



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2021 – 09:25 AM EDT

PDB ID : 3HJ3
Title : Crystal Structure of the ChTS-DHFR F207A Non-Active Site Mutant
Authors : Anderson, K.S.; Martucci, W.E.
Deposited on : 2009-05-20
Resolution : 2.70 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

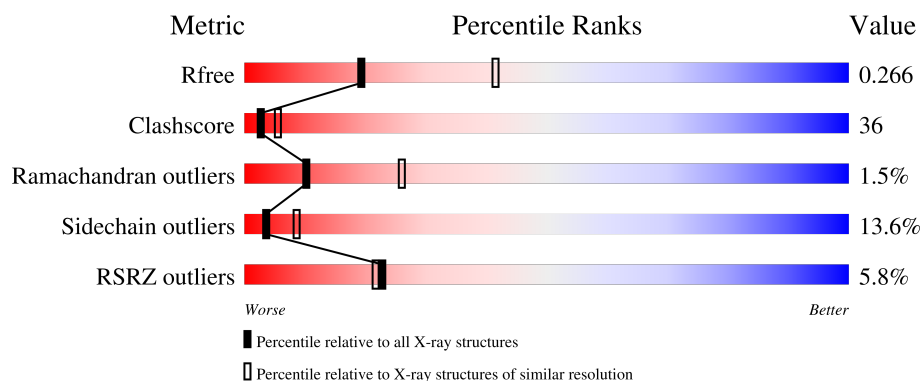
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	521	<div> <div>3%</div> <div>56%</div> <div>32%</div> <div>9%</div> <div>..</div> </div>
1	B	521	<div> <div>3%</div> <div>55%</div> <div>34%</div> <div>8%</div> <div>..</div> </div>
1	C	521	<div> <div>7%</div> <div>47%</div> <div>40%</div> <div>10%</div> <div>..</div> </div>
1	D	521	<div> <div>10%</div> <div>42%</div> <div>45%</div> <div>9%</div> <div>..</div> </div>

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	A	603	-	-	X	X
2	UMP	B	607	-	-	X	X
2	UMP	C	611	-	-	X	-
3	CB3	A	604	X	-	X	-
3	CB3	B	608	X	-	-	X
3	CB3	C	612	X	-	X	X
4	MTX	D	615	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17282 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.

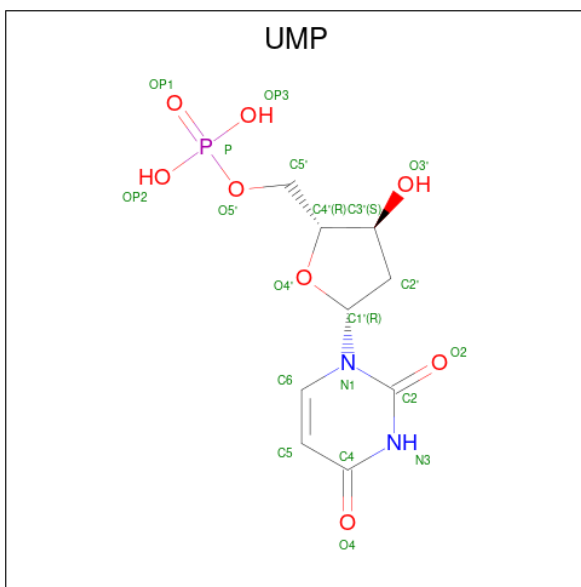
- Molecule 1 is a protein called Chain A, crystal structure of Dhfr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			4131	2638	695	776	22			
1	B	510	Total	C	N	O	S	0	0	0
			4144	2645	698	779	22			
1	C	510	Total	C	N	O	S	0	0	0
			4147	2648	698	779	22			
1	D	505	Total	C	N	O	S	0	0	0
			4104	2622	690	770	22			

There are 4 discrepancies between the modelled and reference sequences:

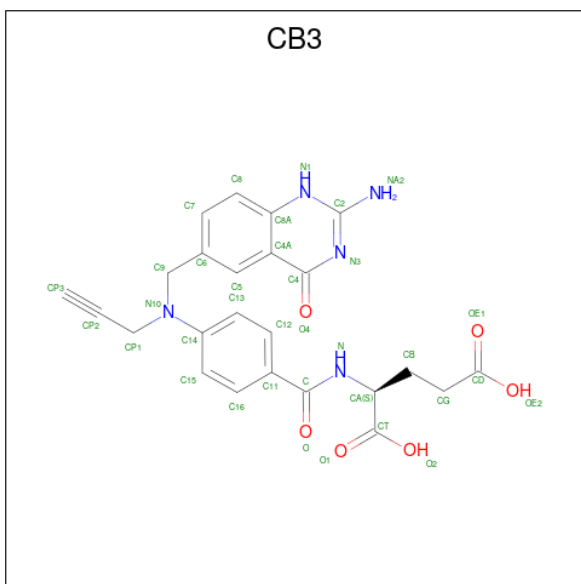
Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ALA	PHE	engineered mutation	UNP Q5CGA3
B	207	ALA	PHE	engineered mutation	UNP Q5CGA3
C	207	ALA	PHE	engineered mutation	UNP Q5CGA3
D	207	ALA	PHE	engineered mutation	UNP Q5CGA3

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



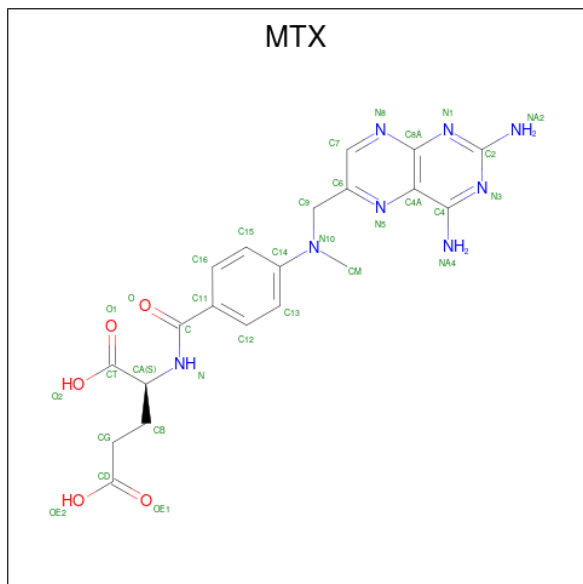
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: $C_{24}H_{23}N_5O_6$).



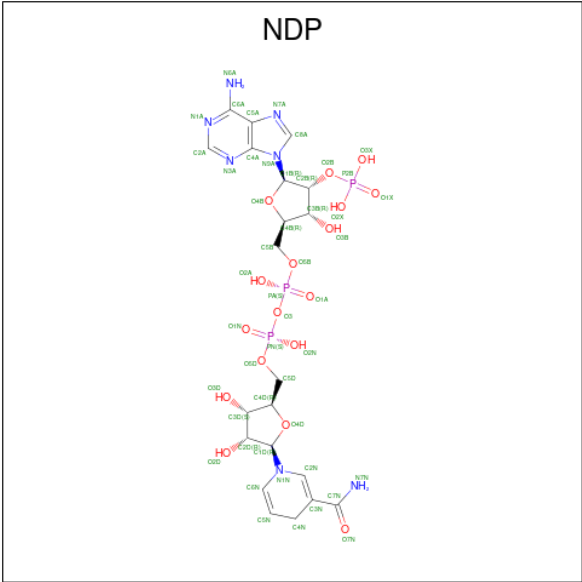
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		

- 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		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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		

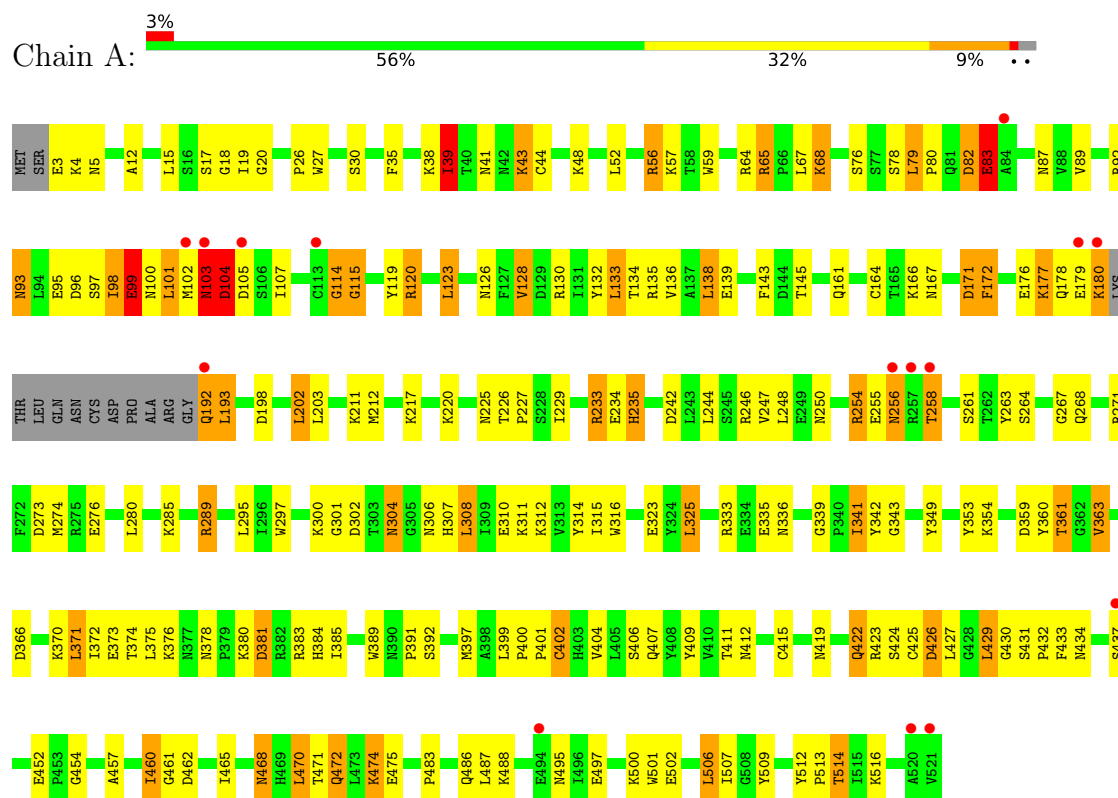
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	98	Total	O	0	0
			98	98		
6	B	86	Total	O	0	0
			86	86		
6	C	47	Total	O	0	0
			47	47		
6	D	36	Total	O	0	0
			36	36		

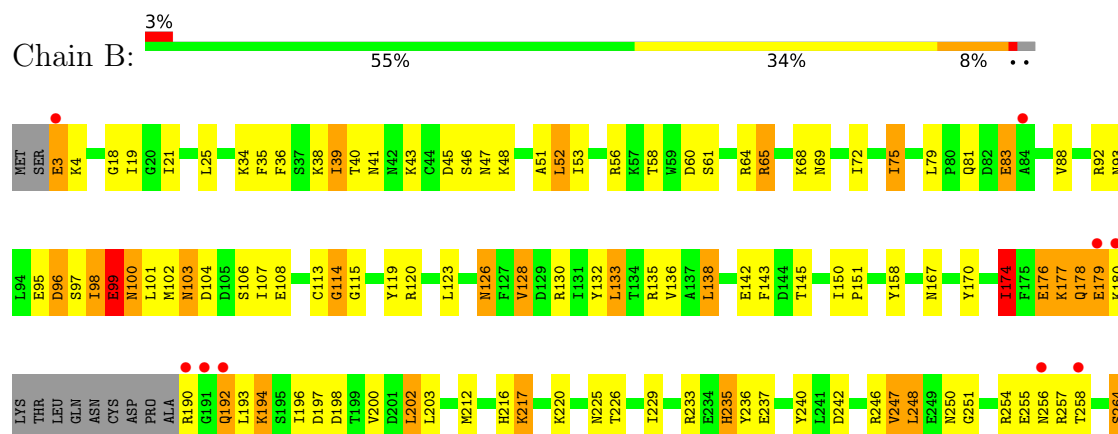
3 Residue-property plots [i](#)

