



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:46 PM UTC

PDB ID : 6PFG / pdb_00006pfg
Title : Crystal structure of TS-DHFR from *Cryptosporidium hominis* in complex with NADPH, FdUMP and 2-(4-((2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl)benzamido)-4-carbamoylbenzoic acid.
Authors : Czyzyk, D.J.; Valhondo, M.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2019-06-21
Resolution : 2.71 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

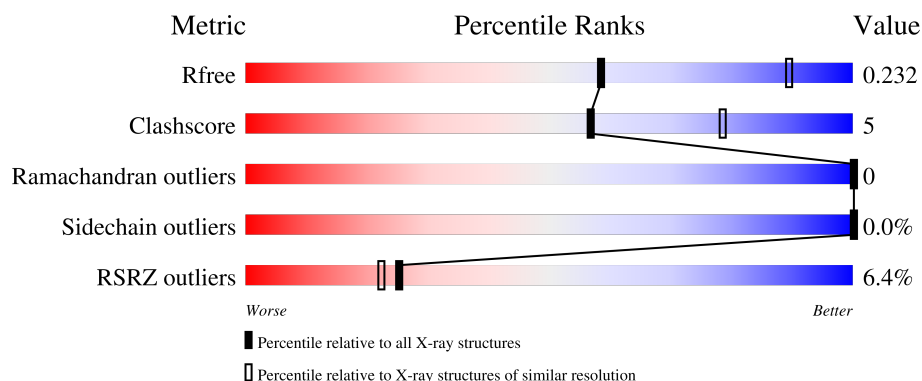
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	521	5% 85% 12%
1	B	521	6% 85% 12%
1	C	521	4% 87% 10%
1	D	521	11% 87% 10%

Continued on next page...

Continued from previous page...

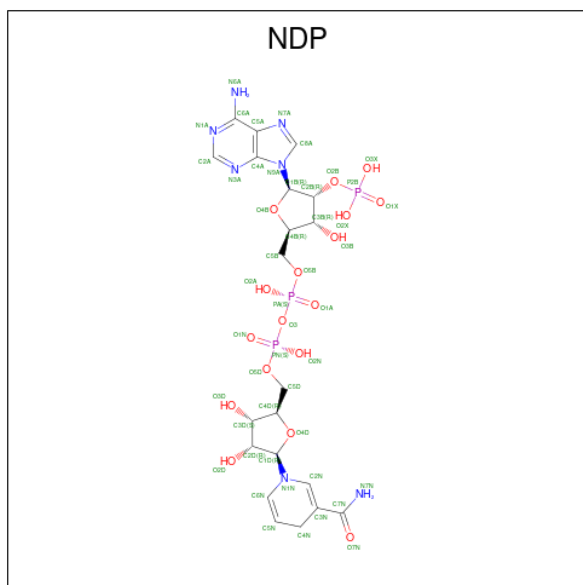
Mol	Chain	Length	Quality of chain
1	E	521	4% 87% 10%

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	505	Total 4064	C 2600	N 684	O 759	S 21	0	0	0
1	B	506	Total 4077	C 2607	N 686	O 763	S 21	0	0	0
1	C	506	Total 4097	C 2619	N 688	O 769	S 21	0	0	0
1	D	506	Total 4039	C 2581	N 676	O 761	S 21	0	0	0
1	E	506	Total 4097	C 2620	N 689	O 767	S 21	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



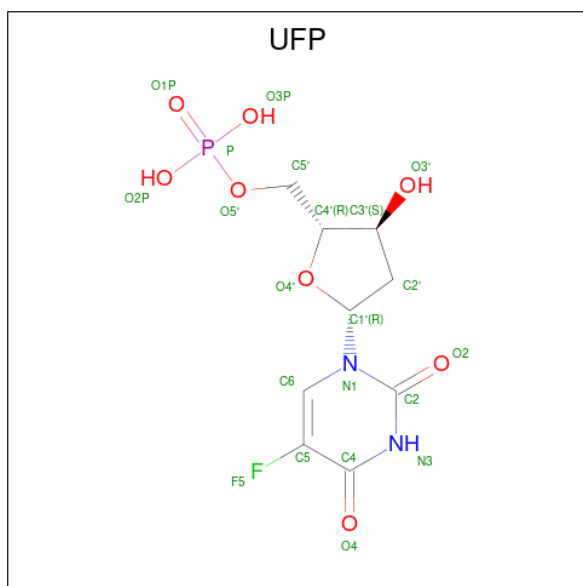
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

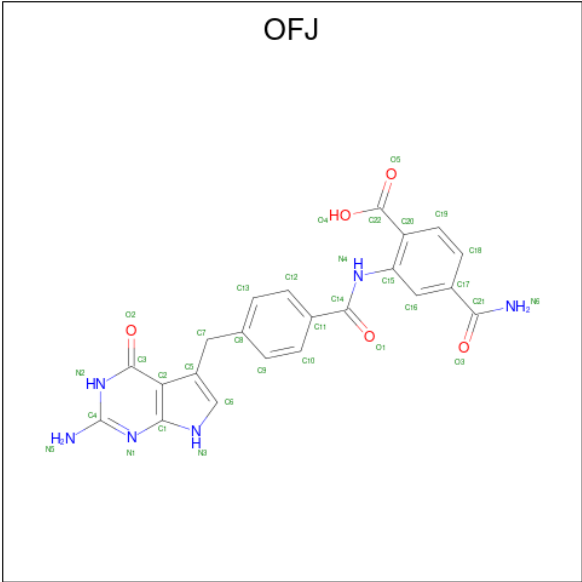
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: UFP) (formula: C₉H₁₂FN₂O₈P).



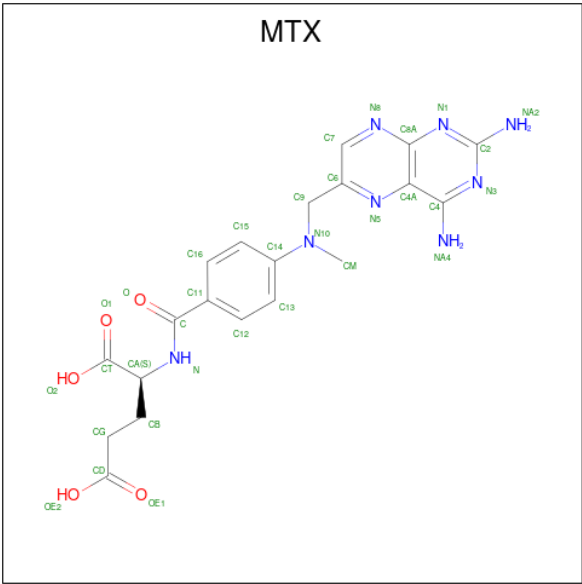
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is 2-({4-[(2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl]benzene-1-carbonyl}amino)-4-carbamoylbenzoic acid (CCD ID: OFJ) (formula: C₂₂H₁₈N₆O₅) (labeled as "Ligand of Interest" by depositor).



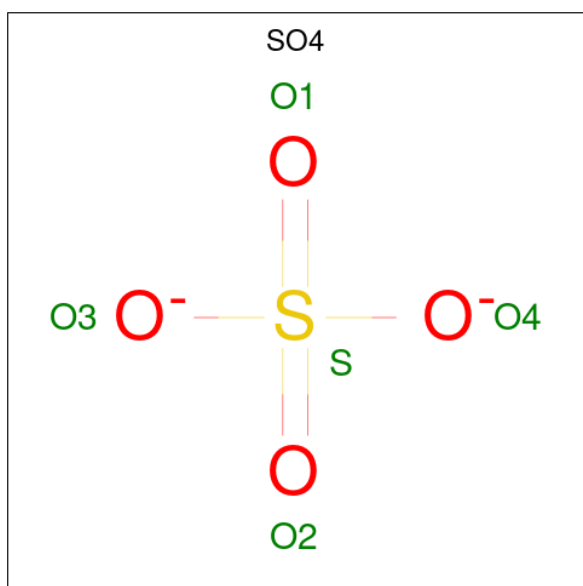
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			33	22	6	5		
4	B	1	Total	C	N	O	0	0
			33	22	6	5		
4	C	1	Total	C	N	O	0	0
			33	22	6	5		
4	D	1	Total	C	N	O	0	0
			33	22	6	5		
4	E	1	Total	C	N	O	0	0
			33	22	6	5		

- Molecule 5 is METHOTREXATE (CCD ID: MTX) (formula: C₂₀H₂₂N₈O₅).



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

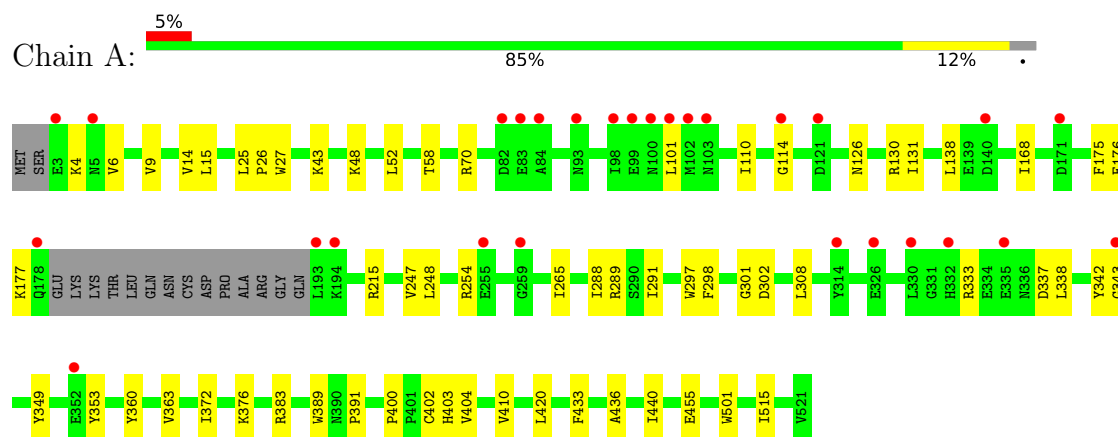
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	66	Total 66	O 66	0	0
7	B	100	Total 100	O 100	0	0
7	C	114	Total 114	O 114	0	0
7	D	20	Total 20	O 20	0	0
7	E	162	Total 162	O 162	0	0

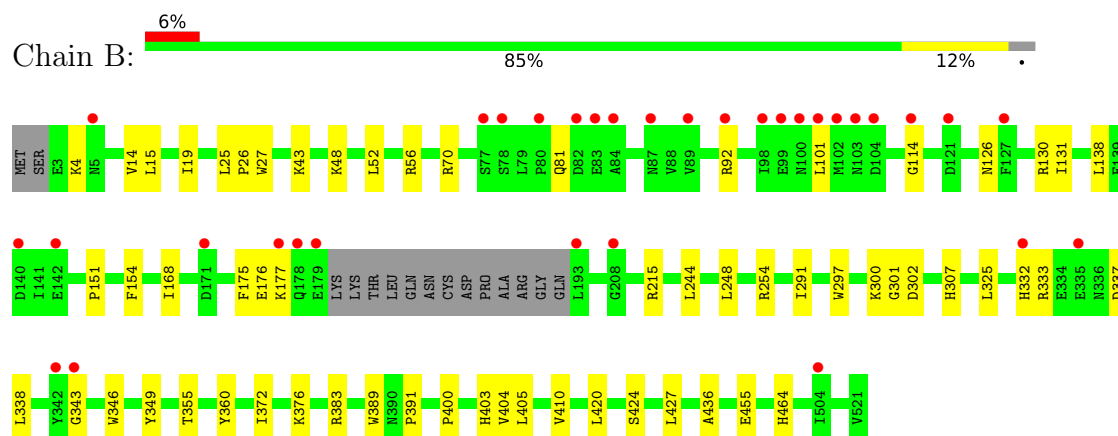
3 Residue-property plots [i](#)

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.

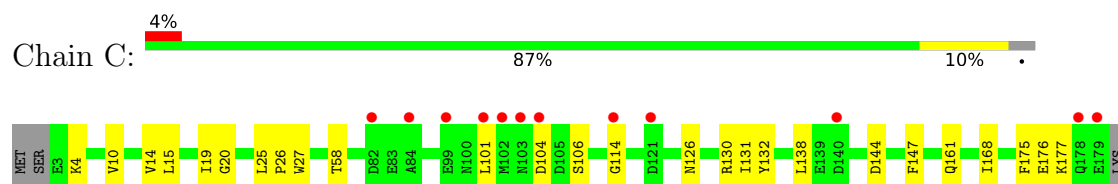
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

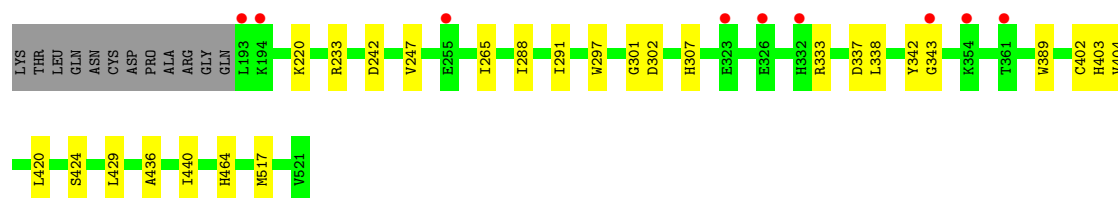


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

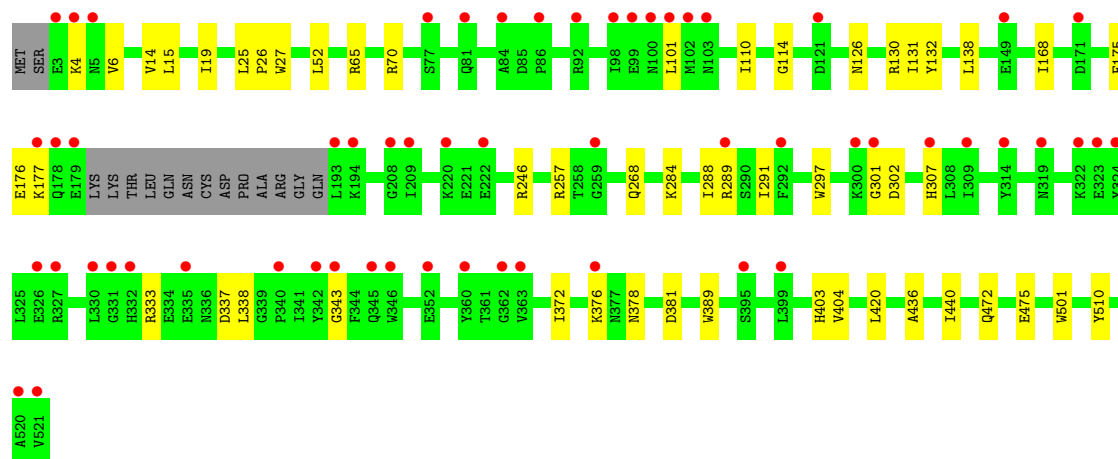
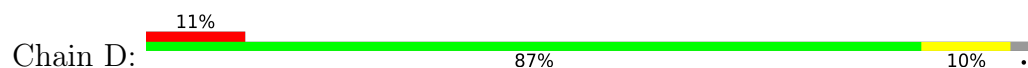


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

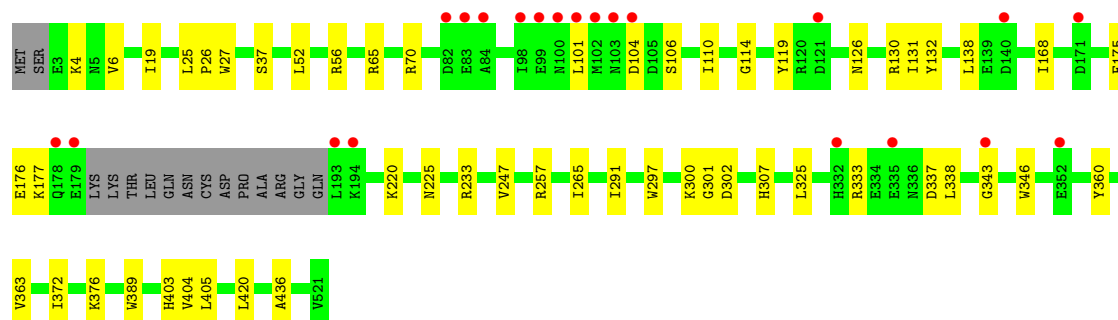
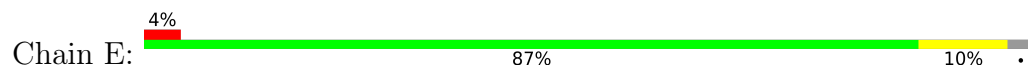




- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.63Å 116.59Å 221.41Å 90.00° 95.21° 90.00°	Depositor
Resolution (Å)	48.64 – 2.71 48.64 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.64-2.71) 99.0 (48.64-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: 000)	Depositor
R, R_{free}	0.201 , 0.231 0.204 , 0.232	Depositor DCC
R_{free} test set	7312 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21541	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: MTX, NDP, SO4, OFJ, UFP

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	0.11	0/4159	0.32	0/5631
1	B	0.11	0/4172	0.33	0/5648
1	C	0.12	0/4192	0.34	0/5671
1	D	0.10	0/4134	0.30	0/5608
1	E	0.12	0/4192	0.36	0/5670
All	All	0.11	0/20849	0.33	0/28228

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	4064	0	3957	44	0
1	B	4077	0	3969	45	0
1	C	4097	0	4003	36	0
1	D	4039	0	3877	34	0
1	E	4097	0	4010	40	0
2	A	48	0	26	1	0
2	B	48	0	26	3	0
2	C	48	0	26	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	26	3	0
2	E	48	0	26	3	0
3	A	21	0	10	0	0
3	B	21	0	10	0	0
3	C	21	0	10	0	0
3	D	21	0	10	1	0
3	E	21	0	10	1	0
4	A	33	0	0	1	0
4	B	33	0	0	0	0
4	C	33	0	0	1	0
4	D	33	0	0	0	0
4	E	33	0	0	0	0
5	A	33	0	20	3	0
5	B	33	0	20	1	0
5	C	33	0	20	3	0
5	D	33	0	20	3	0
5	E	33	0	20	2	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	E	10	0	0	0	0
7	A	66	0	0	0	0
7	B	100	0	0	1	0
7	C	114	0	0	2	0
7	D	20	0	0	0	0
7	E	162	0	0	2	0
All	All	21541	0	20096	191	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 5.

