wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 08:07 AM EDT

PDB ID	:	3DL5
Title	:	Crystal Structure of the A287F Active Site Mutant of TS-DHFR from Cryptosporidium hominis
Authors	:	Vargo, M.A.; Martucci, W.E.; Anderson, K.S.
Deposited on	:	2008-06-26
Resolution	:	2.74 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

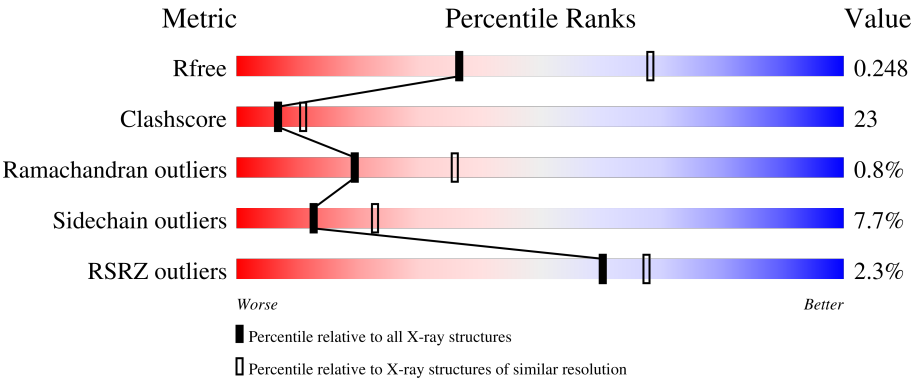
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 <=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	63% 29% 5%
1	B	521	66% 26%
1	C	521	60% 31% 6%
1	D	521	54% 37% 6%
1	E	521	6% 55% 38%

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
3	CB3	D	616	X	-	X	-
3	CB3	E	620	X	-	X	-
4	DHF	A	605	X	-	-	-
4	DHF	B	609	X	-	X	-
4	DHF	C	613	-	-	X	-
4	DHF	D	617	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21793 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.

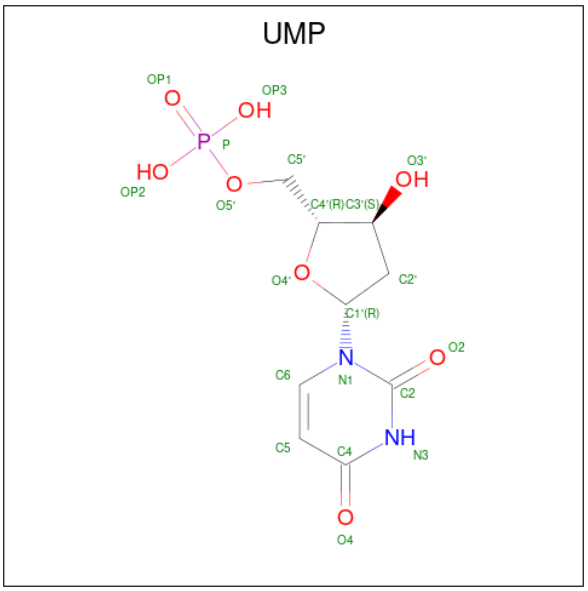
- Molecule 1 is a protein called Dihydrofolate reductase, DHFR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4130	2642	693	773	22			
1	B	508	Total	C	N	O	S	0	0	0
			4143	2650	695	776	22			
1	C	508	Total	C	N	O	S	0	0	0
			4135	2645	694	774	22			
1	D	507	Total	C	N	O	S	0	0	0
			4130	2642	693	773	22			
1	E	508	Total	C	N	O	S	0	0	0
			4135	2645	694	774	22			

There are 5 discrepancies between the modelled and reference sequences:

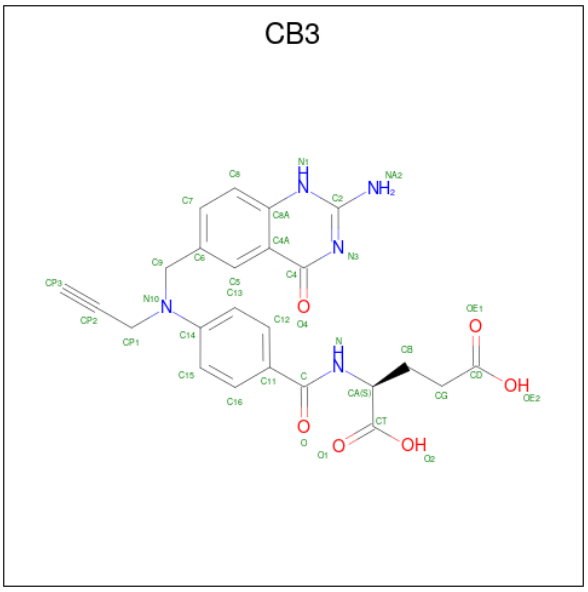
Chain	Residue	Modelled	Actual	Comment	Reference
A	287	PHE	ALA	engineered mutation	UNP Q5CGA3
B	287	PHE	ALA	engineered mutation	UNP Q5CGA3
C	287	PHE	ALA	engineered mutation	UNP Q5CGA3
D	287	PHE	ALA	engineered mutation	UNP Q5CGA3
E	287	PHE	ALA	engineered mutation	UNP Q5CGA3

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



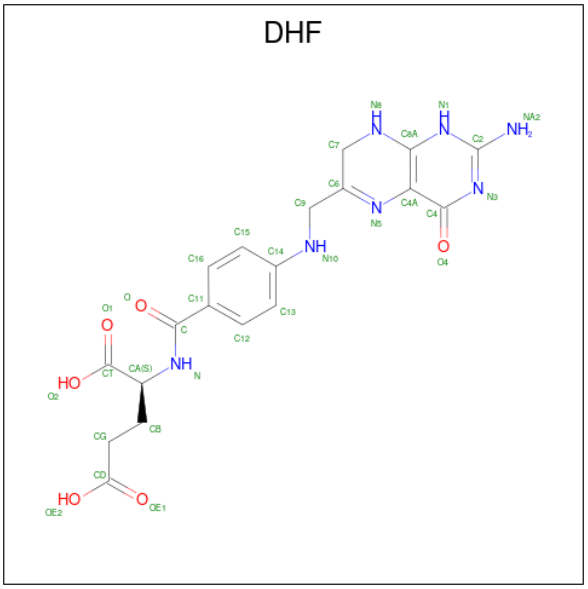
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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



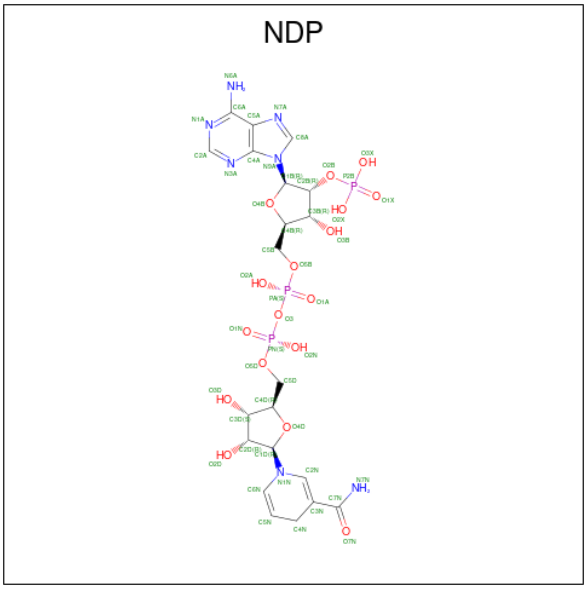
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 35 24 5 6	0	0
3	B	1	Total C N O 35 24 5 6	0	0
3	C	1	Total C N O 35 24 5 6	0	0
3	D	1	Total C N O 35 24 5 6	0	0
3	E	1	Total C N O 35 24 5 6	0	0

- Molecule 4 is DIHYDROFOLIC ACID (three-letter code: DHF) (formula: $C_{19}H_{21}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	19	7	6		
4	B	1	Total	C	N	O	0	0
			32	19	7	6		
4	C	1	Total	C	N	O	0	0
			32	19	7	6		
4	D	1	Total	C	N	O	0	0
			32	19	7	6		
4	E	1	Total	C	N	O	0	0
			32	19	7	6		

- 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		
5	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is water.

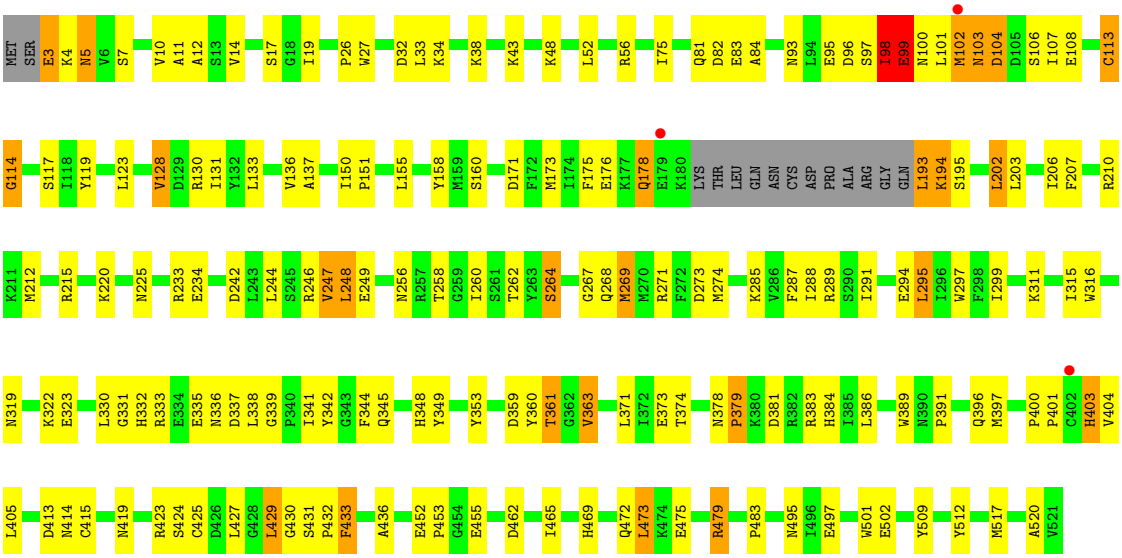
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	114	Total O 114 114	0	0
6	B	150	Total O 150 150	0	0
6	C	95	Total O 95 95	0	0
6	D	62	Total O 62 62	0	0
6	E	24	Total O 24 24	0	0

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.

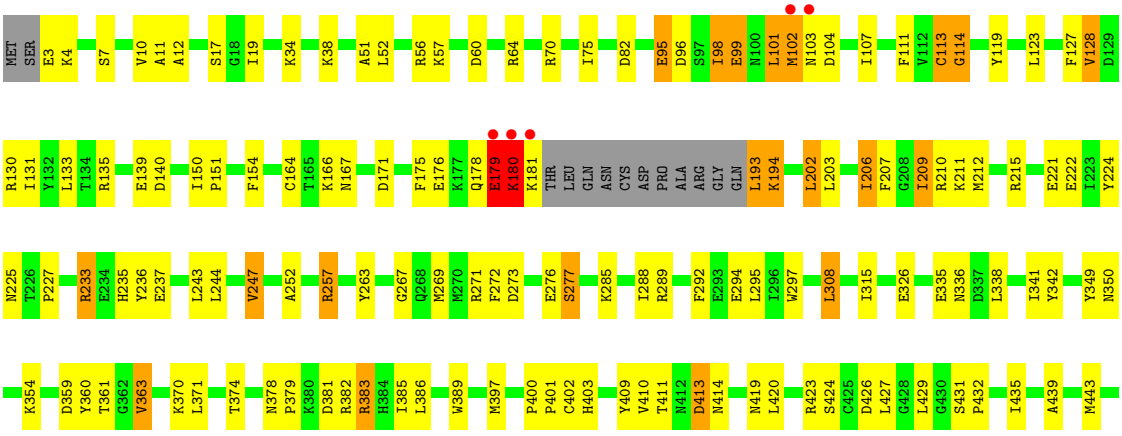
• Molecule 1: Dihydrofolate reductase, DHFR

Chain A:



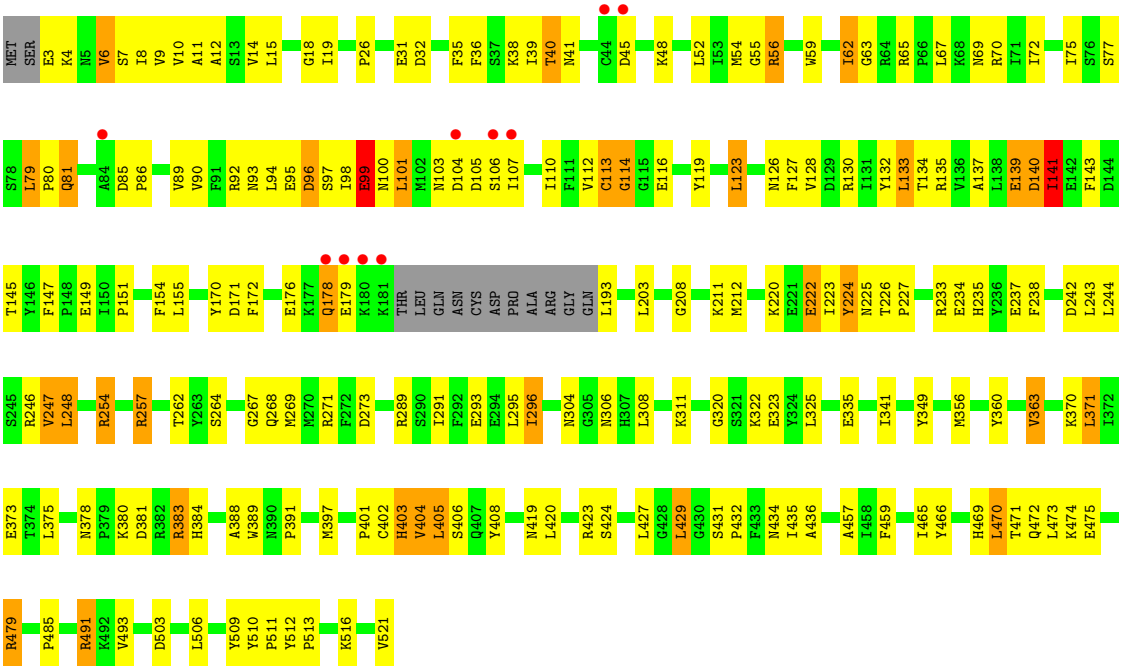
• Molecule 1: Dihydrofolate reductase, DHFR

Chain B:



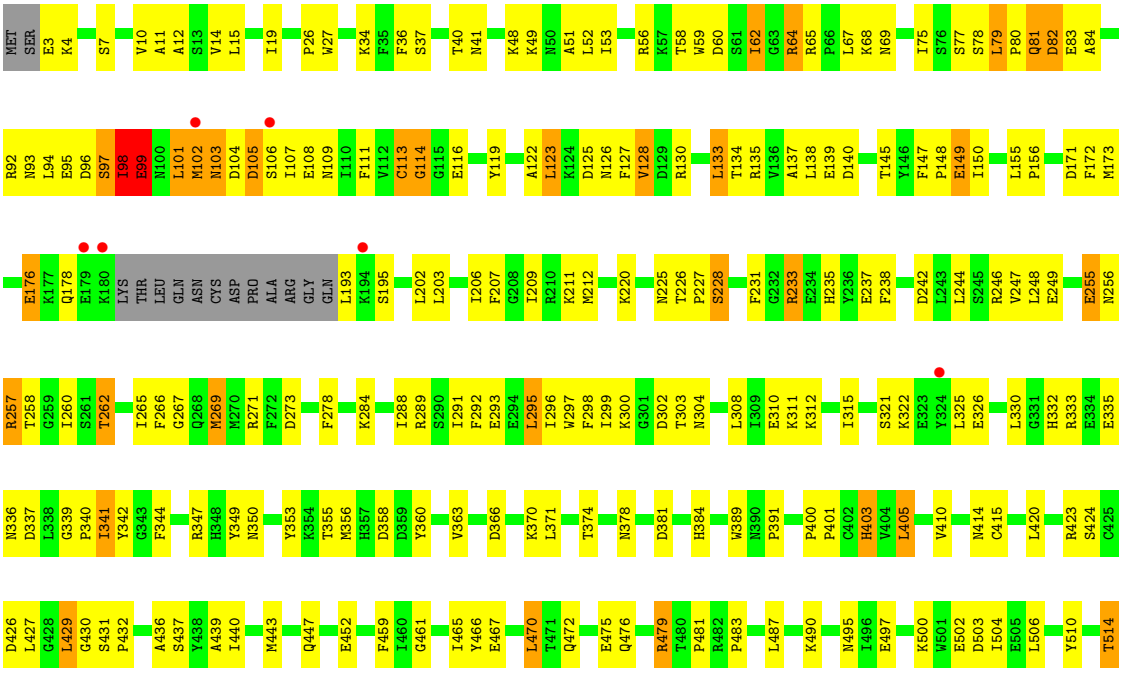
• Molecule 1: Dihydrofolate reductase, DHFR

Chain C:



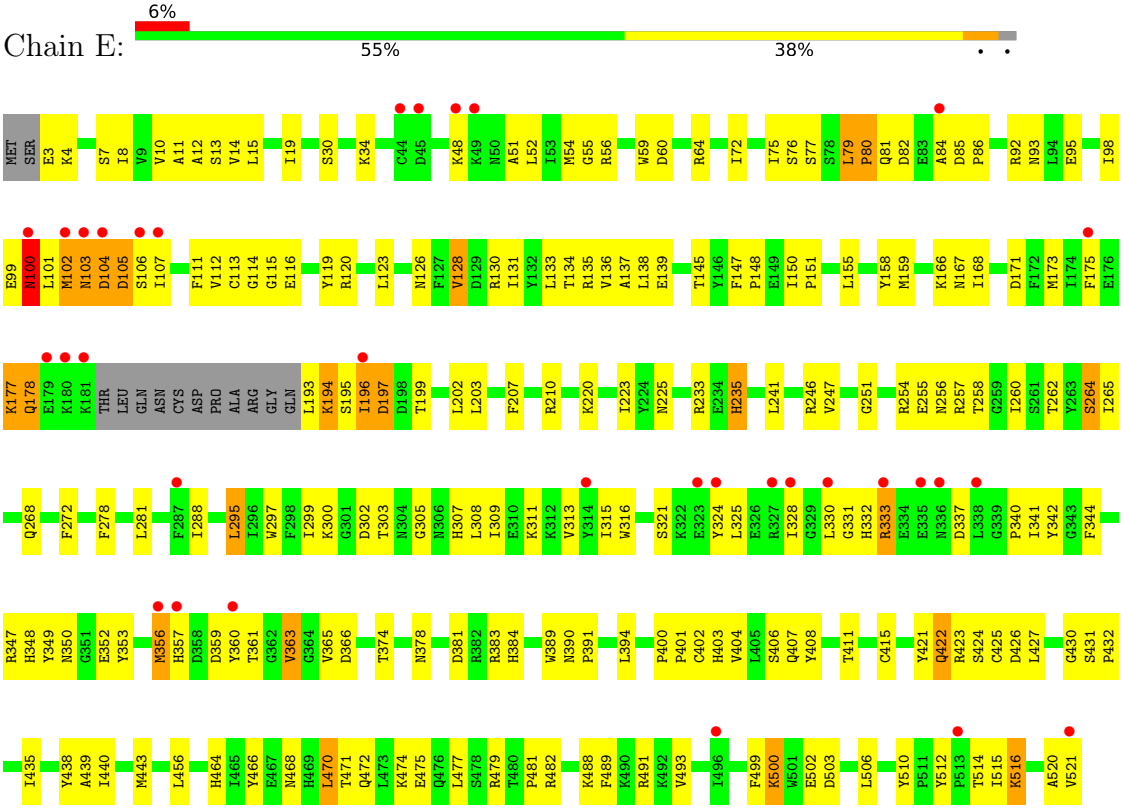
• Molecule 1: Dihydrofolate reductase, DHFR

Chain D:



• Molecule 1: Dihydrofolate reductase, DHFR

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	214.81Å 116.54Å 219.21Å 90.00° 95.21° 90.00°	Depositor
Resolution (Å)	45.40 – 2.74 45.48 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.40-2.74) 99.4 (45.48-2.72)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.245 0.218 , 0.248	Depositor DCC
R_{free} test set	7223 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21793	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.38	0/4226	0.65	0/5711
1	B	0.41	0/4239	0.67	0/5727
1	C	0.36	0/4231	0.62	0/5718
1	D	0.36	0/4226	0.61	0/5711
1	E	0.34	0/4231	0.62	1/5718 (0.0%)
All	All	0.37	0/21153	0.63	1/28585 (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	6
1	B	0	4
1	C	0	5
1	D	0	6
1	E	0	2
All	All	0	23

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	357	HIS	CB-CA-C	-5.04	100.33	110.40

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	206	ILE	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	4130	0	4057	164	0
1	B	4143	0	4074	160	0
1	C	4135	0	4059	193	1
1	D	4130	0	4057	231	0
1	E	4135	0	4059	224	2
2	A	20	0	11	4	0
2	B	20	0	11	3	0
2	C	20	0	11	3	0
2	D	20	0	11	4	0
2	E	20	0	11	6	0
3	A	35	0	21	4	0
3	B	35	0	21	3	0
3	C	35	0	21	2	0
3	D	35	0	21	9	0
3	E	35	0	21	13	0
4	A	32	0	19	6	0
4	B	32	0	19	10	0
4	C	32	0	19	9	0
4	D	32	0	19	9	0
4	E	32	0	19	5	0
5	A	48	0	26	7	0
5	B	48	0	26	8	0
5	C	48	0	26	11	0
5	D	48	0	26	5	0
5	E	48	0	26	12	0
6	A	114	0	0	18	0
6	B	150	0	0	7	0
6	C	95	0	0	9	0
6	D	62	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	24	0	0	5	0
All	All	21793	0	20691	976	2

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 23.