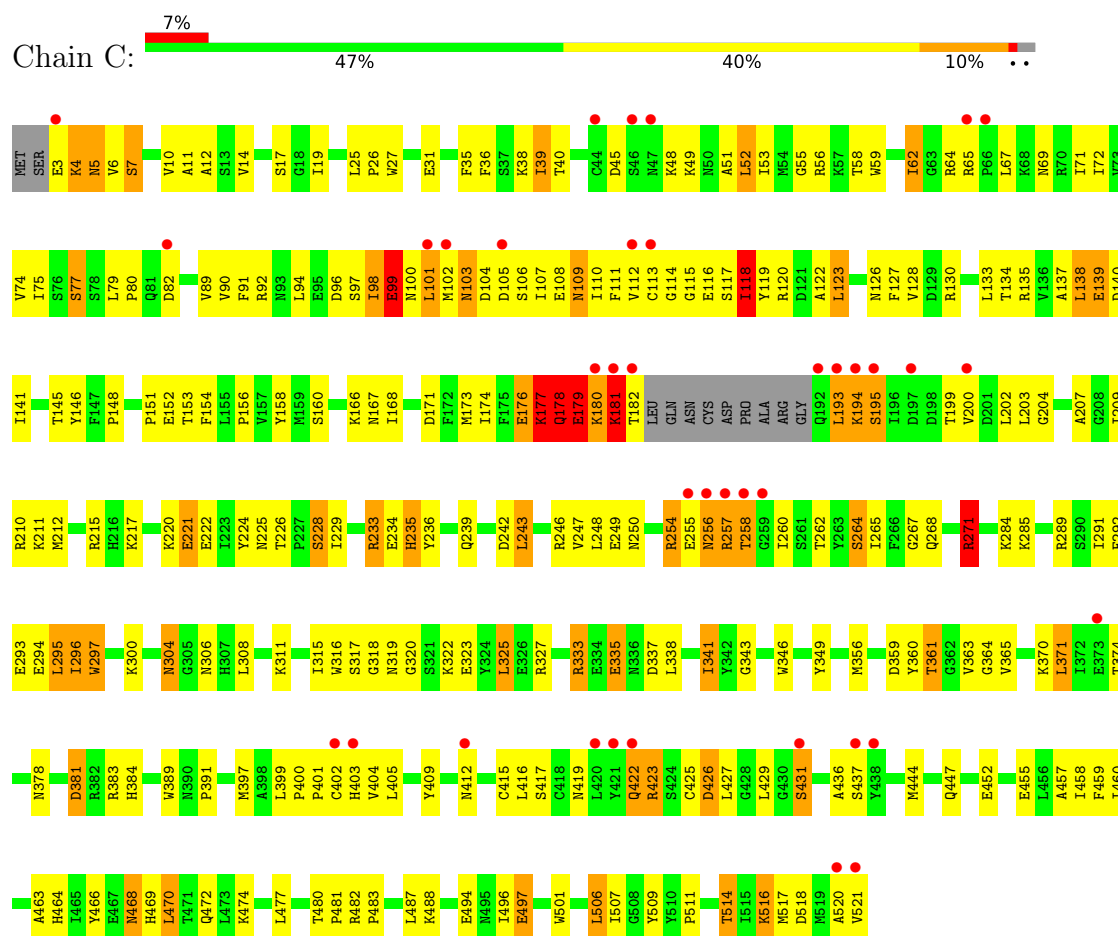
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Chain A, crystal structure of Dhfr



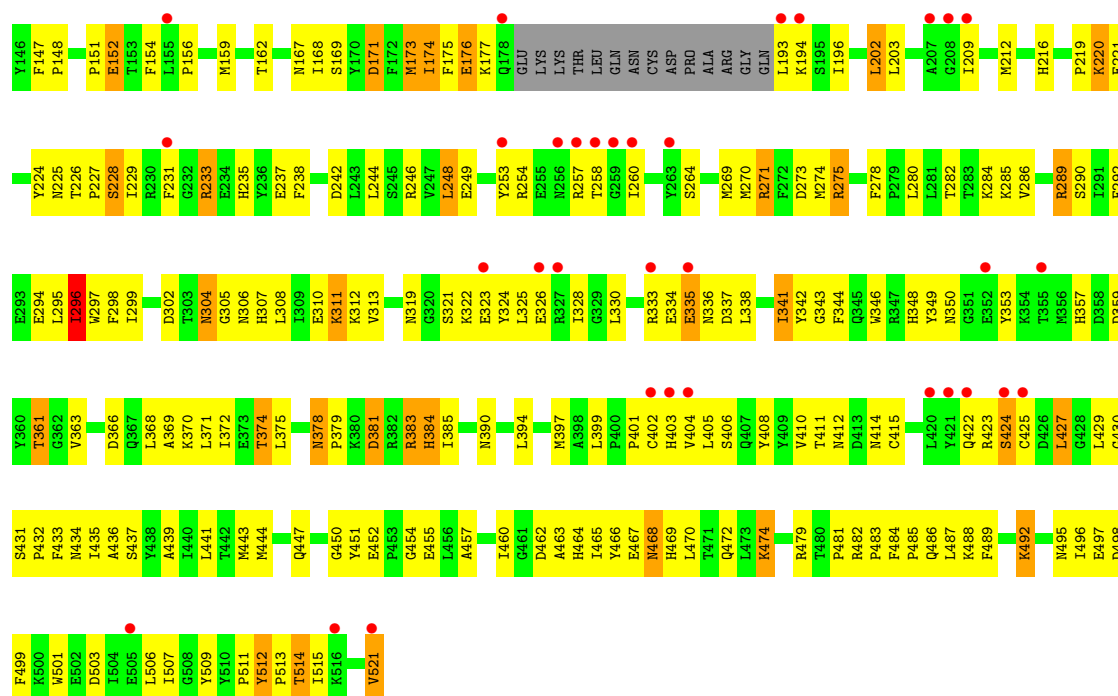
• Molecule 1: Chain A, crystal structure of Dhfr





Chain D:

Category	Percentage
L79	10%
L84	10%
R92	10%
N93	10%
L94	10%
E95	10%
D96	10%
S97	10%
L103	10%
D104	10%
D105	10%
S106	10%
I107	10%
E108	10%
N109	10%
F111	10%
V112	10%
C113	10%
G114	10%
G115	10%
E116	10%
S117	10%
I118	10%
Y119	10%
R120	10%
D121	10%
A122	10%
L123	10%
K124	10%
D125	10%
N126	10%
F127	10%
V128	10%
D129	10%
R130	10%
I131	10%
Y132	10%
L133	10%
F134	10%
R135	10%
V136	10%
A137	10%
L138	10%
E139	10%
D140	10%
I141	10%
E142	10%
F143	10%
D144	10%
F145	10%
MET	42%
SER	42%
E3	42%
K4	42%
N5	42%
V6	42%
S7	42%
I8	42%
L15	42%
G18	42%
I19	42%
G20	42%
I21	42%
G22	42%
G23	42%
Q24	42%
L25	42%
S28	42%
I29	42%
S30	42%
K34	42%
F35	42%
F36	42%
S37	42%
K38	42%
I39	42%
T40	42%
N41	42%
N42	42%
K43	42%
C44	42%
S45	42%
S46	42%
N47	42%
K48	42%
G49	42%
N50	42%
A51	42%
L52	42%
I53	42%
R56	42%
K57	42%
T58	42%
N59	42%
D60	42%
S61	42%
I62	42%
L67	42%
K68	42%
N69	42%
R70	42%
I75	42%
L76	42%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.86Å 121.86Å 342.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 34.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 99.5 (34.47-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.68Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.228 , 0.274 0.219 , 0.266	Depositor DCC
R_{free} test set	4070 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17282	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, UMP, MTX, 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	0.84	1/4225 (0.0%)	0.86	4/5709 (0.1%)
1	B	0.87	2/4238 (0.0%)	0.83	4/5726 (0.1%)
1	C	0.82	1/4241 (0.0%)	0.86	5/5730 (0.1%)
1	D	0.74	1/4198 (0.0%)	0.79	2/5674 (0.0%)
All	All	0.82	5/16902 (0.0%)	0.83	15/22839 (0.1%)

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	6
1	B	0	8
1	C	0	12
1	D	0	6
All	All	0	32

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	CYS	CB-SG	-9.21	1.66	1.82
1	B	402	CYS	CB-SG	-9.01	1.67	1.82
1	D	521	VAL	C-OXT	6.37	1.35	1.23
1	C	521	VAL	C-OXT	6.01	1.34	1.23
1	B	240	TYR	CE1-CZ	5.49	1.45	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	423	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	423	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	B	75	ILE	CG1-CB-CG2	-7.13	95.72	111.40
1	B	402	CYS	CA-CB-SG	-6.15	102.93	114.00
1	A	402	CYS	CA-CB-SG	-5.80	103.55	114.00

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	GLY	Peptide
1	A	171	ASP	Peptide
1	A	192	GLN	Peptide
1	A	98	ILE	Peptide
1	A	99	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4131	0	4066	271	0
1	B	4144	0	4077	280	3
1	C	4147	0	4086	333	3
1	D	4104	0	4039	351	0
2	A	20	0	11	7	0
2	B	20	0	11	9	0
2	C	20	0	11	9	0
3	A	35	0	21	11	0
3	B	35	0	21	8	0
3	C	35	0	21	10	0
4	A	33	0	19	1	0
4	B	33	0	19	4	0
4	C	33	0	19	6	0
4	D	33	0	20	13	0
5	A	48	0	26	4	0
5	B	48	0	26	6	0
5	C	48	0	26	7	0
5	D	48	0	26	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	98	0	0	32	0
6	B	86	0	0	30	0
6	C	47	0	0	29	0
6	D	36	0	0	47	0
All	All	17282	0	16545	1208	3

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 36.

The worst 5 of 1208 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:402:CYS:SG	2:C:611:UMP:C6	2.20	1.33
1:B:65:ARG:HD2	6:B:593:HOH:O	1.41	1.19
1:C:211:LYS:HB3	6:C:561:HOH:O	1.39	1.18
1:C:374:THR:HG22	1:C:384:HIS:CE1	1.81	1.14
1:A:381:ASP:HB2	6:A:591:HOH:O	1.47	1.12

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:OE1	1:C:166:LYS:NZ[5_555]	1.67	0.53
1:B:3:GLU:OE1	1:C:166:LYS:CE[5_555]	1.99	0.21
1:B:3:GLU:CD	1:C:166:LYS:NZ[5_555]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	504/521 (97%)	468 (93%)	28 (6%)	8 (2%)	9 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	506/521 (97%)	473 (94%)	28 (6%)	5 (1%)	15	37
1	C	506/521 (97%)	462 (91%)	37 (7%)	7 (1%)	11	28
1	D	501/521 (96%)	439 (88%)	51 (10%)	11 (2%)	6	17
All	All	2017/2084 (97%)	1842 (91%)	144 (7%)	31 (2%)	10	26

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	C	118	ILE
1	C	178	GLN
1	C	181	LYS
1	D	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	457/469 (97%)	399 (87%)	58 (13%)	4	10
1	B	458/469 (98%)	405 (88%)	53 (12%)	5	12
1	C	459/469 (98%)	385 (84%)	74 (16%)	2	6
1	D	454/469 (97%)	391 (86%)	63 (14%)	3	8
All	All	1828/1876 (97%)	1580 (86%)	248 (14%)	3	8

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	LEU
1	D	308	LEU
1	C	221	GLU
1	D	296	ILE
1	D	412	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	434	ASN
1	D	306	ASN
1	C	468	ASN
1	D	109	ASN
1	D	414	ASN

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](#)

14 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	A	605	-	29,35,35	2.02	10 (34%)	38,49,49	1.90	9 (23%)
3	CB3	A	604	-	30,37,37	2.26	11 (36%)	38,51,51	2.20	6 (15%)
2	UMP	C	611	-	18,21,21	3.74	3 (16%)	21,31,31	1.28	2 (9%)
2	UMP	B	607	-	18,21,21	3.76	3 (16%)	21,31,31	1.29	2 (9%)
5	NDP	C	614	-	45,52,52	1.26	4 (8%)	53,80,80	1.14	4 (7%)
2	UMP	A	603	-	18,21,21	3.82	5 (27%)	21,31,31	1.28	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MTX	C	613	-	29,35,35	1.89	9 (31%)	38,49,49	2.18	13 (34%)
3	CB3	C	612	-	30,37,37	2.09	10 (33%)	38,51,51	2.17	5 (13%)
3	CB3	B	608	-	30,37,37	2.14	9 (30%)	38,51,51	2.18	6 (15%)
5	NDP	D	616	-	45,52,52	1.31	4 (8%)	53,80,80	1.37	8 (15%)
4	MTX	B	609	-	29,35,35	2.06	9 (31%)	38,49,49	2.32	11 (28%)
5	NDP	B	610	-	45,52,52	1.31	4 (8%)	53,80,80	1.19	6 (11%)
4	MTX	D	615	-	29,35,35	1.76	7 (24%)	38,49,49	2.47	15 (39%)
5	NDP	A	606	-	45,52,52	1.44	3 (6%)	53,80,80	1.15	3 (5%)

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	A	605	-	-	4/19/25/25	0/3/3/3
3	CB3	A	604	-	1/1/5/6	1/21/28/28	0/3/3/3
2	UMP	B	607	-	-	1/7/22/22	0/2/2/2
2	UMP	C	611	-	-	1/7/22/22	0/2/2/2
5	NDP	C	614	-	-	7/30/77/77	0/5/5/5
2	UMP	A	603	-	-	1/7/22/22	0/2/2/2
4	MTX	C	613	-	-	5/19/25/25	0/3/3/3
3	CB3	C	612	-	1/1/5/6	1/21/28/28	0/3/3/3
3	CB3	B	608	-	1/1/5/6	1/21/28/28	0/3/3/3
5	NDP	D	616	-	-	4/30/77/77	0/5/5/5
4	MTX	B	609	-	-	4/19/25/25	0/3/3/3
5	NDP	B	610	-	-	6/30/77/77	0/5/5/5
4	MTX	D	615	-	-	5/19/25/25	0/3/3/3
5	NDP	A	606	-	-	2/30/77/77	0/5/5/5

