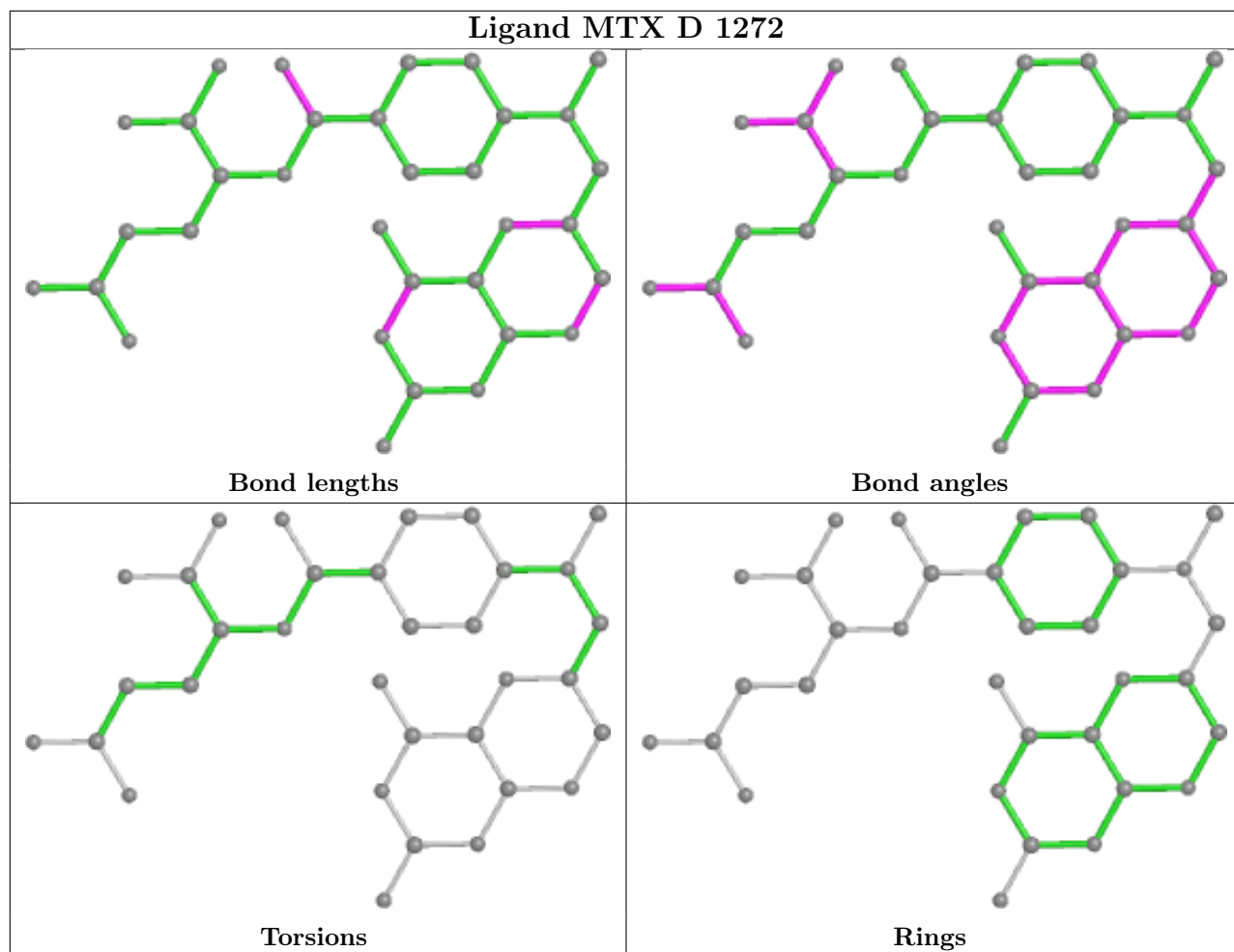


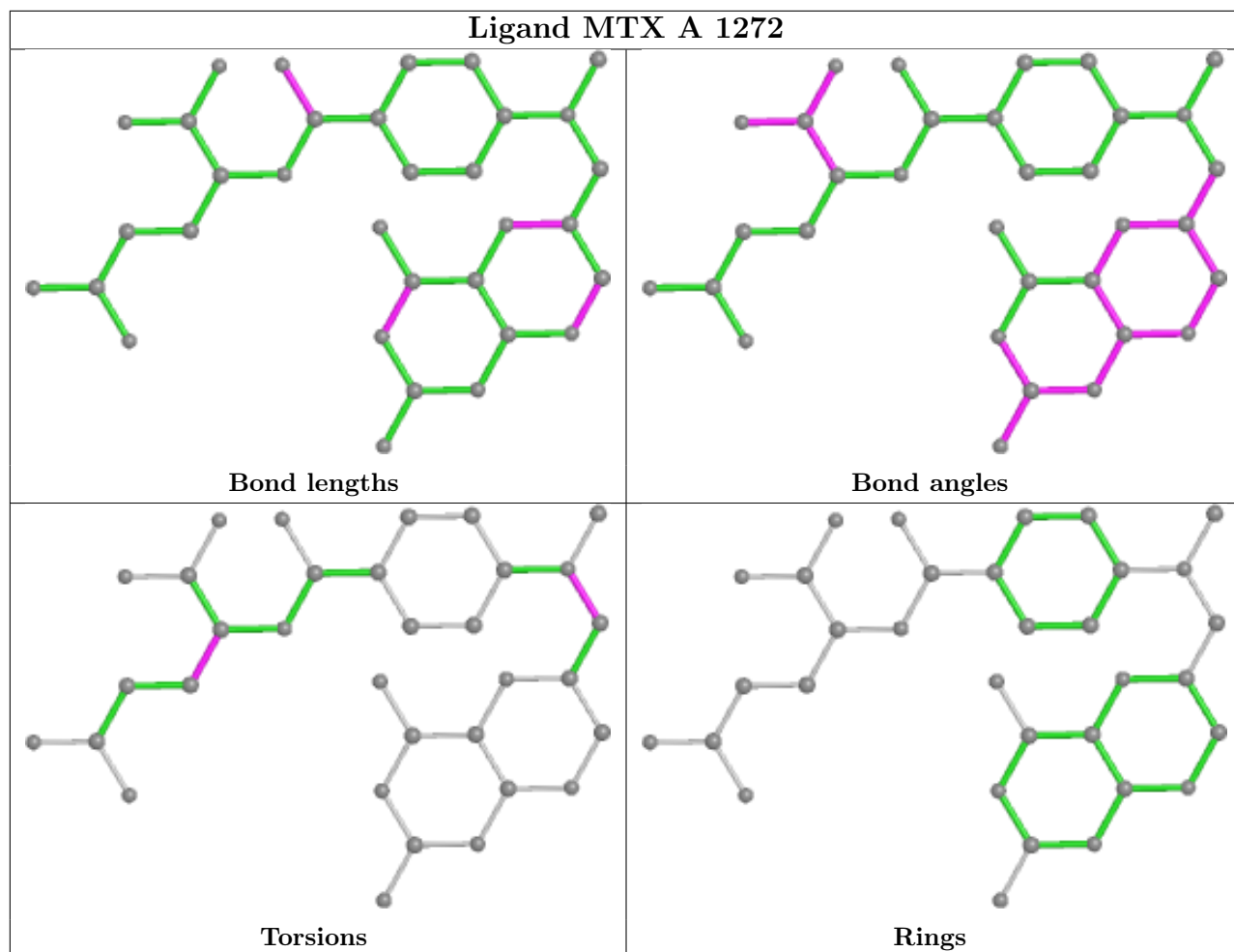


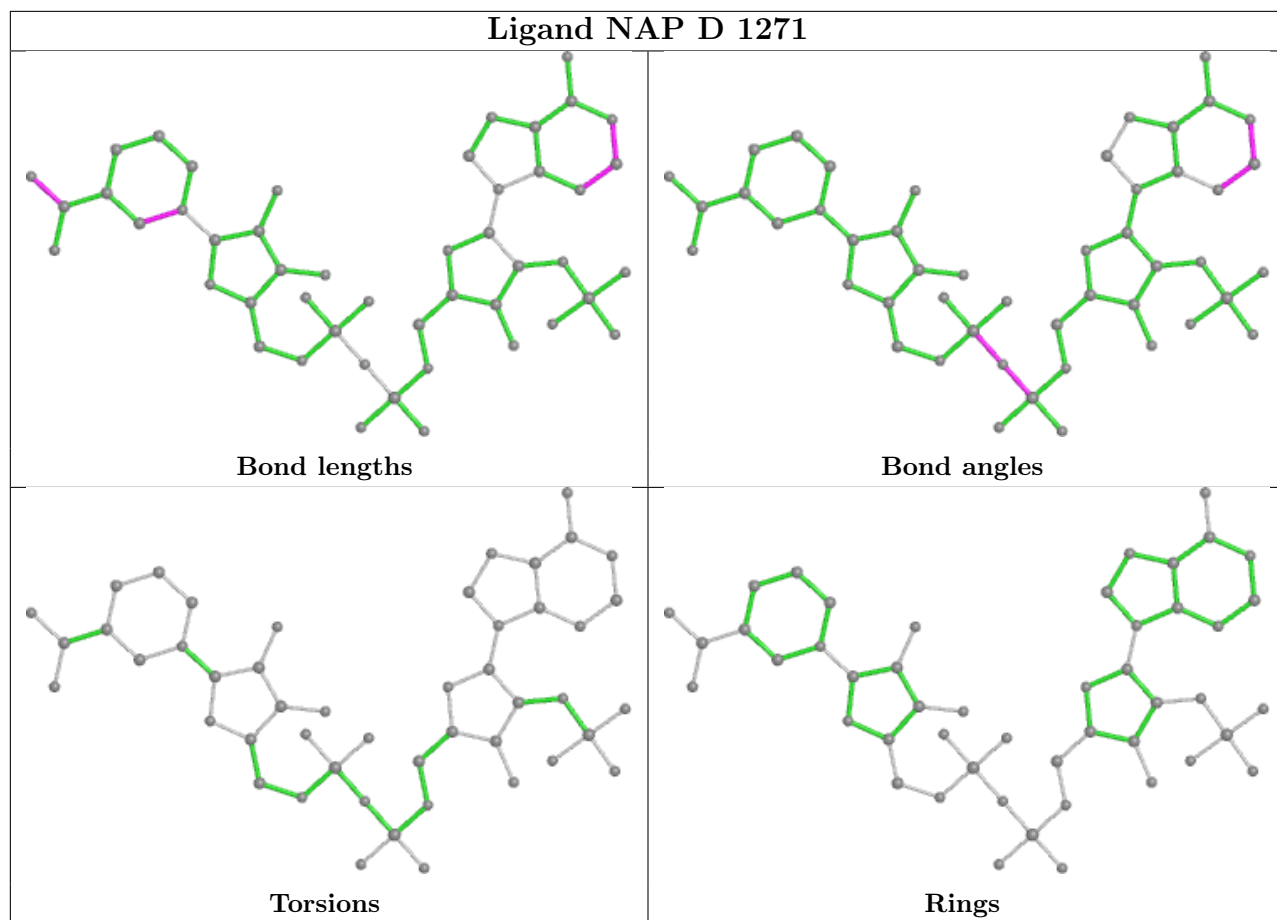


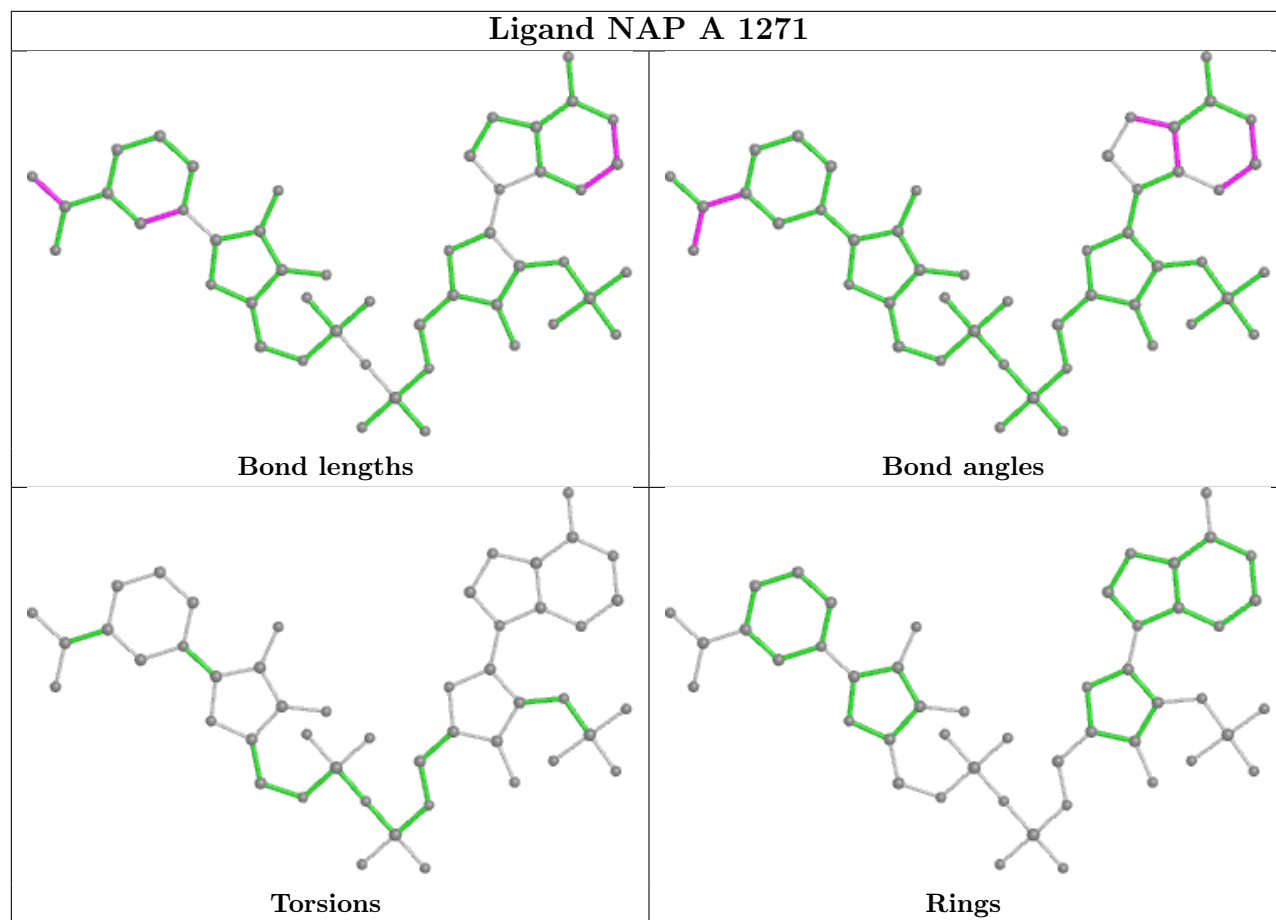












#### 4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	251/268 (93%)	-0.37	8 (3%) 47 45	16, 21, 33, 48	0
1	B	252/268 (94%)	-0.42	7 (2%) 53 51	15, 21, 33, 48	0
1	C	258/268 (96%)	-0.28	10 (3%) 39 37	16, 22, 37, 50	0
