



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2021 – 02:07 PM EDT

PDB ID : 2OIP
Title : Crystal Structure of the S290G Active Site Mutant of TS-DHFR from *Cryptosporidium hominis*
Authors : Martucci, W.E.; Vargo, M.A.
Deposited on : 2007-01-11
Resolution : 2.80 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

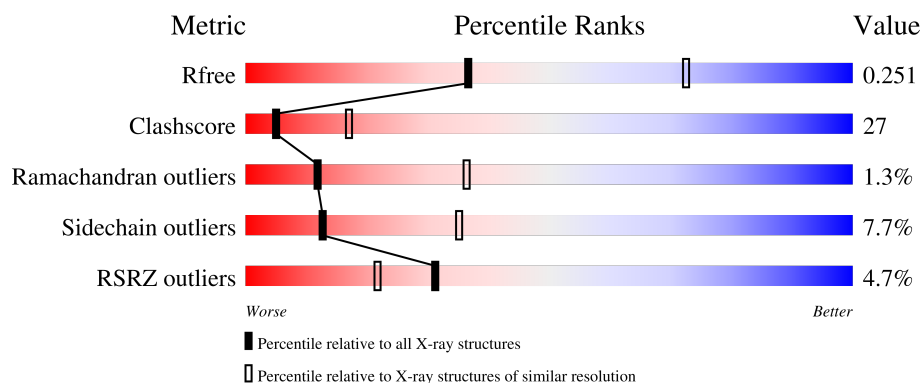
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	519	
1	B	519	
1	C	519	
1	D	519	
1	E	519	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	E	619	-	-	X	-
3	CB3	C	612	X	-	X	-
3	CB3	E	620	X	-	X	X
4	MTX	E	621	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21931 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.

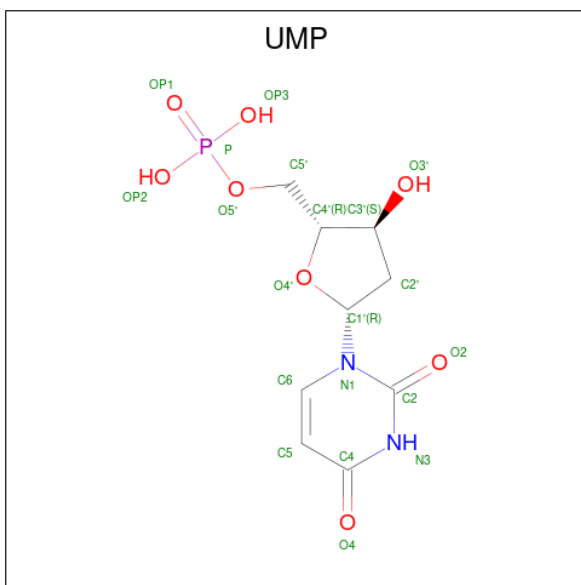
- Molecule 1 is a protein called Chain A, crystal structure of Dhfr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4182	2669	706	784	23			
1	B	516	Total	C	N	O	S	0	0	0
			4189	2674	707	786	22			
1	C	514	Total	C	N	O	S	0	0	0
			4164	2660	703	779	22			
1	D	515	Total	C	N	O	S	0	0	0
			4167	2662	702	781	22			
1	E	511	Total	C	N	O	S	0	0	0
			4145	2648	697	778	22			

There are 5 discrepancies between the modelled and reference sequences:

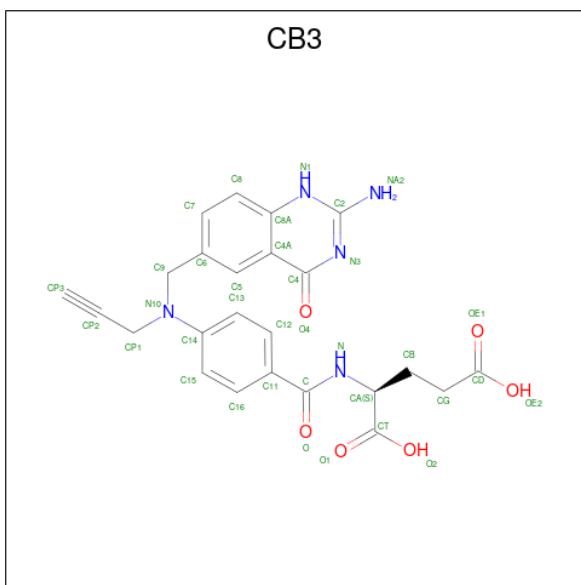
Chain	Residue	Modelled	Actual	Comment	Reference
A	290	GLY	SER	engineered mutation	UNP Q5CGA3
B	290	GLY	SER	engineered mutation	UNP Q5CGA3
C	290	GLY	SER	engineered mutation	UNP Q5CGA3
D	290	GLY	SER	engineered mutation	UNP Q5CGA3
E	290	GLY	SER	engineered mutation	UNP Q5CGA3

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C₉H₁₃N₂O₈P).



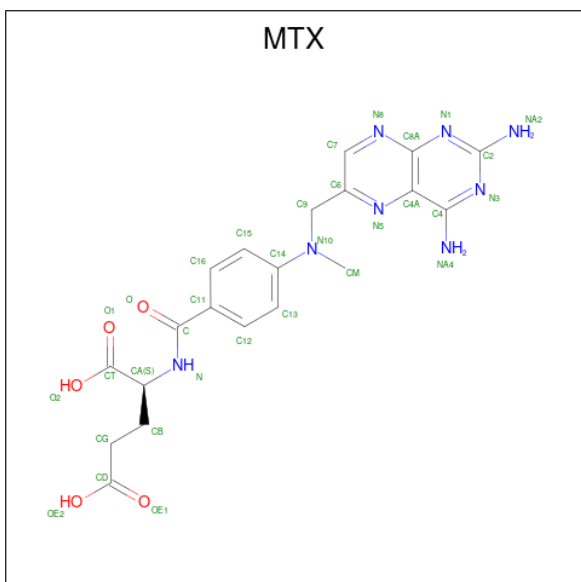
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: C₂₄H₂₃N₅O₆).



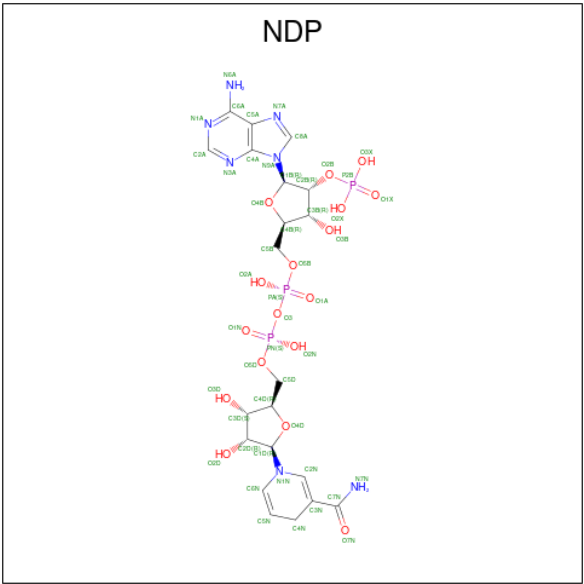
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$).



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

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

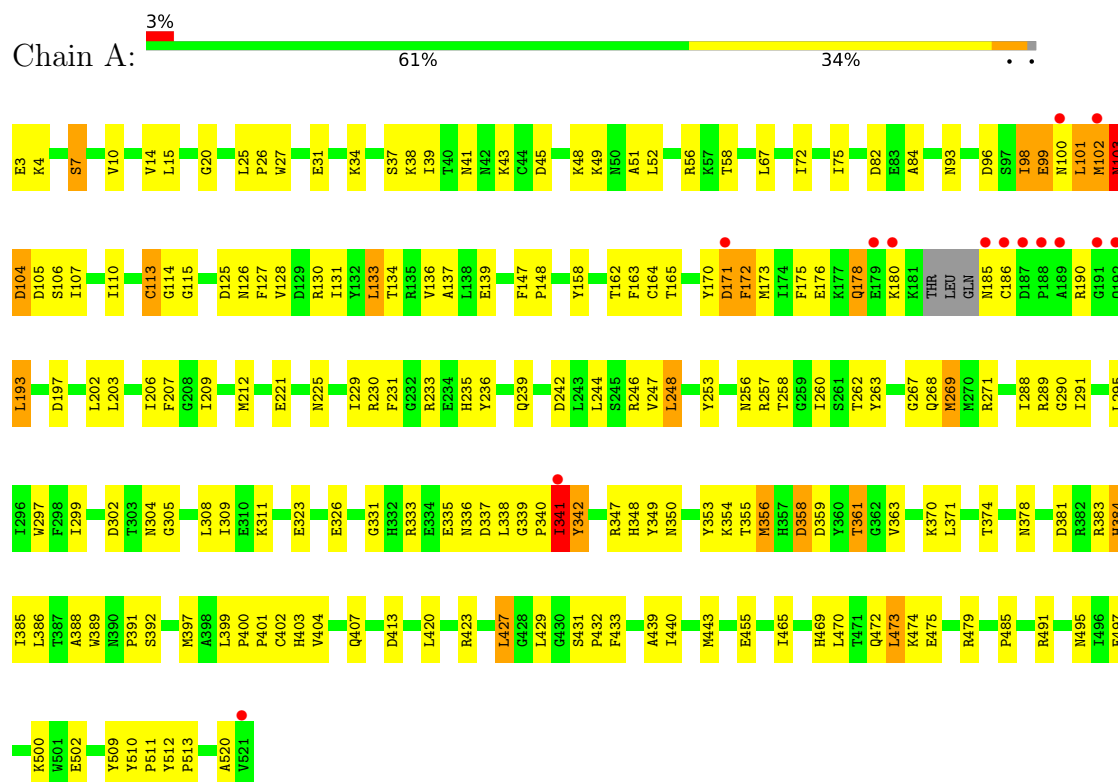
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	113	Total 113	O 113	0	0
6	B	143	Total 143	O 143	0	0
6	C	68	Total 68	O 68	0	0
6	D	61	Total 61	O 61	0	0
6	E	19	Total 19	O 19	0	0

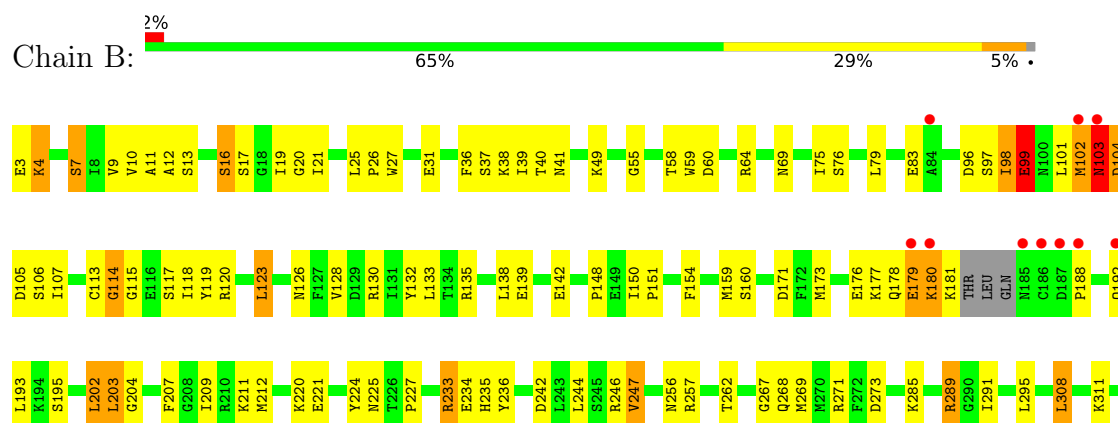
3 Residue-property plots

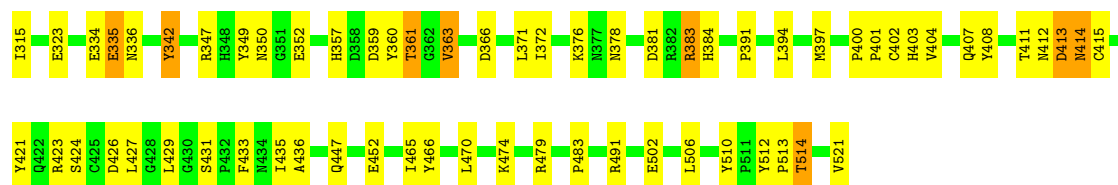
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Chain A, crystal structure of Dhfr

