



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:49 am BST

PDB ID : 6OJS
Title : Crystal structure of TS-DHFR from *Cryptosporidium hominis* in complex with NADPH, FdUMP, MTX and 2-amino-4-oxo-4,7-dihydro-pyrrolo[2,3-d]pyrimidine-methyl-phenyl-D-glutamic acid
Authors : Czyzyk, D.J.; Anderson, K.S.; Jorgensen, W.L.; Valhondo, M.
Deposited on : 2019-04-12
Resolution : 3.21 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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 : 2.11
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) : 2.11

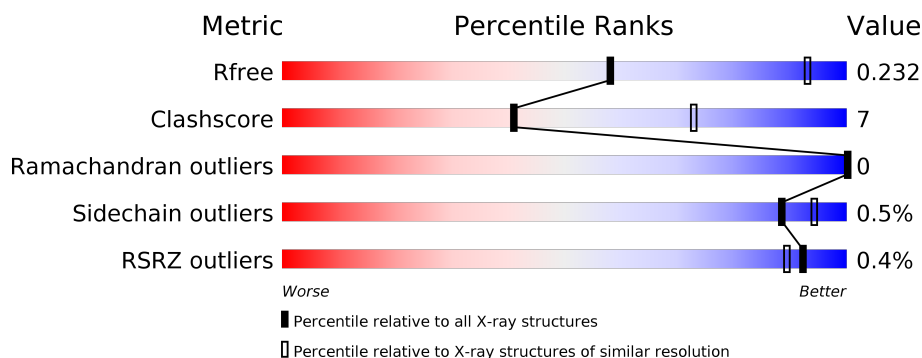
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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 on 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>81%</div> <div>17%</div> <div>•</div> </div>
1	B	521	<div> <div>81%</div> <div>16%</div> <div>•</div> </div>
1	C	521	<div> <div>78%</div> <div>19%</div> <div>•</div> </div>
1	D	521	<div> <div>82%</div> <div>15%</div> <div>•</div> </div>
1	E	521	<div> <div>78%</div> <div>19%</div> <div>•</div> </div>

2 Entry composition [i](#)

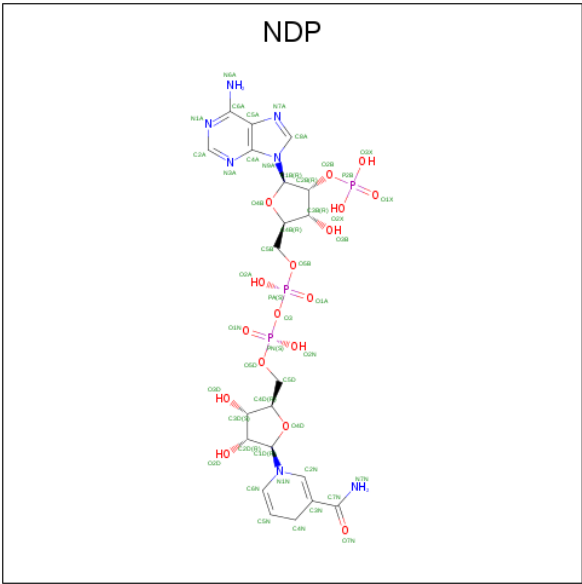
There are 5 unique types of molecules in this entry. The entry contains 20926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			4072	2602	684	765	21			
1	B	508	Total	C	N	O	S	0	0	0
			4056	2591	680	764	21			
1	C	508	Total	C	N	O	S	0	0	0
			4068	2598	682	767	21			
1	D	508	Total	C	N	O	S	0	0	0
			4016	2566	675	754	21			
1	E	508	Total	C	N	O	S	0	0	0
			4054	2591	683	759	21			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



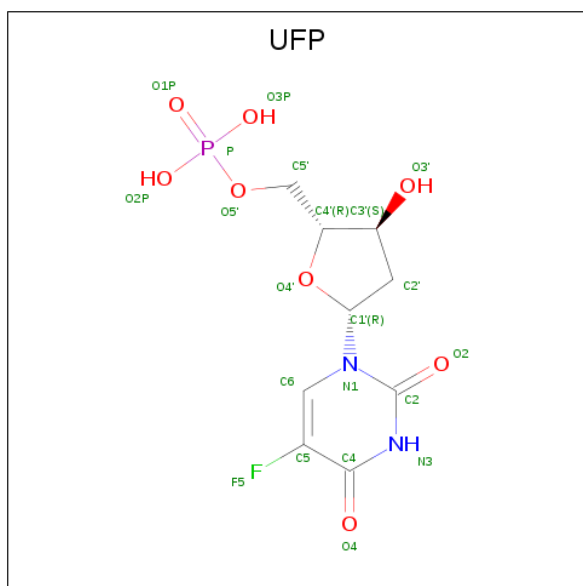
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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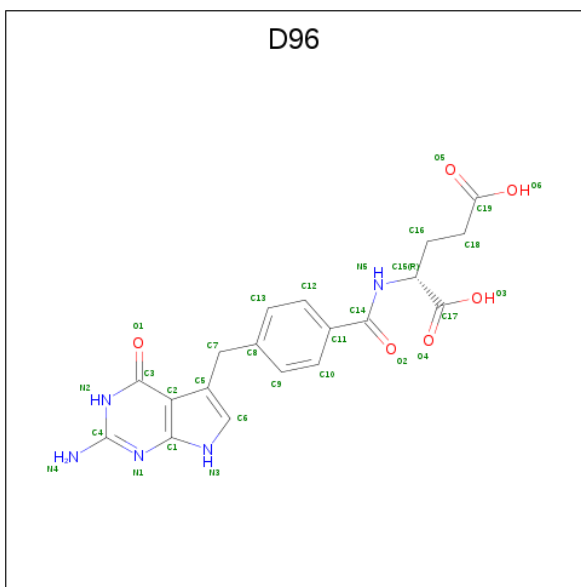
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: C₉H₁₂FN₂O₈P).



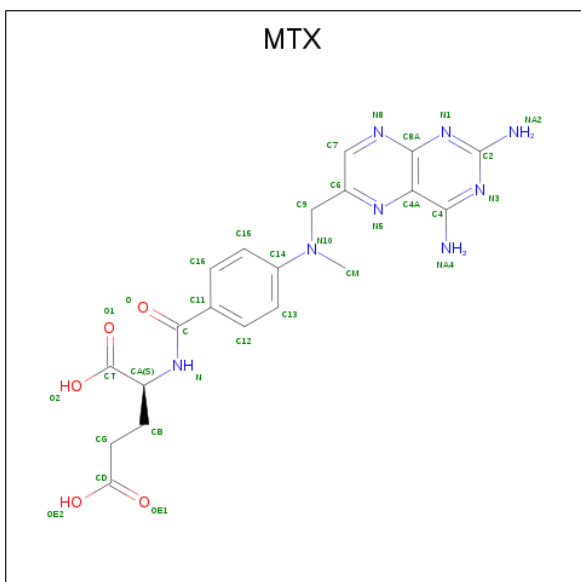
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is N-{4-[(2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl]benzene-1-carbonyl}-D-glutamic acid (three-letter code: D96) (formula: C₁₉H₁₉N₅O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			30	19	5	6		
4	B	1	Total	C	N	O	0	0
			30	19	5	6		
4	C	1	Total	C	N	O	0	0
			30	19	5	6		
4	D	1	Total	C	N	O	0	0
			30	19	5	6		
4	E	1	Total	C	N	O	0	0
			30	19	5	6		

- Molecule 5 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$).

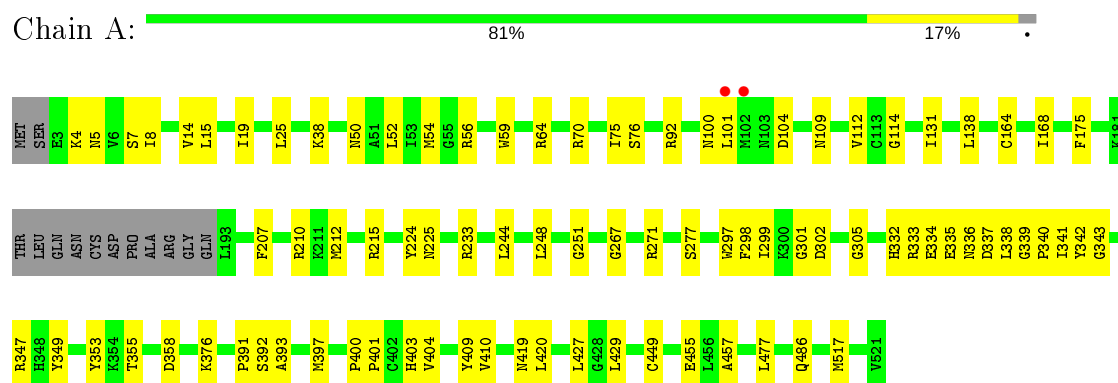


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 33	C 20	N 8	O 5	0	0
5	B	1	Total 33	C 20	N 8	O 5	0	0
5	C	1	Total 33	C 20	N 8	O 5	0	0
5	D	1	Total 33	C 20	N 8	O 5	0	0
5	E	1	Total 33	C 20	N 8	O 5	0	0

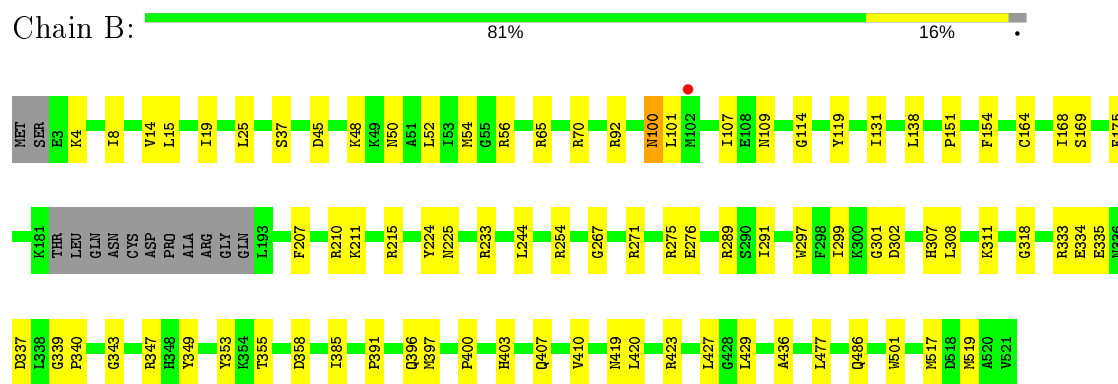
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

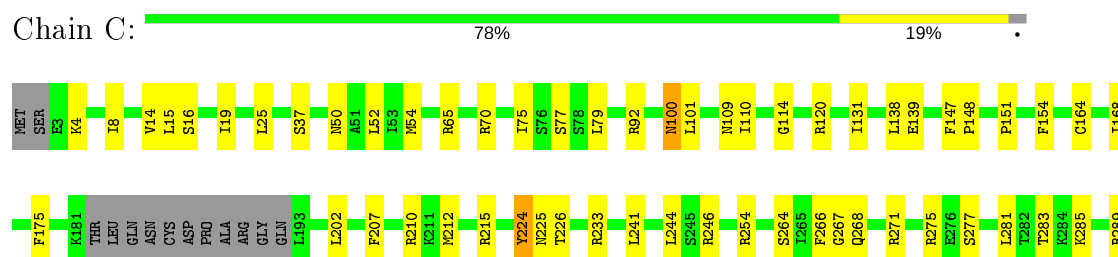
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

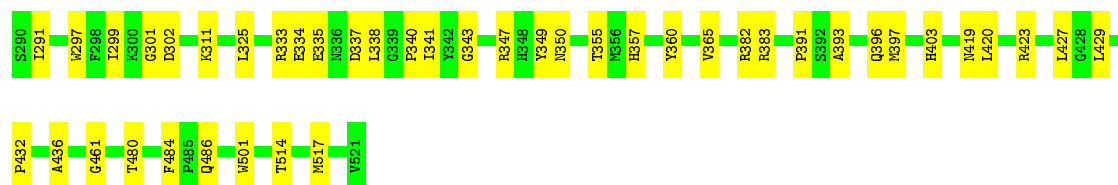


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



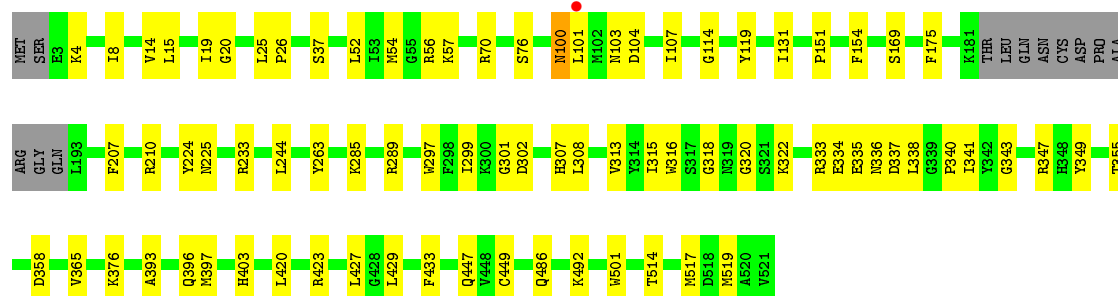
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





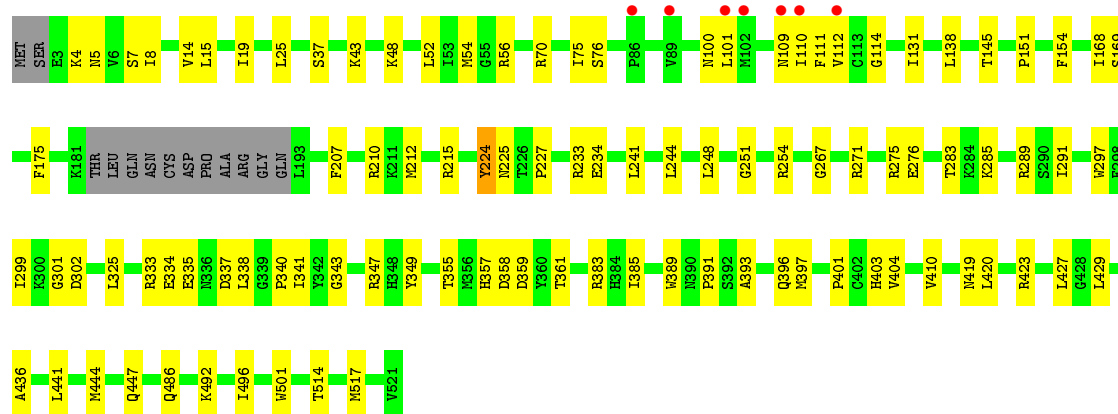
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain D: 82% 15% .



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain E: 78% 19% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.62Å 116.19Å 220.88Å 90.00° 95.48° 90.00°	Depositor
Resolution (Å)	50.12 – 3.21 50.12 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.12-3.21) 98.2 (50.12-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.32	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.218 , 0.232 0.218 , 0.232	Depositor DCC
R_{free} test set	4292 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	90.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20926	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: UFP, NDP, MTX, D96

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	0.25	0/4167	0.43	0/5647
1	B	0.25	0/4151	0.42	0/5630
1	C	0.26	0/4163	0.42	0/5644
1	D	0.25	0/4111	0.42	0/5585
1	E	0.25	0/4149	0.42	0/5626
All	All	0.25	0/20741	0.42	0/28132

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4072	0	3931	63	0
1	B	4056	0	3892	62	0
1	C	4068	0	3913	77	0
1	D	4016	0	3817	52	0
1	E	4054	0	3904	72	0
2	A	48	0	26	3	0
2	B	48	0	26	2	0
2	C	48	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	26	1	0
2	E	48	0	26	2	0
3	A	21	0	10	2	0
3	B	21	0	10	2	0
3	C	21	0	10	1	0
3	D	21	0	10	1	0
3	E	21	0	10	1	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
4	C	30	0	0	0	0
4	D	30	0	0	1	0
4	E	30	0	0	0	0
5	A	33	0	20	2	0
5	B	33	0	20	2	0
5	C	33	0	20	2	0
5	D	33	0	20	2	0
5	E	33	0	20	2	0
All	All	20926	0	19737	289	0

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 7.

