



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:00 AM UTC

PDB ID : 6PF7 / pdb_00006pf7
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)benzoic acid
Authors : Czyzyk, D.J.; Valhondo, M.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2019-06-21
Resolution : 2.79 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

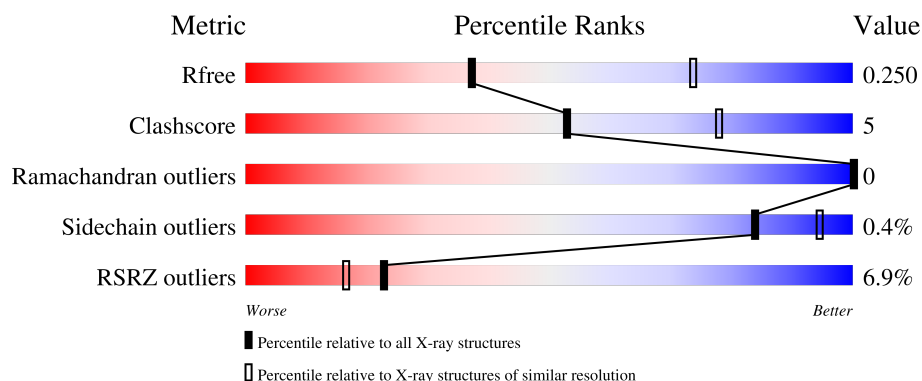
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	521	4% 83% 14% .
1	B	521	5% 82% 15% .
1	C	521	6% 84% 13% .
1	D	521	5% 85% 12% .

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Mol	Chain	Length	Quality of chain
1	E	521	13% 88% 10%

2 Entry composition ⓘ

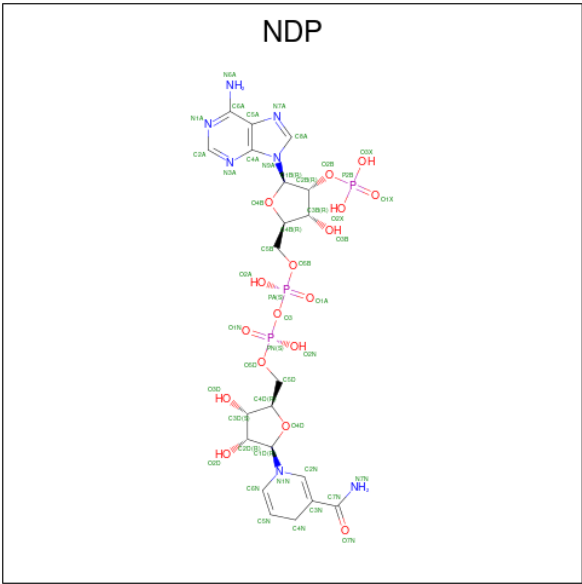
There are 7 unique types of molecules in this entry. The entry contains 21040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	507	Total	C	N	O	S	0	0	0
			4086	2612	686	766	22			
1	B	507	Total	C	N	O	S	0	0	0
			4070	2601	684	764	21			
1	C	508	Total	C	N	O	S	0	0	0
			4044	2587	683	753	21			
1	D	507	Total	C	N	O	S	0	0	0
			4050	2588	681	760	21			
1	E	508	Total	C	N	O	S	0	0	0
			3971	2533	666	751	21			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



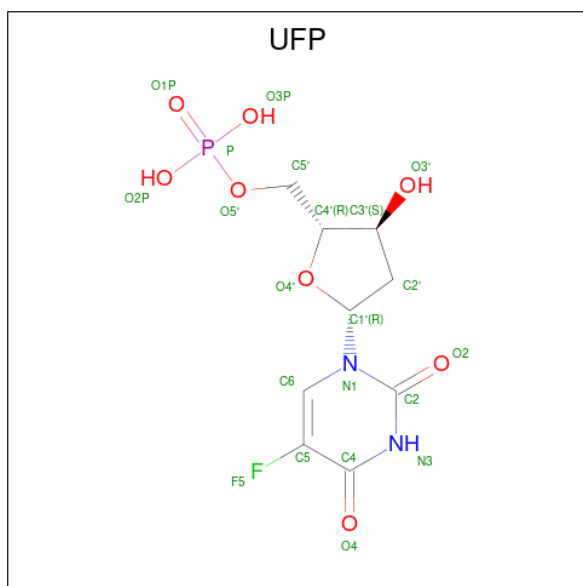
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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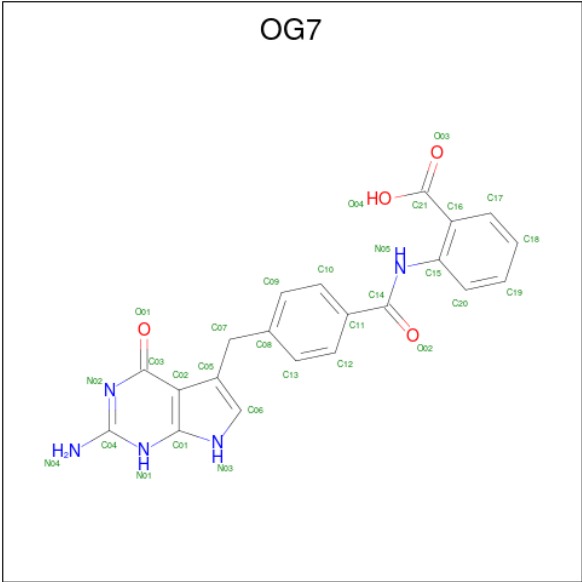
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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