The worst 5 of 976 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:D:104:ASP:O	1:D:106:SER:N	1.63	1.26
1:B:179:GLU:C	1:B:180:LYS:HG3	1.52	1.23
1:E:79:LEU:HD23	1:E:80:PRO:CD	1.68	1.21
1:E:79:LEU:CD2	1:E:80:PRO:HD2	1.71	1.18
1:E:178:GLN:OE1	1:E:178:GLN:HA	1.43	1.16

All (2) 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:C:65:ARG:NH2	1:E:251:GLY:O[2_466]	2.11	0.09
1:E:407:GLN:OE1	1:E:421:TYR:OH[2_457]	2.19	0.01

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	503/521 (96%)	476 (95%)	23 (5%)	4 (1%)	19	36
1	B	504/521 (97%)	477 (95%)	23 (5%)	4 (1%)	19	36
1	C	504/521 (97%)	473 (94%)	28 (6%)	3 (1%)	25	44
1	D	503/521 (96%)	469 (93%)	30 (6%)	4 (1%)	19	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	504/521 (97%)	460 (91%)	38 (8%)	6 (1%)	13 24
All	All	2518/2605 (97%)	2355 (94%)	142 (6%)	21 (1%)	19 36

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	LYS
1	C	99	GLU
1	D	105	ASP
1	E	103	ASN
1	A	99	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	457/471 (97%)	427 (93%)	30 (7%)	16 29
1	B	459/471 (98%)	425 (93%)	34 (7%)	13 24
1	C	457/471 (97%)	413 (90%)	44 (10%)	8 15
1	D	457/471 (97%)	415 (91%)	42 (9%)	9 17
1	E	457/471 (97%)	432 (94%)	25 (6%)	21 37
All	All	2287/2355 (97%)	2112 (92%)	175 (8%)	13 23

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	97	SER
1	D	437	SER
1	D	102	MET
1	D	255	GLU
1	E	79	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	109	ASN
1	D	384	HIS
1	E	348	HIS
1	E	178	GLN
1	B	100	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	DHF	D	617	-	29,34,34	0.92	0	35,47,47	1.78	6 (17%)
2	UMP	D	615	-	21,21,21	2.33	3 (14%)	31,31,31	2.27	8 (25%)
3	CB3	B	608	-	36,37,37	1.29	2 (5%)	46,51,51	2.12	9 (19%)
5	NDP	C	614	-	45,52,52	1.39	3 (6%)	53,80,80	1.12	2 (3%)
3	CB3	C	612	-	36,37,37	1.30	3 (8%)	46,51,51	2.19	9 (19%)
4	DHF	A	605	-	29,34,34	0.89	1 (3%)	35,47,47	1.83	9 (25%)
5	NDP	D	618	-	45,52,52	1.40	3 (6%)	53,80,80	1.13	3 (5%)
5	NDP	E	622	-	45,52,52	1.39	3 (6%)	53,80,80	1.22	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DHF	C	613	-	29,34,34	0.88	0	35,47,47	1.90	7 (20%)
2	UMP	E	619	-	21,21,21	2.34	3 (14%)	31,31,31	2.28	8 (25%)
5	NDP	B	610	-	45,52,52	1.39	5 (11%)	53,80,80	1.20	4 (7%)
4	DHF	E	621	-	29,34,34	0.81	0	35,47,47	1.72	7 (20%)
3	CB3	D	616	-	36,37,37	1.23	2 (5%)	46,51,51	2.08	9 (19%)
3	CB3	E	620	-	36,37,37	1.26	2 (5%)	46,51,51	2.02	10 (21%)
2	UMP	A	603	-	21,21,21	2.31	3 (14%)	31,31,31	2.27	9 (29%)
2	UMP	C	611	-	21,21,21	2.32	3 (14%)	31,31,31	2.28	9 (29%)
3	CB3	A	604	-	36,37,37	1.26	2 (5%)	46,51,51	1.99	8 (17%)
4	DHF	B	609	-	29,34,34	0.93	1 (3%)	35,47,47	1.75	7 (20%)
5	NDP	A	606	-	45,52,52	1.41	5 (11%)	53,80,80	1.10	3 (5%)
2	UMP	B	607	-	21,21,21	2.33	3 (14%)	31,31,31	2.26	8 (25%)

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	DHF	D	617	-	-	2/20/31/31	0/3/3/3
2	UMP	D	615	-	-	4/10/22/22	0/2/2/2
3	CB3	B	608	-	-	6/27/28/28	0/3/3/3
5	NDP	C	614	-	-	6/30/77/77	0/5/5/5
3	CB3	C	612	-	-	4/27/28/28	0/3/3/3
4	DHF	A	605	-	1/1/5/8	5/20/31/31	0/3/3/3
5	NDP	D	618	-	-	2/30/77/77	0/5/5/5
5	NDP	E	622	-	-	5/30/77/77	0/5/5/5
4	DHF	C	613	-	-	4/20/31/31	0/3/3/3
2	UMP	E	619	-	-	4/10/22/22	0/2/2/2
5	NDP	B	610	-	-	4/30/77/77	0/5/5/5
4	DHF	E	621	-	-	2/20/31/31	0/3/3/3
3	CB3	D	616	-	1/1/5/6	5/27/28/28	0/3/3/3
3	CB3	E	620	-	1/1/5/6	6/27/28/28	0/3/3/3
2	UMP	A	603	-	-	1/10/22/22	0/2/2/2
2	UMP	C	611	-	-	2/10/22/22	0/2/2/2
3	CB3	A	604	-	-	6/27/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DHF	B	609	-	1/1/5/8	5/20/31/31	0/3/3/3
5	NDP	A	606	-	-	3/30/77/77	0/5/5/5
2	UMP	B	607	-	-	3/10/22/22	0/2/2/2

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	C6-C5	7.90	1.53	1.35
2	B	607	UMP	C6-C5	7.90	1.53	1.35
2	D	615	UMP	C6-C5	7.89	1.53	1.35
2	A	603	UMP	C6-C5	7.85	1.53	1.35
2	C	611	UMP	C6-C5	7.85	1.53	1.35

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	608	CB3	C4A-C8A-N1	-7.92	119.30	123.60
3	A	604	CB3	C4A-C8A-N1	-7.62	119.46	123.60
3	B	608	CB3	C4A-C4-N3	-7.53	119.16	124.40
3	D	616	CB3	C4A-C4-N3	-7.45	119.20	124.40
3	E	620	CB3	C4A-C4-N3	-7.36	119.27	124.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	616	CB3	CA
3	E	620	CB3	CA
4	A	605	DHF	CA
4	B	609	DHF	CA

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	607	UMP	C5'-O5'-P-OP2
2	B	607	UMP	C5'-O5'-P-OP3
2	D	615	UMP	C5'-O5'-P-OP1
2	D	615	UMP	C5'-O5'-P-OP2
2	D	615	UMP	C5'-O5'-P-OP3

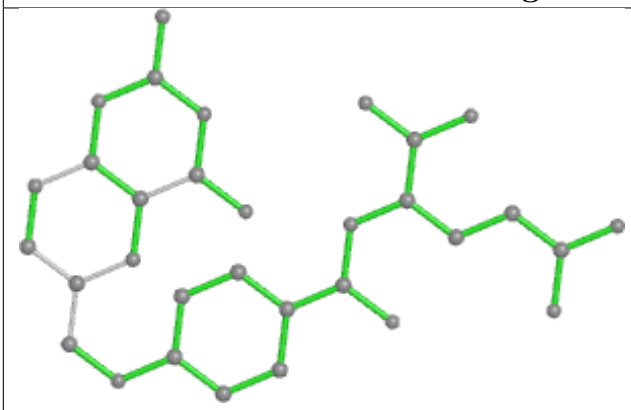
There are no ring outliers.

20 monomers are involved in 115 short contacts:

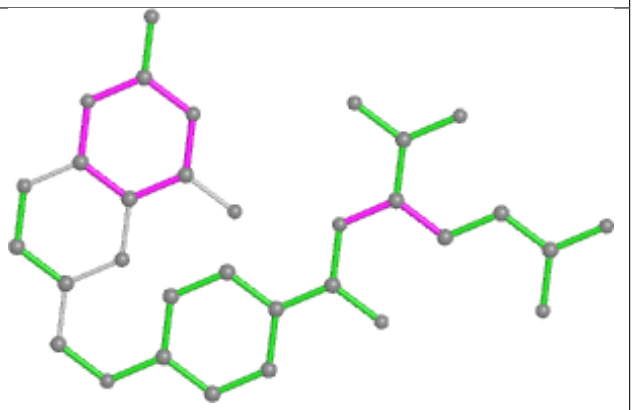
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	617	DHF	9	0
2	D	615	UMP	4	0
3	B	608	CB3	3	0
5	C	614	NDP	11	0
3	C	612	CB3	2	0
4	A	605	DHF	6	0
5	D	618	NDP	5	0
5	E	622	NDP	12	0
4	C	613	DHF	9	0
2	E	619	UMP	6	0
5	B	610	NDP	8	0
4	E	621	DHF	5	0
3	D	616	CB3	9	0
3	E	620	CB3	13	0
2	A	603	UMP	4	0
2	C	611	UMP	3	0
3	A	604	CB3	4	0
4	B	609	DHF	10	0
5	A	606	NDP	7	0
2	B	607	UMP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

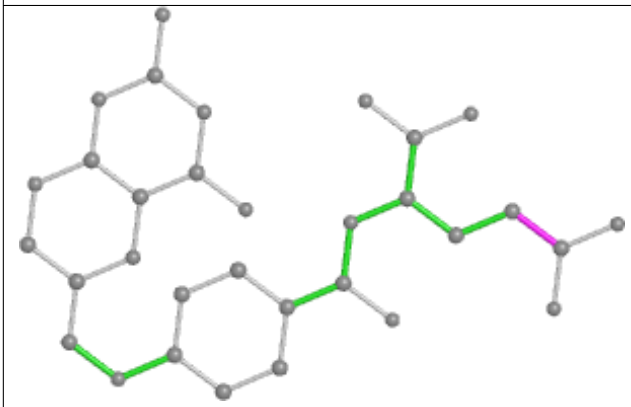
Ligand DHF D 617



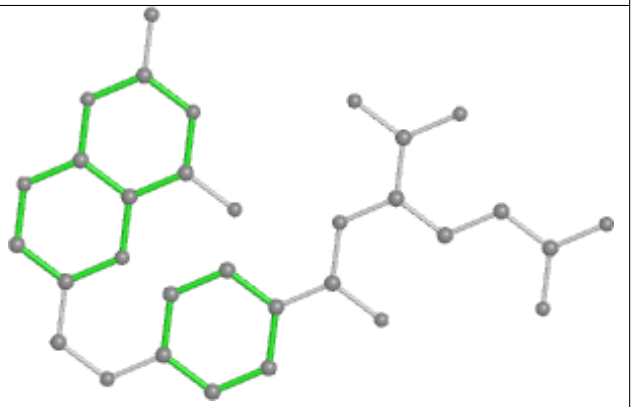
Bond lengths



Bond angles

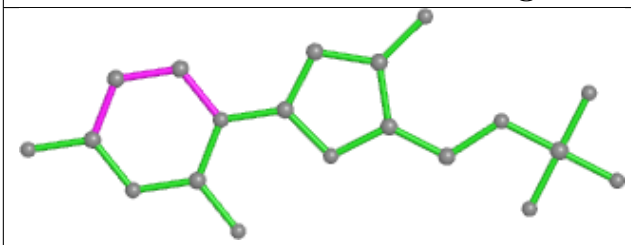


Torsions



Rings

Ligand UMP D 615



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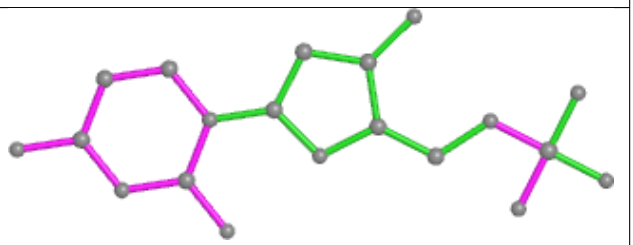
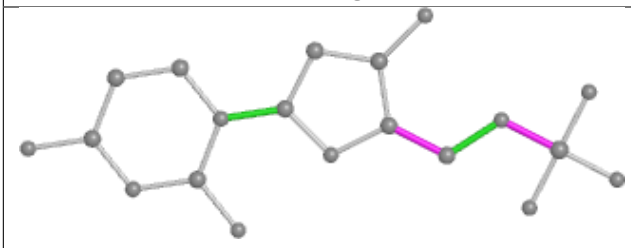


Bond angles



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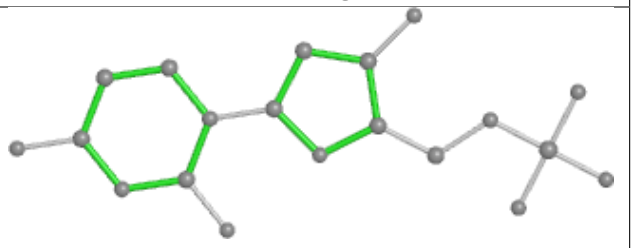
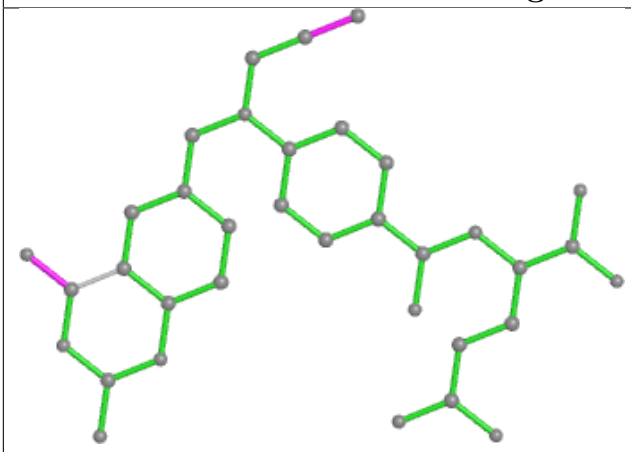


Rings

Ligand CB3 B 608



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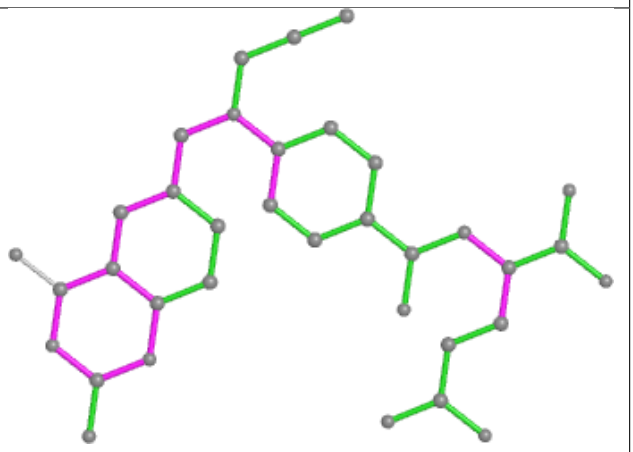

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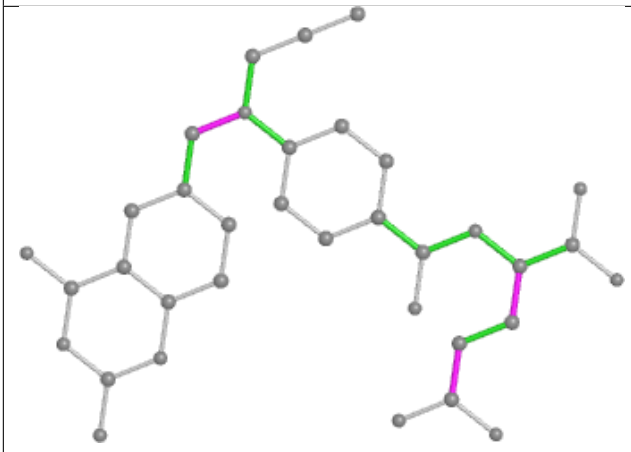