1	D	255/268 (95%)	-0.26	11 (4%) 35 33	14, 22, 37, 62	0
All	All	1016/1072 (94%)	-0.33	36 (3%) 44 42	14, 22, 36, 62	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	ASN	7.8
1	C	144	GLY	6.7
1	D	106	ASP	6.4
1	C	105	GLY	5.9
1	D	107	HIS	5.6
1	D	112	ASN	5.1
1	D	105	GLY	4.8
1	B	104	GLN	4.5
1	B	113	GLY	4.4
1	D	113	GLY	4.4
1	A	113	GLY	3.8
1	D	144	GLY	3.8
1	B	150	THR	3.7
1	D	104	GLN	3.6
1	C	145	THR	3.3
1	C	143	LYS	3.1
1	C	113	GLY	3.0
1	B	143	LYS	2.9
1	B	151	SER	2.8
1	B	2	GLU	2.7
1	A	104	GLN	2.6

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	144	GLY	2.6
1	D	2	GLU	2.4
1	C	2	GLU	2.4
1	A	151	SER	2.4
1	A	152	SER	2.4
1	D	151	SER	2.3
1	D	216	GLU	2.2
1	D	223	ARG	2.2
1	A	51	GLU	2.1
1	C	104[A]	GLN	2.1
1	C	151	SER	2.1
1	C	150	THR	2.1
1	C	148	ASN	2.1
1	A	50	LYS	2.1
1	A	143	LYS	2.1

## 5.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CAF	D	168	10/11	0.90	0.14	27,29,38,39	4
1	CAF	C	168	10/11	0.91	0.16	24,27,37,38	4
1	CAF	A	168	10/11	0.95	0.11	25,27,37,38	4
1	CAF	B	168	10/11	0.96	0.12	23,24,32,32	4
1	CAF	C	59	10/11	0.97	0.11	24,26,34,34	0
1	CAF	B	59	10/11	0.97	0.10	23,25,37,38	0
1	CAF	D	59	10/11	0.97	0.10	24,26,35,37	0
1	CAF	A	59	10/11	0.97	0.10	28,30,44,46	0