All (191) 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	1.74	0.68
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.75	0.67
1:A:410:VAL:O	1:B:254:ARG:NH2	2.27	0.66
1:E:225:ASN:O	1:E:233:ARG:NH2	2.27	0.66
1:C:25:LEU:HD11	5:C:604:MTX:H7	1.79	0.64
1:D:25:LEU:HD11	5:D:604:MTX:H7	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.80	0.64
4:C:603:OFJ:N6	7:C:702:HOH:O	2.31	0.63
1:E:65:ARG:NH1	7:E:701:HOH:O	2.26	0.63
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.81	0.62
1:E:25:LEU:HD11	5:E:604:MTX:H7	1.81	0.62
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.81	0.62
1:B:248:LEU:O	1:E:65:ARG:NH2	2.33	0.61
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.82	0.61
1:E:126:ASN:OD1	1:E:177:LYS:NZ	2.32	0.61
1:A:515:ILE:O	4:A:603:OFJ:N6	2.33	0.61
1:E:114:GLY:HA3	2:E:601:NDP:H5N	1.82	0.61
1:B:126:ASN:OD1	1:B:177:LYS:NZ	2.32	0.60
1:B:130:ARG:NH1	1:B:176:GLU:OE2	2.34	0.60
1:A:25:LEU:HD11	5:A:604:MTX:H7	1.82	0.60
1:C:126:ASN:OD1	1:C:177:LYS:NZ	2.27	0.59
1:C:114:GLY:HA3	2:C:601:NDP:H5N	1.84	0.59
1:B:138:LEU:HD11	1:B:168:ILE:HD13	1.84	0.58
1:D:130:ARG:NH1	1:D:176:GLU:OE2	2.36	0.58
1:E:257:ARG:HH21	3:E:602:UFP:H5'1	1.69	0.58
1:B:52:LEU:HD11	1:B:70:ARG:HD2	1.86	0.58
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.85	0.57
1:C:233:ARG:NH2	1:C:242:ASP:OD1	2.34	0.57
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.87	0.56
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.87	0.56
1:B:301:GLY:HA2	1:B:343:GLY:O	2.06	0.56
1:A:130:ARG:NH1	1:A:176:GLU:OE2	2.39	0.56
1:B:25:LEU:HD11	5:B:604:MTX:H7	1.87	0.55
1:C:288:ILE:HD11	1:C:440:ILE:HD11	1.87	0.55
1:D:126:ASN:OD1	1:D:177:LYS:NZ	2.36	0.55
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.72	0.55
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.88	0.55
1:E:403:HIS:HB2	1:E:420:LEU:HD11	1.89	0.55
1:A:114:GLY:HA3	2:A:601:NDP:H5N	1.89	0.54
1:E:130:ARG:NH1	1:E:176:GLU:OE2	2.41	0.54
1:E:301:GLY:HA2	1:E:343:GLY:O	2.07	0.54
1:E:4:LYS:HG2	1:E:101:LEU:HD23	1.90	0.54
1:A:301:GLY:HA2	1:A:343:GLY:O	2.08	0.53
1:C:4:LYS:H	1:C:101:LEU:HD22	1.73	0.53
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.43	0.53
1:A:254:ARG:NH2	1:B:410:VAL:O	2.39	0.53
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:GLY:HA2	1:C:343:GLY:O	2.08	0.53
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.90	0.53
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.89	0.52
1:D:14:VAL:HG13	1:D:15:LEU:HG	1.90	0.52
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.45	0.52
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.44	0.52
1:C:4:LYS:HG2	1:C:101:LEU:HD23	1.92	0.52
1:A:52:LEU:HD11	1:A:70:ARG:HD2	1.92	0.51
1:A:288:ILE:HD11	1:A:440:ILE:HD11	1.92	0.51
1:E:4:LYS:H	1:E:101:LEU:HD22	1.75	0.51
1:D:403:HIS:H	1:D:403:HIS:CD2	2.28	0.51
1:E:302:ASP:OD2	1:E:307:HIS:ND1	2.31	0.51
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.45	0.51
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.75	0.51
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.45	0.51
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.92	0.51
1:E:297:TRP:HH2	1:E:338:LEU:HD12	1.75	0.51
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.46	0.50
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.76	0.50
1:A:138:LEU:HD11	1:A:168:ILE:HD13	1.93	0.50
1:A:383:ARG:NE	1:B:400:PRO:HG2	2.27	0.50
1:C:26:PRO:HG2	1:C:27:TRP:CZ3	2.47	0.49
1:C:130:ARG:NH1	1:C:176:GLU:OE2	2.45	0.49
1:E:52:LEU:HD11	1:E:70:ARG:HD2	1.94	0.49
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.48	0.49
1:B:43:LYS:NZ	1:B:48:LYS:O	2.33	0.49
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.78	0.49
1:D:372:ILE:O	1:D:376:LYS:HG2	2.13	0.49
1:E:26:PRO:HG2	1:E:27:TRP:CZ3	2.48	0.49
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.93	0.49
1:A:342:TYR:HH	1:A:402:CYS:H	1.55	0.48
1:B:325:LEU:HD23	1:B:333:ARG:HB3	1.95	0.48
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.47	0.48
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.94	0.48
1:C:302:ASP:OD2	1:C:307:HIS:ND1	2.39	0.48
2:D:601:NDP:H42N	5:D:604:MTX:N5	2.29	0.48
1:D:4:LYS:H	1:D:101:LEU:HD22	1.79	0.48
1:C:342:TYR:HH	1:C:402:CYS:H	1.57	0.48
1:A:400:PRO:HG2	1:B:383:ARG:NE	2.30	0.47
1:D:288:ILE:HD11	1:D:440:ILE:HD11	1.96	0.47
1:B:114:GLY:HA3	2:B:601:NDP:H5N	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TRP:CD1	1:C:302:ASP:HB3	2.50	0.47
1:A:14:VAL:HG13	1:A:15:LEU:HG	1.96	0.47
1:A:9:VAL:HG12	5:A:604:MTX:N3	2.30	0.47
1:A:126:ASN:OD1	1:A:177:LYS:NZ	2.36	0.47
1:B:302:ASP:OD2	1:B:307:HIS:ND1	2.37	0.47
1:B:332:HIS:CG	1:C:144:ASP:HB2	2.50	0.47
1:A:26:PRO:HG2	1:A:27:TRP:CZ3	2.50	0.47
1:B:19:ILE:O	2:B:601:NDP:H2N	2.15	0.47
1:B:372:ILE:O	1:B:376:LYS:HG2	2.15	0.46
1:C:104:ASP:OD1	1:C:106:SER:OG	2.29	0.46
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.51	0.46
1:E:297:TRP:CD1	1:E:302:ASP:HB3	2.50	0.46
1:B:291:ILE:HD13	1:B:436:ALA:HB3	1.98	0.46
1:D:6:VAL:HG22	1:D:110:ILE:HB	1.97	0.46
1:E:138:LEU:HD11	1:E:168:ILE:HD13	1.97	0.46
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.97	0.46
1:B:26:PRO:HG2	1:B:27:TRP:CZ3	2.51	0.45
1:D:301:GLY:HA2	1:D:343:GLY:O	2.16	0.45
1:D:138:LEU:HD11	1:D:168:ILE:HD13	1.98	0.45
1:E:325:LEU:HD23	1:E:333:ARG:HB3	1.98	0.45
1:E:291:ILE:HD13	1:E:436:ALA:HB3	1.98	0.45
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.98	0.45
1:E:130:ARG:HD2	1:E:132:TYR:CZ	2.52	0.45
1:E:403:HIS:H	1:E:403:HIS:CD2	2.33	0.45
1:A:248:LEU:O	1:D:65:ARG:NH2	2.49	0.45
1:A:403:HIS:H	1:A:403:HIS:CD2	2.33	0.45
1:B:300:LYS:NZ	7:B:703:HOH:O	2.41	0.45
1:E:104:ASP:OD1	1:E:106:SER:OG	2.35	0.45
1:C:138:LEU:HD11	1:C:168:ILE:HD13	1.98	0.45
1:A:372:ILE:O	1:A:376:LYS:HG2	2.17	0.44
1:D:26:PRO:HG2	1:D:27:TRP:CZ3	2.52	0.44
1:D:302:ASP:OD2	1:D:307:HIS:ND1	2.38	0.44
1:A:6:VAL:HG22	1:A:110:ILE:HB	1.99	0.44
1:B:151:PRO:HG2	1:B:154:PHE:HD1	1.82	0.44
1:E:19:ILE:O	2:E:601:NDP:H2N	2.18	0.44
1:C:19:ILE:O	2:C:601:NDP:H2N	2.16	0.44
1:B:81:GLN:HG3	1:B:92:ARG:NH2	2.33	0.44
1:C:403:HIS:H	1:C:403:HIS:CD2	2.35	0.44
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.99	0.44
1:E:372:ILE:O	1:E:376:LYS:HG2	2.18	0.44
1:B:14:VAL:HG13	1:B:15:LEU:HG	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:VAL:HG22	1:C:265:ILE:HG12	2.00	0.43
1:D:257:ARG:HH21	3:D:602:UFP:H5'1	1.83	0.43
1:E:37:SER:HB2	5:E:604:MTX:HB1	2.00	0.43
1:B:297:TRP:CD1	1:B:302:ASP:HB3	2.54	0.43
1:A:247:VAL:HG22	1:A:265:ILE:HG12	2.01	0.43
1:C:4:LYS:HG2	1:C:101:LEU:CD2	2.47	0.43
1:D:114:GLY:HA3	2:D:601:NDP:H5N	1.99	0.43
1:A:403:HIS:HB2	1:A:420:LEU:HD11	2.00	0.43
1:B:372:ILE:HG22	1:B:376:LYS:HE2	2.01	0.43
1:C:130:ARG:HD2	1:C:132:TYR:CZ	2.54	0.43
1:E:247:VAL:HG22	1:E:265:ILE:HG12	2.01	0.43
1:A:291:ILE:HD13	1:A:436:ALA:HB3	2.01	0.42
1:C:161:GLN:NE2	7:C:703:HOH:O	2.34	0.42
1:D:472:GLN:OE1	1:D:472:GLN:N	2.51	0.42
2:C:601:NDP:H42N	5:C:604:MTX:N5	2.34	0.42
1:E:300:LYS:NZ	7:E:702:HOH:O	2.39	0.42
1:B:244:LEU:HD12	1:B:427:LEU:HD13	2.01	0.42
1:B:405:LEU:O	1:B:420:LEU:HD12	2.20	0.42
1:E:343:GLY:HA2	1:E:346:TRP:HB2	2.01	0.42
1:B:403:HIS:CD2	1:B:403:HIS:H	2.36	0.42
1:D:130:ARG:HD2	1:D:132:TYR:CZ	2.54	0.42
1:A:43:LYS:NZ	1:A:48:LYS:O	2.37	0.42
1:A:58:THR:HG23	5:A:604:MTX:HM2	2.02	0.42
1:D:70:ARG:HH22	5:D:604:MTX:CT	2.32	0.42
1:E:56:ARG:HD3	2:E:601:NDP:O2X	2.20	0.42
1:B:151:PRO:HG2	1:B:154:PHE:CD1	2.54	0.42
1:D:403:HIS:HB2	1:D:420:LEU:HD11	2.01	0.42
1:D:246:ARG:NH2	1:D:268:GLN:OE1	2.38	0.41
1:D:378:ASN:ND2	1:D:381:ASP:HB2	2.35	0.41
1:C:10:VAL:HG21	1:C:147:PHE:CD1	2.55	0.41
1:C:291:ILE:HD13	1:C:436:ALA:HB3	2.01	0.41
1:C:429:LEU:HD21	1:C:517:MET:HB2	2.03	0.41
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.55	0.41
1:D:472:GLN:O	1:D:475:GLU:HB3	2.20	0.41
1:C:14:VAL:HG13	1:C:15:LEU:HG	2.02	0.41
1:A:360:TYR:O	1:A:363:VAL:HG12	2.20	0.41
1:B:355:THR:O	1:B:360:TYR:OH	2.29	0.41
1:E:220:LYS:HE3	1:E:220:LYS:HB2	1.93	0.41
1:B:424:SER:OG	1:B:464:HIS:HE1	2.04	0.41
1:D:19:ILE:O	2:D:601:NDP:H2N	2.21	0.41
1:E:6:VAL:HG22	1:E:110:ILE:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:GLY:HA2	1:E:119:TYR:CZ	2.56	0.41
1:A:4:LYS:H	1:A:101:LEU:HD22	1.86	0.41
1:A:215:ARG:NH1	1:B:455:GLU:OE2	2.54	0.41
1:E:4:LYS:HG2	1:E:101:LEU:CD2	2.50	0.41
1:C:424:SER:OG	1:C:464:HIS:HE1	2.04	0.41
1:B:4:LYS:H	1:B:101:LEU:HD22	1.86	0.40
1:A:337:ASP:OD1	1:A:353:TYR:OH	2.38	0.40
1:A:372:ILE:HG22	1:A:376:LYS:HE2	2.02	0.40
1:A:298:PHE:CE1	1:A:342:TYR:HB2	2.56	0.40
1:B:56:ARG:HD3	2:B:601:NDP:O2X	2.22	0.40
1:B:343:GLY:HA2	1:B:346:TRP:HB2	2.02	0.40
1:C:20:GLY:HA2	1:C:26:PRO:HD3	2.03	0.40
1:C:220:LYS:HE3	1:C:220:LYS:HB2	1.97	0.40
1:E:360:TYR:O	1:E:363:VAL:HG12	2.21	0.40
1:E:405:LEU:O	1:E:420:LEU:HD12	2.21	0.40
1:A:291:ILE:HG12	1:A:433:PHE:CD2	2.57	0.40
1:A:297:TRP:CE3	1:A:308:LEU:HD11	2.56	0.40
1:A:455:GLU:OE2	1:B:215:ARG:NH1	2.55	0.40
1:D:15:LEU:HD11	1:D:510:TYR:HB3	2.03	0.40
1:C:58:THR:HG23	5:C:604:MTX:HM2	2.04	0.40
1:D:289:ARG:HG3	1:D:501:TRP:CE2	2.56	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	501/521 (96%)	475 (95%)	26 (5%)	0	100	100
1	B	502/521 (96%)	476 (95%)	26 (5%)	0	100	100
1	C	502/521 (96%)	475 (95%)	27 (5%)	0	100	100
1	D	502/521 (96%)	476 (95%)	26 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	502/521 (96%)	475 (95%)	27 (5%)	0	100	100
All	All	2509/2605 (96%)	2377 (95%)	132 (5%)	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	443/470 (94%)	443 (100%)	0	100	100
1	B	445/470 (95%)	445 (100%)	0	100	100
1	C	450/470 (96%)	450 (100%)	0	100	100
1	D	436/470 (93%)	435 (100%)	1 (0%)	87	95
1	E	450/470 (96%)	450 (100%)	0	100	100
All	All	2224/2350 (95%)	2223 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	284	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	336	ASN
1	A	486	GLN
1	B	5	ASN
1	B	486	GLN
1	C	336	ASN
1	D	336	ASN
1	D	414	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	486	GLN
1	E	414	ASN
1	E	486	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 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	$\# Z > 2$
2	NDP	C	601	-	51,52,52	1.97	12 (23%)	71,80,80	1.48	11 (15%)
6	SO4	A	605	-	4,4,4	0.23	0	6,6,6	0.08	0
5	MTX	C	604	-	35,35,35	1.59	5 (14%)	47,49,49	1.79	8 (17%)
6	SO4	E	605	-	4,4,4	0.25	0	6,6,6	0.06	0
5	MTX	E	604	-	35,35,35	1.62	5 (14%)	47,49,49	1.79	9 (19%)
6	SO4	E	606	-	4,4,4	0.25	0	6,6,6	0.09	0
4	OFJ	C	603	-	36,36,36	1.38	4 (11%)	48,52,52	1.19	5 (10%)
4	OFJ	E	603	-	36,36,36	1.42	3 (8%)	48,52,52	1.34	6 (12%)
3	UFP	E	602	-	22,22,22	1.05	0	32,33,33	2.68	11 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OFJ	A	603	-	36,36,36	1.35	2 (5%)	48,52,52	1.17	4 (8%)
5	MTX	A	604	-	35,35,35	1.60	5 (14%)	47,49,49	1.75	7 (14%)
2	NDP	D	601	-	51,52,52	1.96	12 (23%)	71,80,80	1.53	12 (16%)
4	OFJ	D	603	-	36,36,36	1.36	2 (5%)	48,52,52	1.13	4 (8%)
6	SO4	D	605	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	B	605	-	4,4,4	0.25	0	6,6,6	0.06	0
5	MTX	B	604	-	35,35,35	1.62	5 (14%)	47,49,49	1.78	7 (14%)
2	NDP	B	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.50	11 (15%)
3	UFP	A	602	-	22,22,22	1.04	0	32,33,33	2.61	11 (34%)
3	UFP	D	602	-	22,22,22	1.05	0	32,33,33	2.66	11 (34%)
5	MTX	D	604	-	35,35,35	1.61	5 (14%)	47,49,49	1.75	7 (14%)
3	UFP	C	602	-	22,22,22	1.28	1 (4%)	32,33,33	2.69	11 (34%)
6	SO4	C	605	-	4,4,4	0.25	0	6,6,6	0.08	0
2	NDP	A	601	-	51,52,52	1.97	12 (23%)	71,80,80	1.51	10 (14%)
2	NDP	E	601	-	51,52,52	1.98	12 (23%)	71,80,80	1.50	11 (15%)
3	UFP	B	602	-	22,22,22	1.04	0	32,33,33	2.66	11 (34%)
4	OFJ	B	603	-	36,36,36	1.39	3 (8%)	48,52,52	1.25	5 (10%)

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
2	NDP	C	601	-	-	3/34/77/77	0/5/5/5
5	MTX	C	604	-	-	7/25/25/25	0/3/3/3
5	MTX	E	604	-	-	6/25/25/25	0/3/3/3
4	OFJ	C	603	-	-	2/20/20/20	0/4/4/4
4	OFJ	E	603	-	-	2/20/20/20	0/4/4/4
3	UFP	E	602	-	-	6/10/22/22	0/2/2/2
4	OFJ	A	603	-	-	2/20/20/20	0/4/4/4
5	MTX	A	604	-	-	7/25/25/25	0/3/3/3
2	NDP	D	601	-	-	5/34/77/77	0/5/5/5
4	OFJ	D	603	-	-	2/20/20/20	0/4/4/4
5	MTX	B	604	-	-	7/25/25/25	0/3/3/3
2	NDP	B	601	-	-	5/34/77/77	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UFP	A	602	-	-	5/10/22/22	0/2/2/2
3	UFP	D	602	-	-	5/10/22/22	0/2/2/2
5	MTX	D	604	-	-	7/25/25/25	0/3/3/3
3	UFP	C	602	-	-	3/10/22/22	0/2/2/2
2	NDP	A	601	-	-	4/34/77/77	0/5/5/5
2	NDP	E	601	-	-	3/34/77/77	0/5/5/5
3	UFP	B	602	-	-	5/10/22/22	0/2/2/2
4	OFJ	B	603	-	-	2/20/20/20	0/4/4/4

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NDP	C6A-N6A	5.80	1.49	1.34
2	A	601	NDP	C6A-N6A	5.78	1.49	1.34
2	B	601	NDP	C6A-N6A	5.72	1.48	1.34
2	E	601	NDP	C6A-N6A	5.72	1.48	1.34
2	C	601	NDP	C6A-N6A	5.71	1.48	1.34
5	E	604	MTX	C2-NA2	5.33	1.44	1.33
5	A	604	MTX	C2-NA2	5.27	1.44	1.33
5	D	604	MTX	C2-NA2	5.26	1.44	1.33
5	B	604	MTX	C2-NA2	5.25	1.44	1.33
5	C	604	MTX	C2-NA2	5.15	1.44	1.33
2	E	601	NDP	C4N-C3N	-4.83	1.40	1.50
5	D	604	MTX	C-N	4.78	1.45	1.34
5	B	604	MTX	C-N	4.77	1.45	1.34
5	E	604	MTX	C-N	4.75	1.45	1.34
2	C	601	NDP	C4N-C3N	-4.74	1.41	1.50
5	C	604	MTX	C-N	4.74	1.45	1.34
2	A	601	NDP	C4N-C3N	-4.73	1.41	1.50
5	A	604	MTX	C-N	4.68	1.45	1.34
2	D	601	NDP	C4N-C3N	-4.68	1.41	1.50
2	B	601	NDP	C4N-C3N	-4.68	1.41	1.50
2	C	601	NDP	C2D-C3D	-4.01	1.42	1.53
2	A	601	NDP	C2D-C3D	-3.97	1.42	1.53
2	E	601	NDP	C3B-C2B	-3.96	1.44	1.53
2	E	601	NDP	C2D-C3D	-3.96	1.42	1.53
2	B	601	NDP	C2D-C3D	-3.95	1.42	1.53
2	D	601	NDP	C3B-C2B	-3.93	1.44	1.53
2	D	601	NDP	C2D-C3D	-3.91	1.42	1.53
2	A	601	NDP	C3B-C2B	-3.91	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NDP	C3B-C2B	-3.85	1.44	1.53
2	B	601	NDP	C3B-C2B	-3.83	1.44	1.53
2	A	601	NDP	C7N-N7N	3.69	1.44	1.33
2	E	601	NDP	C7N-N7N	3.68	1.44	1.33
2	B	601	NDP	C7N-N7N	3.67	1.44	1.33
2	C	601	NDP	C7N-N7N	3.65	1.44	1.33
2	D	601	NDP	C7N-N7N	3.65	1.43	1.33
4	B	603	OFJ	C2-C1	-3.59	1.37	1.45
4	D	603	OFJ	C2-C1	-3.53	1.37	1.45
4	C	603	OFJ	C2-C1	-3.52	1.37	1.45
4	E	603	OFJ	C2-C1	-3.52	1.37	1.45
4	A	603	OFJ	C2-C1	-3.50	1.37	1.45
3	C	602	UFP	P-O1P	3.37	1.60	1.50
2	D	601	NDP	C4N-C5N	-3.34	1.40	1.49
2	E	601	NDP	C4N-C5N	-3.33	1.40	1.49
2	C	601	NDP	C4N-C5N	-3.32	1.40	1.49
2	A	601	NDP	C4N-C5N	-3.32	1.40	1.49
2	B	601	NDP	C4N-C5N	-3.31	1.40	1.49
2	A	601	NDP	C2B-C1B	-3.12	1.45	1.53
2	B	601	NDP	C2B-C1B	-3.09	1.45	1.53
2	C	601	NDP	C2B-C1B	-3.08	1.45	1.53
2	D	601	NDP	C2B-C1B	-3.06	1.45	1.53
2	E	601	NDP	C2B-C1B	-3.03	1.45	1.53
5	B	604	MTX	C4-NA4	2.57	1.43	1.34
5	A	604	MTX	C4-NA4	2.57	1.43	1.34
5	D	604	MTX	C4-NA4	2.54	1.43	1.34
5	C	604	MTX	C4-NA4	2.54	1.43	1.34
5	E	604	MTX	C4-NA4	2.52	1.43	1.34
5	E	604	MTX	C14-N10	2.50	1.45	1.38
2	A	601	NDP	C3B-C4B	-2.48	1.46	1.53
2	B	601	NDP	C3B-C4B	-2.48	1.46	1.53
5	B	604	MTX	C14-N10	2.48	1.45	1.38
2	D	601	NDP	C3B-C4B	-2.46	1.46	1.53
2	E	601	NDP	C3B-C4B	-2.46	1.46	1.53
2	C	601	NDP	C3B-C4B	-2.45	1.46	1.53
5	D	604	MTX	C14-N10	2.43	1.45	1.38
5	A	604	MTX	C14-N10	2.41	1.45	1.38
2	D	601	NDP	C4A-N3A	2.41	1.38	1.34
2	A	601	NDP	C4A-N3A	2.37	1.38	1.34
2	C	601	NDP	C3D-C4D	-2.35	1.47	1.53
2	E	601	NDP	C4A-N3A	2.34	1.38	1.34
4	E	603	OFJ	O4-C22	2.33	1.37	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NDP	C4A-N3A	2.33	1.38	1.34
2	C	601	NDP	C4A-N3A	2.32	1.38	1.34
2	A	601	NDP	C3D-C4D	-2.32	1.47	1.53
2	E	601	NDP	C3D-C4D	-2.31	1.47	1.53
2	D	601	NDP	C3D-C4D	-2.30	1.47	1.53
4	B	603	OFJ	O4-C22	2.30	1.37	1.30
5	E	604	MTX	C7-N8	2.29	1.35	1.31
2	B	601	NDP	C3D-C4D	-2.29	1.47	1.53
4	A	603	OFJ	O4-C22	2.26	1.37	1.30
4	C	603	OFJ	O4-C22	2.26	1.37	1.30
5	B	604	MTX	C7-N8	2.25	1.35	1.31
5	C	604	MTX	C14-N10	2.25	1.45	1.38
5	D	604	MTX	C7-N8	2.24	1.35	1.31
5	C	604	MTX	C7-N8	2.23	1.35	1.31
4	D	603	OFJ	O4-C22	2.23	1.37	1.30
5	A	604	MTX	C7-N8	2.22	1.35	1.31
2	D	601	NDP	C6N-C5N	2.17	1.39	1.33
2	B	601	NDP	C6N-C5N	2.16	1.39	1.33
2	A	601	NDP	C6N-C5N	2.12	1.39	1.33
2	C	601	NDP	C6N-C5N	2.12	1.39	1.33
2	D	601	NDP	C2N-C3N	2.06	1.40	1.35
2	E	601	NDP	C2N-C3N	2.05	1.40	1.35
2	E	601	NDP	C6N-C5N	2.05	1.39	1.33
2	C	601	NDP	C2N-C3N	2.03	1.40	1.35
2	A	601	NDP	C2N-C3N	2.03	1.40	1.35
2	B	601	NDP	C2N-C3N	2.02	1.40	1.35
4	B	603	OFJ	C3-N2	-2.02	1.35	1.38
4	E	603	OFJ	C2-C3	2.01	1.48	1.44
4	C	603	OFJ	C3-N2	-2.01	1.35	1.38
4	C	603	OFJ	C2-C3	2.01	1.48	1.44