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	UMP	C6-N1	12.98	1.51	1.35
2	B	607	UMP	C6-N1	12.91	1.51	1.35
2	C	611	UMP	C6-N1	12.88	1.51	1.35
2	B	607	UMP	C6-C5	7.55	1.54	1.38
2	A	603	UMP	C6-C5	7.54	1.54	1.38

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	CB3	C4A-C8A-N1	-7.57	119.49	123.60
4	D	615	MTX	CB-CA-N	-7.53	99.23	110.19
3	B	608	CB3	C4A-C8A-N1	-7.15	119.72	123.60
3	C	612	CB3	C4A-C8A-N1	-6.86	119.88	123.60
3	A	604	CB3	C4A-C4-N3	-6.74	119.70	124.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	604	CB3	CA
3	B	608	CB3	CA
3	C	612	CB3	CA

5 of 43 torsion outliers are listed below:

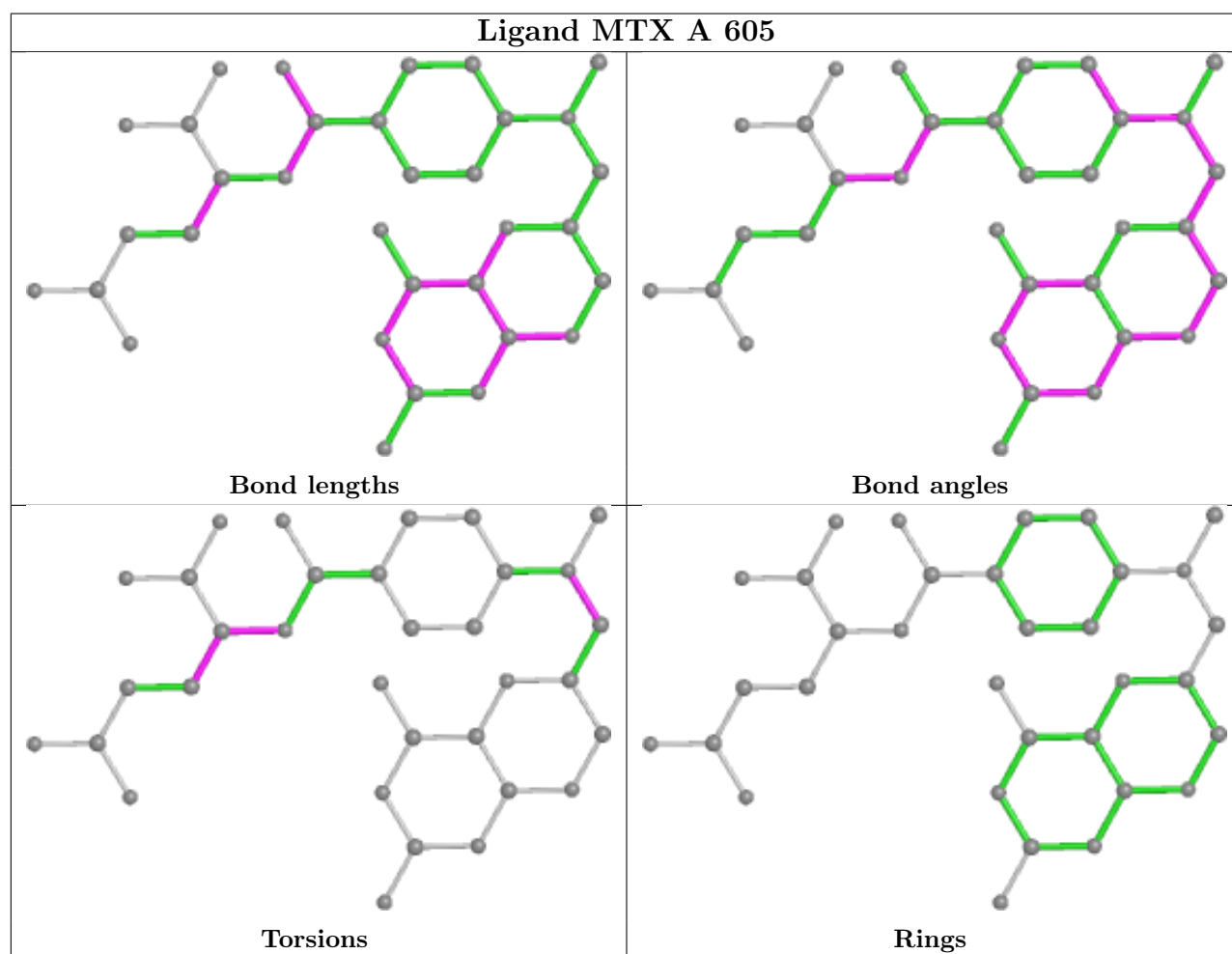
Mol	Chain	Res	Type	Atoms
3	A	604	CB3	CB-CA-N-C
3	B	608	CB3	CB-CA-N-C
3	C	612	CB3	CB-CA-N-C
4	A	605	MTX	CT-CA-CB-CG
4	B	609	MTX	CT-CA-N-C

There are no ring outliers.

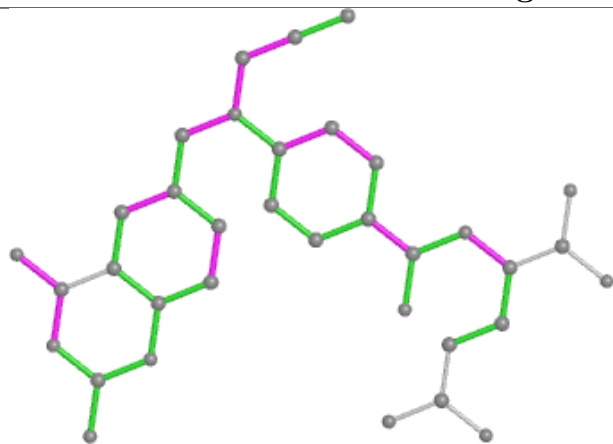
14 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	MTX	1	0
3	A	604	CB3	11	0
2	C	611	UMP	9	0
2	B	607	UMP	9	0
5	C	614	NDP	7	0
2	A	603	UMP	7	0
4	C	613	MTX	6	0
3	C	612	CB3	10	0
3	B	608	CB3	8	0
5	D	616	NDP	8	0
4	B	609	MTX	4	0
5	B	610	NDP	6	0
4	D	615	MTX	13	0
5	A	606	NDP	4	0

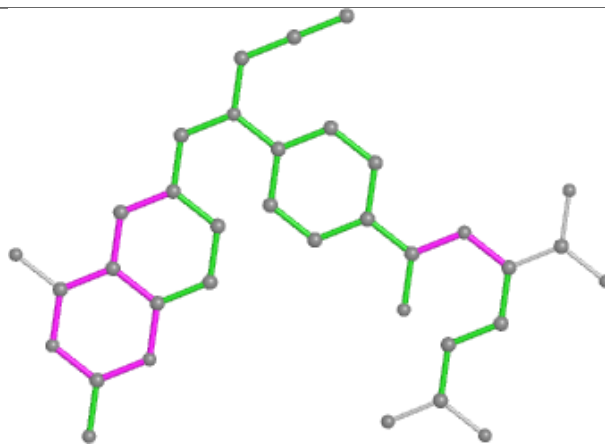
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



