wwPDB X-ray Structure Validation Summary Report (i)

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 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 (1)) were used in the production of this report:

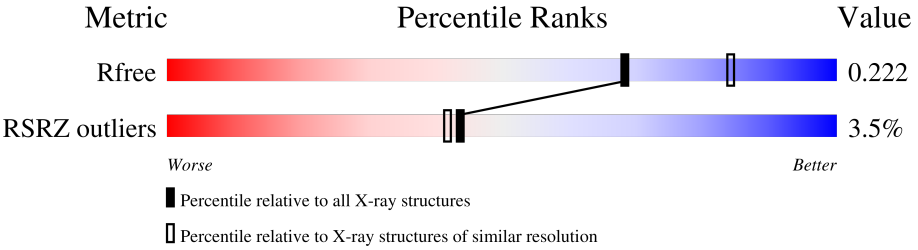
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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)

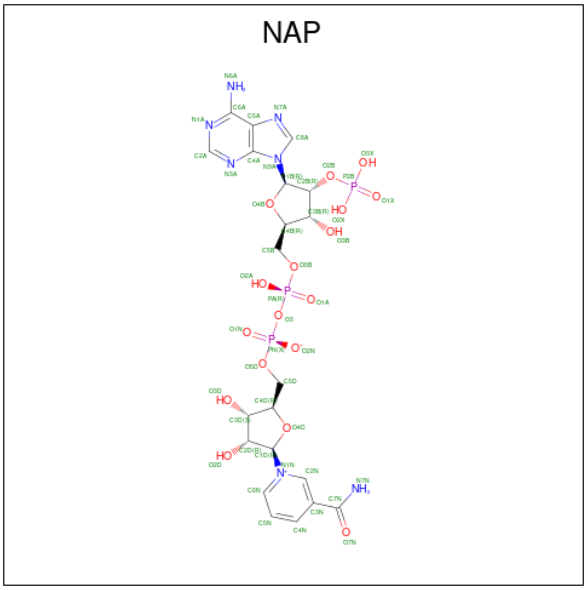
There are 6 unique types of molecules in this entry. The entry contains 8945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1933	2	1215	341	364	11	0	7	0
1	B	254	1945	2	1220	342	370	11	0	7	0
1	C	260	1984	2	1242	352	376	12	0	7	0
1	D	257	1950	2	1225	342	370	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	48	21	7	17	3	0	0
2	B	1	48	21	7	17	3	0	0

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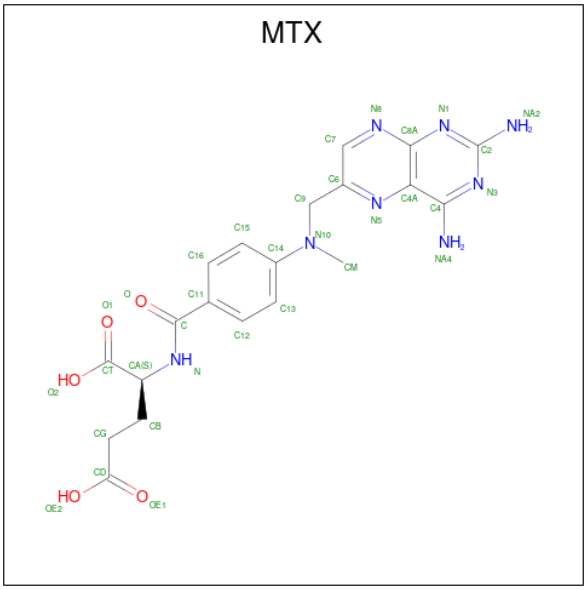
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	D	1	48	21	7	17	3	0	0

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$).

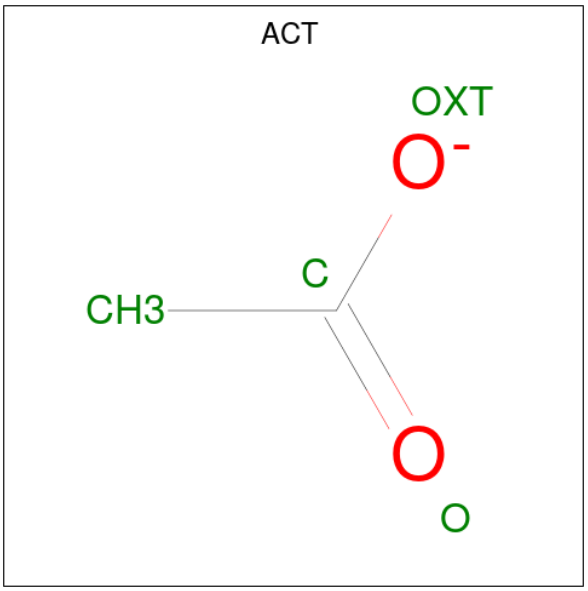


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	20	8	5	0	0
			Total	C	N	O		
3	B	1	33	20	8	5	0	0
			Total	C	N	O		
3	C	1	33	20	8	5	0	0
			Total	C	N	O		
3	D	1	33	20	8	5	0	0

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

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

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

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

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.79 (at 2.20Å)	Xtriage
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^2)	22.1	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8945	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage'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.*

[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.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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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)

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

4.3.3 RNA (i)

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

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

The worst 5 of 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

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

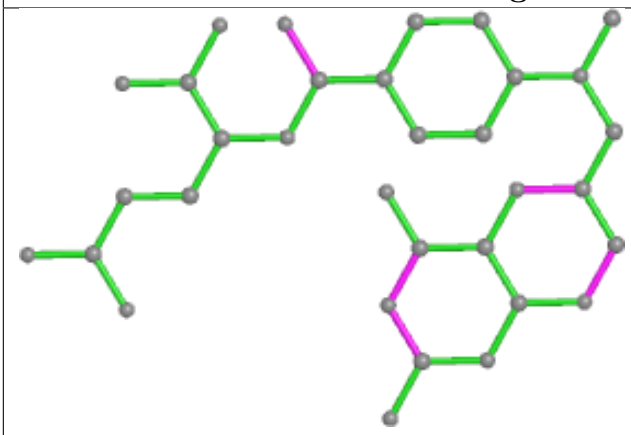
Mol	Chain	Res	Type	Atoms
3	C	1272	MTX	N-CA-CB-CG
3	C	1272	MTX	CT-CA-CB-CG
3	A	1272	MTX	C6-C9-N10-CM
3	B	1272	MTX	C6-C9-N10-CM
3	C	1272	MTX	OE1-CD-CG-CB

There are no ring outliers.