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	UFP	C5-C4-N3	6.95	119.00	112.64
3	C	602	UFP	C5-C4-N3	6.94	118.98	112.64
3	B	602	UFP	C5-C4-N3	6.89	118.94	112.64
3	E	602	UFP	C5-C4-N3	6.87	118.92	112.64
3	A	602	UFP	C5-C4-N3	6.83	118.88	112.64
3	C	602	UFP	O4-C4-C5	-6.17	120.44	125.69
3	D	602	UFP	O4-C4-C5	-6.09	120.50	125.69
3	A	602	UFP	O4-C4-C5	-6.03	120.56	125.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	UFP	O4-C4-C5	-5.97	120.60	125.69
3	E	602	UFP	O4-C4-C5	-5.73	120.81	125.69
2	A	601	NDP	C5A-C4A-N3A	-5.37	119.32	126.72
2	D	601	NDP	C5A-C4A-N3A	-5.36	119.34	126.72
3	E	602	UFP	F5-C5-C4	5.34	121.15	116.47
2	B	601	NDP	C5A-C4A-N3A	-5.30	119.41	126.72
5	E	604	MTX	C6-C7-N8	-5.27	118.08	123.14
3	A	602	UFP	F5-C5-C4	5.22	121.05	116.47
5	B	604	MTX	C6-C7-N8	-5.20	118.15	123.14
3	D	602	UFP	F5-C5-C4	5.17	121.00	116.47
5	A	604	MTX	C6-C7-N8	-5.15	118.20	123.14
2	C	601	NDP	C5A-C4A-N3A	-5.12	119.66	126.72
5	C	604	MTX	C6-C7-N8	-5.12	118.23	123.14
5	D	604	MTX	C6-C7-N8	-5.10	118.25	123.14
2	E	601	NDP	C5A-C4A-N3A	-5.08	119.72	126.72
3	B	602	UFP	F5-C5-C4	5.07	120.91	116.47
3	C	602	UFP	F5-C5-C4	4.83	120.70	116.47
3	D	602	UFP	C4-N3-C2	-4.63	121.27	127.34
3	E	602	UFP	C4-N3-C2	-4.62	121.28	127.34
3	C	602	UFP	C4-N3-C2	-4.61	121.29	127.34
3	B	602	UFP	C4-N3-C2	-4.60	121.31	127.34
3	A	602	UFP	C4-N3-C2	-4.51	121.43	127.34
3	C	602	UFP	N3-C2-N1	4.45	120.68	114.89
3	E	602	UFP	C1'-N1-C2	4.44	126.34	117.66
3	E	602	UFP	N3-C2-N1	4.41	120.63	114.89
3	B	602	UFP	N3-C2-N1	4.34	120.54	114.89
3	B	602	UFP	C1'-N1-C2	4.33	126.13	117.66
4	E	603	OFJ	C5-C2-C1	-4.30	107.75	112.68
3	D	602	UFP	N3-C2-N1	4.29	120.47	114.89
4	A	603	OFJ	C5-C2-C1	-4.29	107.77	112.68
4	C	603	OFJ	C5-C2-C1	-4.27	107.79	112.68
4	D	603	OFJ	C5-C2-C1	-4.26	107.80	112.68
3	A	602	UFP	N3-C2-N1	4.23	120.40	114.89
3	D	602	UFP	C6-C5-C4	-4.22	118.72	122.57
3	A	602	UFP	C6-C5-C4	-4.21	118.73	122.57
3	C	602	UFP	C1'-N1-C2	4.21	125.89	117.66
3	C	602	UFP	C6-C5-C4	-4.18	118.76	122.57
3	D	602	UFP	C1'-N1-C2	4.17	125.82	117.66
4	B	603	OFJ	C5-C2-C1	-4.16	107.91	112.68
3	E	602	UFP	C6-C5-C4	-4.12	118.81	122.57
5	E	604	MTX	N8-C8A-N1	4.12	120.26	115.77
3	B	602	UFP	C6-C5-C4	-4.11	118.82	122.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	604	MTX	N1-C2-N3	-3.97	122.16	127.21
5	A	604	MTX	N1-C2-N3	-3.97	122.16	127.21
5	E	604	MTX	N1-C2-N3	-3.94	122.20	127.21
5	B	604	MTX	N1-C2-N3	-3.94	122.20	127.21
5	C	604	MTX	N8-C8A-N1	3.93	120.05	115.77
3	A	602	UFP	C1'-N1-C2	3.93	125.34	117.66
5	C	604	MTX	N1-C2-N3	-3.91	122.24	127.21
2	E	601	NDP	N3A-C2A-N1A	-3.90	122.67	128.58
2	D	601	NDP	N3A-C2A-N1A	-3.87	122.73	128.58
2	A	601	NDP	N3A-C2A-N1A	-3.86	122.74	128.58
5	B	604	MTX	CG-CB-CA	3.86	120.27	113.16
5	D	604	MTX	N8-C8A-N1	3.85	119.97	115.77
5	B	604	MTX	N8-C8A-N1	3.85	119.96	115.77
5	E	604	MTX	C2-N1-C8A	3.82	119.60	115.48
5	B	604	MTX	C2-N1-C8A	3.80	119.58	115.48
2	C	601	NDP	N3A-C2A-N1A	-3.79	122.84	128.58
5	C	604	MTX	C2-N1-C8A	3.79	119.57	115.48
5	A	604	MTX	N8-C8A-N1	3.79	119.90	115.77
2	B	601	NDP	N3A-C2A-N1A	-3.76	122.90	128.58
5	D	604	MTX	C2-N1-C8A	3.75	119.53	115.48
2	A	601	NDP	N3A-C4A-N9A	3.72	133.49	127.17
5	A	604	MTX	C2-N1-C8A	3.68	119.45	115.48
2	D	601	NDP	N3A-C4A-N9A	3.67	133.41	127.17
3	E	602	UFP	C1'-N1-C6	-3.62	114.67	120.74
2	C	601	NDP	N3A-C4A-N9A	3.62	133.32	127.17
5	C	604	MTX	CG-CB-CA	3.61	119.82	113.16
3	B	602	UFP	C1'-N1-C6	-3.58	114.74	120.74
2	B	601	NDP	N3A-C4A-N9A	3.57	133.24	127.17
2	E	601	NDP	N3A-C4A-N9A	3.52	133.15	127.17
5	D	604	MTX	CG-CB-CA	3.51	119.64	113.16
5	A	604	MTX	CG-CB-CA	3.48	119.58	113.16
3	D	602	UFP	C1'-N1-C6	-3.48	114.90	120.74
5	E	604	MTX	CG-CB-CA	3.48	119.57	113.16
4	E	603	OFJ	C15-C20-C22	3.44	125.55	121.72
2	D	601	NDP	C2A-N3A-C4A	3.39	120.12	111.83
2	A	601	NDP	C2A-N3A-C4A	3.39	120.10	111.83
2	B	601	NDP	C2A-N3A-C4A	3.35	120.02	111.83
2	E	601	NDP	N9A-C8A-N7A	-3.34	109.19	113.94
2	C	601	NDP	N9A-C8A-N7A	-3.33	109.21	113.94
2	E	601	NDP	C2A-N3A-C4A	3.31	119.92	111.83
3	C	602	UFP	C1'-N1-C6	-3.30	115.21	120.74
2	A	601	NDP	N9A-C8A-N7A	-3.28	109.29	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NDP	N9A-C8A-N7A	-3.26	109.31	113.94
2	C	601	NDP	C2A-N3A-C4A	3.25	119.78	111.83
2	B	601	NDP	C4A-C5A-N7A	-3.22	106.90	110.58
2	B	601	NDP	N9A-C8A-N7A	-3.22	109.37	113.94
3	A	602	UFP	C1'-N1-C6	-3.17	115.41	120.74
2	D	601	NDP	C4A-C5A-N7A	-3.15	106.98	110.58
2	D	601	NDP	C5A-N7A-C8A	3.09	108.31	103.45
2	A	601	NDP	C4A-C5A-N7A	-3.07	107.07	110.58
2	B	601	NDP	C5A-N7A-C8A	3.06	108.26	103.45
2	A	601	NDP	C5A-N7A-C8A	3.06	108.26	103.45
3	C	602	UFP	O2-C2-N3	-3.03	115.89	121.49
2	E	601	NDP	C4A-C5A-N7A	-3.01	107.14	110.58
2	E	601	NDP	C5A-N7A-C8A	3.01	108.18	103.45
3	E	602	UFP	O2-C2-N3	-3.00	115.95	121.49
3	C	602	UFP	O4'-C1'-C2'	-2.99	100.66	106.25
2	C	601	NDP	C5A-N7A-C8A	2.97	108.12	103.45
3	B	602	UFP	O2-C2-N3	-2.96	116.02	121.49
4	E	603	OFJ	C20-C15-N4	2.93	123.98	118.70
2	C	601	NDP	C4A-C5A-N7A	-2.93	107.23	110.58
4	B	603	OFJ	C15-C20-C22	2.77	124.81	121.72
3	D	602	UFP	O2-C2-N3	-2.73	116.45	121.49
4	E	603	OFJ	N5-C4-N2	-2.72	111.02	116.76
3	B	602	UFP	O4'-C1'-C2'	-2.64	101.31	106.25
4	B	603	OFJ	N5-C4-N2	-2.63	111.20	116.76
4	C	603	OFJ	N5-C4-N2	-2.61	111.25	116.76
2	B	601	NDP	O5D-C5D-C4D	2.60	117.85	108.99
4	B	603	OFJ	C20-C15-N4	2.59	123.37	118.70
3	E	602	UFP	O4'-C1'-C2'	-2.58	101.42	106.25
2	D	601	NDP	O5D-C5D-C4D	2.58	117.78	108.99
4	A	603	OFJ	N5-C4-N2	-2.58	111.32	116.76
3	A	602	UFP	O4'-C1'-C2'	-2.57	101.45	106.25
3	A	602	UFP	O2-C2-N3	-2.57	116.75	121.49
2	C	601	NDP	C4A-N9A-C8A	2.55	108.41	105.74
3	D	602	UFP	O4'-C1'-C2'	-2.54	101.51	106.25
5	D	604	MTX	C7-N8-C8A	2.53	120.72	117.20
5	B	604	MTX	C7-N8-C8A	2.51	120.69	117.20
4	D	603	OFJ	N5-C4-N2	-2.51	111.47	116.76
2	E	601	NDP	C4A-N9A-C8A	2.50	108.36	105.74
5	E	604	MTX	C7-N8-C8A	2.49	120.67	117.20
4	E	603	OFJ	N5-C4-N1	2.47	124.50	119.67
4	C	603	OFJ	N5-C4-N1	2.45	124.45	119.67
5	A	604	MTX	C7-N8-C8A	2.43	120.58	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	604	MTX	C7-N8-C8A	2.43	120.58	117.20
3	C	602	UFP	C6-N1-C2	-2.41	118.90	121.30
4	B	603	OFJ	N5-C4-N1	2.41	124.38	119.67
2	A	601	NDP	O5D-C5D-C4D	2.40	117.18	108.99
2	A	601	NDP	O5B-C5B-C4B	2.39	117.14	108.99
4	A	603	OFJ	N5-C4-N1	2.36	124.28	119.67
4	C	603	OFJ	C15-C20-C22	2.36	124.35	121.72
2	D	601	NDP	C2B-C1B-N9A	-2.35	109.89	113.75
2	D	601	NDP	O5B-C5B-C4B	2.35	116.98	108.99
2	A	601	NDP	C4A-N9A-C8A	2.33	108.19	105.74
5	C	604	MTX	CM-N10-C9	2.32	121.15	115.11
3	E	602	UFP	C6-N1-C2	-2.32	118.99	121.30
2	D	601	NDP	C4A-N9A-C8A	2.30	108.15	105.74
4	D	603	OFJ	N5-C4-N1	2.28	124.13	119.67
2	B	601	NDP	C4A-N9A-C8A	2.26	108.11	105.74
2	B	601	NDP	O5B-C5B-C4B	2.26	116.68	108.99
4	A	603	OFJ	C15-C20-C22	2.26	124.23	121.72
2	E	601	NDP	C3N-C7N-N7N	2.25	121.67	117.67
2	E	601	NDP	C2B-C1B-N9A	-2.25	110.05	113.75
2	E	601	NDP	O5D-C5D-C4D	2.24	116.64	108.99
2	C	601	NDP	O5D-C5D-C4D	2.21	116.52	108.99
3	B	602	UFP	C6-N1-C2	-2.18	119.13	121.30
2	C	601	NDP	C3N-C7N-N7N	2.15	121.49	117.67
5	E	604	MTX	C6-C9-N10	-2.11	109.33	112.95
5	B	604	MTX	O2-CT-CA	2.10	120.63	113.51
4	C	603	OFJ	C20-C15-N4	2.08	122.44	118.70
4	E	603	OFJ	C15-N4-C14	2.07	132.67	126.90
2	D	601	NDP	C3N-C7N-N7N	2.07	121.34	117.67
5	A	604	MTX	O2-CT-CA	2.07	120.51	113.51
2	C	601	NDP	O4D-C1D-N1N	2.07	112.03	108.08
5	E	604	MTX	CM-N10-C9	2.06	120.48	115.11
5	E	604	MTX	O2-CT-CA	2.06	120.49	113.51
3	A	602	UFP	C6-N1-C2	-2.06	119.25	121.30
5	D	604	MTX	O2-CT-CA	2.03	120.38	113.51
3	D	602	UFP	C6-N1-C2	-2.03	119.28	121.30
2	B	601	NDP	O4D-C1D-N1N	2.02	111.95	108.08
4	D	603	OFJ	C15-C20-C22	2.02	123.97	121.72
5	C	604	MTX	O2-CT-CA	2.02	120.34	113.51

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	UFP	C5'-O5'-P-O2P
5	D	604	MTX	N-CA-CB-CG
5	B	604	MTX	N-CA-CB-CG
5	E	604	MTX	N-CA-CB-CG
5	A	604	MTX	CT-CA-CB-CG
5	B	604	MTX	CT-CA-CB-CG
5	D	604	MTX	CT-CA-CB-CG
3	D	602	UFP	C3'-C4'-C5'-O5'
3	E	602	UFP	C3'-C4'-C5'-O5'
5	C	604	MTX	CT-CA-CB-CG
5	E	604	MTX	CT-CA-CB-CG
2	B	601	NDP	C3D-C4D-C5D-O5D
3	A	602	UFP	C3'-C4'-C5'-O5'
3	D	602	UFP	O4'-C4'-C5'-O5'
3	E	602	UFP	O4'-C4'-C5'-O5'
5	A	604	MTX	C13-C14-N10-CM
5	A	604	MTX	C15-C14-N10-CM
5	B	604	MTX	C15-C14-N10-CM
5	D	604	MTX	C15-C14-N10-CM
5	C	604	MTX	N-CA-CB-CG
3	A	602	UFP	O4'-C4'-C5'-O5'
3	C	602	UFP	C2'-C1'-N1-C2
5	B	604	MTX	C13-C14-N10-CM
5	D	604	MTX	C13-C14-N10-CM
2	B	601	NDP	O4D-C4D-C5D-O5D
3	B	602	UFP	C2'-C1'-N1-C2
3	E	602	UFP	C2'-C1'-N1-C2
5	C	604	MTX	C15-C14-N10-CM
5	E	604	MTX	C15-C14-N10-CM
3	D	602	UFP	C2'-C1'-N1-C2
3	B	602	UFP	C2'-C1'-N1-C6
3	C	602	UFP	C2'-C1'-N1-C6
5	C	604	MTX	C13-C14-N10-CM
3	E	602	UFP	C5'-O5'-P-O3P
5	A	604	MTX	C6-C9-N10-CM
5	B	604	MTX	C6-C9-N10-CM
5	C	604	MTX	C6-C9-N10-CM
5	D	604	MTX	C6-C9-N10-CM
5	E	604	MTX	C13-C14-N10-CM
4	A	603	OFJ	C16-C15-N4-C14
2	D	601	NDP	C3D-C4D-C5D-O5D
4	C	603	OFJ	C16-C15-N4-C14
4	D	603	OFJ	C16-C15-N4-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	603	OFJ	C16-C15-N4-C14
5	A	604	MTX	N-CA-CB-CG
3	A	602	UFP	C2'-C1'-N1-C2
4	B	603	OFJ	C16-C15-N4-C14
3	D	602	UFP	C2'-C1'-N1-C6
3	E	602	UFP	C2'-C1'-N1-C6
3	B	602	UFP	O4'-C4'-C5'-O5'
2	A	601	NDP	C3D-C4D-C5D-O5D
3	B	602	UFP	C3'-C4'-C5'-O5'
4	C	603	OFJ	C20-C15-N4-C14
2	E	601	NDP	O4D-C1D-N1N-C2N
4	A	603	OFJ	C20-C15-N4-C14
4	D	603	OFJ	C20-C15-N4-C14
4	E	603	OFJ	C20-C15-N4-C14
4	B	603	OFJ	C20-C15-N4-C14
5	C	604	MTX	OE2-CD-CG-CB
2	A	601	NDP	O4D-C1D-N1N-C2N
5	A	604	MTX	OE2-CD-CG-CB
5	B	604	MTX	OE2-CD-CG-CB
2	B	601	NDP	O4D-C1D-N1N-C2N
2	C	601	NDP	O4D-C1D-N1N-C2N
2	D	601	NDP	O4D-C4D-C5D-O5D
2	D	601	NDP	O4D-C1D-N1N-C2N
5	A	604	MTX	OE1-CD-CG-CB
5	B	604	MTX	OE1-CD-CG-CB
5	C	604	MTX	OE1-CD-CG-CB
5	D	604	MTX	OE1-CD-CG-CB
5	E	604	MTX	OE1-CD-CG-CB
5	D	604	MTX	OE2-CD-CG-CB
2	C	601	NDP	C2D-C1D-N1N-C2N
2	D	601	NDP	C2D-C1D-N1N-C2N
2	E	601	NDP	C2D-C1D-N1N-C2N
3	A	602	UFP	C5'-O5'-P-O2P
3	B	602	UFP	C5'-O5'-P-O2P
3	D	602	UFP	C5'-O5'-P-O2P
3	E	602	UFP	C5'-O5'-P-O2P
5	E	604	MTX	OE2-CD-CG-CB
2	A	601	NDP	C2D-C1D-N1N-C2N
2	A	601	NDP	C4D-C5D-O5D-PN
2	D	601	NDP	C4D-C5D-O5D-PN
2	B	601	NDP	C2D-C1D-N1N-C2N
2	B	601	NDP	C4D-C5D-O5D-PN

Continued on next page...

Continued from previous page...