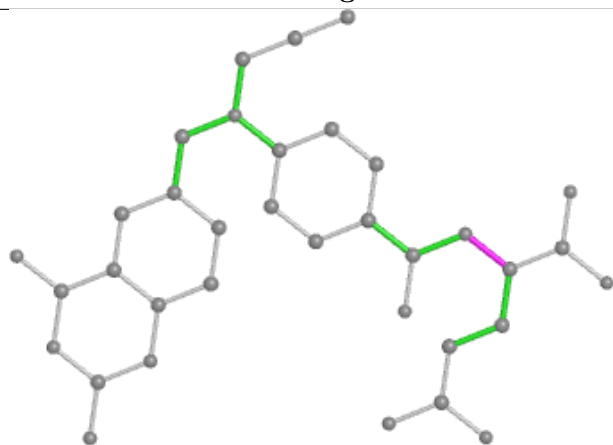
Ligand CB3 A 604



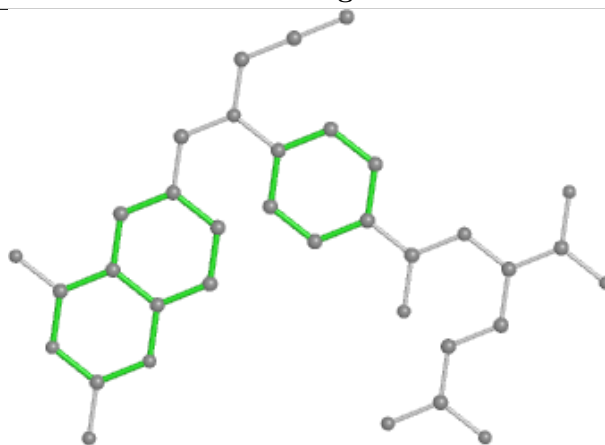
Bond lengths



Bond angles

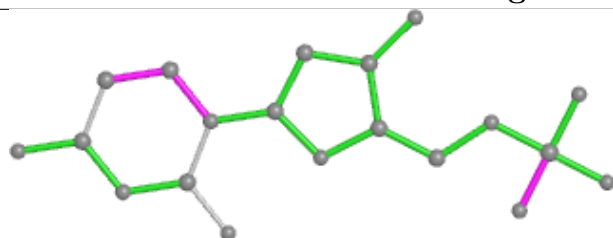


Torsions

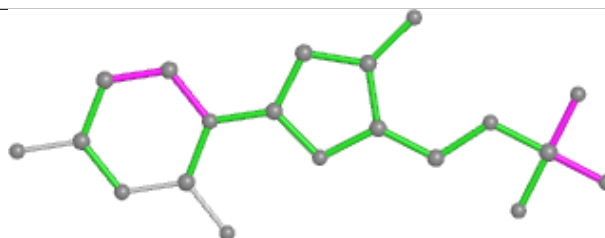


Rings

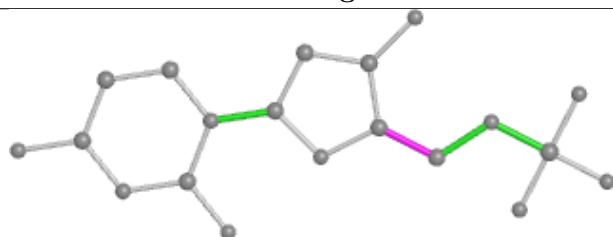
Ligand UMP C 611



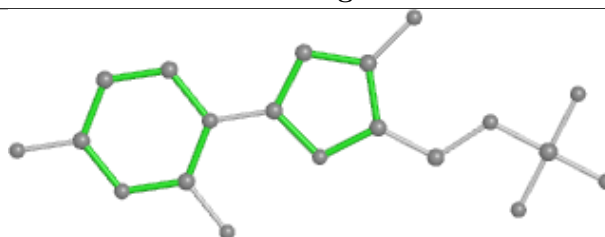
Bond lengths



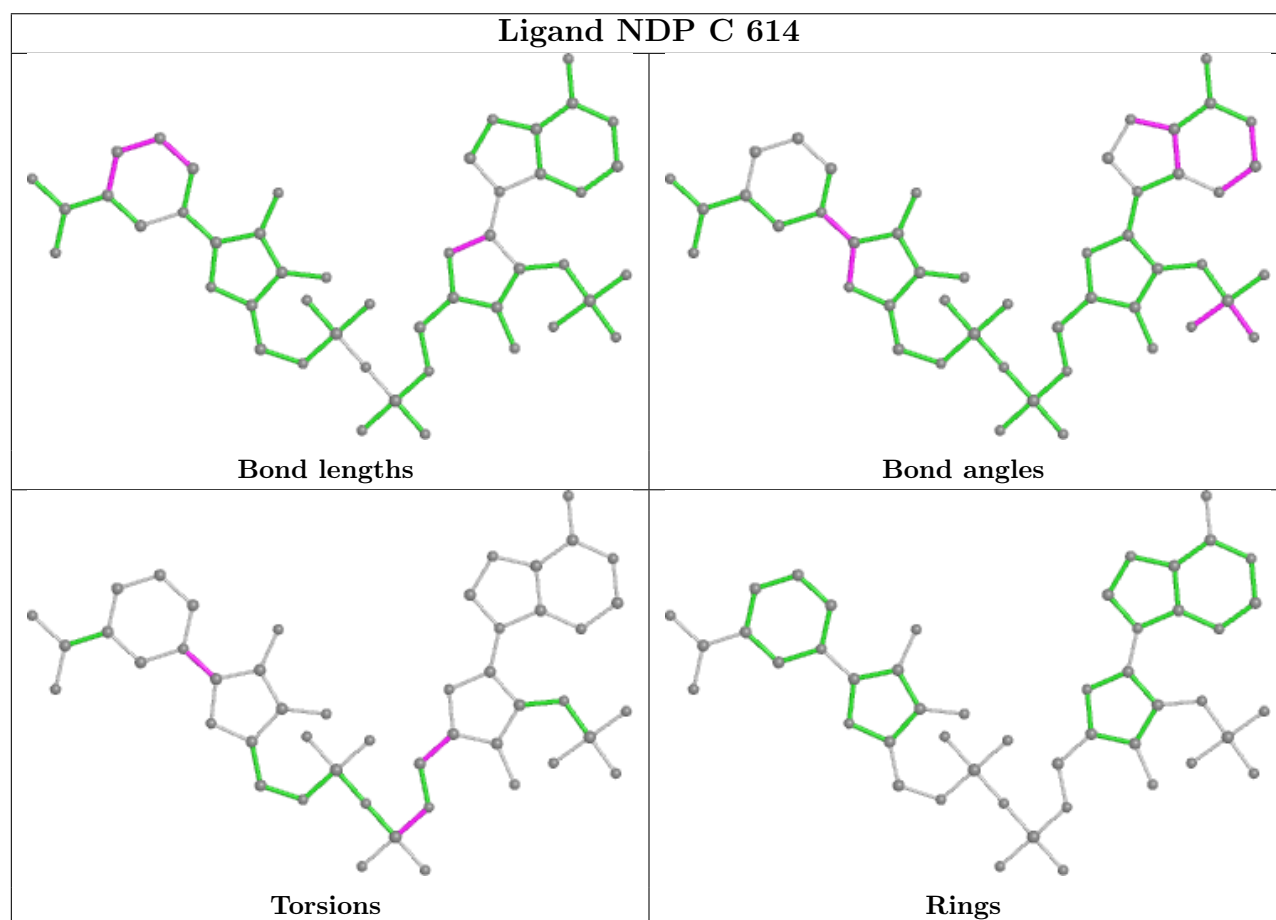
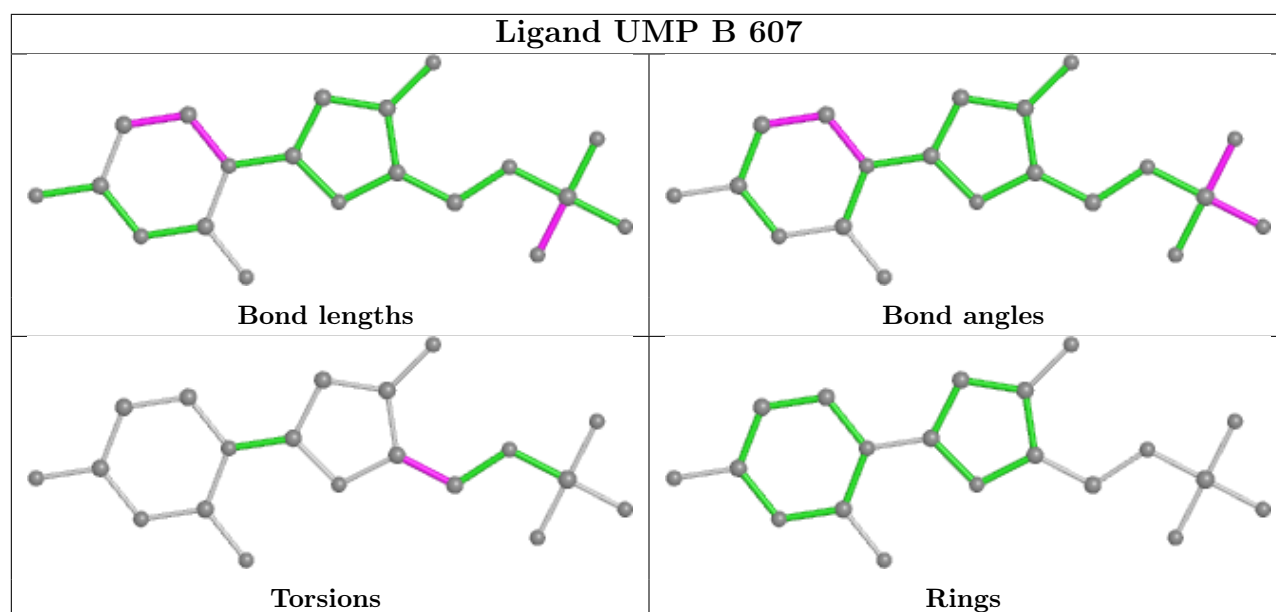
Bond angles

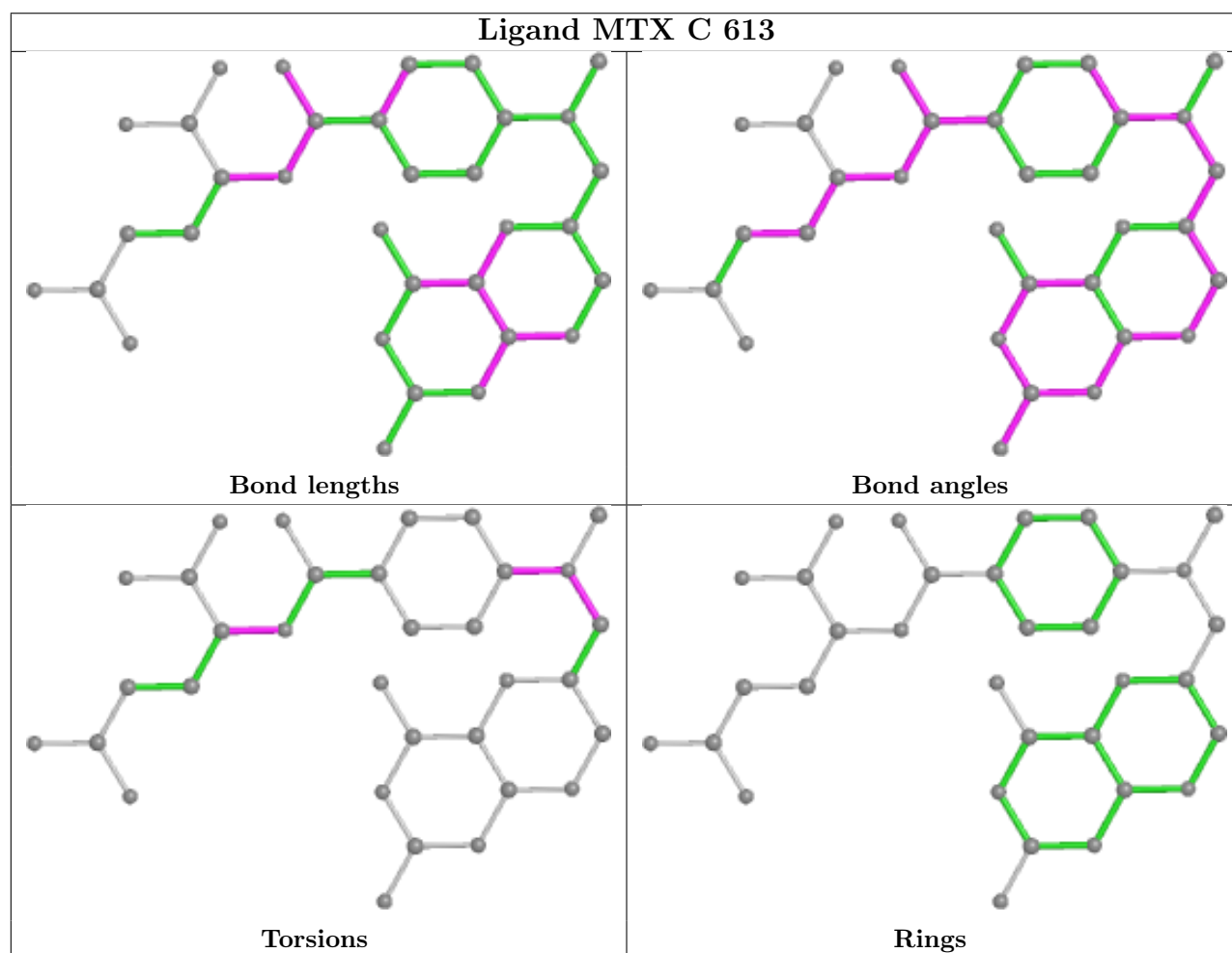
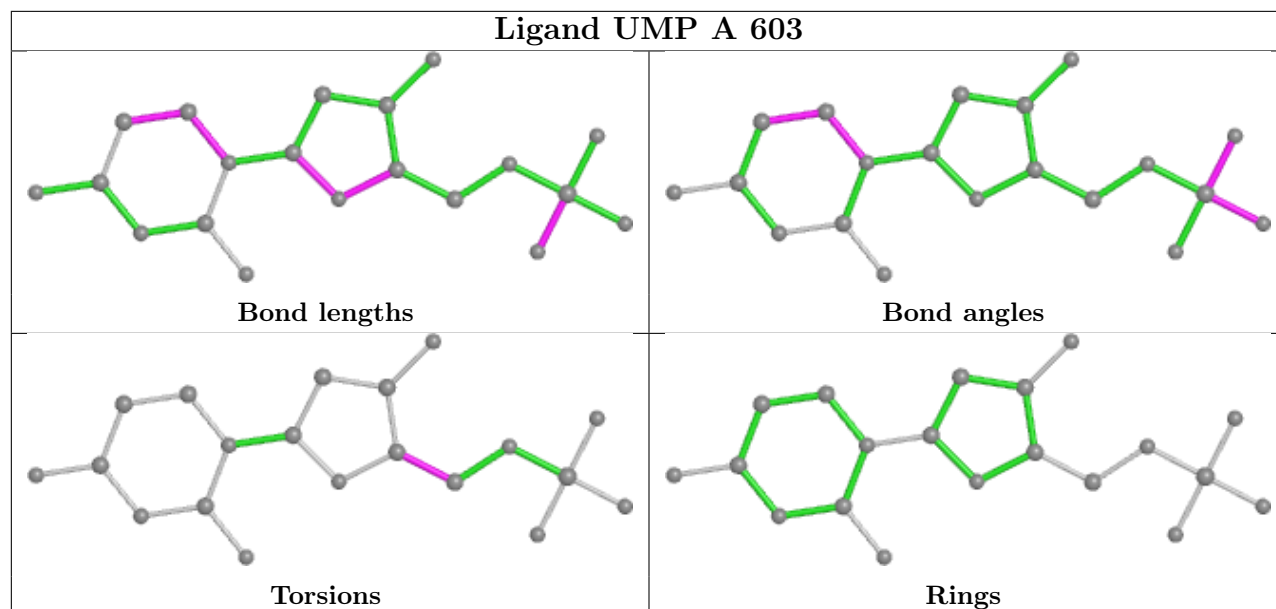