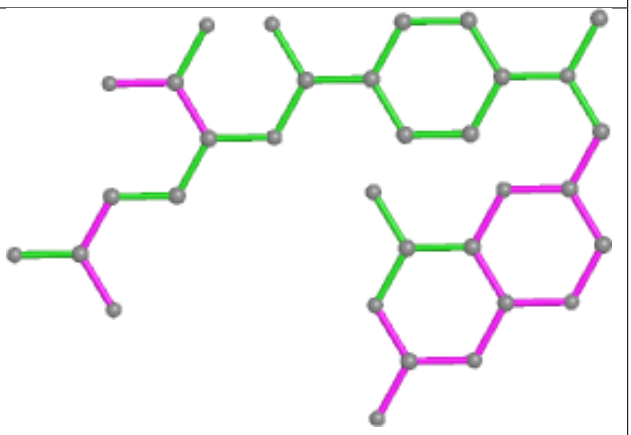
No monomer is involved in short contacts.

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 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.

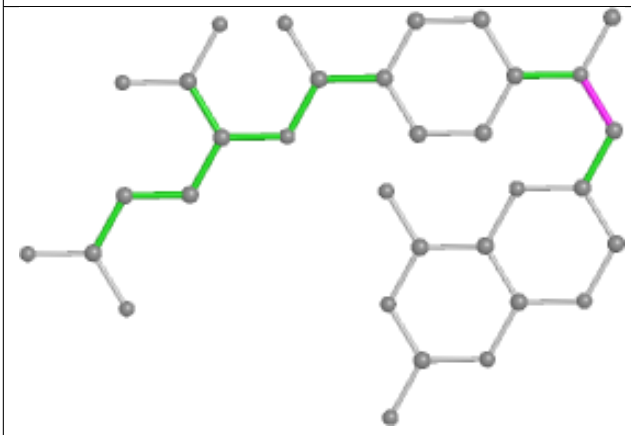
Ligand MTX B 1272



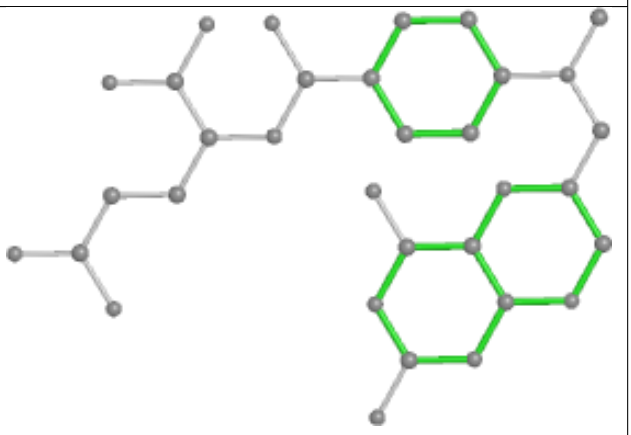
Bond lengths



Bond angles

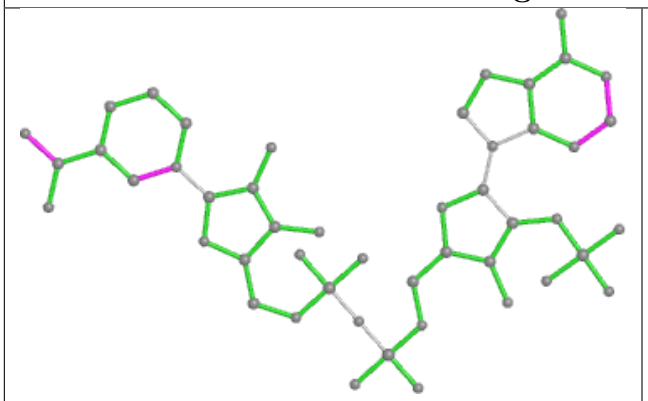


Torsions

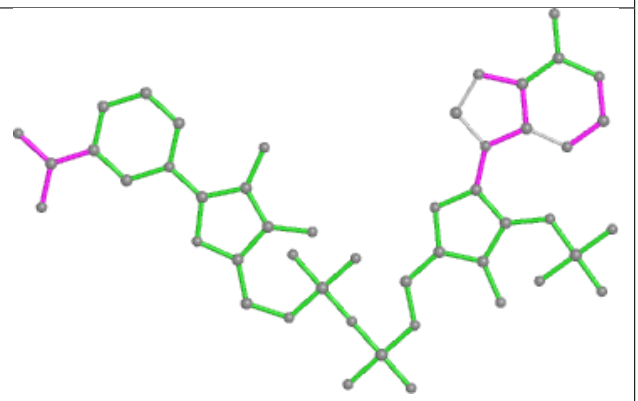


Rings

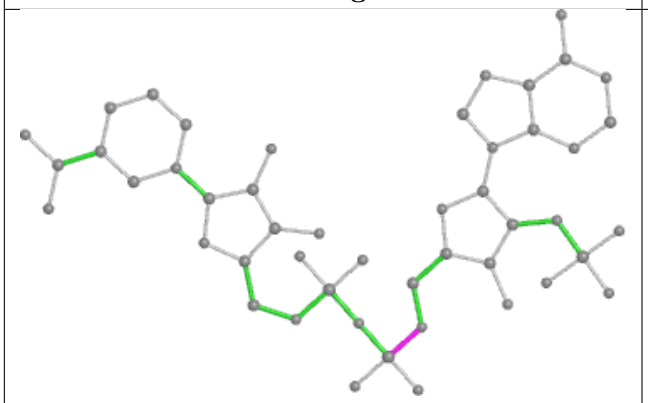
Ligand NAP C 1271



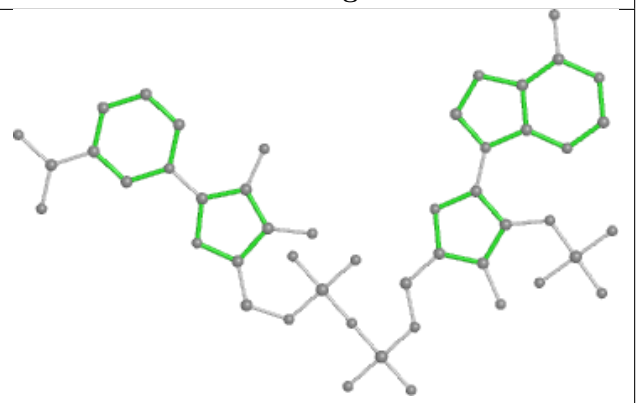