All (289) 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:E:333:ARG:HG3	1:E:337:ASP:HB3	1.65	0.78
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.64	0.77
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.68	0.75
1:B:400:PRO:HG2	1:E:383:ARG:HE	1.52	0.74
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.69	0.73
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.69	0.72
1:B:267:GLY:O	1:E:271:ARG:NH2	2.23	0.72
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.72	0.71
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.73	0.71
1:C:225:ASN:O	1:C:233:ARG:NH2	2.25	0.70
1:D:225:ASN:O	1:D:233:ARG:NH2	2.25	0.69
1:A:400:PRO:HG2	1:C:383:ARG:HE	1.58	0.69
3:A:602:UFP:O3P	1:C:383:ARG:NH2	2.26	0.69
1:B:334:GLU:HG2	1:B:335:GLU:H	1.58	0.68
1:C:246:ARG:NH2	1:C:268:GLN:OE1	2.26	0.68
1:A:271:ARG:NH2	1:C:267:GLY:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ASN:O	1:B:233:ARG:NH2	2.27	0.67
1:A:267:GLY:O	1:C:271:ARG:NH2	2.27	0.67
1:D:8:ILE:HG22	1:D:131:ILE:HA	1.77	0.67
1:E:54:MET:HA	1:E:114:GLY:HA3	1.76	0.66
1:E:334:GLU:OE1	1:E:357:HIS:NE2	2.26	0.66
1:E:8:ILE:HG22	1:E:112:VAL:HB	1.76	0.66
1:A:225:ASN:O	1:A:233:ARG:NH2	2.27	0.65
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.77	0.65
1:D:100:ASN:N	1:D:100:ASN:OD1	2.30	0.64
1:E:423:ARG:NH1	3:E:602:UFP:O1P	2.27	0.64
1:B:25:LEU:HD11	5:B:604:MTX:H7	1.80	0.64
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.80	0.64
1:C:100:ASN:OD1	1:C:100:ASN:N	2.31	0.64
1:C:301:GLY:HA2	1:C:343:GLY:O	1.97	0.64
1:B:271:ARG:NH2	1:E:267:GLY:O	2.29	0.63
1:B:100:ASN:OD1	1:B:100:ASN:N	2.28	0.63
1:B:54:MET:HA	1:B:114:GLY:HA3	1.80	0.63
1:C:54:MET:HA	1:C:114:GLY:HA3	1.80	0.63
1:A:54:MET:HA	1:A:114:GLY:HA3	1.79	0.63
1:E:207:PHE:HB3	1:E:210:ARG:HB2	1.81	0.63
1:E:301:GLY:HA2	1:E:343:GLY:O	1.99	0.63
1:C:429:LEU:HD21	1:C:517:MET:HB2	1.80	0.63
1:D:54:MET:HA	1:D:114:GLY:HA3	1.81	0.63
1:A:25:LEU:HD11	5:A:604:MTX:H7	1.80	0.63
1:D:318:GLY:HA3	1:D:519:MET:HE1	1.81	0.62
1:A:4:LYS:H	1:A:101:LEU:HD22	1.65	0.62
1:A:429:LEU:HD21	1:A:517:MET:HB2	1.81	0.61
1:A:341:ILE:HG22	1:A:397:MET:HE3	1.83	0.61
1:C:341:ILE:HG22	1:C:397:MET:HE3	1.83	0.61
1:C:25:LEU:HD11	5:C:604:MTX:H7	1.82	0.61
1:D:207:PHE:HB3	1:D:210:ARG:HB2	1.82	0.61
1:D:25:LEU:HD11	5:D:604:MTX:H7	1.83	0.61
1:E:244:LEU:HD12	1:E:427:LEU:HD13	1.83	0.61
1:C:138:LEU:HD11	1:C:168:ILE:HD13	1.82	0.60
1:D:341:ILE:HG22	1:D:397:MET:HE2	1.82	0.60
1:C:244:LEU:HD12	1:C:427:LEU:HD13	1.84	0.60
1:E:341:ILE:HG22	1:E:397:MET:HE3	1.84	0.60
1:E:403:HIS:HB2	1:E:420:LEU:HD11	1.84	0.60
1:D:56:ARG:HH12	1:D:57:LYS:HE3	1.67	0.60
1:B:100:ASN:HB3	1:B:107:ILE:HD12	1.84	0.59
1:B:207:PHE:HB3	1:B:210:ARG:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:PHE:HB3	1:C:210:ARG:HB2	1.84	0.59
1:A:138:LEU:HD11	1:A:168:ILE:HD13	1.85	0.59
1:A:59:TRP:NE1	1:A:64:ARG:HG3	2.18	0.58
1:A:409:TYR:OH	1:C:264:SER:OG	2.22	0.58
1:D:334:GLU:HG2	1:D:335:GLU:H	1.69	0.58
1:B:244:LEU:HD12	1:B:427:LEU:HD13	1.86	0.58
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.85	0.58
1:E:138:LEU:HD11	1:E:168:ILE:HD13	1.85	0.57
1:E:325:LEU:HD23	1:E:333:ARG:HB3	1.87	0.57
1:A:207:PHE:HB3	1:A:210:ARG:HB2	1.86	0.57
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.86	0.57
1:E:52:LEU:HD11	1:E:70:ARG:HD2	1.85	0.56
1:C:52:LEU:HD11	1:C:70:ARG:HD2	1.87	0.56
1:A:301:GLY:HA2	1:A:343:GLY:O	2.05	0.56
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.88	0.56
1:C:65:ARG:NH2	1:E:248:LEU:O	2.39	0.56
1:E:333:ARG:NH2	1:E:396:GLN:O	2.32	0.56
1:A:4:LYS:NZ	1:A:104:ASP:O	2.39	0.56
1:D:320:GLY:O	1:D:336:ASN:ND2	2.39	0.56
1:B:297:TRP:CE2	1:B:308:LEU:HD11	2.41	0.56
1:B:349:TYR:OH	1:E:349:TYR:OH	2.21	0.55
1:E:100:ASN:OD1	1:E:110:ILE:HD11	2.06	0.55
1:A:455:GLU:OE2	1:C:215:ARG:NH1	2.40	0.55
1:B:423:ARG:NH1	3:B:602:UFP:O3P	2.36	0.55
1:B:52:LEU:HD11	1:B:70:ARG:HD2	1.87	0.55
1:D:301:GLY:HA2	1:D:343:GLY:O	2.06	0.55
1:B:301:GLY:HA2	1:B:343:GLY:O	2.06	0.55
1:C:334:GLU:OE1	1:C:357:HIS:NE2	2.36	0.55
1:E:25:LEU:HD11	5:E:604:MTX:H7	1.89	0.55
1:C:423:ARG:NH1	3:C:602:UFP:O1P	2.31	0.55
1:E:299:ILE:O	1:E:347:ARG:NH1	2.38	0.55
1:A:334:GLU:HG2	1:A:335:GLU:H	1.71	0.55
1:A:52:LEU:HD11	1:A:70:ARG:HD2	1.88	0.55
1:B:297:TRP:CD2	1:B:308:LEU:HD11	2.42	0.55
1:B:254:ARG:NH2	1:E:410:VAL:O	2.39	0.55
1:A:248:LEU:O	1:B:65:ARG:NH2	2.40	0.54
1:D:244:LEU:HD12	1:D:427:LEU:HD13	1.90	0.54
1:A:19:ILE:O	2:A:601:NDP:H2N	2.07	0.54
1:E:429:LEU:HD21	1:E:517:MET:HB2	1.89	0.54
1:E:225:ASN:O	1:E:233:ARG:NH2	2.41	0.54
1:B:138:LEU:HD11	1:B:168:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:PRO:O	1:C:397:MET:HG2	2.09	0.53
1:B:4:LYS:H	1:B:101:LEU:HD22	1.73	0.53
1:C:65:ARG:NH1	1:E:251:GLY:O	2.40	0.53
1:B:340:PRO:O	1:B:397:MET:HG2	2.09	0.53
1:D:340:PRO:O	1:D:397:MET:HG2	2.08	0.53
1:A:403:HIS:HB2	1:A:420:LEU:HD11	1.91	0.53
1:B:349:TYR:CE2	1:E:391:PRO:HD2	2.44	0.53
1:C:120:ARG:HG2	1:C:148:PRO:HB3	1.91	0.53
1:C:4:LYS:HG2	1:C:101:LEU:HD23	1.91	0.53
1:D:297:TRP:CD2	1:D:308:LEU:HD11	2.44	0.53
1:D:8:ILE:HD11	1:D:119:TYR:CD1	2.44	0.52
1:C:299:ILE:O	1:C:347:ARG:NH1	2.41	0.52
1:C:50:ASN:HD22	1:C:109:ASN:H	1.56	0.52
1:D:103:ASN:OD1	1:D:104:ASP:N	2.42	0.52
1:D:151:PRO:HG2	1:D:154:PHE:HD1	1.74	0.52
1:B:267:GLY:HA2	1:E:419:ASN:HD21	1.75	0.52
1:A:251:GLY:O	1:B:65:ARG:NH1	2.42	0.52
1:D:299:ILE:O	1:D:347:ARG:NH1	2.39	0.52
1:D:423:ARG:NH1	3:D:602:UFP:O3P	2.35	0.51
1:A:376:LYS:HD3	1:A:449:CYS:HA	1.92	0.51
1:B:410:VAL:O	1:E:254:ARG:NH2	2.41	0.51
1:C:349:TYR:HB3	1:C:365:VAL:HB	1.91	0.51
1:E:340:PRO:O	1:E:397:MET:HG2	2.09	0.51
1:A:50:ASN:HD22	1:A:109:ASN:H	1.57	0.51
1:B:419:ASN:HD21	1:E:267:GLY:HA2	1.75	0.51
1:A:164:CYS:O	1:C:210:ARG:NH2	2.44	0.51
1:B:299:ILE:O	1:B:347:ARG:NH1	2.38	0.51
1:E:297:TRP:HH2	1:E:338:LEU:HD12	1.76	0.51
1:D:349:TYR:HB3	1:D:365:VAL:HB	1.92	0.50
1:B:429:LEU:HD21	1:B:517:MET:HB2	1.92	0.50
1:B:391:PRO:HD2	1:E:349:TYR:CE2	2.46	0.50
1:A:215:ARG:CZ	1:C:275:ARG:HD2	2.42	0.50
1:A:392:SER:HG	1:C:350:ASN:HD22	1.59	0.50
1:E:444:MET:HB3	1:E:496:ILE:HD11	1.93	0.50
1:C:285:LYS:HB3	1:C:514:THR:HB	1.94	0.50
1:A:299:ILE:O	1:A:347:ARG:NH1	2.43	0.50
1:A:393:ALA:O	1:A:397:MET:HG3	2.12	0.50
1:A:340:PRO:HD3	1:A:353:TYR:CD2	2.47	0.49
1:E:43:LYS:NZ	1:E:48:LYS:O	2.46	0.49
1:A:340:PRO:O	1:A:397:MET:HG2	2.13	0.49
1:E:151:PRO:HG2	1:E:154:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ILE:O	2:E:601:NDP:H2N	2.12	0.49
1:B:164:CYS:O	1:E:210:ARG:NH2	2.45	0.49
1:A:410:VAL:O	1:C:254:ARG:NH2	2.42	0.49
1:C:19:ILE:O	2:C:601:NDP:H2N	2.13	0.49
1:B:215:ARG:CZ	1:E:275:ARG:HD2	2.42	0.49
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.93	0.49
1:A:244:LEU:HD12	1:A:427:LEU:HD13	1.93	0.48
1:B:291:ILE:HD13	1:B:436:ALA:HB3	1.94	0.48
1:A:349:TYR:OH	1:C:349:TYR:OH	2.29	0.48
1:A:267:GLY:HA2	1:C:419:ASN:HD21	1.78	0.48
1:B:14:VAL:HG13	1:B:15:LEU:HG	1.95	0.48
1:D:447:GLN:NE2	1:D:492:LYS:HA	2.27	0.48
1:C:100:ASN:HB2	1:C:110:ILE:HD11	1.96	0.48
1:A:392:SER:OG	1:C:350:ASN:ND2	2.39	0.48
1:C:334:GLU:HG2	1:C:335:GLU:H	1.76	0.48
1:D:315:ILE:HD11	1:D:433:PHE:HE2	1.76	0.48
1:E:299:ILE:HD11	1:E:441:LEU:HD13	1.96	0.48
1:B:50:ASN:HD22	1:B:109:ASN:H	1.62	0.48
1:B:275:ARG:HD2	1:E:215:ARG:CZ	2.44	0.48
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.95	0.47
1:E:276:GLU:O	1:E:486:GLN:NE2	2.37	0.47
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.49	0.47
1:D:315:ILE:HG23	4:D:603:D96:C9	2.44	0.47
1:A:391:PRO:HD2	1:C:349:TYR:CE2	2.49	0.47
1:B:8:ILE:HD11	1:B:119:TYR:CD1	2.49	0.47
1:B:19:ILE:O	2:B:601:NDP:H2N	2.14	0.47
3:B:602:UFP:O2P	1:E:383:ARG:NH2	2.47	0.47
1:B:271:ARG:HG2	1:E:212:MET:HE1	1.96	0.47
1:C:297:TRP:CD1	1:C:302:ASP:HB3	2.50	0.47
1:E:389:TRP:HE3	1:E:401:PRO:HG2	1.79	0.47
1:A:349:TYR:CE2	1:C:391:PRO:HD2	2.49	0.47
1:B:151:PRO:HG2	1:B:154:PHE:HD1	1.79	0.47
1:A:14:VAL:HG13	1:A:15:LEU:HG	1.97	0.47
1:C:14:VAL:HG13	1:C:15:LEU:HG	1.97	0.47
1:D:289:ARG:HG3	1:D:501:TRP:CE2	2.49	0.47
1:E:393:ALA:O	1:E:397:MET:HG3	2.15	0.47
1:B:355:THR:OG1	1:B:358:ASP:OD2	2.27	0.47
1:E:14:VAL:HG13	1:E:15:LEU:HG	1.95	0.47
1:A:56:ARG:HB2	1:A:76:SER:HB2	1.97	0.46
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.98	0.46
1:E:289:ARG:HG3	1:E:501:TRP:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:PRO:HG2	1:C:154:PHE:HD1	1.80	0.46
1:E:359:ASP:OD1	1:E:361:THR:OG1	2.31	0.46
1:D:56:ARG:HB2	1:D:76:SER:HB2	1.98	0.46
1:E:5:ASN:ND2	1:E:7:SER:OG	2.47	0.46
1:D:333:ARG:NH2	1:D:396:GLN:O	2.35	0.46
1:C:325:LEU:HD23	1:C:333:ARG:HB3	1.98	0.46
1:B:92:ARG:HA	1:B:92:ARG:HD3	1.77	0.46
1:E:291:ILE:HD13	1:E:436:ALA:HB3	1.97	0.46
1:C:8:ILE:HD11	1:C:147:PHE:HE1	1.80	0.46
1:D:355:THR:OG1	1:D:358:ASP:OD2	2.29	0.46
1:E:401:PRO:HG2	1:E:404:VAL:HG12	1.98	0.45
1:E:4:LYS:H	1:E:101:LEU:HD22	1.80	0.45
1:D:322:LYS:N	1:D:335:GLU:OE2	2.49	0.45
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.82	0.45
3:A:602:UFP:O1P	1:C:382:ARG:NH1	2.50	0.45
1:E:19:ILE:HD11	1:E:145:THR:HG22	1.98	0.45
1:D:316:TRP:HB3	1:D:338:LEU:HD11	1.97	0.45
1:D:37:SER:OG	5:D:604:MTX:HB1	2.16	0.45
1:A:419:ASN:ND2	1:A:457:ALA:HB3	2.32	0.45
1:A:210:ARG:NH2	1:C:164:CYS:O	2.49	0.45
1:C:289:ARG:HG3	1:C:501:TRP:CE2	2.52	0.45
1:B:297:TRP:CD1	1:B:302:ASP:HB3	2.52	0.44
1:A:38:LYS:HB3	1:C:202:LEU:HD13	1.99	0.44
1:C:212:MET:HG3	1:C:215:ARG:NH1	2.31	0.44
1:C:393:ALA:O	1:C:397:MET:HG3	2.18	0.44
1:B:45:ASP:HB3	1:B:48:LYS:HB2	2.00	0.44
1:C:333:ARG:NH2	1:C:396:GLN:O	2.41	0.44
1:D:14:VAL:HG13	1:D:15:LEU:HG	1.98	0.44
1:C:77:SER:OG	2:C:601:NDP:O3X	2.27	0.44
1:A:75:ILE:O	2:A:601:NDP:H1B	2.18	0.44
1:C:92:ARG:HA	1:C:92:ARG:HD3	1.72	0.44
1:D:297:TRP:CE2	1:D:308:LEU:HD11	2.53	0.44
1:D:169:SER:OG	1:D:486:GLN:HG2	2.18	0.43
1:B:385:ILE:HD13	1:B:407:GLN:HB2	2.00	0.43
1:B:164:CYS:HB2	1:B:486:GLN:NE2	2.33	0.43
1:A:8:ILE:HG12	1:A:112:VAL:HB	2.00	0.43
1:E:37:SER:OG	5:E:604:MTX:HB1	2.19	0.43
1:C:37:SER:OG	5:C:604:MTX:HB1	2.19	0.43
1:D:285:LYS:HB3	1:D:514:THR:HB	2.00	0.43
1:D:429:LEU:HD21	1:D:517:MET:HB2	2.01	0.43
1:D:151:PRO:HG2	1:D:154:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASN:ND2	1:A:7:SER:OG	2.52	0.43
1:B:307:HIS:O	1:B:311:LYS:HG3	2.18	0.43
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.84	0.43
1:A:225:ASN:ND2	1:A:477:LEU:O	2.51	0.43
1:B:56:ARG:NH1	2:B:601:NDP:O1X	2.43	0.43
1:C:16:SER:N	1:C:139:GLU:OE2	2.39	0.42
1:E:297:TRP:CD1	1:E:302:ASP:HB3	2.53	0.42
1:E:341:ILE:HA	1:E:397:MET:HE3	2.01	0.42
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.54	0.42
1:A:337:ASP:OD1	1:A:353:TYR:OH	2.30	0.42
1:C:79:LEU:HA	1:C:79:LEU:HD23	1.93	0.42
1:A:298:PHE:CE1	1:A:342:TYR:HB2	2.53	0.42
1:C:75:ILE:O	2:C:601:NDP:H1B	2.19	0.42
1:D:376:LYS:HD3	1:D:449:CYS:HA	2.01	0.42
1:A:277:SER:HA	1:A:486:GLN:OE1	2.19	0.42
2:A:601:NDP:H42N	5:A:604:MTX:N5	2.35	0.42
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.55	0.42
1:A:212:MET:HE1	1:C:271:ARG:HG2	2.01	0.42
1:D:19:ILE:O	2:D:601:NDP:H2N	2.19	0.42
1:E:56:ARG:HB3	1:E:76:SER:HB2	2.01	0.42
1:A:164:CYS:SG	1:A:486:GLN:NE2	2.93	0.42
1:B:276:GLU:O	1:B:486:GLN:NE2	2.37	0.42
1:D:393:ALA:O	1:D:397:MET:HG3	2.20	0.42
1:D:4:LYS:NZ	1:D:107:ILE:O	2.34	0.42
1:B:423:ARG:HB3	1:E:385:ILE:HD11	2.02	0.42
1:C:277:SER:HA	1:C:486:GLN:OE1	2.20	0.42
1:C:79:LEU:O	1:C:92:ARG:NH2	2.51	0.42
1:D:315:ILE:HD11	1:D:433:PHE:CE2	2.54	0.41
1:B:37:SER:OG	5:B:604:MTX:HB1	2.20	0.41
1:D:20:GLY:HA2	1:D:26:PRO:HD3	2.02	0.41
1:D:302:ASP:OD2	1:D:307:HIS:ND1	2.33	0.41
1:A:401:PRO:HG2	1:A:404:VAL:HG12	2.03	0.41
1:B:339:GLY:HA2	1:B:353:TYR:CZ	2.55	0.41
1:A:339:GLY:HA2	1:A:353:TYR:CE2	2.56	0.41
1:C:50:ASN:ND2	1:C:109:ASN:H	2.17	0.41
1:B:211:LYS:HE2	1:E:234:GLU:OE2	2.20	0.41
1:A:305:GLY:HA3	1:A:336:ASN:HB3	2.02	0.41
1:A:355:THR:OG1	1:A:358:ASP:OD2	2.31	0.41
1:B:333:ARG:NH2	1:B:396:GLN:O	2.36	0.41
1:C:8:ILE:HG23	1:C:131:ILE:HA	2.03	0.41
1:E:5:ASN:HB3	1:E:109:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HA	1:A:92:ARG:HD3	1.79	0.41
1:B:225:ASN:ND2	1:B:477:LEU:O	2.54	0.41
1:C:355:THR:O	1:C:360:TYR:OH	2.26	0.41
1:E:355:THR:OG1	1:E:358:ASP:OD2	2.37	0.41
1:B:385:ILE:HB	1:E:389:TRP:CZ2	2.56	0.41
1:E:334:GLU:HG2	1:E:335:GLU:H	1.84	0.41
1:E:447:GLN:NE2	1:E:492:LYS:HA	2.36	0.41
1:D:4:LYS:HE3	1:D:101:LEU:HA	2.03	0.41
1:E:7:SER:O	1:E:111:PHE:HA	2.20	0.41
1:E:75:ILE:O	2:E:601:NDP:H1B	2.21	0.41
1:C:224:TYR:HD1	1:C:224:TYR:HA	1.78	0.41
1:C:277:SER:HB2	1:C:484:PHE:HB2	2.03	0.41
1:E:285:LYS:HB3	1:E:514:THR:HB	2.02	0.41
1:A:59:TRP:CE2	1:A:64:ARG:HG3	2.56	0.40
1:C:289:ARG:NH2	1:C:311:LYS:O	2.52	0.40
1:D:403:HIS:H	1:D:403:HIS:CD2	2.39	0.40
1:E:169:SER:OG	1:E:486:GLN:HG2	2.21	0.40
1:C:241:LEU:HD11	1:C:283:THR:HG21	2.04	0.40
1:B:318:GLY:HA3	1:B:519:MET:HE1	2.02	0.40
1:E:224:TYR:HB3	1:E:227:PRO:HB3	2.02	0.40
1:E:241:LEU:HD11	1:E:283:THR:HG21	2.04	0.40
1:A:403:HIS:CD2	1:A:403:HIS:H	2.38	0.40
1:C:266:PHE:HA	1:C:461:GLY:O	2.21	0.40
1:C:226:THR:OG1	1:C:480:THR:HG22	2.20	0.40
1:D:308:LEU:HB3	1:D:313:VAL:HB	2.03	0.40
1:B:169:SER:OG	1:B:486:GLN:HG2	2.21	0.40
1:C:281:LEU:HD12	1:C:432:PRO:HB3	2.03	0.40

There are no symmetry-related clashes.

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%)	474 (94%)	30 (6%)	0	100	100
1	B	504/521 (97%)	472 (94%)	32 (6%)	0	100	100
1	C	504/521 (97%)	475 (94%)	29 (6%)	0	100	100
1	D	504/521 (97%)	475 (94%)	29 (6%)	0	100	100
1	E	504/521 (97%)	472 (94%)	32 (6%)	0	100	100
All	All	2520/2605 (97%)	2368 (94%)	152 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	441/470 (94%)	438 (99%)	3 (1%)	84	93
1	B	437/470 (93%)	435 (100%)	2 (0%)	88	94
1	C	440/470 (94%)	438 (100%)	2 (0%)	88	94
1	D	427/470 (91%)	424 (99%)	3 (1%)	84	93
1	E	437/470 (93%)	436 (100%)	1 (0%)	93	97
All	All	2182/2350 (93%)	2171 (100%)	11 (0%)	88	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	224	TYR
1	A	332	HIS
1	B	100	ASN
1	B	224	TYR
1	C	100	ASN
1	C	224	TYR
1	D	100	ASN
1	D	224	TYR
1	D	263	TYR

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Mol	Chain	Res	Type
1	E	224	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	24	GLN
1	A	50	ASN
1	A	332	HIS
1	A	336	ASN
1	A	422	GLN
1	A	486	GLN
1	B	50	ASN
1	B	126	ASN
1	B	336	ASN
1	B	422	GLN
1	C	5	ASN
1	C	50	ASN
1	C	336	ASN
1	C	422	GLN
1	C	486	GLN
1	D	336	ASN
1	D	422	GLN
1	E	5	ASN
1	E	336	ASN
1	E	403	HIS
1	E	422	GLN
1	E	447	GLN

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 carbohydrates 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
5	MTX	A	604	-	29,35,35	1.78	7 (24%)	38,49,49	1.87	8 (21%)
4	D96	C	603	-	25,32,32	1.55	3 (12%)	26,45,45	3.79	10 (38%)
5	MTX	B	604	-	29,35,35	1.77	7 (24%)	38,49,49	1.88	8 (21%)
4	D96	B	603	-	25,32,32	1.55	3 (12%)	26,45,45	3.85	9 (34%)
2	NDP	D	601	-	45,52,52	1.96	10 (22%)	53,80,80	1.17	5 (9%)
3	UFP	E	602	-	19,22,22	1.37	3 (15%)	24,33,33	2.13	5 (20%)
3	UFP	C	602	-	19,22,22	1.13	1 (5%)	24,33,33	2.13	5 (20%)
2	NDP	B	601	-	45,52,52	1.96	10 (22%)	53,80,80	1.18	5 (9%)
5	MTX	D	604	-	29,35,35	1.78	7 (24%)	38,49,49	1.92	9 (23%)
5	MTX	E	604	-	29,35,35	1.78	7 (24%)	38,49,49	1.86	8 (21%)
3	UFP	A	602	-	19,22,22	1.36	2 (10%)	24,33,33	2.16	4 (16%)
3	UFP	B	602	-	19,22,22	1.15	2 (10%)	24,33,33	2.15	4 (16%)
4	D96	E	603	-	25,32,32	1.56	3 (12%)	26,45,45	3.79	7 (26%)
4	D96	A	603	-	25,32,32	1.56	3 (12%)	26,45,45	3.82	10 (38%)
2	NDP	E	601	-	45,52,52	1.95	10 (22%)	53,80,80	1.17	6 (11%)
3	UFP	D	602	-	19,22,22	1.15	1 (5%)	24,33,33	2.08	5 (20%)
5	MTX	C	604	-	29,35,35	1.78	7 (24%)	38,49,49	1.89	7 (18%)
2	NDP	C	601	-	45,52,52	1.96	11 (24%)	53,80,80	1.17	7 (13%)
2	NDP	A	601	-	45,52,52	1.98	10 (22%)	53,80,80	1.16	6 (11%)
4	D96	D	603	-	25,32,32	1.54	3 (12%)	26,45,45	3.89	7 (26%)