## 5.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

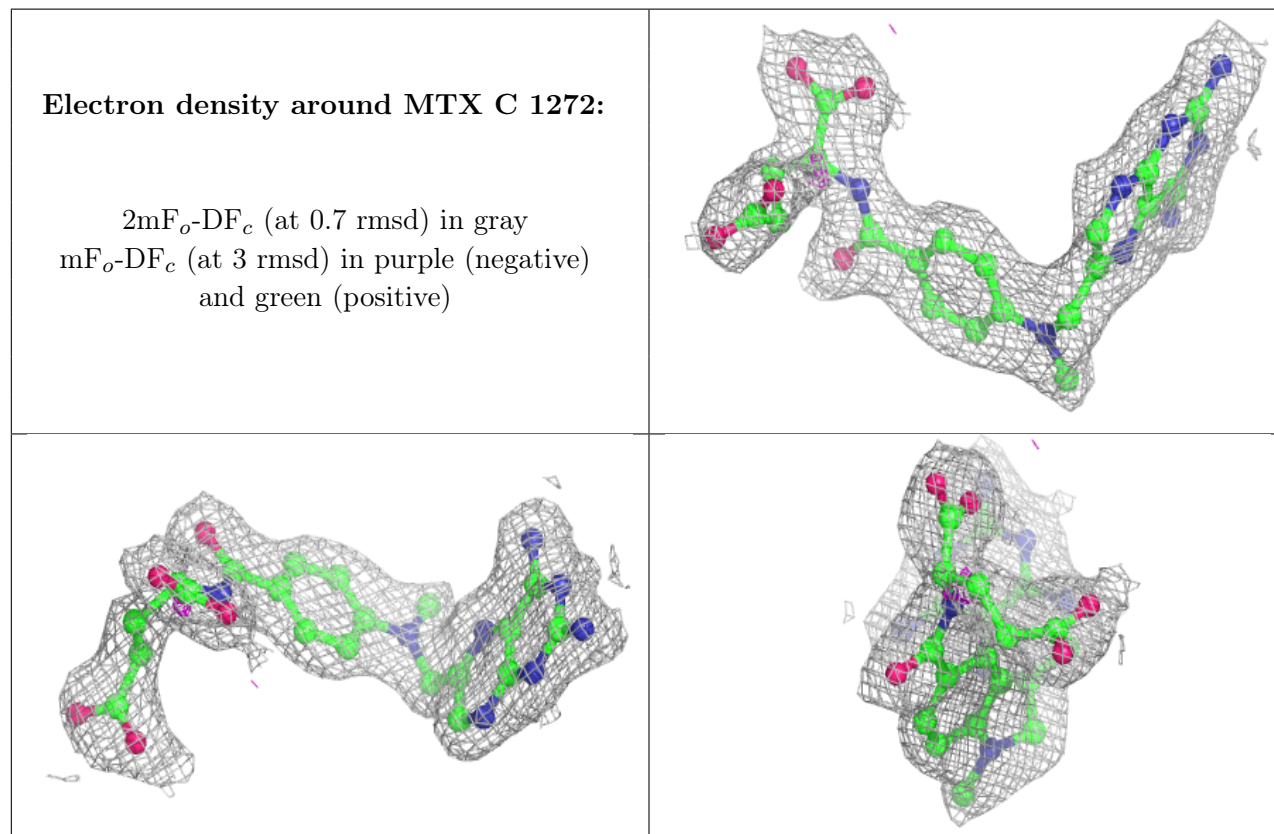
## 5.4 Ligands [i](#)

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<sup>th</sup> 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.

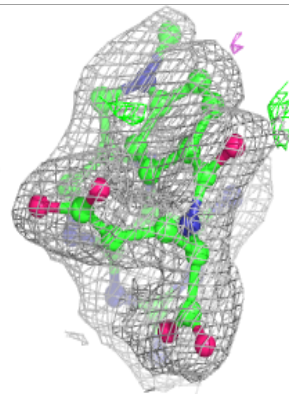
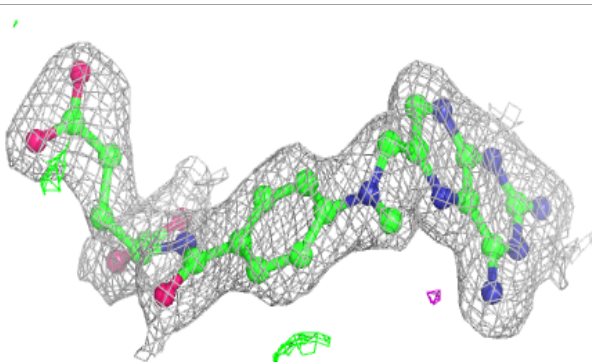
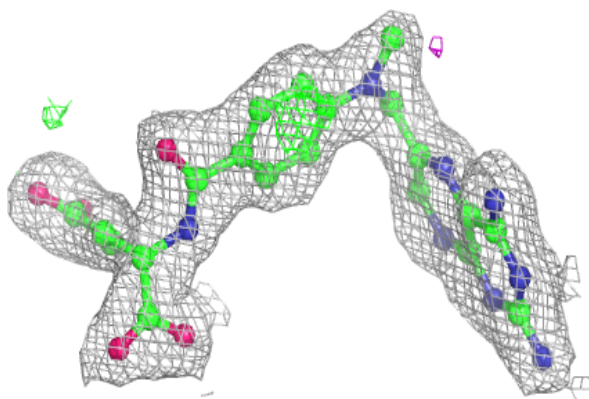
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ACT	A	1274	4/4	0.91	0.17	37,38,38,38	0
3	MTX	C	1272	33/33	0.92	0.14	16,25,36,37	0
3	MTX	D	1272	33/33	0.93	0.13	16,26,35,37	0
3	MTX	A	1272	33/33	0.94	0.11	19,24,30,32	0
4	NI	A	1273	1/1	0.95	0.21	49,49,49,49	1
3	MTX	B	1272	33/33	0.95	0.10	14,22,30,32	0
5	ACT	B	1274	4/4	0.95	0.13	23,23,23,24	0
2	NAP	C	1271	48/48	0.97	0.09	14,17,20,21	0
2	NAP	A	1271	48/48	0.98	0.08	14,19,21,22	0
2	NAP	D	1271	48/48	0.98	0.08	15,18,22,24	0
2	NAP	B	1271	48/48	0.98	0.09	14,17,20,21	0
4	NI	B	1273	1/1	0.99	0.13	43,43,43,43	1