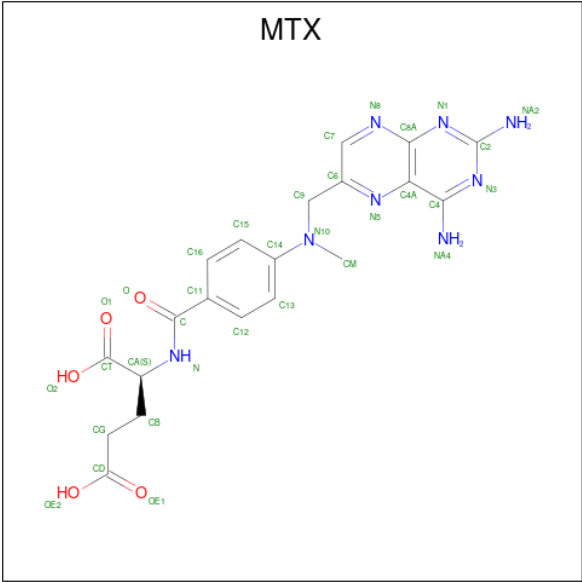
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is 2-({4-[(2-amino-4-oxo-4,7-dihydro-1H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl]benzene-1-carbonyl}amino)benzoic acid (CCD ID: OG7) (formula: C₂₁H₁₇N₅O₄) (labeled as "Ligand of Interest" by depositor).



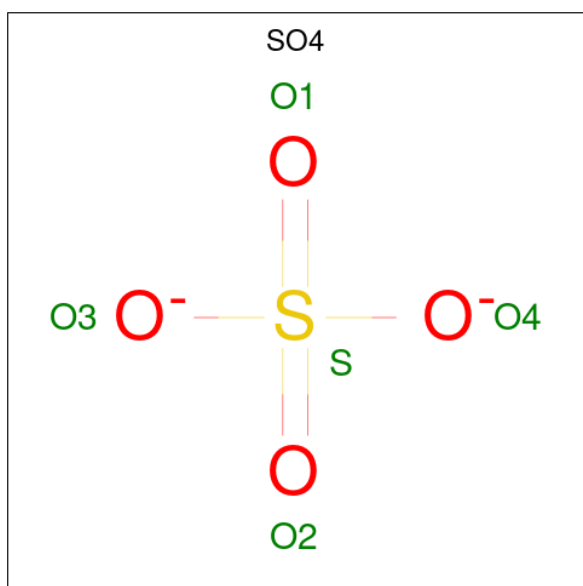
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			30	21	5	4		
4	B	1	Total	C	N	O	0	0
			30	21	5	4		
4	C	1	Total	C	N	O	0	0
			30	21	5	4		
4	D	1	Total	C	N	O	0	0
			30	21	5	4		
4	E	1	Total	C	N	O	0	0
			30	21	5	4		

- 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		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	55	Total	O	0	0
			55	55		

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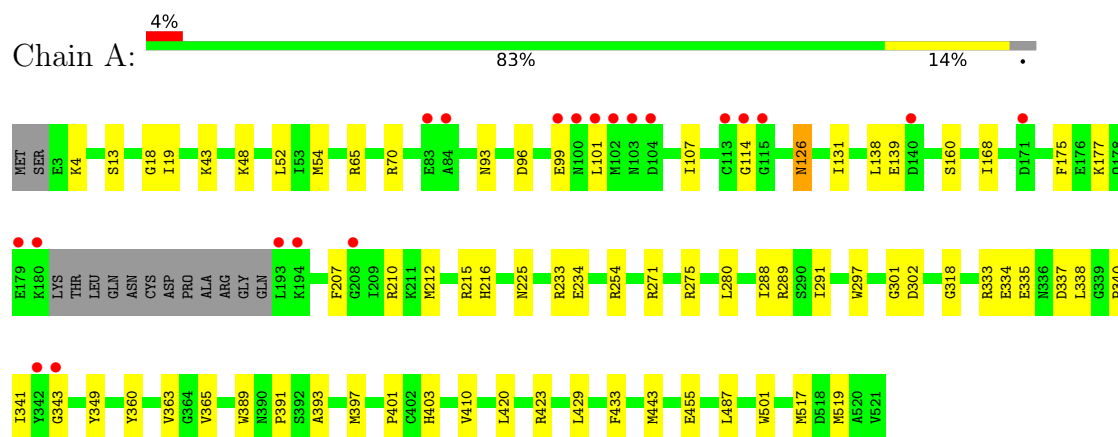
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	27	Total 27	O 27	0	0
7	C	28	Total 28	O 28	0	0
7	D	25	Total 25	O 25	0	0
7	E	4	Total 4	O 4	0	0

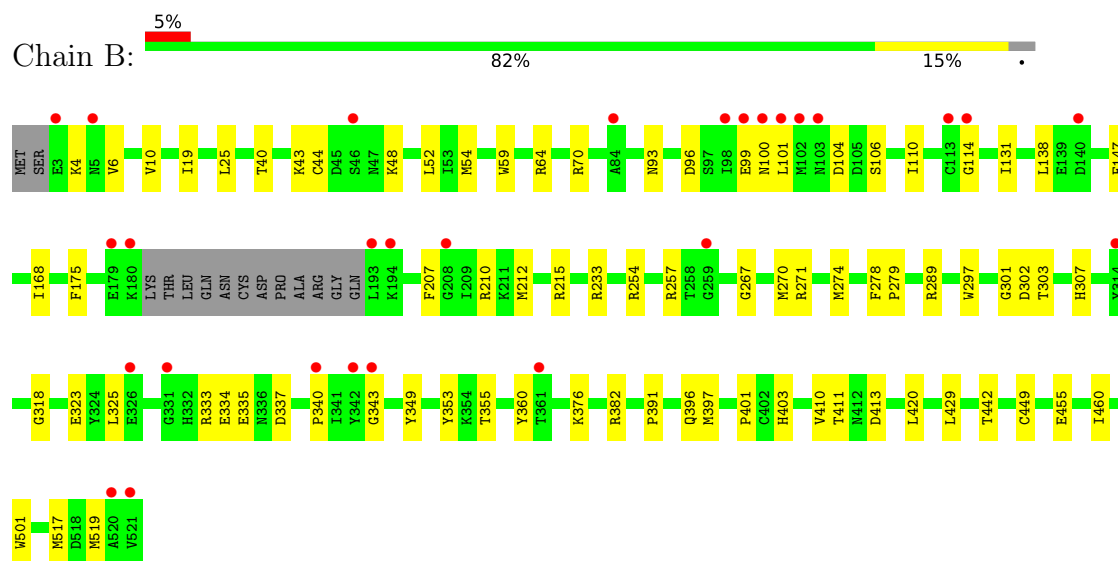
3 Residue-property plots [i](#)

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.