Bond lengths



Bond angles

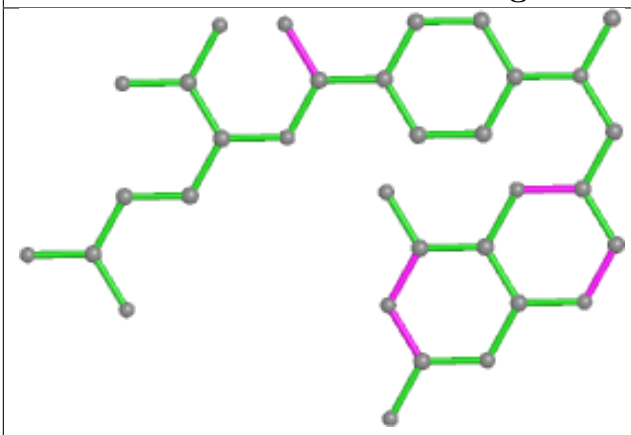


Torsions

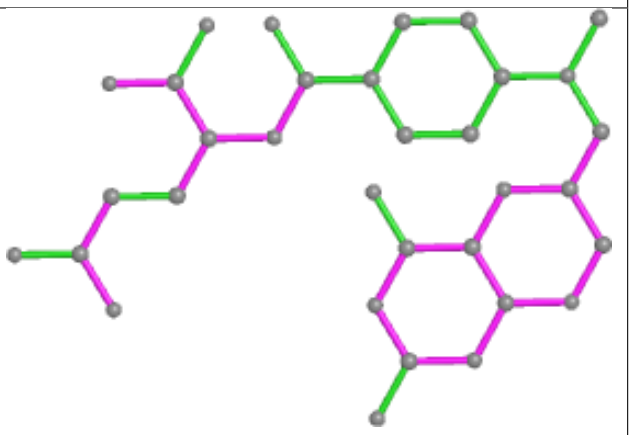


Rings

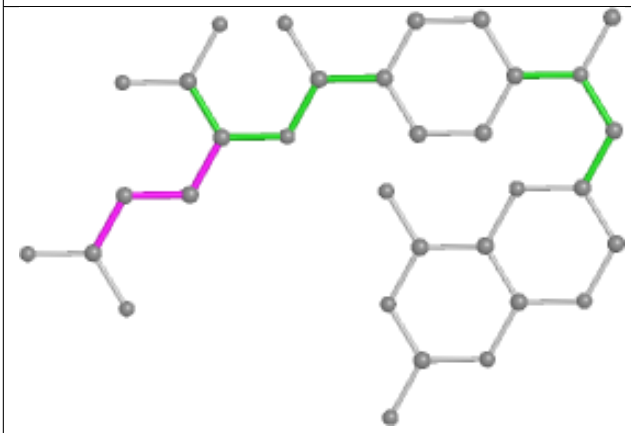
Ligand MTX C 1272



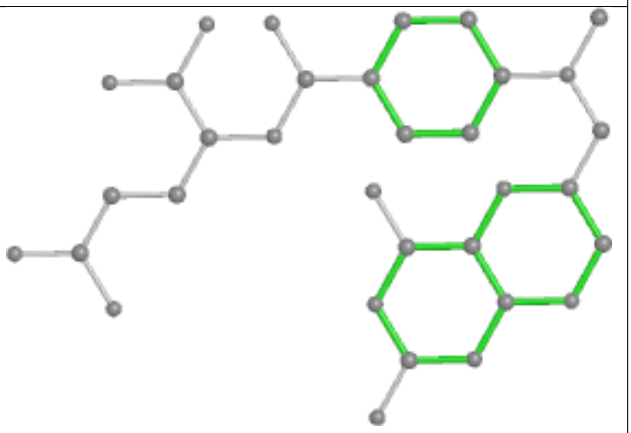
Bond lengths



Bond angles

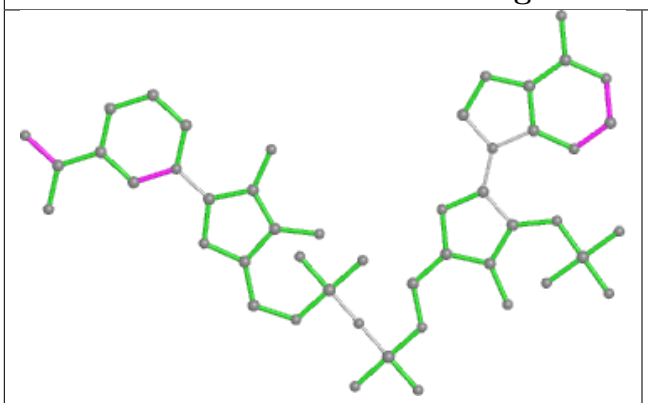


Torsions

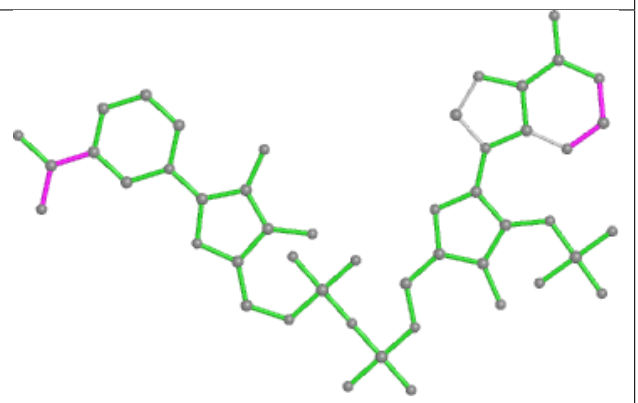


Rings

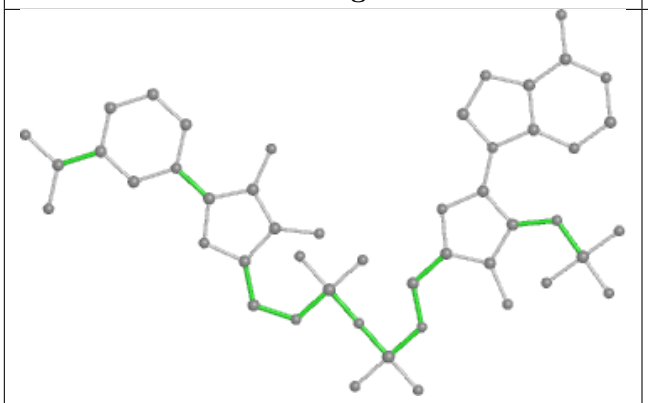
Ligand NAP B 1271



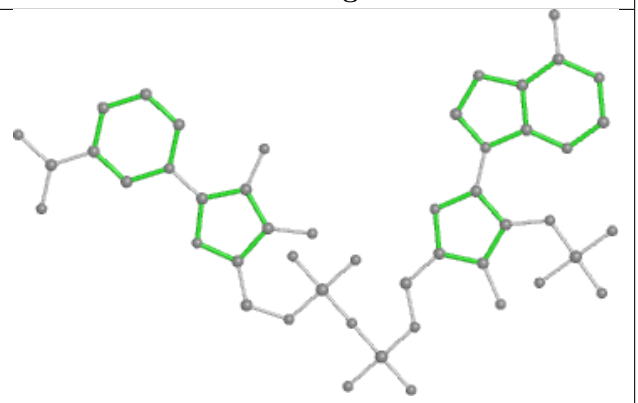
Bond lengths



Bond angles