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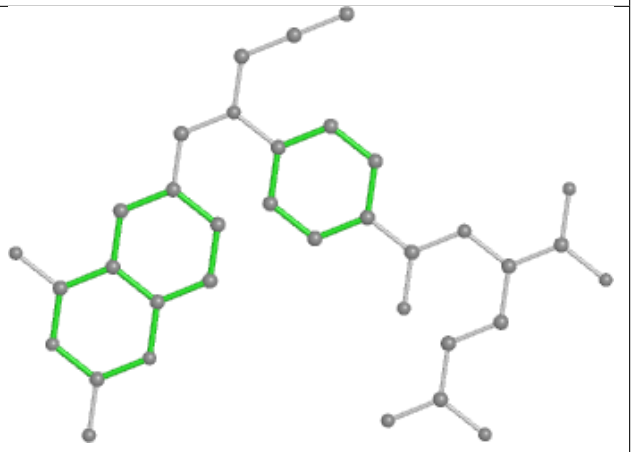
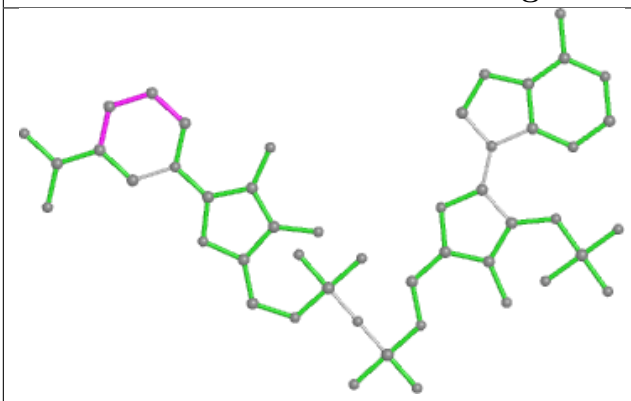
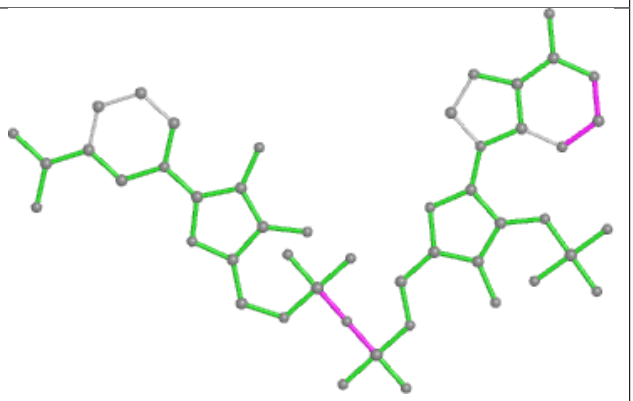


Rings

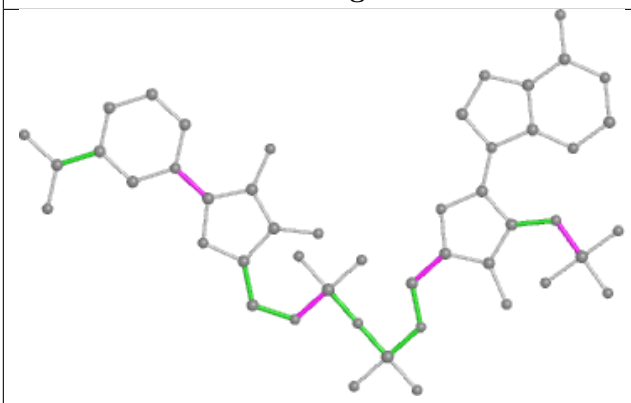
Ligand NDP C 614



Bond lengths



Bond angles



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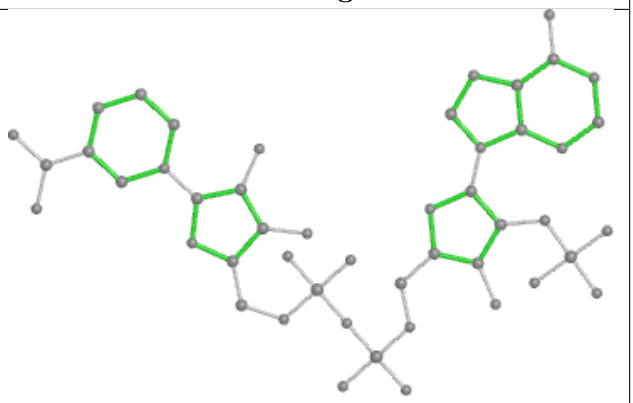
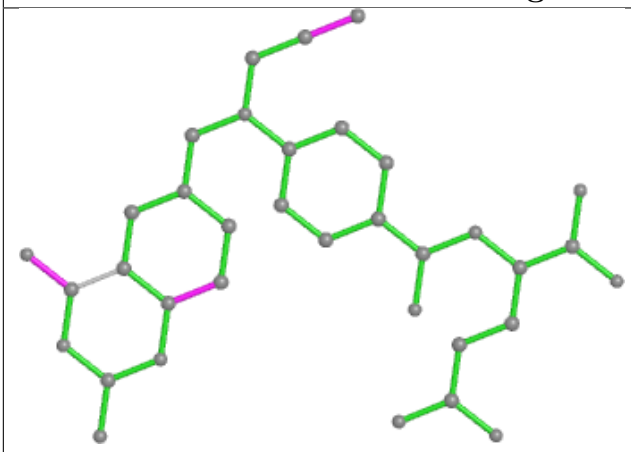


Rings

Ligand CB3 C 612



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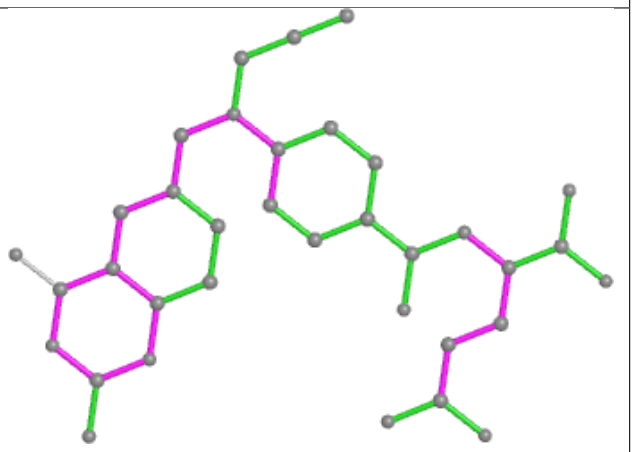
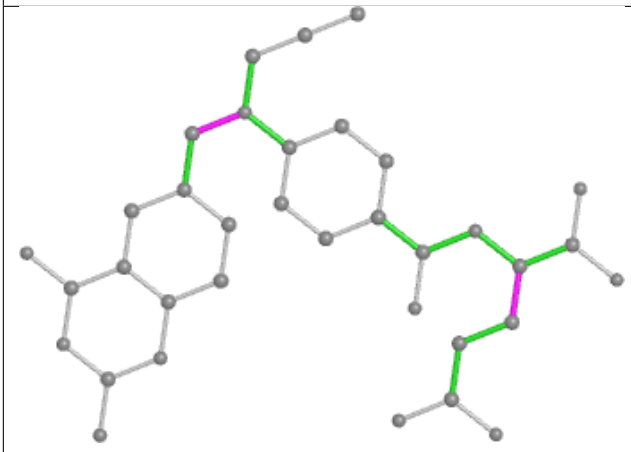


Bond angles



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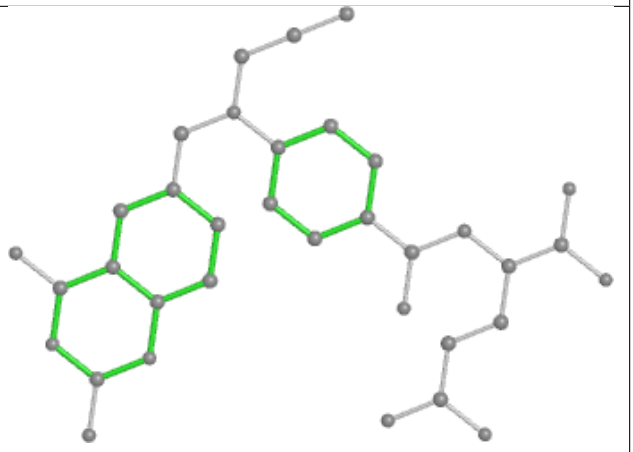
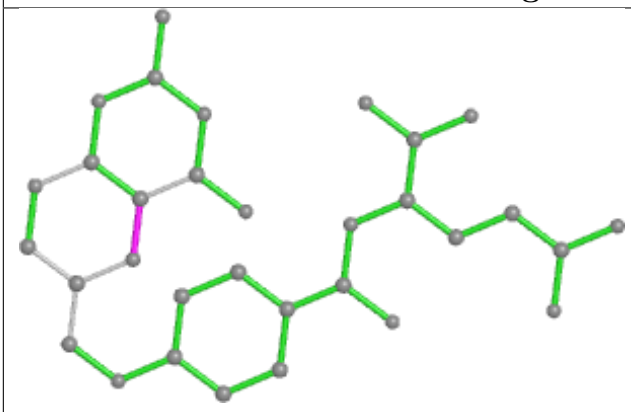


Rings

Ligand DHF A 605



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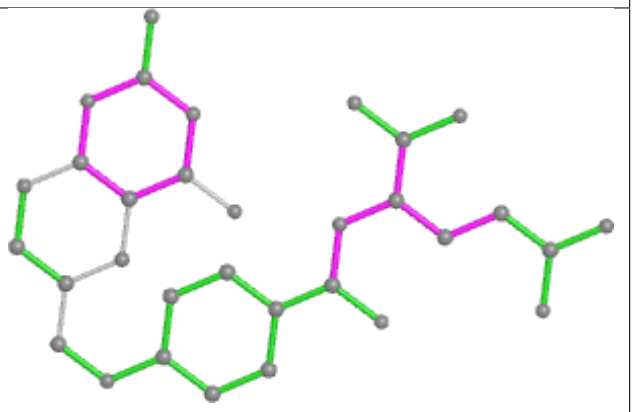
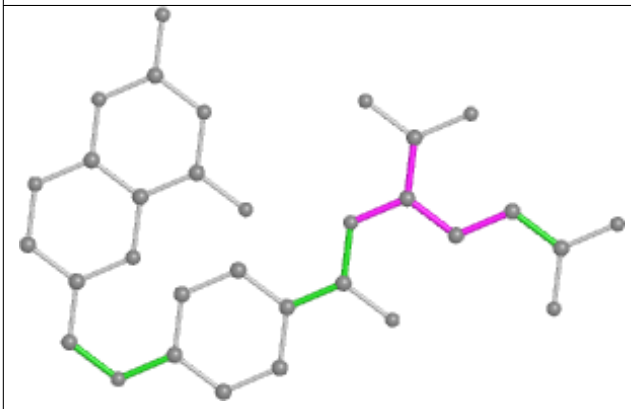


Bond angles



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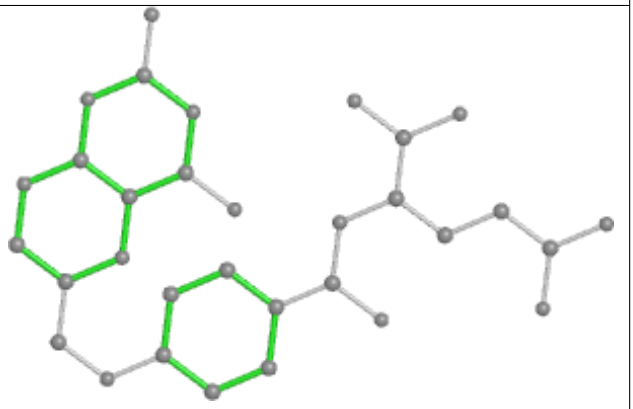
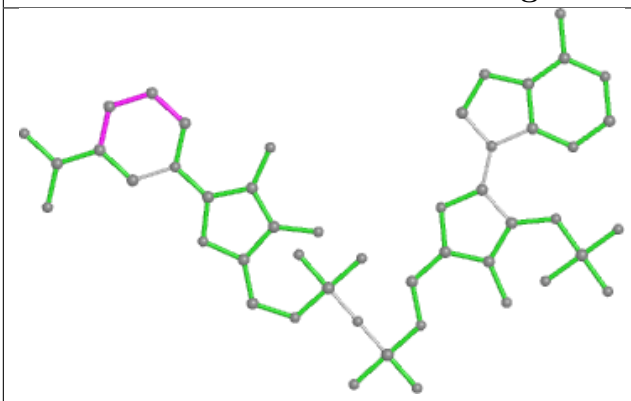
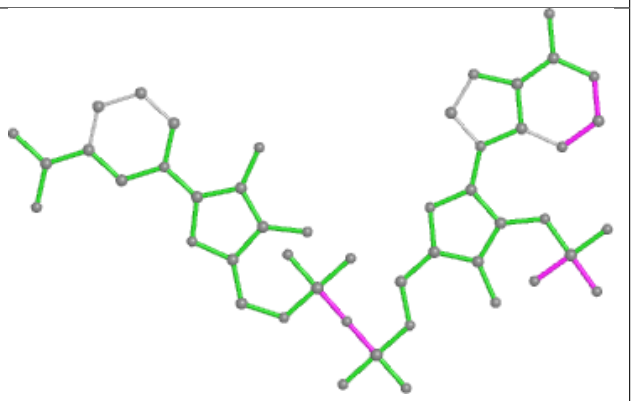


Rings

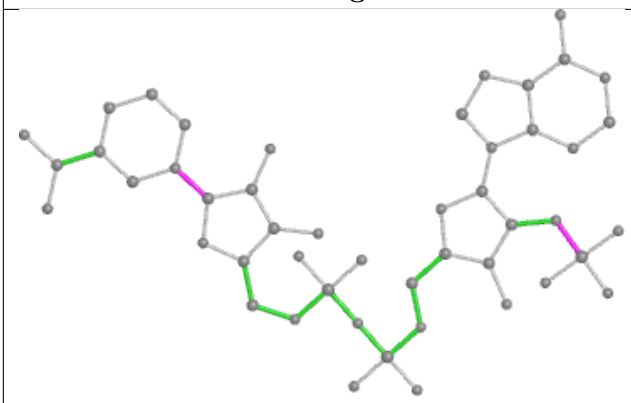
Ligand NDP D 618



Bond lengths



Bond angles



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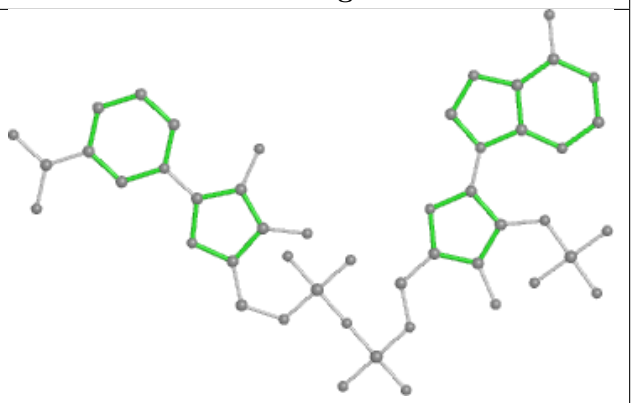
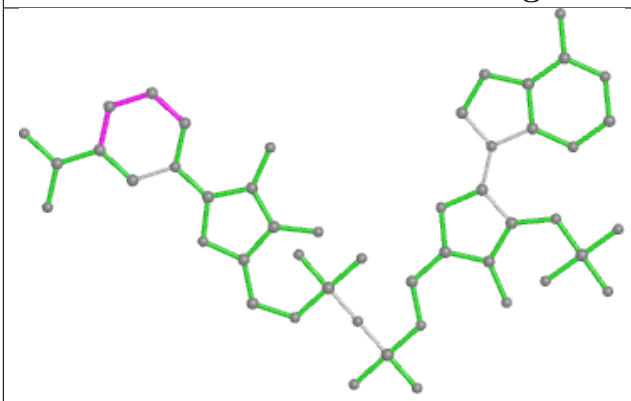
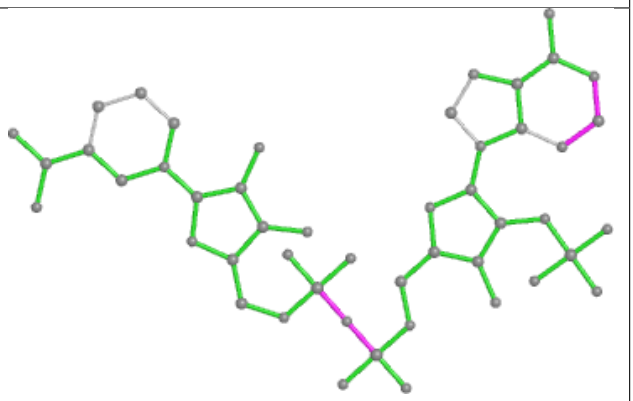


Rings

Ligand NDP E 622



Bond lengths



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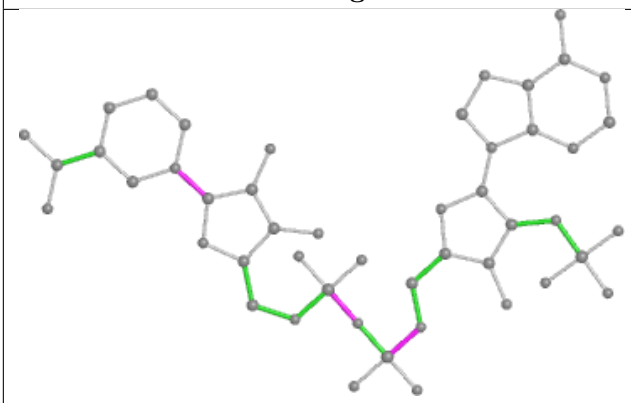
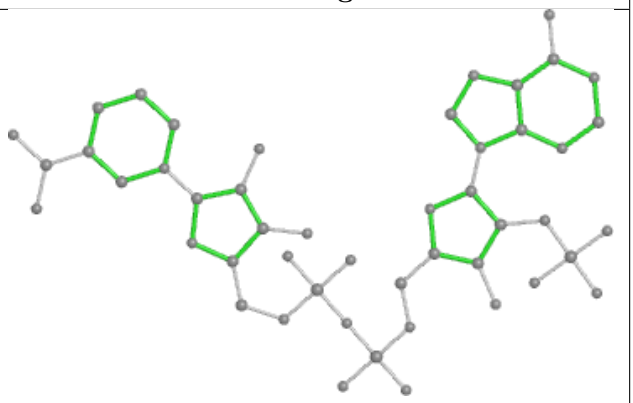
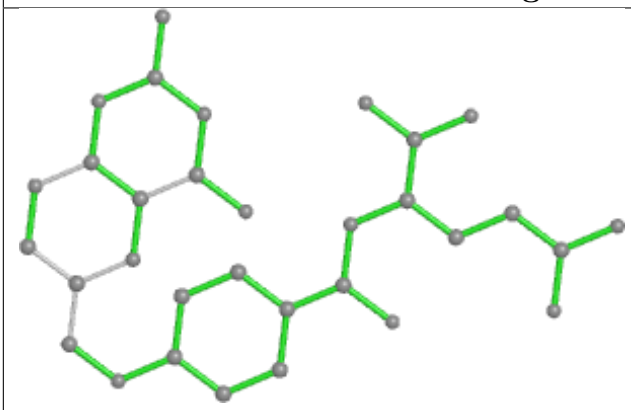