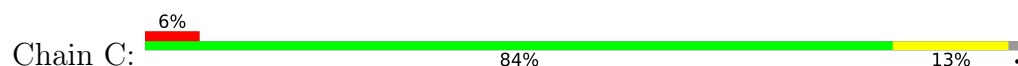
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

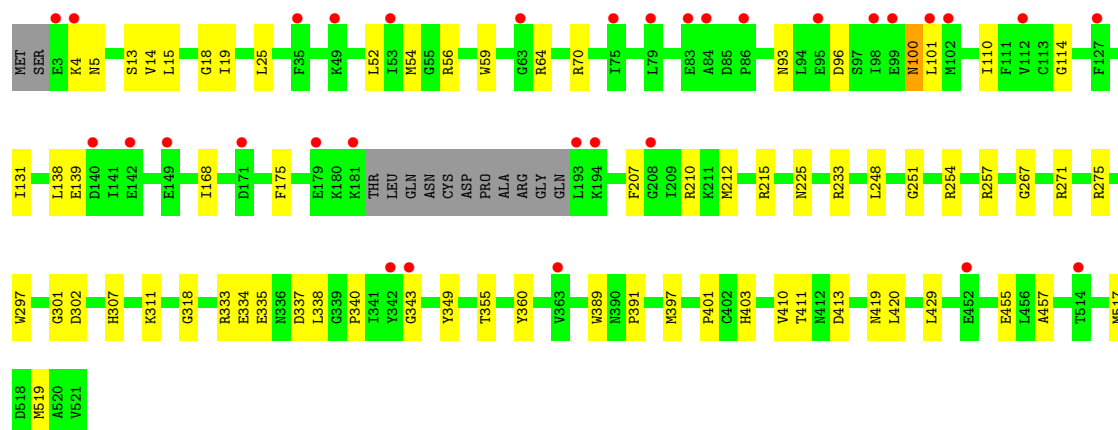


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

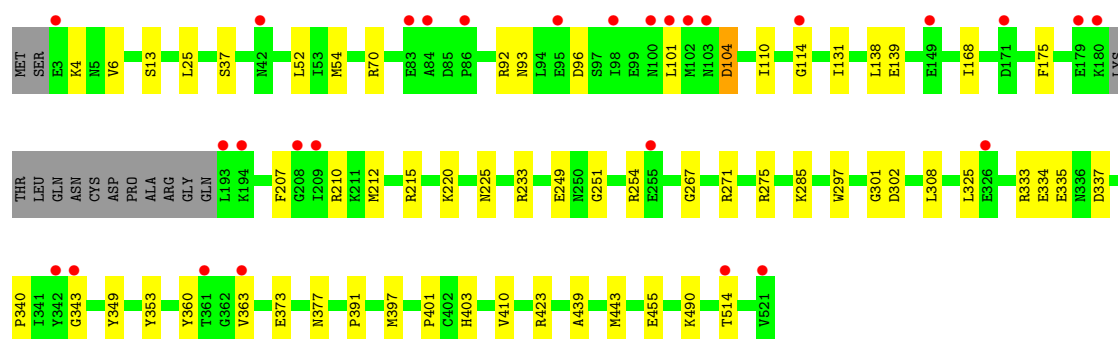
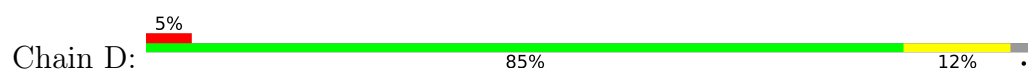


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

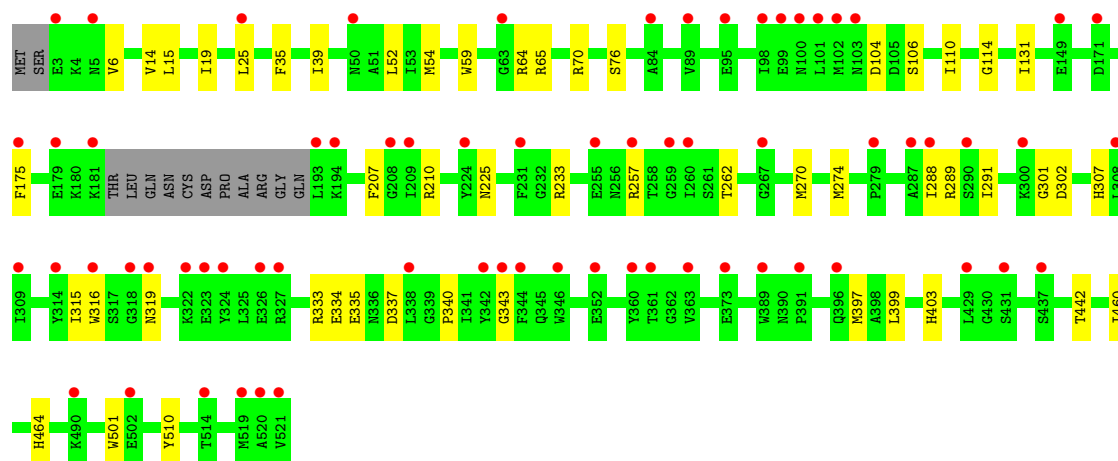
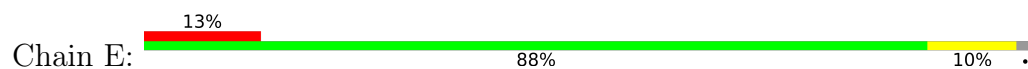




- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



- 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	214.77Å 115.79Å 220.14Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	49.09 – 2.79 49.09 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.09-2.79) 99.6 (49.09-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472)	Depositor
R, R_{free}	0.222 , 0.253 0.225 , 0.250	Depositor DCC
R_{free} test set	2002 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21040	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OG7, UFP, MTX, NDP, SO4

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	0.12	0/4181	0.32	0/5660
1	B	0.11	0/4165	0.31	0/5643
1	C	0.11	0/4139	0.30	0/5613
1	D	0.11	0/4145	0.31	0/5621
1	E	0.10	0/4066	0.28	0/5533
All	All	0.11	0/20696	0.31	0/28070

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

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	4086	0	3973	51	0
1	B	4070	0	3938	53	0
1	C	4044	0	3896	48	0
1	D	4050	0	3897	43	0
1	E	3971	0	3707	30	0
2	A	48	0	26	1	0
2	B	48	0	26	1	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	0	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	1	0
4	C	30	0	0	0	0
4	D	30	0	0	0	0
4	E	30	0	0	0	0
5	A	33	0	20	0	0
5	B	33	0	20	1	0
5	C	33	0	20	2	0
5	D	33	0	20	2	0
5	E	33	0	20	1	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
7	A	55	0	0	0	0
7	B	27	0	0	4	0
7	C	28	0	0	1	0
7	D	25	0	0	2	0
7	E	4	0	0	0	0
All	All	21040	0	19691	204	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 (204) 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:A:225:ASN:O	1:A:233:ARG:NH2	2.20	0.74
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.72	0.72
1:C:207:PHE:HB3	1:C:210:ARG:HB2	1.73	0.71
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.73	0.69
1:D:4:LYS:H	1:D:101:LEU:HD22	1.57	0.69
1:C:100:ASN:N	1:C:100:ASN:OD1	2.27	0.68
1:C:271:ARG:NH2	1:D:267:GLY:O	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ASN:O	1:D:233:ARG:NH2	2.26	0.67
1:D:25:LEU:HD11	5:D:604:MTX:H7	1.77	0.67
1:A:341:ILE:HA	1:A:397:MET:HE3	1.76	0.67
1:C:54:MET:HA	1:C:114:GLY:HA3	1.77	0.66
1:D:207:PHE:HB3	1:D:210:ARG:HB2	1.78	0.66
1:B:4:LYS:NZ	1:B:104:ASP:O	2.29	0.65
1:D:54:MET:HA	1:D:114:GLY:HA3	1.80	0.64
1:E:54:MET:HA	1:E:114:GLY:HA3	1.79	0.64
1:A:207:PHE:HB3	1:A:210:ARG:HB2	1.78	0.64
1:E:207:PHE:HB3	1:E:210:ARG:HB2	1.80	0.64
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.79	0.64
1:A:254:ARG:NH2	1:B:410:VAL:O	2.30	0.63
1:B:54:MET:HA	1:B:114:GLY:HA3	1.80	0.63
1:B:207:PHE:HB3	1:B:210:ARG:HB2	1.81	0.63
1:B:25:LEU:HD11	5:B:604:MTX:H7	1.80	0.62
1:C:267:GLY:O	1:D:271:ARG:NH2	2.30	0.62
1:A:52:LEU:HD11	1:A:70:ARG:HD2	1.82	0.62
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.80	0.62
1:C:301:GLY:HA2	1:C:343:GLY:O	1.99	0.62
1:A:54:MET:HA	1:A:114:GLY:HA3	1.80	0.62
1:A:301:GLY:HA2	1:A:343:GLY:O	2.01	0.61
1:C:225:ASN:O	1:C:233:ARG:NH2	2.33	0.61
1:B:325:LEU:HD23	1:B:333:ARG:HB3	1.83	0.60
1:C:100:ASN:HB2	1:C:110:ILE:HD11	1.83	0.60
1:E:225:ASN:O	1:E:233:ARG:NH2	2.34	0.60
1:A:410:VAL:O	1:B:254:ARG:NH2	2.34	0.60
1:D:301:GLY:HA2	1:D:343:GLY:O	2.02	0.59
1:D:423:ARG:NH1	3:D:602:UFP:O3P	2.31	0.59
1:B:301:GLY:HA2	1:B:343:GLY:O	2.03	0.58
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.85	0.57
1:B:93:ASN:ND2	1:B:96:ASP:OD2	2.35	0.57
1:D:13:SER:OG	1:D:139:GLU:OE2	2.22	0.56
1:D:251:GLY:O	1:E:65:ARG:NH1	2.38	0.56
1:E:25:LEU:HD11	5:E:604:MTX:H7	1.85	0.56
1:C:59:TRP:NE1	1:C:64:ARG:HG3	2.20	0.56
1:C:410:VAL:O	1:D:254:ARG:NH2	2.33	0.56
1:B:59:TRP:NE1	1:B:64:ARG:HG3	2.20	0.55