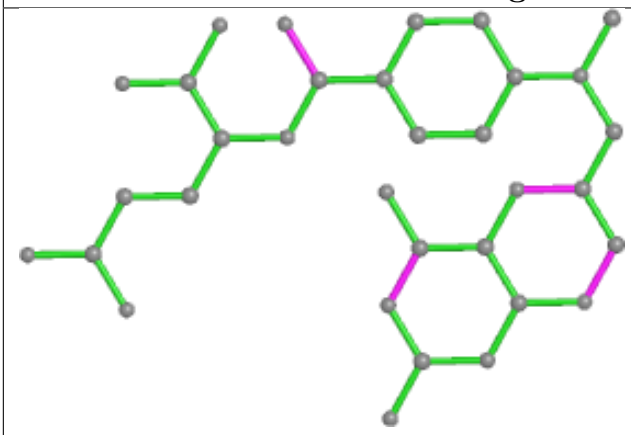


Torsions

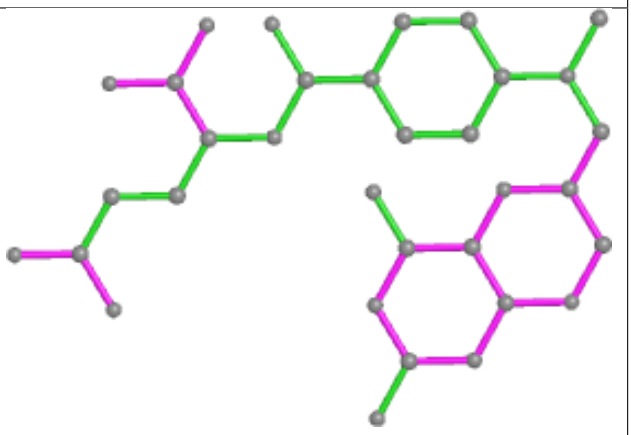


Rings

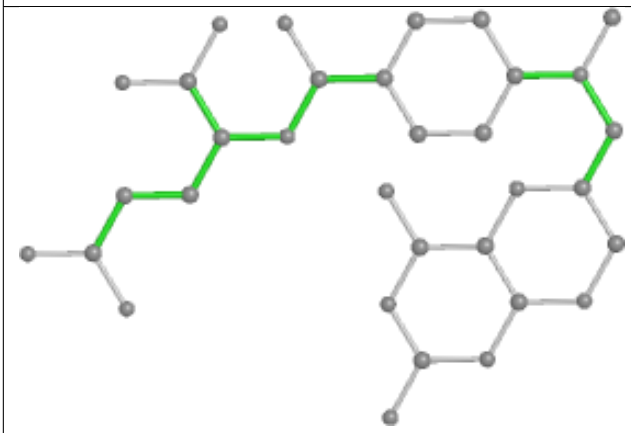
Ligand MTX D 1272



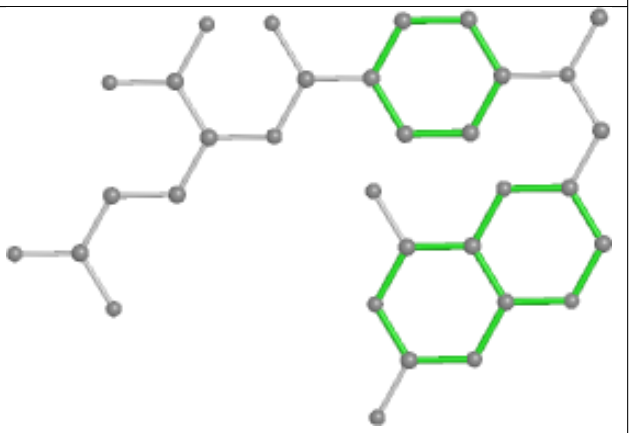
Bond lengths



Bond angles

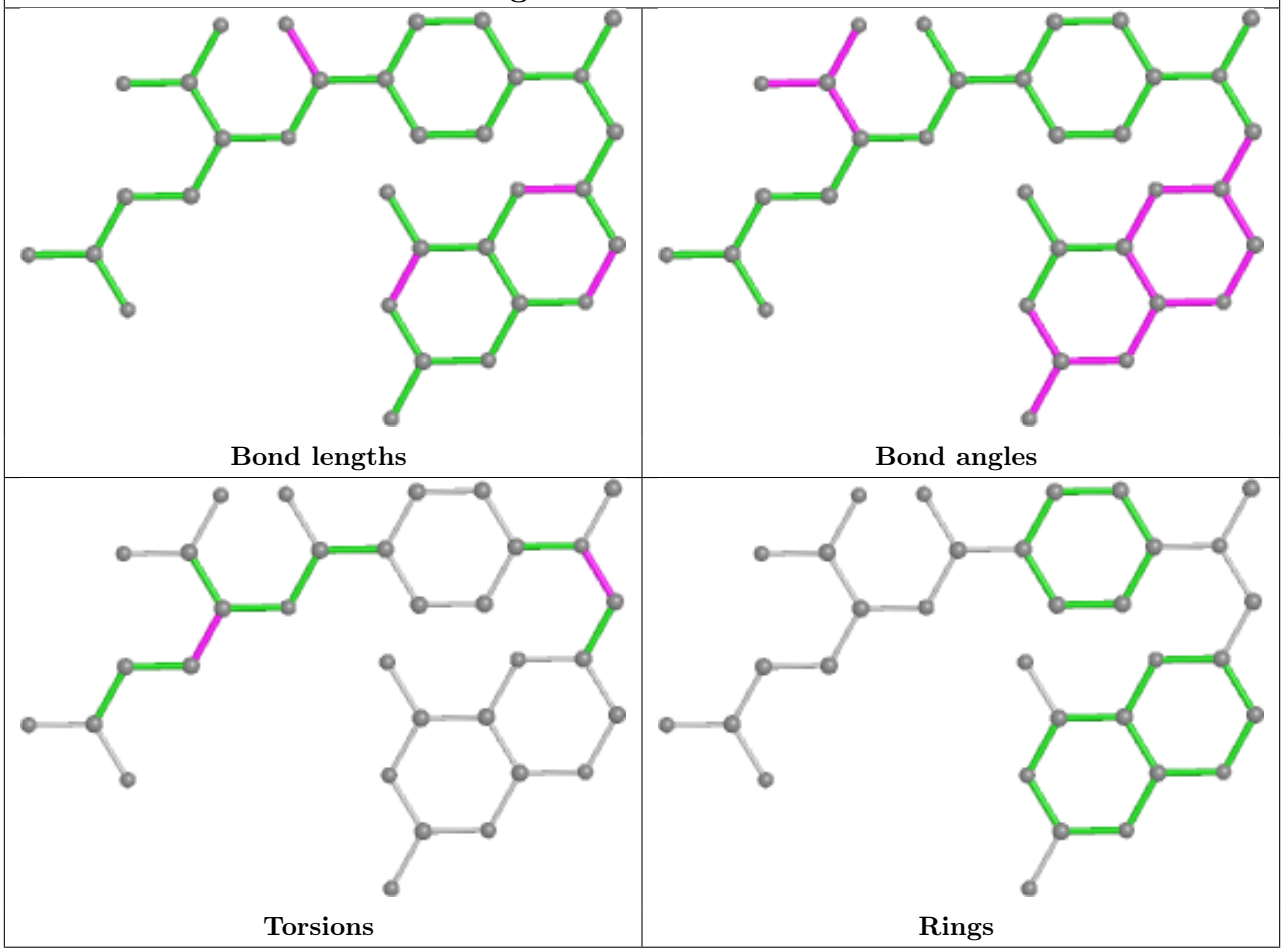


Torsions

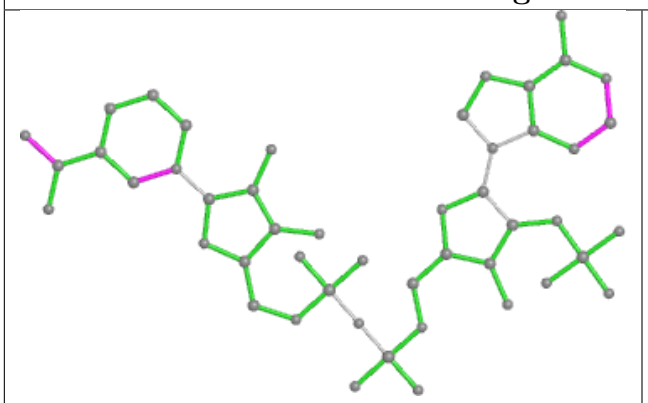


Rings

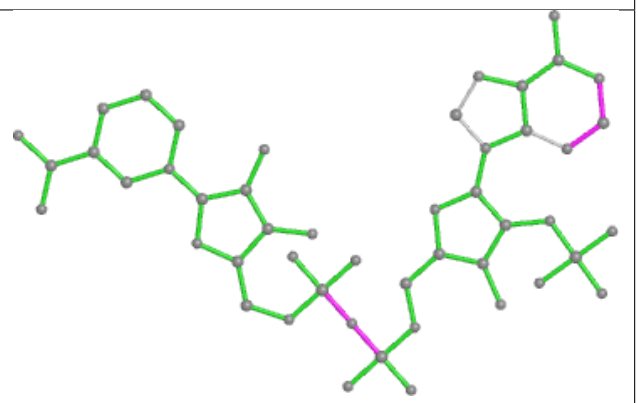
Ligand MTX A 1272



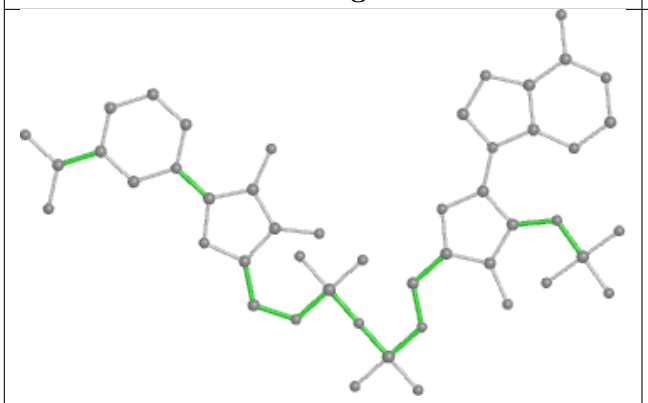
Ligand NAP D 1271



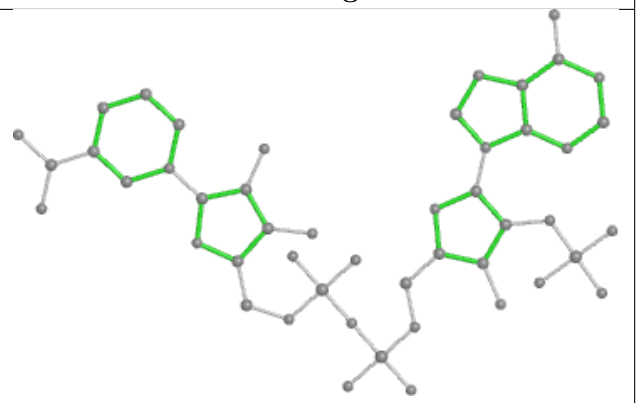
Bond lengths



Bond angles