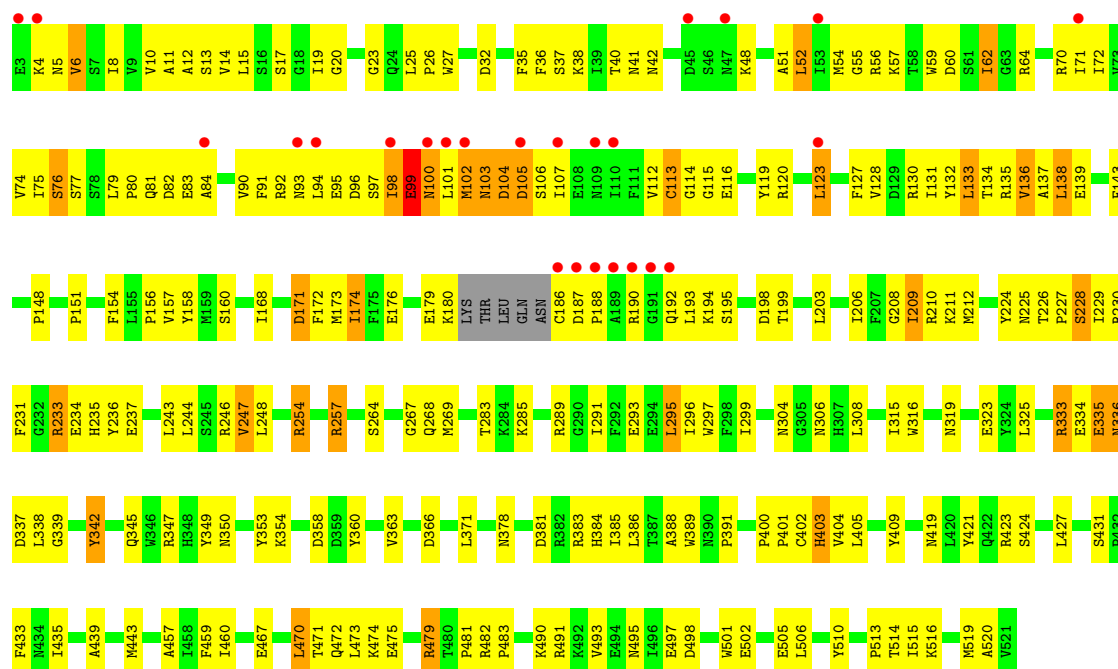


• Molecule 1: Chain A, crystal structure of Dhfr

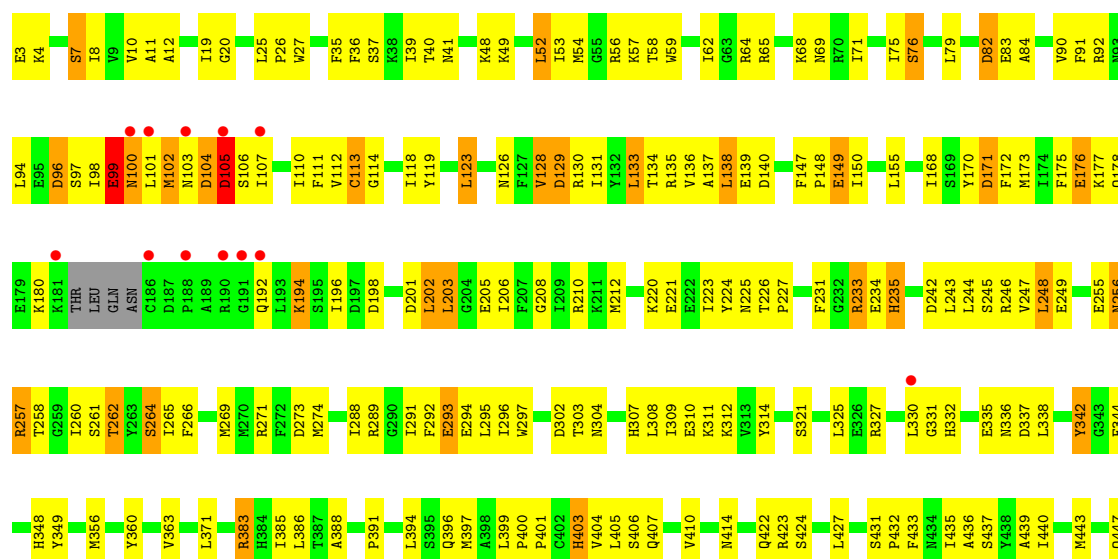




• Molecule 1: Chain A, crystal structure of Dhfr

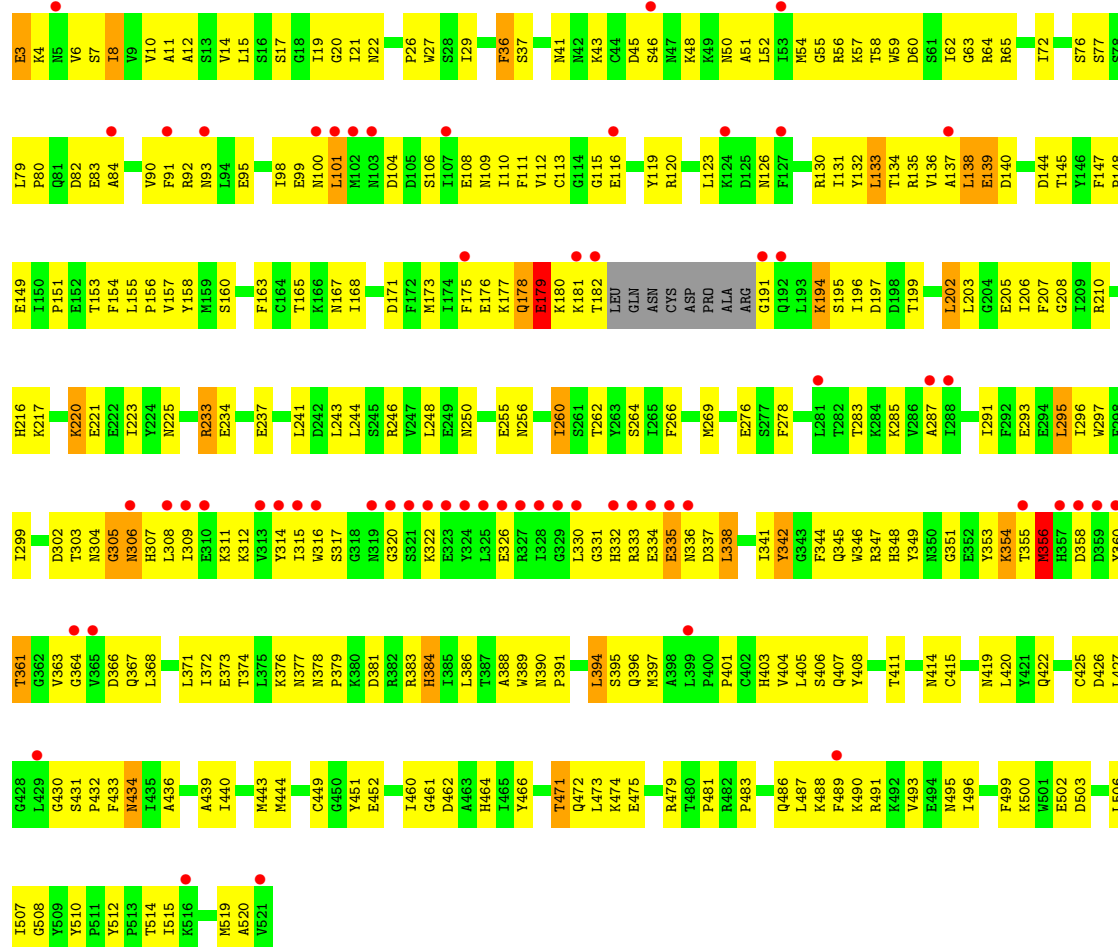
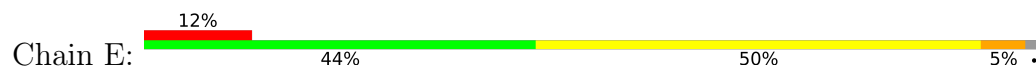


• Molecule 1: Chain A, crystal structure of Dhfr





• Molecule 1: Chain A, crystal structure of Dhfr



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.03Å 116.20Å 216.60Å 90.00° 94.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.80) 99.3 (49.74-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.259 0.215 , 0.251	Depositor DCC
R_{free} test set	6550 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21931	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, MTX, NDP, CB3

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	0.40	0/4278	0.66	0/5782
1	B	0.43	0/4285	0.68	2/5790 (0.0%)
1	C	0.37	0/4260	0.61	0/5758
1	D	0.36	0/4263	0.62	0/5763
1	E	0.35	0/4240	0.63	0/5730
All	All	0.38	0/21326	0.64	2/28823 (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	5
1	B	0	4
1	C	0	6
1	D	0	3
1	E	0	5
All	All	0	23

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	B	104	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	CYS	Peptide
1	A	114	GLY	Peptide
1	A	171	ASP	Peptide
1	A	340	PRO	Peptide
1	A	341	ILE	Peptide

5.2 Too-close contacts

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	4182	0	4100	201	0
1	B	4189	0	4112	159	0
1	C	4164	0	4085	266	0
1	D	4167	0	4082	226	0
1	E	4145	0	4064	291	1
2	A	20	0	11	3	0
2	B	20	0	11	2	0
2	C	20	0	11	5	0
2	D	20	0	11	5	0
2	E	20	0	11	8	0
3	A	35	0	21	2	0
3	B	35	0	21	7	0
3	C	35	0	20	9	0
3	D	35	0	21	4	0
3	E	35	0	21	17	0
4	A	33	0	19	6	0
4	B	33	0	19	8	0
4	C	33	0	20	6	0
4	D	33	0	20	7	0
4	E	33	0	20	10	0
5	A	48	0	26	5	0
5	B	48	0	26	8	0
5	C	48	0	26	12	0
5	D	48	0	26	7	0
5	E	48	0	26	12	0
6	A	113	0	0	12	0
6	B	143	0	0	6	0
6	C	68	0	0	9	0
6	D	61	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	19	0	0	3	0
All	All	21931	0	20830	1148	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 1148 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:100:ASN:CA	1:C:103:ASN:HB2	1.03	1.50
1:C:100:ASN:HA	1:C:103:ASN:CB	0.91	1.36
1:A:43:LYS:HE3	1:A:48:LYS:O	1.36	1.23
1:C:100:ASN:C	1:C:103:ASN:HB2	1.64	1.16
1:C:99:GLU:CD	1:C:103:ASN:HD21	1.49	1.16

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:TYR:OH	1:E:349:TYR:OH[2_457]	1.93	0.27

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	512/519 (99%)	481 (94%)	24 (5%)	7 (1%)	11	34
1	B	512/519 (99%)	482 (94%)	25 (5%)	5 (1%)	15	44
1	C	510/519 (98%)	468 (92%)	37 (7%)	5 (1%)	15	44
1	D	511/519 (98%)	464 (91%)	38 (7%)	9 (2%)	8	28
1	E	507/519 (98%)	458 (90%)	42 (8%)	7 (1%)	11	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2552/2595 (98%)	2353 (92%)	166 (6%)	33 (1%)	12	36

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	MET
1	A	103	ASN
1	B	103	ASN
1	B	342	TYR
1	C	103	ASN

5.3.2 Protein sidechains ⓘ

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	460/467 (98%)	427 (93%)	33 (7%)	14	38
1	B	461/467 (99%)	423 (92%)	38 (8%)	11	33
1	C	457/467 (98%)	420 (92%)	37 (8%)	11	33
1	D	457/467 (98%)	419 (92%)	38 (8%)	11	32
1	E	456/467 (98%)	425 (93%)	31 (7%)	16	42
All	All	2291/2335 (98%)	2114 (92%)	177 (8%)	13	35

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	99	GLU
1	D	437	SER
1	D	128	VAL
1	D	235	HIS
1	E	99	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	69	ASN
1	E	384	HIS
1	E	126	ASN
1	E	307	HIS
1	E	403	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MTX	B	609	-	29,35,35	1.45	3 (10%)	38,49,49	1.91	9 (23%)
5	NDP	A	606	-	45,52,52	1.42	3 (6%)	53,80,80	1.14	3 (5%)
4	MTX	E	621	-	29,35,35	1.34	2 (6%)	38,49,49	1.86	8 (21%)
4	MTX	D	617	-	29,35,35	1.42	2 (6%)	38,49,49	1.99	10 (26%)
4	MTX	C	613	-	29,35,35	1.36	2 (6%)	38,49,49	1.87	8 (21%)
5	NDP	C	614	-	45,52,52	1.31	3 (6%)	53,80,80	1.29	3 (5%)
3	CB3	C	612	-	30,37,37	2.73	18 (60%)	38,51,51	3.16	18 (47%)
3	CB3	A	604	-	30,37,37	2.34	13 (43%)	38,51,51	3.05	19 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CB3	E	620	-	30,37,37	1.26	2 (6%)	38,51,51	2.27	7 (18%)
2	UMP	E	619	-	18,21,21	3.14	3 (16%)	21,31,31	1.08	1 (4%)
5	NDP	B	610	-	45,52,52	1.45	3 (6%)	53,80,80	1.14	3 (5%)
2	UMP	B	607	-	18,21,21	3.11	3 (16%)	21,31,31	0.92	1 (4%)
2	UMP	D	615	1	18,21,21	3.10	3 (16%)	21,31,31	0.93	2 (9%)
3	CB3	D	616	-	30,37,37	2.22	16 (53%)	38,51,51	2.35	12 (31%)
2	UMP	C	611	-	18,21,21	3.10	3 (16%)	21,31,31	0.97	1 (4%)
4	MTX	A	605	-	29,35,35	1.46	3 (10%)	38,49,49	2.08	12 (31%)
3	CB3	B	608	-	30,37,37	3.37	24 (80%)	38,51,51	3.18	17 (44%)
5	NDP	D	618	-	45,52,52	1.42	3 (6%)	53,80,80	1.21	3 (5%)
2	UMP	A	603	1	18,21,21	3.09	3 (16%)	21,31,31	0.96	2 (9%)
5	NDP	E	622	-	45,52,52	1.38	3 (6%)	53,80,80	1.19	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MTX	B	609	-	-	7/19/25/25	0/3/3/3
5	NDP	A	606	-	-	4/30/77/77	0/5/5/5
4	MTX	E	621	-	-	8/19/25/25	0/3/3/3
4	MTX	D	617	-	-	7/19/25/25	0/3/3/3
4	MTX	C	613	-	-	6/19/25/25	0/3/3/3
5	NDP	C	614	-	-	15/30/77/77	0/5/5/5
3	CB3	C	612	-	1/1/5/6	5/21/28/28	0/3/3/3
3	CB3	A	604	-	-	5/21/28/28	0/3/3/3
3	CB3	E	620	-	1/1/5/6	6/21/28/28	0/3/3/3
2	UMP	E	619	-	-	5/7/22/22	0/2/2/2
5	NDP	B	610	-	-	3/30/77/77	0/5/5/5
2	UMP	B	607	-	-	2/7/22/22	0/2/2/2
2	UMP	D	615	1	-	5/7/22/22	0/2/2/2
3	CB3	D	616	-	-	5/21/28/28	0/3/3/3
2	UMP	C	611	-	-	2/7/22/22	0/2/2/2
4	MTX	A	605	-	-	5/19/25/25	0/3/3/3
3	CB3	B	608	-	-	6/21/28/28	0/3/3/3

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NDP	D	618	-	-	2/30/77/77	0/5/5/5
2	UMP	A	603	1	-	3/7/22/22	0/2/2/2
5	NDP	E	622	-	-	14/30/77/77	0/5/5/5

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	C6-N1	9.99	1.48	1.35
2	B	607	UMP	C6-N1	9.92	1.48	1.35
2	D	615	UMP	C6-N1	9.89	1.48	1.35
2	C	611	UMP	C6-N1	9.88	1.48	1.35
2	A	603	UMP	C6-N1	9.87	1.48	1.35

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	CB3	C4A-C8A-N1	-12.96	116.56	123.60
3	C	612	CB3	C4A-C8A-N1	-11.18	117.53	123.60
3	D	616	CB3	C4A-C4-N3	-8.14	118.73	124.40
3	B	608	CB3	C4A-C4-N3	-7.79	118.97	124.40
3	E	620	CB3	C4A-C8A-N1	-7.45	119.56	123.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	612	CB3	CA
3	E	620	CB3	CA

5 of 115 torsion outliers are listed below:

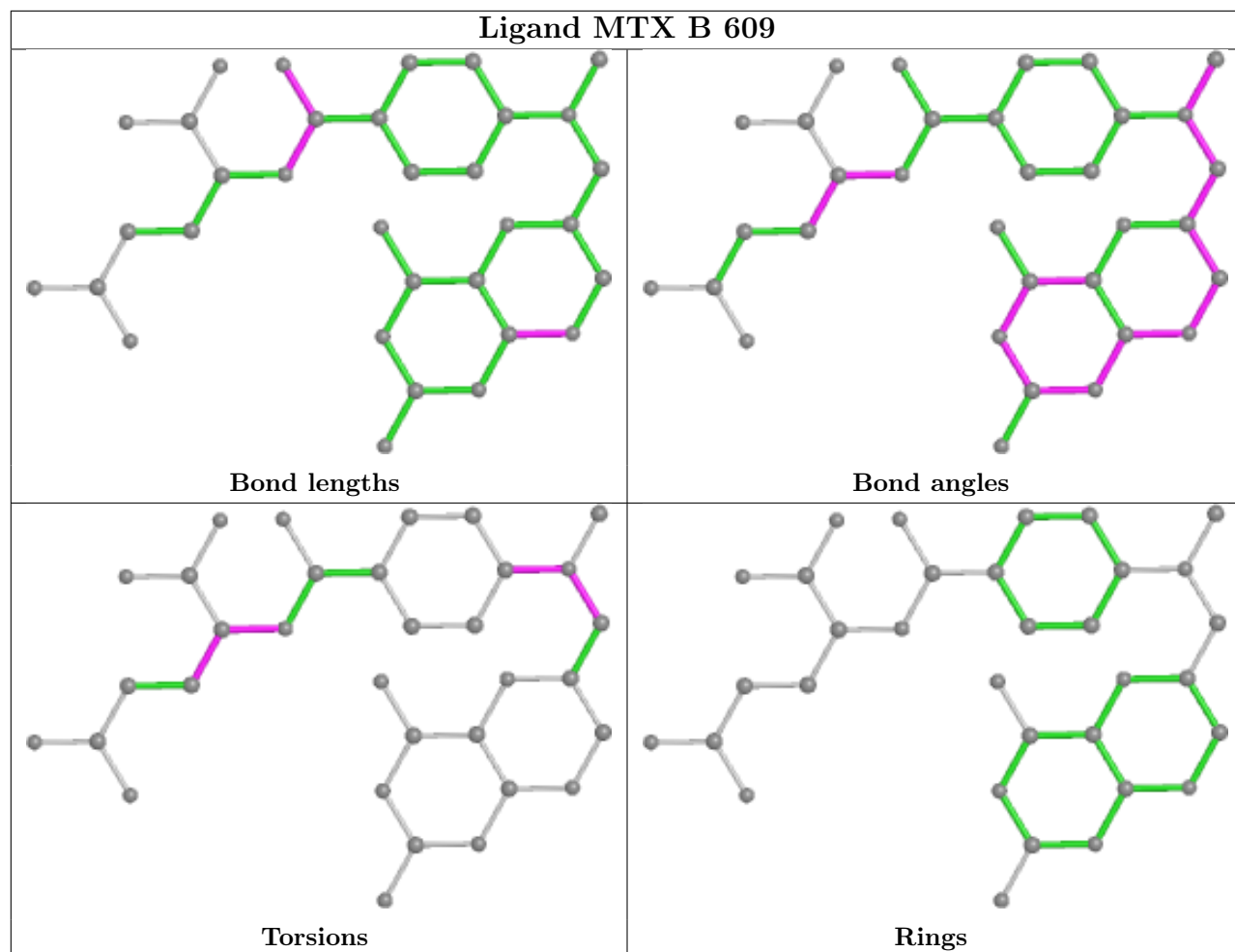
Mol	Chain	Res	Type	Atoms
2	D	615	UMP	C3'-C4'-C5'-O5'
2	D	615	UMP	C5'-O5'-P-OP1
2	D	615	UMP	C5'-O5'-P-OP2
2	D	615	UMP	C5'-O5'-P-OP3
2	E	619	UMP	C3'-C4'-C5'-O5'

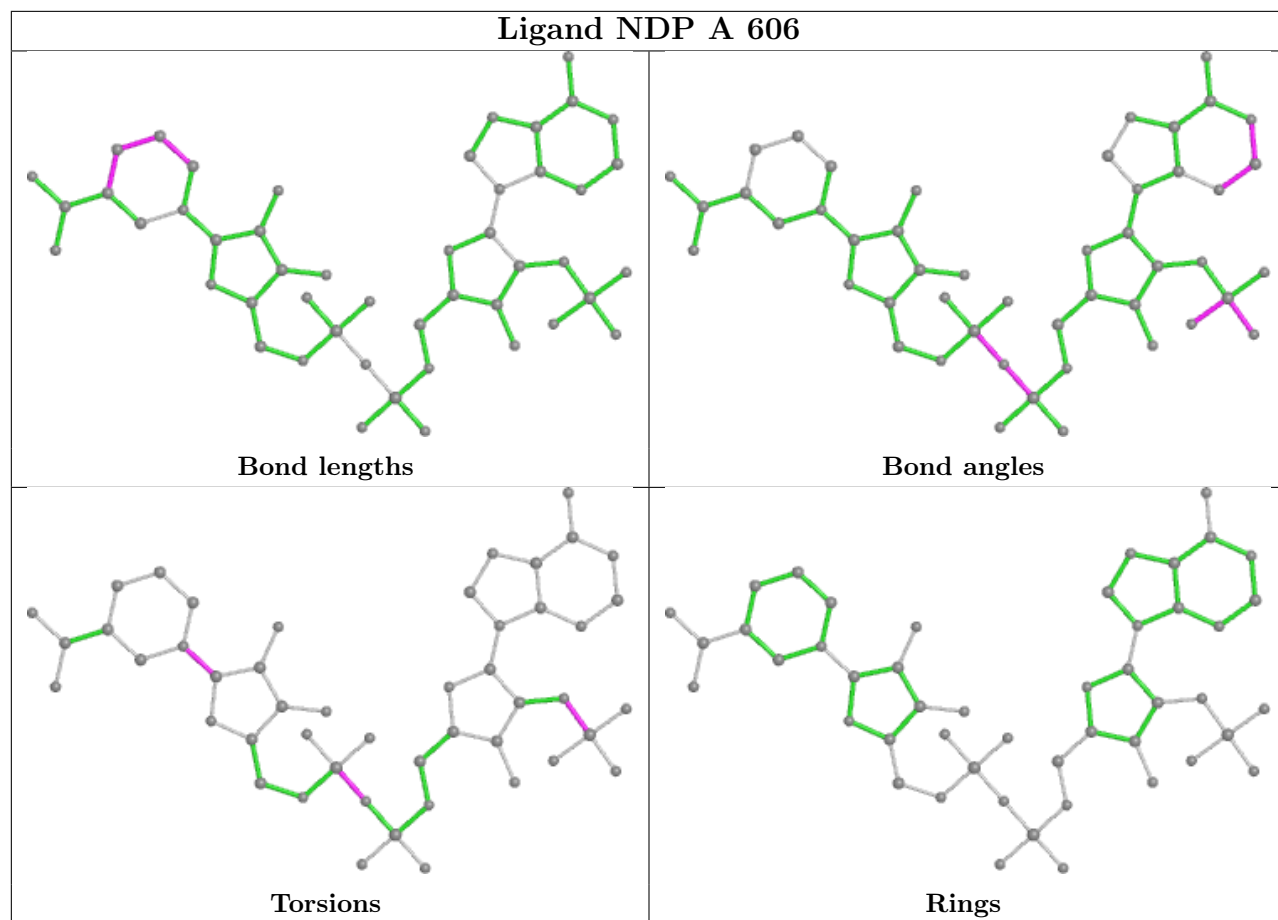
There are no ring outliers.