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.

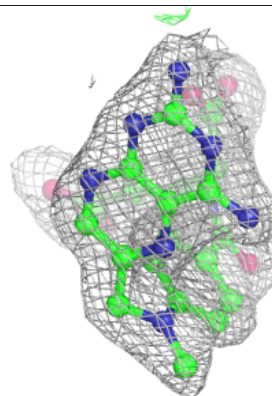
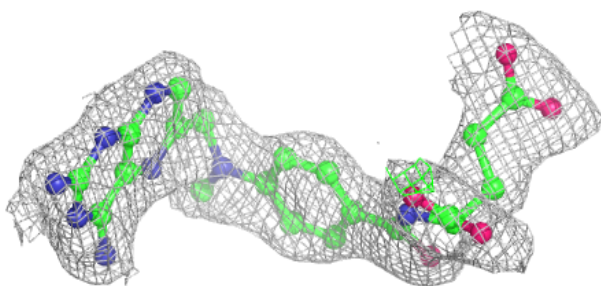
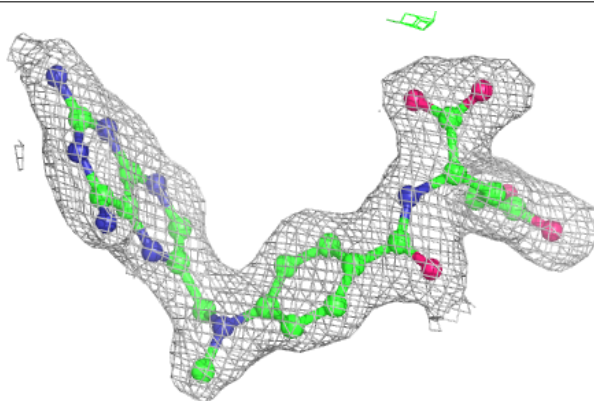


**Electron density around MTX D 1272:**

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

**Electron density around MTX A 1272:**

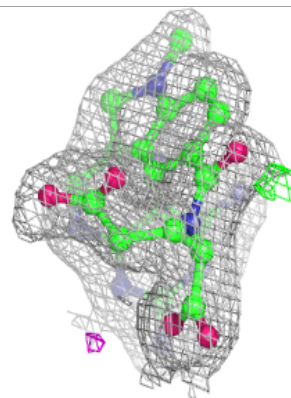
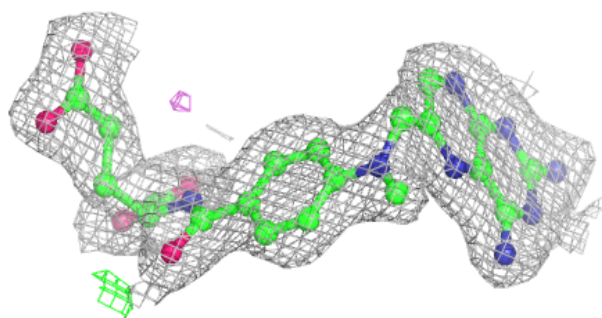
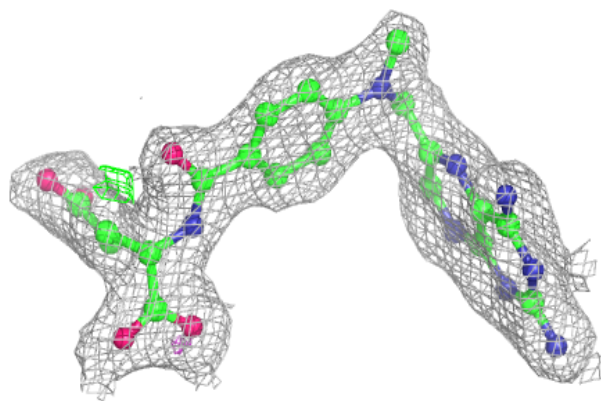
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