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
5	MTX	A	604	-	-	5/19/25/25	0/3/3/3
4	D96	C	603	-	-	2/15/21/21	0/3/3/3
5	MTX	B	604	-	-	6/19/25/25	0/3/3/3
4	D96	B	603	-	-	4/15/21/21	0/3/3/3
2	NDP	D	601	-	-	8/30/77/77	0/5/5/5
3	UFP	E	602	-	-	1/7/22/22	0/2/2/2
3	UFP	C	602	-	-	1/7/22/22	0/2/2/2
2	NDP	B	601	-	-	6/30/77/77	0/5/5/5
5	MTX	D	604	-	-	6/19/25/25	0/3/3/3
5	MTX	E	604	-	-	5/19/25/25	0/3/3/3
3	UFP	A	602	-	-	1/7/22/22	0/2/2/2
3	UFP	B	602	-	-	1/7/22/22	0/2/2/2
4	D96	E	603	-	-	0/15/21/21	0/3/3/3
4	D96	A	603	-	-	0/15/21/21	0/3/3/3
2	NDP	E	601	-	-	9/30/77/77	0/5/5/5
3	UFP	D	602	-	-	1/7/22/22	0/2/2/2
5	MTX	C	604	-	-	6/19/25/25	0/3/3/3
2	NDP	C	601	-	-	5/30/77/77	0/5/5/5
2	NDP	A	601	-	-	5/30/77/77	0/5/5/5
4	D96	D	603	-	-	4/15/21/21	0/3/3/3

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	D96	C4-N4	6.25	1.46	1.33
4	B	603	D96	C4-N4	6.24	1.46	1.33
4	C	603	D96	C4-N4	6.23	1.46	1.33
4	A	603	D96	C4-N4	6.23	1.46	1.33
4	E	603	D96	C4-N4	6.21	1.46	1.33
5	E	604	MTX	C2-NA2	5.34	1.44	1.33
5	B	604	MTX	C2-NA2	5.31	1.44	1.33
5	D	604	MTX	C2-NA2	5.30	1.44	1.33
5	C	604	MTX	C2-NA2	5.28	1.44	1.33
5	A	604	MTX	C2-NA2	5.25	1.44	1.33
5	C	604	MTX	C-N	4.88	1.44	1.34
5	A	604	MTX	C-N	4.88	1.44	1.34
5	B	604	MTX	C-N	4.86	1.44	1.34
5	E	604	MTX	C-N	4.84	1.44	1.34
5	D	604	MTX	C-N	4.84	1.44	1.34
2	C	601	NDP	C4N-C3N	-4.57	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NDP	C4N-C3N	-4.55	1.41	1.49
2	A	601	NDP	C4N-C3N	-4.53	1.41	1.49
2	D	601	NDP	C4N-C3N	-4.52	1.41	1.49
2	B	601	NDP	C4N-C3N	-4.48	1.41	1.49
2	B	601	NDP	C6A-N6A	4.11	1.49	1.34
2	A	601	NDP	C6A-N6A	4.08	1.49	1.34
2	C	601	NDP	C6A-N6A	4.07	1.48	1.34
2	D	601	NDP	C6A-N6A	4.07	1.48	1.34
2	A	601	NDP	C2D-C3D	-4.06	1.42	1.53
2	E	601	NDP	C6A-N6A	4.05	1.48	1.34
2	E	601	NDP	C7N-N7N	3.98	1.44	1.33
2	B	601	NDP	C2D-C3D	-3.97	1.42	1.53
2	B	601	NDP	C7N-N7N	3.97	1.44	1.33
2	D	601	NDP	C2D-C3D	-3.96	1.42	1.53
2	C	601	NDP	C7N-N7N	3.96	1.43	1.33
2	B	601	NDP	C3B-C2B	-3.95	1.44	1.52
2	A	601	NDP	C7N-N7N	3.95	1.43	1.33
2	D	601	NDP	C7N-N7N	3.94	1.43	1.33
2	C	601	NDP	C2D-C3D	-3.94	1.42	1.53
2	E	601	NDP	C2D-C3D	-3.93	1.42	1.53
2	A	601	NDP	C3B-C2B	-3.89	1.44	1.52
2	D	601	NDP	C3B-C2B	-3.82	1.44	1.52
2	E	601	NDP	C3B-C2B	-3.80	1.44	1.52
2	C	601	NDP	C3B-C2B	-3.78	1.44	1.52
2	A	601	NDP	C6N-C5N	3.63	1.39	1.33
2	E	601	NDP	C6N-C5N	3.60	1.39	1.33
2	D	601	NDP	C6N-C5N	3.57	1.39	1.33
2	C	601	NDP	C6N-C5N	3.57	1.39	1.33
2	B	601	NDP	C6N-C5N	3.56	1.39	1.33
5	A	604	MTX	CB-CA	-3.32	1.49	1.53
5	E	604	MTX	CB-CA	-3.29	1.49	1.53
2	E	601	NDP	C4N-C5N	-3.24	1.40	1.48
5	C	604	MTX	CB-CA	-3.23	1.49	1.53
3	E	602	UFP	P-O1P	3.23	1.61	1.50
3	A	602	UFP	P-O1P	3.23	1.60	1.50
5	B	604	MTX	CB-CA	-3.22	1.49	1.53
2	C	601	NDP	C4N-C5N	-3.21	1.40	1.48
2	B	601	NDP	C4N-C5N	-3.20	1.40	1.48
2	A	601	NDP	C4N-C5N	-3.20	1.40	1.48
2	D	601	NDP	C4N-C5N	-3.19	1.40	1.48
5	D	604	MTX	CB-CA	-3.17	1.49	1.53
3	E	602	UFP	C4-C5	2.68	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	UFP	C4-C5	2.61	1.41	1.38
3	C	602	UFP	C4-C5	2.59	1.41	1.38
4	E	603	D96	C16-C15	-2.58	1.50	1.53
3	D	602	UFP	C4-C5	2.55	1.41	1.38
3	A	602	UFP	C4-C5	2.52	1.41	1.38
5	D	604	MTX	C4-NA4	2.51	1.43	1.34
5	B	604	MTX	C4-NA4	2.50	1.43	1.34
5	A	604	MTX	C4-NA4	2.50	1.43	1.34
5	C	604	MTX	C4-NA4	2.49	1.43	1.34
5	E	604	MTX	C4-NA4	2.48	1.43	1.34
4	A	603	D96	C16-C15	-2.47	1.50	1.53
2	B	601	NDP	C3B-C4B	-2.46	1.46	1.53
4	C	603	D96	C16-C15	-2.44	1.50	1.53
2	D	601	NDP	C3B-C4B	-2.44	1.46	1.53
2	C	601	NDP	C3B-C4B	-2.42	1.46	1.53
2	A	601	NDP	C3B-C4B	-2.42	1.46	1.53
2	E	601	NDP	C3B-C4B	-2.40	1.46	1.53
2	A	601	NDP	C3D-C4D	-2.39	1.46	1.53
4	A	603	D96	C3-N2	2.38	1.37	1.33
2	B	601	NDP	C3D-C4D	-2.38	1.46	1.53
4	B	603	D96	C16-C15	-2.37	1.50	1.53
4	B	603	D96	C3-N2	2.37	1.37	1.33
4	E	603	D96	C3-N2	2.37	1.37	1.33
4	D	603	D96	C3-N2	2.36	1.37	1.33
2	D	601	NDP	C3D-C4D	-2.31	1.47	1.53
4	C	603	D96	C3-N2	2.30	1.37	1.33
2	D	601	NDP	C4A-N3A	2.29	1.38	1.35
2	C	601	NDP	C3D-C4D	-2.29	1.47	1.53
5	D	604	MTX	C7-N8	2.29	1.35	1.31
5	C	604	MTX	C14-N10	2.29	1.45	1.39
5	E	604	MTX	C7-N8	2.28	1.35	1.31
5	C	604	MTX	C7-N8	2.27	1.35	1.31
5	B	604	MTX	C7-N8	2.27	1.35	1.31
5	A	604	MTX	C7-N8	2.27	1.35	1.31
5	A	604	MTX	C14-N10	2.25	1.45	1.39
5	E	604	MTX	C14-N10	2.25	1.45	1.39
2	E	601	NDP	C3D-C4D	-2.25	1.47	1.53
2	B	601	NDP	C4A-N3A	2.24	1.38	1.35
5	D	604	MTX	C14-N10	2.24	1.45	1.39
2	E	601	NDP	C4A-N3A	2.22	1.38	1.35
5	D	604	MTX	CA-N	-2.21	1.43	1.46
5	B	604	MTX	C14-N10	2.20	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NDP	C4A-N3A	2.16	1.38	1.35
5	A	604	MTX	CA-N	-2.16	1.43	1.46
5	B	604	MTX	CA-N	-2.15	1.43	1.46
3	E	602	UFP	C6-C5	-2.07	1.34	1.38
2	C	601	NDP	C5D-C4D	-2.06	1.45	1.51
2	C	601	NDP	C4A-N3A	2.06	1.38	1.35
4	D	603	D96	C16-C15	-2.04	1.50	1.53
5	C	604	MTX	CA-N	-2.04	1.43	1.46
3	B	602	UFP	C6-C5	-2.01	1.34	1.38
5	E	604	MTX	CA-N	-2.01	1.44	1.46

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	D96	C2-C3-N2	-15.45	110.39	124.09
4	B	603	D96	C2-C3-N2	-15.25	110.56	124.09
4	A	603	D96	C2-C3-N2	-15.15	110.65	124.09
4	C	603	D96	C2-C3-N2	-15.12	110.68	124.09
4	E	603	D96	C2-C3-N2	-15.06	110.73	124.09
3	A	602	UFP	C4-N3-C2	8.03	121.93	115.14
3	B	602	UFP	C4-N3-C2	7.96	121.86	115.14
3	C	602	UFP	C4-N3-C2	7.74	121.68	115.14
3	E	602	UFP	C4-N3-C2	7.61	121.57	115.14
4	D	603	D96	C3-N2-C4	7.59	127.98	115.93
3	D	602	UFP	C4-N3-C2	7.56	121.53	115.14
4	C	603	D96	C3-N2-C4	7.56	127.94	115.93
4	B	603	D96	C3-N2-C4	7.55	127.93	115.93
4	A	603	D96	C3-N2-C4	7.53	127.90	115.93
4	E	603	D96	C3-N2-C4	7.50	127.84	115.93
4	D	603	D96	C3-C2-C1	6.52	118.69	115.01
4	B	603	D96	C3-C2-C1	6.19	118.50	115.01
4	E	603	D96	C3-C2-C1	5.98	118.39	115.01
4	A	603	D96	C3-C2-C1	5.93	118.36	115.01
4	C	603	D96	C3-C2-C1	5.67	118.21	115.01
5	D	604	MTX	C6-C7-N8	-5.00	118.23	123.13
5	E	604	MTX	C6-C7-N8	-4.97	118.26	123.13
5	C	604	MTX	C6-C7-N8	-4.92	118.31	123.13
5	A	604	MTX	C6-C7-N8	-4.88	118.35	123.13
5	B	604	MTX	C6-C7-N8	-4.85	118.38	123.13
4	C	603	D96	N1-C4-N2	-4.57	121.12	127.22
4	E	603	D96	N1-C4-N2	-4.55	121.16	127.22
4	B	603	D96	N1-C4-N2	-4.51	121.21	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	D96	N1-C4-N2	-4.50	121.22	127.22
4	D	603	D96	N1-C4-N2	-4.45	121.29	127.22
5	E	604	MTX	N8-C8A-N1	4.02	120.41	115.82
5	D	604	MTX	C7-N8-C8A	4.00	120.71	116.69
5	D	604	MTX	N8-C8A-N1	3.97	120.36	115.82
2	D	601	NDP	N3A-C2A-N1A	-3.88	122.61	128.68
5	B	604	MTX	C7-N8-C8A	3.86	120.58	116.69
2	B	601	NDP	N3A-C2A-N1A	-3.86	122.64	128.68
5	C	604	MTX	N8-C8A-N1	3.86	120.22	115.82
5	E	604	MTX	C7-N8-C8A	3.82	120.53	116.69
5	C	604	MTX	N1-C2-N3	-3.82	122.13	127.22
5	A	604	MTX	N1-C2-N3	-3.77	122.19	127.22
5	A	604	MTX	C7-N8-C8A	3.77	120.48	116.69
5	C	604	MTX	C7-N8-C8A	3.77	120.48	116.69
5	D	604	MTX	CG-CB-CA	3.75	120.62	113.04
3	E	602	UFP	P-O5'-C5'	-3.75	107.97	118.30
5	E	604	MTX	N1-C2-N3	-3.75	122.23	127.22
2	E	601	NDP	N3A-C2A-N1A	-3.74	122.83	128.68
2	A	601	NDP	N3A-C2A-N1A	-3.73	122.86	128.68
5	B	604	MTX	N8-C8A-N1	3.72	120.07	115.82
5	D	604	MTX	N1-C2-N3	-3.72	122.26	127.22
5	B	604	MTX	N1-C2-N3	-3.70	122.28	127.22
5	A	604	MTX	N8-C8A-N1	3.70	120.04	115.82
2	C	601	NDP	N3A-C2A-N1A	-3.68	122.92	128.68
5	B	604	MTX	CG-CB-CA	3.68	120.47	113.04
5	C	604	MTX	C2-N1-C8A	3.67	119.55	115.36
3	A	602	UFP	C5-C4-N3	-3.66	118.53	122.39
3	B	602	UFP	C5-C4-N3	-3.64	118.55	122.39
5	D	604	MTX	C2-N1-C8A	3.64	119.52	115.36
2	A	601	NDP	PN-O3-PA	-3.62	120.39	132.83
5	E	604	MTX	C2-N1-C8A	3.62	119.49	115.36
2	C	601	NDP	PN-O3-PA	-3.61	120.44	132.83
5	A	604	MTX	C2-N1-C8A	3.56	119.42	115.36
3	C	602	UFP	P-O5'-C5'	-3.54	108.54	118.30
3	D	602	UFP	P-O5'-C5'	-3.50	108.64	118.30
5	B	604	MTX	C2-N1-C8A	3.48	119.33	115.36
3	C	602	UFP	C5-C4-N3	-3.48	118.72	122.39
3	E	602	UFP	C5-C4-N3	-3.47	118.73	122.39
3	A	602	UFP	P-O5'-C5'	-3.45	108.79	118.30
5	A	604	MTX	CG-CB-CA	3.44	120.00	113.04
2	B	601	NDP	PN-O3-PA	-3.44	121.03	132.83
3	B	602	UFP	P-O5'-C5'	-3.39	108.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	UFP	C5-C4-N3	-3.38	118.82	122.39
5	C	604	MTX	CG-CB-CA	3.24	119.59	113.04
2	E	601	NDP	PN-O3-PA	-3.22	121.78	132.83
2	D	601	NDP	PN-O3-PA	-3.19	121.88	132.83
5	E	604	MTX	CG-CB-CA	3.18	119.47	113.04
4	D	603	D96	C5-C7-C8	-2.93	107.18	114.21
2	B	601	NDP	O5B-C5B-C4B	2.91	119.02	108.99
2	E	601	NDP	O5B-C5B-C4B	2.89	118.95	108.99
4	E	603	D96	C5-C7-C8	-2.84	107.41	114.21
2	D	601	NDP	O5B-C5B-C4B	2.80	118.62	108.99
5	A	604	MTX	C4A-C4-N3	-2.57	119.32	121.01
5	B	604	MTX	C4A-C4-N3	-2.56	119.33	121.01
2	E	601	NDP	O5D-C5D-C4D	2.54	117.74	108.99
2	C	601	NDP	O5B-C5B-C4B	2.49	117.57	108.99
5	D	604	MTX	C4A-C4-N3	-2.49	119.37	121.01
2	A	601	NDP	O5B-C5B-C4B	2.48	117.54	108.99
3	E	602	UFP	O4'-C1'-C2'	-2.48	101.56	106.25
5	C	604	MTX	C4A-C4-N3	-2.44	119.41	121.01
2	B	601	NDP	C4A-C5A-N7A	-2.43	106.86	109.40
4	E	603	D96	C18-C16-C15	-2.43	108.14	113.04
4	A	603	D96	C11-C14-N5	-2.43	112.41	117.06
4	B	603	D96	N4-C4-N1	2.42	121.73	117.79
4	A	603	D96	O2-C14-C11	2.41	125.24	120.94
2	D	601	NDP	O5D-C5D-C4D	2.41	117.29	108.99
2	C	601	NDP	C4A-C5A-N7A	-2.39	106.91	109.40
3	E	602	UFP	C6-N1-C1'	-2.37	113.91	119.24
4	C	603	D96	C16-C18-C19	-2.37	108.50	113.59
2	E	601	NDP	C4A-C5A-N7A	-2.37	106.93	109.40
4	D	603	D96	N4-C4-N1	2.36	121.64	117.79
2	A	601	NDP	C4A-C5A-N7A	-2.36	106.94	109.40
2	B	601	NDP	O5D-C5D-C4D	2.35	117.08	108.99
2	D	601	NDP	C4A-C5A-N7A	-2.34	106.96	109.40
4	C	603	D96	C15-N5-C14	2.34	125.36	122.34
3	C	602	UFP	O4'-C1'-C2'	-2.34	101.84	106.25
5	E	604	MTX	C4A-C4-N3	-2.33	119.48	121.01
4	C	603	D96	N4-C4-N1	2.32	121.58	117.79
4	A	603	D96	N4-C4-N1	2.32	121.58	117.79
4	B	603	D96	C5-C7-C8	-2.31	108.66	114.21
4	E	603	D96	N4-C4-N1	2.28	121.51	117.79
3	C	602	UFP	C6-N1-C1'	-2.22	114.25	119.24
2	A	601	NDP	O5D-C5D-C4D	2.20	116.57	108.99
4	B	603	D96	O2-C14-C11	2.19	124.84	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604	MTX	CM-N10-C9	2.18	120.64	114.84
2	C	601	NDP	O5D-C5D-C4D	2.18	116.48	108.99
3	B	602	UFP	C6-N1-C1'	-2.17	114.37	119.24
4	B	603	D96	C11-C14-N5	-2.16	112.93	117.06
3	A	602	UFP	C6-N1-C1'	-2.15	114.41	119.24
3	D	602	UFP	O4'-C1'-C2'	-2.13	102.22	106.25
4	A	603	D96	C5-C7-C8	-2.11	109.15	114.21
3	D	602	UFP	C6-N1-C1'	-2.10	114.51	119.24
5	D	604	MTX	CB-CA-N	-2.10	107.14	110.19
2	C	601	NDP	C3N-C7N-N7N	2.10	121.39	117.67
4	B	603	D96	C15-N5-C14	2.09	125.03	122.34
5	A	604	MTX	CM-N10-C9	2.07	120.34	114.84
2	E	601	NDP	C3N-C7N-N7N	2.07	121.34	117.67
4	C	603	D96	O2-C14-C11	2.07	124.63	120.94
4	C	603	D96	C5-C7-C8	-2.07	109.25	114.21
4	C	603	D96	C11-C14-N5	-2.06	113.12	117.06
4	A	603	D96	C18-C16-C15	-2.06	108.89	113.04
5	E	604	MTX	CM-N10-C9	2.05	120.29	114.84
4	D	603	D96	O2-C14-C11	2.05	124.59	120.94
5	D	604	MTX	CM-N10-C9	2.04	120.26	114.84
2	C	601	NDP	C1D-N1N-C2N	-2.03	117.73	121.11
4	A	603	D96	C15-N5-C14	2.02	124.95	122.34
2	A	601	NDP	C1D-N1N-C2N	-2.01	117.77	121.11

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	604	MTX	N-CA-CB-CG
5	B	604	MTX	CT-CA-CB-CG
5	A	604	MTX	N-CA-CB-CG
5	A	604	MTX	CT-CA-CB-CG
5	D	604	MTX	CT-CA-N-C
5	D	604	MTX	N-CA-CB-CG
5	D	604	MTX	CT-CA-CB-CG
5	E	604	MTX	N-CA-CB-CG
5	E	604	MTX	CT-CA-CB-CG
2	E	601	NDP	C5D-O5D-PN-O1N
5	C	604	MTX	N-CA-CB-CG
5	C	604	MTX	CT-CA-CB-CG
4	D	603	D96	N5-C15-C16-C18
4	D	603	D96	C17-C15-C16-C18