1:C:254:ARG:NH2	1:D:410:VAL:O	2.38	0.55
1:C:25:LEU:HD11	5:C:604:MTX:H7	1.89	0.55
1:A:271:ARG:NH2	1:B:267:GLY:O	2.36	0.55
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HD11	1:B:70:ARG:HD2	1.87	0.54
1:A:4:LYS:H	1:A:101:LEU:HD22	1.71	0.54
1:B:302:ASP:OD2	1:B:307:HIS:ND1	2.32	0.54
1:C:318:GLY:HA3	1:C:519:MET:HE1	1.89	0.54
1:B:59:TRP:CE2	1:B:64:ARG:HG3	2.42	0.54
1:B:43:LYS:NZ	1:B:48:LYS:O	2.34	0.54
1:C:334:GLU:HG2	1:C:335:GLU:H	1.73	0.54
1:B:257:ARG:HH21	3:B:602:UFP:H5'2	1.72	0.53
1:A:126:ASN:ND2	1:A:177:LYS:HE3	2.24	0.53
1:A:138:LEU:HD11	1:A:168:ILE:HD13	1.91	0.53
1:A:13:SER:OG	1:A:139:GLU:OE2	2.23	0.53
1:A:443:MET:HE1	1:A:487:LEU:HD22	1.90	0.53
1:B:340:PRO:O	1:B:397:MET:HG2	2.09	0.53
1:C:52:LEU:HD11	1:C:70:ARG:HD2	1.90	0.53
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.43	0.53
1:A:93:ASN:ND2	1:A:96:ASP:OD2	2.36	0.53
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.90	0.53
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.90	0.52
1:E:59:TRP:NE1	1:E:64:ARG:HG3	2.23	0.52
1:A:126:ASN:HD21	1:A:177:LYS:HE3	1.74	0.52
1:C:19:ILE:O	2:C:601:NDP:H2N	2.09	0.52
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.90	0.52
1:D:325:LEU:HD23	1:D:333:ARG:HB3	1.91	0.52
1:E:301:GLY:HA2	1:E:343:GLY:O	2.10	0.52
1:B:138:LEU:HD11	1:B:168:ILE:HD13	1.91	0.52
1:B:323:GLU:OE1	1:B:323:GLU:N	2.39	0.52
1:D:138:LEU:HD11	1:D:168:ILE:HD13	1.92	0.52
1:D:490:LYS:NZ	7:D:703:HOH:O	2.43	0.51
1:A:455:GLU:CD	1:B:212:MET:HE3	2.35	0.51
1:E:334:GLU:HG2	1:E:335:GLU:H	1.76	0.51
1:C:13:SER:OG	1:C:139:GLU:OE2	2.28	0.50
1:C:212:MET:HE3	1:D:455:GLU:CD	2.37	0.50
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.47	0.50
1:B:289:ARG:NH1	7:B:702:HOH:O	2.44	0.50
1:A:212:MET:HE3	1:B:455:GLU:CD	2.36	0.50
1:A:334:GLU:HG2	1:A:335:GLU:H	1.75	0.50
1:C:349:TYR:HH	1:D:349:TYR:HH	1.58	0.50
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.47	0.50
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.47	0.50
1:A:341:ILE:HG22	1:A:397:MET:HE3	1.94	0.50
1:E:35:PHE:CZ	1:E:39:ILE:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HD2	1:B:215:ARG:CZ	2.42	0.49
1:B:334:GLU:HG2	1:B:335:GLU:H	1.75	0.49
1:A:423:ARG:NH1	3:A:602:UFP:O3P	2.39	0.49
1:E:59:TRP:CE2	1:E:64:ARG:HG3	2.47	0.49
1:B:318:GLY:HA3	1:B:519:MET:HE1	1.95	0.49
1:E:14:VAL:HG13	1:E:15:LEU:HG	1.95	0.49
1:E:52:LEU:HD11	1:E:70:ARG:HD2	1.93	0.49
1:B:297:TRP:CD1	1:B:302:ASP:HB3	2.46	0.49
1:D:334:GLU:HG2	1:D:335:GLU:H	1.76	0.49
1:A:397:MET:HE1	1:A:401:PRO:HD3	1.94	0.49
1:C:138:LEU:HD11	1:C:168:ILE:HD13	1.94	0.49
1:A:318:GLY:HA3	1:A:519:MET:HE1	1.95	0.48
1:C:455:GLU:CD	1:D:212:MET:HE3	2.38	0.48
1:B:4:LYS:H	1:B:101:LEU:HD22	1.78	0.48
1:A:19:ILE:O	2:A:601:NDP:H2N	2.13	0.48
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.78	0.48
1:B:44:CYS:SG	7:B:727:HOH:O	2.60	0.48
1:C:59:TRP:CE2	1:C:64:ARG:HG3	2.48	0.48
1:D:340:PRO:O	1:D:397:MET:HG2	2.12	0.48
1:E:403:HIS:H	1:E:403:HIS:CD2	2.30	0.48
1:C:389:TRP:HE3	1:C:401:PRO:HG2	1.78	0.48
1:C:56:ARG:HD3	2:C:601:NDP:O2X	2.14	0.48
1:C:311:LYS:NZ	7:C:703:HOH:O	2.46	0.48
1:B:6:VAL:HG22	1:B:110:ILE:HB	1.96	0.48
1:A:403:HIS:H	1:A:403:HIS:CD2	2.32	0.48
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.95	0.47
1:D:6:VAL:HG22	1:D:110:ILE:HB	1.96	0.47
1:C:340:PRO:O	1:C:397:MET:HG2	2.15	0.47
1:E:340:PRO:O	1:E:397:MET:HG2	2.14	0.47
1:E:15:LEU:HD11	1:E:510:TYR:HB3	1.97	0.47
1:A:280:LEU:HD22	1:A:288:ILE:HD12	1.96	0.47
1:A:349:TYR:HB3	1:A:365:VAL:HB	1.96	0.46
1:A:403:HIS:HB2	1:A:420:LEU:HD11	1.97	0.46
1:B:337:ASP:OD1	1:B:353:TYR:OH	2.32	0.46