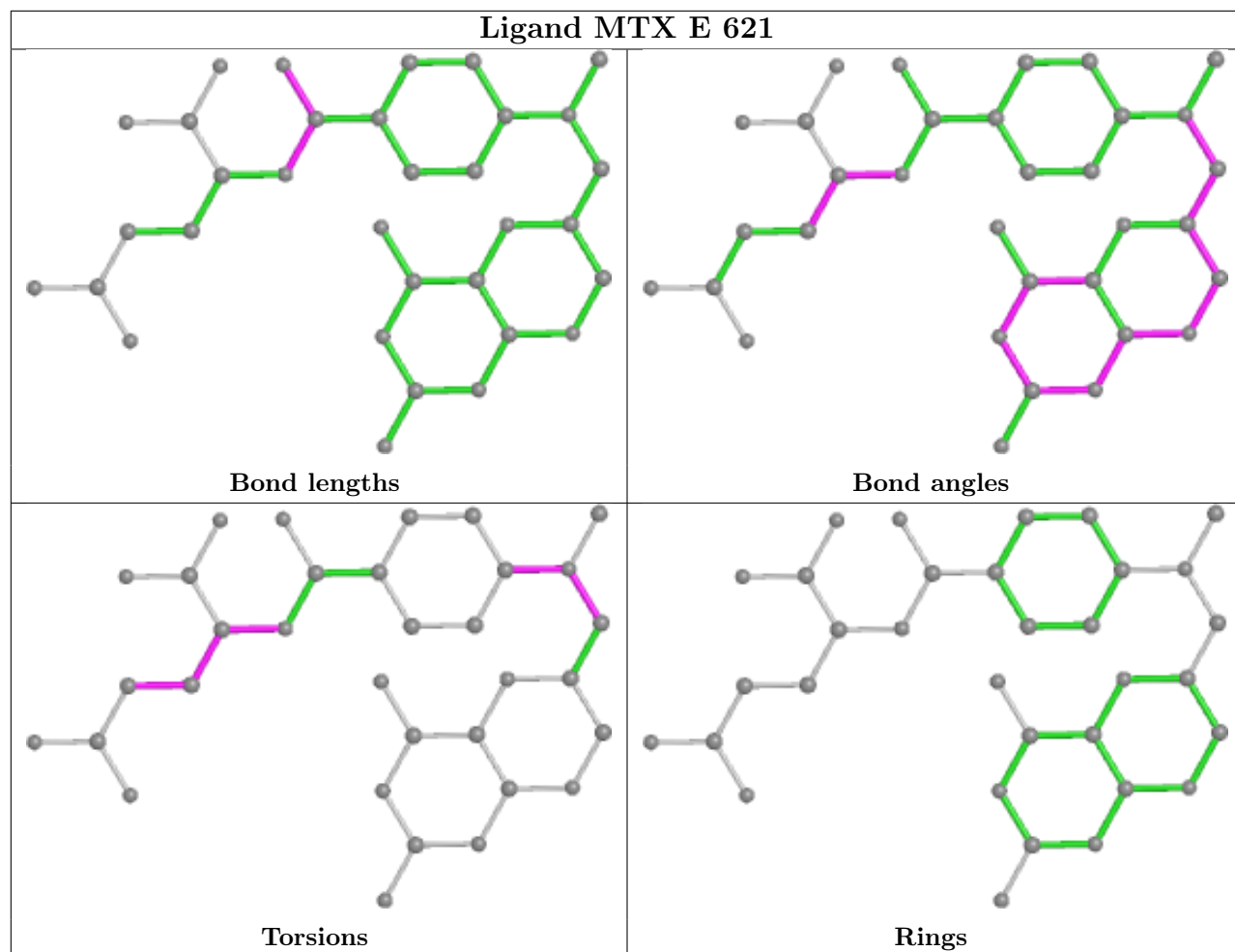
20 monomers are involved in 132 short contacts:

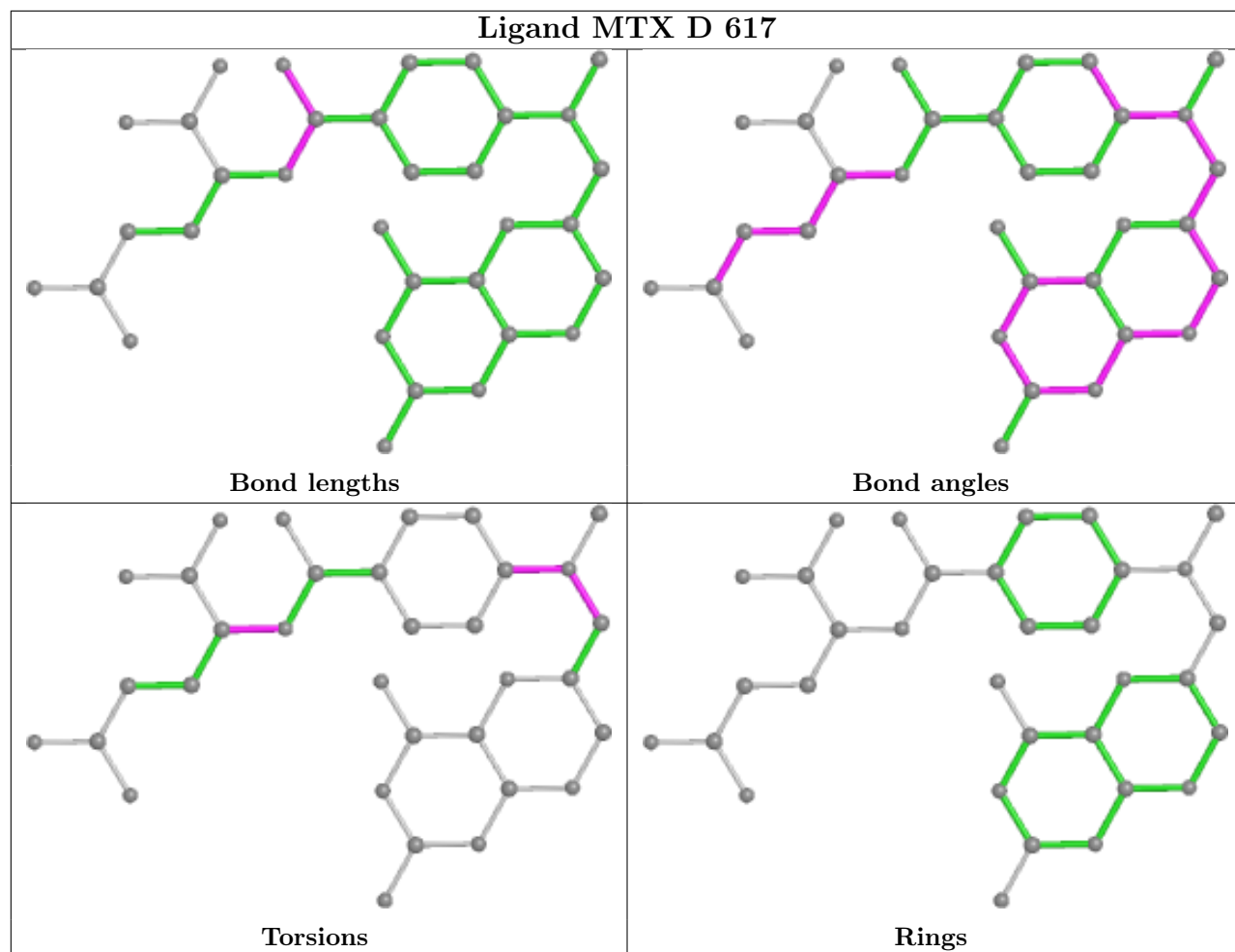
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	609	MTX	8	0
5	A	606	NDP	5	0
4	E	621	MTX	10	0
4	D	617	MTX	7	0
4	C	613	MTX	6	0
5	C	614	NDP	12	0
3	C	612	CB3	9	0
3	A	604	CB3	2	0
3	E	620	CB3	17	0
2	E	619	UMP	8	0
5	B	610	NDP	8	0
2	B	607	UMP	2	0
2	D	615	UMP	5	0
3	D	616	CB3	4	0
2	C	611	UMP	5	0
4	A	605	MTX	6	0
3	B	608	CB3	7	0
5	D	618	NDP	7	0
2	A	603	UMP	3	0
5	E	622	NDP	12	0

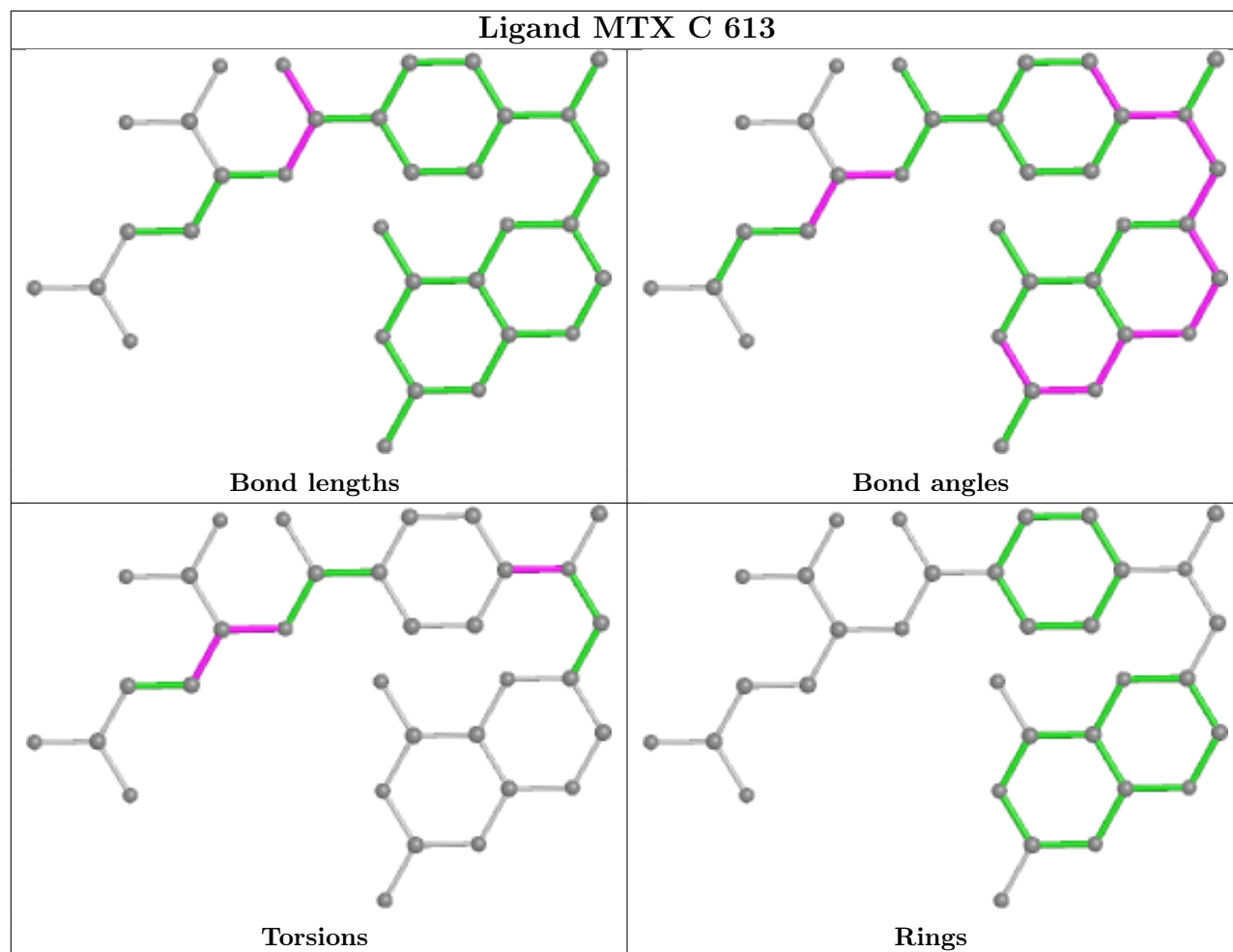
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