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Mol	Chain	Res	Type	Atoms
2	D	601	NDP	C3D-C4D-C5D-O5D
2	E	601	NDP	C3D-C4D-C5D-O5D
2	D	601	NDP	O4D-C4D-C5D-O5D
2	E	601	NDP	O4D-C4D-C5D-O5D
5	B	604	MTX	CT-CA-N-C
5	A	604	MTX	CT-CA-N-C
5	E	604	MTX	CT-CA-N-C
5	C	604	MTX	CT-CA-N-C
4	C	603	D96	N5-C15-C16-C18
4	B	603	D96	C10-C11-C14-N5
4	B	603	D96	C10-C11-C14-O2
4	B	603	D96	C12-C11-C14-N5
4	B	603	D96	C12-C11-C14-O2
4	C	603	D96	C15-C16-C18-C19
4	D	603	D96	C15-C16-C18-C19
2	D	601	NDP	PA-O3-PN-O5D
2	B	601	NDP	PA-O3-PN-O5D
2	C	601	NDP	PA-O3-PN-O5D
2	E	601	NDP	PA-O3-PN-O5D
2	A	601	NDP	PA-O3-PN-O5D
2	D	601	NDP	C2B-O2B-P2B-O1X
2	B	601	NDP	C2B-O2B-P2B-O1X
2	C	601	NDP	C2B-O2B-P2B-O1X
2	E	601	NDP	C2B-O2B-P2B-O1X
2	A	601	NDP	C2B-O2B-P2B-O1X
2	D	601	NDP	C5D-O5D-PN-O3
2	E	601	NDP	C5D-O5D-PN-O3
2	D	601	NDP	C5D-O5D-PN-O2N
2	E	601	NDP	C5D-O5D-PN-O2N
4	D	603	D96	C17-C15-N5-C14
5	B	604	MTX	C6-C9-N10-CM
5	A	604	MTX	C6-C9-N10-CM
5	D	604	MTX	C6-C9-N10-CM
5	E	604	MTX	C6-C9-N10-CM
5	C	604	MTX	C6-C9-N10-CM
2	E	601	NDP	O4D-C1D-N1N-C2N
2	A	601	NDP	O4D-C1D-N1N-C2N
2	D	601	NDP	C4D-C5D-O5D-PN
2	D	601	NDP	O4D-C1D-N1N-C2N
2	B	601	NDP	O4D-C1D-N1N-C2N
2	C	601	NDP	O4D-C1D-N1N-C2N
2	B	601	NDP	C4D-C5D-O5D-PN

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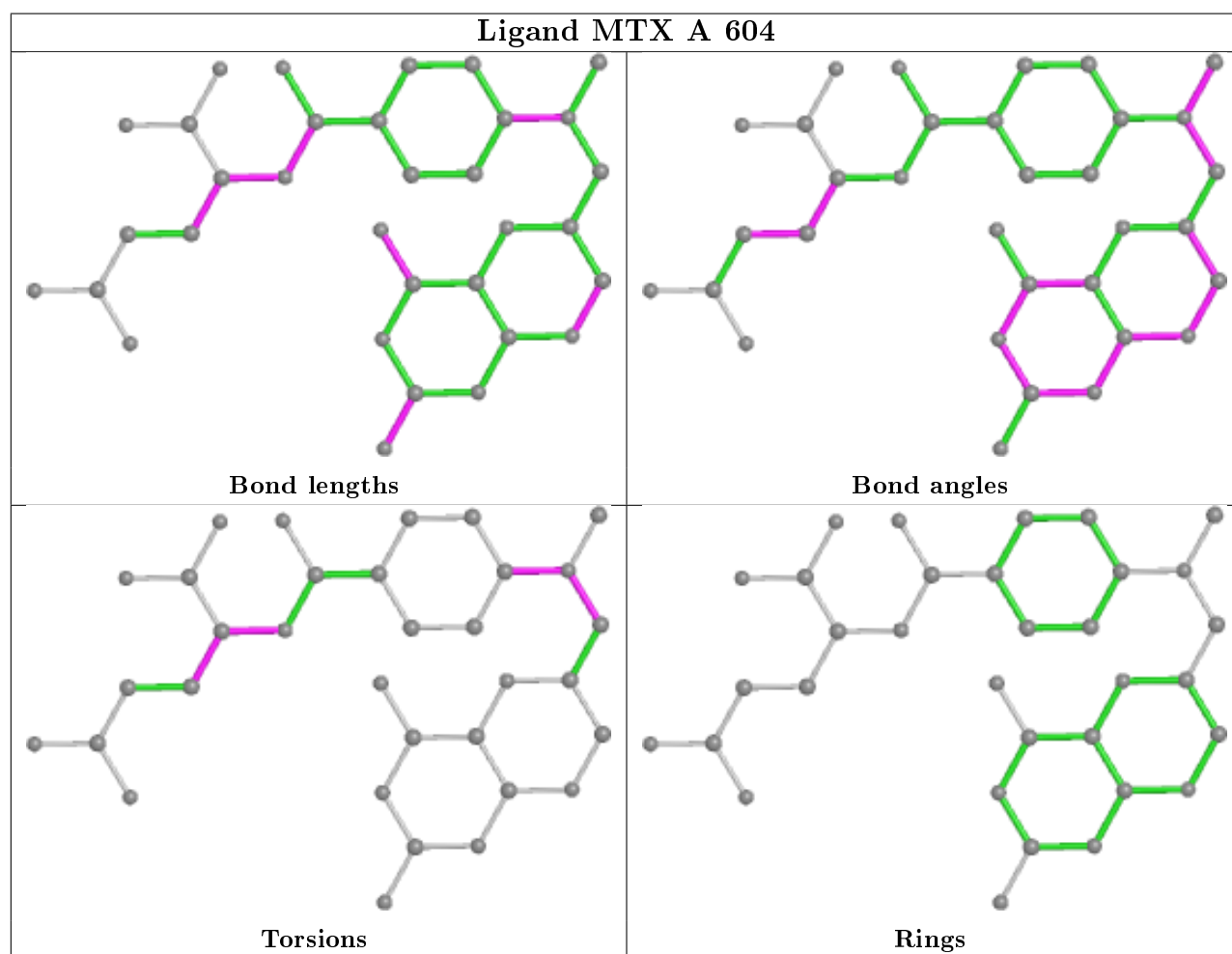
Mol	Chain	Res	Type	Atoms
2	C	601	NDP	C4D-C5D-O5D-PN
2	E	601	NDP	C4D-C5D-O5D-PN
2	A	601	NDP	C4D-C5D-O5D-PN
2	B	601	NDP	C2D-C1D-N1N-C2N
2	A	601	NDP	C2D-C1D-N1N-C2N
5	D	604	MTX	C15-C14-N10-CM
2	B	601	NDP	C3D-C4D-C5D-O5D
5	B	604	MTX	C15-C14-N10-CM
5	D	604	MTX	C13-C14-N10-CM
5	C	604	MTX	C15-C14-N10-CM
3	E	602	UFP	O4'-C4'-C5'-O5'
2	C	601	NDP	C3D-C4D-C5D-O5D
5	B	604	MTX	C13-C14-N10-CM
5	C	604	MTX	C13-C14-N10-CM
3	C	602	UFP	O4'-C4'-C5'-O5'
3	A	602	UFP	O4'-C4'-C5'-O5'
3	D	602	UFP	O4'-C4'-C5'-O5'
3	B	602	UFP	O4'-C4'-C5'-O5'
5	A	604	MTX	C13-C14-N10-CM
5	E	604	MTX	C13-C14-N10-CM

There are no ring outliers.

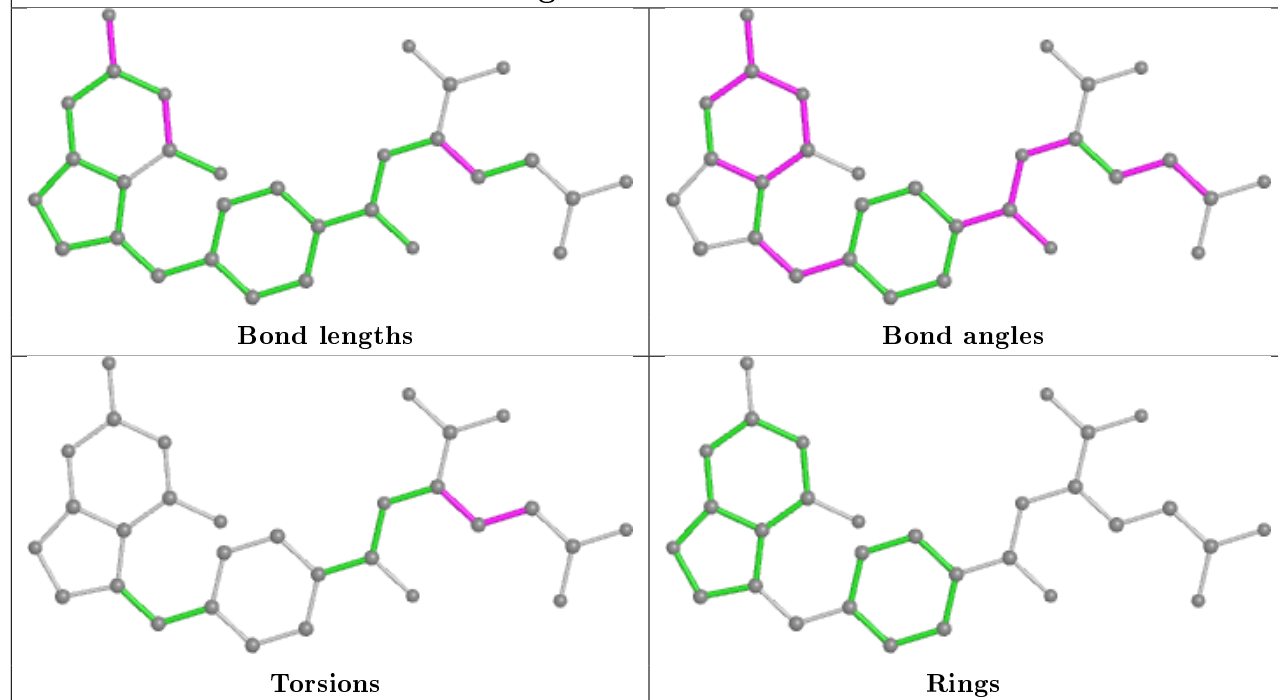
16 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	MTX	2	0
5	B	604	MTX	2	0
2	D	601	NDP	1	0
3	E	602	UFP	1	0
3	C	602	UFP	1	0
2	B	601	NDP	2	0
5	D	604	MTX	2	0
5	E	604	MTX	2	0
3	A	602	UFP	2	0
3	B	602	UFP	2	0
2	E	601	NDP	2	0
3	D	602	UFP	1	0
5	C	604	MTX	2	0
2	C	601	NDP	3	0
2	A	601	NDP	3	0
4	D	603	D96	1	0

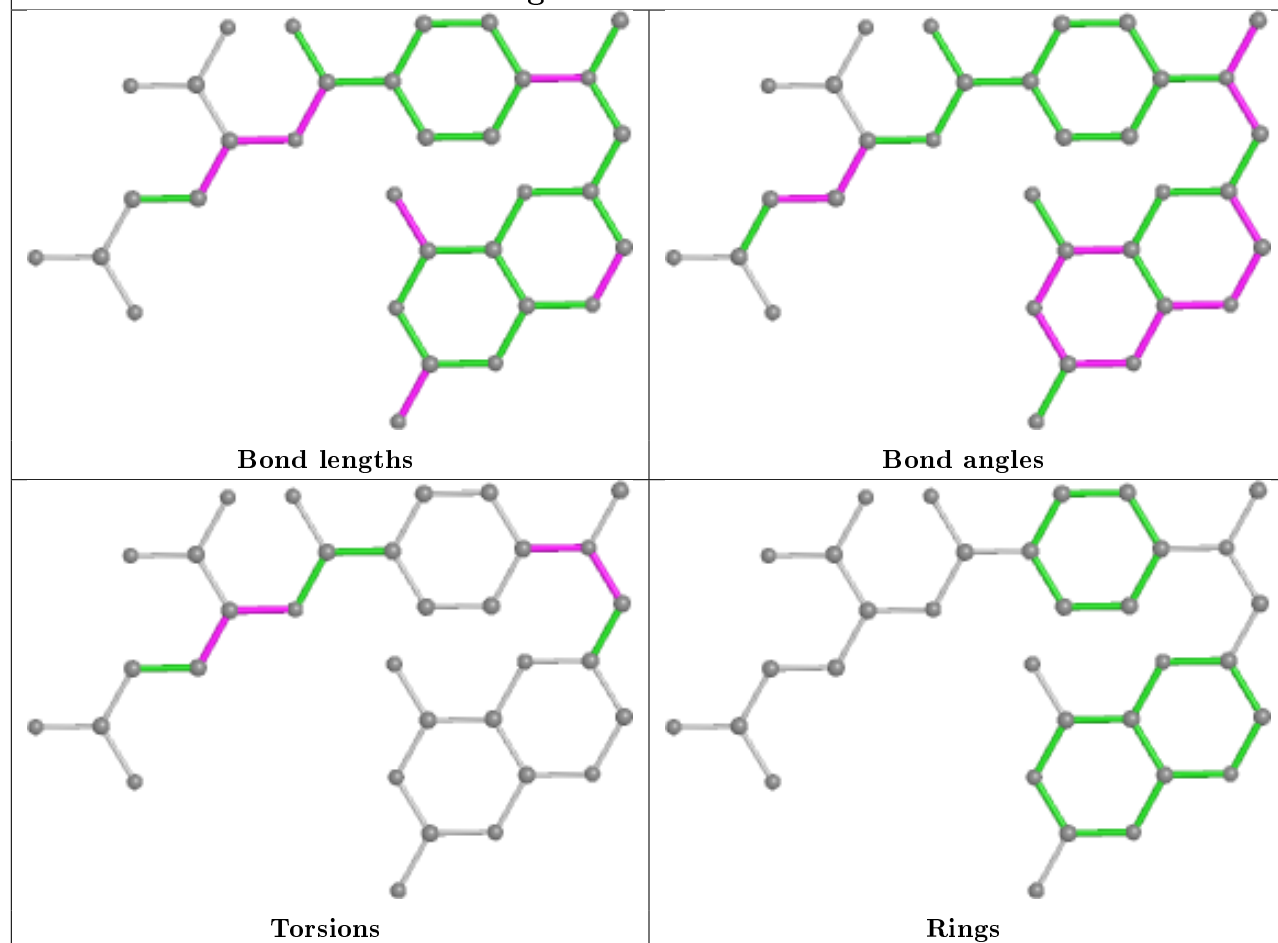
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