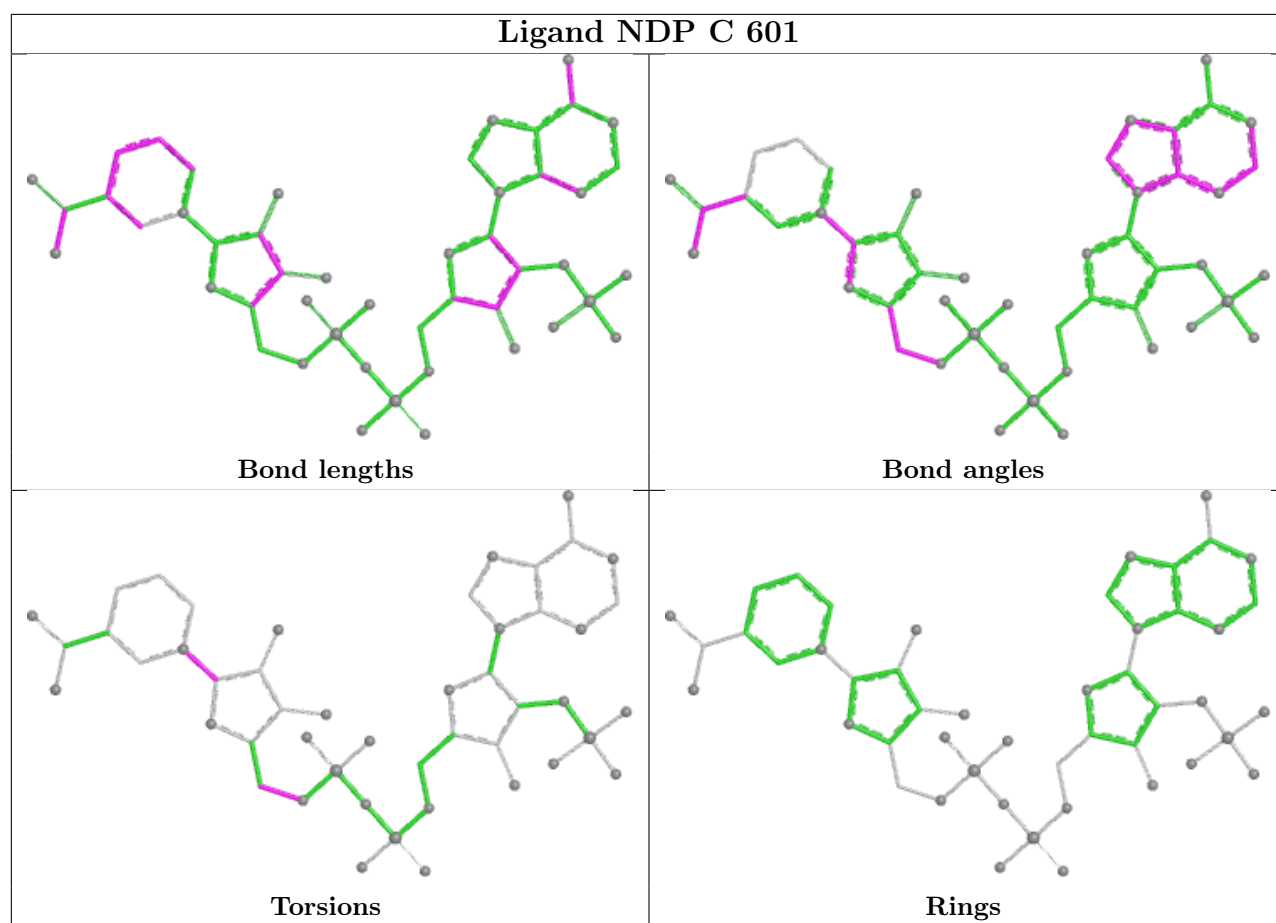
Mol	Chain	Res	Type	Atoms
2	C	601	NDP	C4D-C5D-O5D-PN
2	E	601	NDP	C4D-C5D-O5D-PN
3	A	602	UFP	C2'-C1'-N1-C6

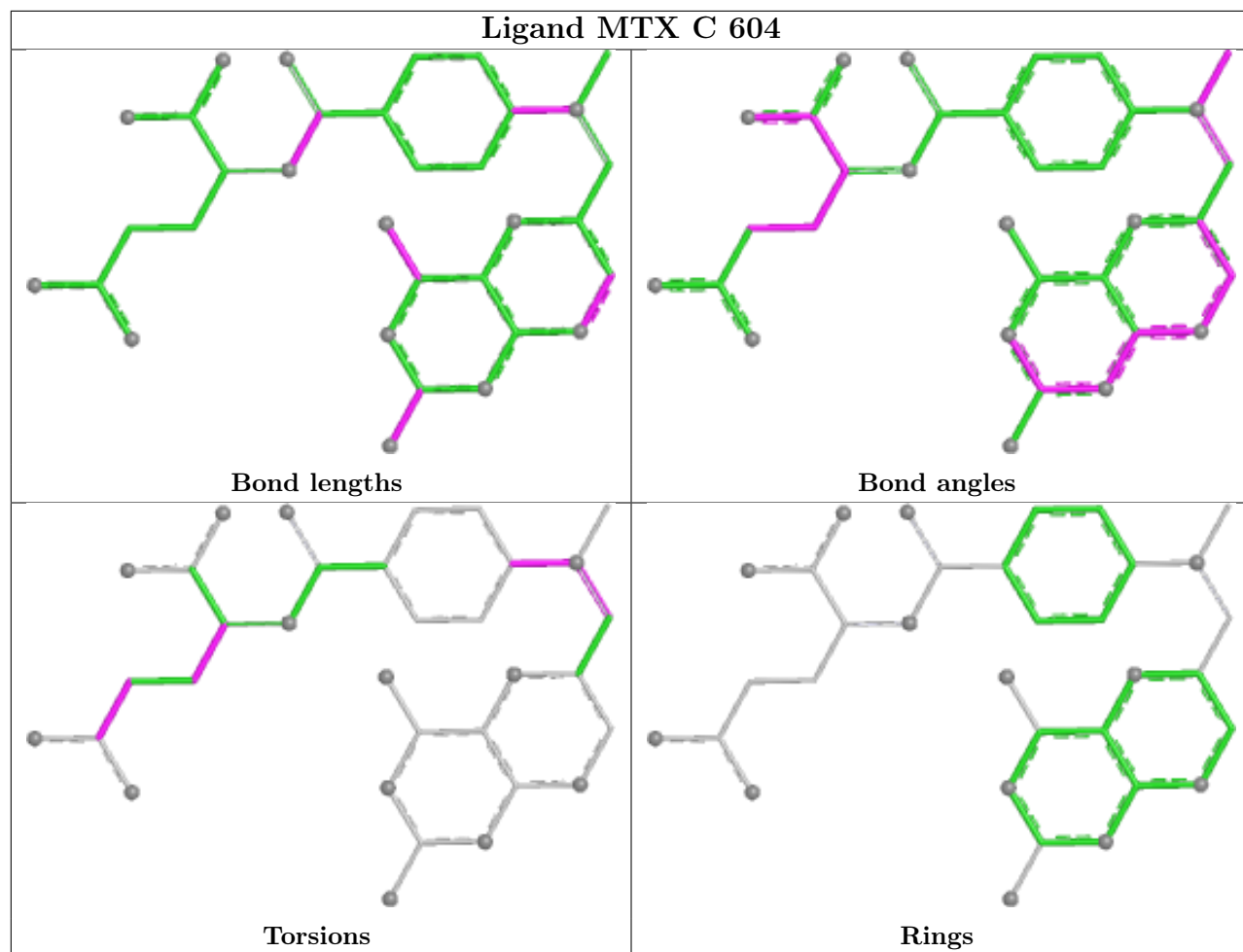
There are no ring outliers.

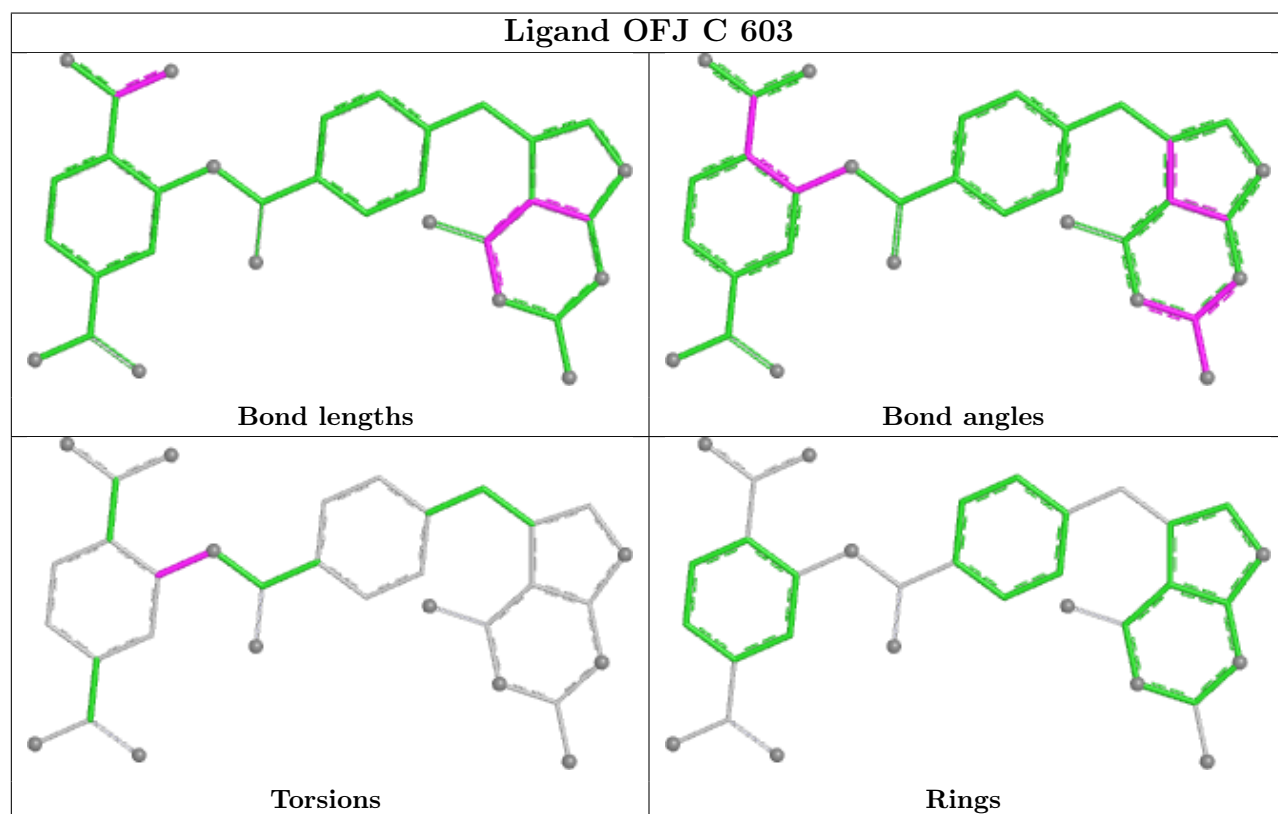
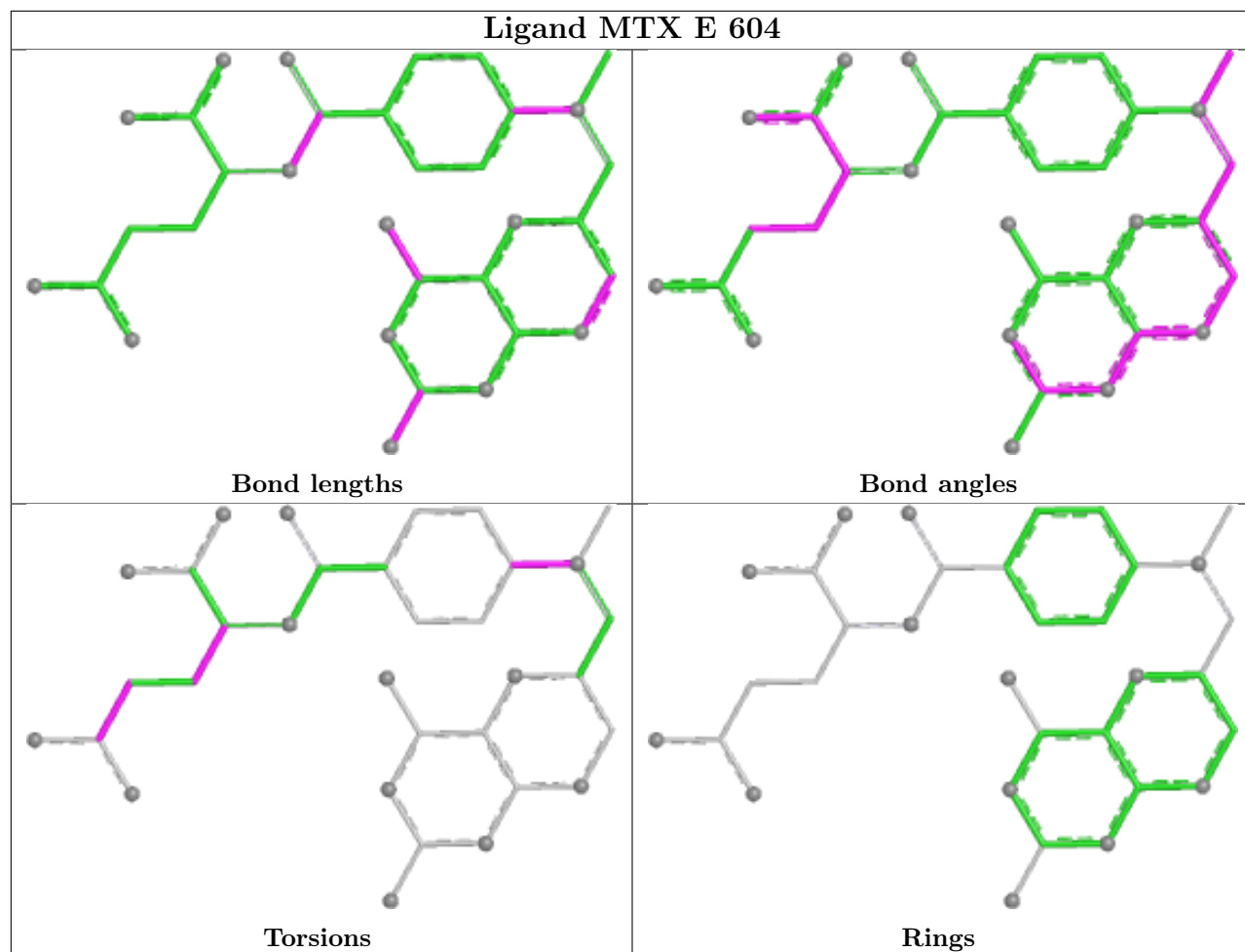
14 monomers are involved in 27 short contacts:

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

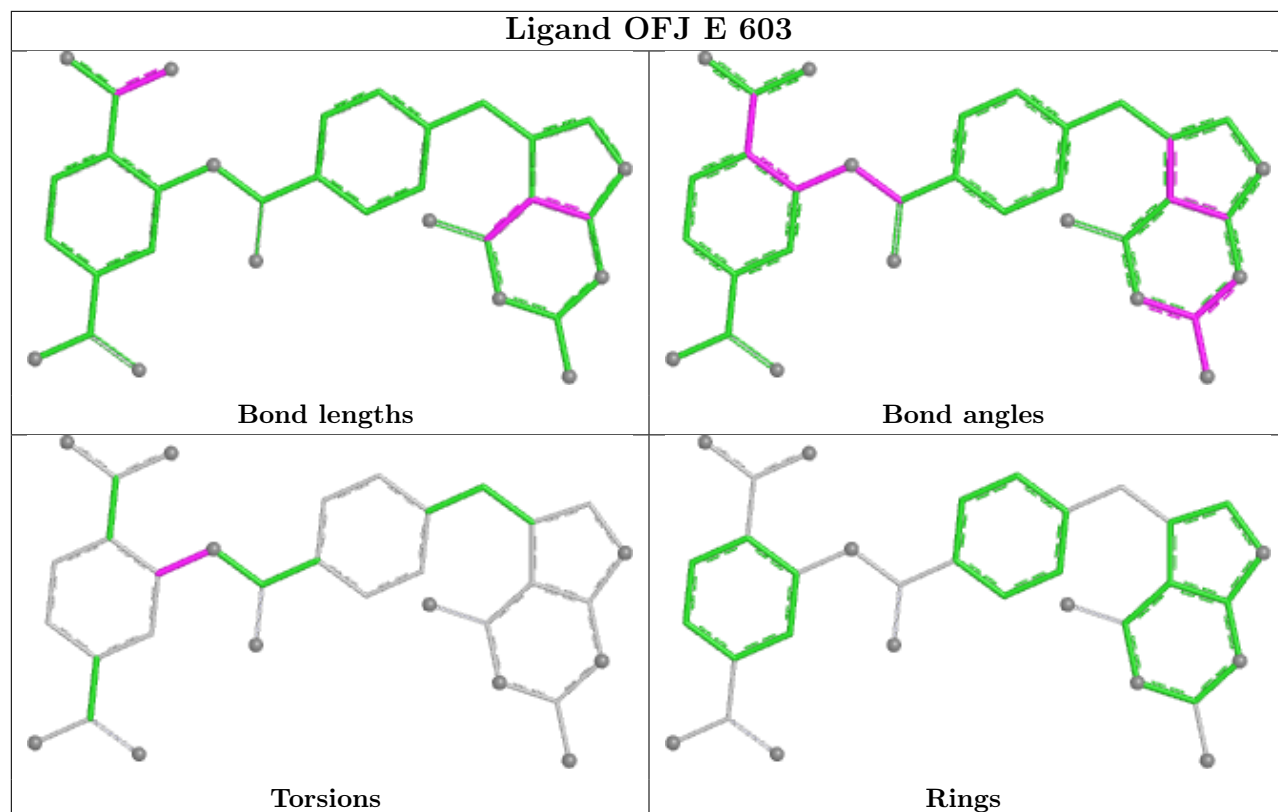
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



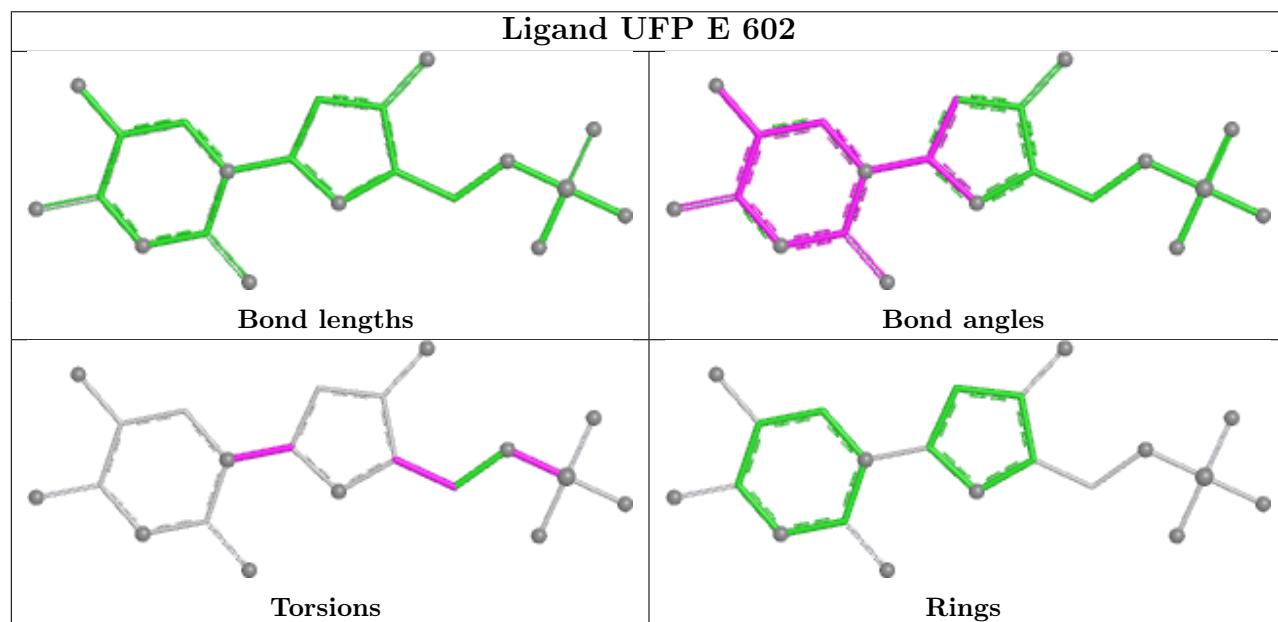


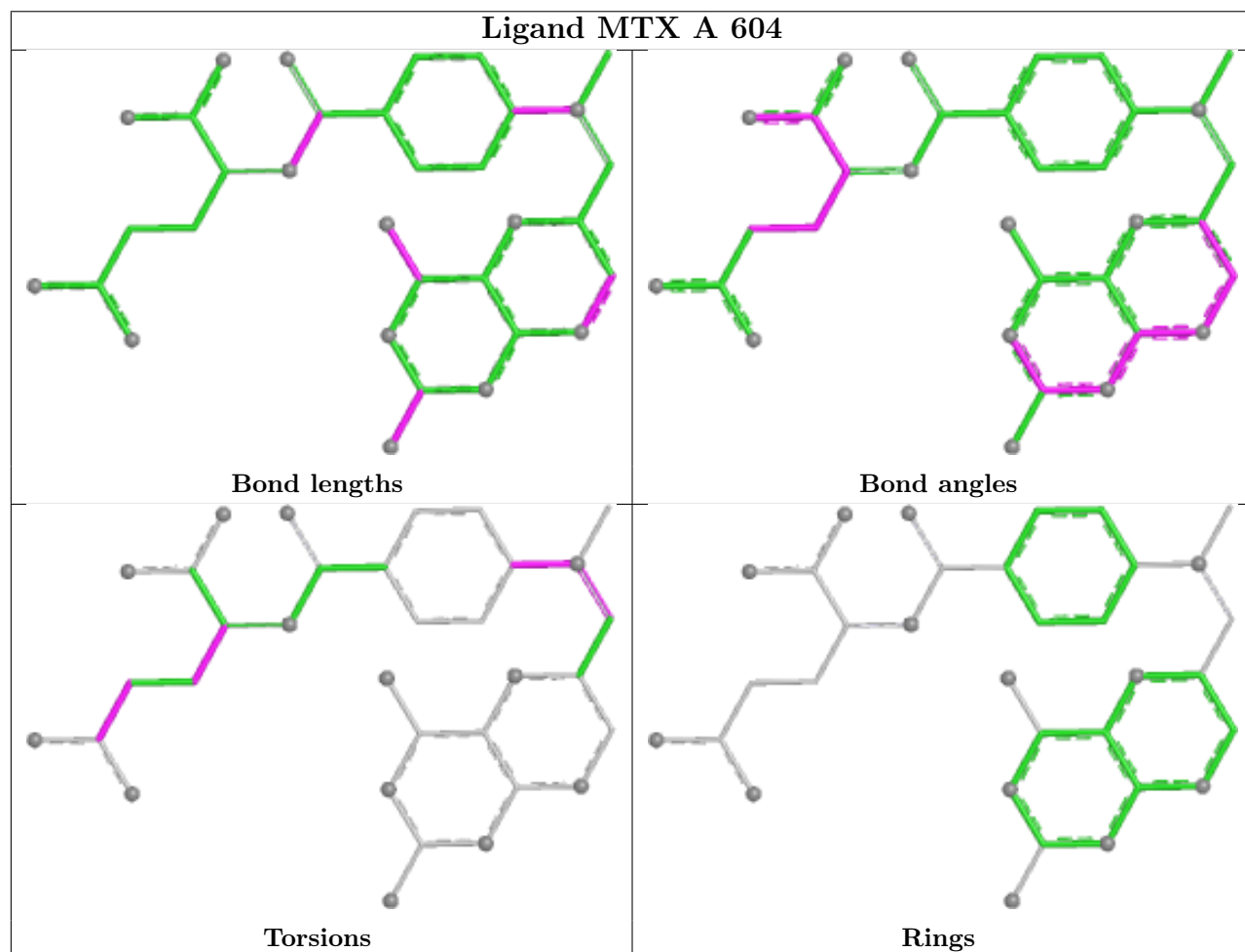
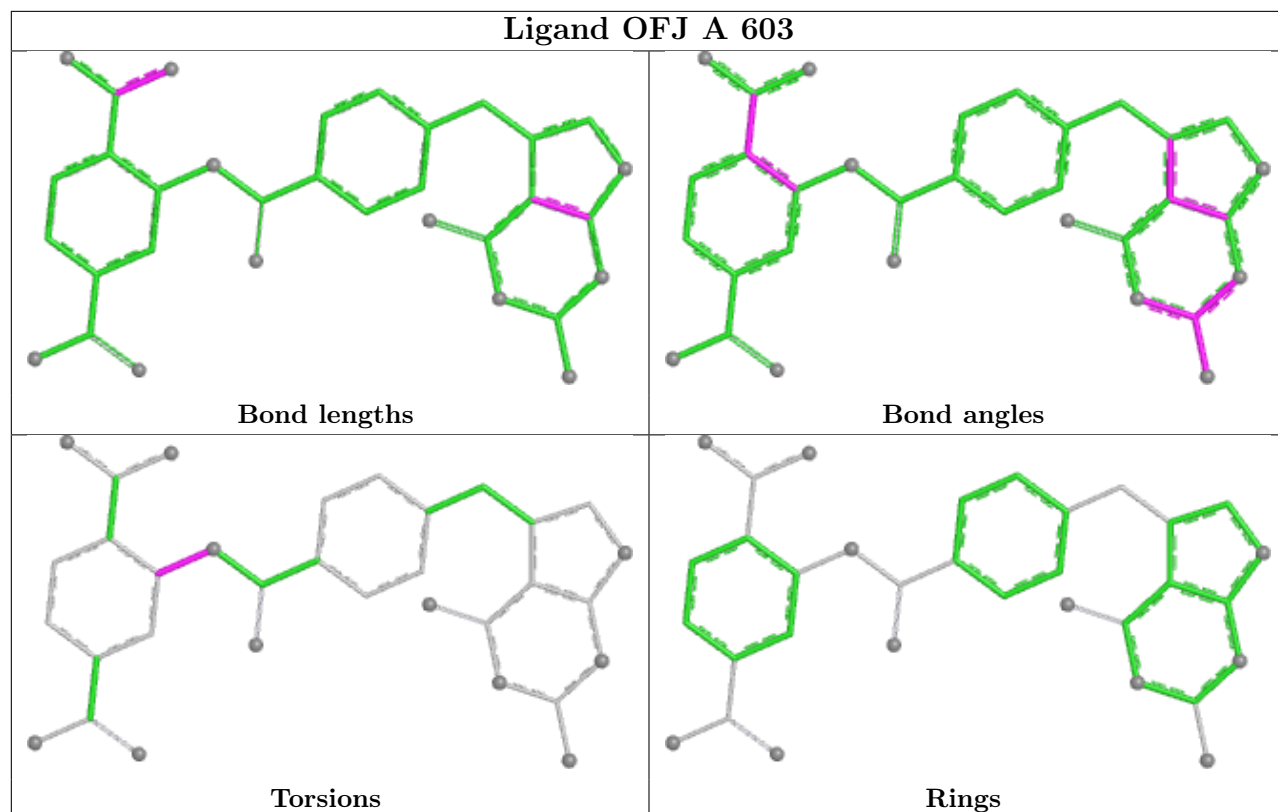