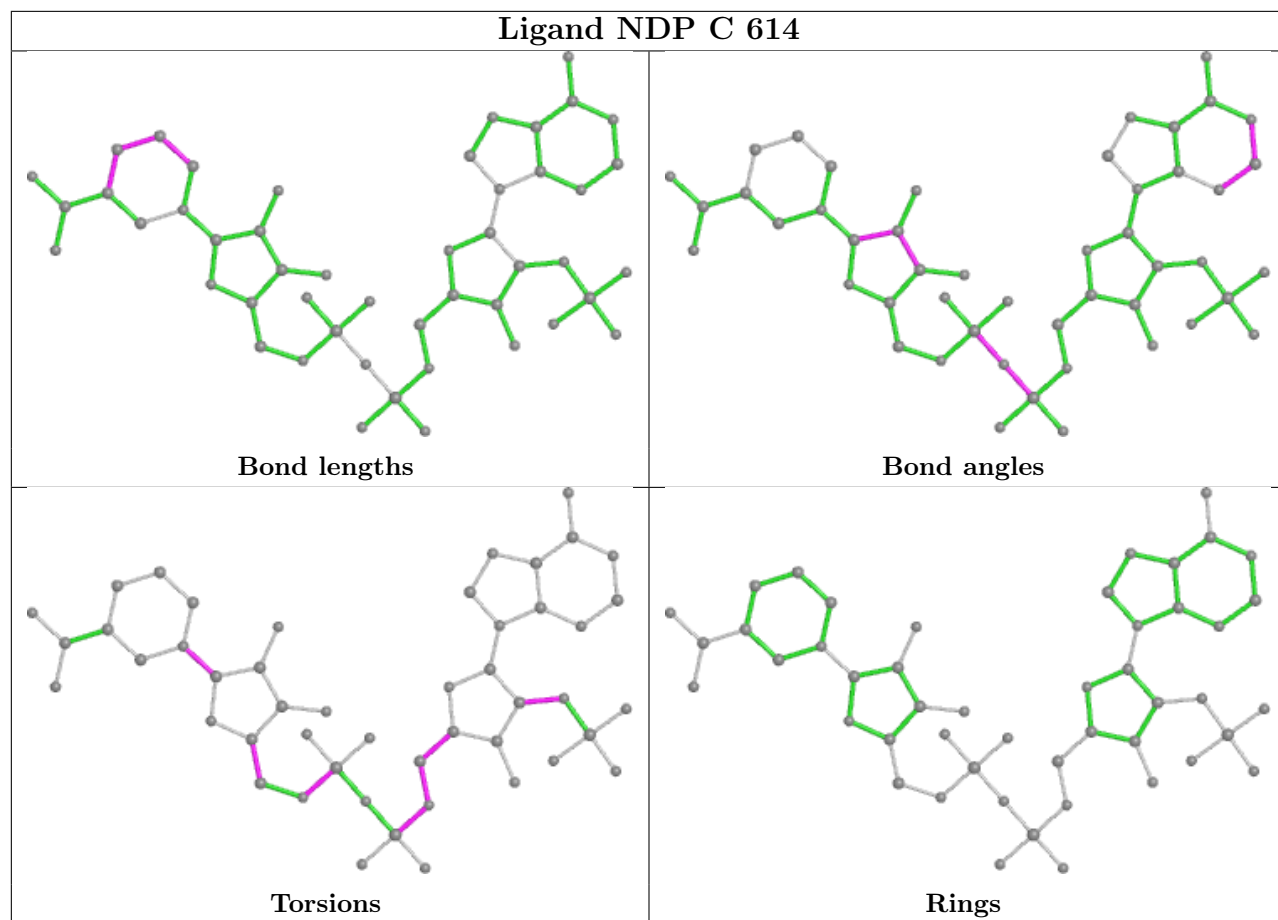




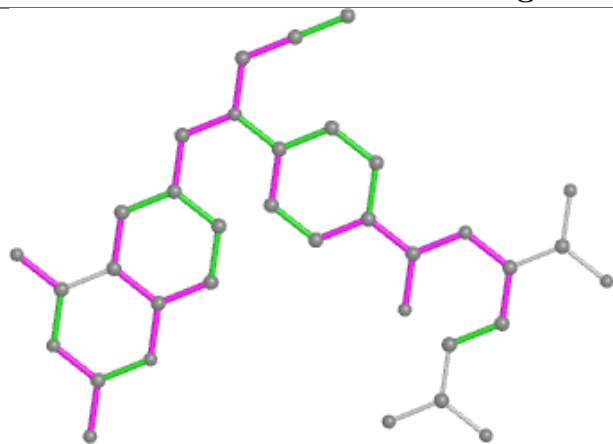




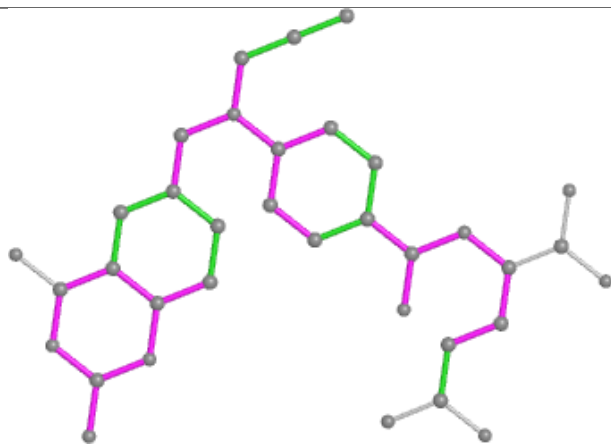




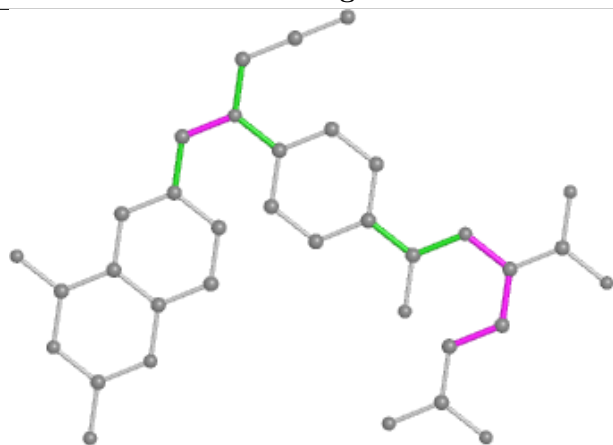
Ligand CB3 C 612



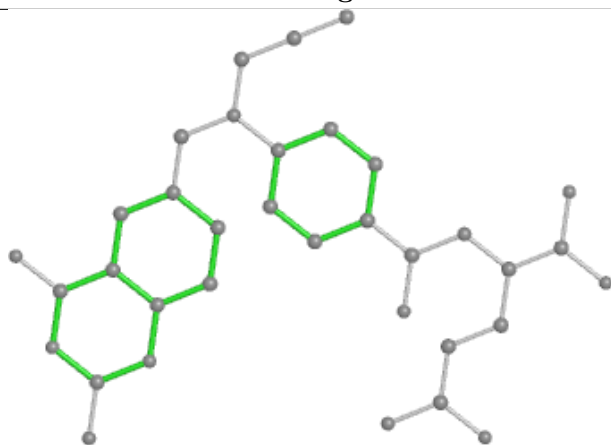
Bond lengths



Bond angles

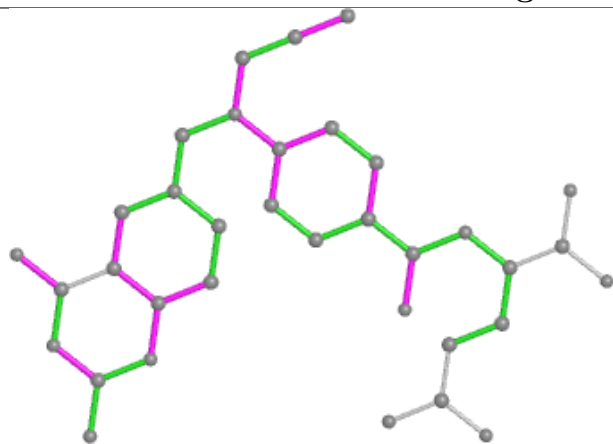


Torsions

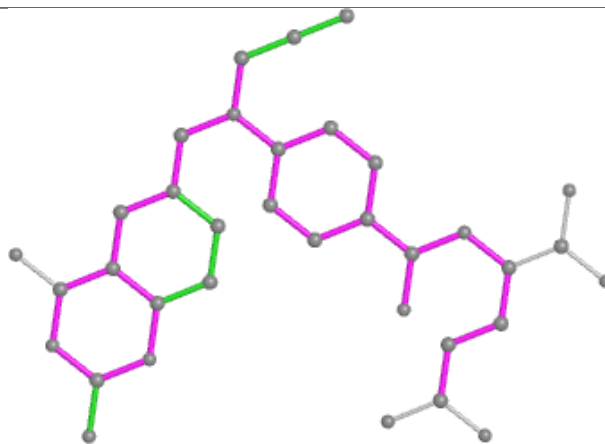


Rings

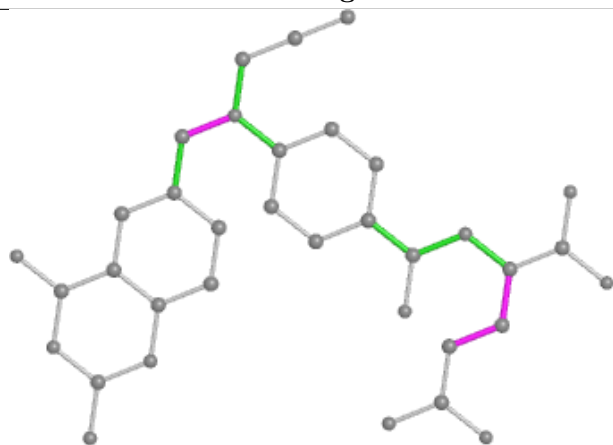
Ligand CB3 A 604



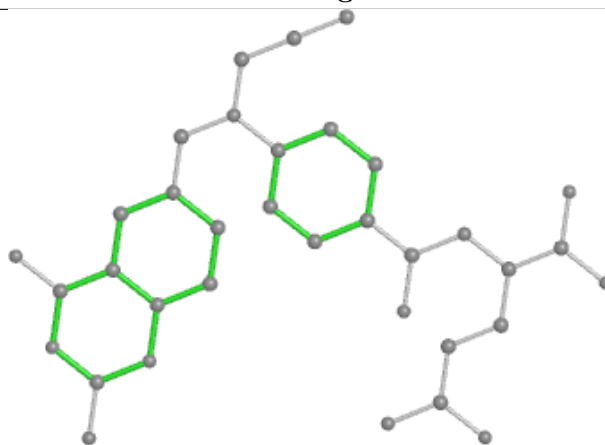
Bond lengths



Bond angles

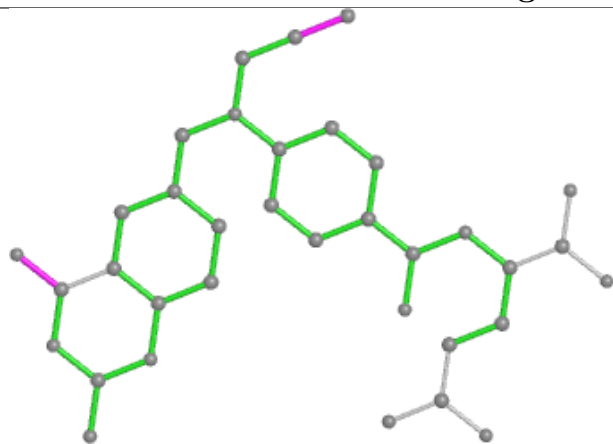


Torsions

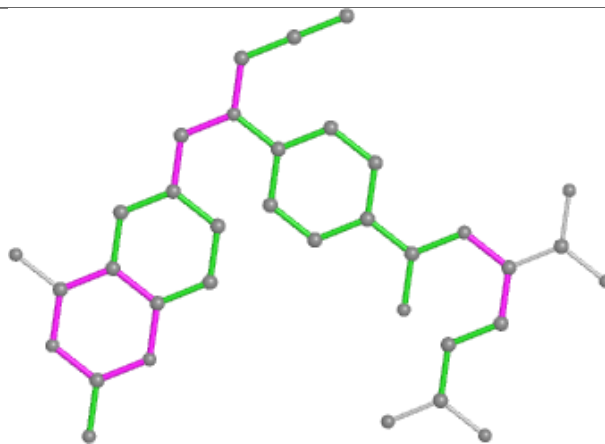


Rings

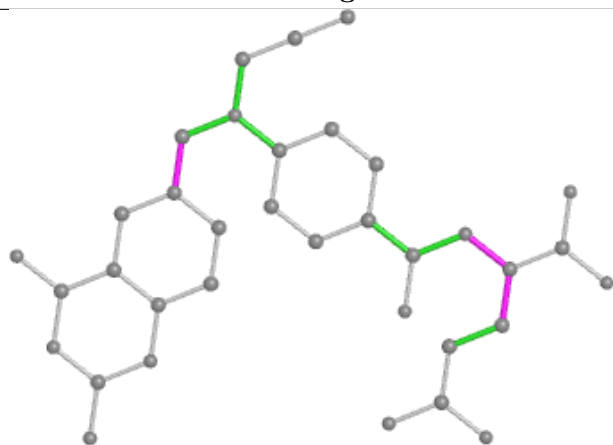
Ligand CB3 E 620



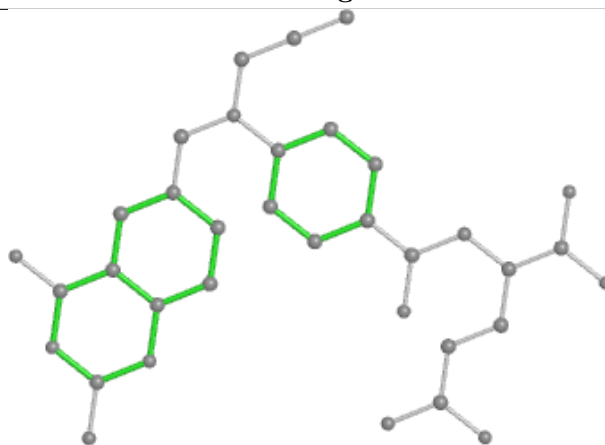
Bond lengths



Bond angles

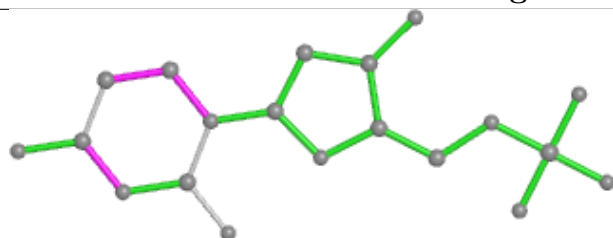


Torsions

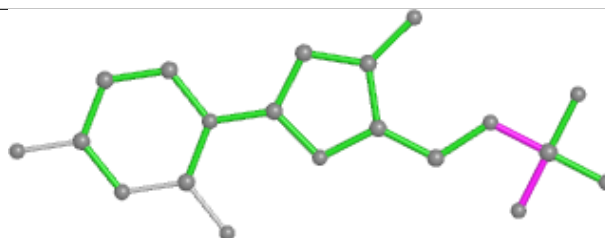


Rings

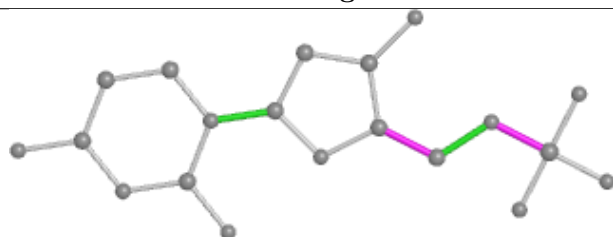
Ligand UMP E 619



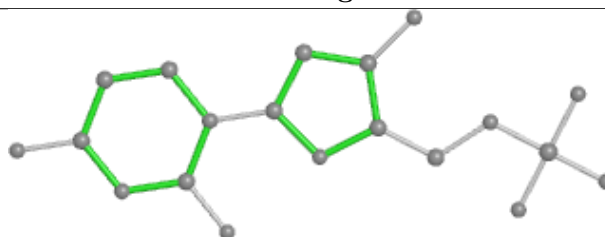
Bond lengths



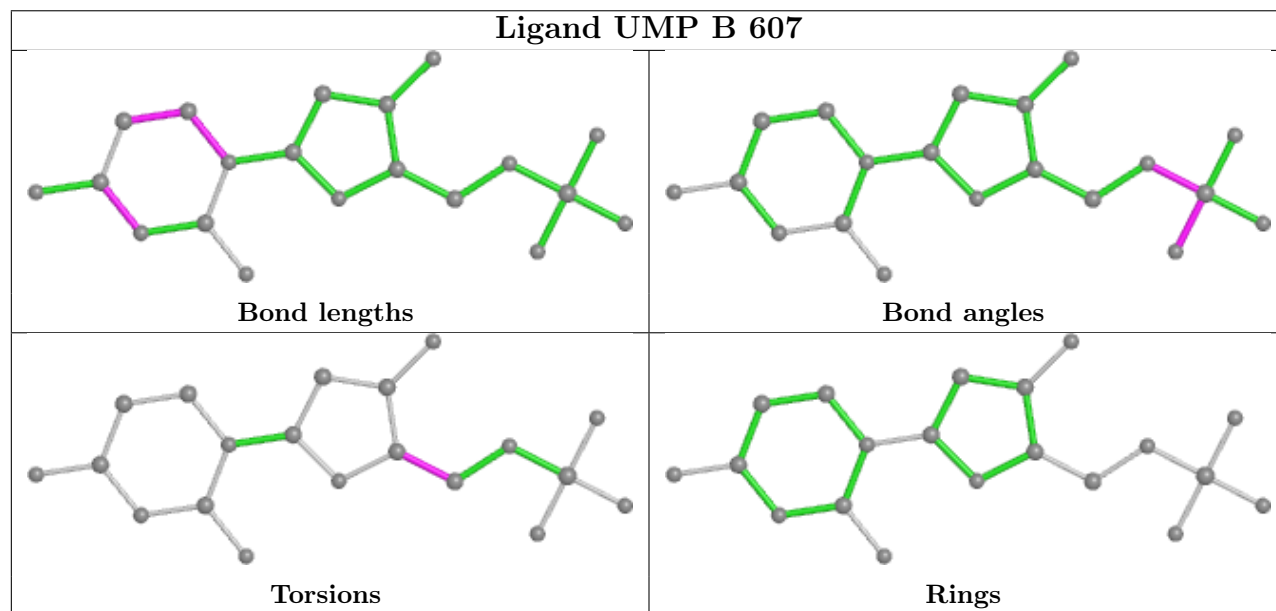
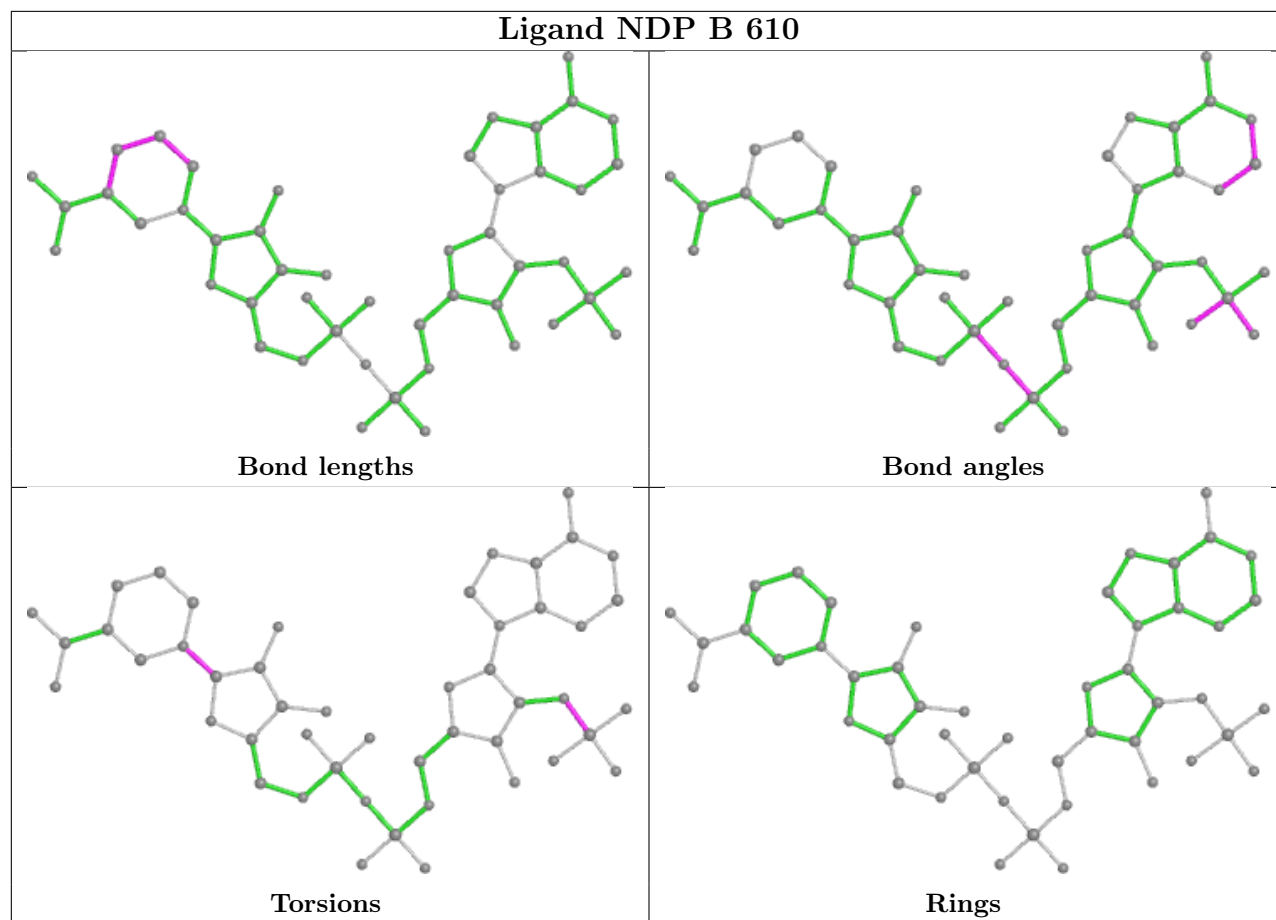
Bond angles