Torsions



Rings

Ligand DHF C 613



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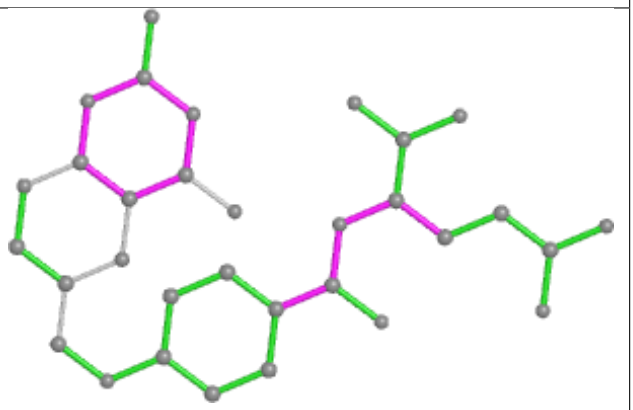
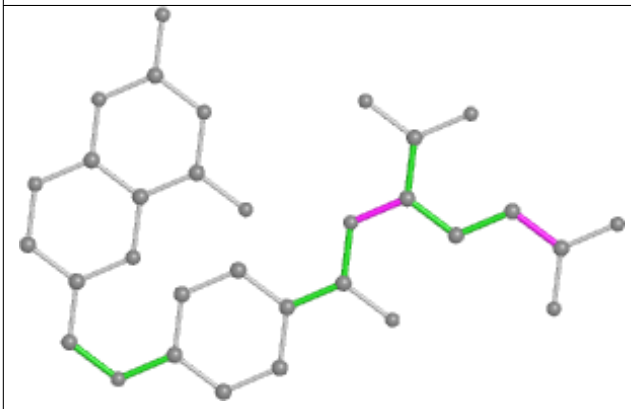
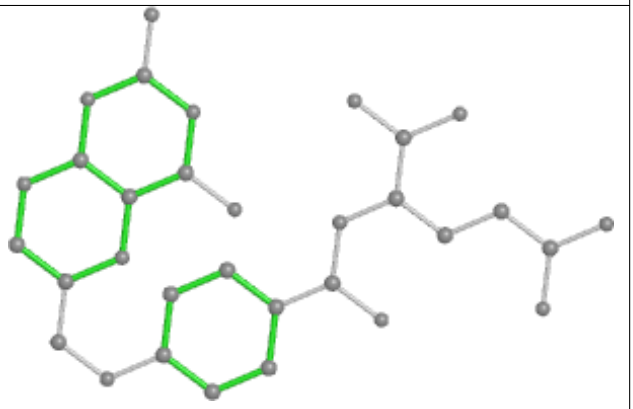