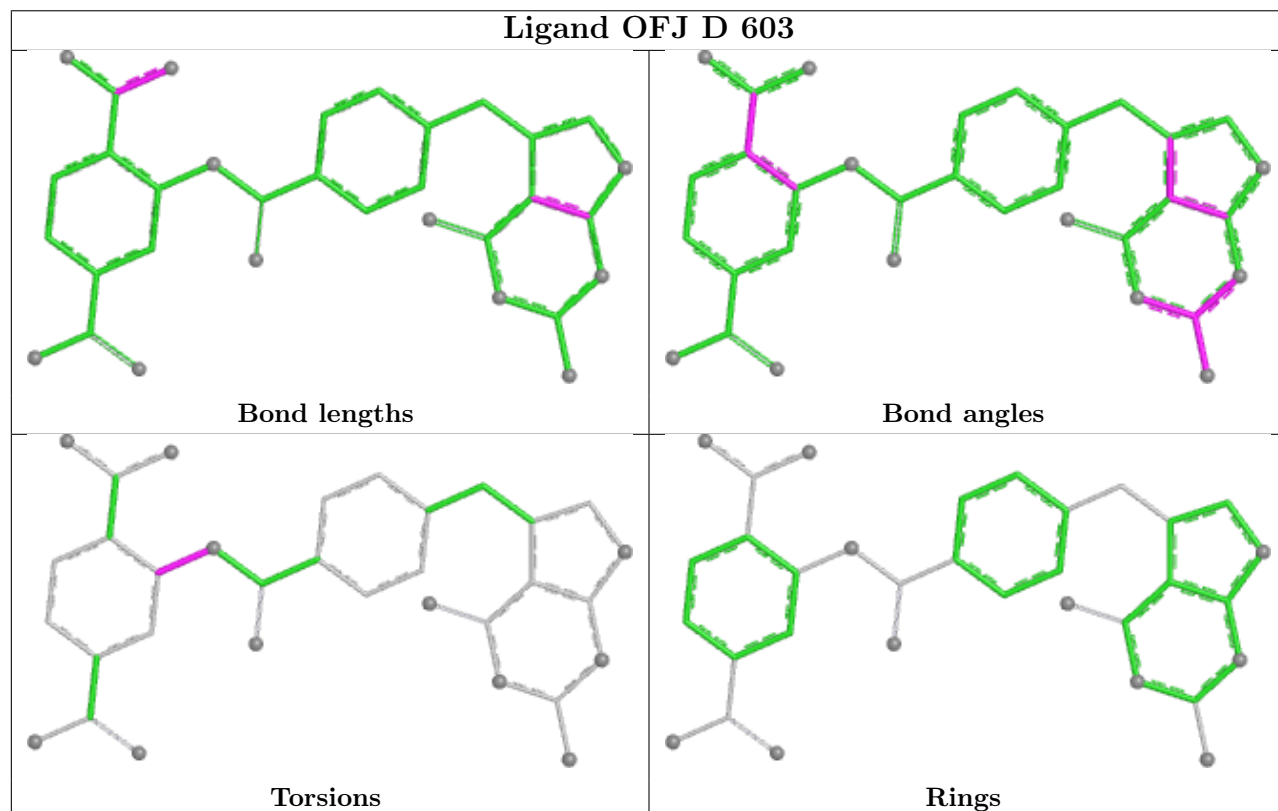
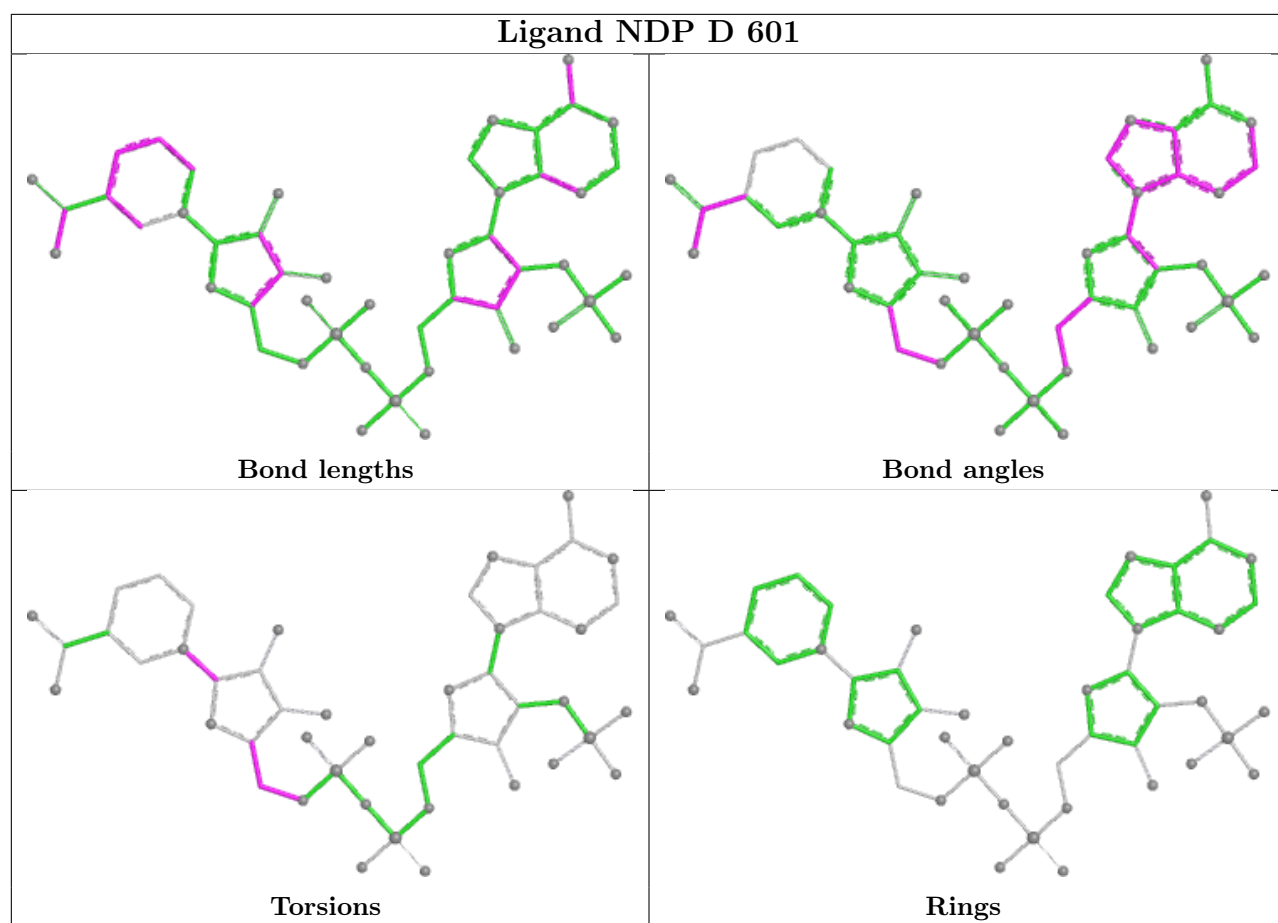
Ligand OFJ E 603

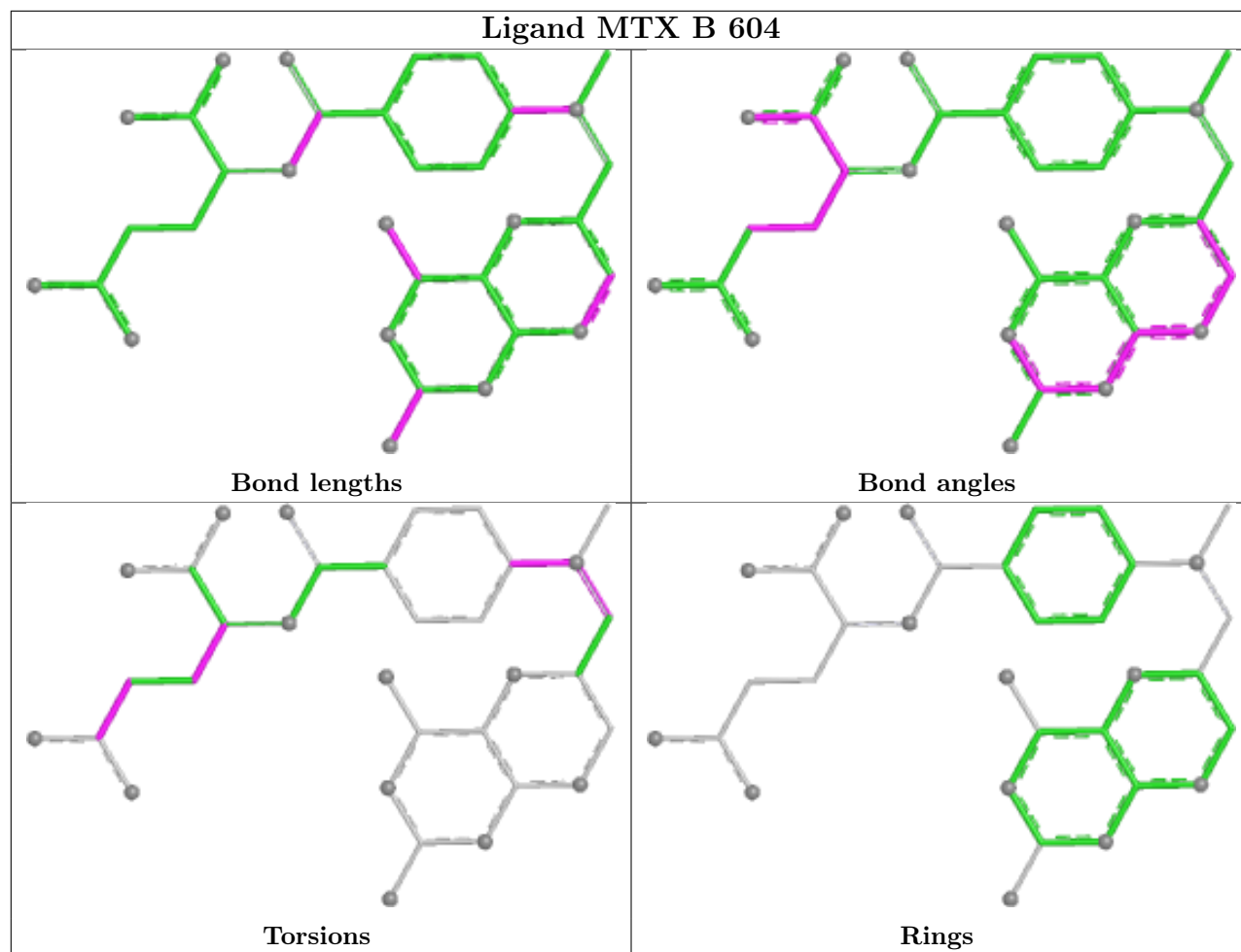


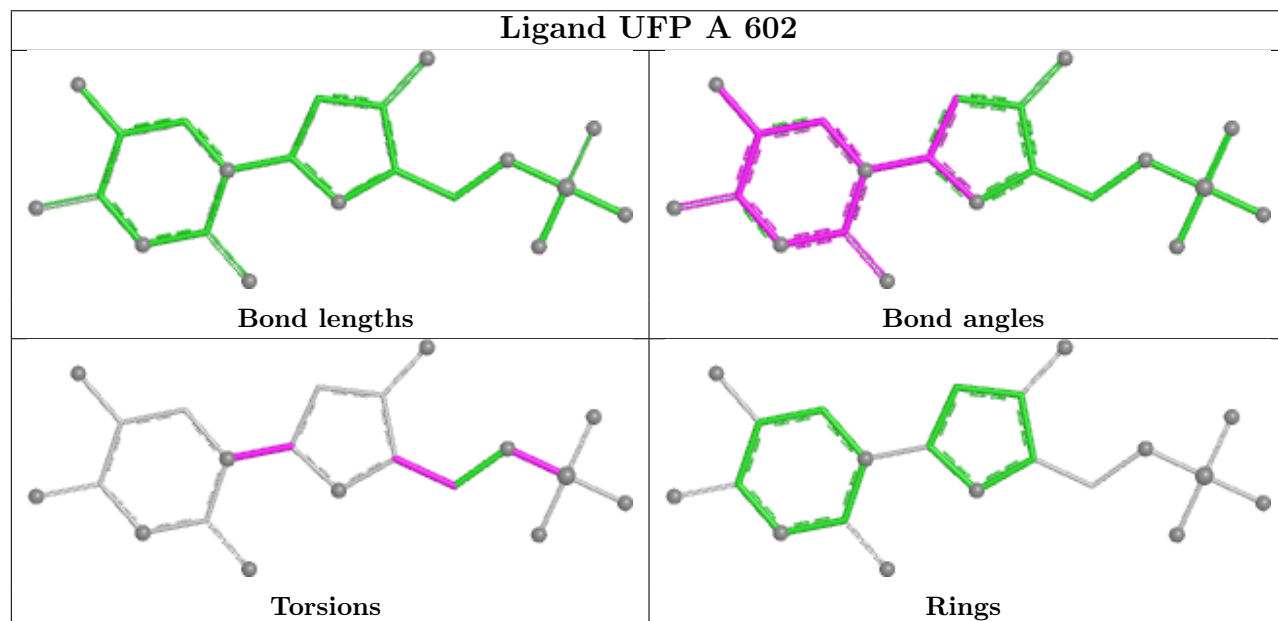
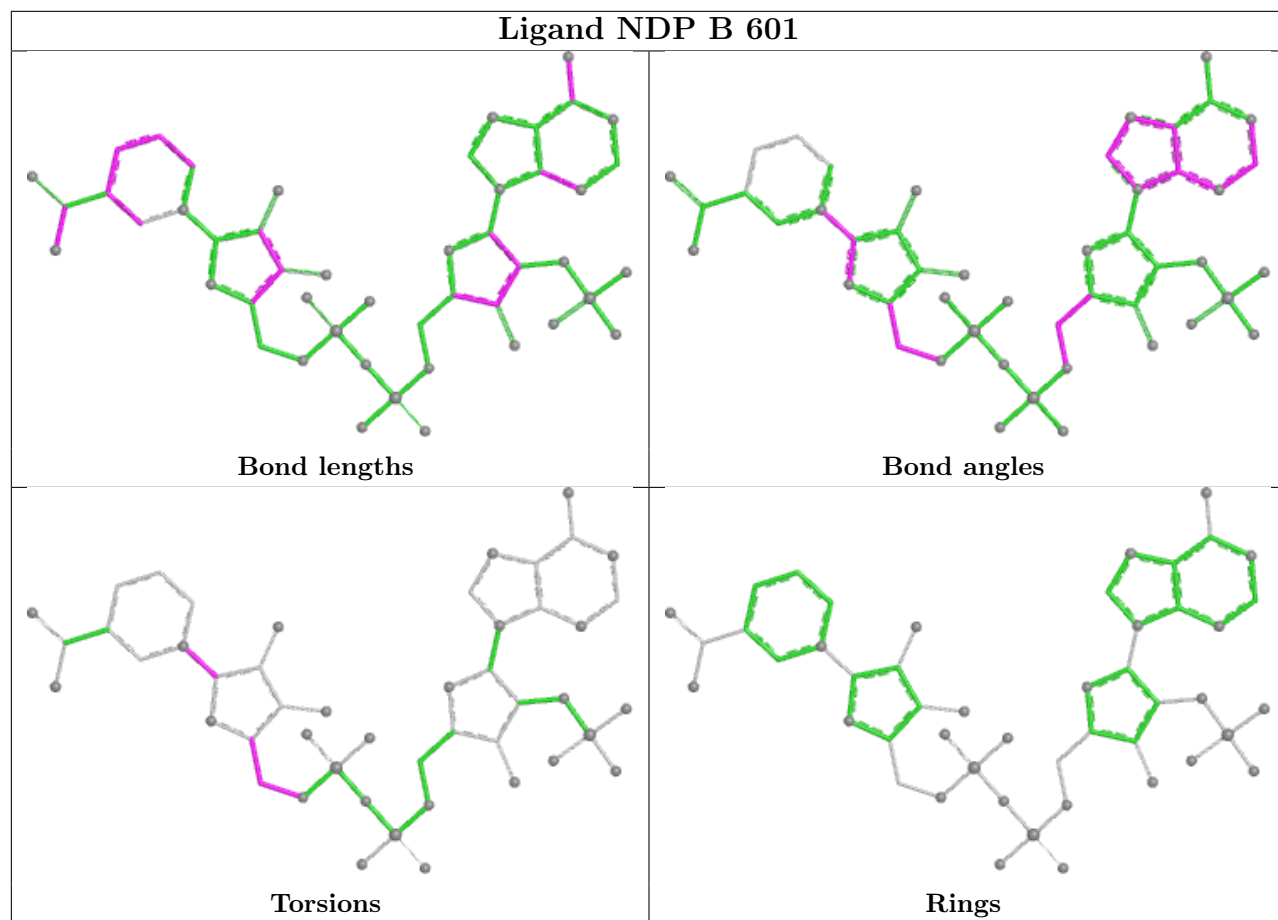
Ligand UFP E 602