Torsions

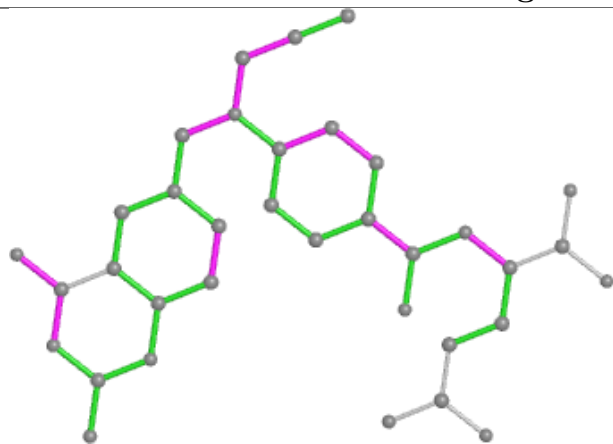


Rings

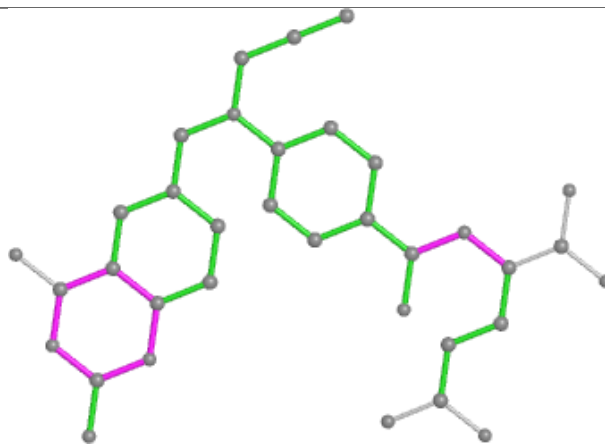




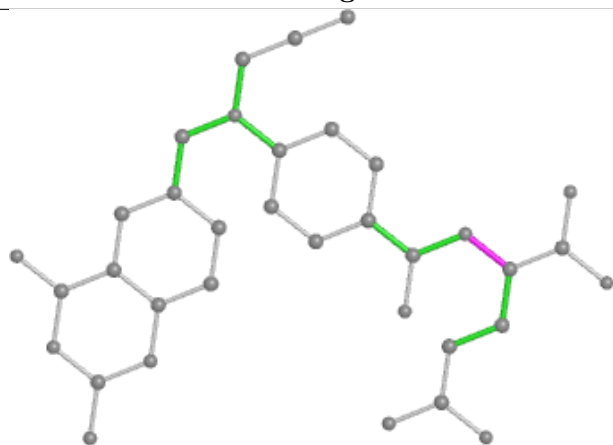
Ligand CB3 C 612



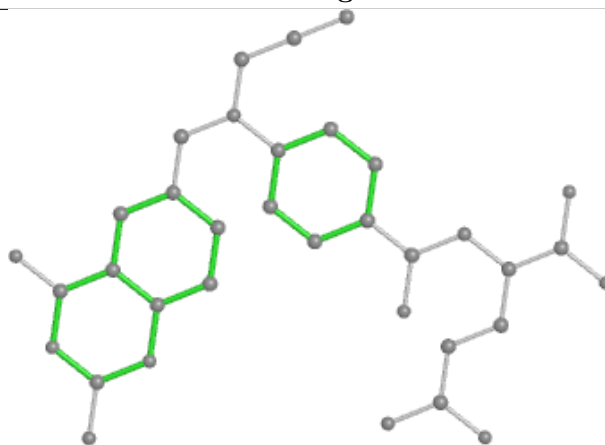
Bond lengths



Bond angles

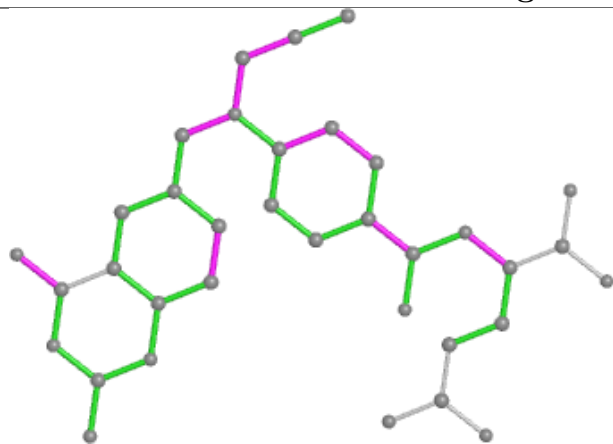


Torsions

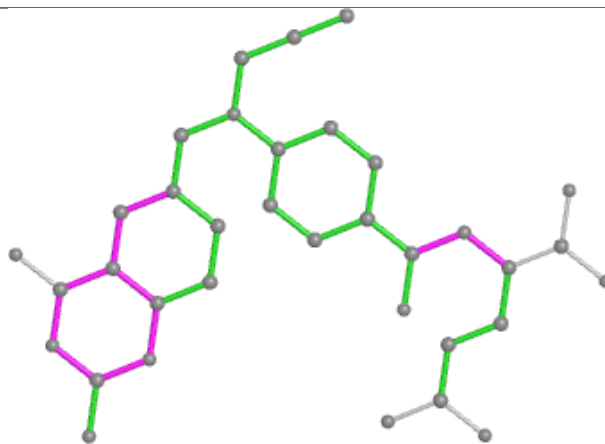


Rings

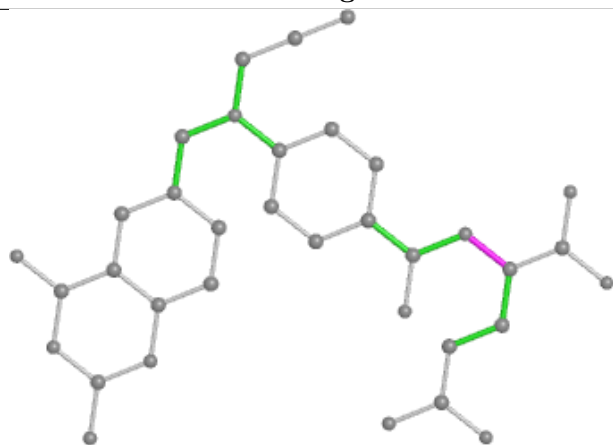
Ligand CB3 B 608



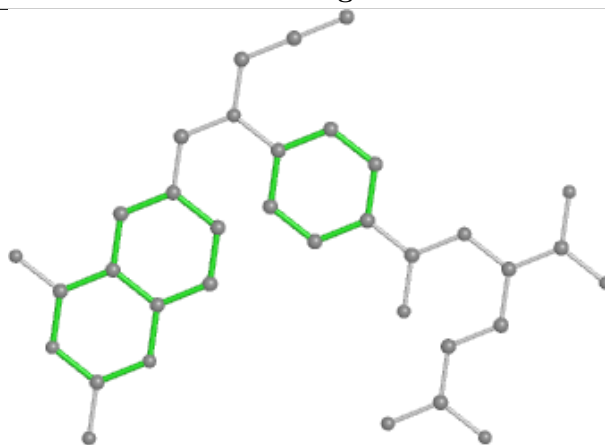
Bond lengths



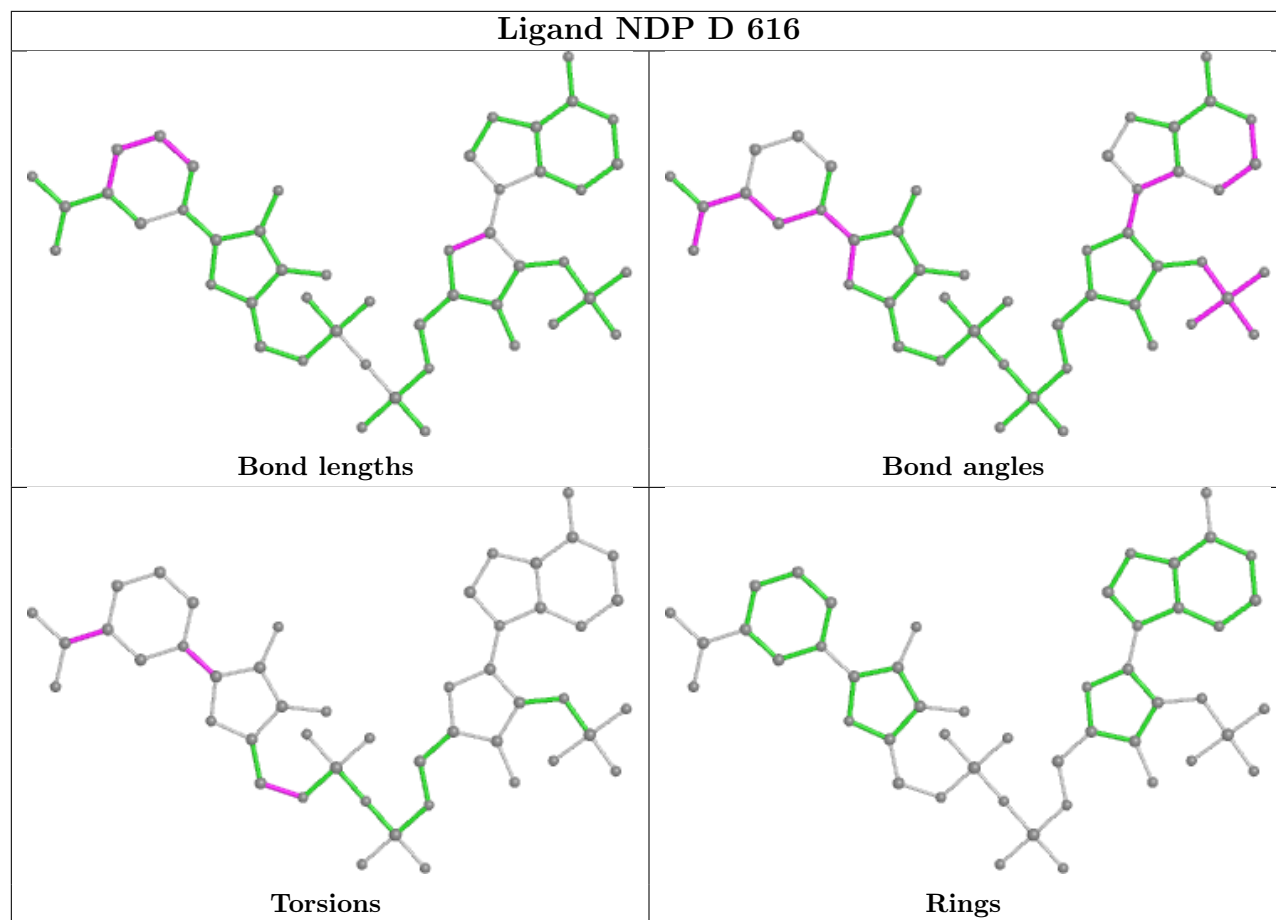
Bond angles

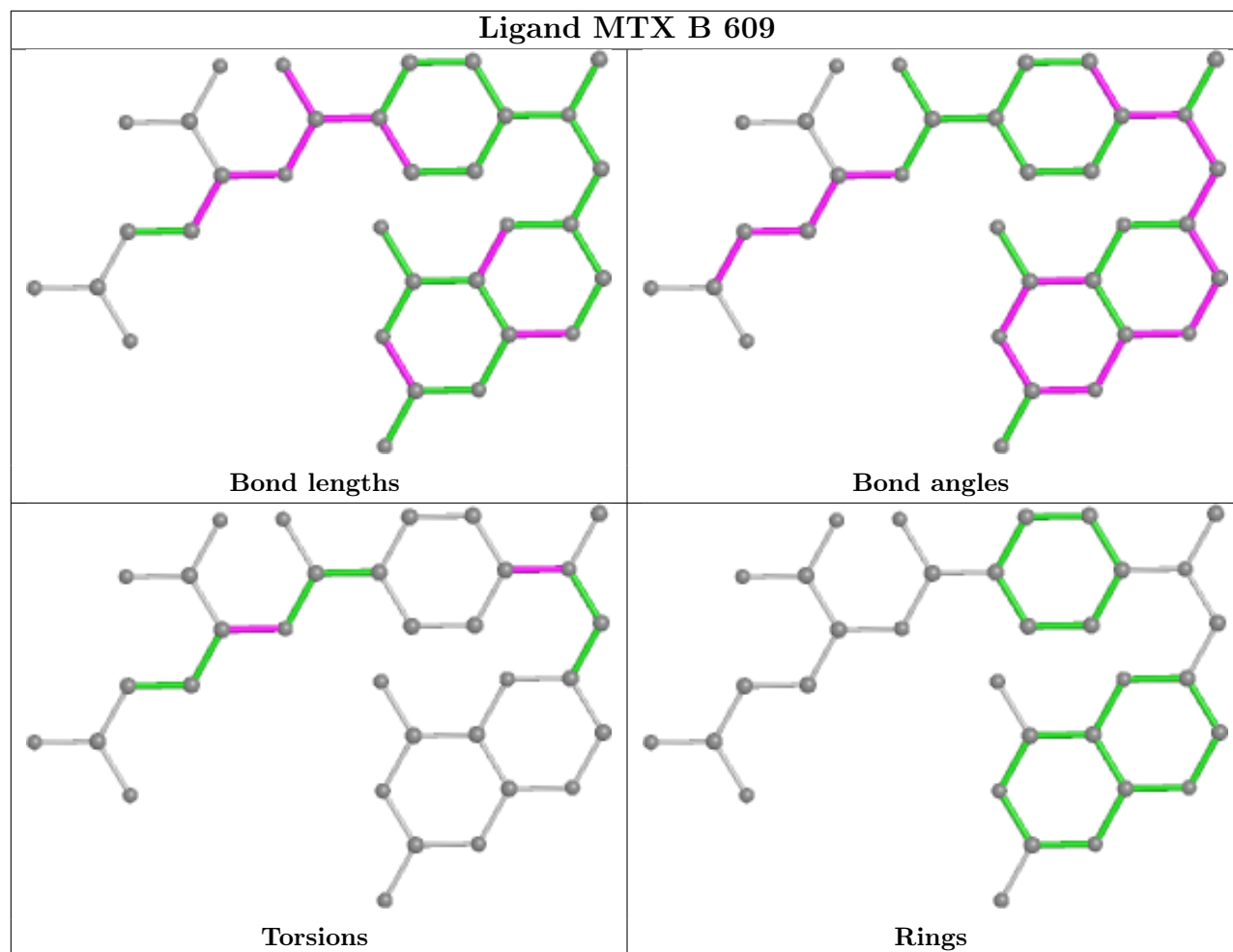


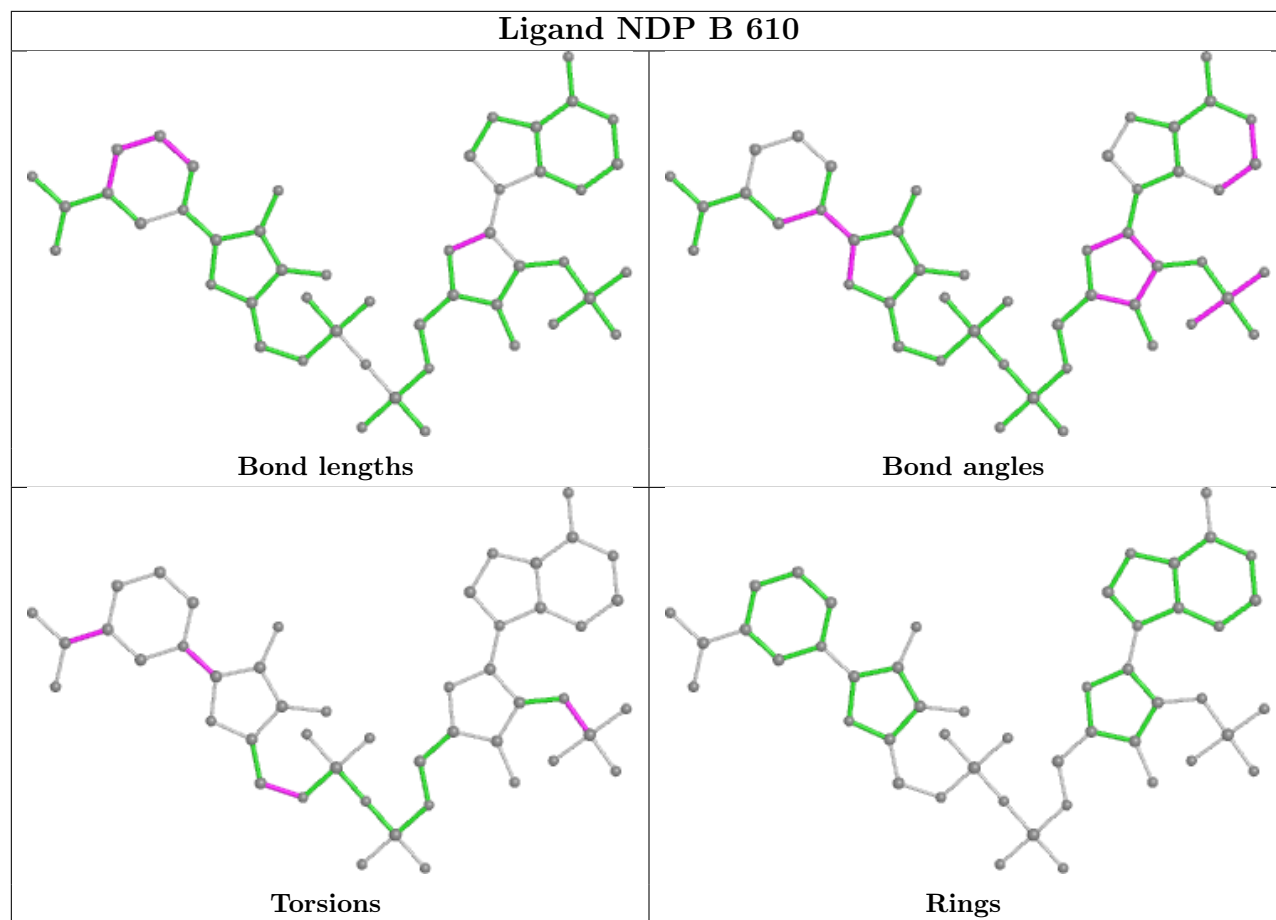
Torsions

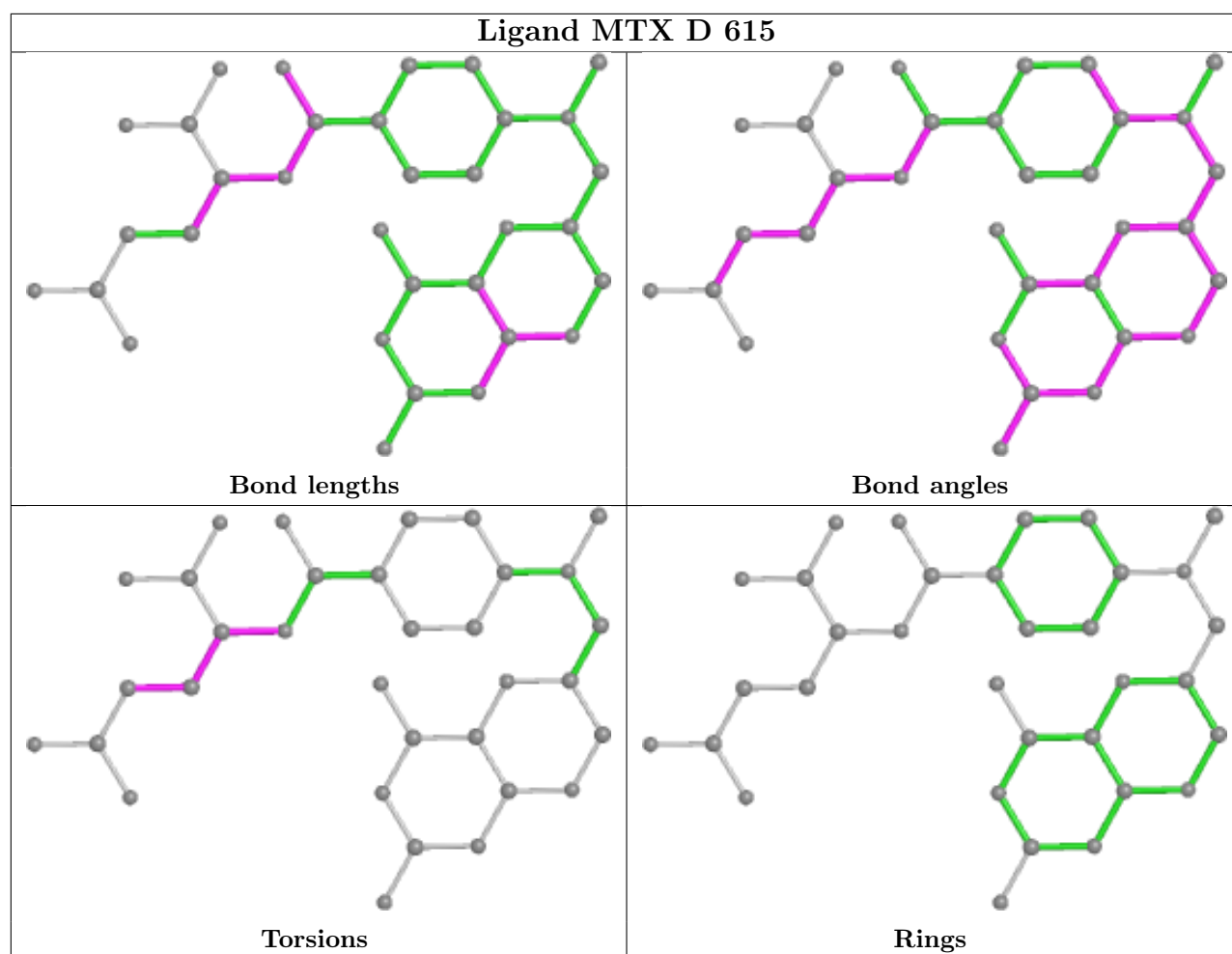


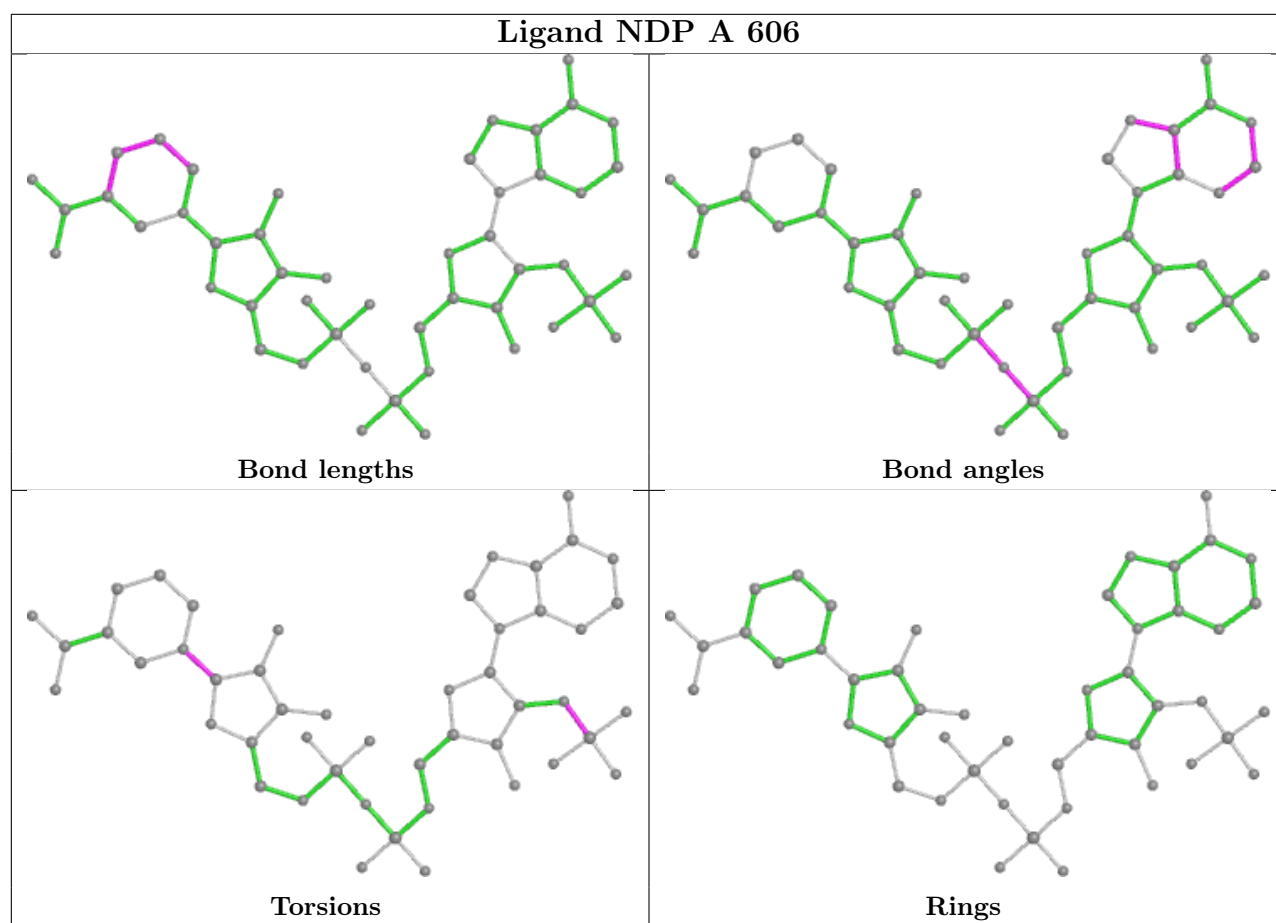
Rings











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	508/521 (97%)	-0.15	15 (2%)	50	51	19, 38, 67, 100	0
1	B	510/521 (97%)	-0.13	15 (2%)	51	52	22, 39, 75, 129	0
1	C	510/521 (97%)	0.37	38 (7%)	14	12	33, 54, 98, 126	0
1	D	505/521 (96%)	0.67	50 (9%)	7	5	41, 73, 101, 126	0