1:C:411:THR:OG1	1:C:413:ASP:OD1	2.33	0.46
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.51	0.46
1:A:429:LEU:HD21	1:A:517:MET:HB2	1.97	0.46
1:B:270:MET:HE2	1:B:460:ILE:HD11	1.98	0.46
1:E:104:ASP:OD1	1:E:106:SER:OG	2.28	0.46
1:C:215:ARG:CZ	1:D:275:ARG:HD2	2.45	0.46
1:E:6:VAL:HG22	1:E:110:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:NH2	1:C:248:LEU:O	2.50	0.45
1:A:216:HIS:CE1	1:B:271:ARG:HH12	2.33	0.45
1:C:4:LYS:H	1:C:101:LEU:HD22	1.82	0.45
1:B:396:GLN:NE2	7:B:703:HOH:O	2.47	0.45
1:C:275:ARG:HD2	1:D:215:ARG:CZ	2.47	0.45
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.52	0.45
1:D:104:ASP:OD1	7:D:701:HOH:O	2.21	0.45
1:B:303:THR:HG22	7:B:722:HOH:O	2.17	0.45
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.99	0.45
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.52	0.44
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.99	0.44
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.52	0.44
1:A:4:LYS:NZ	1:A:107:ILE:O	2.44	0.44
1:A:393:ALA:O	1:A:397:MET:HG3	2.18	0.44
1:D:220:LYS:HG3	1:D:249:GLU:OE1	2.18	0.44
1:E:257:ARG:NE	3:E:602:UFP:O1P	2.29	0.44
1:E:270:MET:HE2	1:E:460:ILE:HD11	2.00	0.44
1:A:291:ILE:HG12	1:A:433:PHE:CD2	2.53	0.43
1:B:403:HIS:CD2	1:B:403:HIS:H	2.35	0.43
1:D:397:MET:SD	1:D:401:PRO:HD3	2.58	0.43
1:C:403:HIS:H	1:C:403:HIS:CD2	2.35	0.43
1:D:373:GLU:O	1:D:377:ASN:ND2	2.51	0.43
1:A:13:SER:HB3	1:A:18:GLY:H	1.81	0.43
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.99	0.43
1:E:76:SER:OG	2:E:601:NDP:O2X	2.34	0.43
1:E:274:MET:HE1	1:E:442:THR:HG21	2.00	0.43
1:A:389:TRP:HE3	1:A:401:PRO:HG2	1.84	0.43
1:C:429:LEU:HD21	1:C:517:MET:HB2	2.01	0.43
1:D:340:PRO:HD3	1:D:353:TYR:CD2	2.53	0.43
1:C:257:ARG:NE	3:C:602:UFP:O1P	2.46	0.43
1:D:403:HIS:CD2	1:D:403:HIS:H	2.36	0.43
1:D:285:LYS:HB3	1:D:514:THR:HB	2.01	0.42
1:D:297:TRP:CE3	1:D:308:LEU:HD11	2.54	0.42
1:E:19:ILE:O	2:E:601:NDP:H2N	2.18	0.42
1:C:333:ARG:CG	1:C:337:ASP:HB3	2.47	0.42
1:C:403:HIS:HB2	1:C:420:LEU:HD11	2.01	0.42
1:B:19:ILE:O	2:B:601:NDP:H2N	2.20	0.42
1:D:93:ASN:ND2	1:D:96:ASP:OD2	2.53	0.42
1:D:360:TYR:O	1:D:363:VAL:HG12	2.20	0.42
1:E:288:ILE:HD12	1:E:291:ILE:HD12	2.02	0.42
1:E:302:ASP:OD2	1:E:307:HIS:ND1	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:LEU:HD21	1:B:517:MET:HB2	2.02	0.42
1:A:43:LYS:NZ	1:A:48:LYS:O	2.48	0.41
2:C:601:NDP:H42N	5:C:604:MTX:N5	2.34	0.41
1:A:360:TYR:O	1:A:363:VAL:HG12	2.20	0.41
3:A:602:UFP:O2P	1:B:382:ARG:NH1	2.53	0.41
1:C:355:THR:O	1:C:360:TYR:OH	2.34	0.41
1:D:37:SER:HB2	5:D:604:MTX:HB1	2.03	0.41
1:E:289:ARG:HG3	1:E:501:TRP:CE2	2.55	0.41
1:A:212:MET:HG3	1:A:215:ARG:NH1	2.36	0.41
1:A:289:ARG:HG3	1:A:501:TRP:CD2	2.55	0.41
1:A:340:PRO:O	1:A:397:MET:HG2	2.20	0.41
1:B:355:THR:O	1:B:360:TYR:OH	2.35	0.41
1:B:40:THR:HB	1:B:52:LEU:HD21	2.02	0.41
1:D:92:ARG:HD3	1:D:92:ARG:HA	1.87	0.41
1:E:262:THR:HB	1:E:464:HIS:HB2	2.03	0.41
1:A:65:ARG:NH1	1:C:251:GLY:O	2.53	0.41
1:A:160:SER:HA	1:A:234:GLU:HB3	2.03	0.41
1:B:411:THR:OG1	1:B:413:ASP:OD1	2.30	0.41
1:B:10:VAL:HG21	1:B:147:PHE:CD1	2.55	0.41
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.94	0.41
1:B:376:LYS:HD3	1:B:449:CYS:HA	2.03	0.41
1:E:319:ASN:ND2	1:E:399:LEU:HD22	2.36	0.41
1:C:13:SER:HB3	1:C:18:GLY:H	1.85	0.41
1:C:14:VAL:HG13	1:C:15:LEU:HG	2.01	0.41
1:B:104:ASP:OD1	1:B:106:SER:OG	2.33	0.40
1:E:315:ILE:HG13	1:E:316:TRP:CD1	2.56	0.40
1:B:274:MET:HE1	1:B:442:THR:HG21	2.03	0.40
3:B:602:UFP:H4'	4:B:603:OG7:N04	2.37	0.40
1:C:302:ASP:OD2	1:C:307:HIS:ND1	2.34	0.40
1:D:439:ALA:O	1:D:443:MET:HG3	2.21	0.40