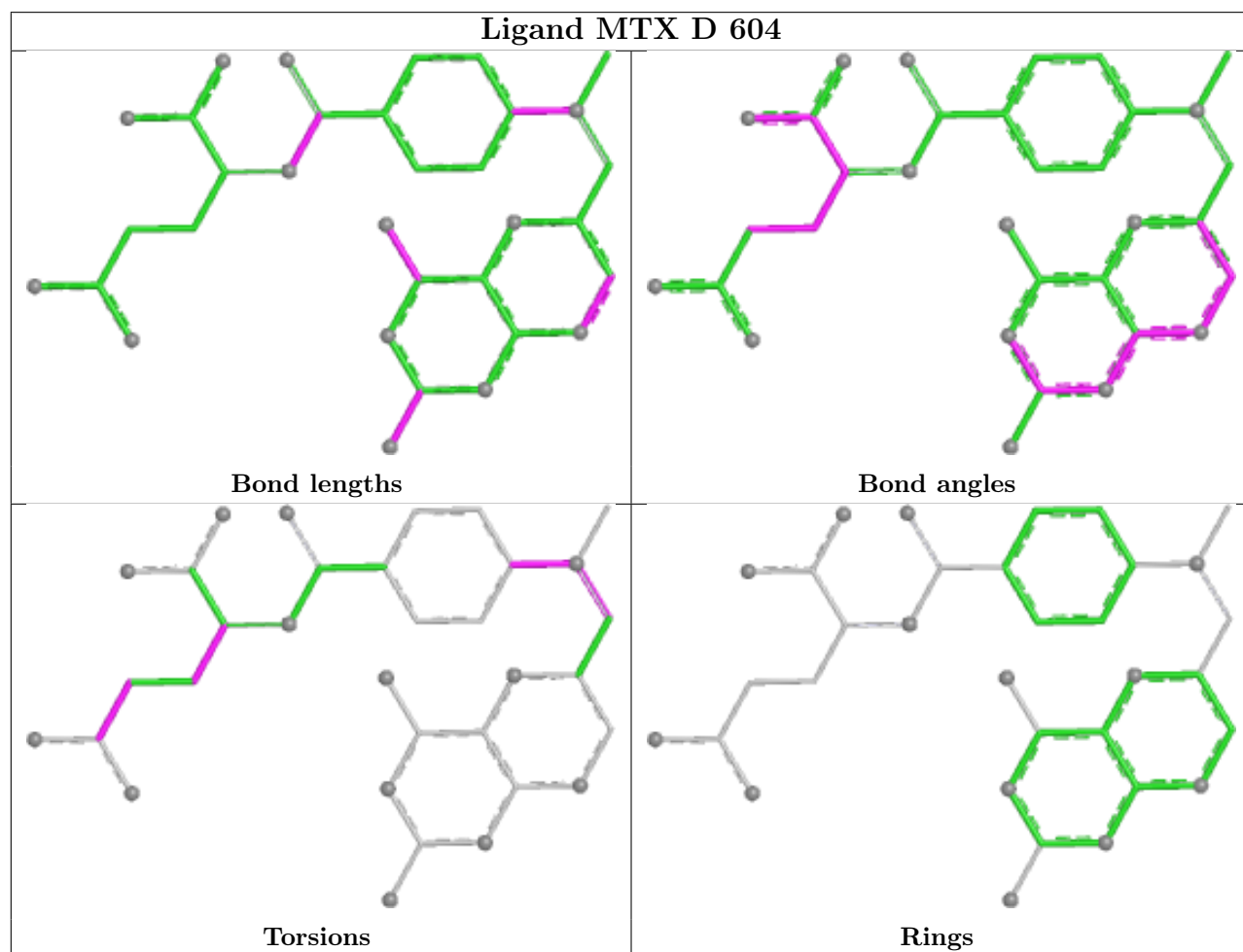
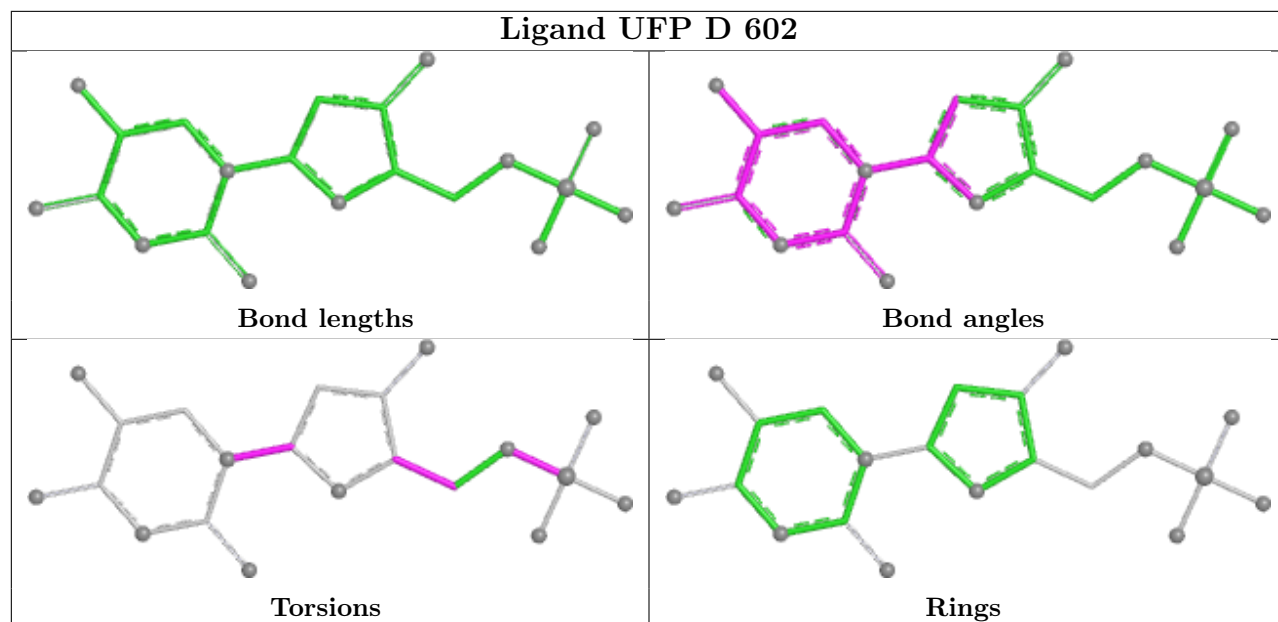


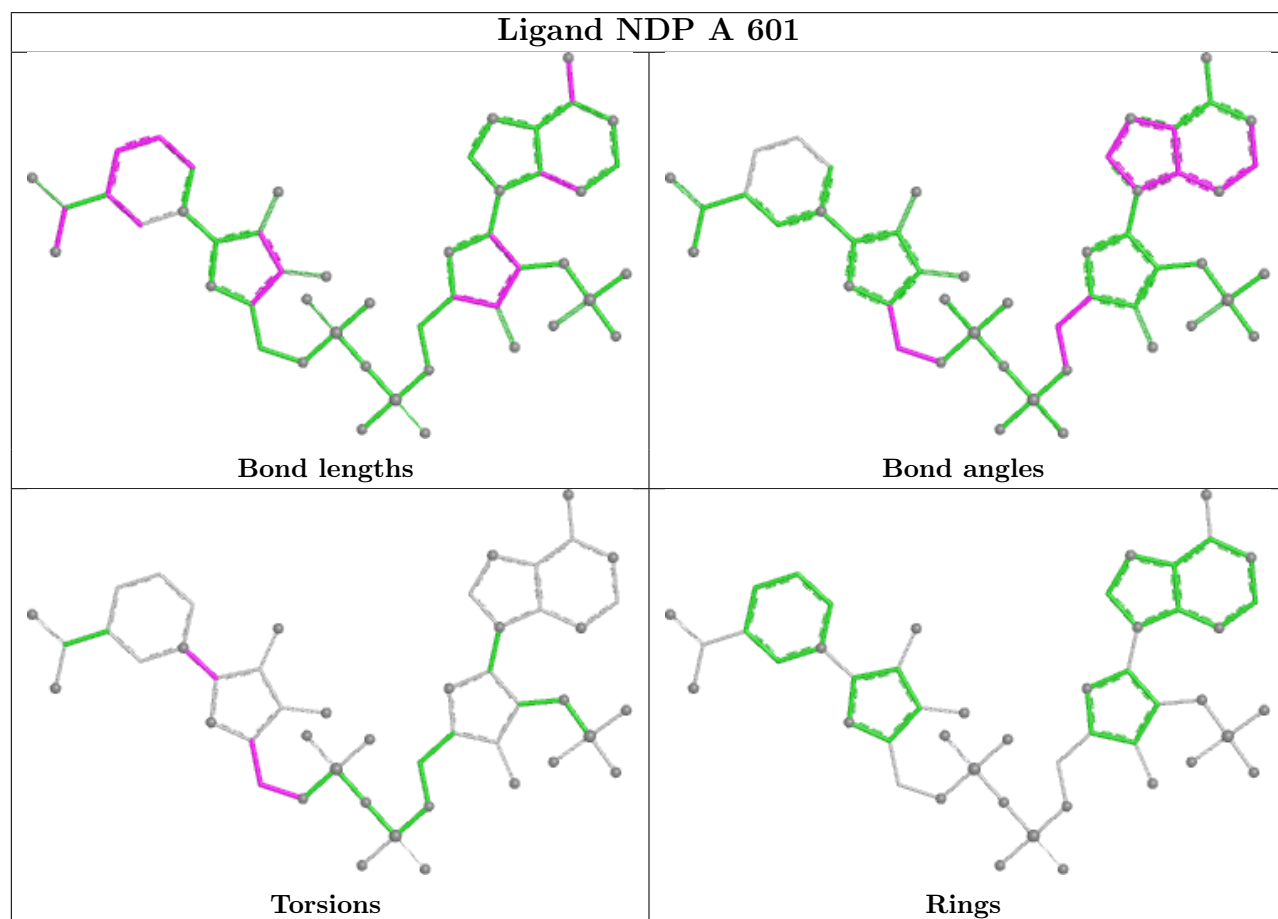
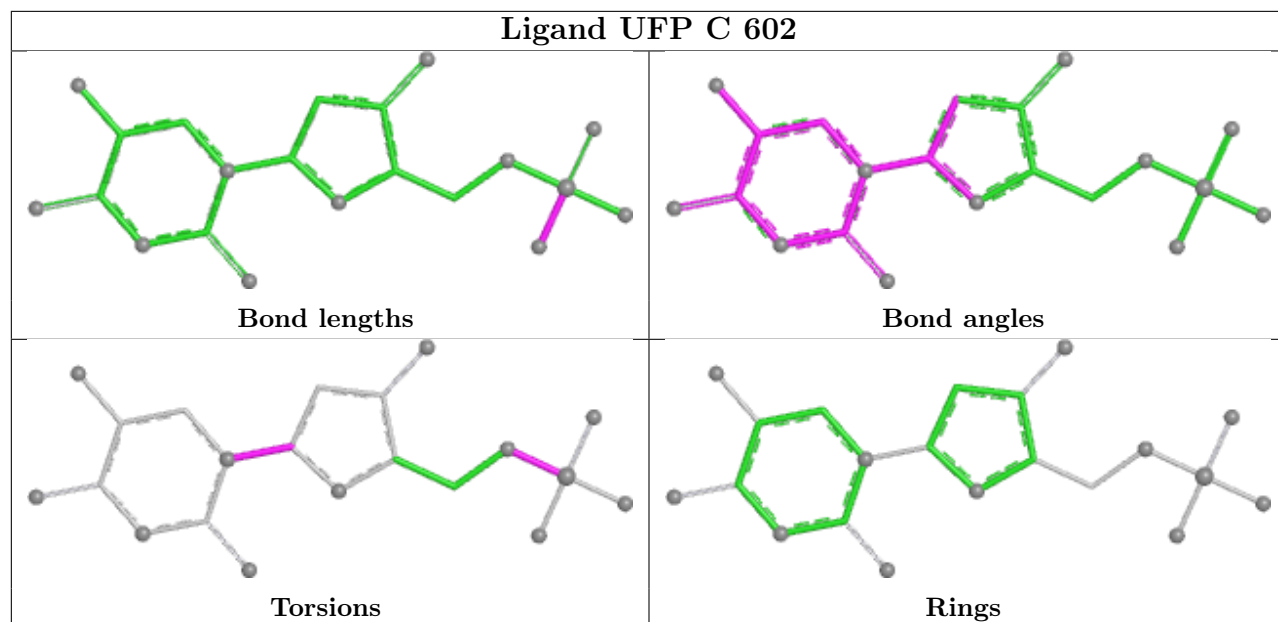


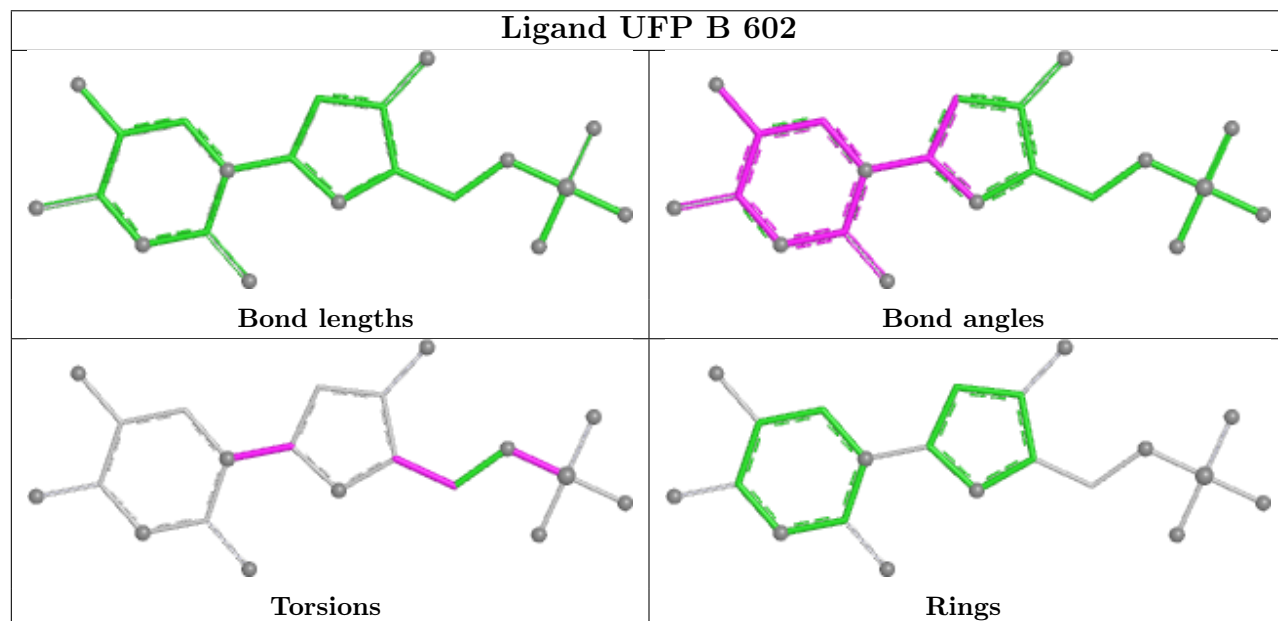
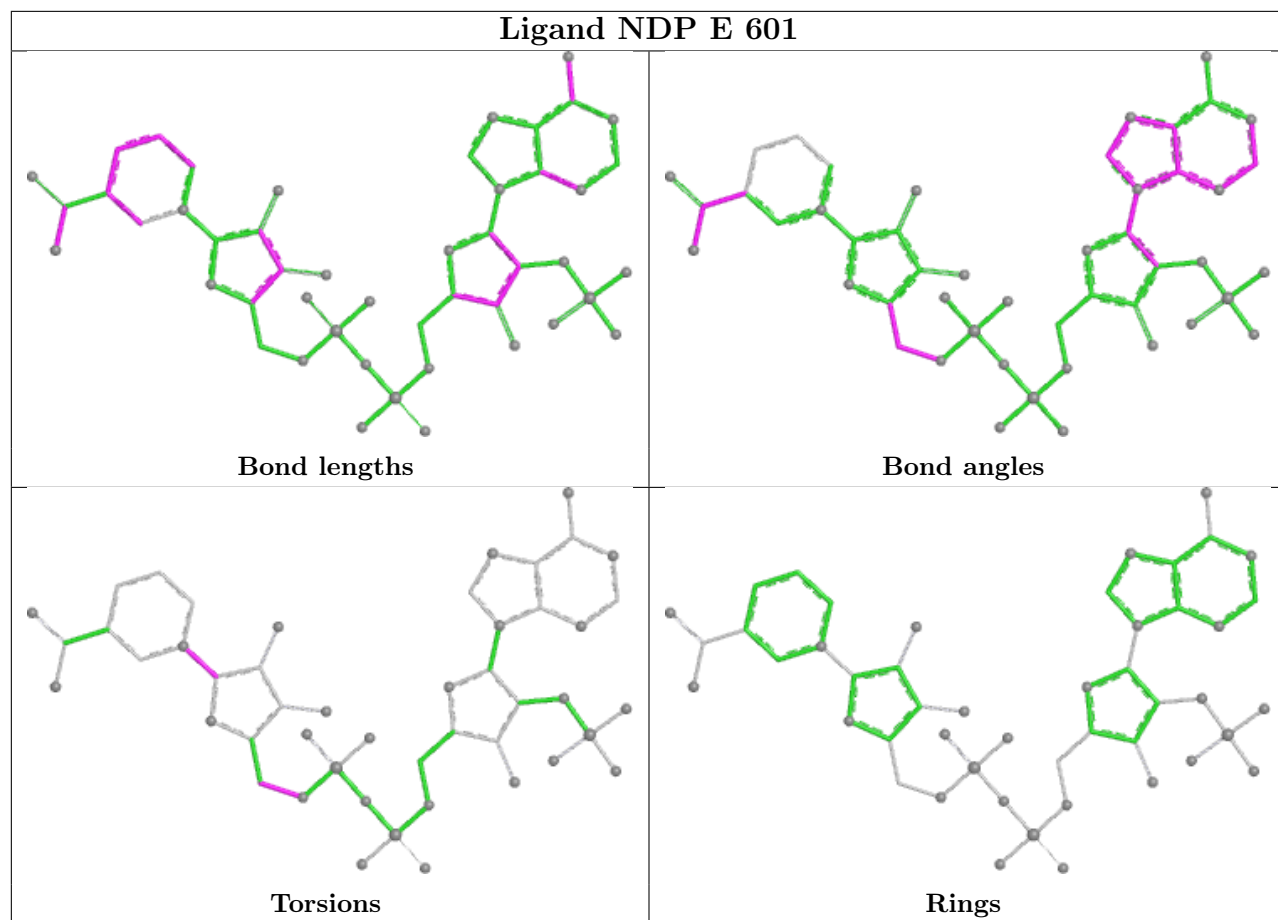