Bond angles

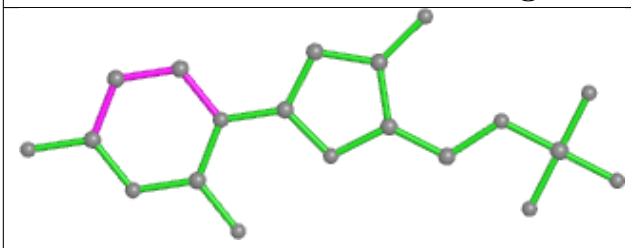


Torsions

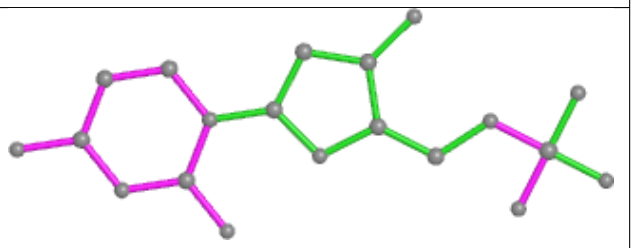


Rings

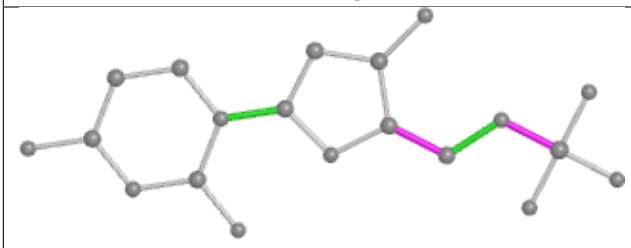
Ligand UMP E 619



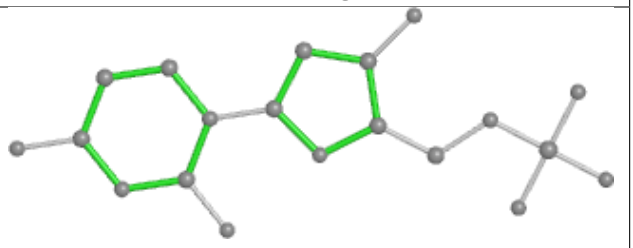
Bond lengths



Bond angles

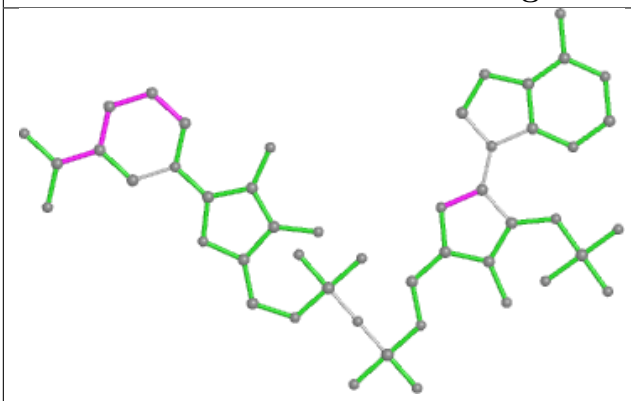


Torsions

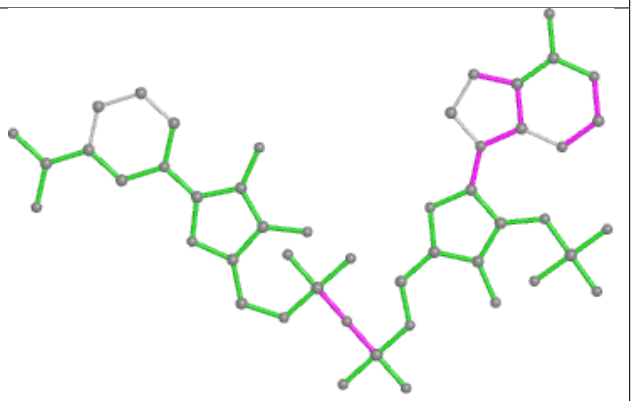


Rings

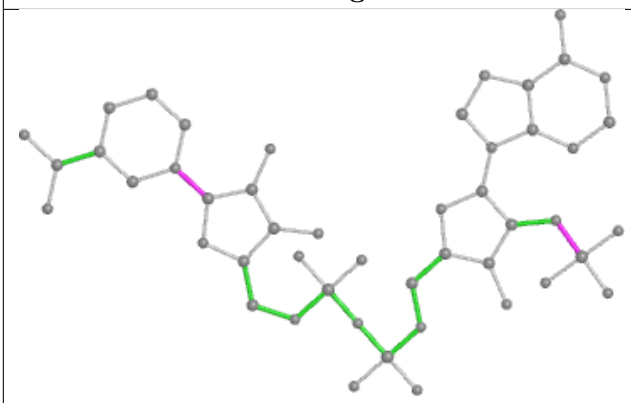
Ligand NDP B 610



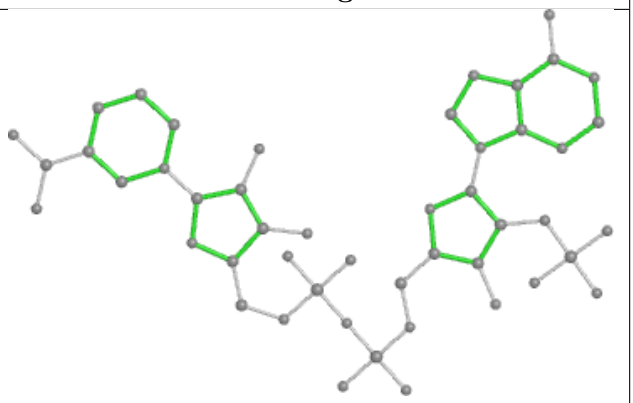
Bond lengths



Bond angles

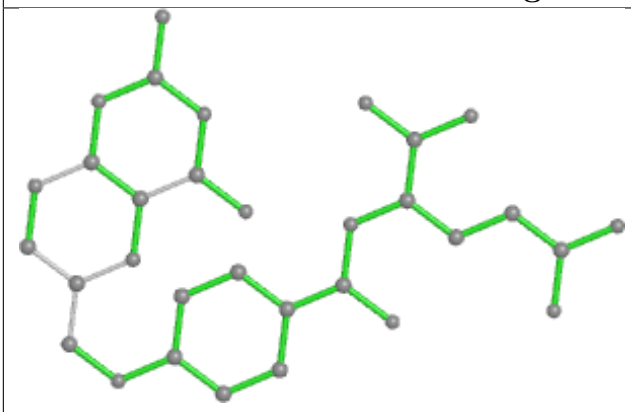


Torsions

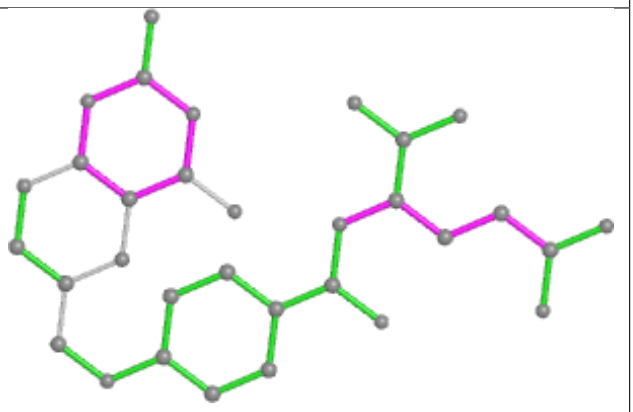


Rings

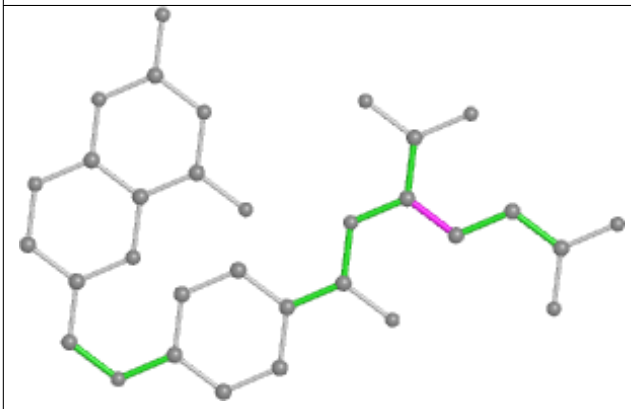
Ligand DHF E 621



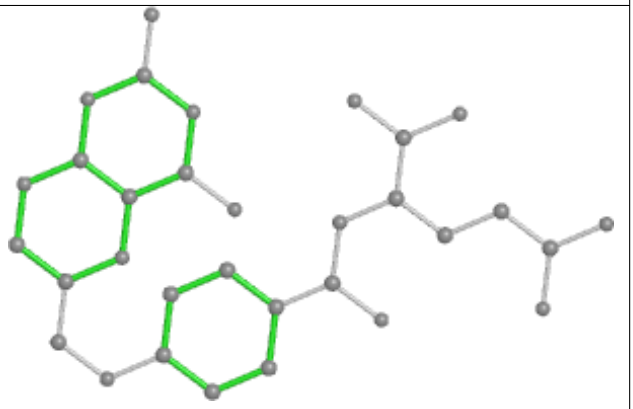
Bond lengths



Bond angles

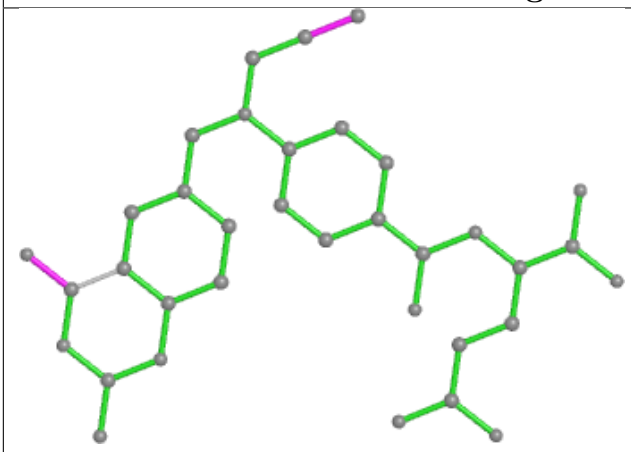


Torsions

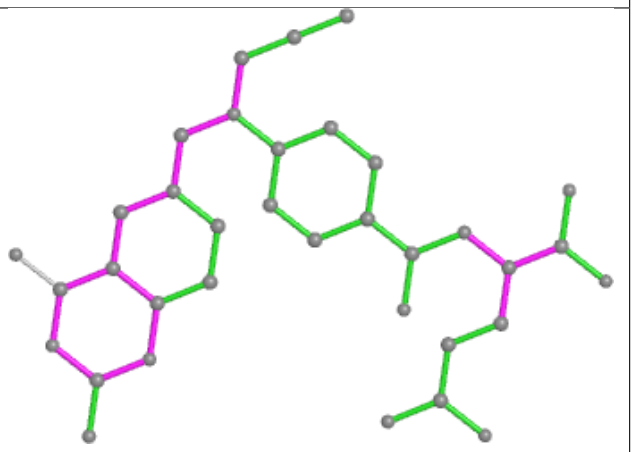


Rings

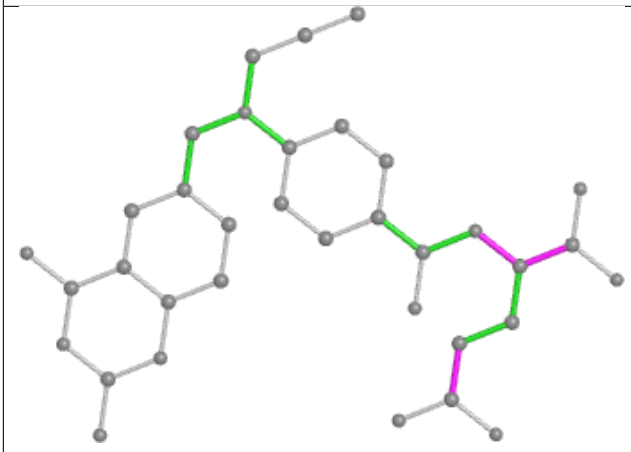
Ligand CB3 D 616



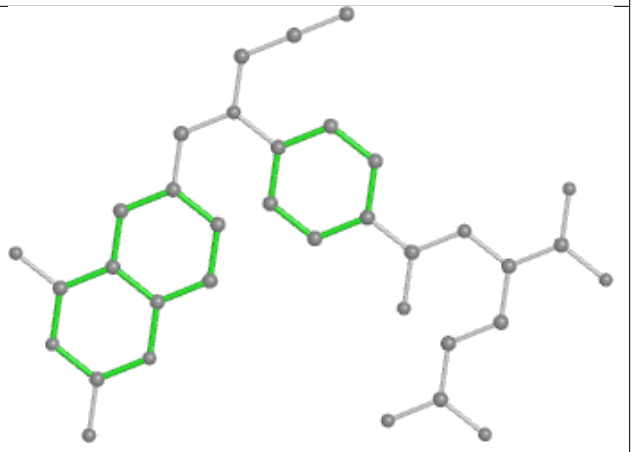
Bond lengths



Bond angles

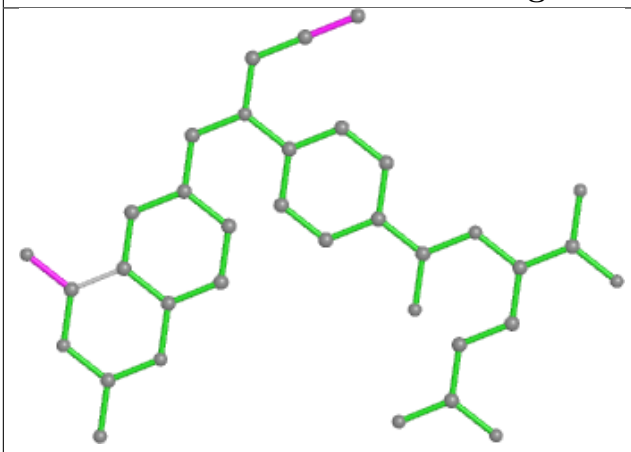


Torsions

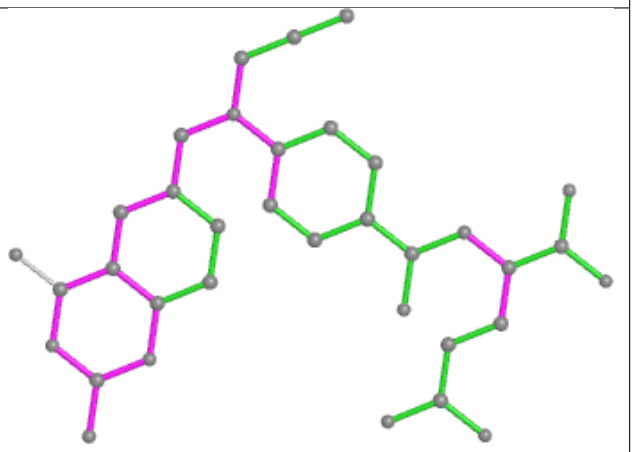


Rings

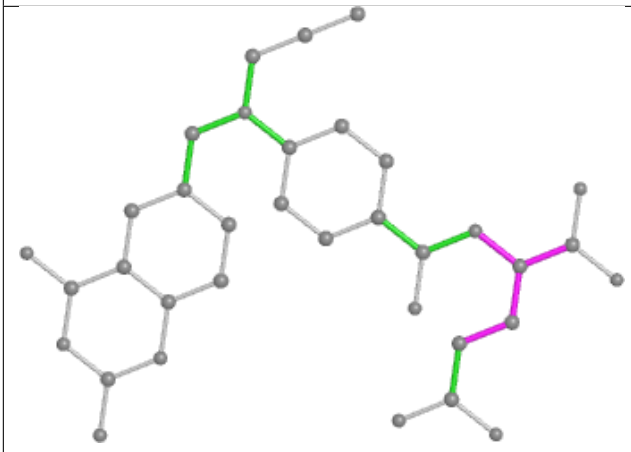
Ligand CB3 E 620



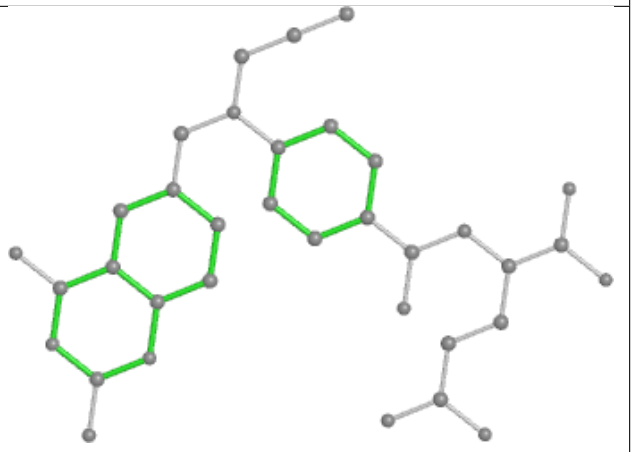
Bond lengths



Bond angles

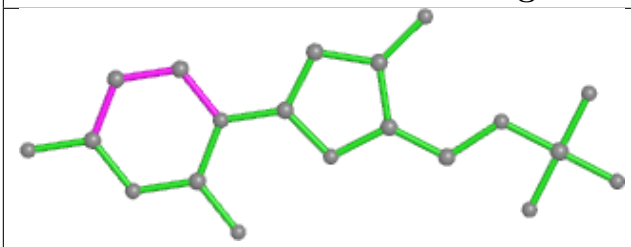


Torsions

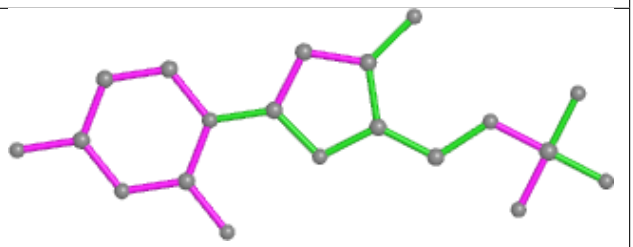


Rings

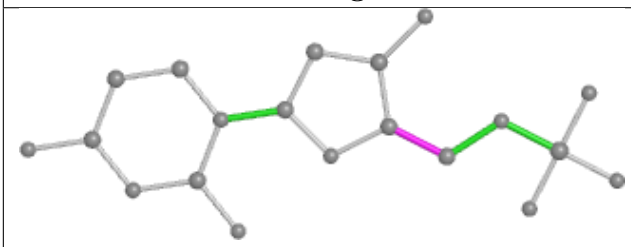
Ligand UMP A 603



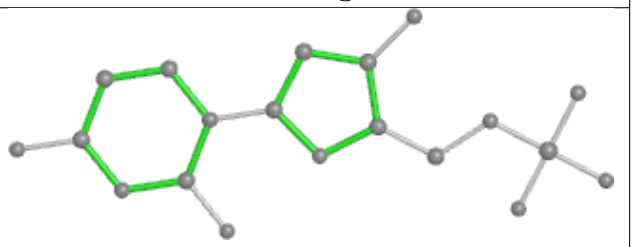
Bond lengths



Bond angles

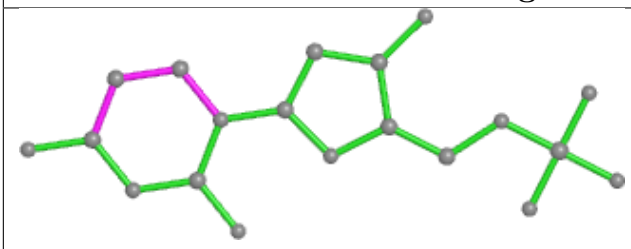


Torsions

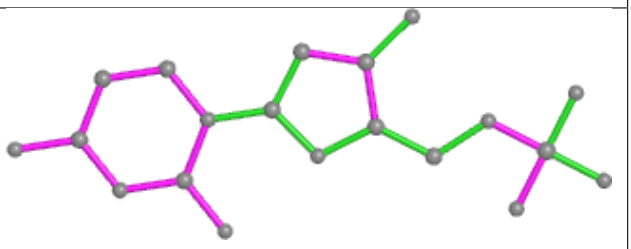


Rings

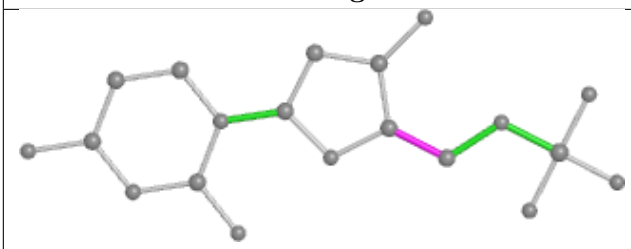
Ligand UMP C 611



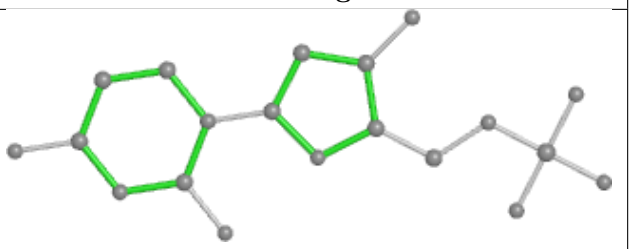
Bond lengths



Bond angles

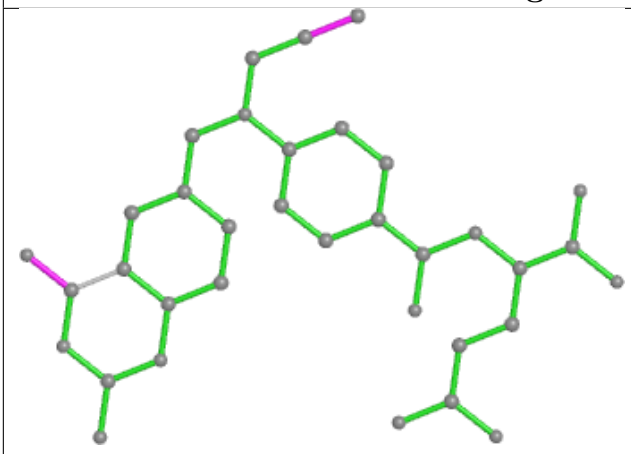


Torsions

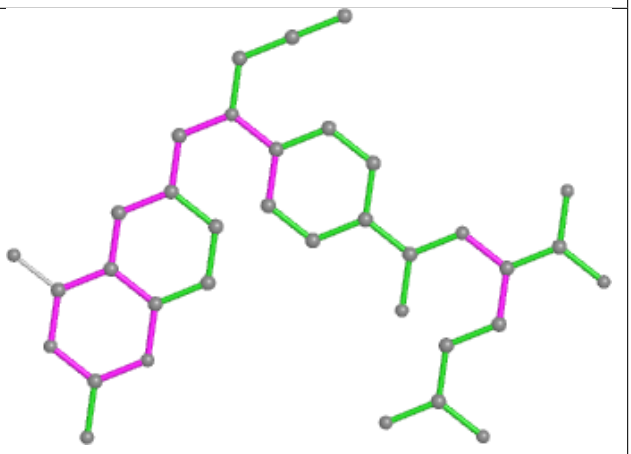


Rings

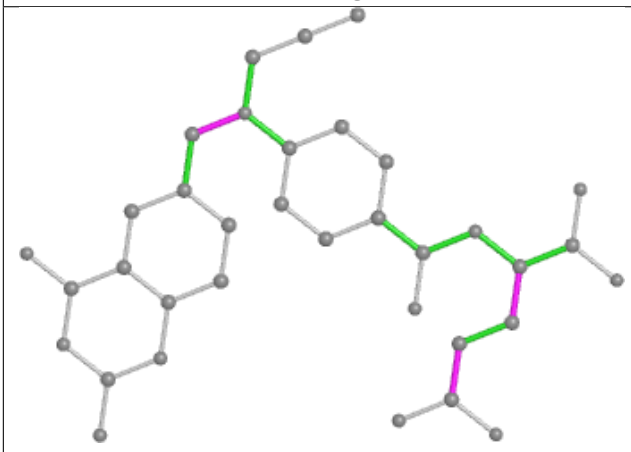
Ligand CB3 A 604



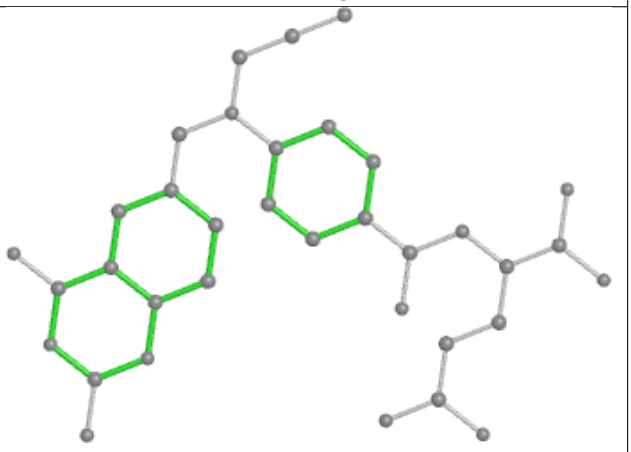
Bond lengths



Bond angles

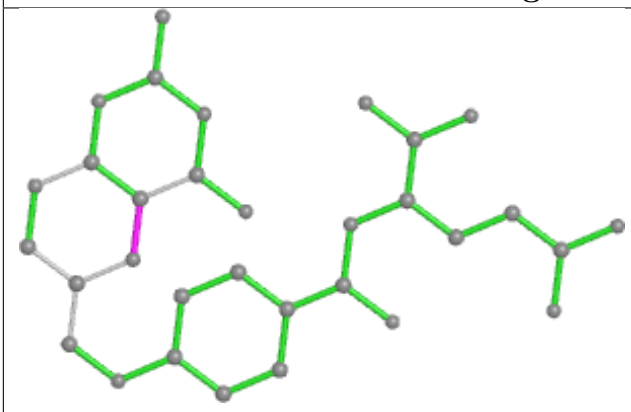


Torsions

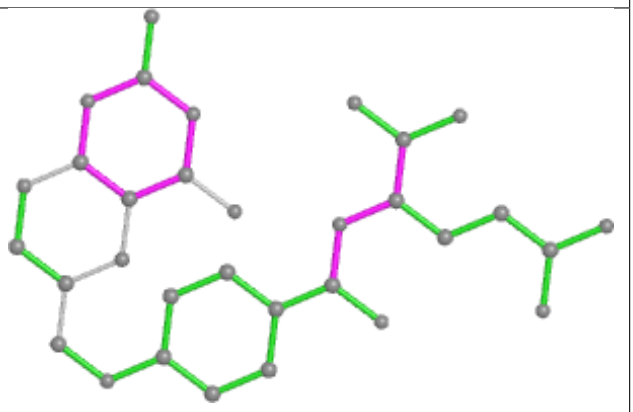


Rings

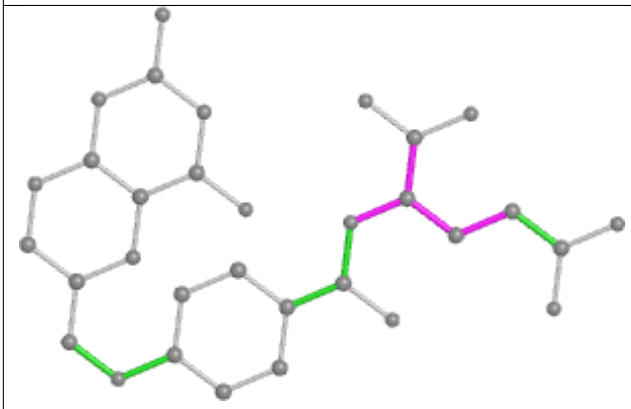
Ligand DHF B 609



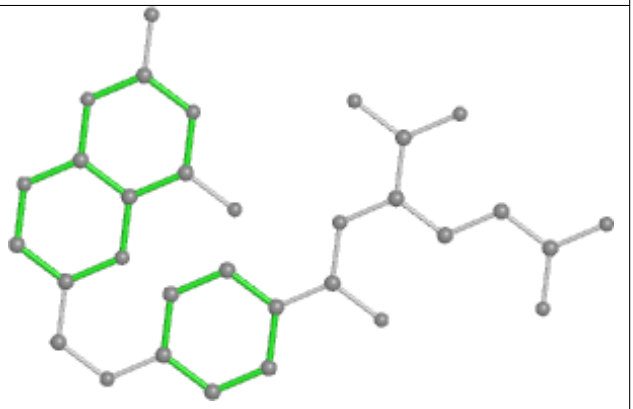
Bond lengths



Bond angles

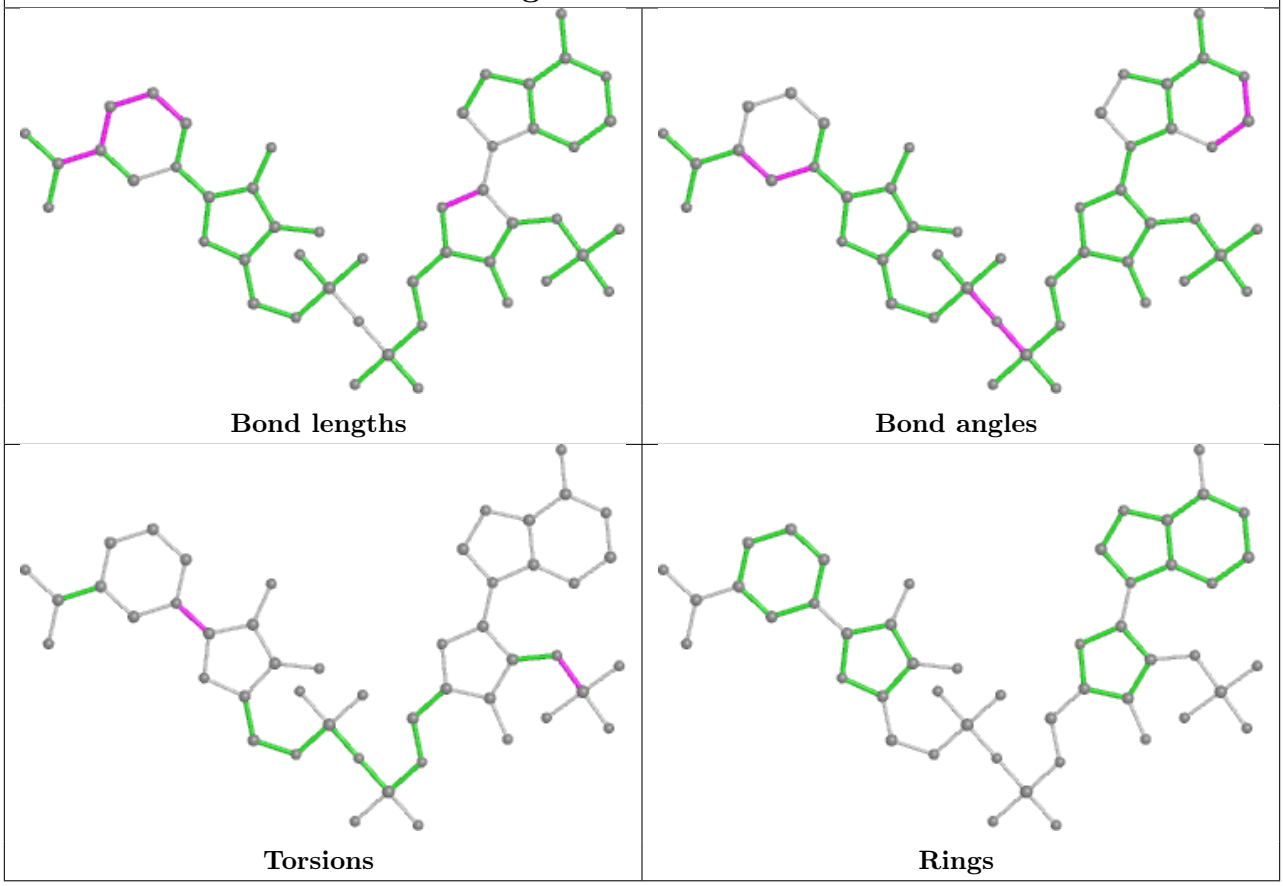


Torsions

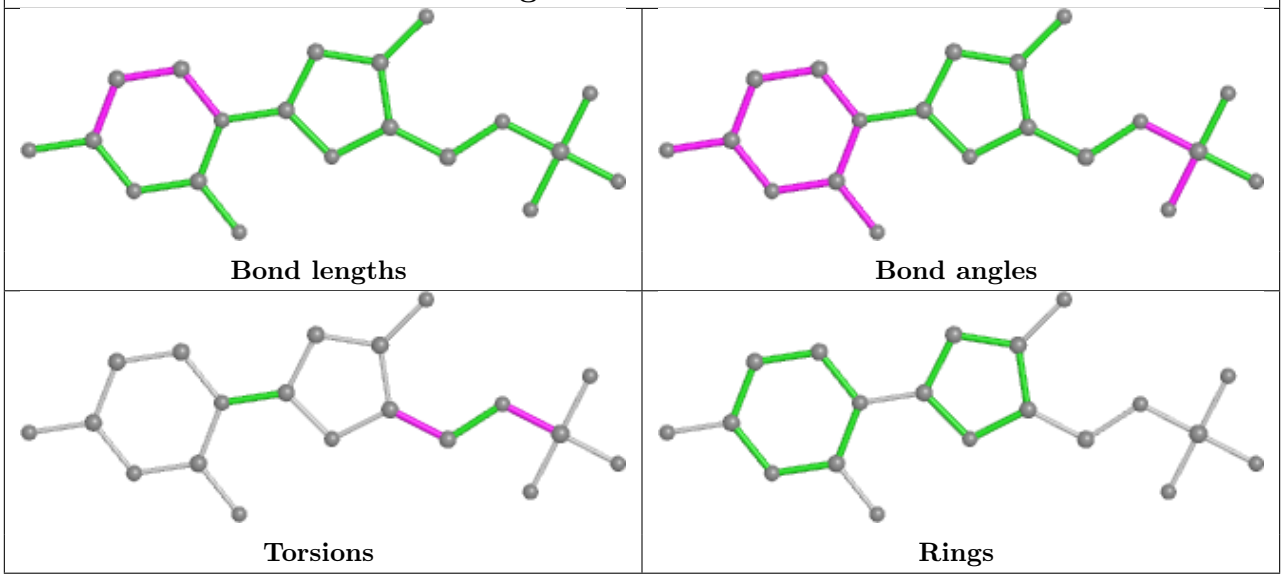


Rings

Ligand NDP A 606



Ligand UMP B 607



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	507/521 (97%)	-0.16	3 (0%)	89	91	23, 39, 74, 118	0
1	B	508/521 (97%)	-0.30	5 (0%)	82	86	20, 34, 62, 135	0
1	C	508/521 (97%)	-0.09	10 (1%)	65	72	26, 47, 90, 131	0
1	D	507/521 (97%)	0.01	7 (1%)	75	80	29, 50, 84, 158	0
1	E	508/521 (97%)	0.49	33 (6%)	18	21	45, 72, 112, 149	0
All	All	2538/2605 (97%)	-0.01	58 (2%)	60	67	20, 48, 96, 158	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	521	VAL	5.1
1	E	324	TYR	3.9
1	E	179	GLU	3.8
1	E	106	SER	3.6
1	C	181	LYS	3.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

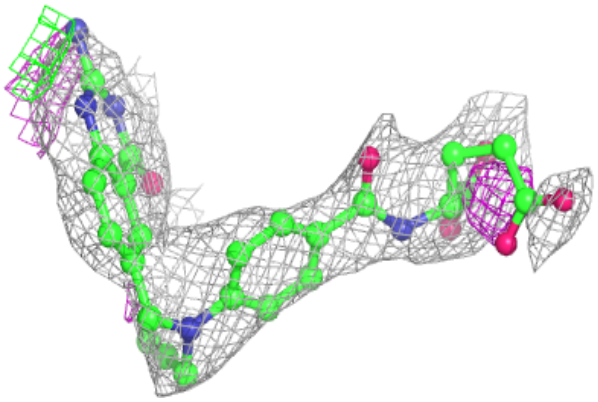
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