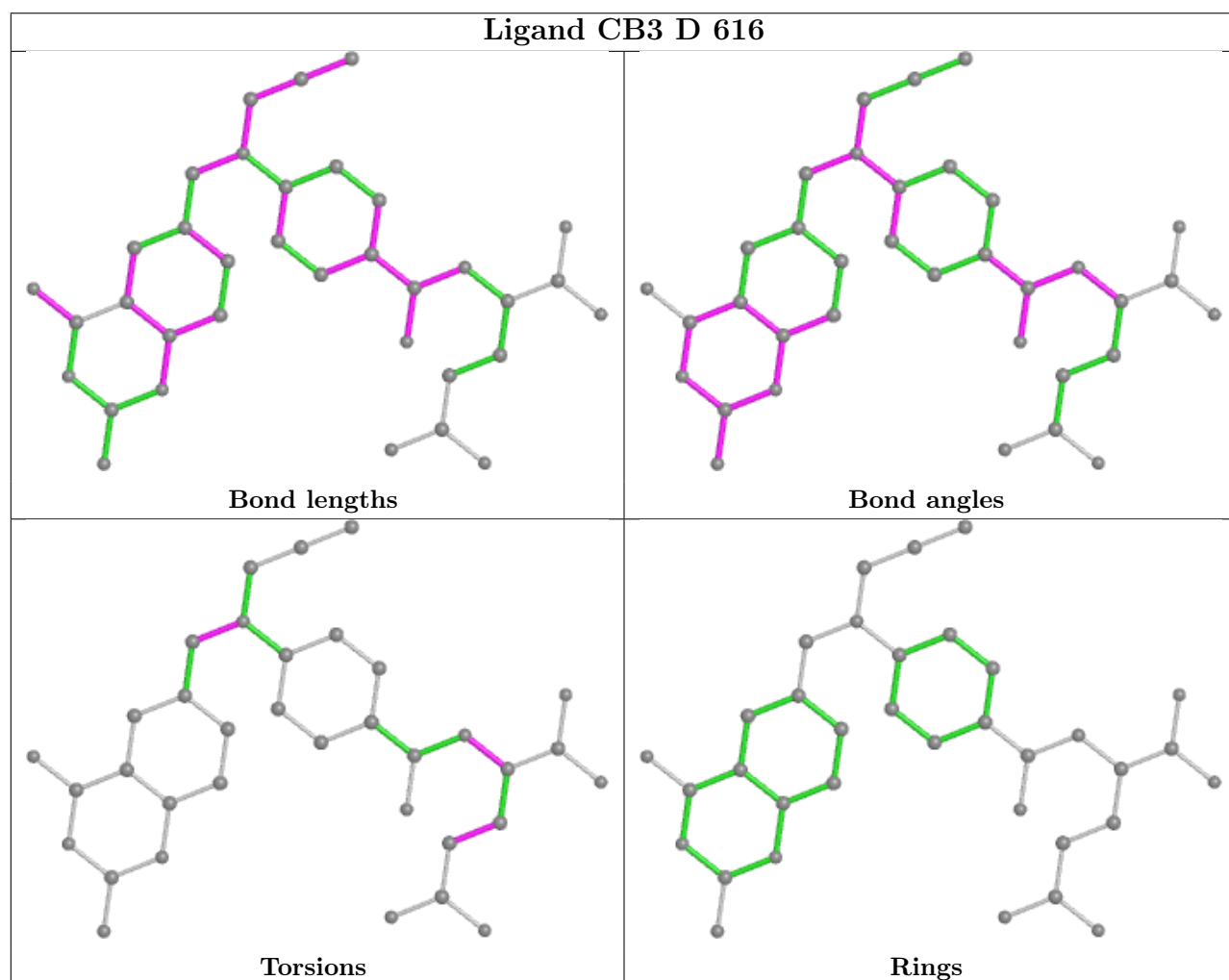
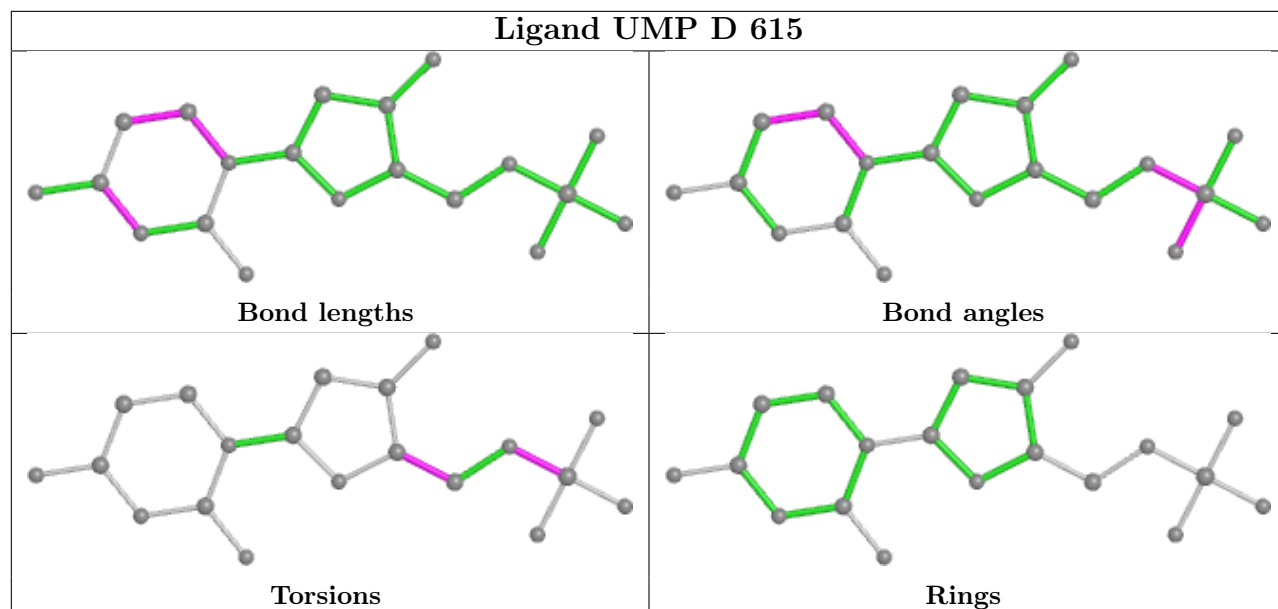


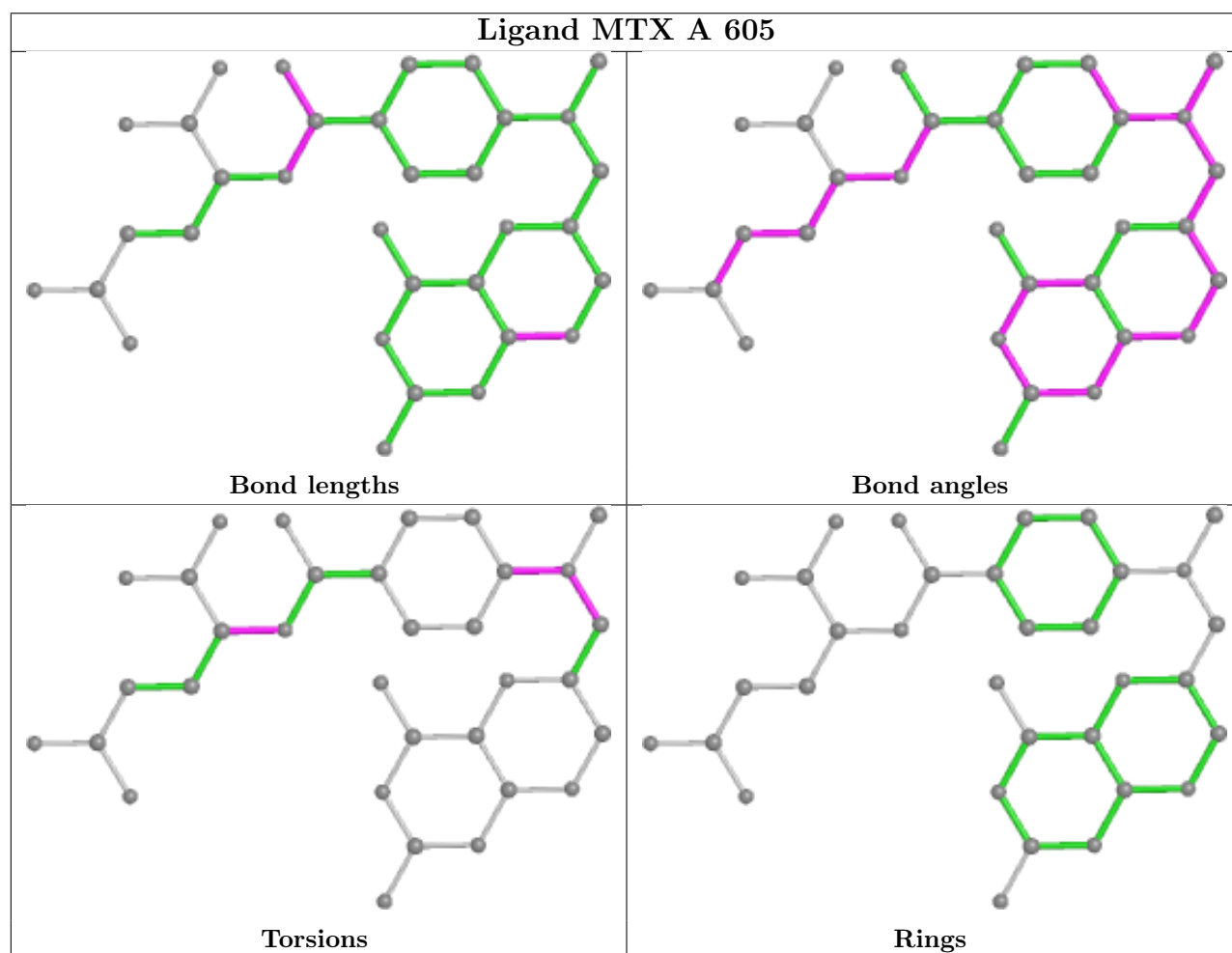
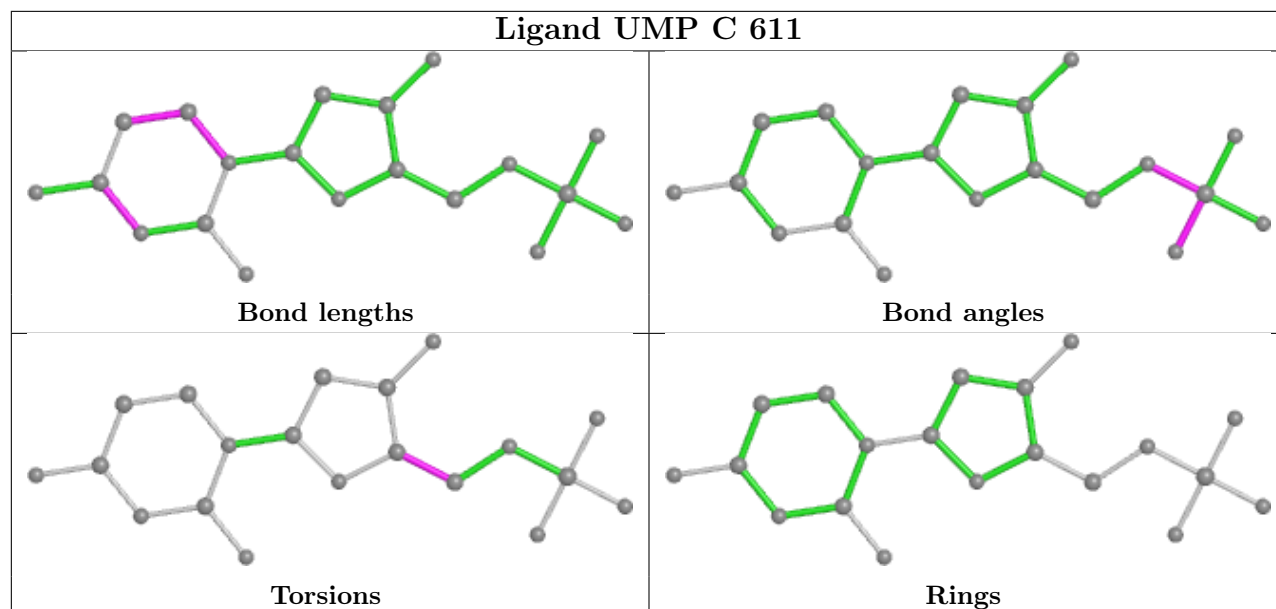
Torsions