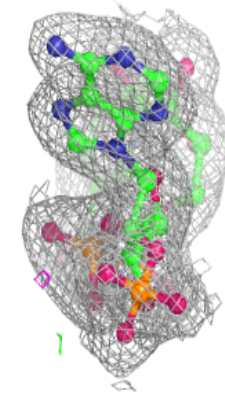
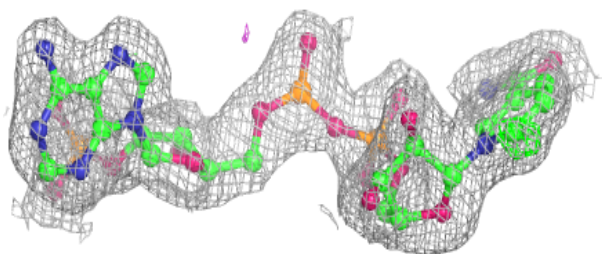
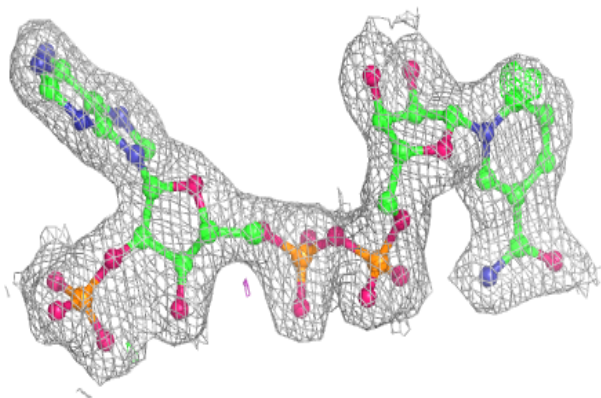


**Electron density around MTX B 1272:**

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

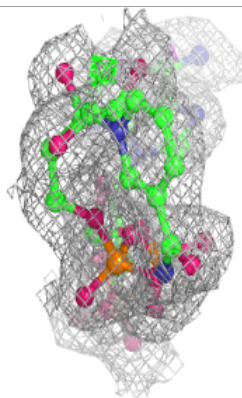
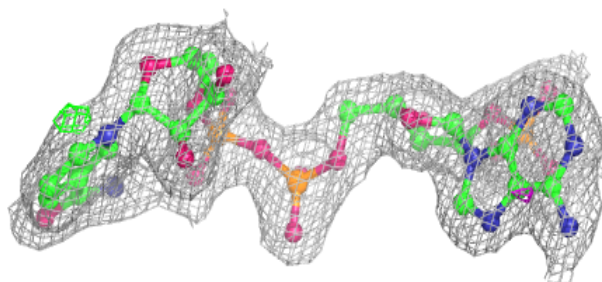
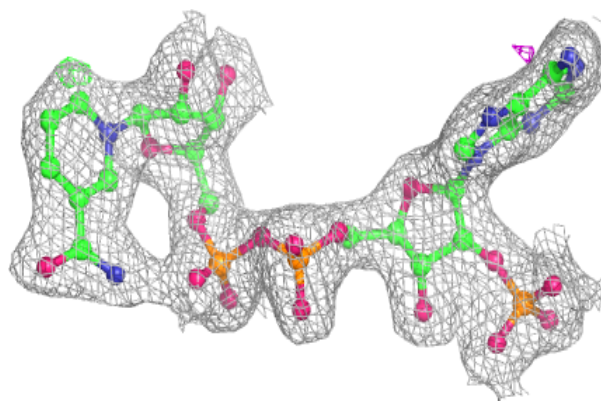
**Electron density around NAP C 1271:**