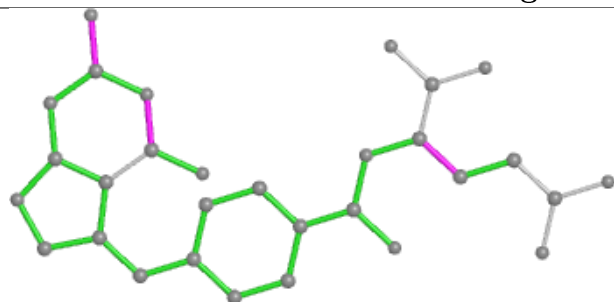
Ligand D96 C 603



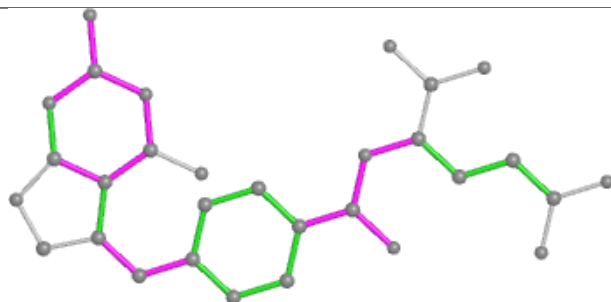
Ligand MTX B 604



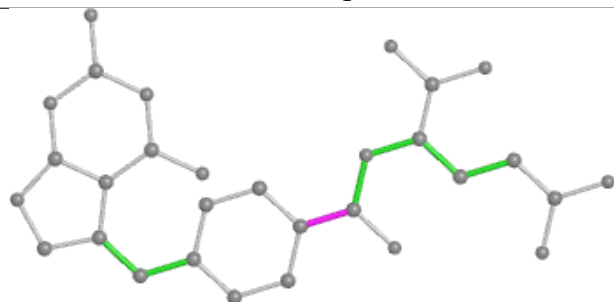
Ligand D96 B 603



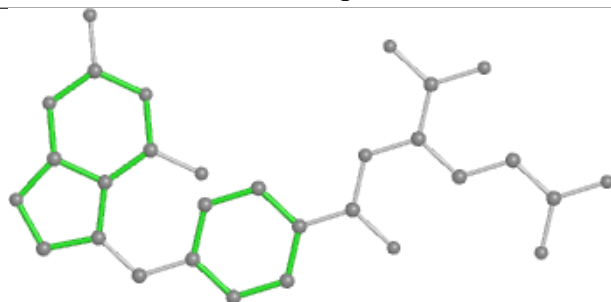
Bond lengths



Bond angles

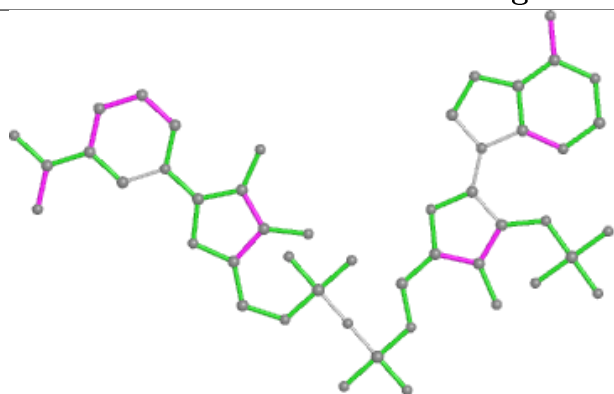


Torsions

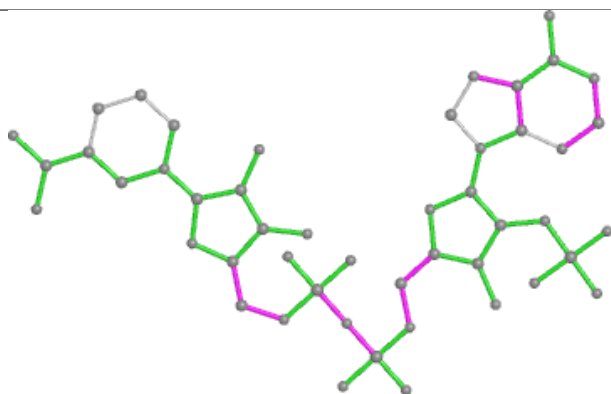


Rings

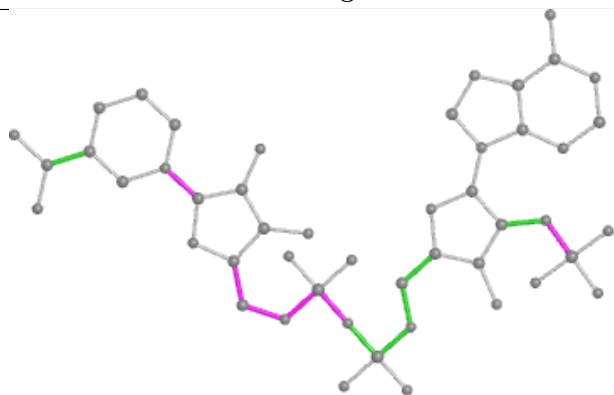
Ligand NDP D 601



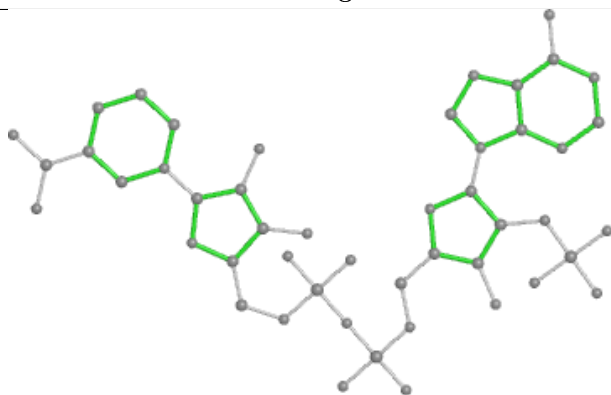
Bond lengths



Bond angles

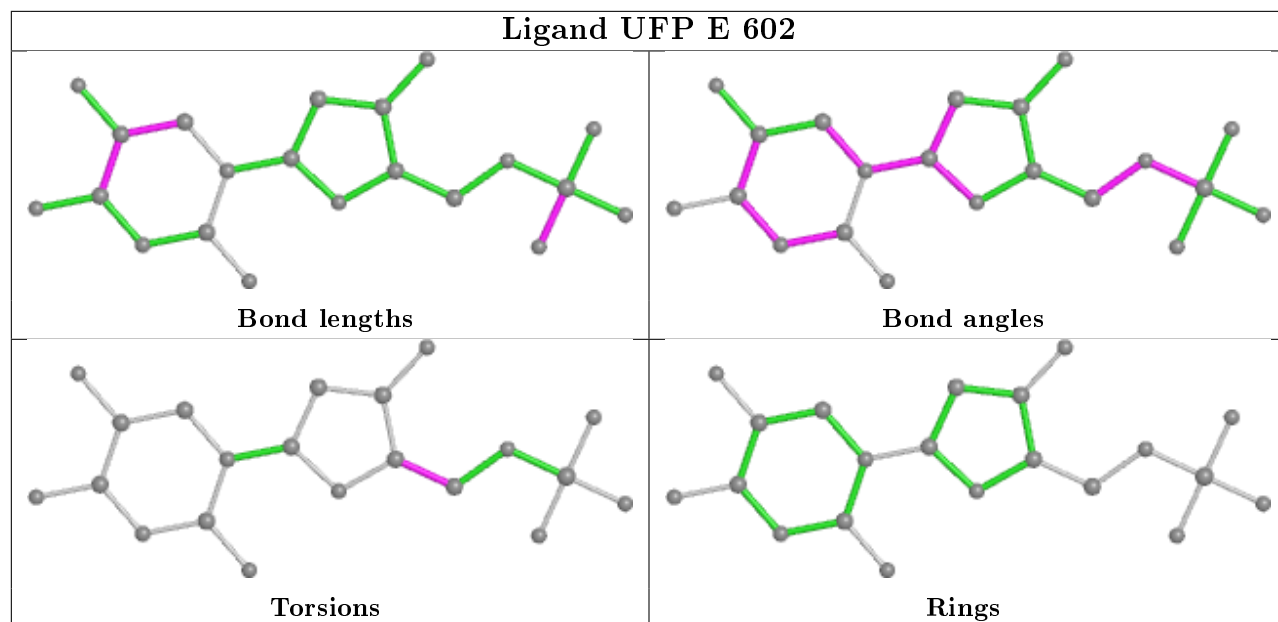


Torsions

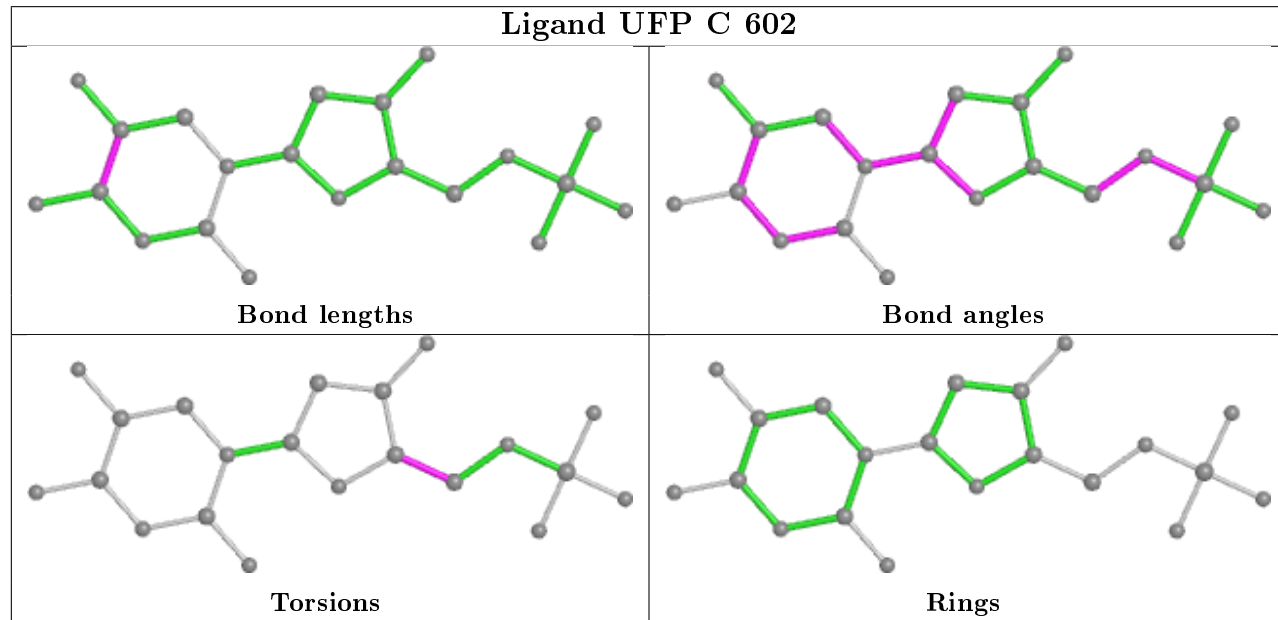


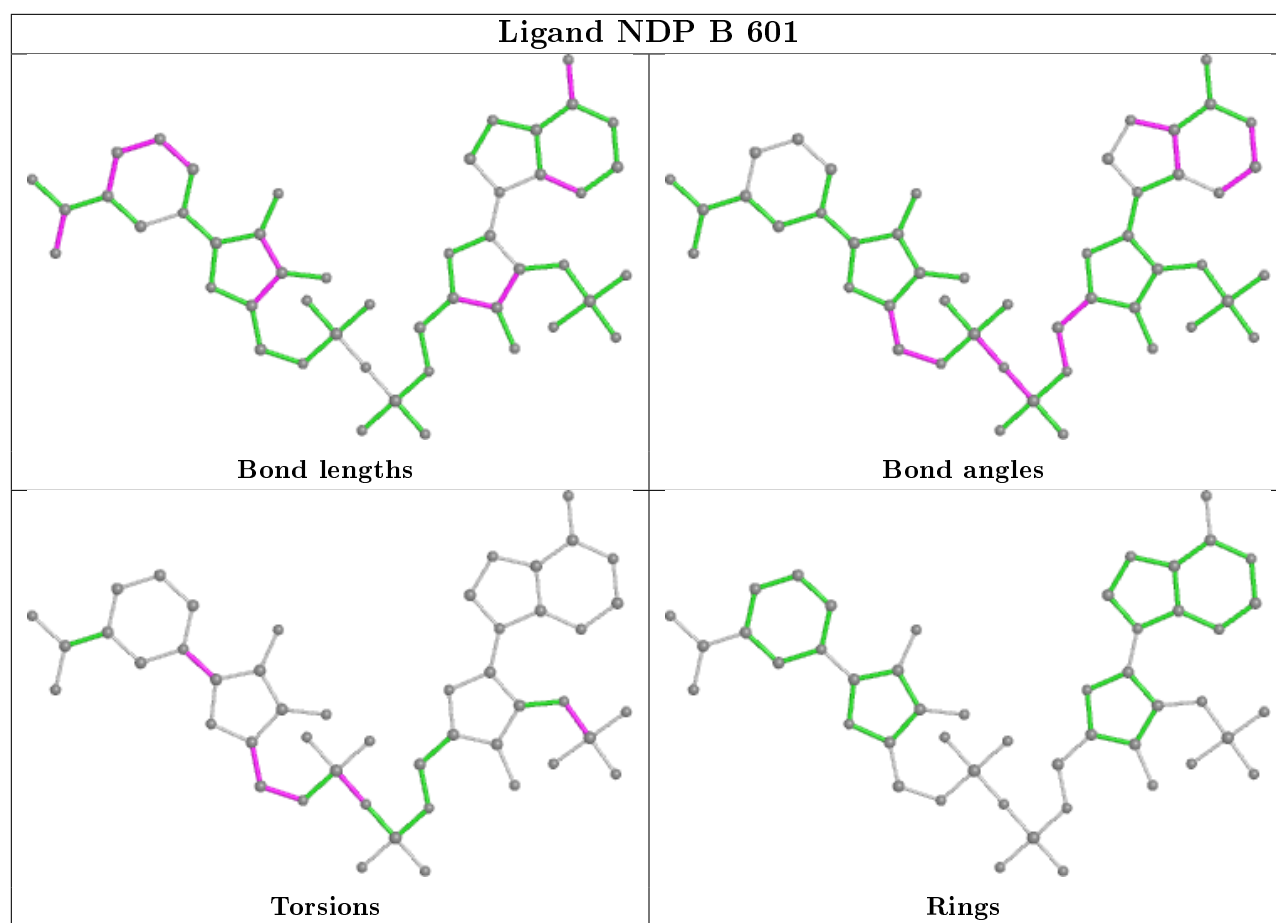
Rings

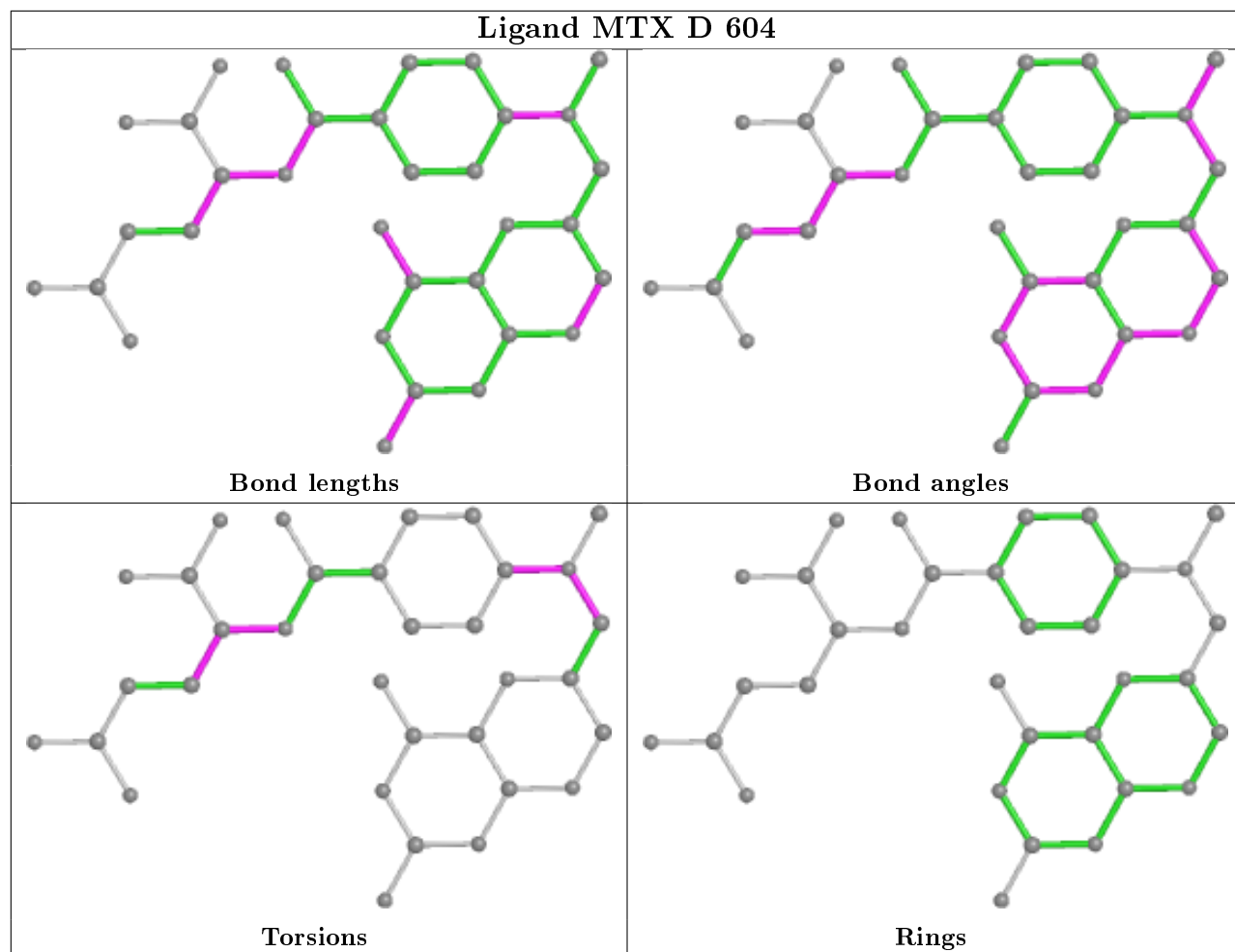
Ligand UFP E 602

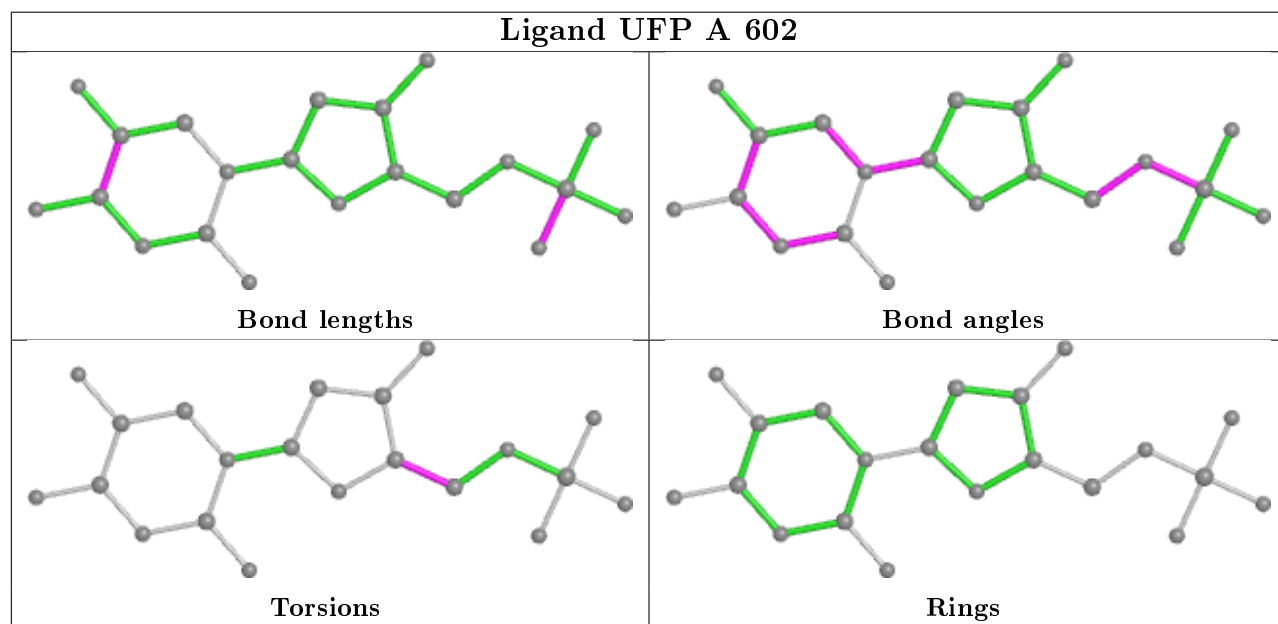
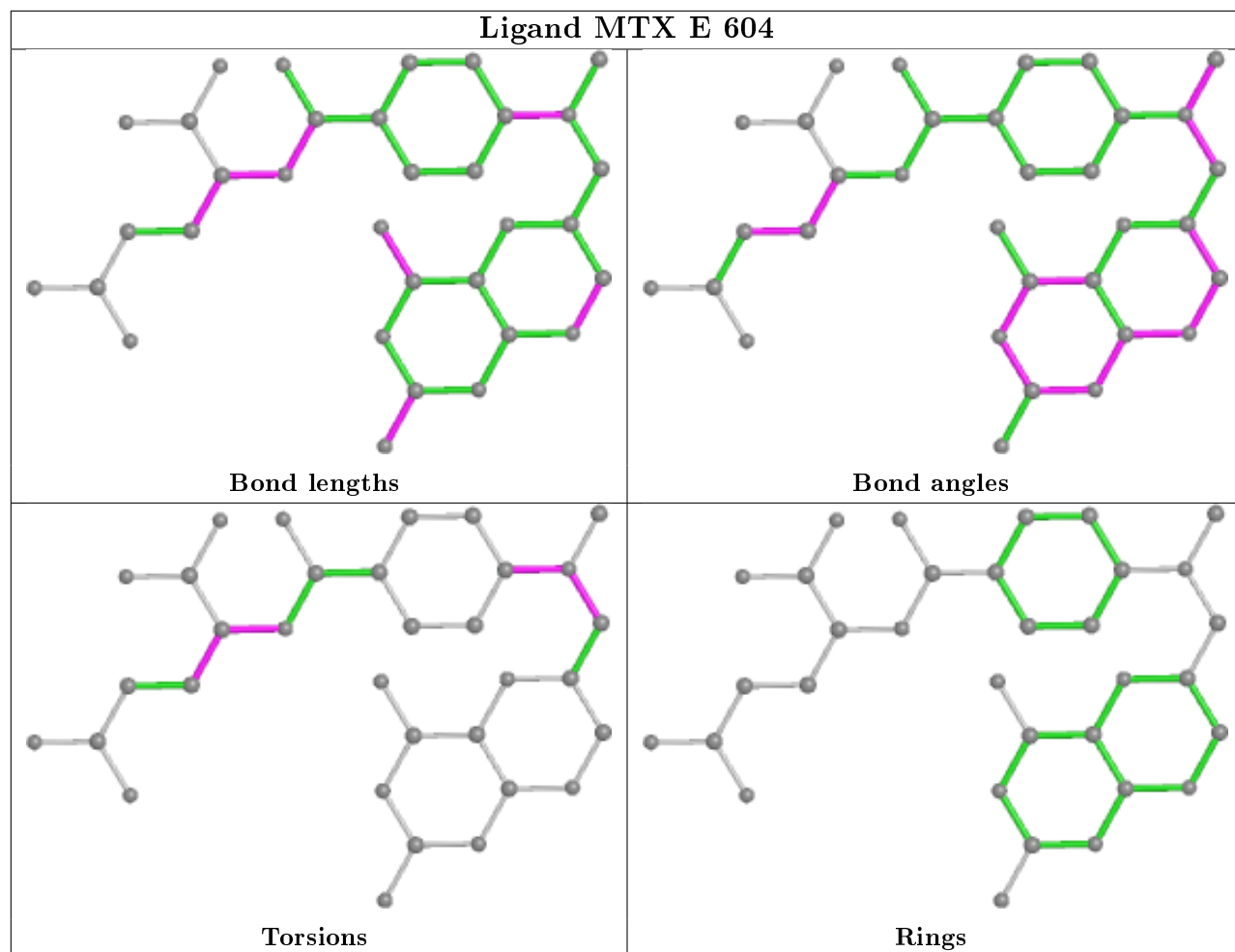