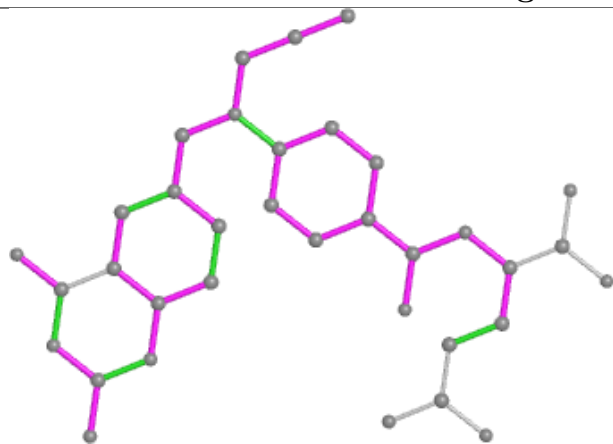
Rings



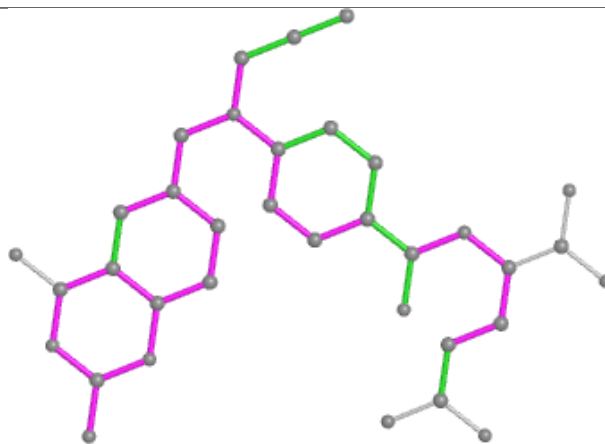




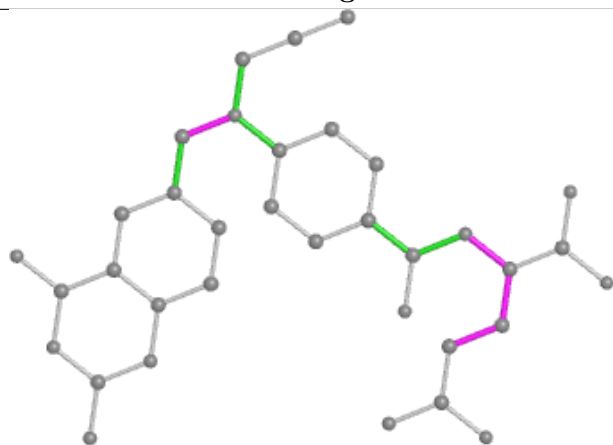
Ligand CB3 B 608



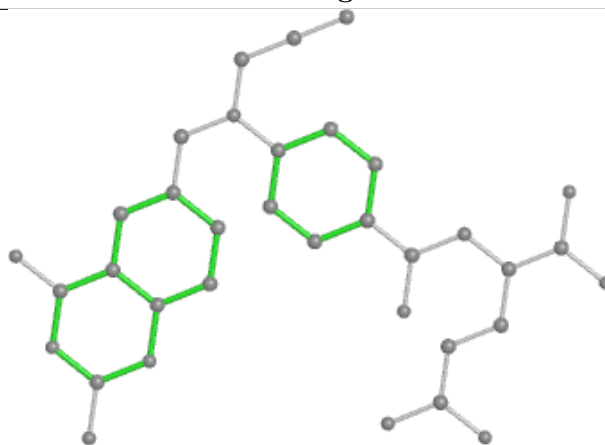
Bond lengths



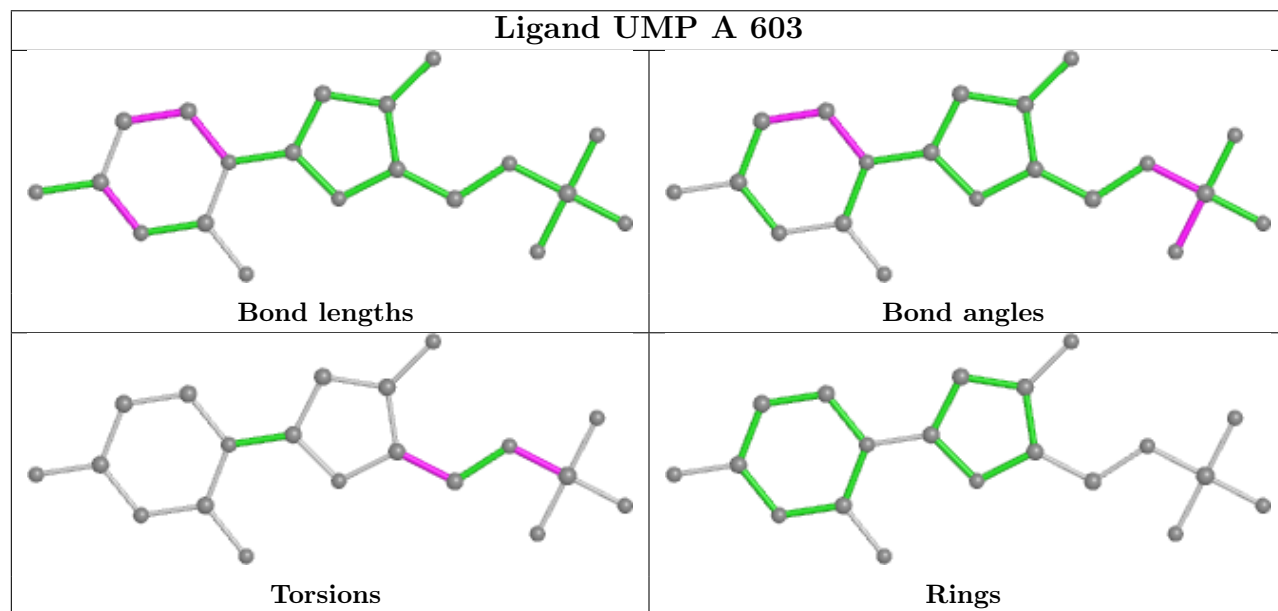
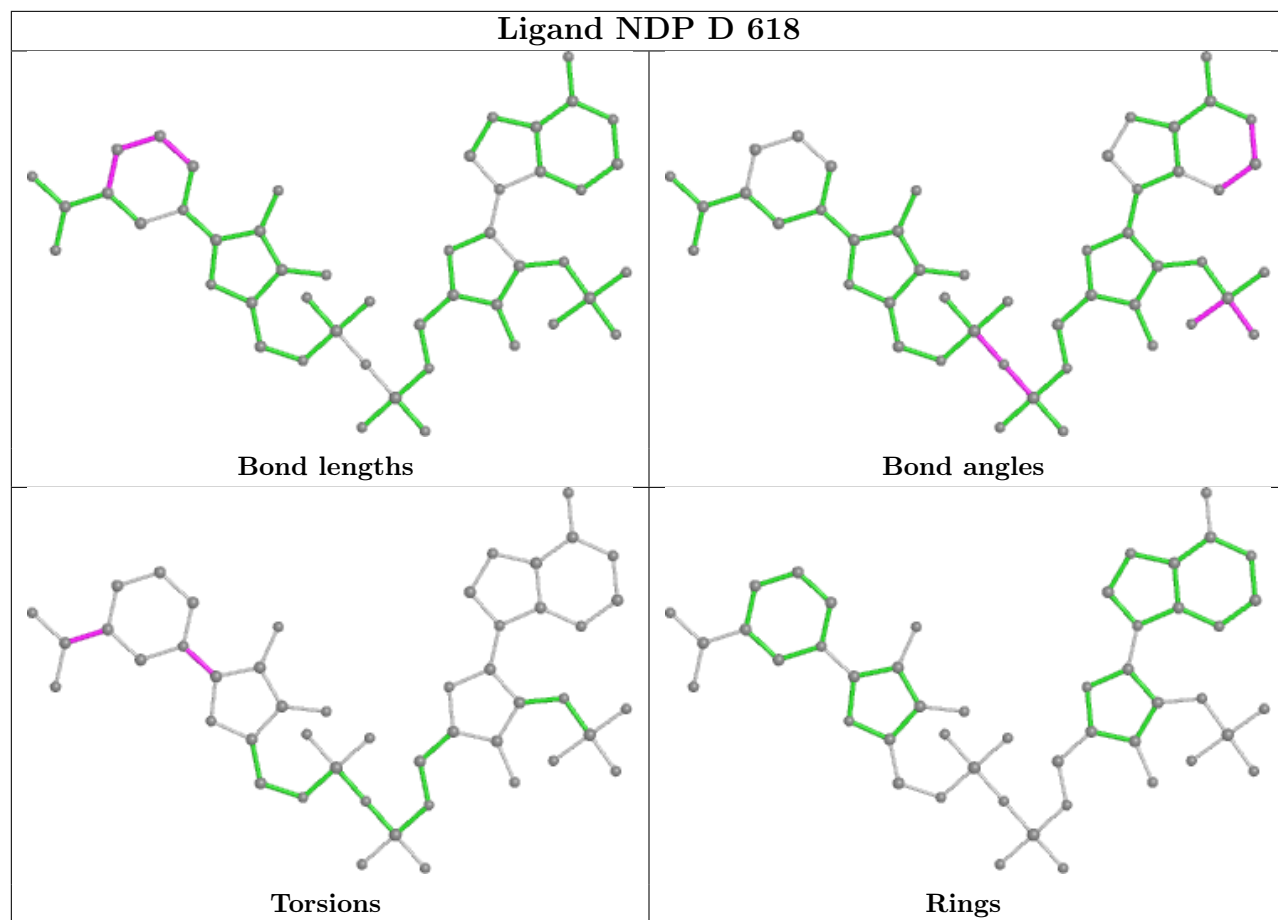
Bond angles

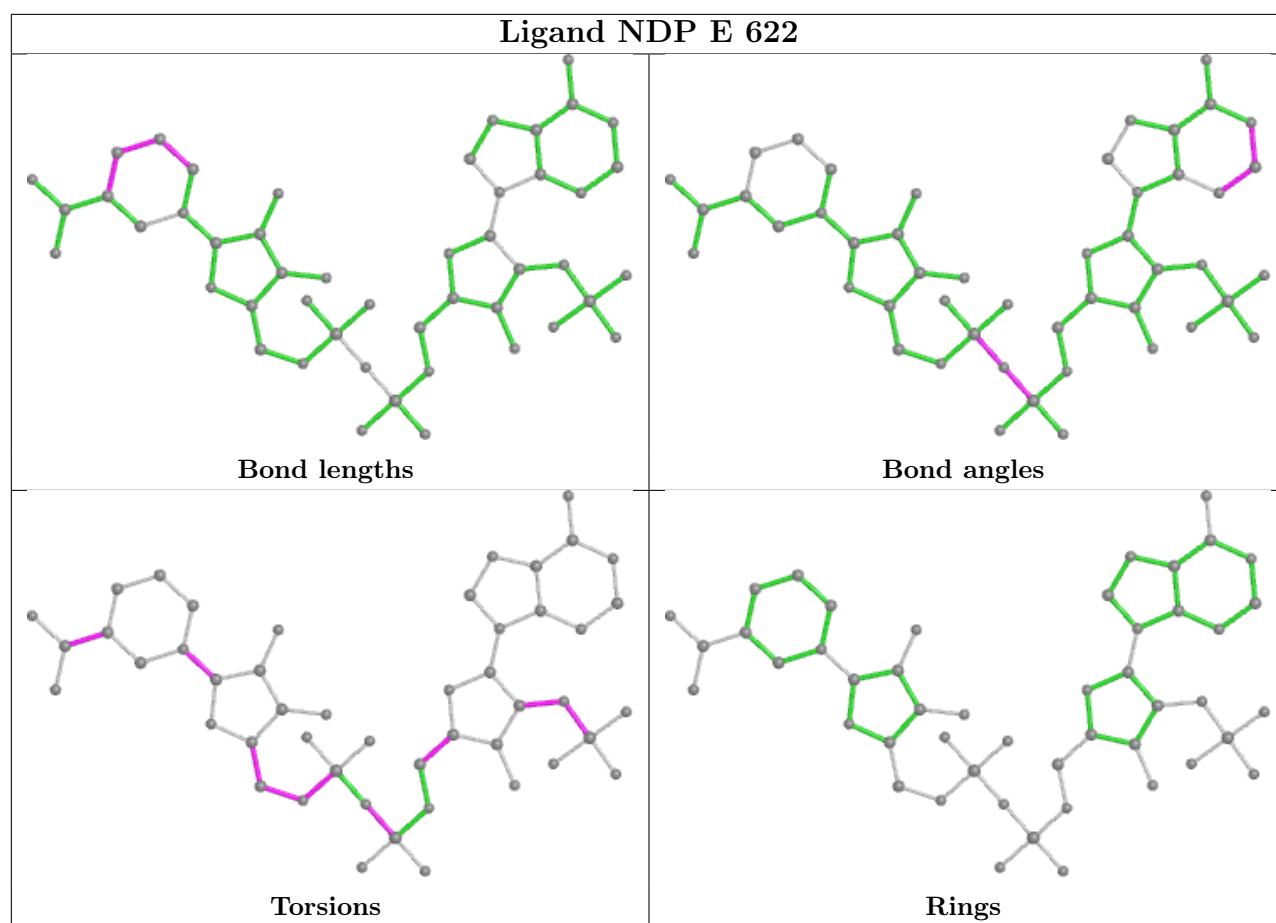


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

6.1 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	516/519 (99%)	-0.07	14 (2%) 54 44	26, 45, 92, 140	0
1	B	516/519 (99%)	-0.20	10 (1%) 66 59	23, 39, 77, 139	0
1	C	514/519 (99%)	0.06	25 (4%) 29 20	34, 60, 111, 148	0
1	D	515/519 (99%)	0.06	12 (2%) 60 51	36, 60, 103, 136	0
1	E	511/519 (98%)	0.69	60 (11%) 4 2	65, 101, 146, 167	0
All	All	2572/2595 (99%)	0.11	121 (4%) 31 22	23, 58, 123, 167	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	CYS	7.7
1	E	103	ASN	6.5
1	D	103	ASN	6.2
1	E	364	GLY	6.1
1	D	192	GLN	5.9

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

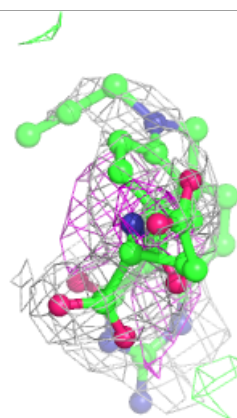
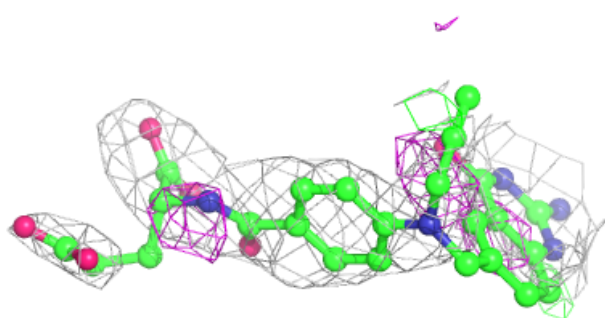
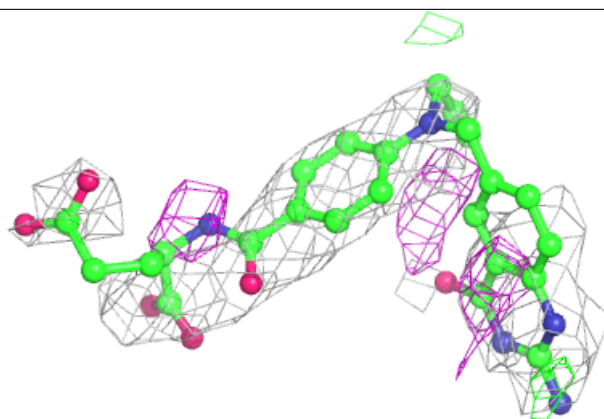
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CB3	E	620	35/35	0.65	0.53	131,134,135,135	0
3	CB3	D	616	35/35	0.82	0.34	107,110,114,115	0
4	MTX	C	613	33/33	0.85	0.27	75,83,87,87	0
2	UMP	E	619	20/20	0.86	0.18	125,131,135,135	0
4	MTX	E	621	33/33	0.86	0.25	96,102,103,104	0
5	NDP	C	614	48/48	0.86	0.24	92,96,111,112	0
3	CB3	A	604	35/35	0.88	0.30	68,77,89,90	0
3	CB3	C	612	35/35	0.89	0.23	59,71,80,82	0
5	NDP	E	622	48/48	0.90	0.18	85,89,105,106	0
2	UMP	D	615	20/20	0.93	0.18	77,82,86,88	0
3	CB3	B	608	35/35	0.93	0.21	44,52,63,66	0
4	MTX	D	617	33/33	0.93	0.21	61,68,71,71	0
5	NDP	D	618	48/48	0.94	0.17	49,64,75,75	0
2	UMP	B	607	20/20	0.95	0.18	37,43,46,50	0
2	UMP	A	603	20/20	0.95	0.17	53,58,63,68	0
4	MTX	B	609	33/33	0.95	0.19	44,50,51,54	0
2	UMP	C	611	20/20	0.96	0.19	44,62,68,70	0
4	MTX	A	605	33/33	0.96	0.18	42,48,50,52	0
5	NDP	B	610	48/48	0.96	0.15	33,41,45,46	0
5	NDP	A	606	48/48	0.97	0.15	41,46,50,50	0

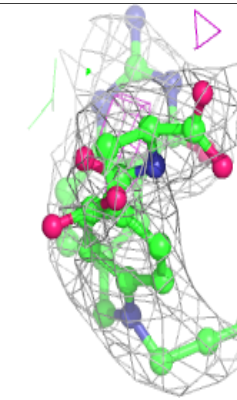
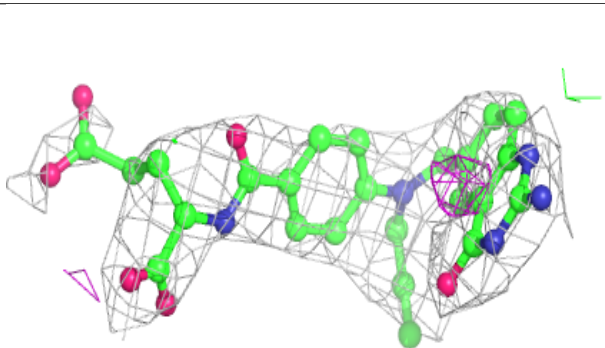
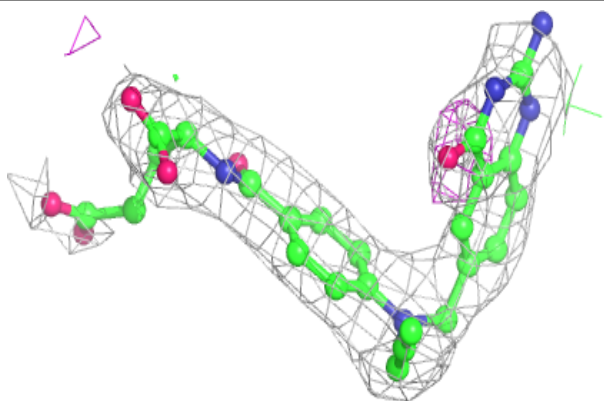
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CB3 E 620:

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

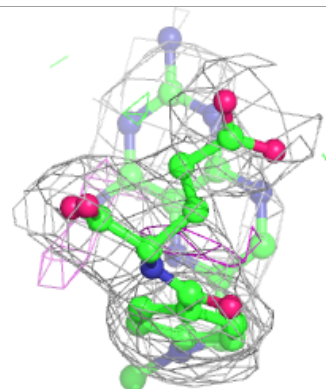
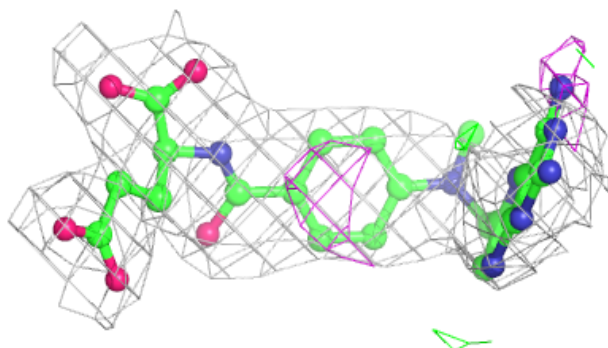
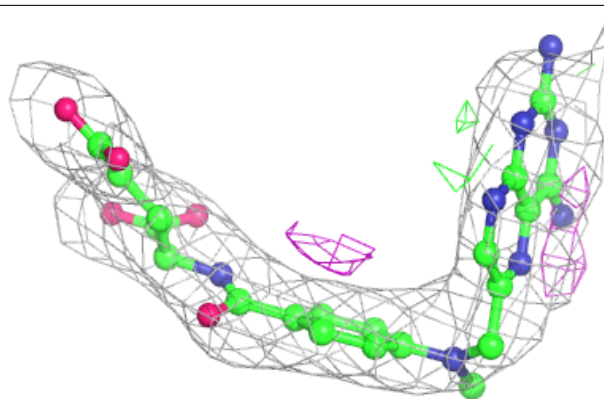
**Electron density around CB3 D 616:**

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

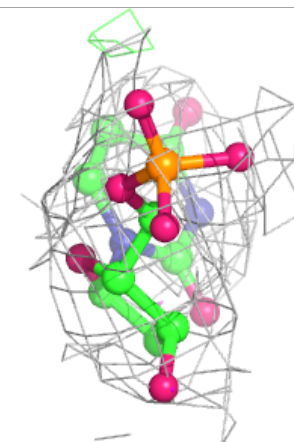
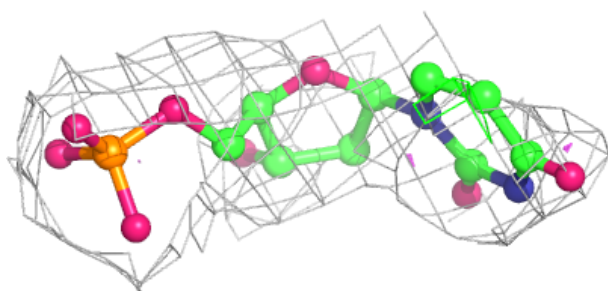
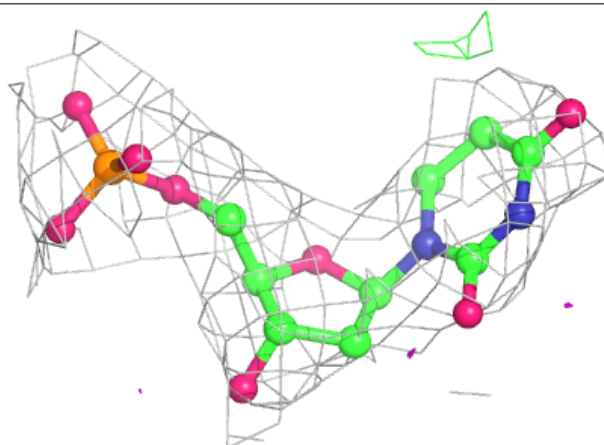


Electron density around MTX C 613:

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

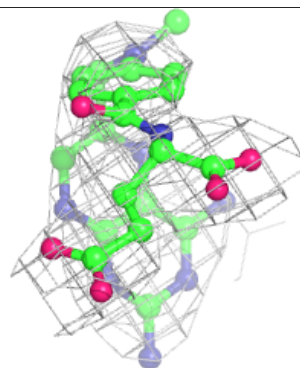
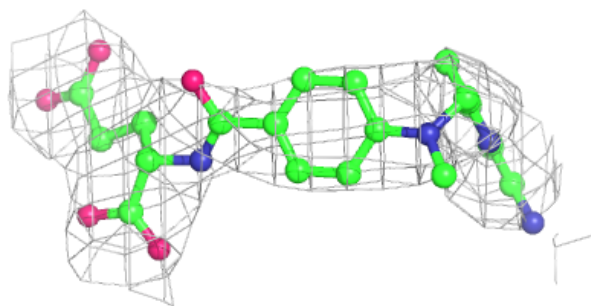
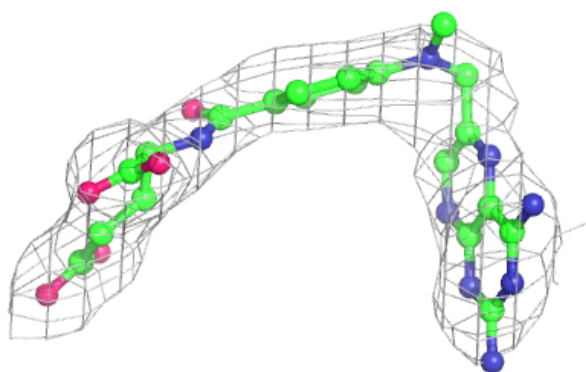
**Electron density around UMP E 619:**

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

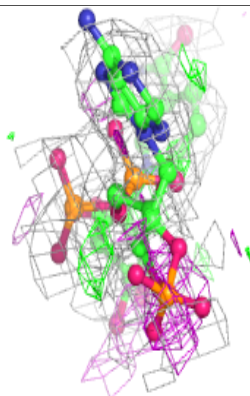
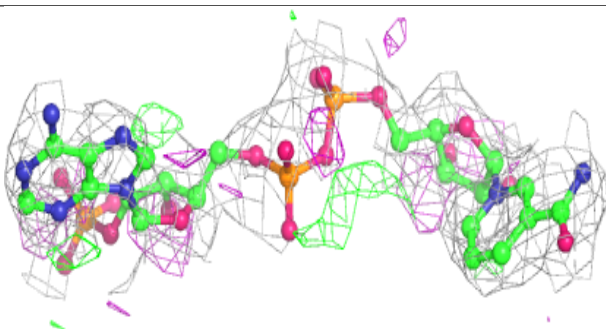
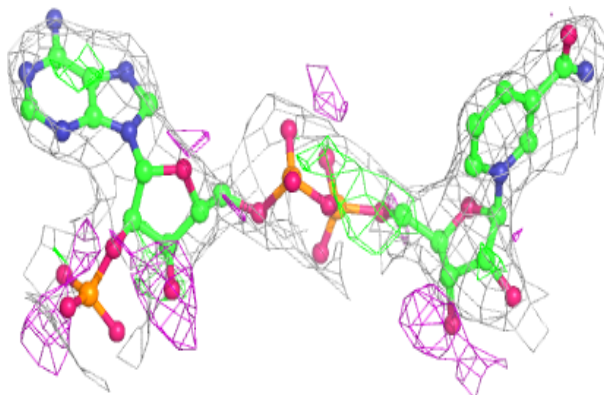


Electron density around MTX E 621:

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

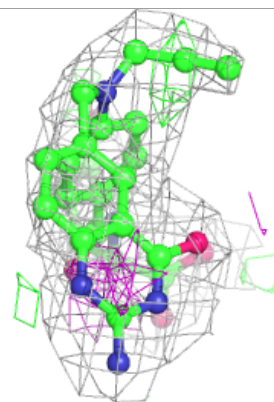
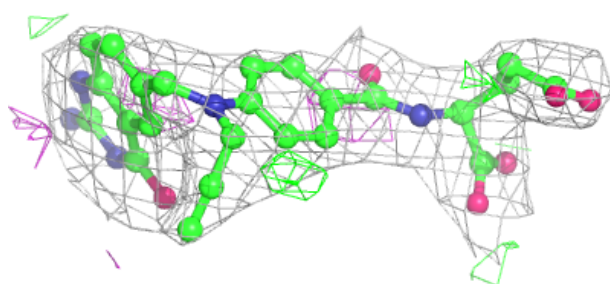
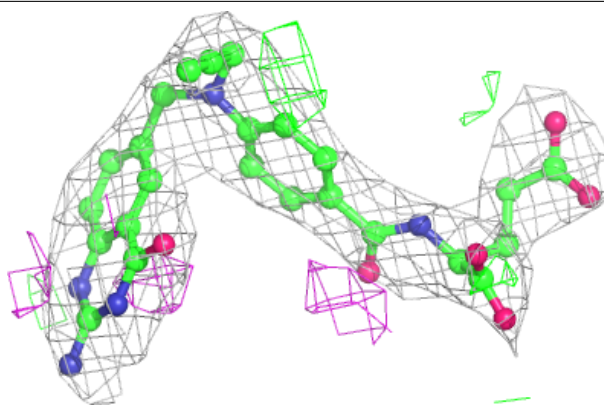
**Electron density around NDP C 614:**

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

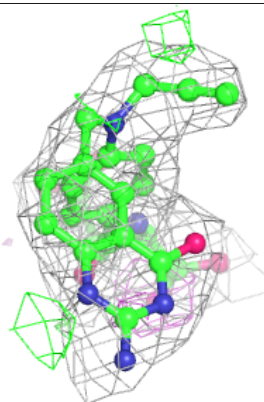
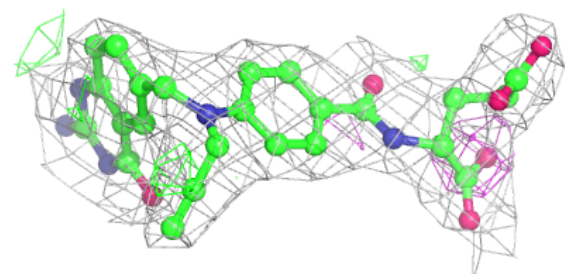
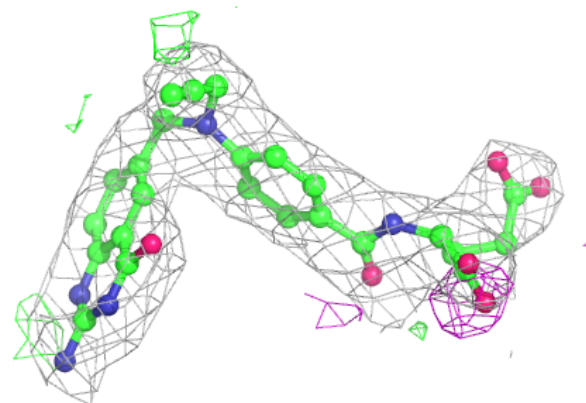


Electron density around CB3 A 604:

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

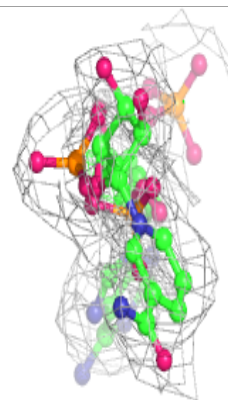
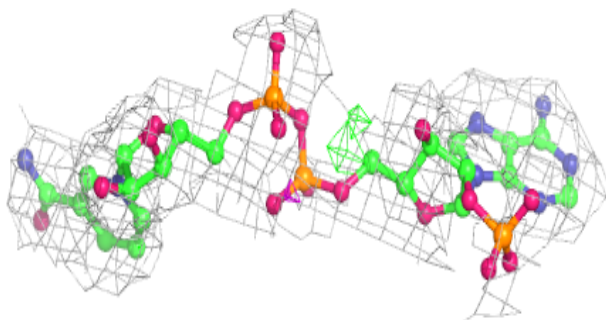
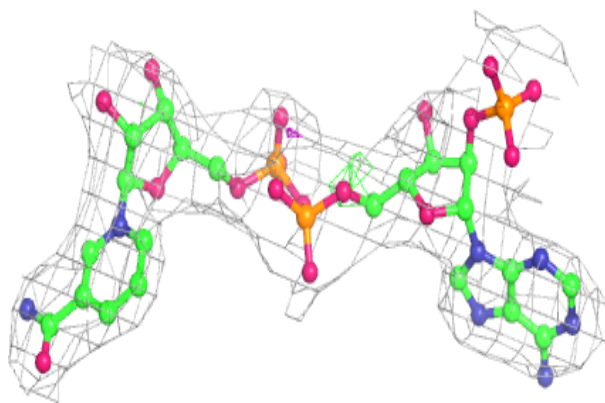
**Electron density around CB3 C 612:**

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

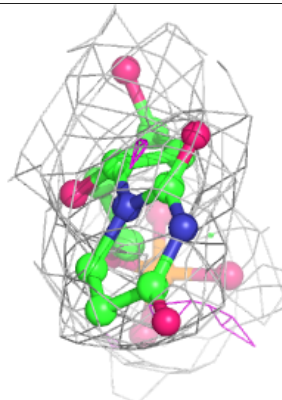
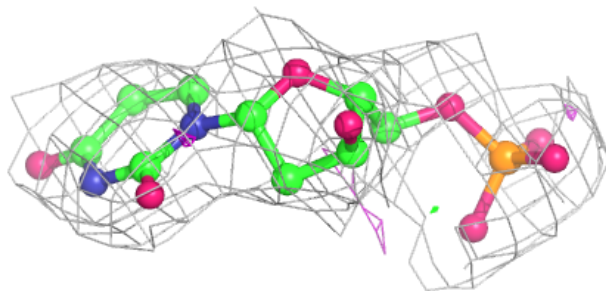
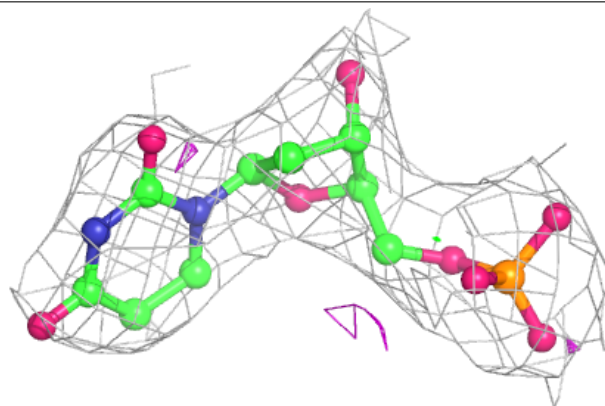


Electron density around NDP E 622:

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

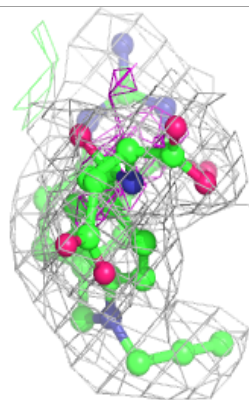
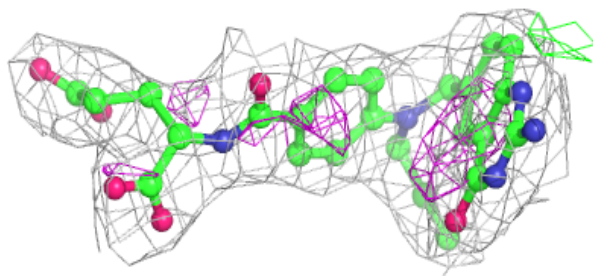
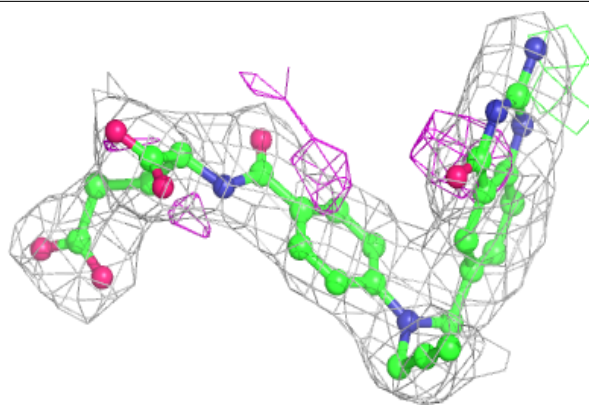
**Electron density around UMP D 615:**