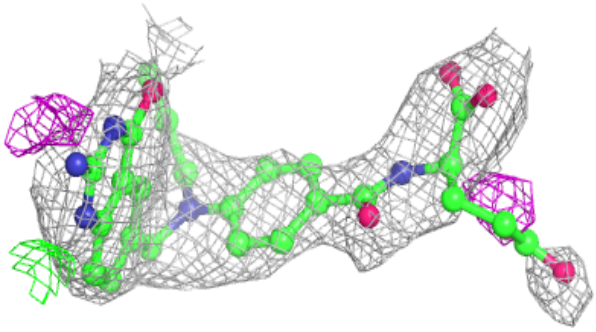
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CB3	E	620	35/35	0.73	0.31	93,98,107,108	0
3	CB3	D	616	35/35	0.78	0.33	69,75,87,89	0
3	CB3	A	604	35/35	0.84	0.24	60,67,76,77	0
2	UMP	E	619	20/20	0.88	0.19	80,88,89,89	0
3	CB3	C	612	35/35	0.90	0.21	49,60,71,73	0
4	DHF	B	609	32/32	0.91	0.18	23,26,39,44	0
4	DHF	C	613	32/32	0.91	0.22	29,35,44,48	0
5	NDP	C	614	48/48	0.91	0.18	65,77,95,95	0
4	DHF	A	605	32/32	0.92	0.16	23,28,38,48	0
2	UMP	A	603	20/20	0.92	0.22	46,57,61,63	0
2	UMP	D	615	20/20	0.92	0.20	53,66,73,73	0
4	DHF	D	617	32/32	0.92	0.16	23,31,41,47	0
3	CB3	B	608	35/35	0.92	0.20	45,50,68,69	0
5	NDP	E	622	48/48	0.92	0.18	66,77,90,92	0
4	DHF	E	621	32/32	0.93	0.22	30,33,42,47	0
2	UMP	C	611	20/20	0.93	0.18	39,50,55,58	0
5	NDP	D	618	48/48	0.93	0.18	50,61,74,76	0
2	UMP	B	607	20/20	0.93	0.19	27,44,48,51	0
5	NDP	A	606	48/48	0.96	0.14	31,40,43,44	0
5	NDP	B	610	48/48	0.97	0.15	31,37,42,43	0

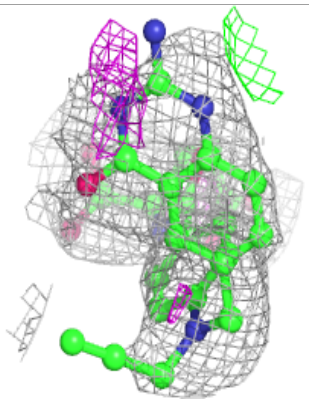
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

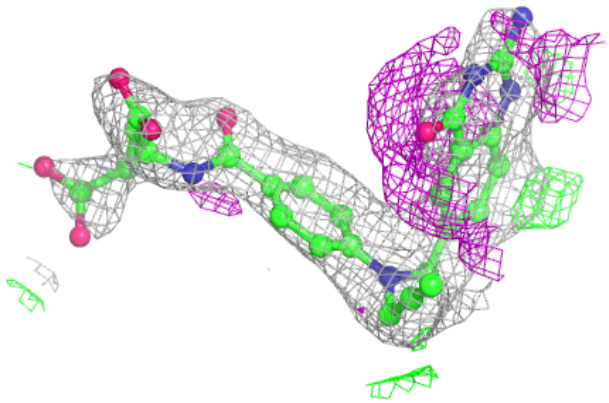


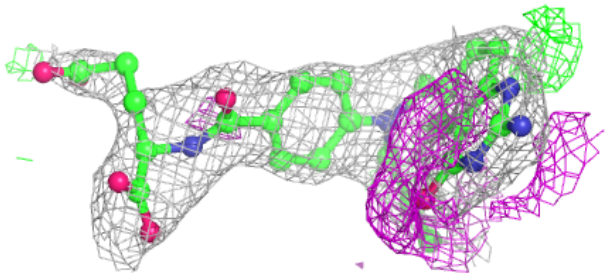


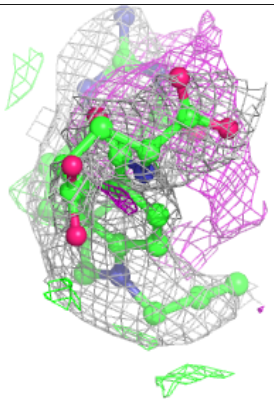


Electron density around CB3 D 616:

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

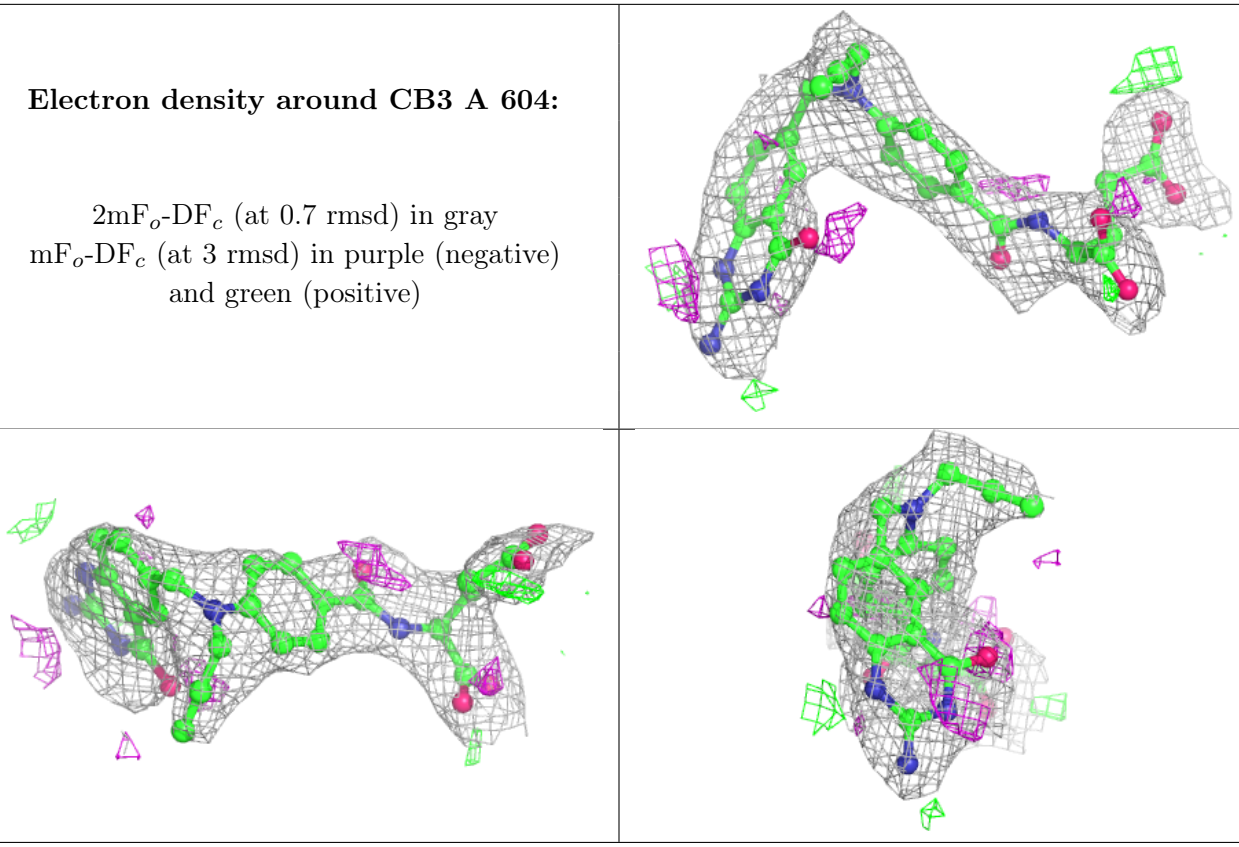






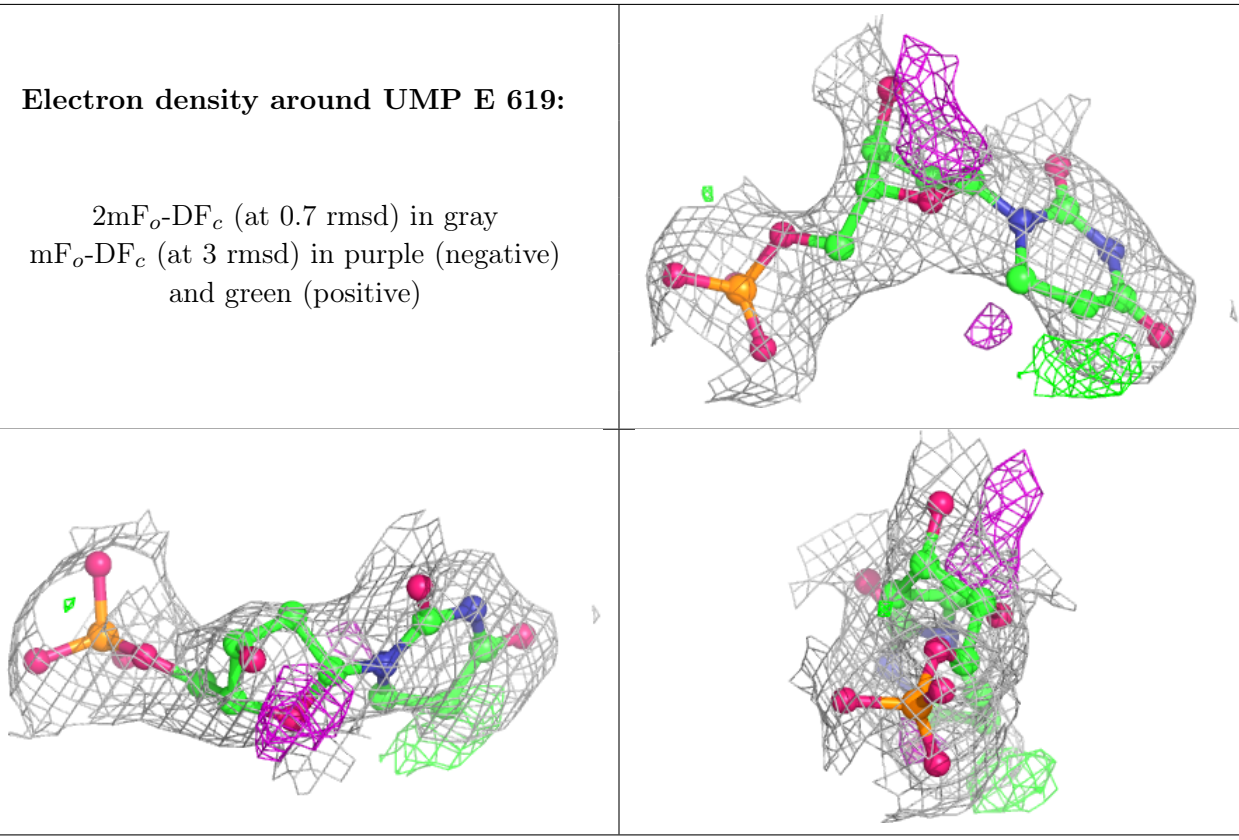
Electron density around CB3 A 604:

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



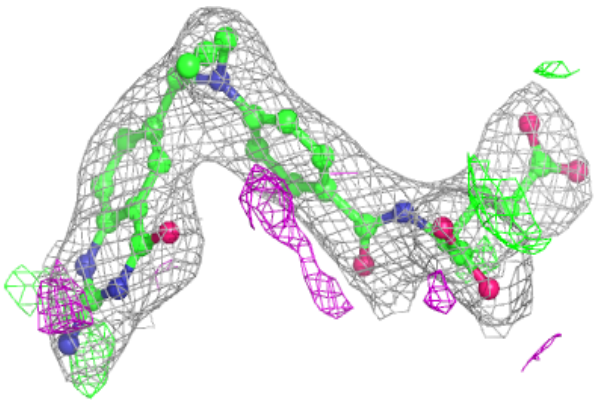
Electron density around UMP E 619:

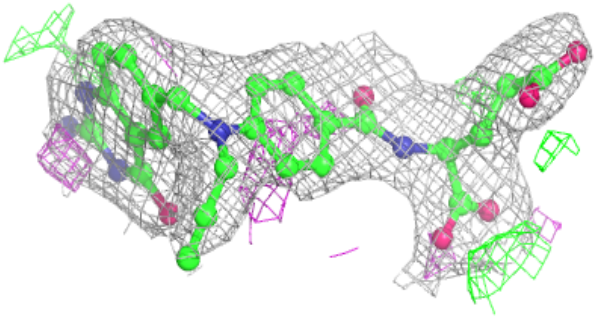
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

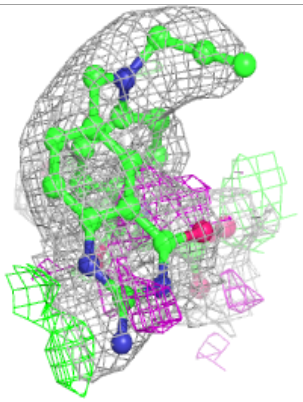


Electron density around CB3 C 612:

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

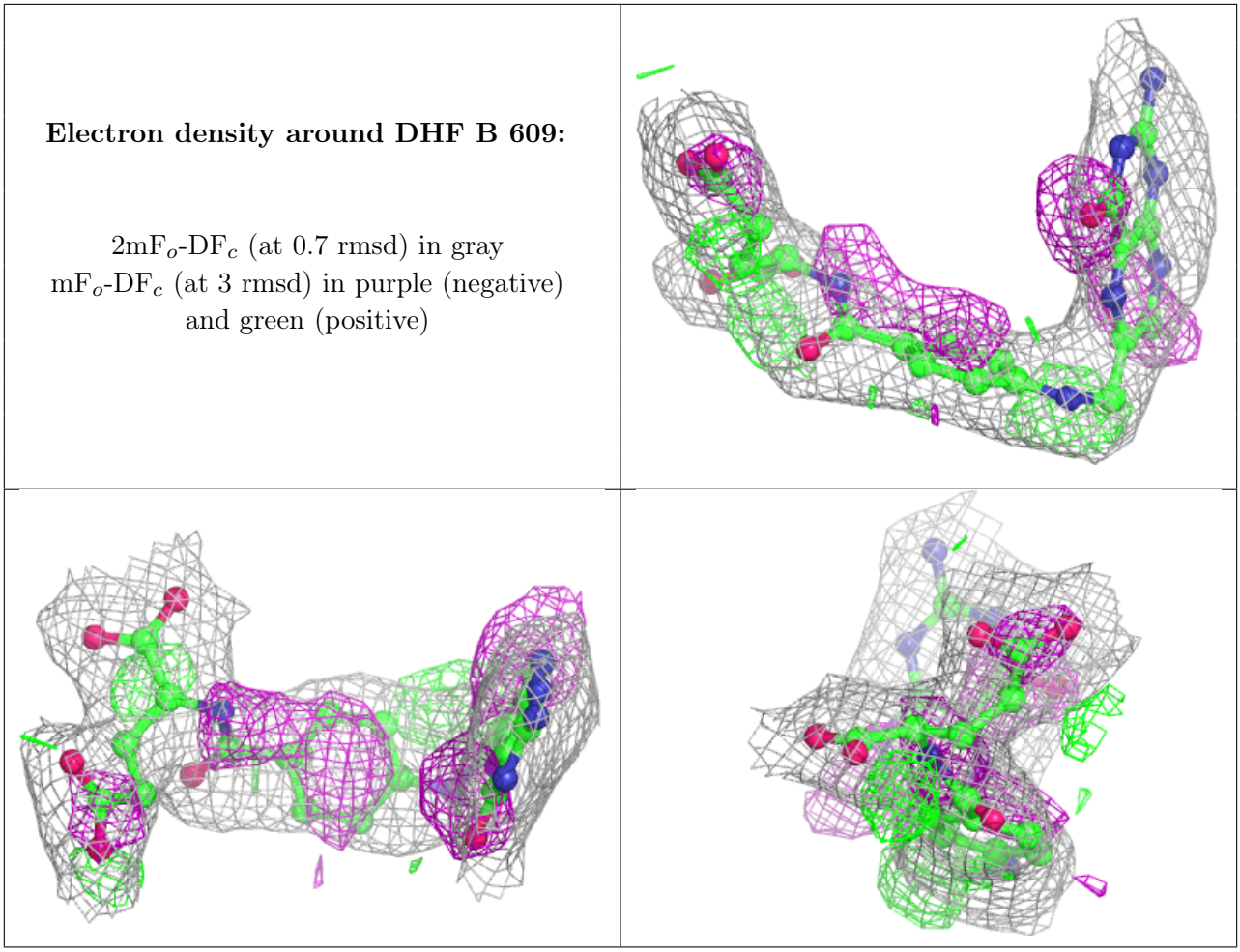






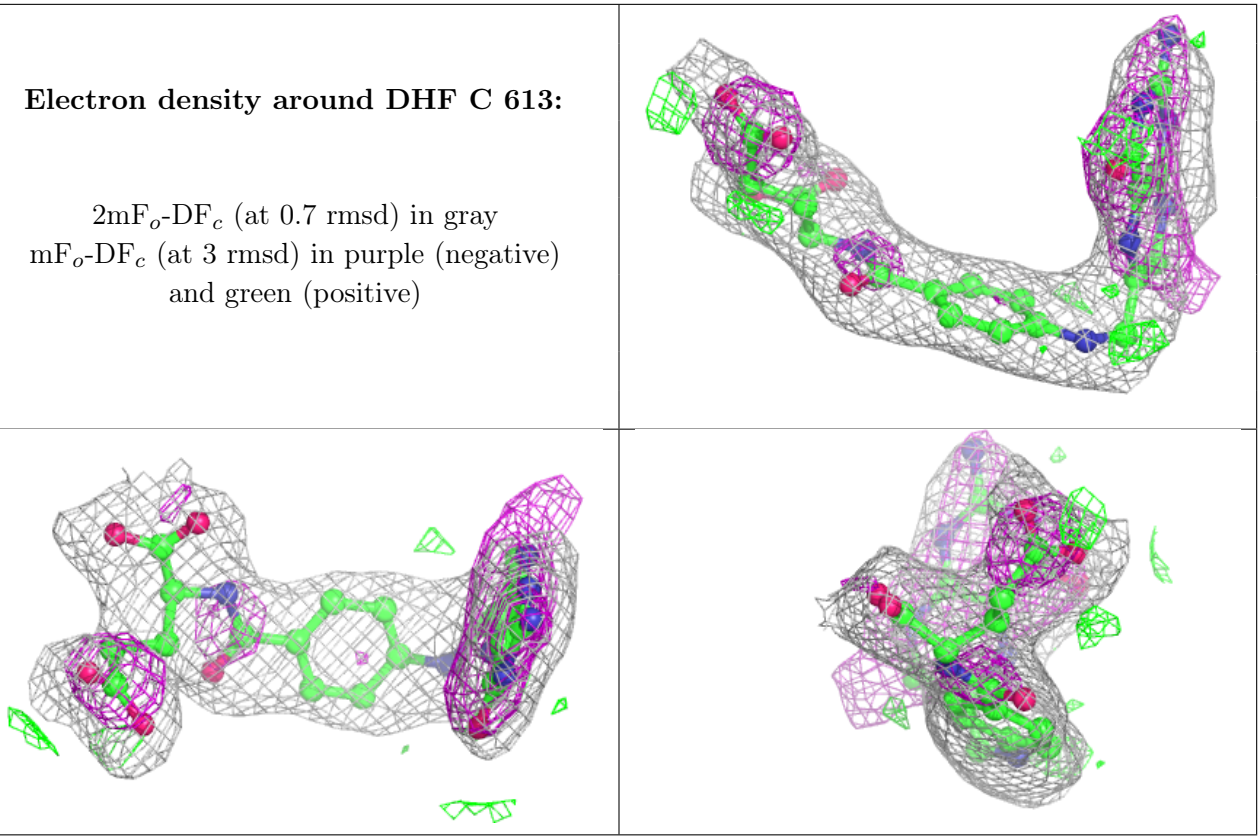
Electron density around DHF B 609:

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



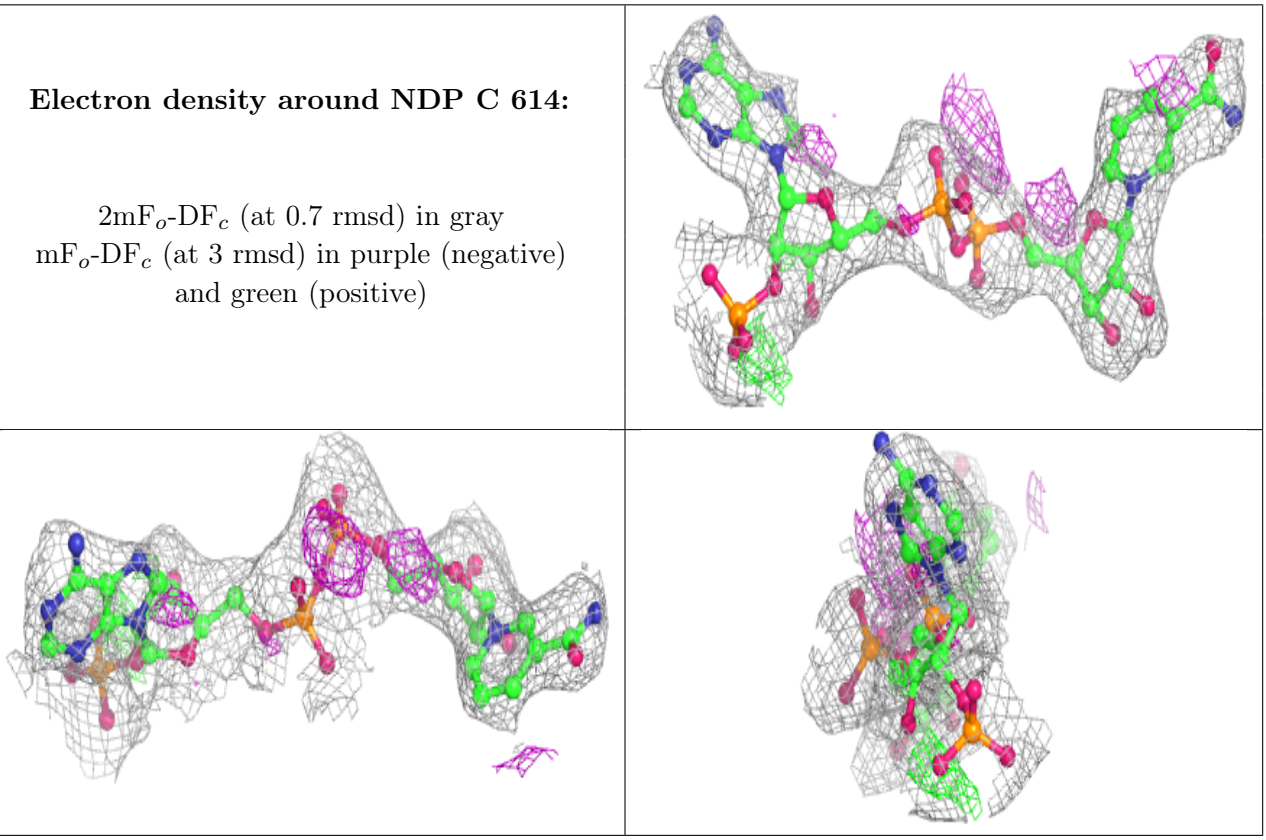
Electron density around DHF C 613:

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



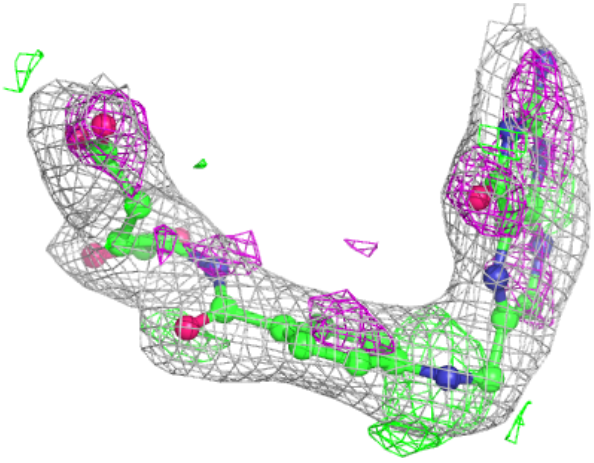
Electron density around NDP C 614:

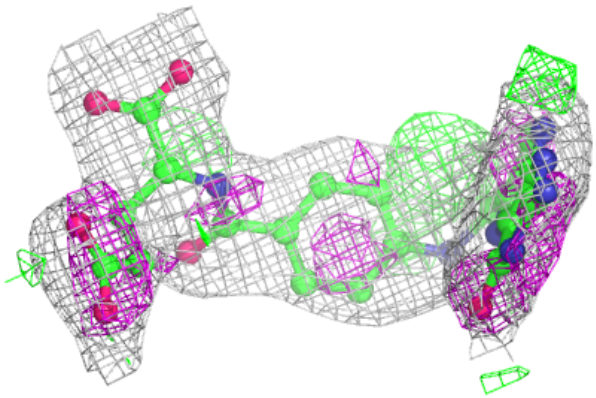
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

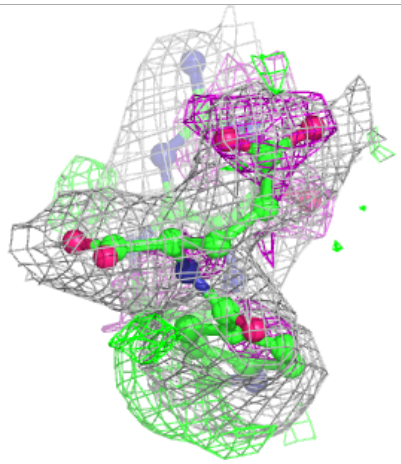


Electron density around DHF A 605:

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

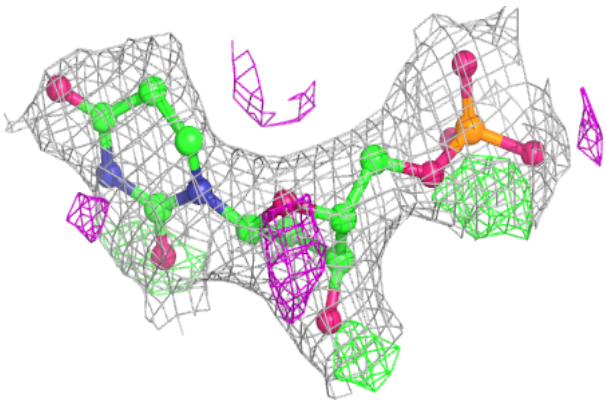


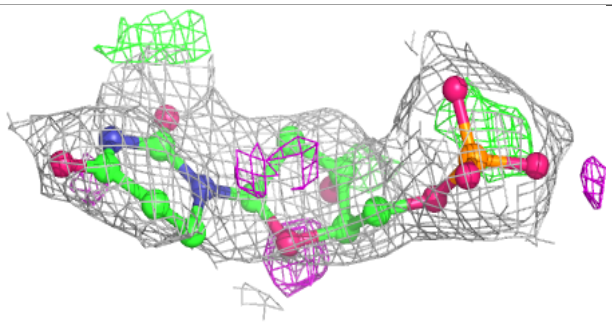


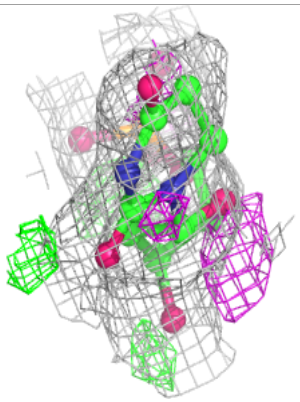


Electron density around UMP A 603:

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

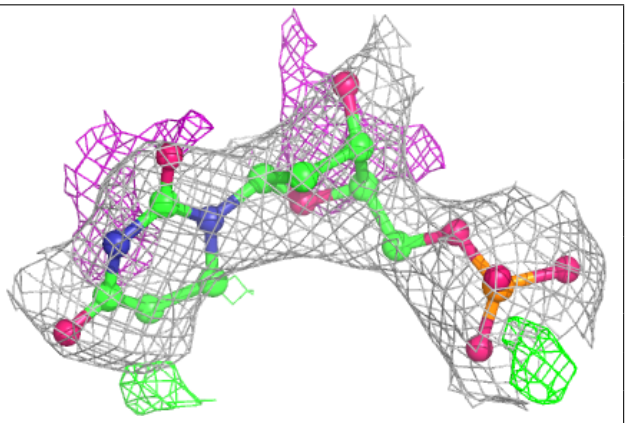


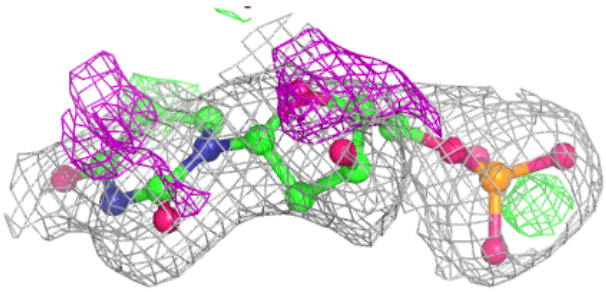


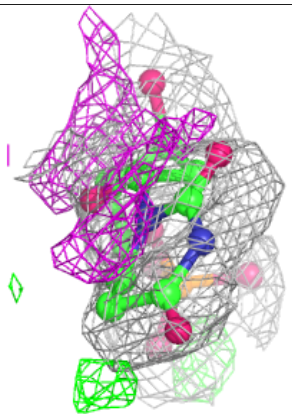


Electron density around UMP D 615:

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

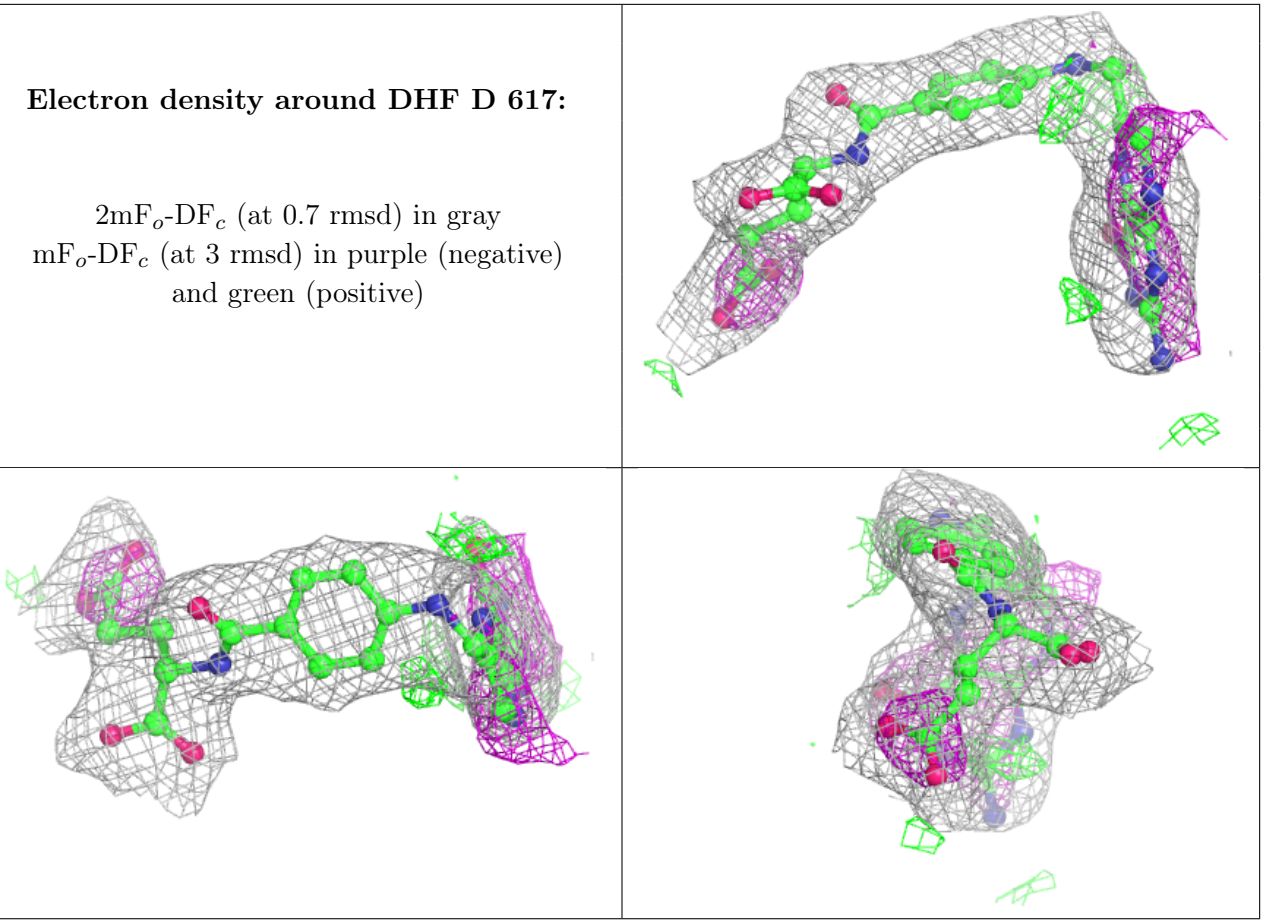






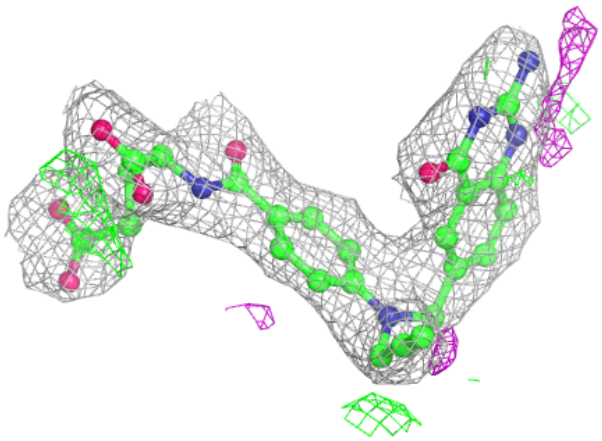
Electron density around DHF D 617:

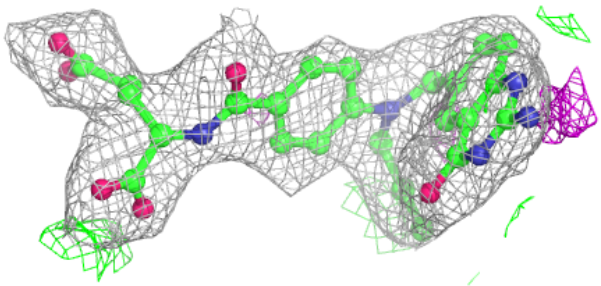
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

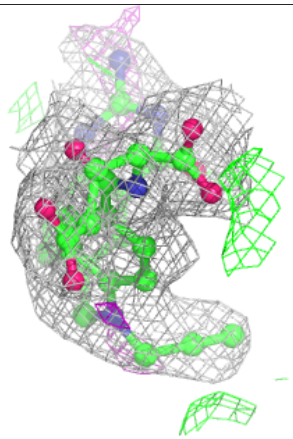


Electron density around CB3 B 608:

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

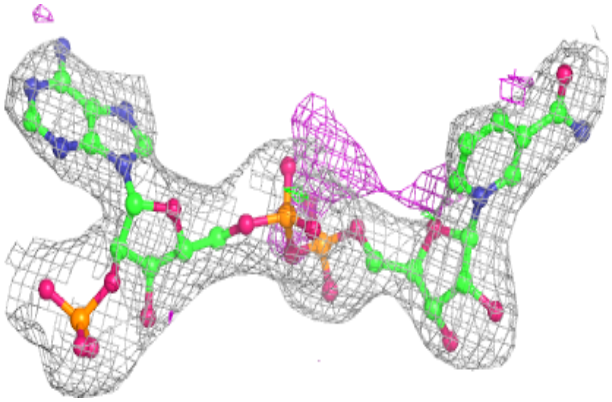


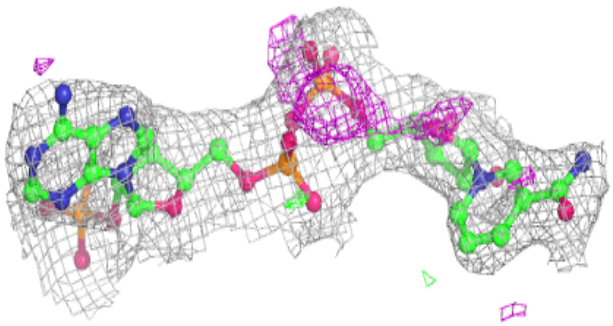


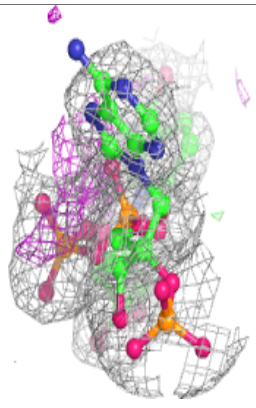


Electron density around NDP E 622:

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

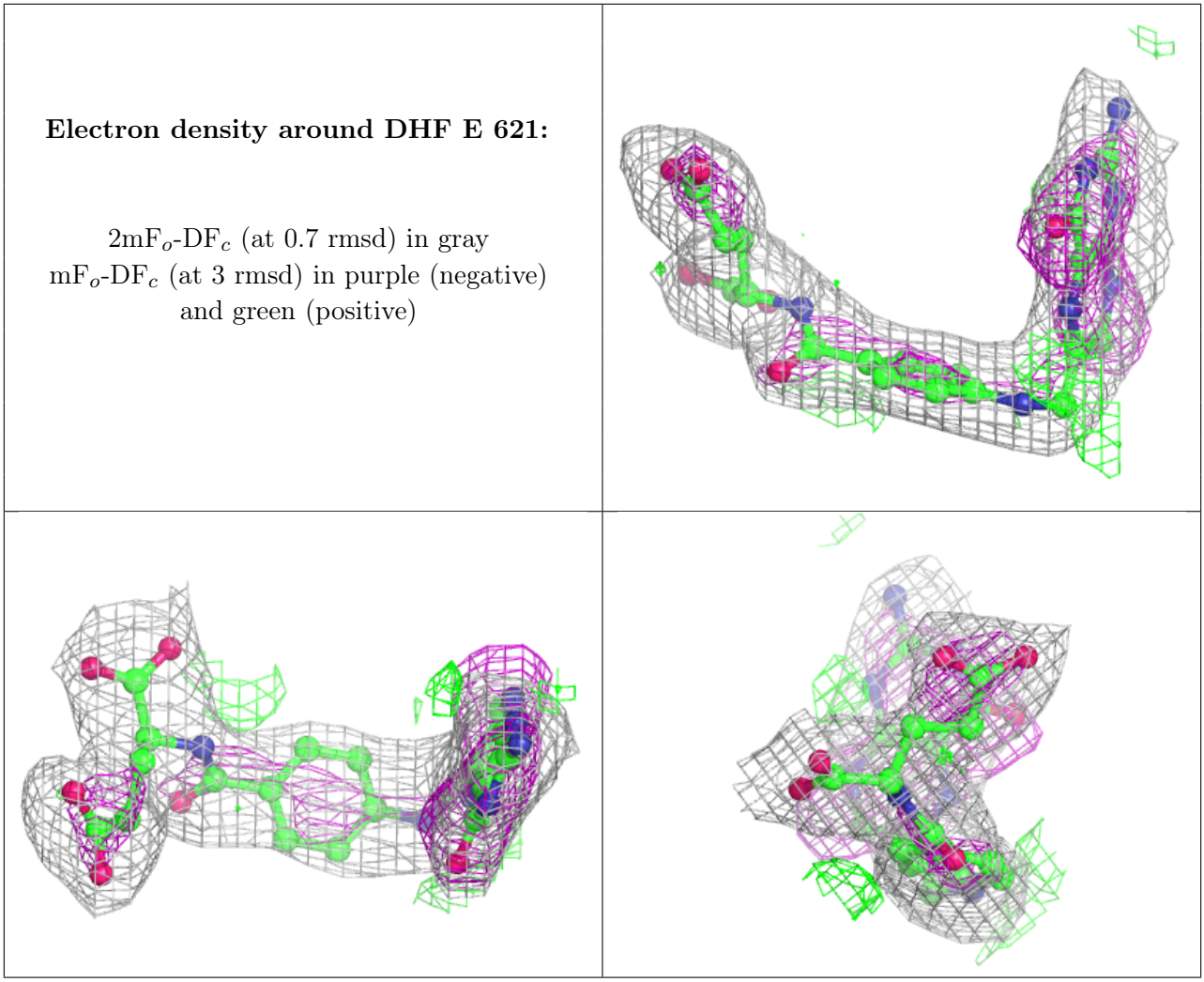






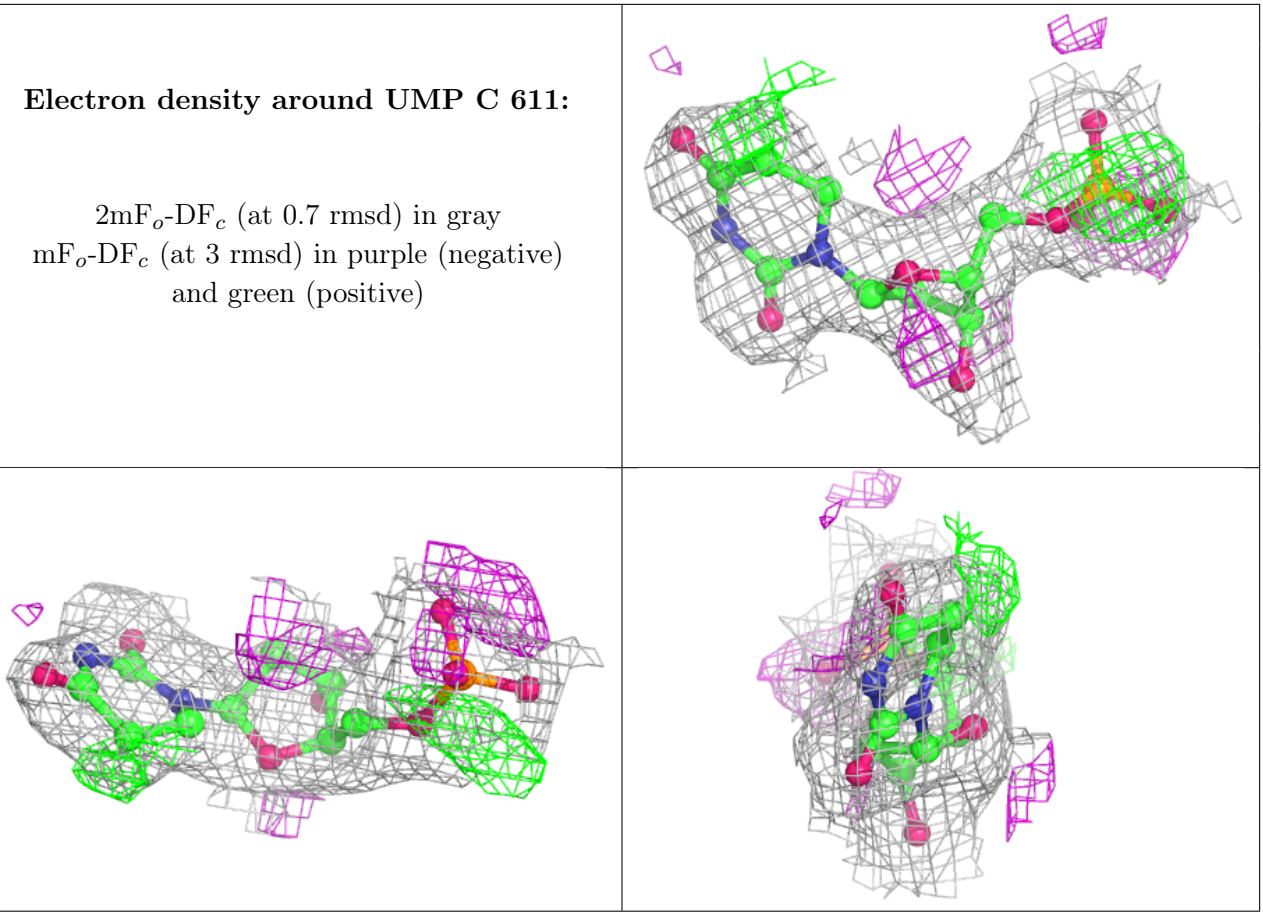
Electron density around DHF E 621:

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



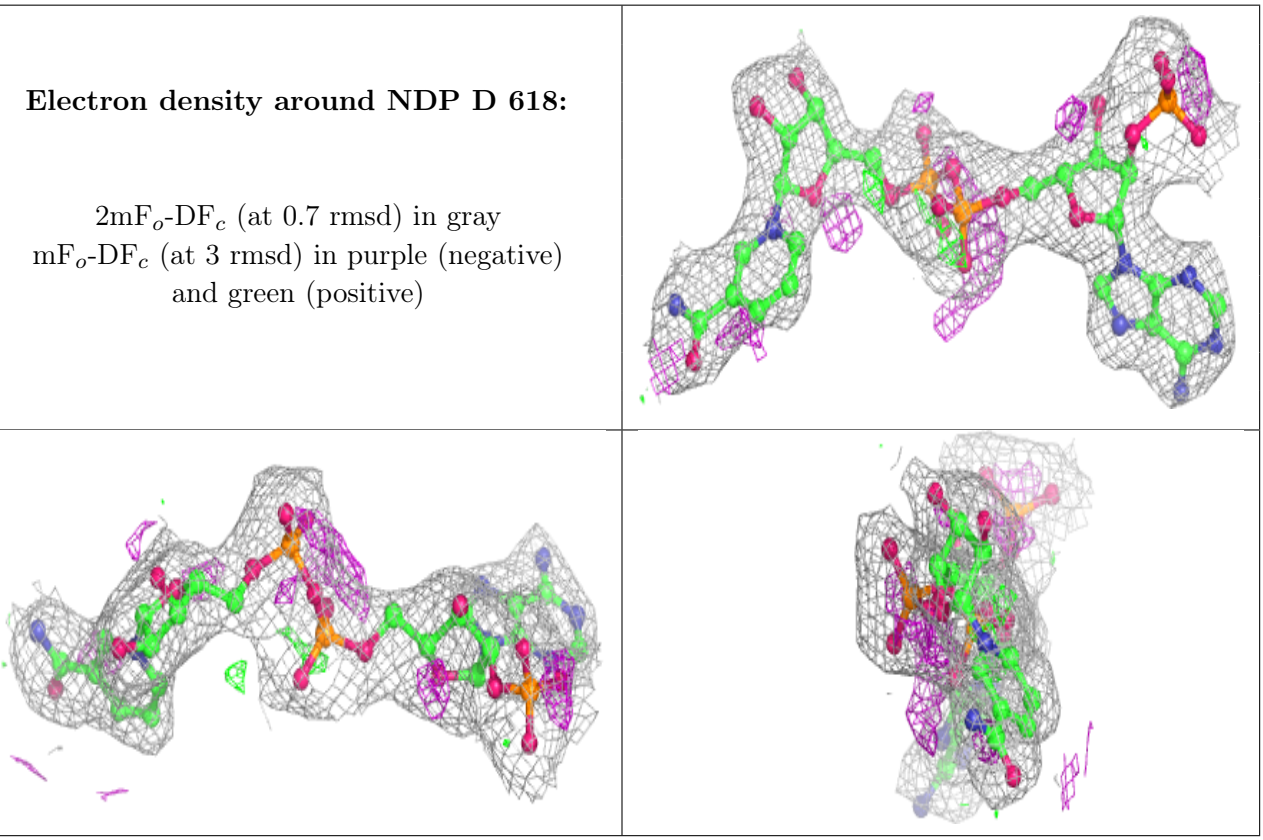
Electron density around UMP C 611:

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



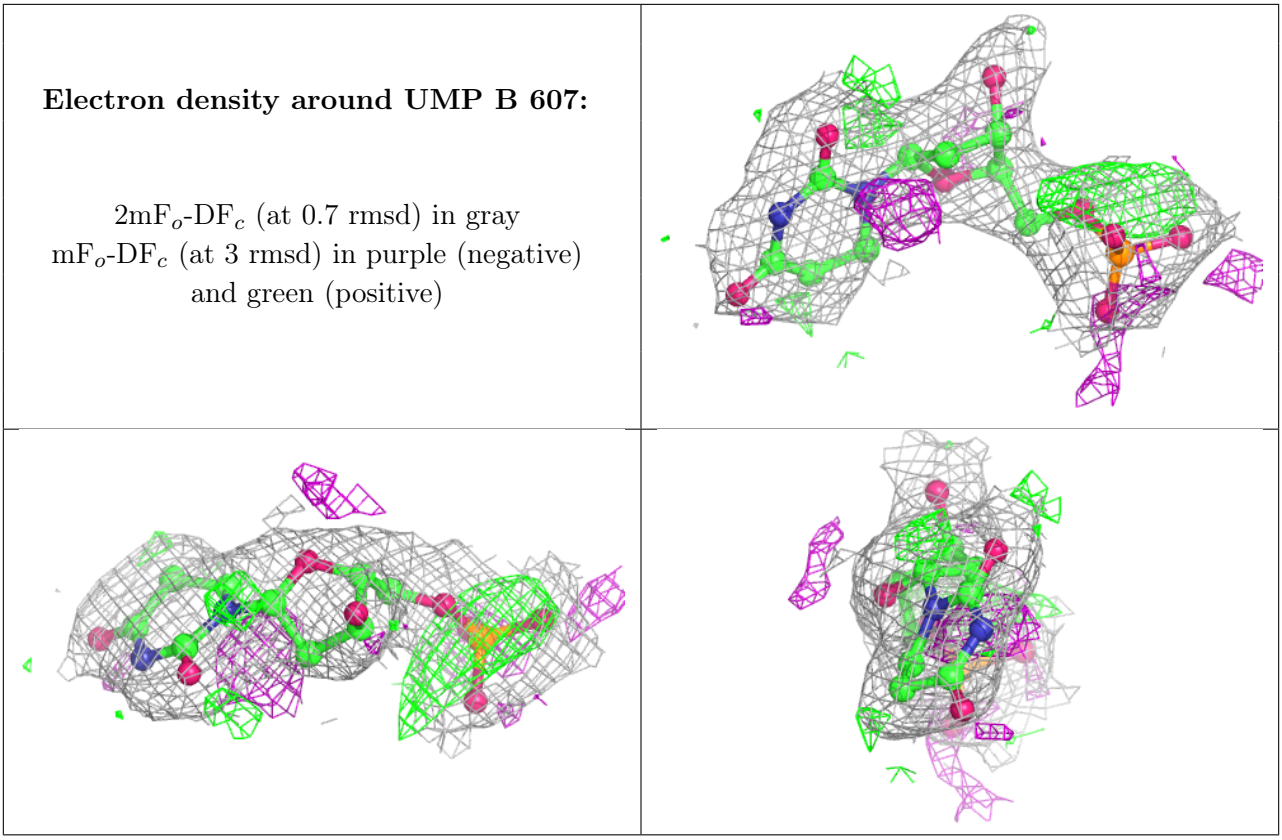
Electron density around NDP D 618:

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



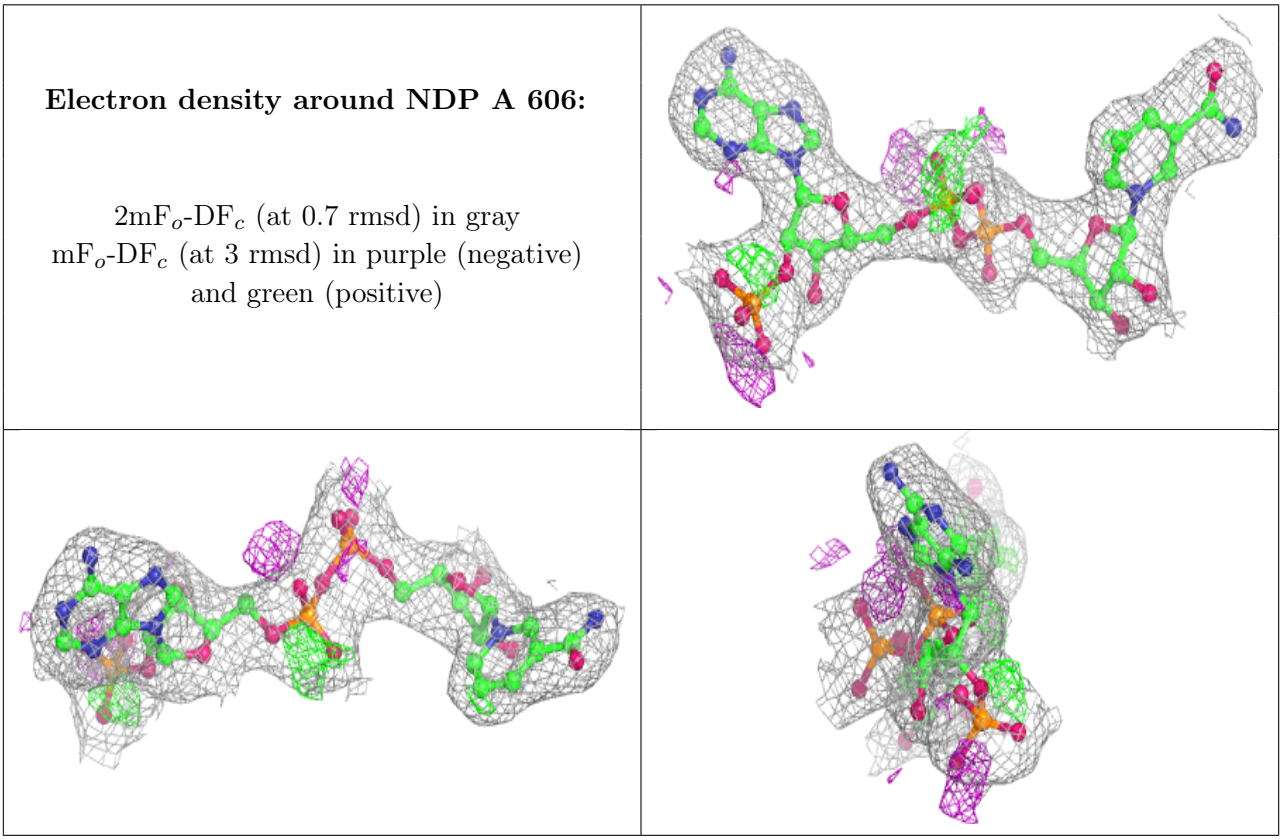
Electron density around UMP B 607:

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



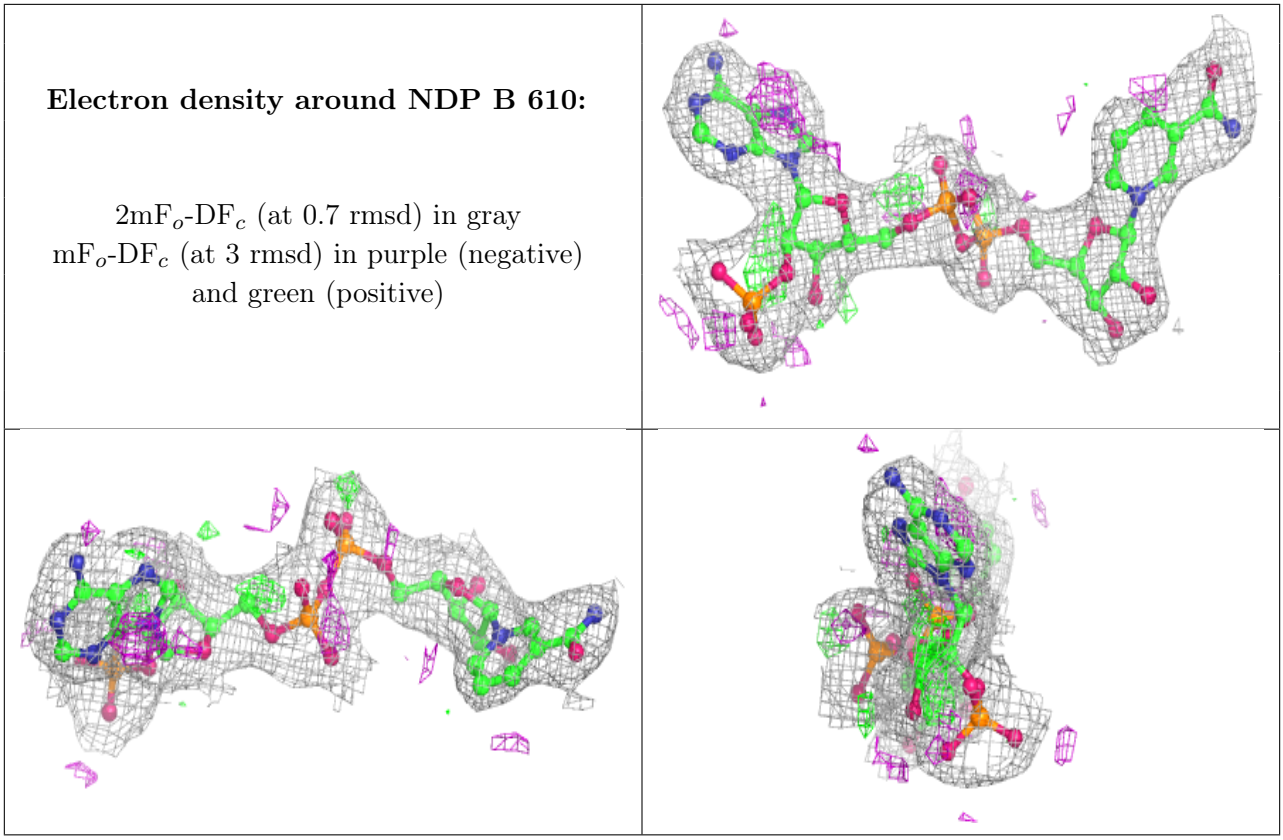
Electron density around NDP A 606:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.