Ligand UFP C 602

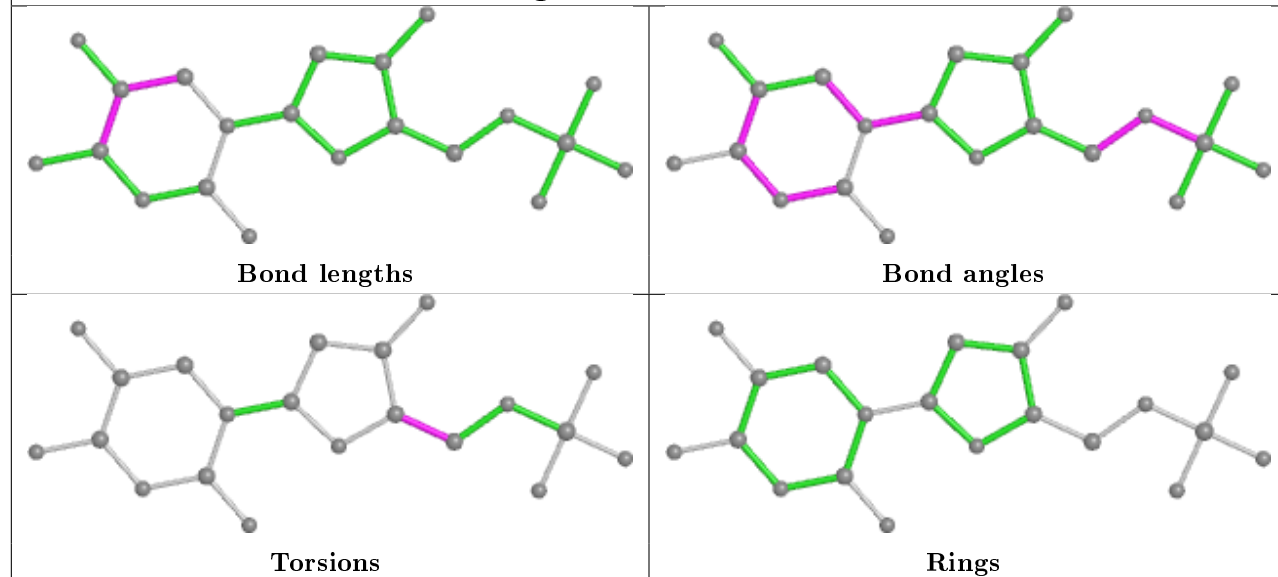




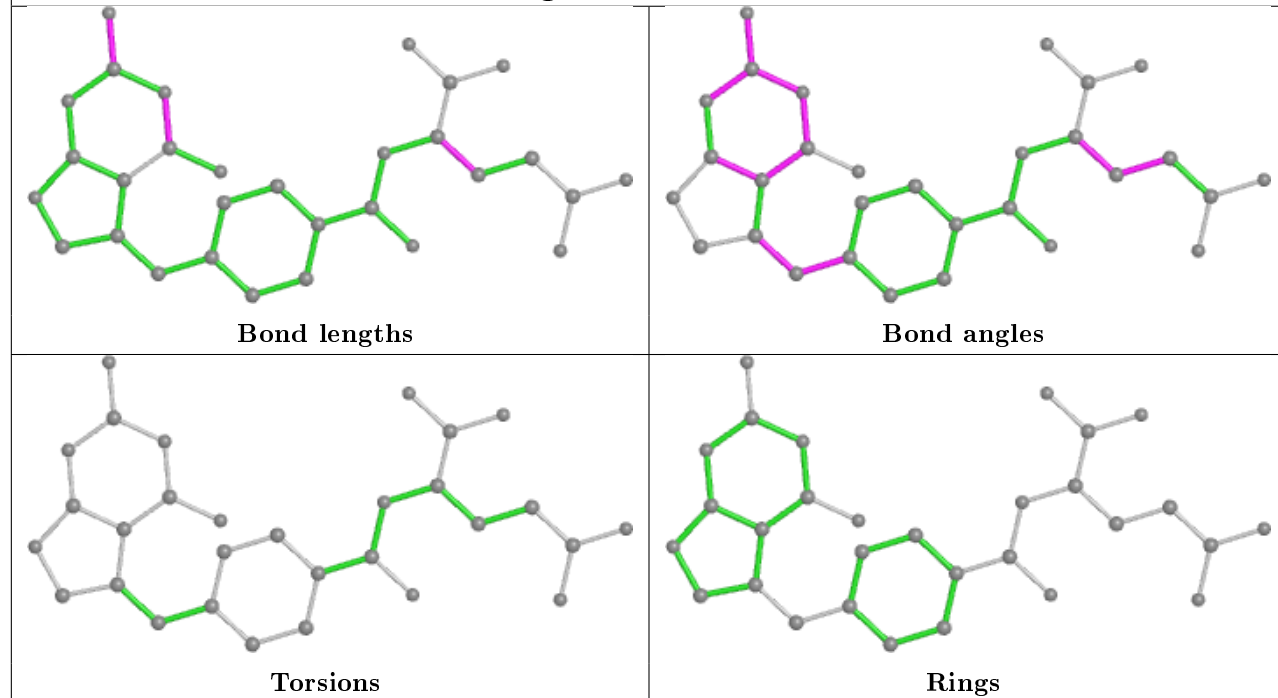




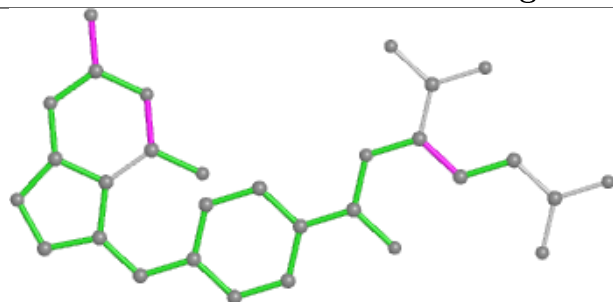
Ligand UFP B 602



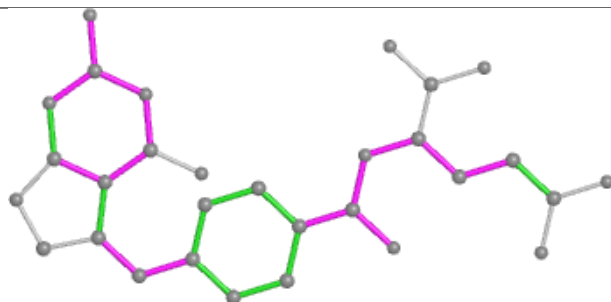
Ligand D96 E 603



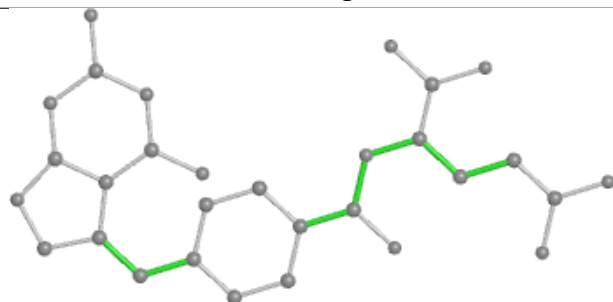
Ligand D96 A 603



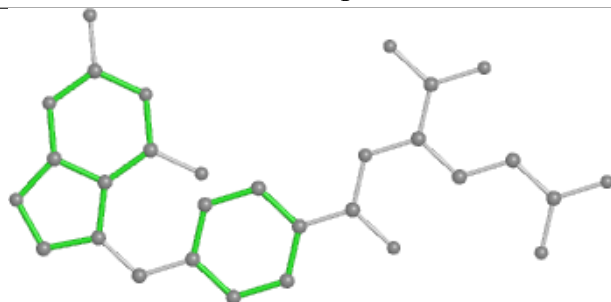
Bond lengths



Bond angles

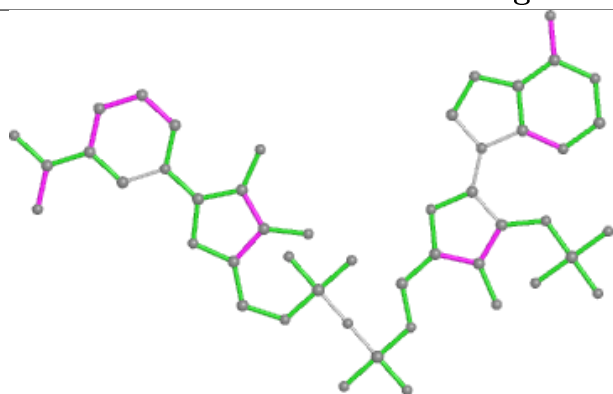


Torsions

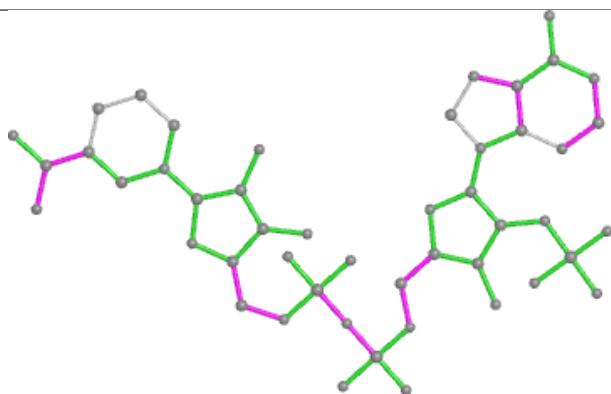


Rings

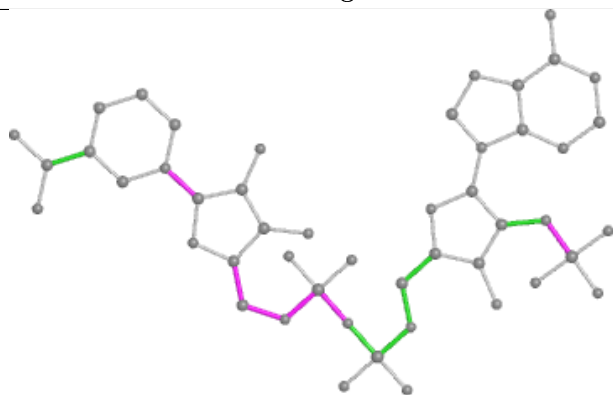
Ligand NDP E 601



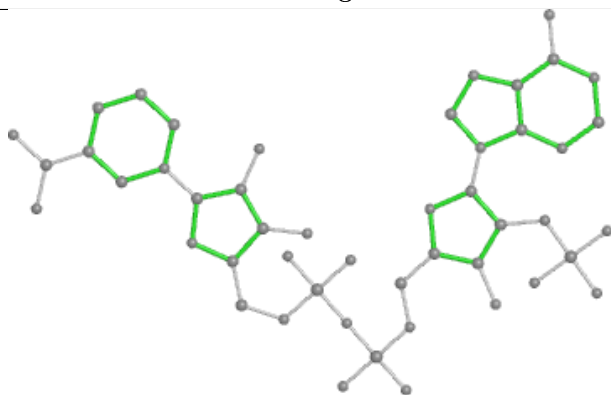
Bond lengths



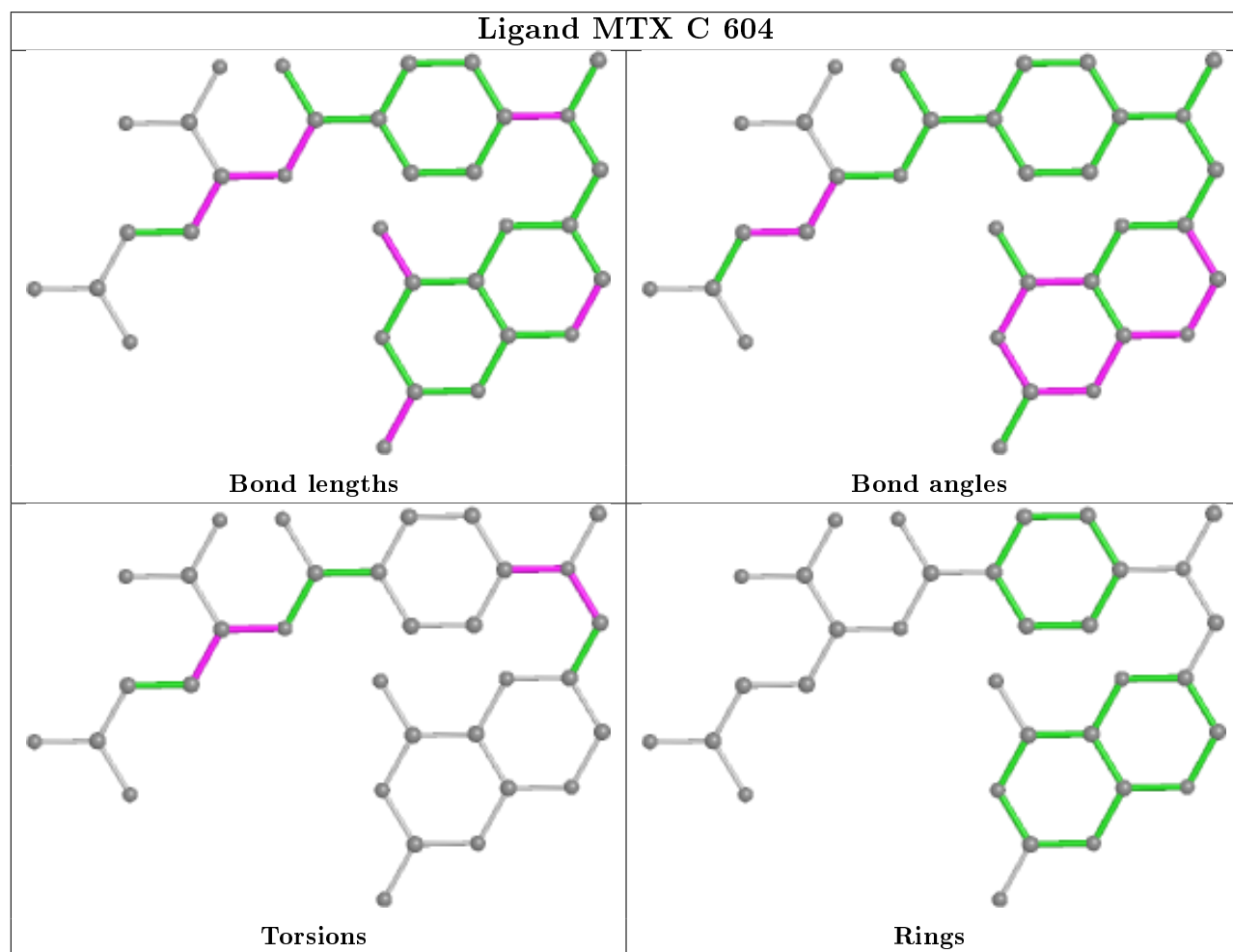
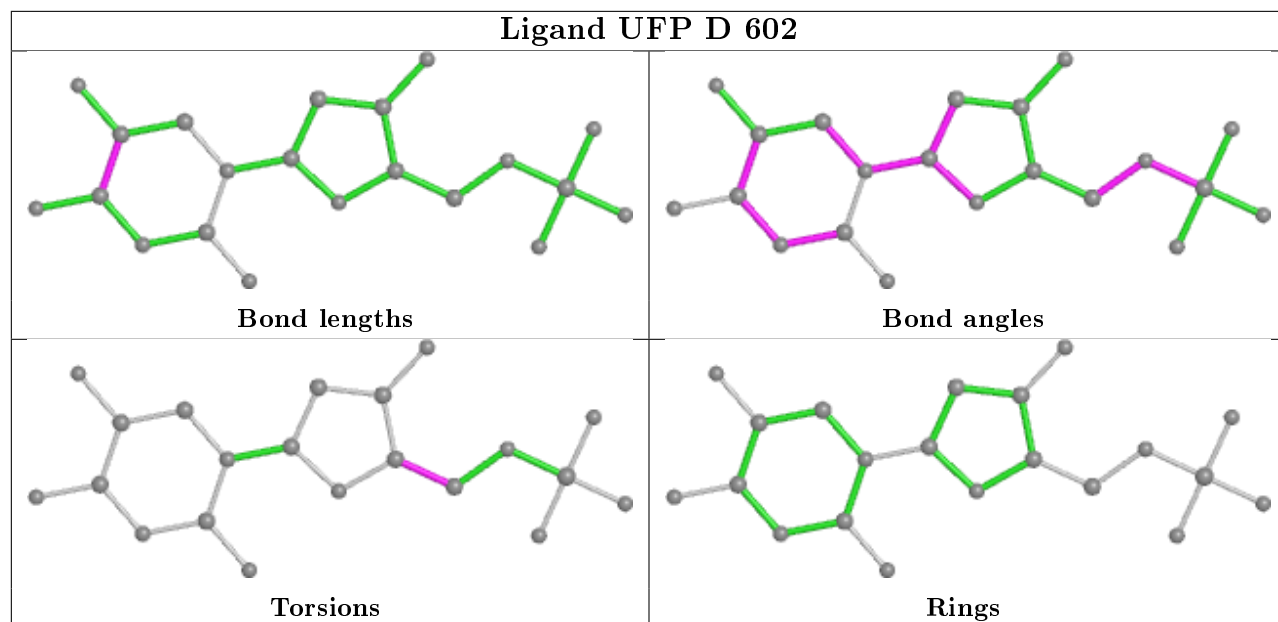
Bond angles

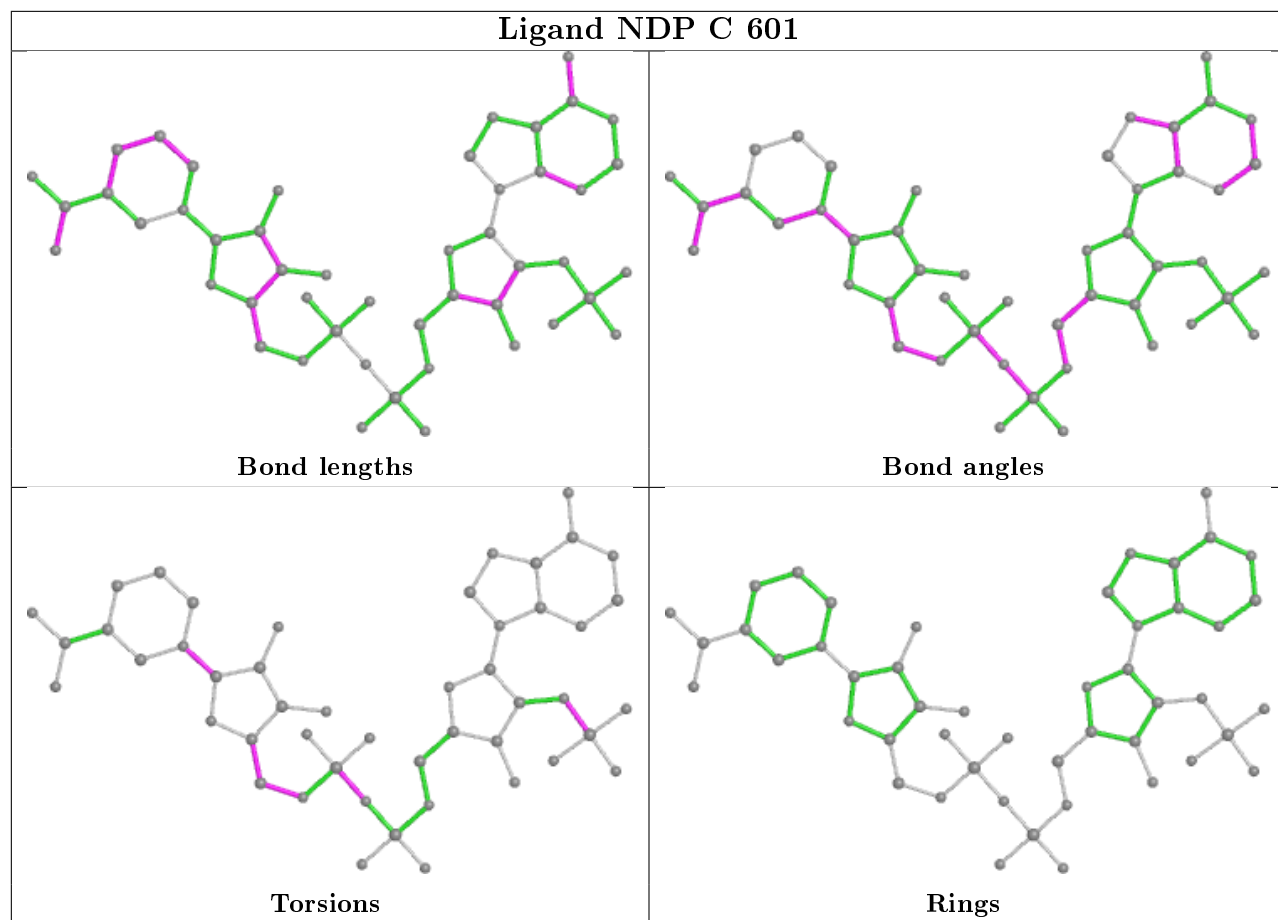


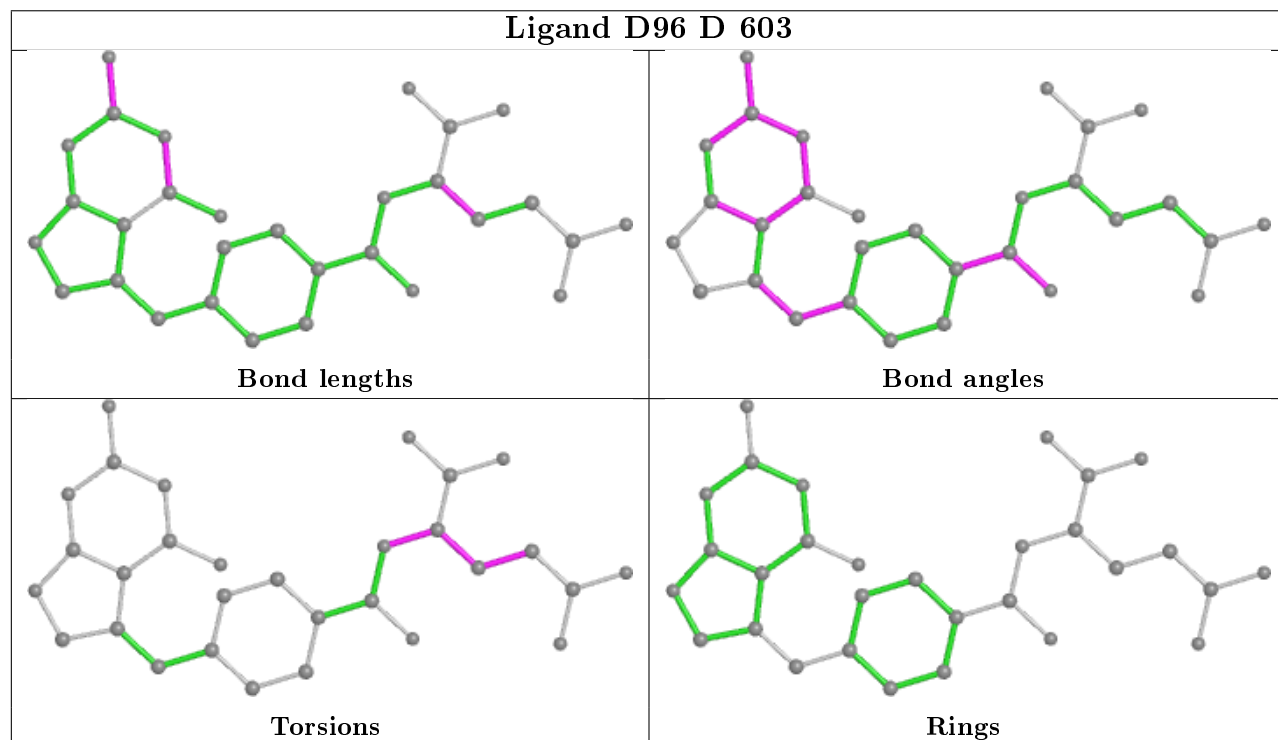
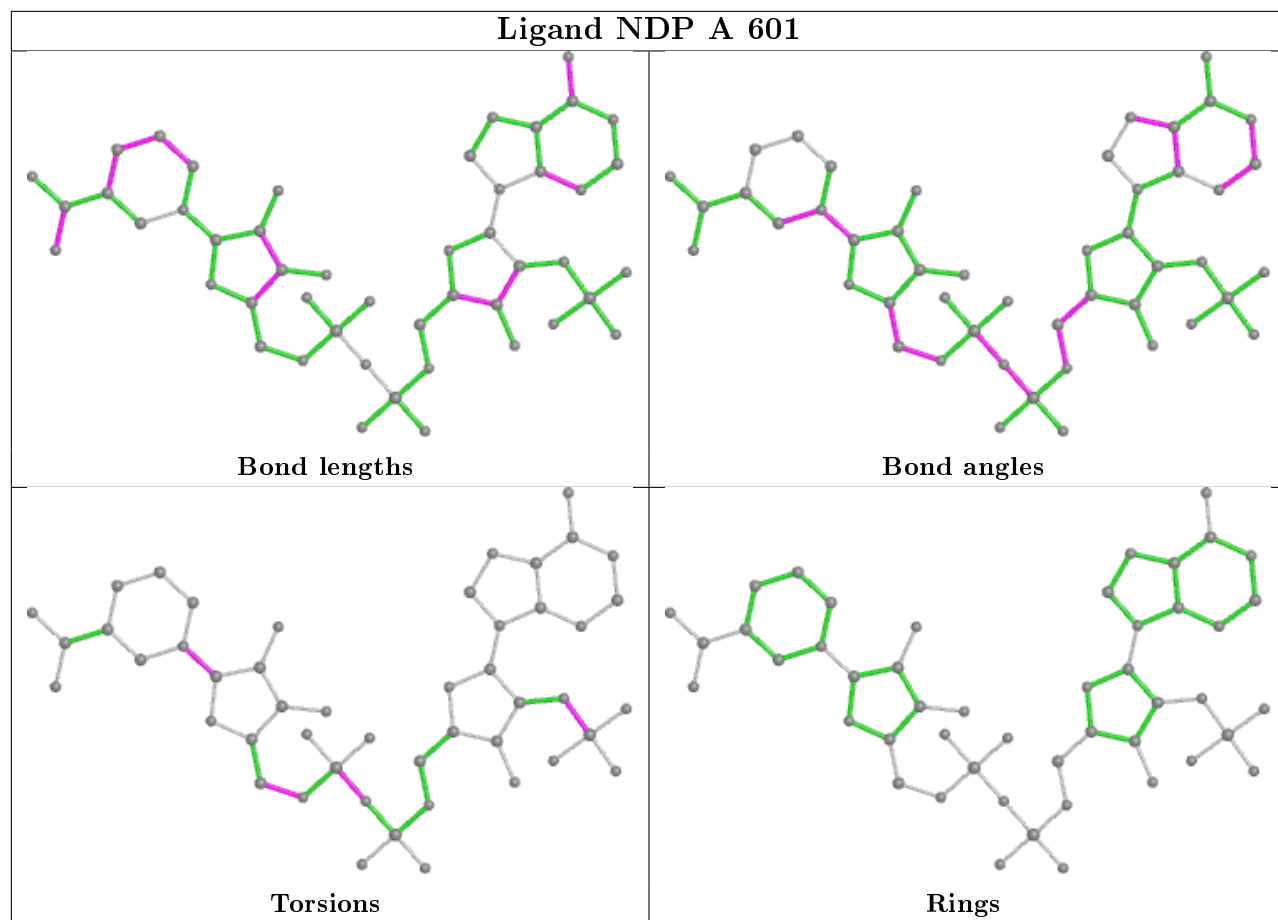
Torsions