1:C:93:ASN:ND2	1:C:96:ASP:OD2	2.51	0.40
1:C:419:ASN:OD1	1:C:457:ALA:HB3	2.21	0.40
1:B:397:MET:SD	1:B:401:PRO:HD3	2.60	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	503/521 (96%)	480 (95%)	23 (5%)	0	100	100
1	B	503/521 (96%)	478 (95%)	25 (5%)	0	100	100
1	C	504/521 (97%)	480 (95%)	24 (5%)	0	100	100
1	D	503/521 (96%)	480 (95%)	23 (5%)	0	100	100
1	E	504/521 (97%)	480 (95%)	24 (5%)	0	100	100
All	All	2517/2605 (97%)	2398 (95%)	119 (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	446/470 (95%)	444 (100%)	2 (0%)	84	94
1	B	442/470 (94%)	439 (99%)	3 (1%)	76	91
1	C	434/470 (92%)	432 (100%)	2 (0%)	81	93
1	D	437/470 (93%)	436 (100%)	1 (0%)	87	96
1	E	415/470 (88%)	415 (100%)	0	100	100
All	All	2174/2350 (92%)	2166 (100%)	8 (0%)	84	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLU
1	A	126	ASN
1	B	99	GLU
1	B	100	ASN
1	B	233	ARG
1	C	5	ASN
1	C	100	ASN
1	D	104	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	126	ASN
1	A	495	ASN
1	B	5	ASN
1	B	214	ASN
1	B	319	ASN
1	B	336	ASN
1	B	345	GLN
1	B	486	GLN
1	B	495	ASN
1	C	214	ASN
1	C	348	HIS
1	C	350	ASN
1	C	390	ASN
1	C	447	GLN
1	C	495	ASN
1	D	22	ASN
1	D	178	GLN
1	D	214	ASN
1	D	336	ASN
1	D	350	ASN
1	D	390	ASN
1	D	447	GLN
1	D	486	GLN
1	E	214	ASN
1	E	336	ASN
1	E	486	GLN
1	E	495	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	OG7	E	603	-	32,33,33	1.26	1 (3%)	42,47,47	1.26	4 (9%)
3	UFP	A	602	-	22,22,22	1.22	1 (4%)	32,33,33	2.75	11 (34%)
6	SO4	D	605	-	4,4,4	0.24	0	6,6,6	0.08	0
5	MTX	E	604	-	35,35,35	1.03	1 (2%)	47,49,49	1.94	15 (31%)
4	OG7	D	603	-	32,33,33	1.27	1 (3%)	42,47,47	1.29	4 (9%)
2	NDP	B	601	-	51,52,52	1.96	12 (23%)	71,80,80	1.52	13 (18%)
3	UFP	B	602	-	22,22,22	1.30	2 (9%)	32,33,33	2.75	11 (34%)
2	NDP	D	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.50	10 (14%)
5	MTX	A	604	-	35,35,35	1.02	1 (2%)	47,49,49	1.88	14 (29%)
2	NDP	A	601	-	51,52,52	1.95	11 (21%)	71,80,80	1.50	11 (15%)
6	SO4	C	605	-	4,4,4	0.24	0	6,6,6	0.08	0
2	NDP	E	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.50	11 (15%)
5	MTX	D	604	-	35,35,35	1.02	1 (2%)	47,49,49	1.93	15 (31%)
3	UFP	D	602	-	22,22,22	1.26	1 (4%)	32,33,33	2.67	11 (34%)
2	NDP	C	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.51	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OG7	B	603	-	32,33,33	1.29	1 (3%)	42,47,47	1.33	5 (11%)
6	SO4	B	605	-	4,4,4	0.23	0	6,6,6	0.06	0
3	UFP	E	602	-	22,22,22	1.26	1 (4%)	32,33,33	2.65	10 (31%)
4	OG7	A	603	-	32,33,33	1.30	1 (3%)	42,47,47	1.42	5 (11%)
6	SO4	A	605	-	4,4,4	0.23	0	6,6,6	0.07	0
5	MTX	C	604	-	35,35,35	1.03	1 (2%)	47,49,49	1.89	14 (29%)
3	UFP	C	602	-	22,22,22	1.26	1 (4%)	32,33,33	2.71	11 (34%)
5	MTX	B	604	-	35,35,35	1.01	1 (2%)	47,49,49	1.89	14 (29%)
4	OG7	C	603	-	32,33,33	1.28	1 (3%)	42,47,47	1.32	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OG7	E	603	-	-	2/16/16/16	0/4/4/4
3	UFP	A	602	-	-	5/10/22/22	0/2/2/2
5	MTX	E	604	-	-	7/25/25/25	0/3/3/3
4	OG7	D	603	-	-	2/16/16/16	0/4/4/4
2	NDP	B	601	-	-	3/34/77/77	0/5/5/5
3	UFP	B	602	-	-	5/10/22/22	0/2/2/2
2	NDP	D	601	-	-	5/34/77/77	0/5/5/5
5	MTX	A	604	-	-	5/25/25/25	0/3/3/3
2	NDP	A	601	-	-	3/34/77/77	0/5/5/5
2	NDP	E	601	-	-	5/34/77/77	0/5/5/5
5	MTX	D	604	-	-	7/25/25/25	0/3/3/3
3	UFP	D	602	-	-	5/10/22/22	0/2/2/2
2	NDP	C	601	-	-	3/34/77/77	0/5/5/5
4	OG7	B	603	-	-	2/16/16/16	0/4/4/4
3	UFP	E	602	-	-	6/10/22/22	0/2/2/2
4	OG7	A	603	-	-	2/16/16/16	0/4/4/4
5	MTX	C	604	-	-	7/25/25/25	0/3/3/3
3	UFP	C	602	-	-	6/10/22/22	0/2/2/2
5	MTX	B	604	-	-	5/25/25/25	0/3/3/3
4	OG7	C	603	-	-	2/16/16/16	0/4/4/4