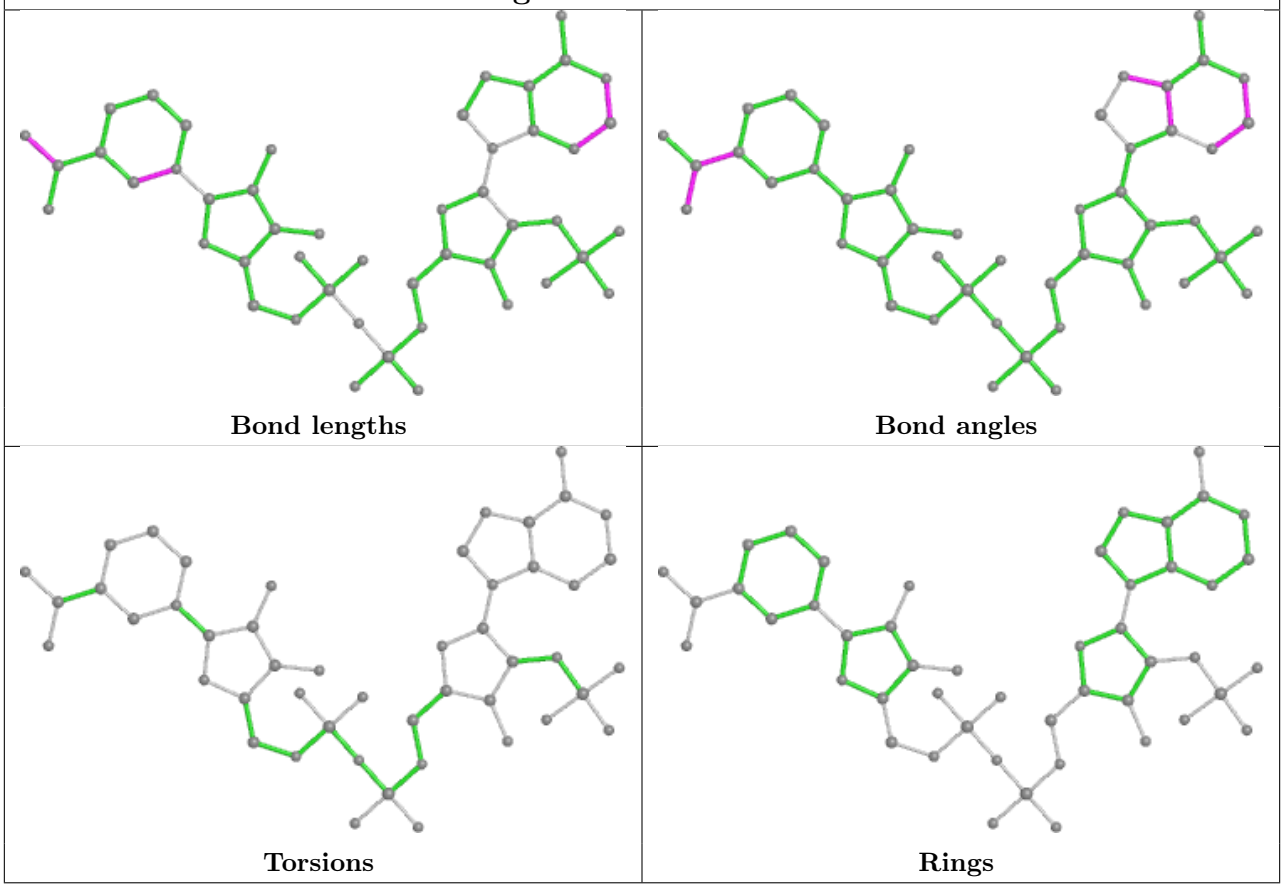


Torsions



Rings

Ligand NAP A 1271



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, 95th 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	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

The worst 5 of 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

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, 95th 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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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)