Rings







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.09	2 (0%) 92 89	65, 80, 107, 163	0
1	B	508/521 (97%)	-0.09	1 (0%) 95 94	71, 88, 114, 164	0
1	C	508/521 (97%)	-0.14	0 100 100	63, 78, 104, 146	0
1	D	508/521 (97%)	0.01	1 (0%) 95 94	82, 99, 129, 165	0
1	E	508/521 (97%)	-0.07	7 (1%) 75 64	68, 85, 116, 158	0
All	All	2540/2605 (97%)	-0.08	11 (0%) 92 89	63, 86, 120, 165	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	MET	3.7
1	A	101	LEU	3.3
1	B	102	MET	3.1
1	E	102	MET	2.6
1	E	101	LEU	2.6
1	E	110	ILE	2.5
1	E	109	ASN	2.4
1	E	112	VAL	2.2
1	E	86	PRO	2.2
1	E	89	VAL	2.2
1	D	101	LEU	2.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

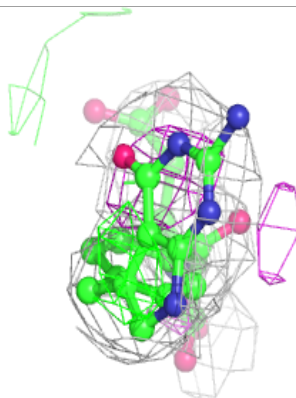
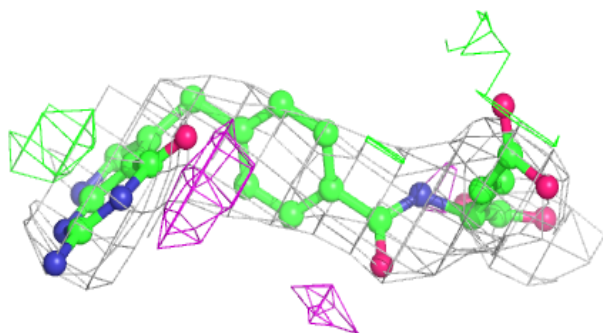
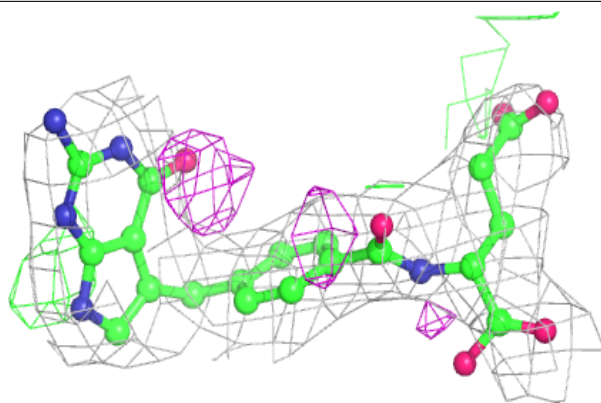
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	D96	B	603	30/30	0.83	0.29	93,100,114,125	0
4	D96	D	603	30/30	0.83	0.34	105,113,119,120	0
4	D96	A	603	30/30	0.85	0.31	90,96,112,127	0
4	D96	C	603	30/30	0.87	0.31	78,86,97,105	0
5	MTX	E	604	33/33	0.88	0.23	78,87,95,97	0
3	UFP	A	602	21/21	0.90	0.23	76,88,100,122	0
4	D96	E	603	30/30	0.90	0.29	84,88,107,119	0
5	MTX	D	604	33/33	0.91	0.27	89,97,100,103	0
3	UFP	B	602	21/21	0.93	0.22	83,93,102,123	0
2	NDP	E	601	48/48	0.94	0.20	82,95,112,114	0
3	UFP	D	602	21/21	0.94	0.19	101,110,118,127	0
5	MTX	C	604	33/33	0.94	0.24	65,72,82,83	0
5	MTX	A	604	33/33	0.94	0.21	68,74,81,85	0
5	MTX	B	604	33/33	0.94	0.23	72,82,88,93	0
2	NDP	B	601	48/48	0.95	0.16	81,90,101,103	0
2	NDP	D	601	48/48	0.95	0.18	85,96,104,113	0
3	UFP	C	602	21/21	0.95	0.18	69,81,90,113	0
3	UFP	E	602	21/21	0.96	0.19	74,81,91,110	0
2	NDP	A	601	48/48	0.97	0.15	67,80,90,96	0
2	NDP	C	601	48/48	0.97	0.15	65,78,86,97	0

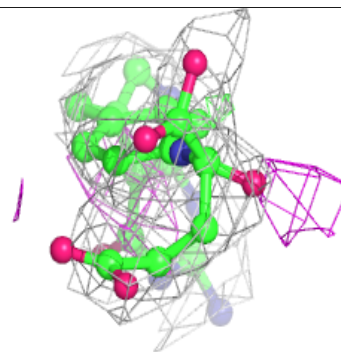
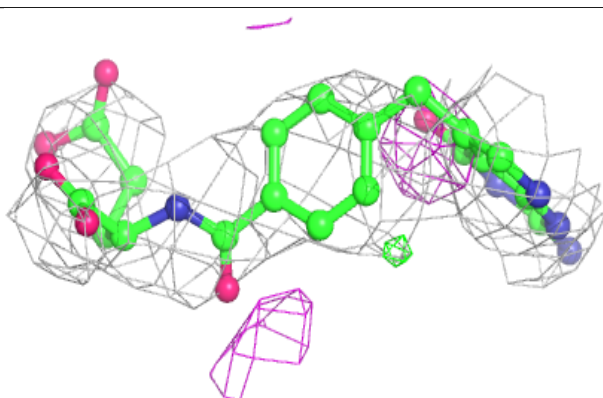
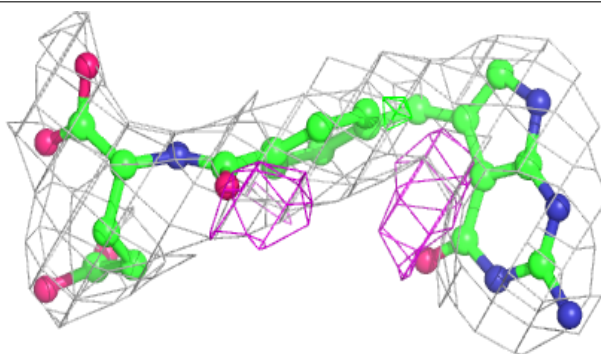
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around D96 B 603:

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

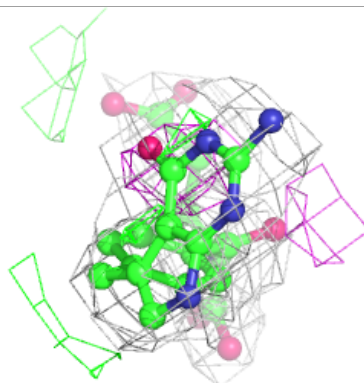
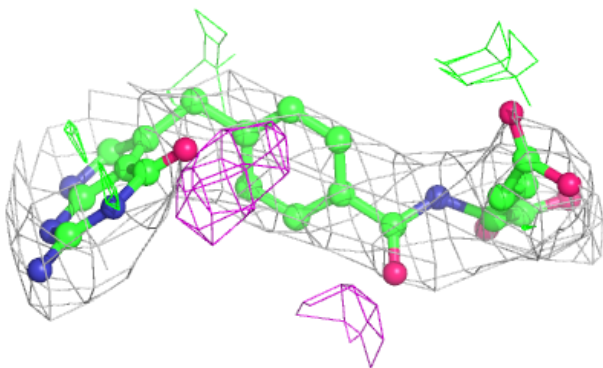
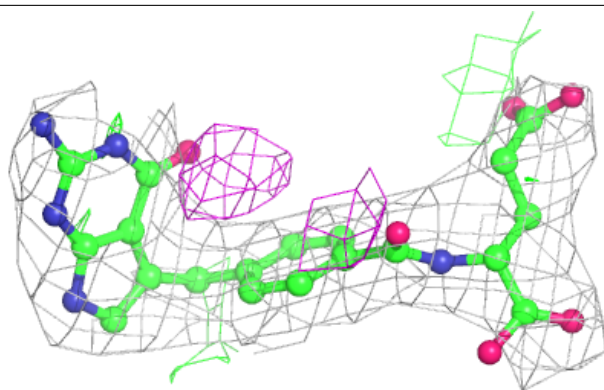
**Electron density around D96 D 603:**

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

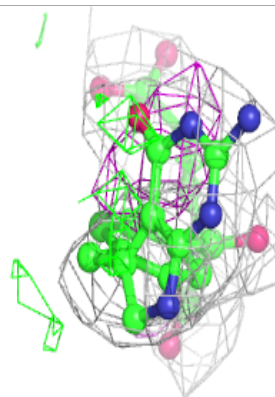
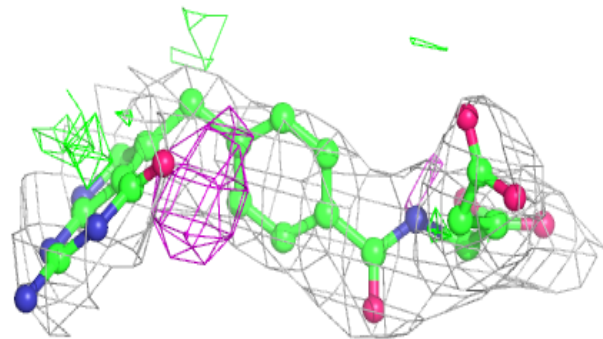
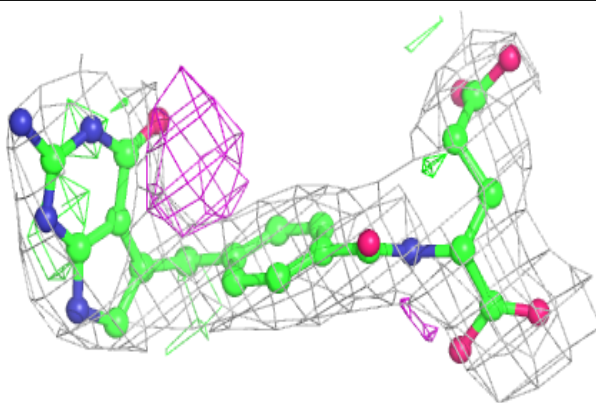


Electron density around D96 A 603:

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

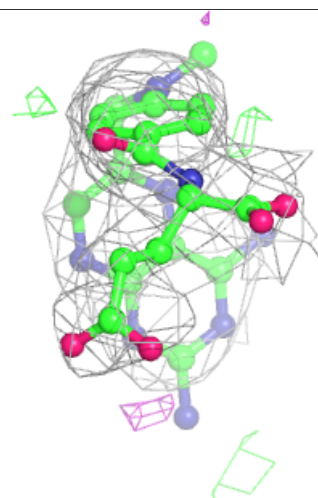
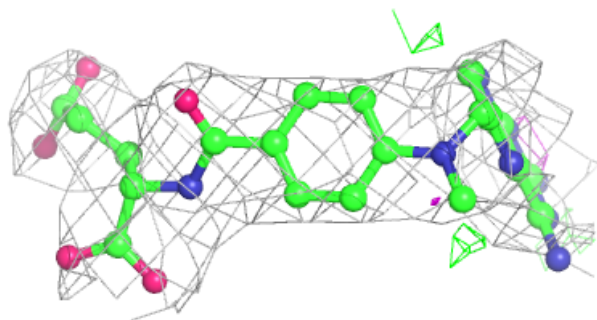
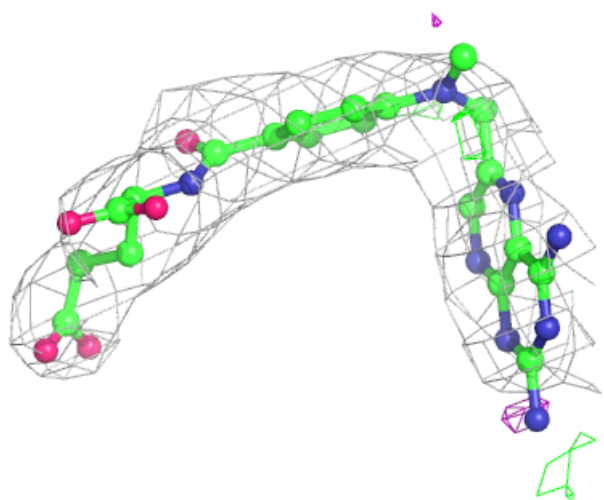
**Electron density around D96 C 603:**

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



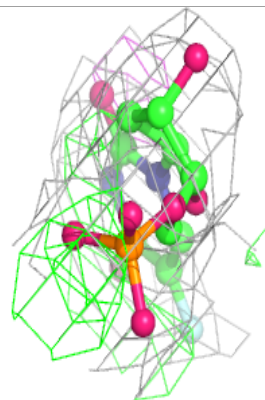
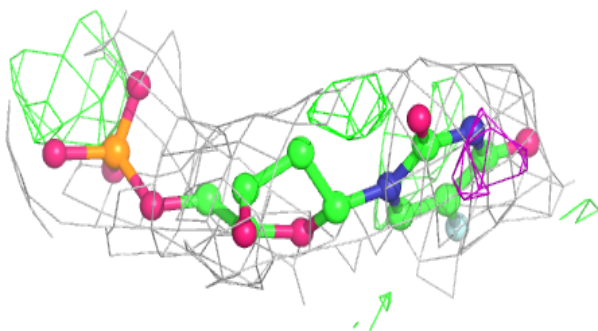
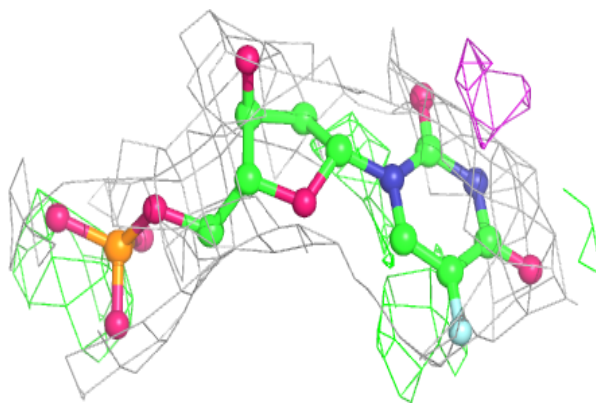
Electron density around MTX E 604:

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

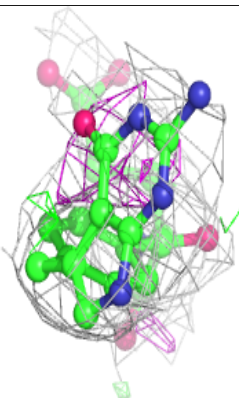
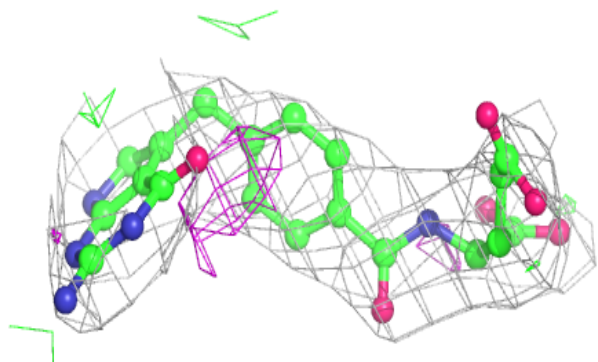
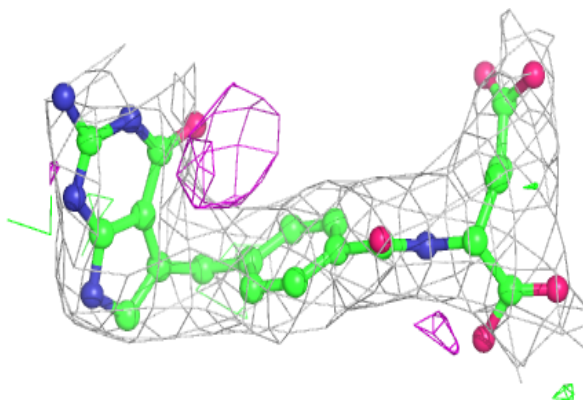


Electron density around UFP A 602:

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

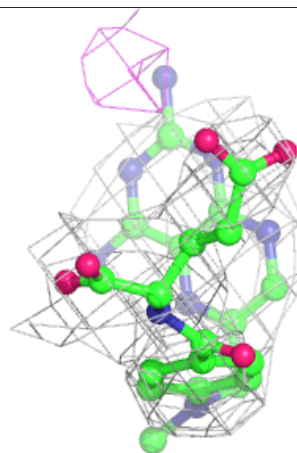
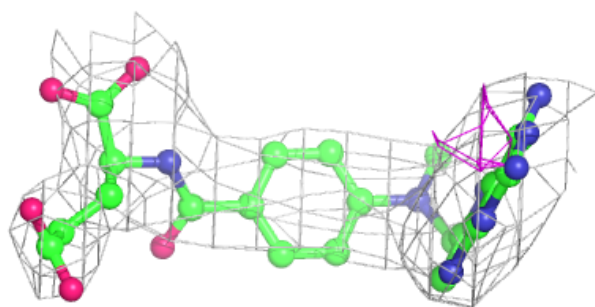
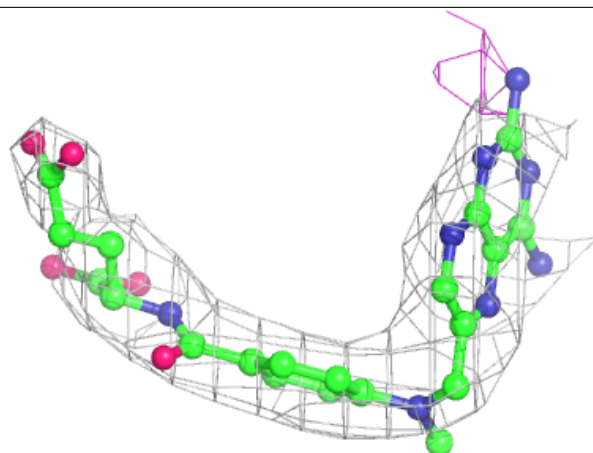
**Electron density around D96 E 603:**

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

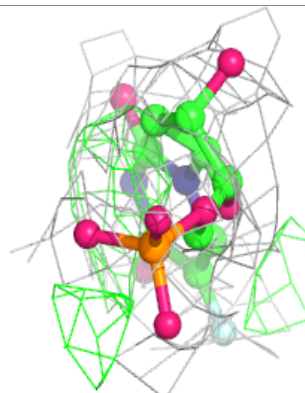
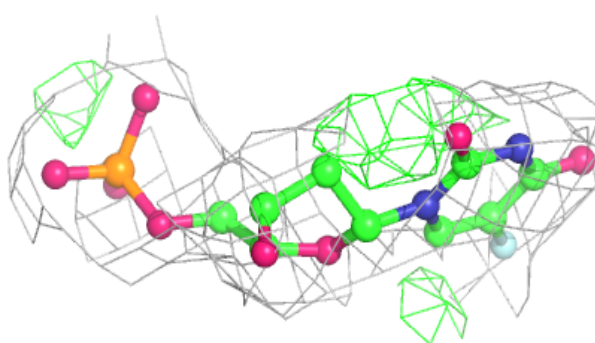
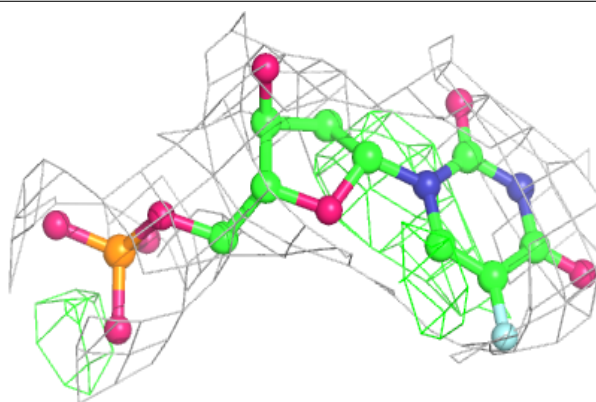


Electron density around MTX D 604:

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

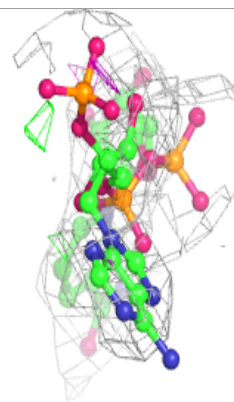
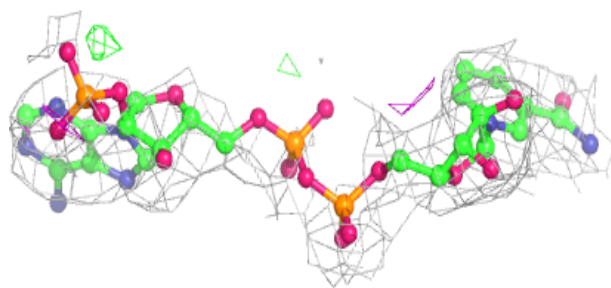
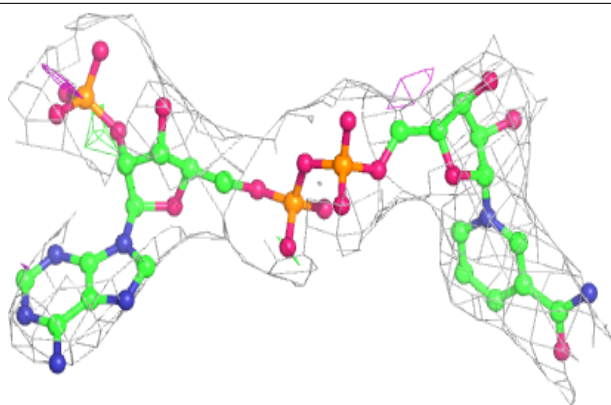
**Electron density around UFP B 602:**

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

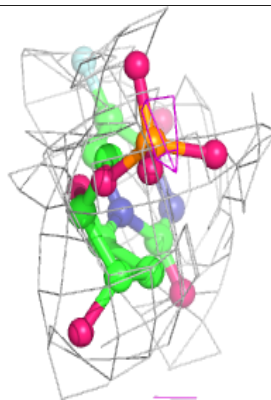
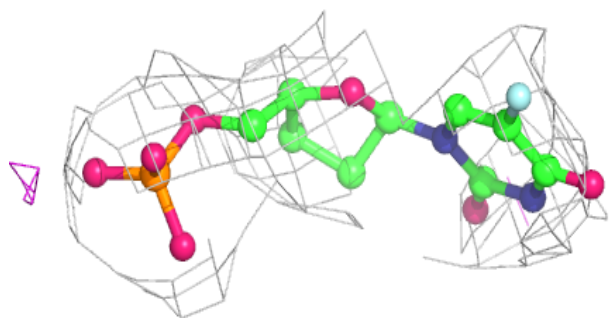
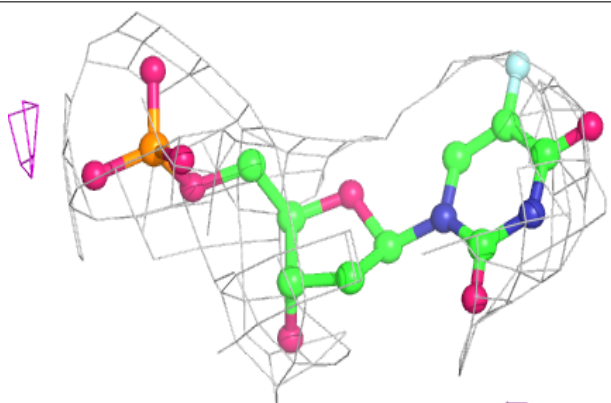


Electron density around NDP E 601:

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

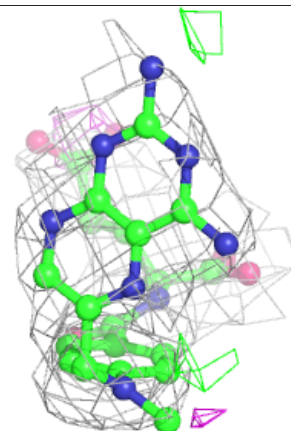
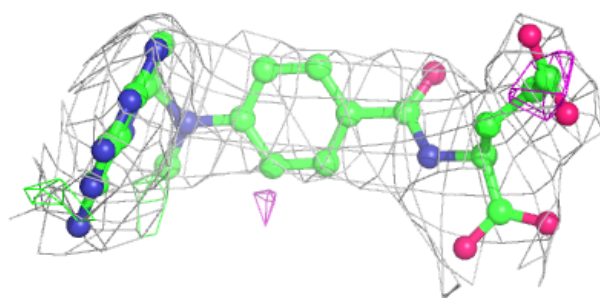
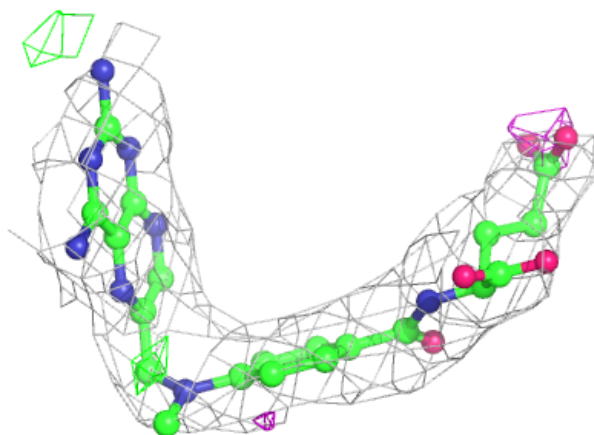
**Electron density around UFP D 602:**

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



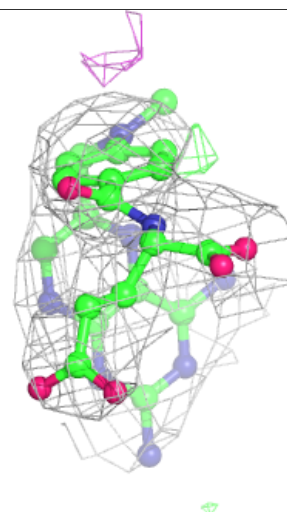
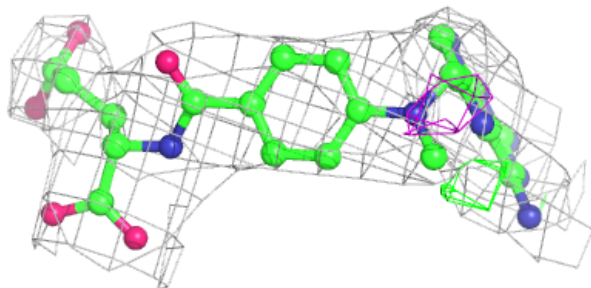
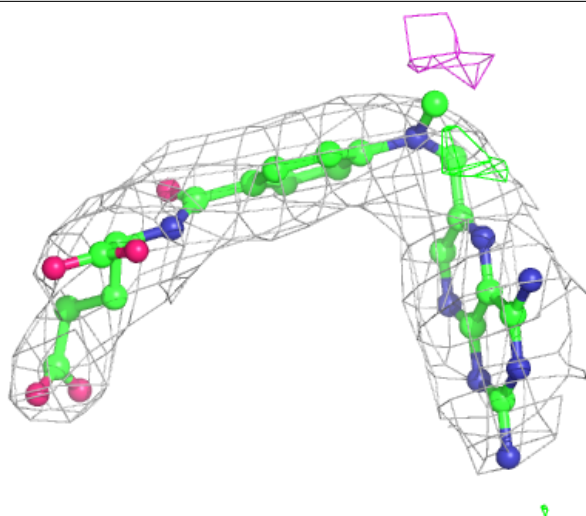
Electron density around MTX C 604:

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



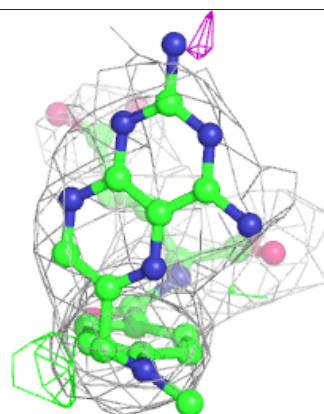
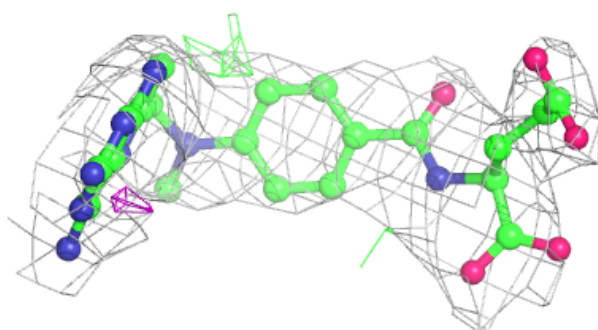
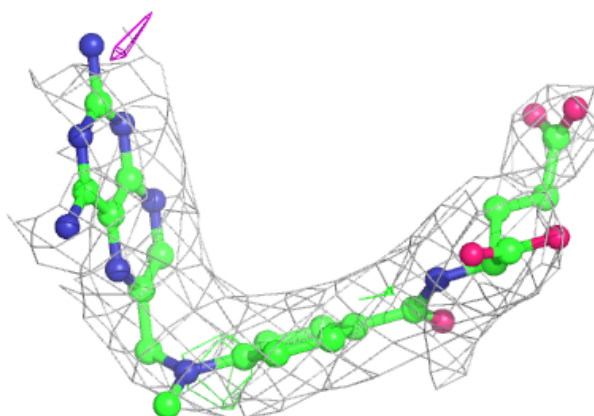
Electron density around MTX A 604:

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

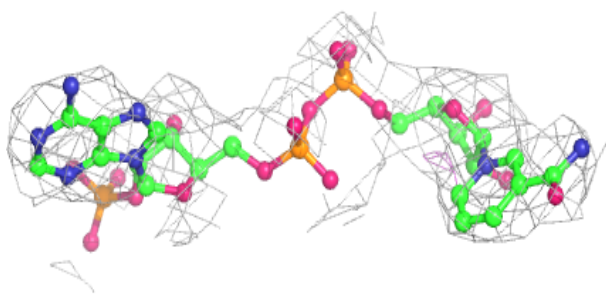
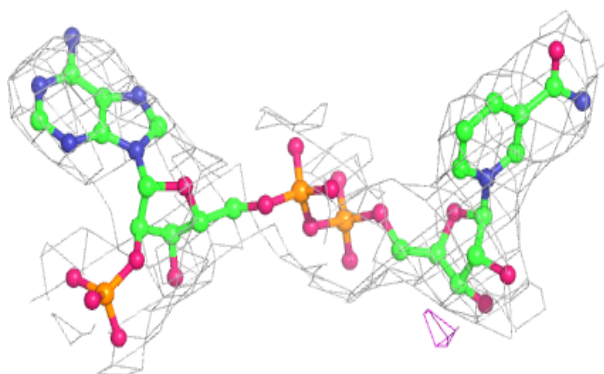


Electron density around MTX B 604:

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

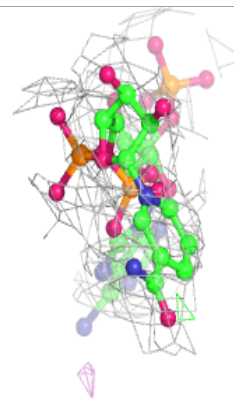
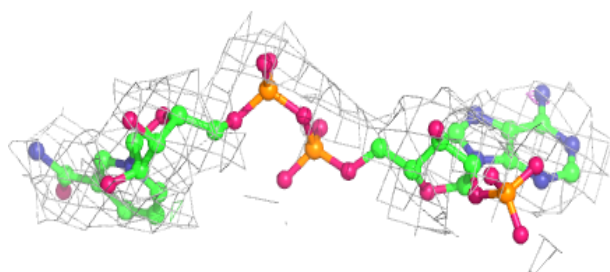
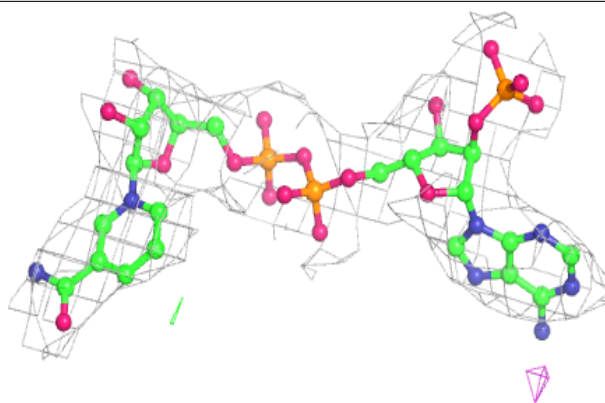
**Electron density around NDP B 601:**

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

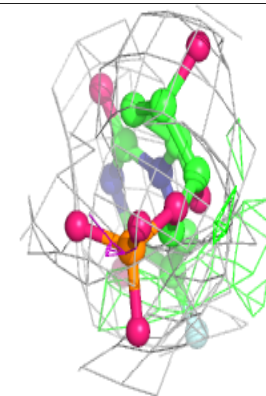
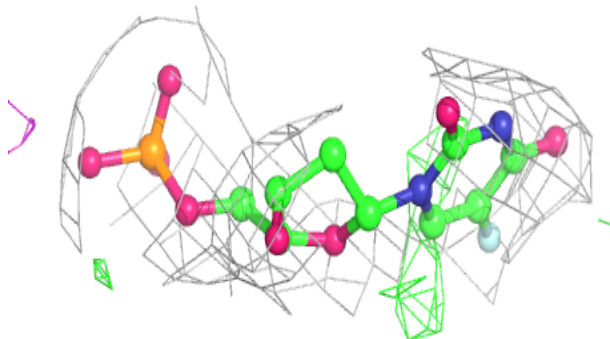
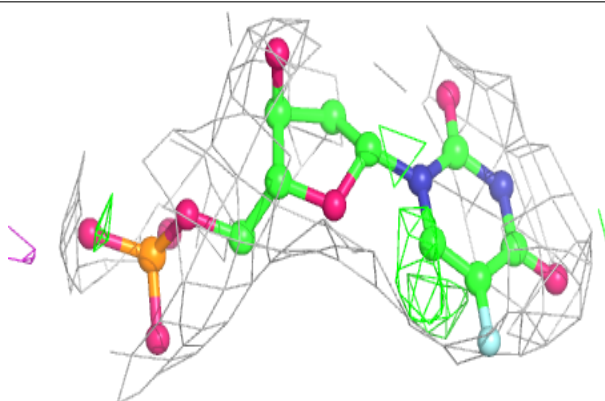


Electron density around NDP D 601:

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

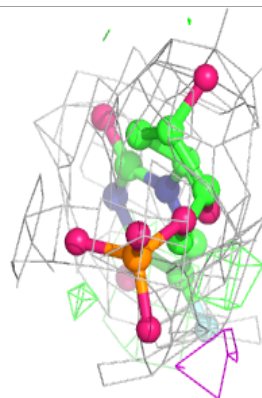
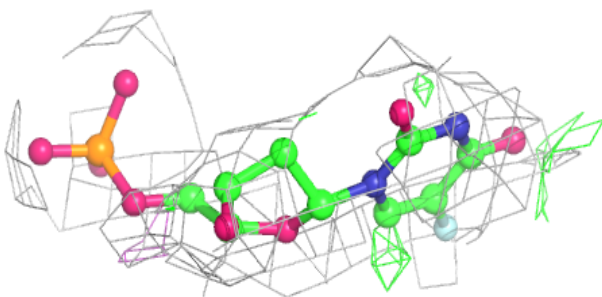
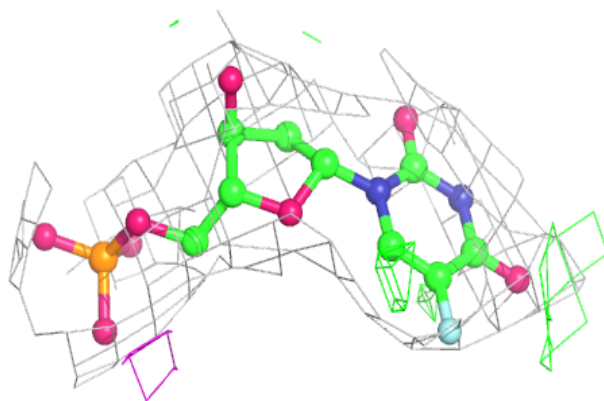
**Electron density around UFP C 602:**

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

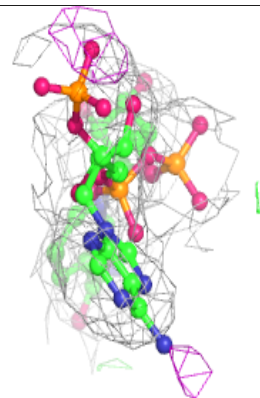
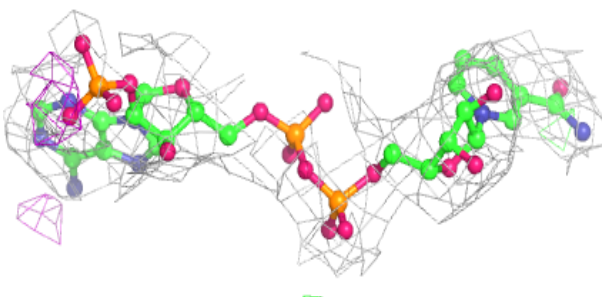
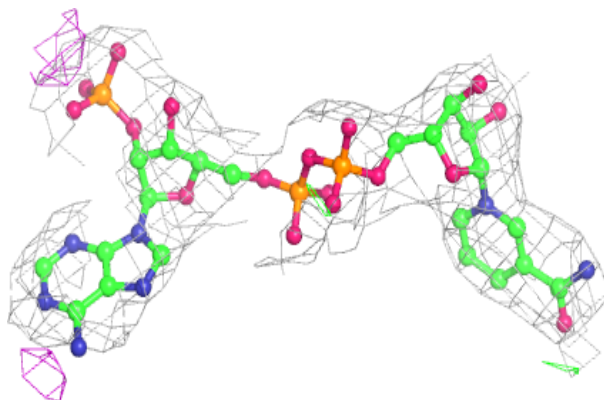


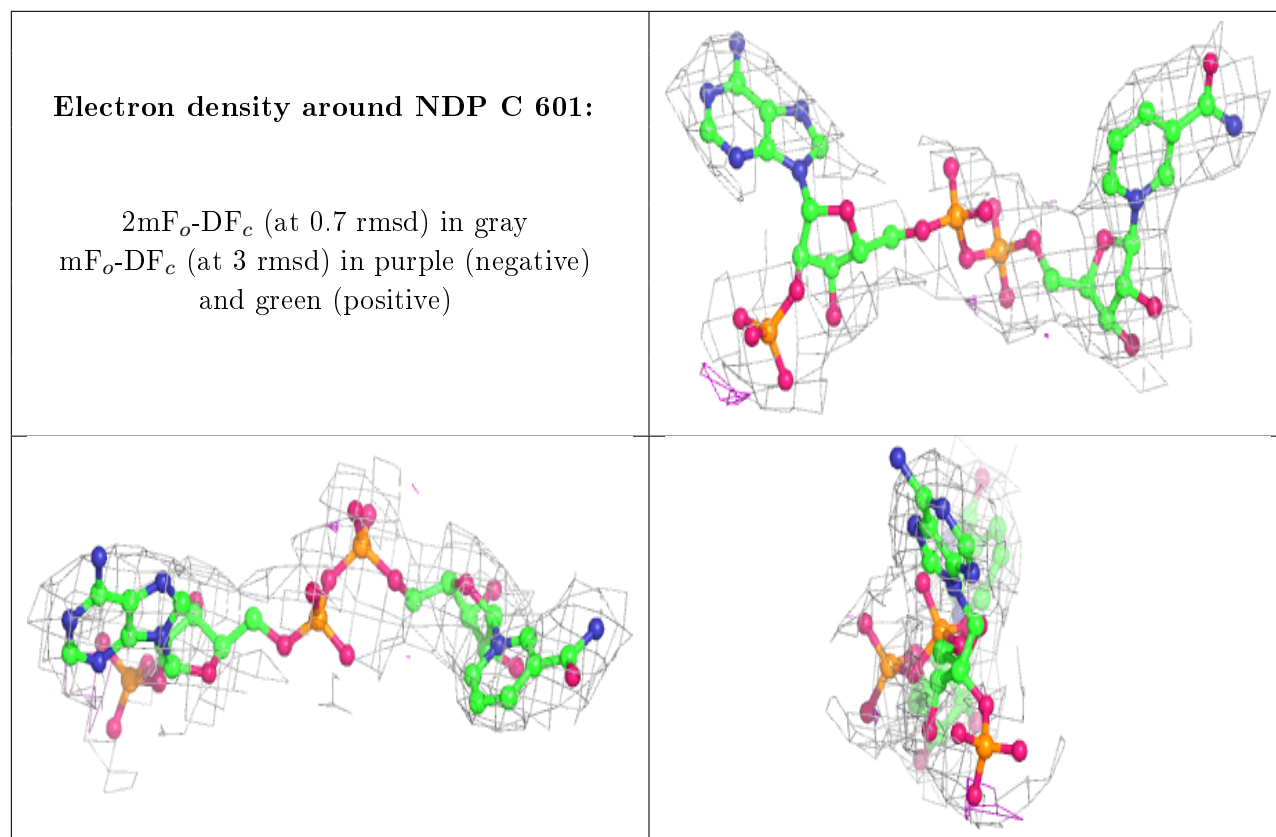
Electron density around UFP E 602:

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

**Electron density around NDP A 601:**

$2mF_o-DF_c$ (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.