All	All	2033/2084 (97%)	0.19	118 (5%)	23	22	19, 50, 94, 129	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	GLN	9.6
1	B	191	GLY	8.2
1	C	182	THR	7.1
1	D	257	ARG	6.9
1	C	256	ASN	6.8

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](#)

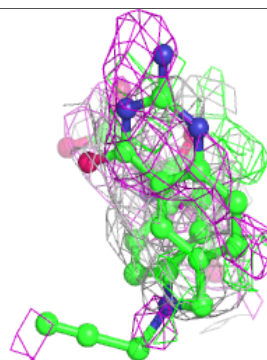
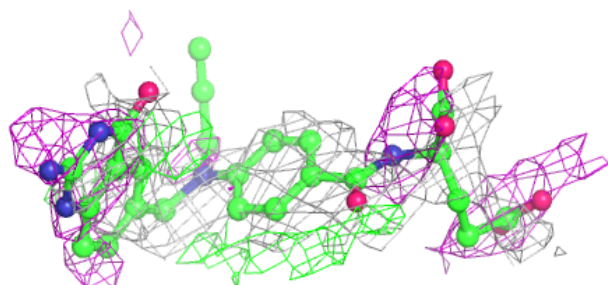
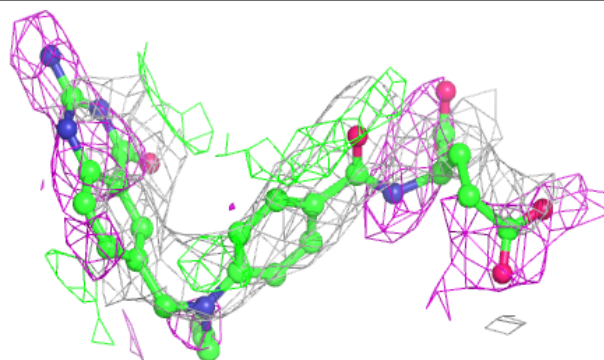
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CB3	C	612	35/35	0.57	0.54	65,69,76,76	0
2	UMP	B	607	20/20	0.65	0.54	52,66,72,72	0
3	CB3	B	608	35/35	0.66	0.43	63,69,76,76	0
3	CB3	A	604	35/35	0.70	0.38	66,71,77,78	0
2	UMP	A	603	20/20	0.76	0.45	55,68,73,73	0
2	UMP	C	611	20/20	0.78	0.36	55,66,73,73	0
4	MTX	D	615	33/33	0.87	0.21	65,70,133,151	0
5	NDP	D	616	48/48	0.88	0.20	54,74,151,159	0
4	MTX	C	613	33/33	0.90	0.19	52,63,100,144	0
5	NDP	C	614	48/48	0.91	0.17	50,74,118,195	0
4	MTX	A	605	33/33	0.94	0.18	28,40,56,79	0
4	MTX	B	609	33/33	0.95	0.14	27,38,51,73	0
5	NDP	A	606	48/48	0.97	0.14	27,38,50,69	0
5	NDP	B	610	48/48	0.98	0.11	24,33,46,49	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.