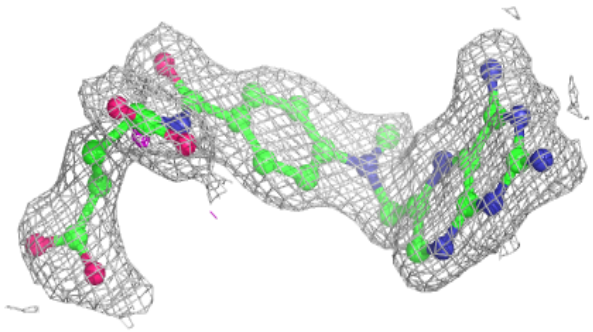
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

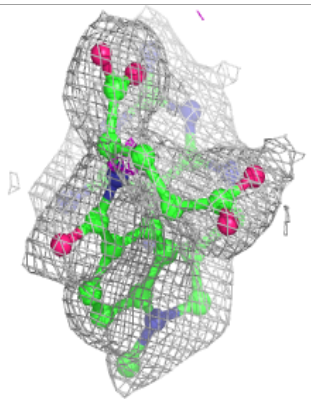
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	A	1274	4/4	0.91	0.17	37,38,38,38	0
3	MTX	C	1272	33/33	0.92	0.14	16,25,36,37	0
3	MTX	D	1272	33/33	0.93	0.13	16,26,35,37	0
3	MTX	A	1272	33/33	0.94	0.11	19,24,30,32	0
4	NI	A	1273	1/1	0.95	0.21	49,49,49,49	1
3	MTX	B	1272	33/33	0.95	0.10	14,22,30,32	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 C 1272:

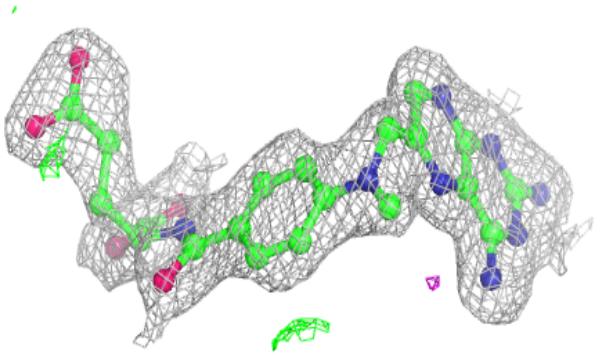
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

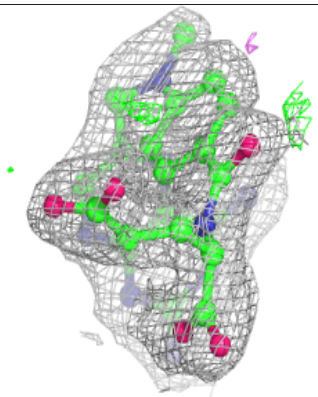




Electron density around MTX D 1272:

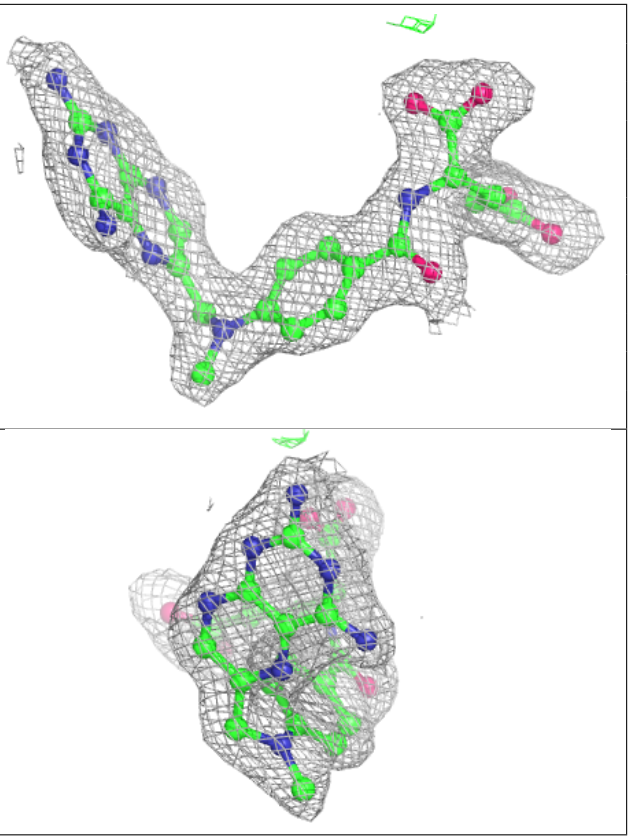
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

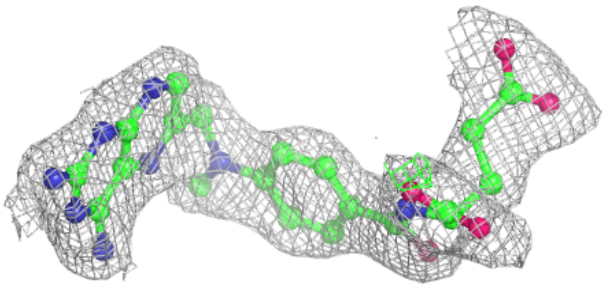




Electron density around MTX A 1272:

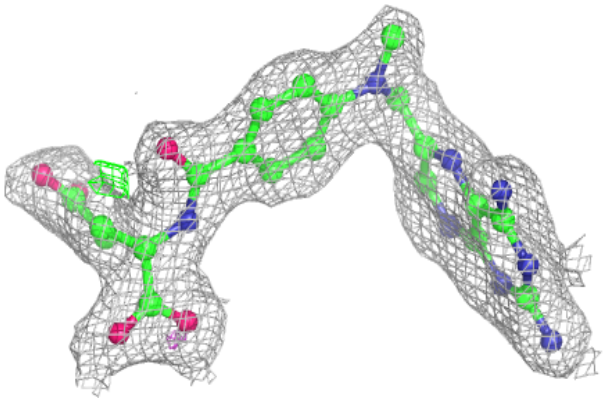
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

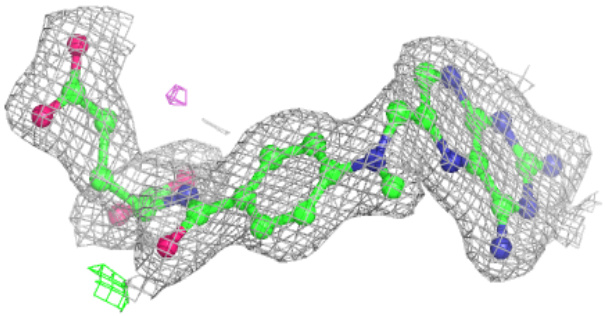


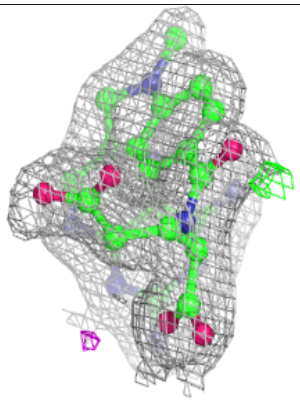


Electron density around MTX B 1272:

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

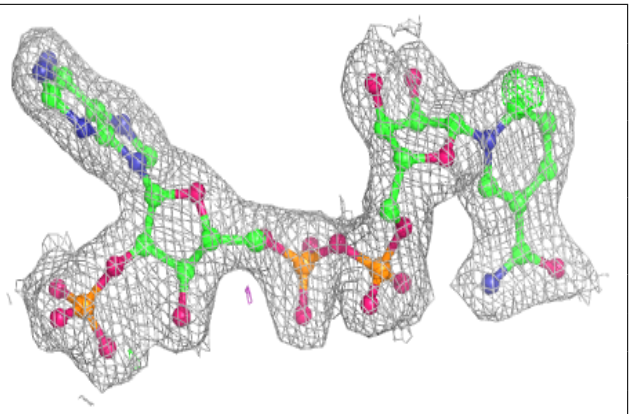


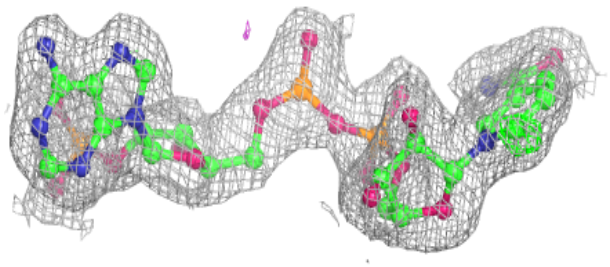


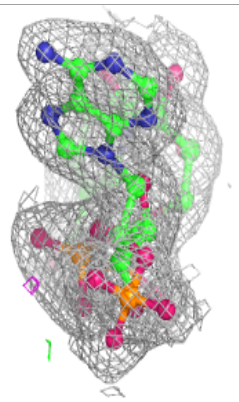


Electron density around NAP C 1271:

$2mF_o$-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:

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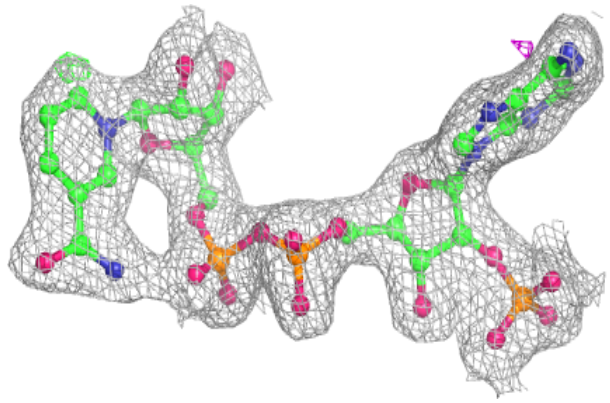
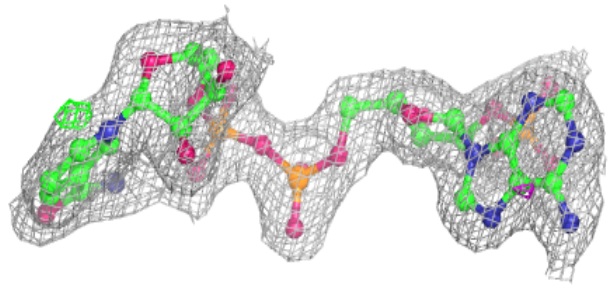
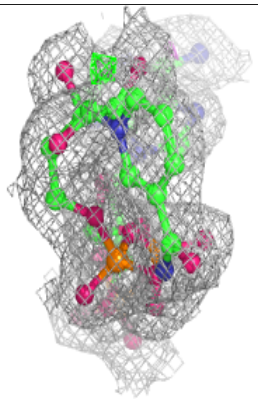
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

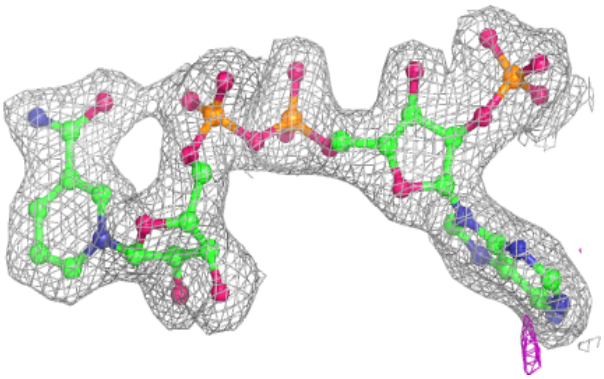


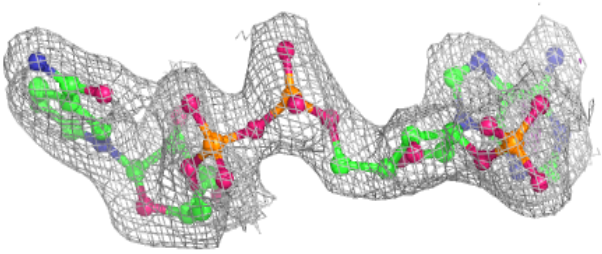


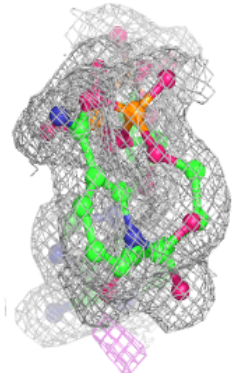


Electron density around NAP D 1271:

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

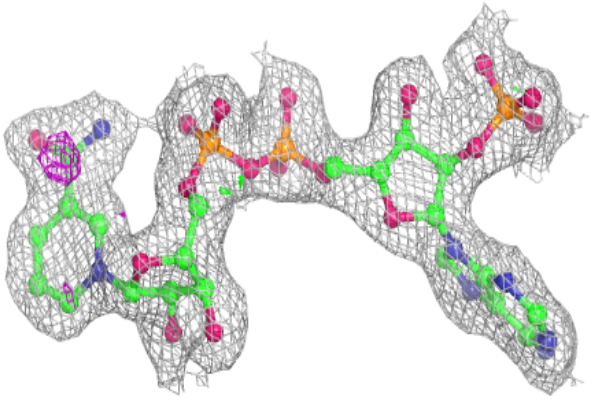


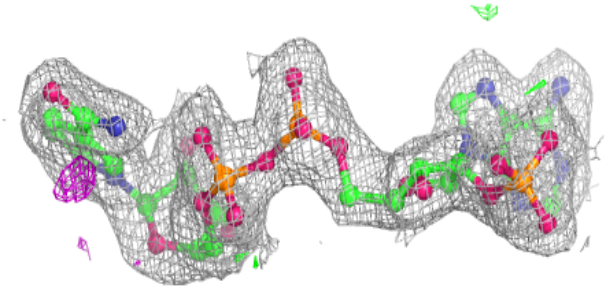


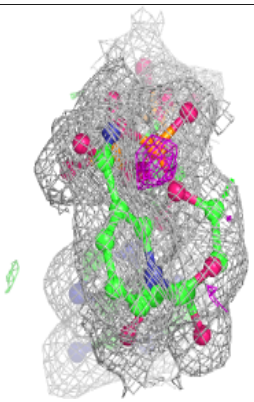


Electron density around NAP B 1271:

$2mF_o$-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.