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

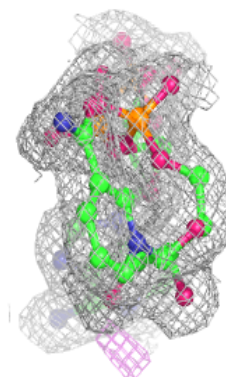
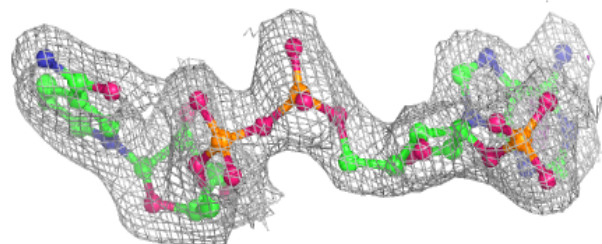
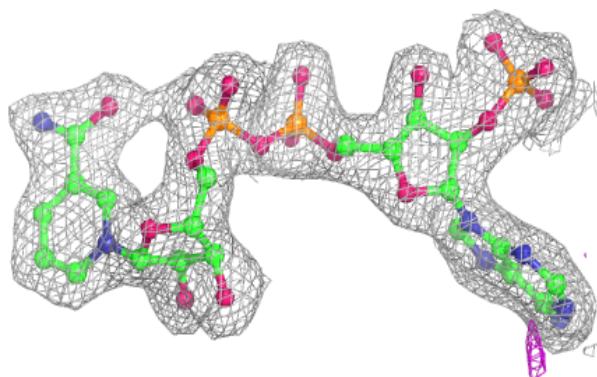


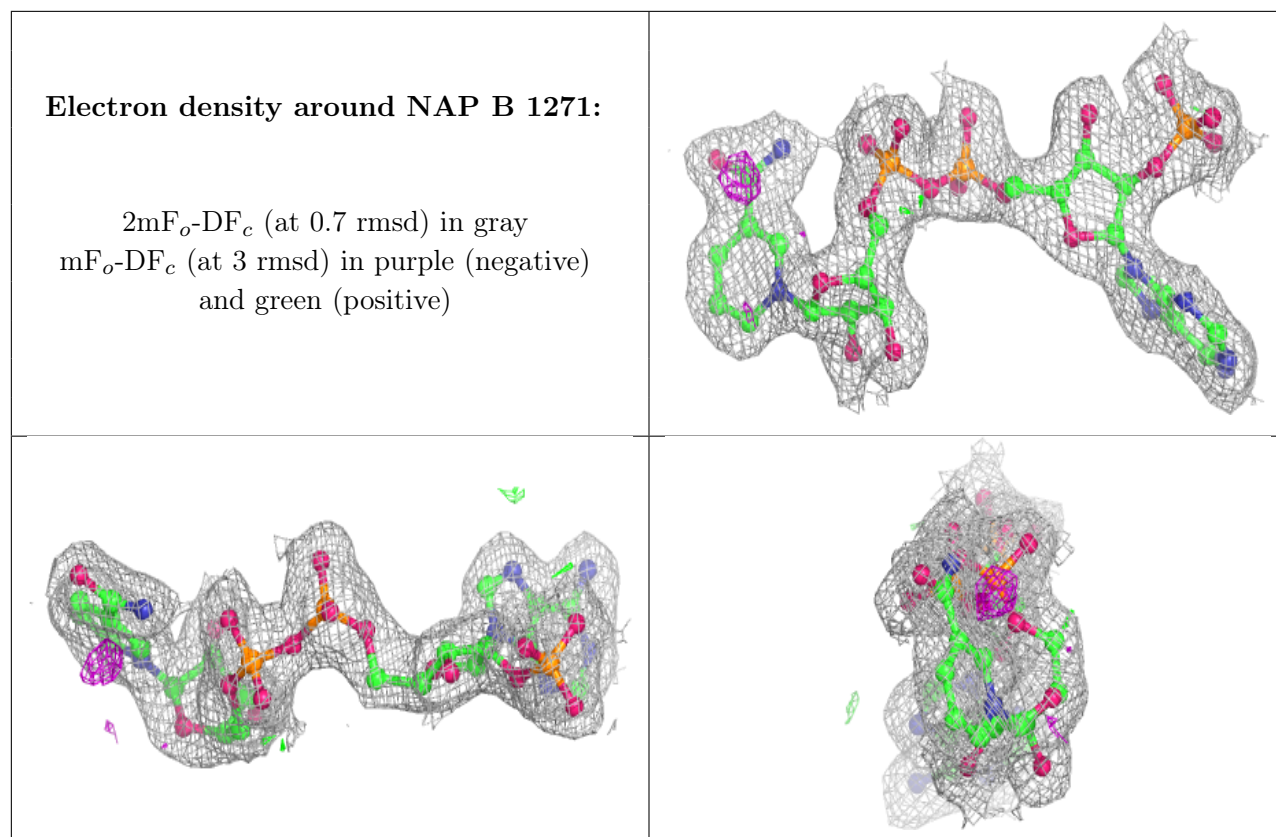
**Electron density around NAP A 1271:**

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

**Electron density around NAP D 1271:**

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





## 5.5 Other polymers [i](#)

There are no such residues in this entry.