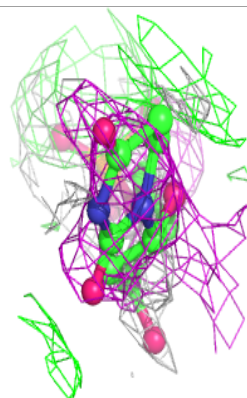
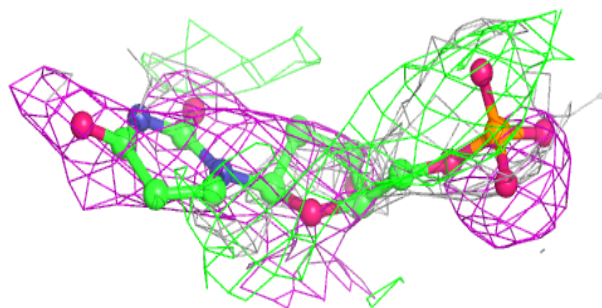
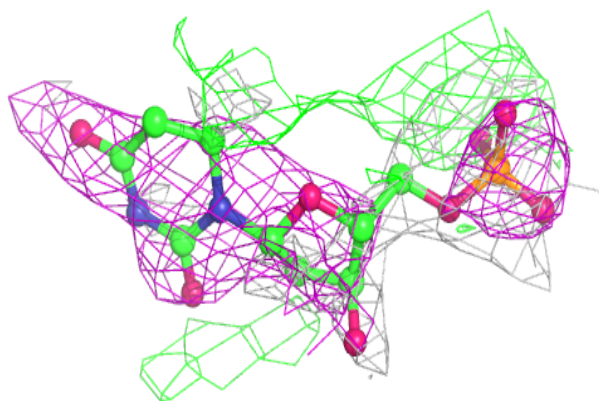
Electron density around CB3 C 612:

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

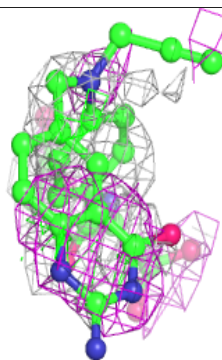
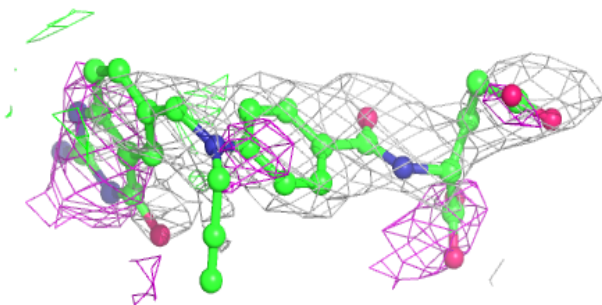
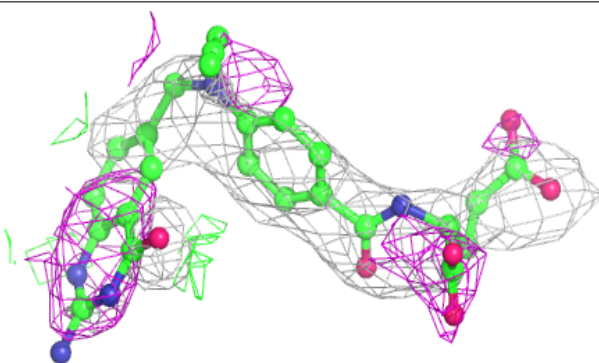


Electron density around UMP B 607:

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

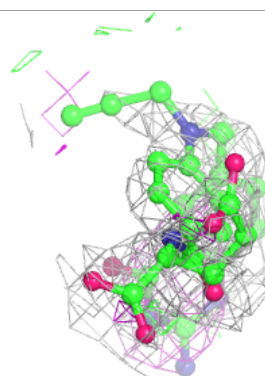
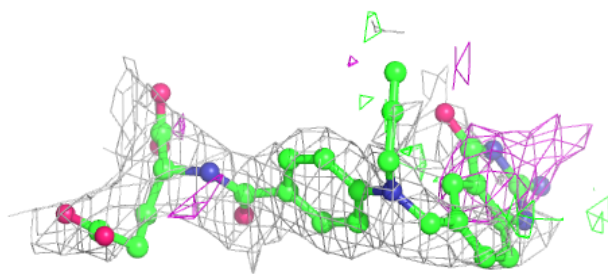
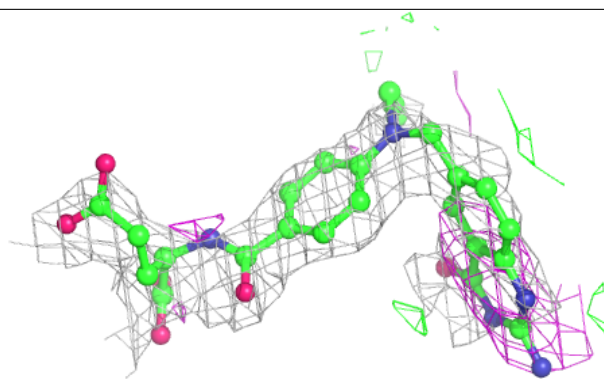
**Electron density around CB3 B 608:**

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

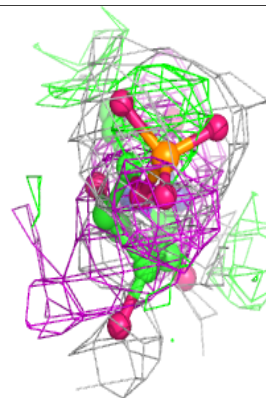
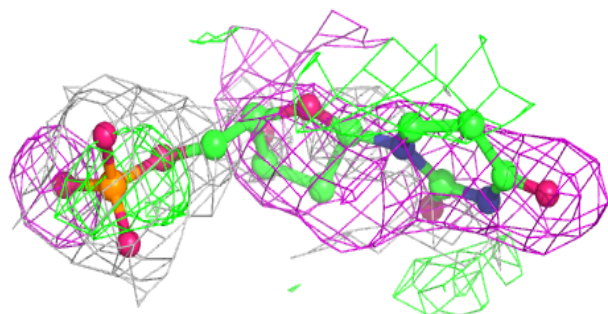
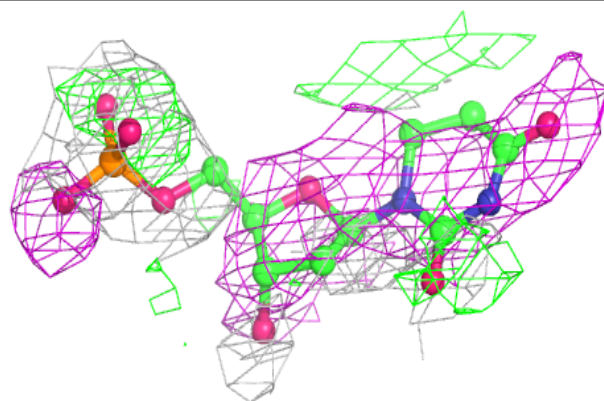


Electron density around CB3 A 604:

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

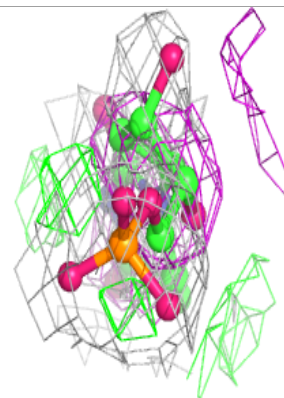
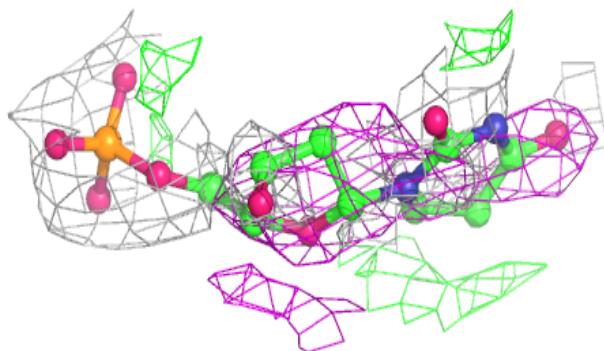
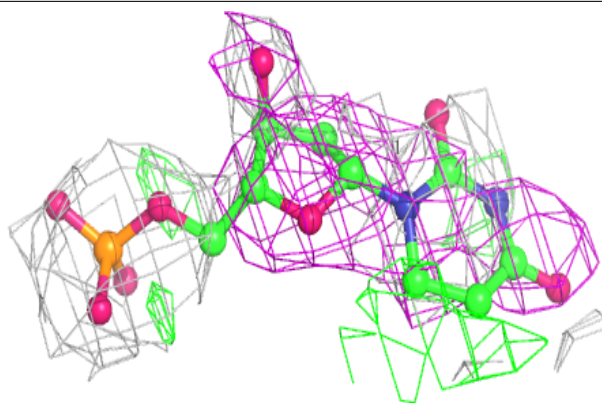
**Electron density around UMP A 603:**

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



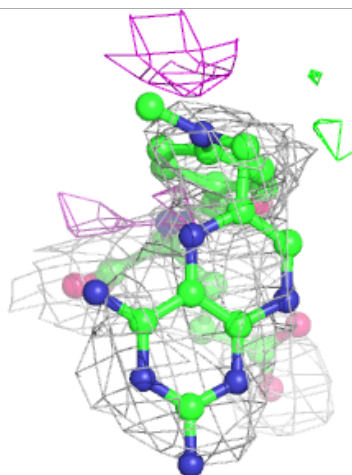
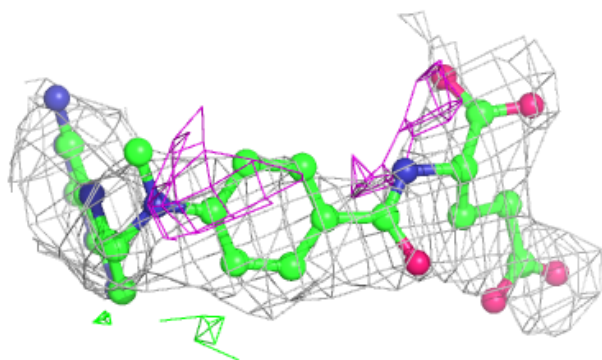
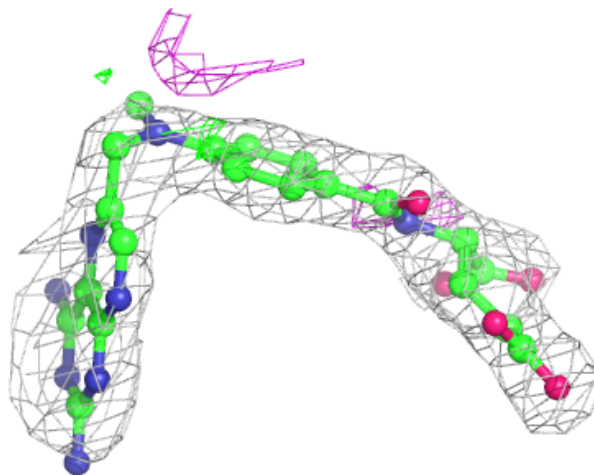
Electron density around UMP C 611:

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



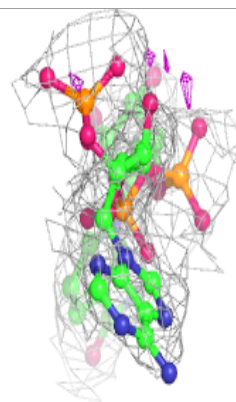
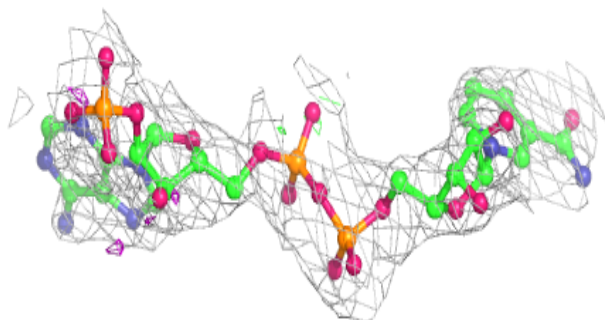
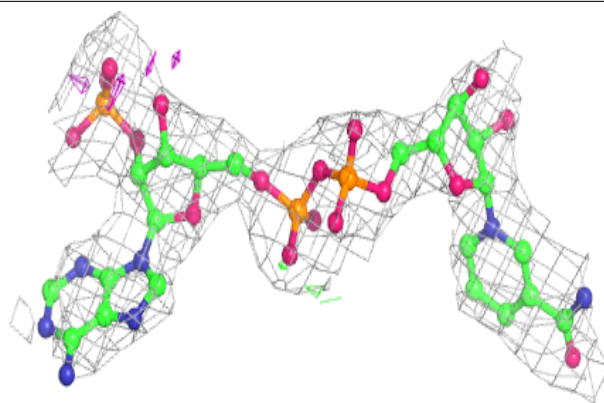
Electron density around MTX D 615:

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

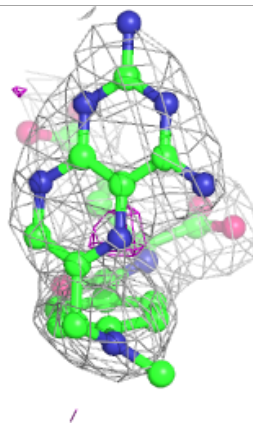
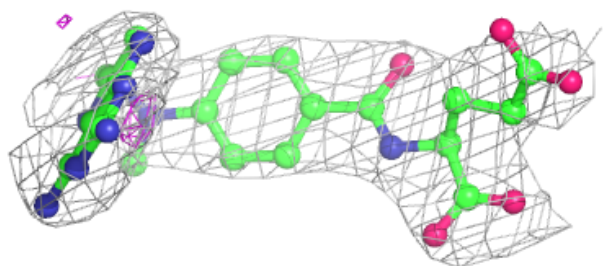
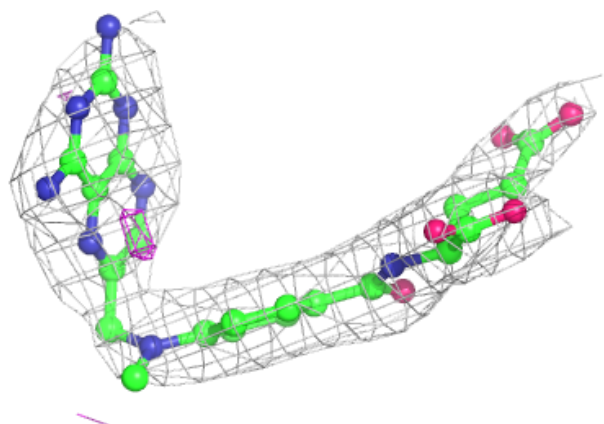


Electron density around NDP D 616:

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

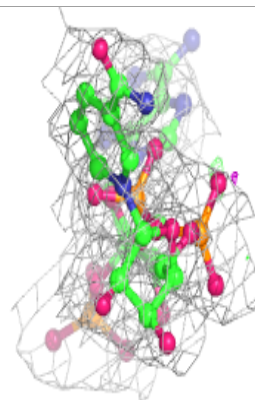
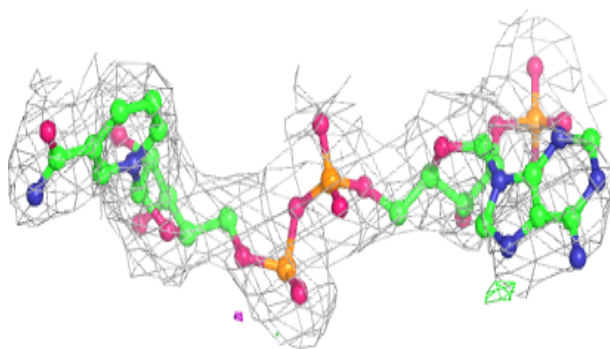
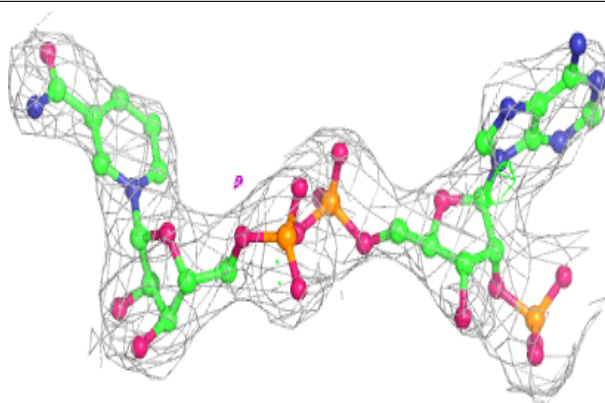
**Electron density around MTX C 613:**

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and green (positive)

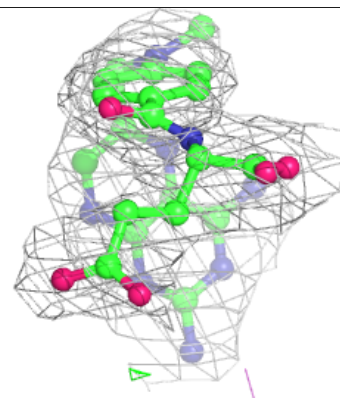
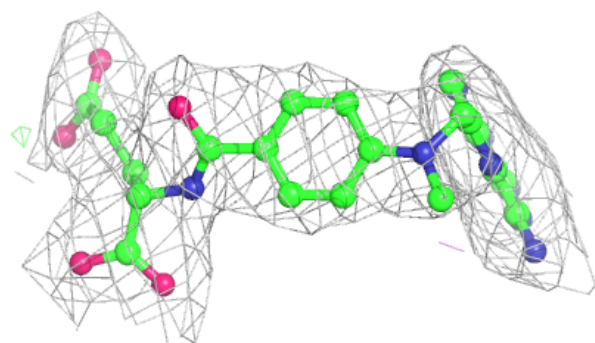
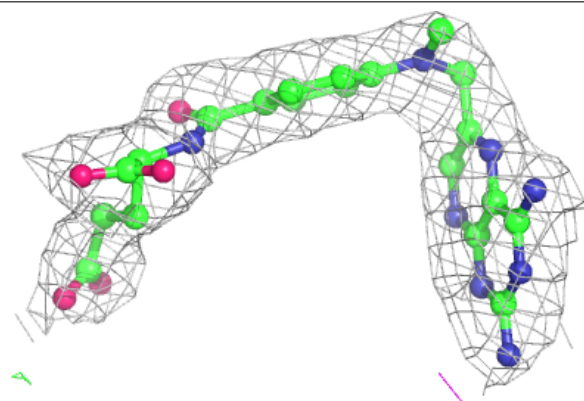


Electron density around NDP C 614:

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

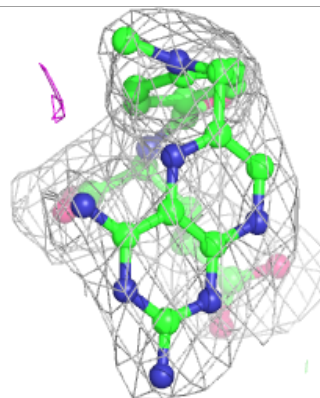
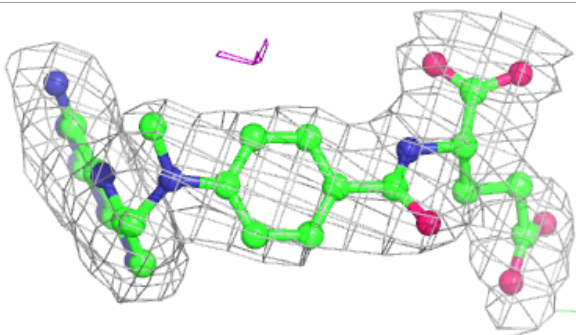
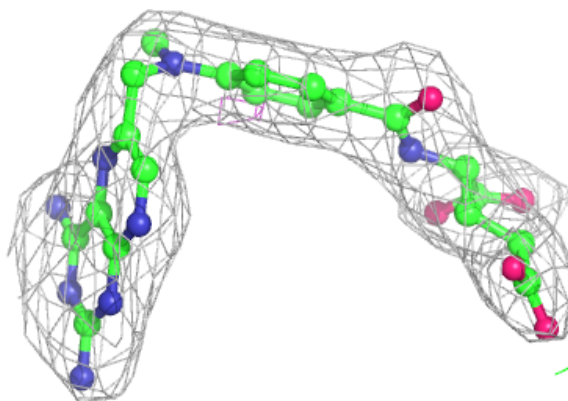
**Electron density around MTX A 605:**

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

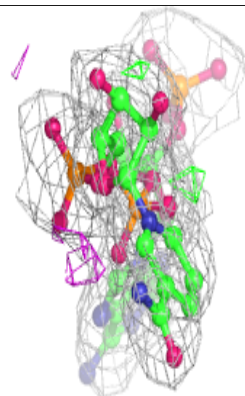
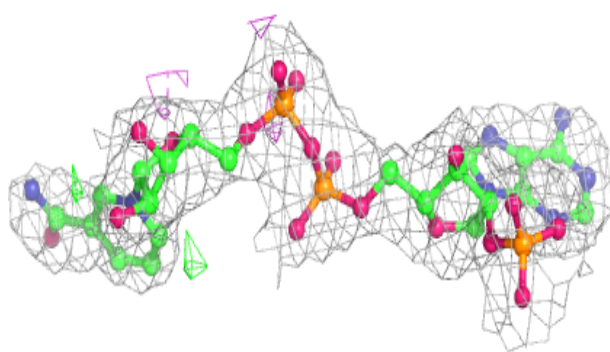
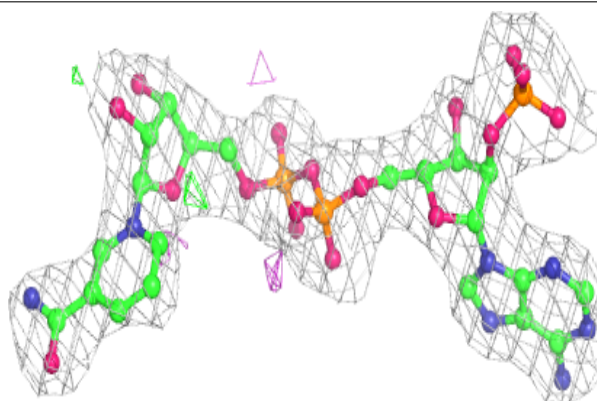


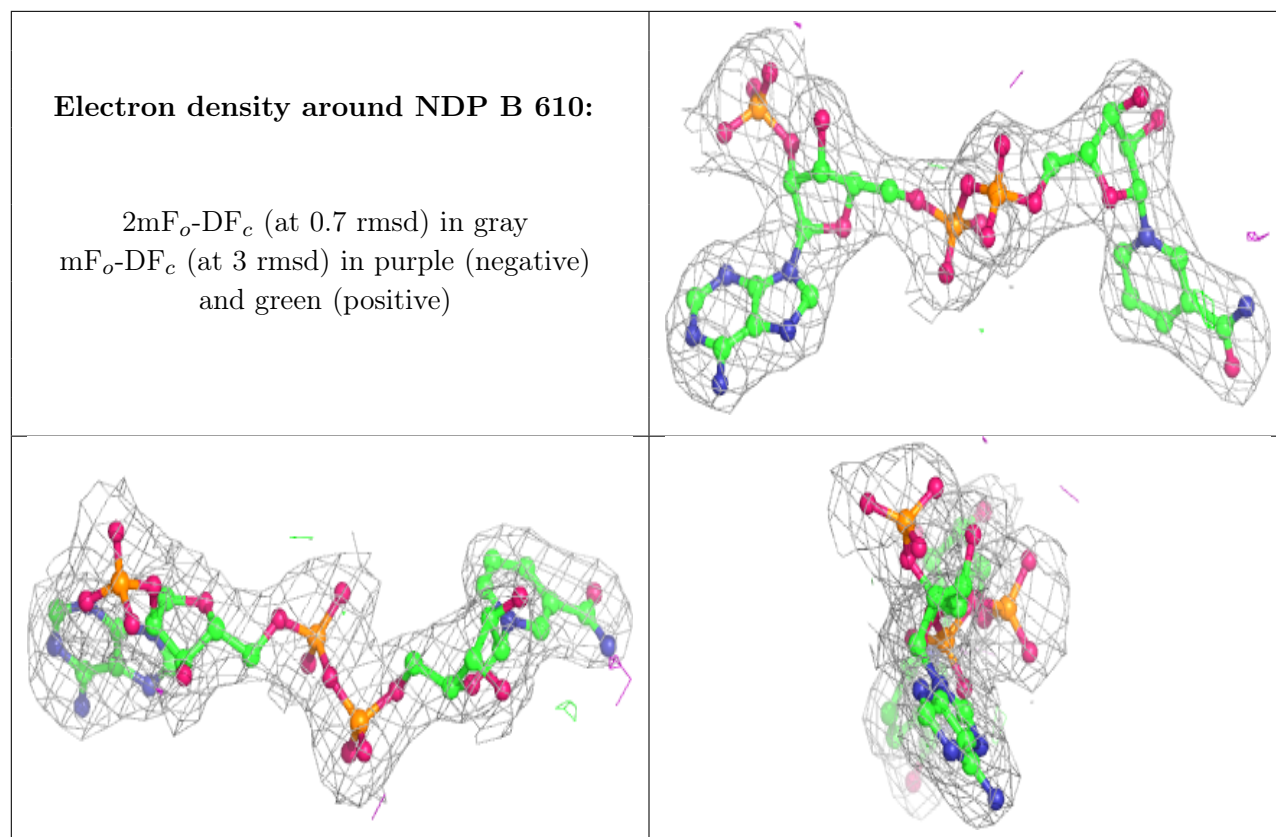
Electron density around MTX B 609:

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

**Electron density around 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.