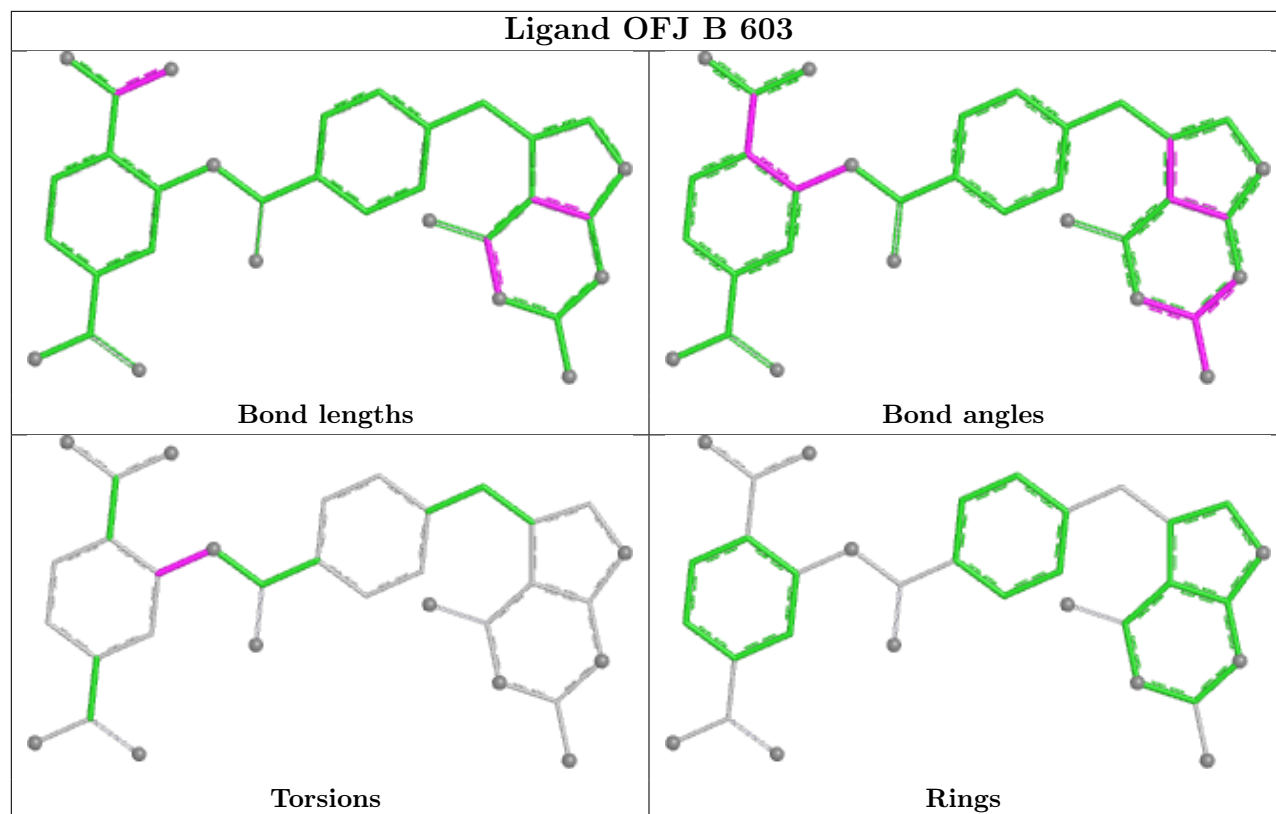












5.7 Other polymers [i](#)

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, 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	505/521 (96%)	0.48	28 (5%)	30	27	36, 55, 83, 118	0
1	B	506/521 (97%)	0.41	33 (6%)	25	22	36, 53, 90, 116	0
1	C	506/521 (97%)	0.25	21 (4%)	40	37	33, 46, 76, 106	0
1	D	506/521 (97%)	1.03	58 (11%)	9	8	54, 71, 102, 123	0
1	E	506/521 (97%)	0.10	21 (4%)	40	37	30, 42, 67, 110	0
All	All	2529/2605 (97%)	0.46	161 (6%)	25	22	30, 54, 92, 123	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	MET	7.8
1	C	102	MET	7.8
1	D	193	LEU	7.5
1	E	179	GLU	7.2
1	E	102	MET	7.2
1	A	102	MET	7.1
1	C	179	GLU	6.7
1	A	193	LEU	6.7
1	E	193	LEU	6.3
1	C	193	LEU	6.1
1	D	179	GLU	6.1
1	B	193	LEU	5.7
1	B	179	GLU	5.7
1	B	99	GLU	5.4
1	A	178	GLN	5.2
1	B	102	MET	4.9
1	E	103	ASN	4.9
1	D	343	GLY	4.8
1	C	103	ASN	4.8
1	B	343	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	103	ASN	4.3
1	E	178	GLN	4.2
1	E	84	ALA	4.1
1	B	84	ALA	4.0
1	E	121	ASP	4.0
1	C	194	LYS	4.0
1	A	101	LEU	4.0
1	C	121	ASP	4.0
1	E	99	GLU	3.9
1	A	121	ASP	3.9
1	A	99	GLU	3.9
1	D	101	LEU	3.9
1	B	103	ASN	3.8
1	D	100	ASN	3.8
1	A	103	ASN	3.7
1	D	342	TYR	3.7
1	E	82	ASP	3.6
1	C	178	GLN	3.6
1	D	84	ALA	3.6
1	D	194	LYS	3.6
1	A	84	ALA	3.5
1	C	99	GLU	3.5
1	B	171	ASP	3.4
1	E	194	LYS	3.4
1	B	121	ASP	3.4
1	E	83	GLU	3.3
1	D	121	ASP	3.3
1	A	343	GLY	3.3
1	C	343	GLY	3.3
1	C	84	ALA	3.3
1	D	178	GLN	3.3
1	B	127	PHE	3.3
1	D	5	ASN	3.2
1	D	326	GLU	3.2
1	B	178	GLN	3.2
1	D	521	VAL	3.1
1	D	300	LYS	3.1
1	A	100	ASN	3.1
1	E	352	GLU	3.1
1	D	208	GLY	3.1
1	A	83	GLU	3.0
1	D	346	TRP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	100	ASN	3.0
1	D	99	GLU	3.0
1	D	323	GLU	2.9
1	A	259	GLY	2.9
1	D	520	ALA	2.9
1	B	332	HIS	2.9
1	D	171	ASP	2.9
1	D	259	GLY	2.8
1	B	101	LEU	2.8
1	B	83	GLU	2.8
1	B	77	SER	2.8
1	A	255	GLU	2.8
1	D	352	GLU	2.8
1	D	340	PRO	2.7
1	D	314	TYR	2.7
1	A	82	ASP	2.7
1	E	104	ASP	2.7
1	B	98	ILE	2.6
1	C	140	ASP	2.6
1	A	326	GLU	2.6
1	D	149	GLU	2.6
1	E	335	GLU	2.6
1	B	5	ASN	2.6
1	D	220	LYS	2.6
1	D	363	VAL	2.6
1	E	343	GLY	2.6
1	B	142	GLU	2.5
1	A	114	GLY	2.5
1	D	77	SER	2.5
1	D	395	SER	2.5
1	A	3	GLU	2.5
1	D	324	TYR	2.5
1	C	114	GLY	2.5
1	D	345	GLN	2.5
1	B	140	ASP	2.5
1	B	342	TYR	2.5
1	C	82	ASP	2.5
1	A	98	ILE	2.4
1	A	5	ASN	2.4
1	C	101	LEU	2.4
1	D	319	ASN	2.4
1	B	104	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	100	ASN	2.4
1	A	171	ASP	2.4
1	E	171	ASP	2.4
1	A	194	LYS	2.4
1	D	81	GLN	2.4
1	D	98	ILE	2.3
1	A	140	ASP	2.3
1	D	86	PRO	2.3
1	B	89	VAL	2.3
1	D	3	GLU	2.3
1	D	331	GLY	2.3
1	D	177	LYS	2.3
1	E	140	ASP	2.3
1	D	327	ARG	2.3
1	B	114	GLY	2.3
1	D	209	ILE	2.3
1	A	332	HIS	2.3
1	D	322	LYS	2.2
1	D	332	HIS	2.2
1	C	255	GLU	2.2
1	C	326	GLU	2.2
1	D	362	GLY	2.2
1	D	307	HIS	2.2
1	B	87	ASN	2.2
1	D	335	GLU	2.2
1	A	314	TYR	2.2
1	C	104	ASP	2.2
1	B	335	GLU	2.1
1	C	323	GLU	2.1
1	A	335	GLU	2.1
1	D	222	GLU	2.1
1	D	4	LYS	2.1
1	D	376	LYS	2.1
1	D	301	GLY	2.1
1	B	504	ILE	2.1
1	C	332	HIS	2.1
1	B	92	ARG	2.1
1	D	289	ARG	2.1
1	C	354	LYS	2.1
1	B	208	GLY	2.1
1	E	332	HIS	2.1
1	E	98	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	82	ASP	2.1
1	B	78	SER	2.1
1	A	330	LEU	2.1
1	A	93	ASN	2.1
1	D	360	TYR	2.1
1	B	177	LYS	2.0
1	C	361	THR	2.0
1	B	80	PRO	2.0
1	E	101	LEU	2.0
1	A	352	GLU	2.0
1	D	292	PHE	2.0
1	D	330	LEU	2.0
1	D	399	LEU	2.0
1	D	309	ILE	2.0
1	D	92	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OFJ	D	603	33/33	0.72	0.27	70,106,120,127	0
4	OFJ	A	603	33/33	0.75	0.24	65,85,106,109	0
4	OFJ	C	603	33/33	0.77	0.24	56,74,100,104	0
4	OFJ	E	603	33/33	0.81	0.22	36,56,82,93	0
4	OFJ	B	603	33/33	0.83	0.22	44,66,94,104	0
6	SO4	D	605	5/5	0.88	0.13	66,77,85,94	0
3	UFP	D	602	21/21	0.90	0.13	76,93,103,110	0
5	MTX	D	604	33/33	0.91	0.13	52,67,77,81	0

Continued on next page...

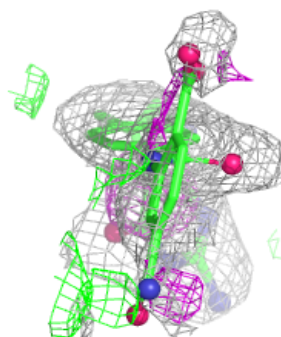
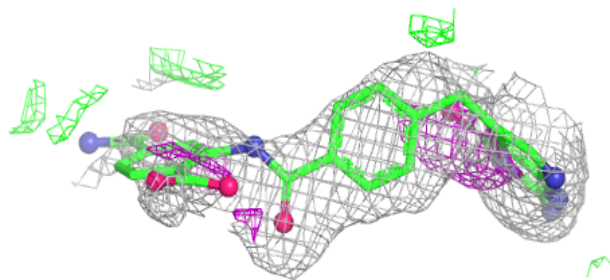
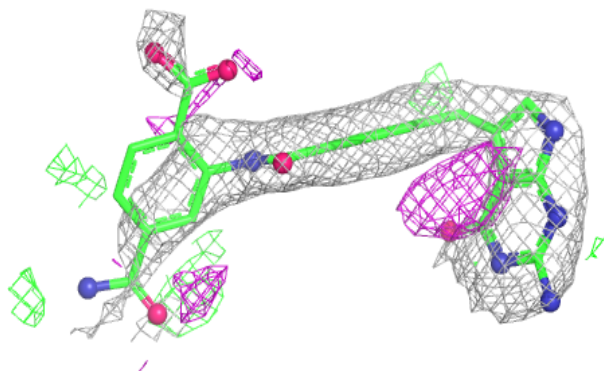
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MTX	B	604	33/33	0.91	0.13	41,58,70,73	0
6	SO4	E	606	5/5	0.91	0.19	55,61,80,88	0
2	NDP	B	601	48/48	0.92	0.11	56,78,100,107	0
2	NDP	D	601	48/48	0.92	0.12	60,78,91,101	0
3	UFP	A	602	21/21	0.93	0.12	53,67,81,84	0
3	UFP	C	602	21/21	0.93	0.12	49,59,70,80	0
5	MTX	E	604	33/33	0.94	0.10	28,41,63,73	0
6	SO4	A	605	5/5	0.94	0.12	61,62,79,81	0
2	NDP	A	601	48/48	0.94	0.10	50,67,82,90	0
5	MTX	A	604	33/33	0.94	0.11	40,55,67,71	0
3	UFP	E	602	21/21	0.95	0.11	33,46,62,67	0
6	SO4	E	605	5/5	0.95	0.11	47,59,64,76	0
6	SO4	B	605	5/5	0.95	0.09	56,67,70,78	0
5	MTX	C	604	33/33	0.96	0.09	31,41,67,72	0
3	UFP	B	602	21/21	0.96	0.10	41,55,66,72	0
2	NDP	E	601	48/48	0.97	0.07	37,47,56,64	0
2	NDP	C	601	48/48	0.97	0.07	34,47,55,60	0
6	SO4	C	605	5/5	0.97	0.09	41,46,64,69	0

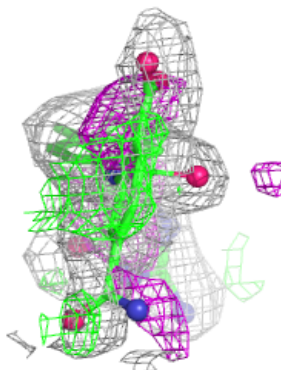
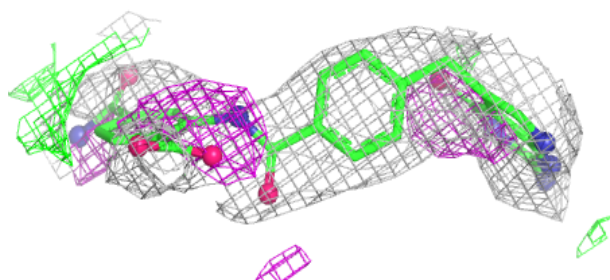
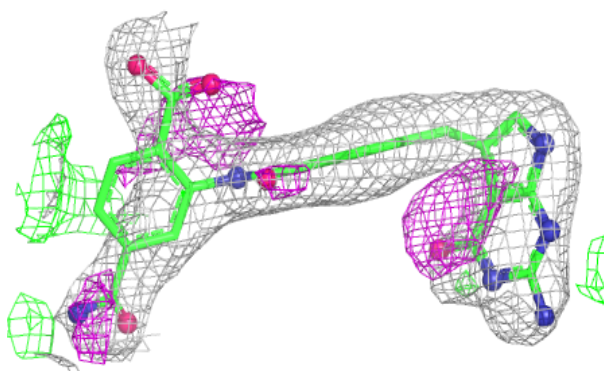
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OFJ 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)

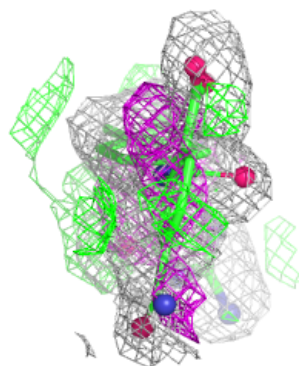
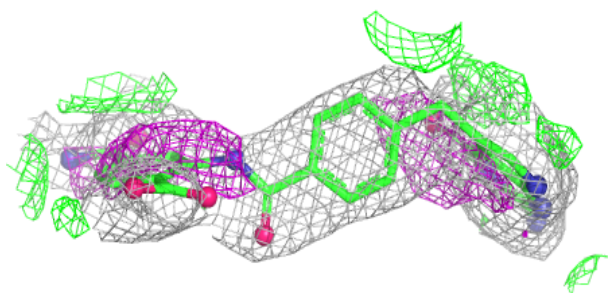
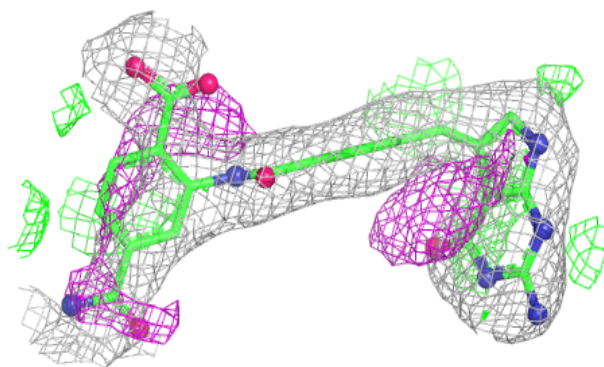
**Electron density around OFJ A 603:**

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

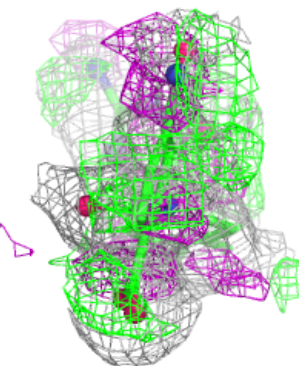
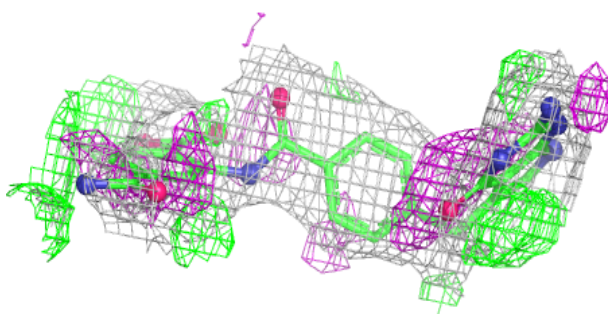
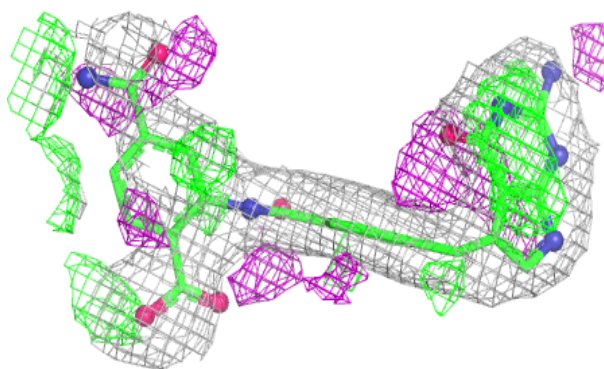


Electron density around OFJ C 603:

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

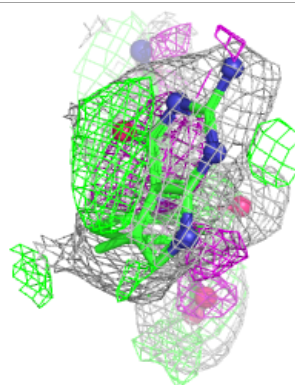
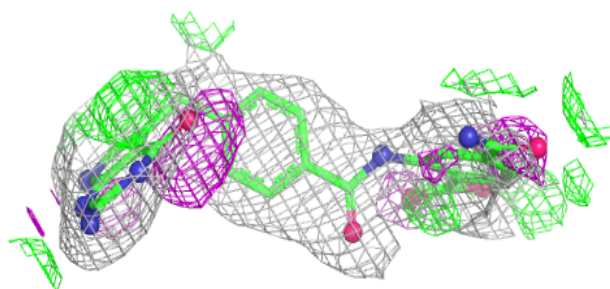
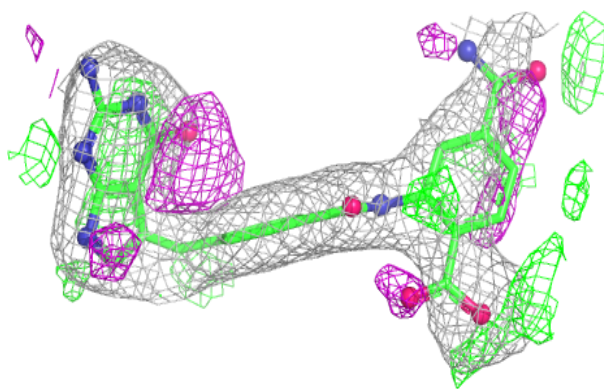
**Electron density around OFJ E 603:**

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

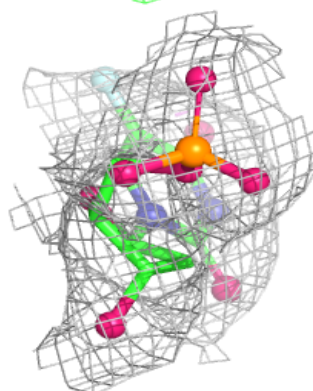
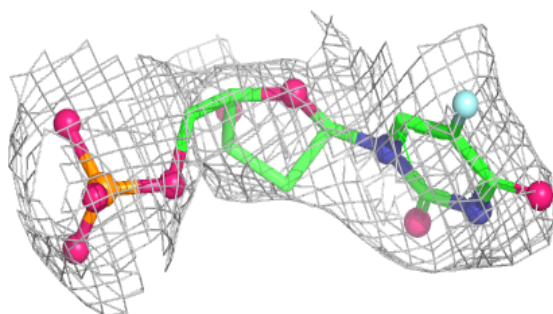
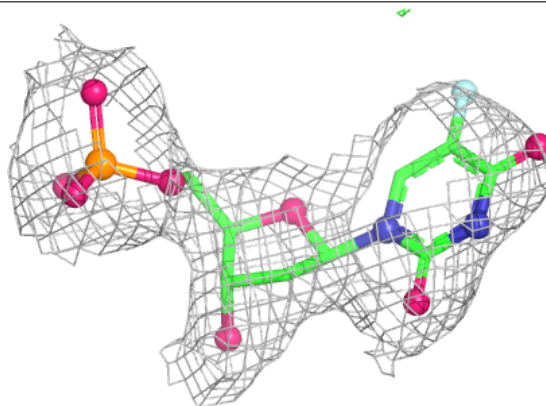


Electron density around OFJ B 603:

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

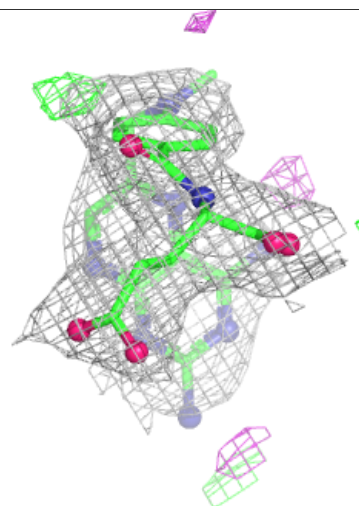
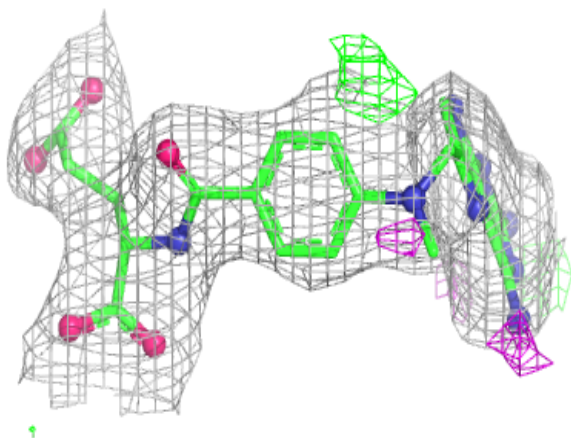
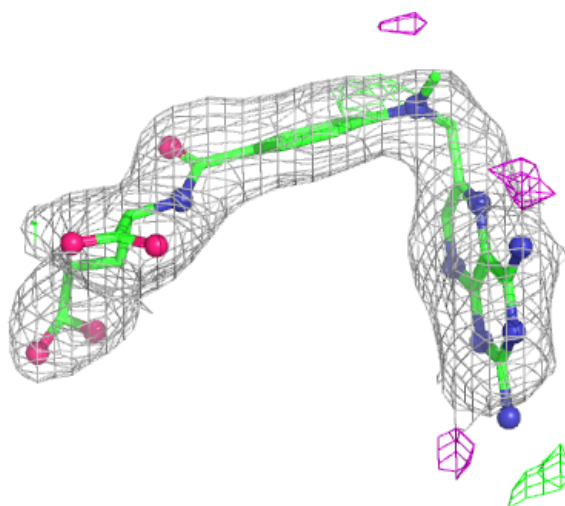
**Electron density around UFP D 602:**

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



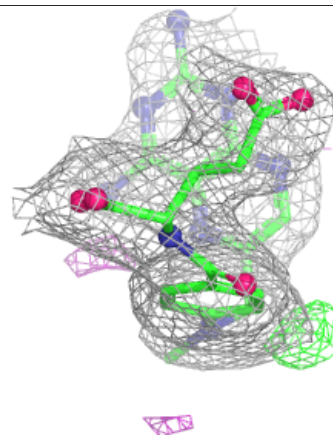
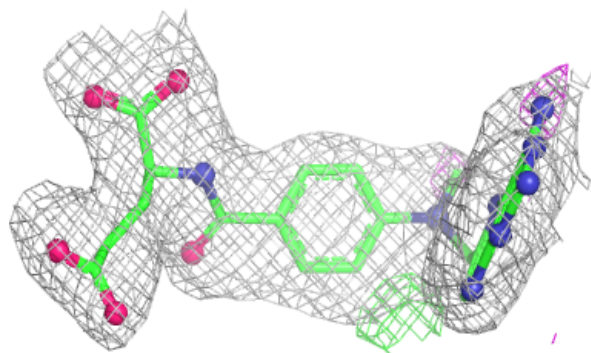
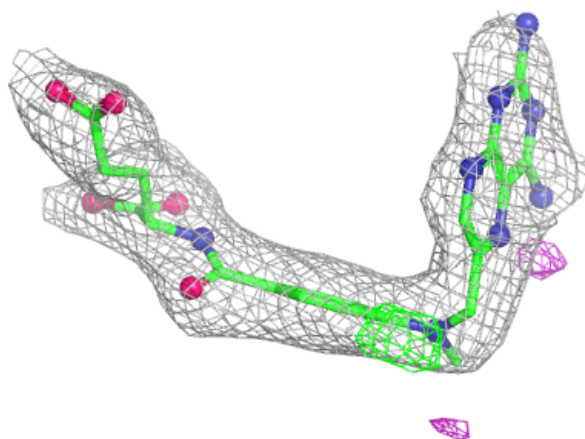
Electron density around MTX D 604:

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

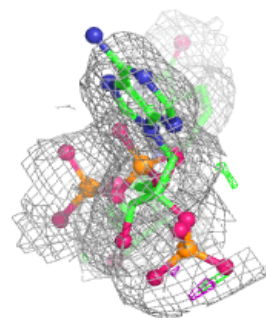
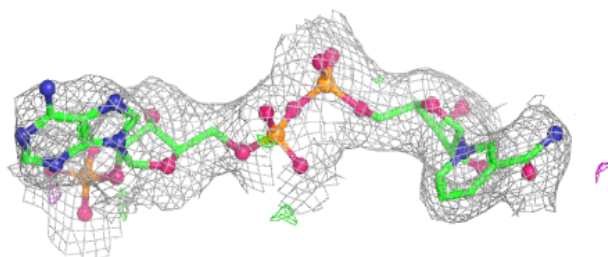
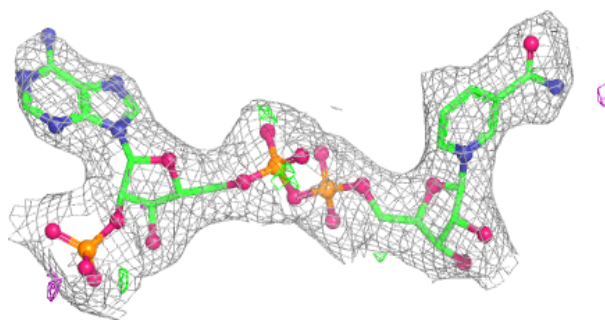


Electron density around MTX B 604:

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

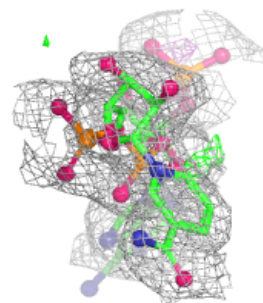
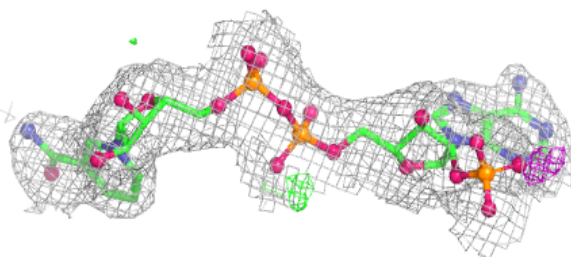
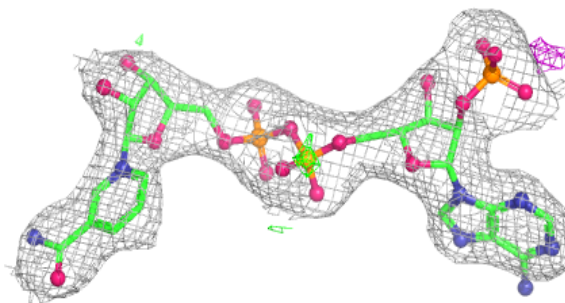
**Electron density around NDP B 601:**

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

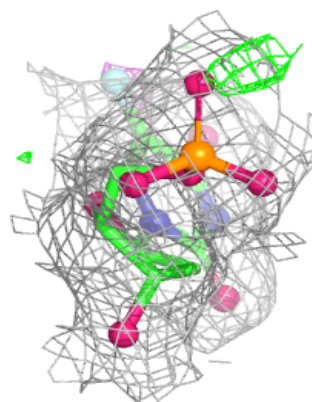
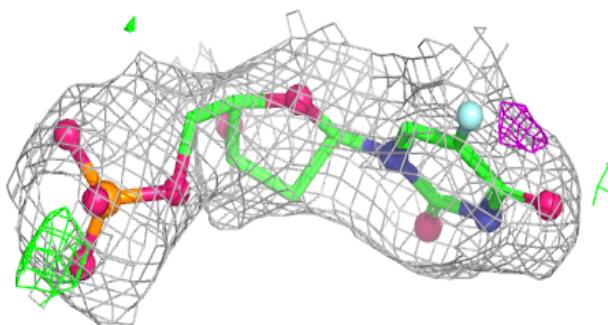
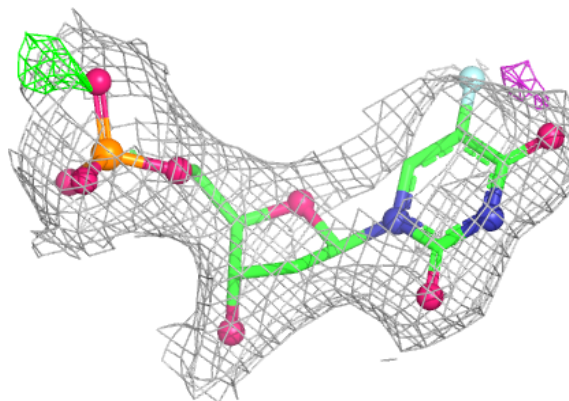


Electron density around NDP D 601:

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

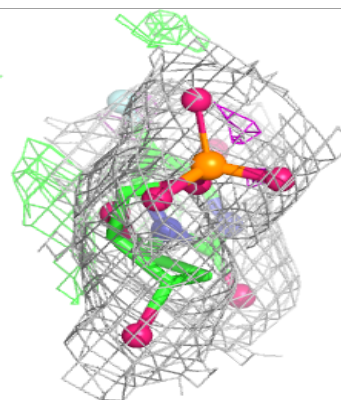
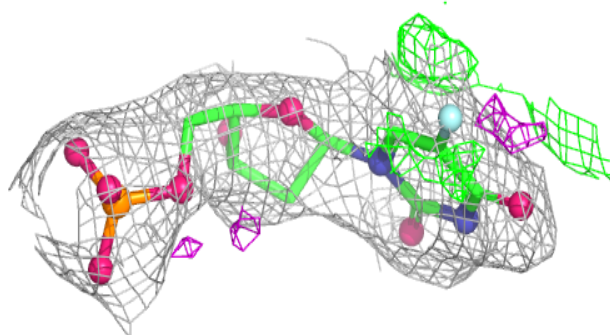
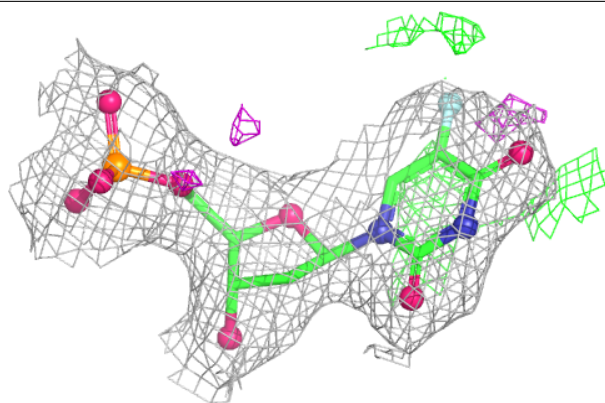
**Electron density around UFP A 602:**

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

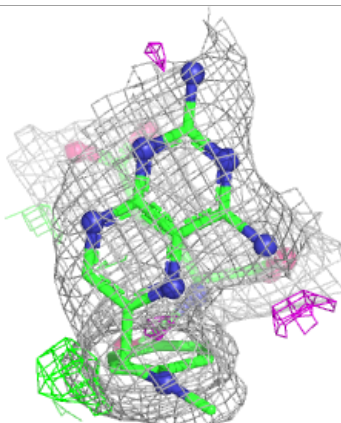
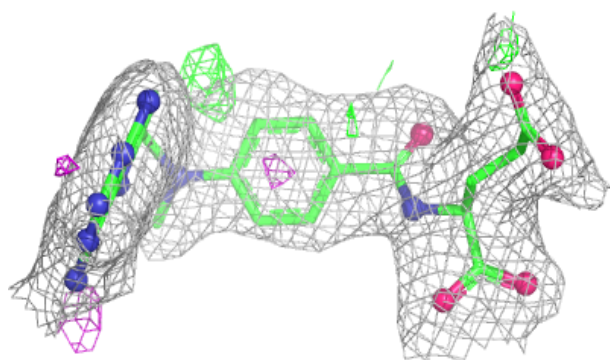
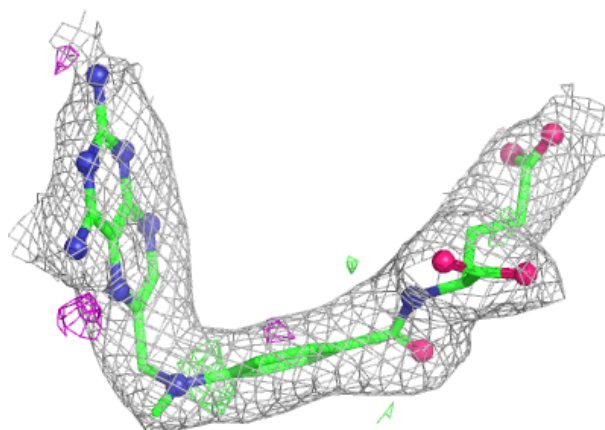


Electron density around UFP C 602:

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

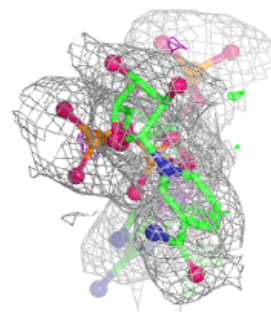
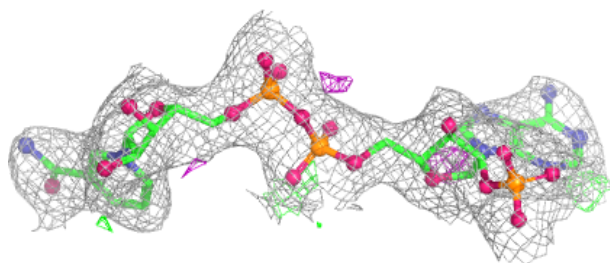
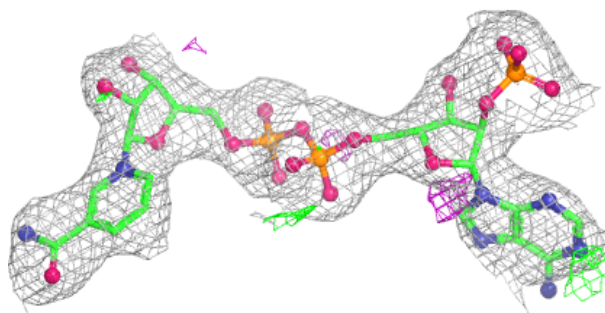
**Electron density around MTX E 604:**

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



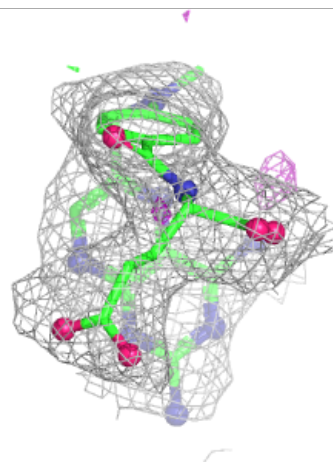
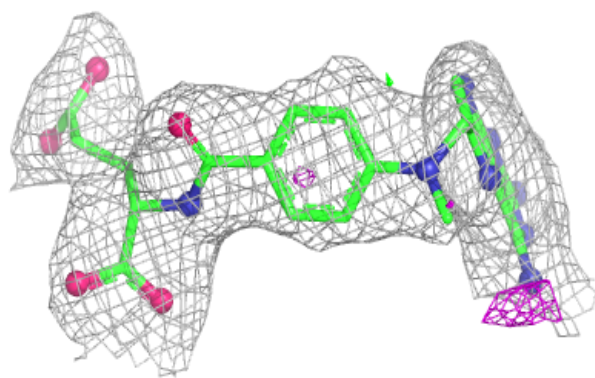
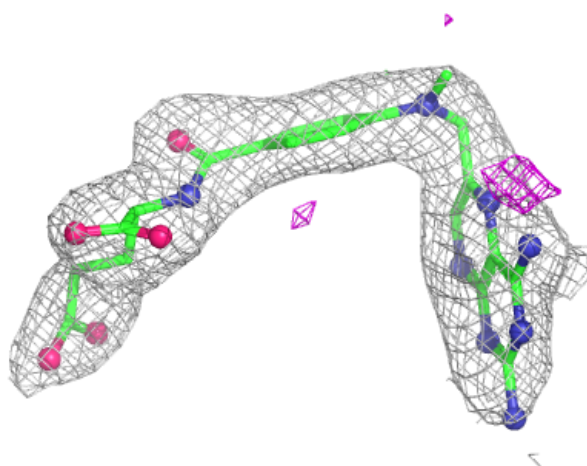
Electron density around NDP A 601:

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



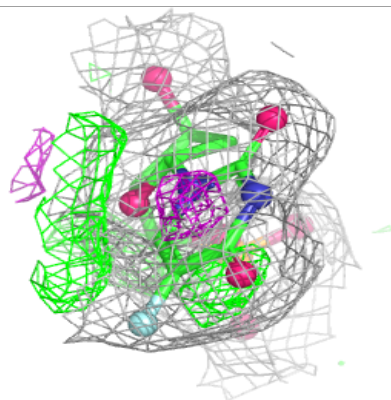
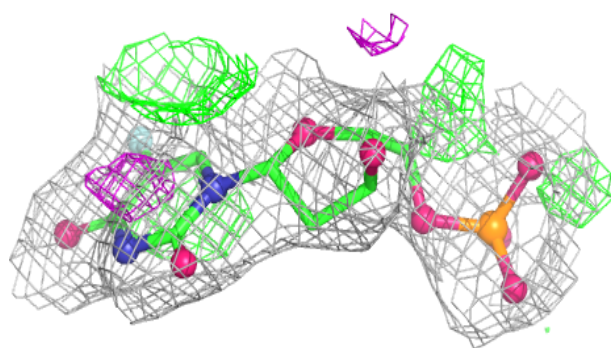
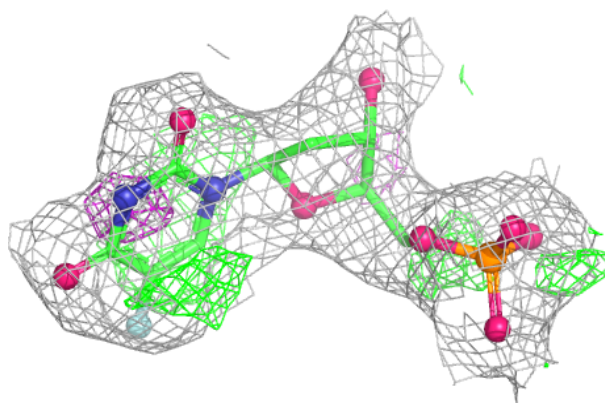
Electron density around MTX A 604:

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



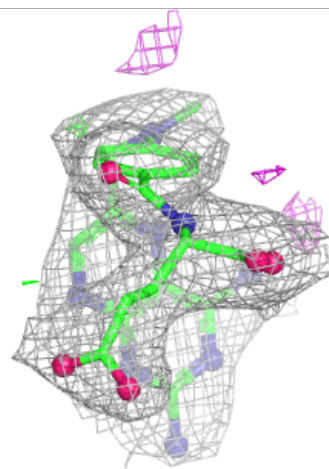
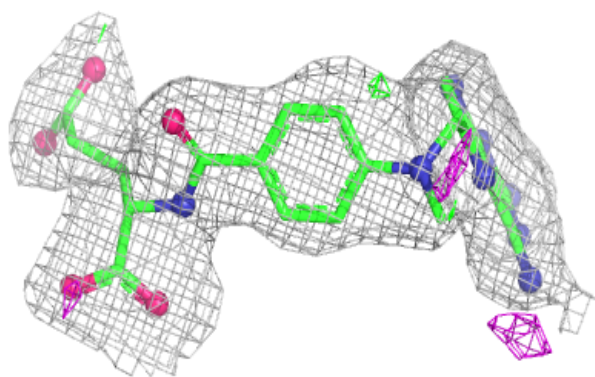
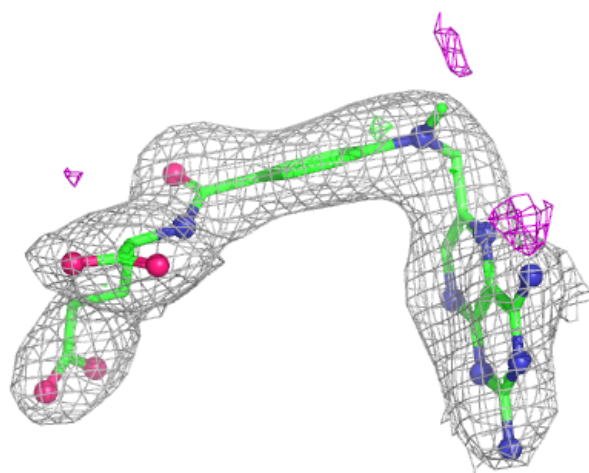
Electron density around UFP E 602:

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



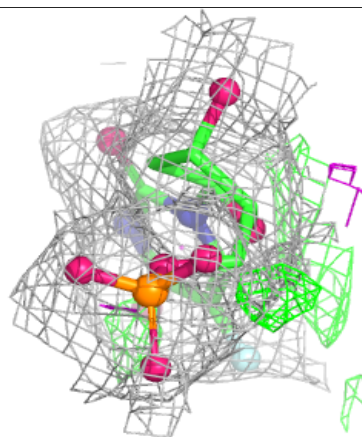
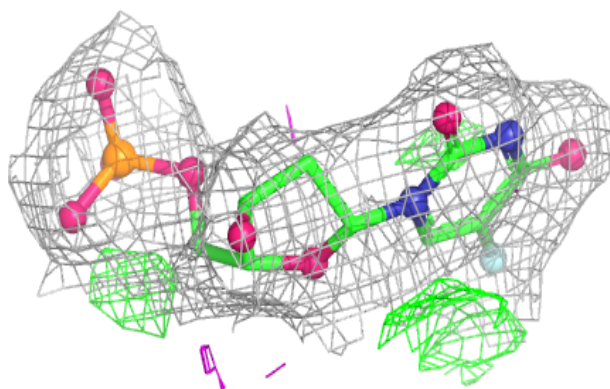
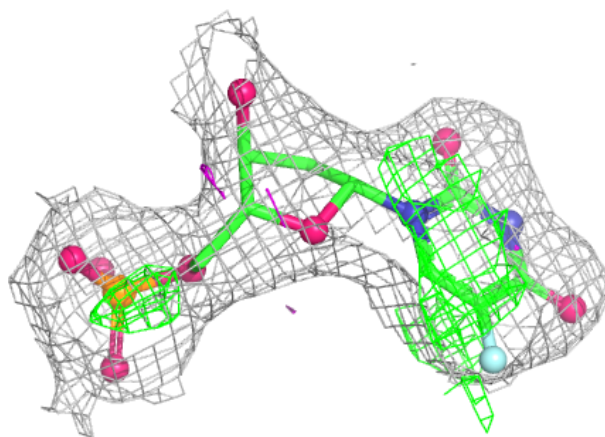
Electron density around MTX C 604:

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

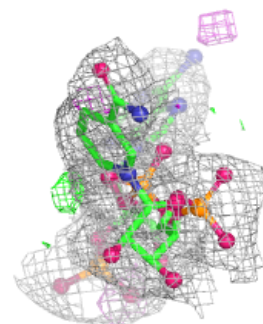
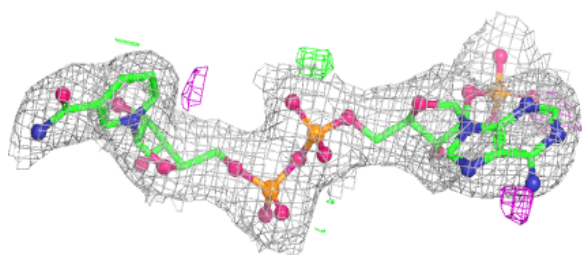
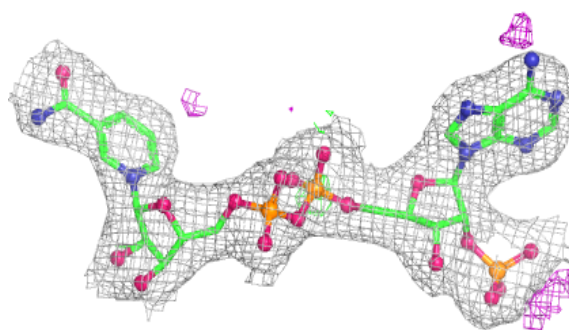


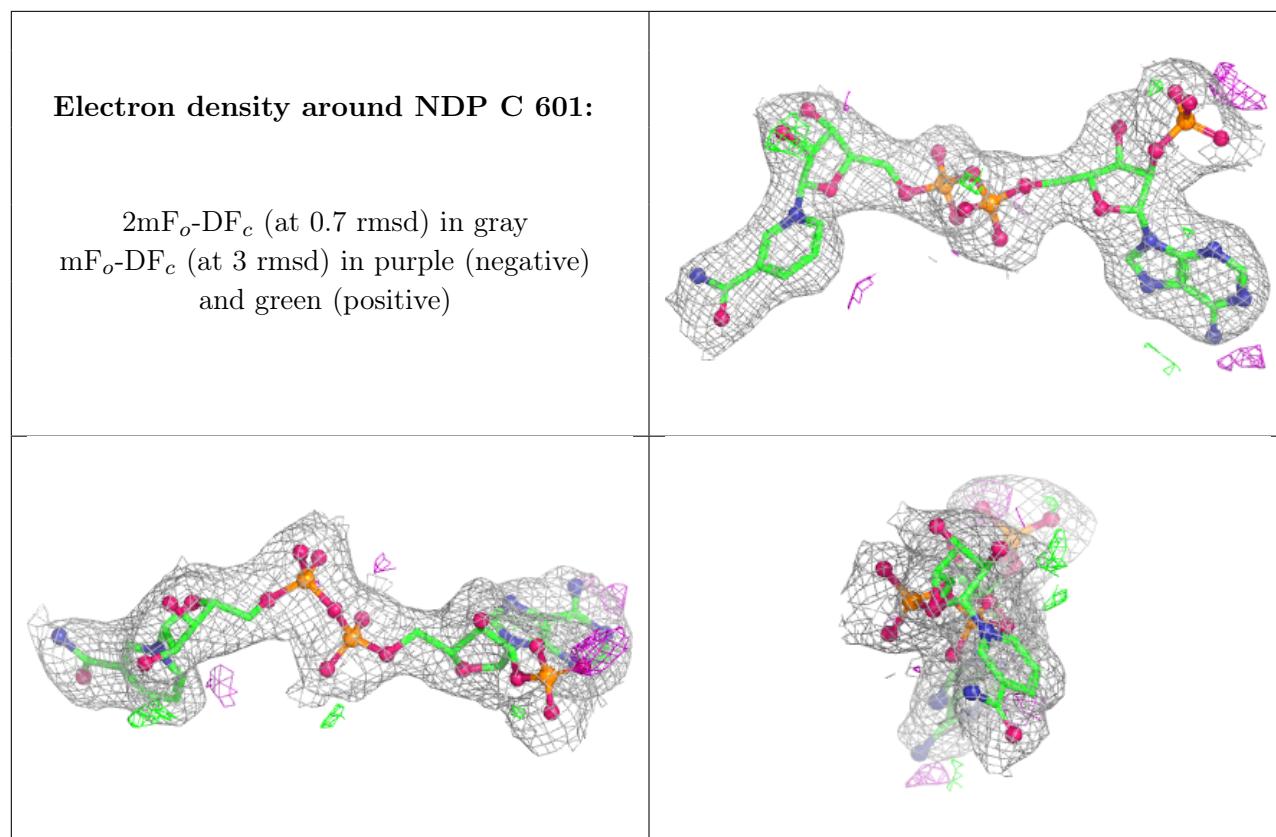
Electron density around UFP B 602:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.