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



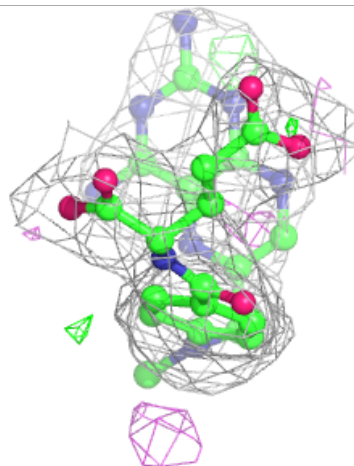
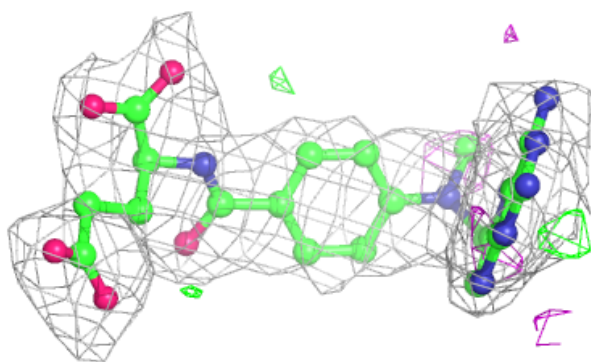
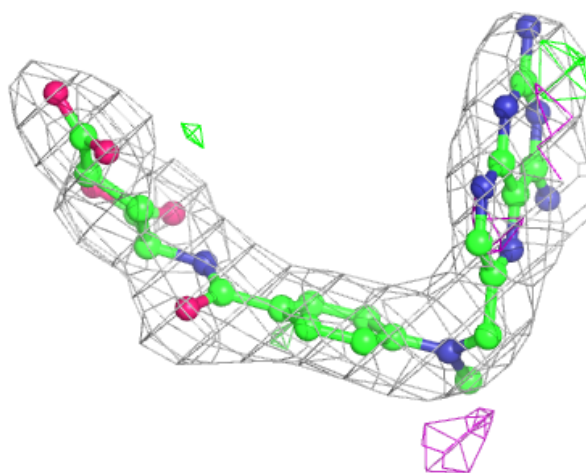
Electron density around CB3 B 608:

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



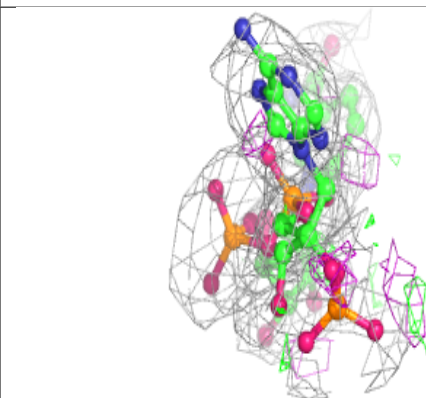
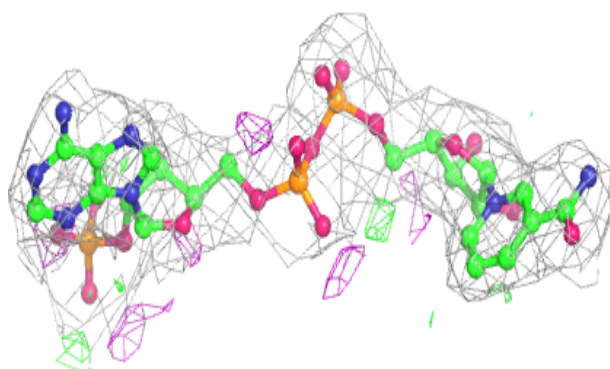
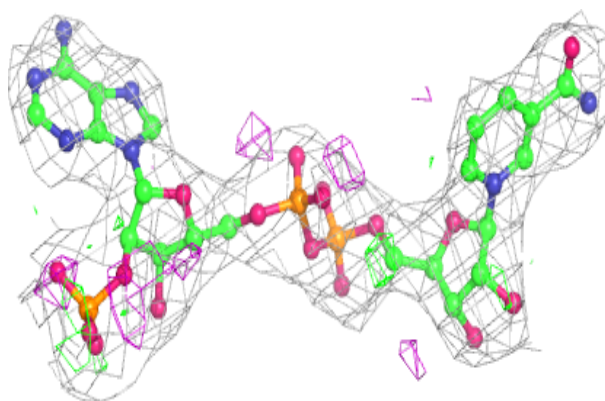
Electron density around MTX D 617:

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

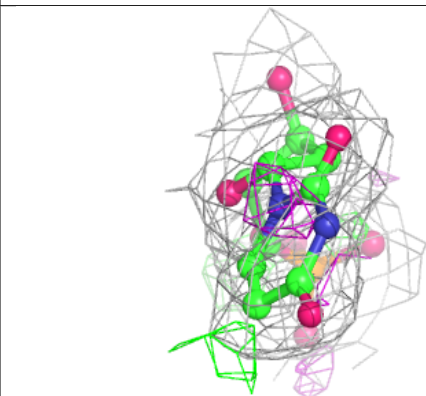
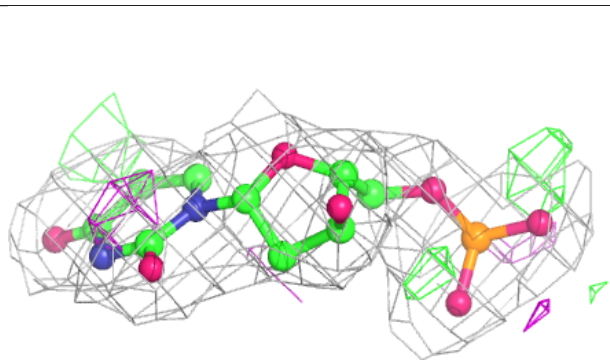
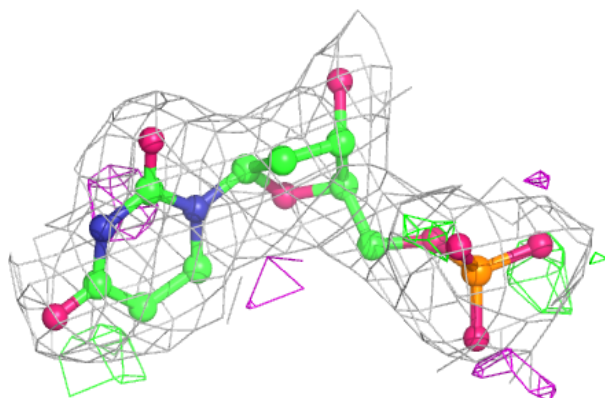


Electron density around NDP D 618:

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

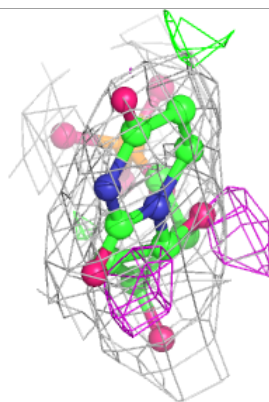
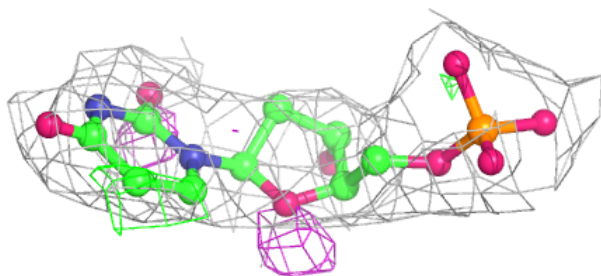
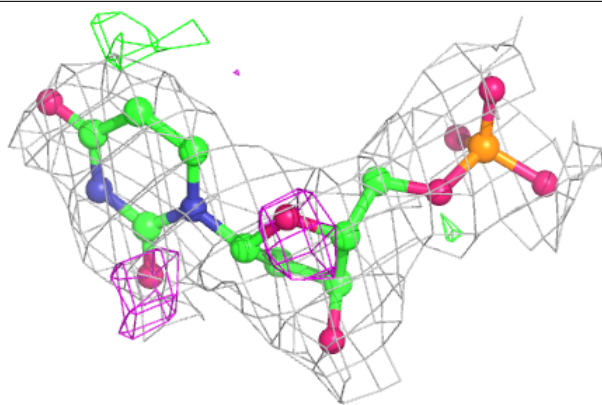
**Electron density around UMP B 607:**

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

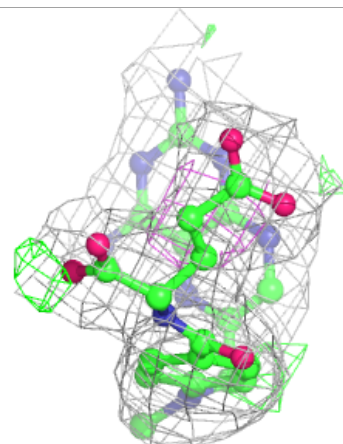
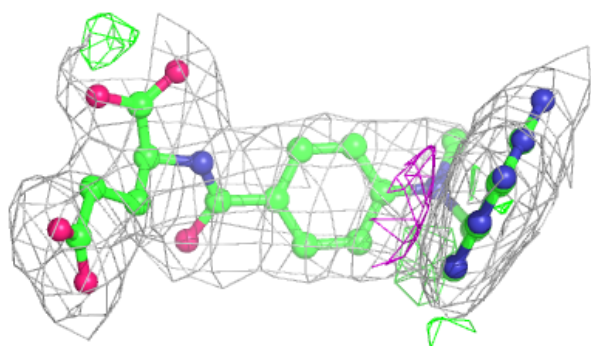
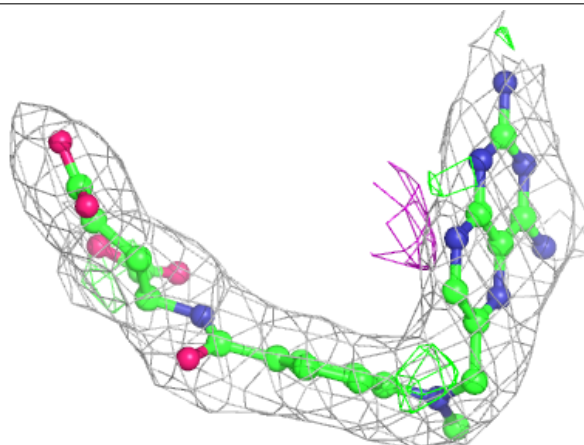


Electron density around UMP A 603:

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

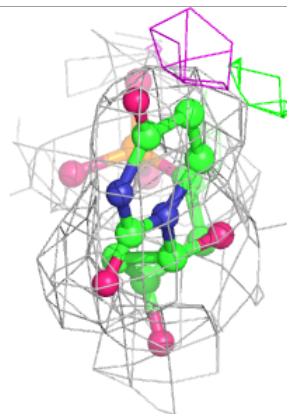
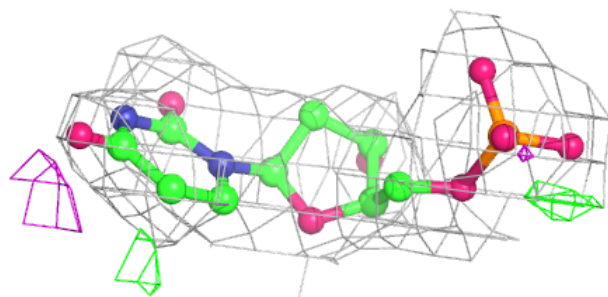
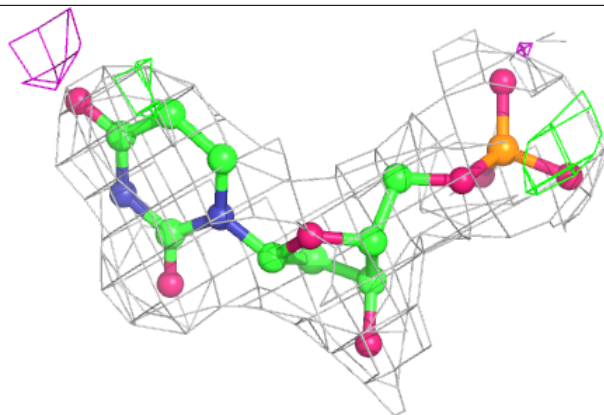
**Electron density around MTX B 609:**

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



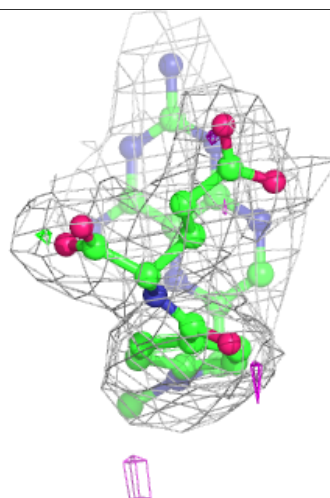
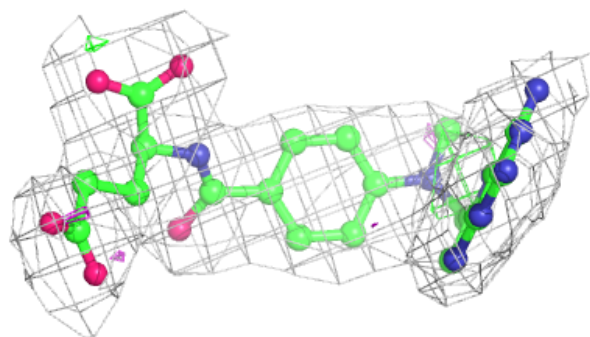
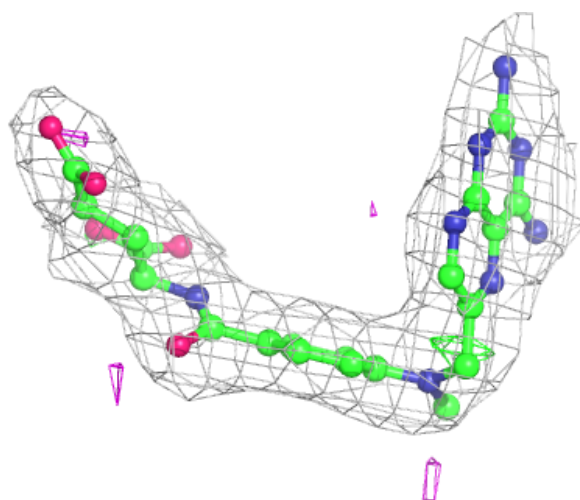
Electron density around UMP C 611:

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



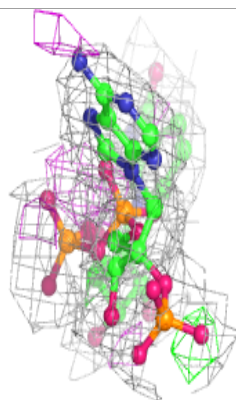
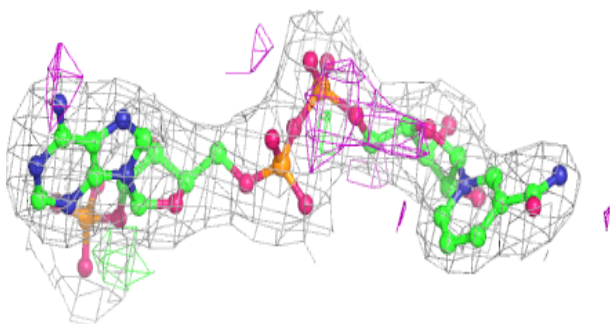
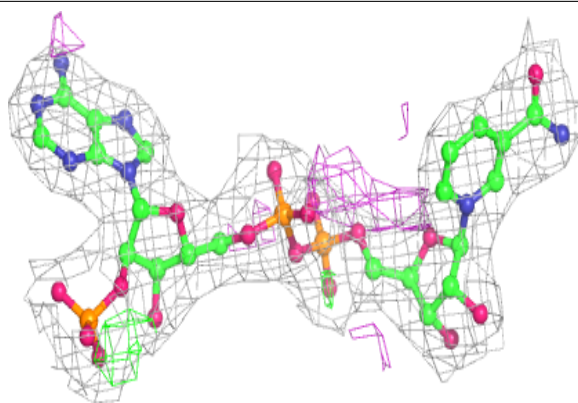
Electron density around MTX A 605:

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

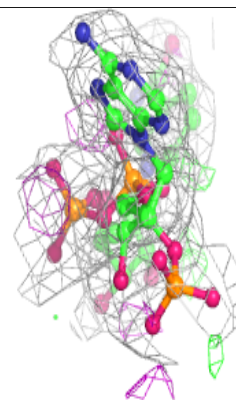
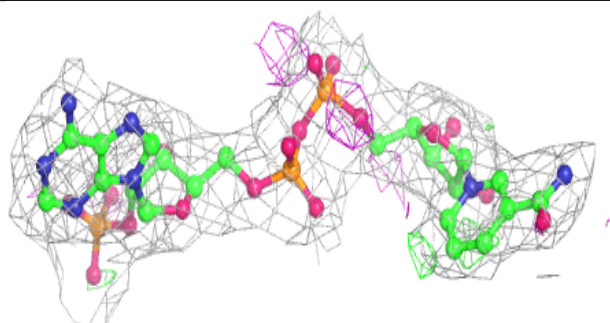
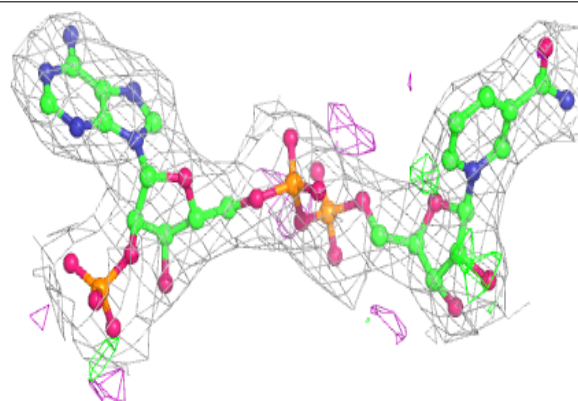


Electron density around NDP B 610:

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

**Electron density around NDP A 606:**

$2mF_o-DF_c$ (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.