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NDP	C6A-N6A	5.79	1.49	1.34
2	B	601	NDP	C6A-N6A	5.77	1.48	1.34
2	E	601	NDP	C6A-N6A	5.76	1.48	1.34
2	C	601	NDP	C6A-N6A	5.73	1.48	1.34
2	A	601	NDP	C6A-N6A	5.70	1.48	1.34
2	C	601	NDP	C4N-C3N	-4.74	1.41	1.50
2	D	601	NDP	C4N-C3N	-4.71	1.41	1.50
2	B	601	NDP	C4N-C3N	-4.69	1.41	1.50
2	E	601	NDP	C4N-C3N	-4.68	1.41	1.50
2	A	601	NDP	C4N-C3N	-4.66	1.41	1.50
2	B	601	NDP	C2D-C3D	-3.97	1.42	1.53
2	A	601	NDP	C2D-C3D	-3.94	1.42	1.53
2	E	601	NDP	C2D-C3D	-3.90	1.42	1.53
2	D	601	NDP	C2D-C3D	-3.89	1.42	1.53
2	C	601	NDP	C2D-C3D	-3.87	1.42	1.53
2	C	601	NDP	C3B-C2B	-3.84	1.44	1.53
2	E	601	NDP	C3B-C2B	-3.84	1.44	1.53
2	A	601	NDP	C3B-C2B	-3.83	1.44	1.53
2	D	601	NDP	C3B-C2B	-3.82	1.44	1.53
2	B	601	NDP	C3B-C2B	-3.82	1.44	1.53
2	B	601	NDP	C7N-N7N	3.69	1.44	1.33
2	D	601	NDP	C7N-N7N	3.68	1.44	1.33
2	E	601	NDP	C7N-N7N	3.66	1.44	1.33
2	C	601	NDP	C7N-N7N	3.66	1.44	1.33
2	A	601	NDP	C7N-N7N	3.66	1.44	1.33
3	B	602	UFP	P-O1P	3.43	1.61	1.50
3	D	602	UFP	P-O1P	3.41	1.61	1.50
3	E	602	UFP	P-O1P	3.40	1.61	1.50
3	C	602	UFP	P-O1P	3.36	1.60	1.50
3	A	602	UFP	P-O1P	3.33	1.60	1.50
2	C	601	NDP	C4N-C5N	-3.30	1.40	1.49
2	A	601	NDP	C4N-C5N	-3.26	1.40	1.49
2	E	601	NDP	C4N-C5N	-3.26	1.40	1.49
2	D	601	NDP	C4N-C5N	-3.26	1.40	1.49
2	B	601	NDP	C4N-C5N	-3.24	1.40	1.49
2	B	601	NDP	C2B-C1B	-3.21	1.45	1.53
2	A	601	NDP	C2B-C1B	-3.12	1.45	1.53
2	D	601	NDP	C2B-C1B	-3.12	1.45	1.53
2	C	601	NDP	C2B-C1B	-3.01	1.45	1.53
2	E	601	NDP	C2B-C1B	-2.98	1.45	1.53
2	C	601	NDP	C3B-C4B	-2.44	1.46	1.53
5	C	604	MTX	C7-C6	2.41	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NDP	C4A-N3A	2.40	1.38	1.34
5	E	604	MTX	C7-C6	2.40	1.43	1.39
2	A	601	NDP	C3B-C4B	-2.39	1.46	1.53
2	E	601	NDP	C4A-N3A	2.38	1.38	1.34
2	D	601	NDP	C4A-N3A	2.38	1.38	1.34
5	D	604	MTX	C7-C6	2.38	1.43	1.39
2	E	601	NDP	C3B-C4B	-2.37	1.47	1.53
5	A	604	MTX	C7-C6	2.36	1.43	1.39
2	B	601	NDP	C3B-C4B	-2.35	1.47	1.53
2	C	601	NDP	C4A-N3A	2.33	1.38	1.34
2	D	601	NDP	C3D-C4D	-2.31	1.47	1.53
5	B	604	MTX	C7-C6	2.30	1.43	1.39
2	C	601	NDP	C3D-C4D	-2.30	1.47	1.53
2	A	601	NDP	C3D-C4D	-2.30	1.47	1.53
2	D	601	NDP	C3B-C4B	-2.30	1.47	1.53
2	A	601	NDP	C4A-N3A	2.28	1.38	1.34
4	A	603	OG7	C16-C15	2.27	1.44	1.41
2	B	601	NDP	C3D-C4D	-2.26	1.47	1.53
2	E	601	NDP	C3D-C4D	-2.26	1.47	1.53
2	B	601	NDP	C6N-C5N	2.24	1.39	1.33
2	D	601	NDP	C6N-C5N	2.23	1.39	1.33
2	A	601	NDP	C6N-C5N	2.22	1.39	1.33
2	E	601	NDP	C6N-C5N	2.22	1.39	1.33
2	C	601	NDP	C6N-C5N	2.21	1.39	1.33
4	D	603	OG7	C16-C15	2.08	1.44	1.41
2	E	601	NDP	C2N-C3N	2.06	1.40	1.35
4	B	603	OG7	C16-C15	2.06	1.44	1.41
4	E	603	OG7	C16-C15	2.05	1.44	1.41
2	D	601	NDP	C2N-C3N	2.04	1.40	1.35
2	B	601	NDP	C2N-C3N	2.02	1.40	1.35
2	C	601	NDP	C2N-C3N	2.02	1.40	1.35
4	C	603	OG7	C10-C11	2.00	1.42	1.39
3	B	602	UFP	C4-N3	-2.00	1.35	1.38

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	UFP	C5-C4-N3	6.84	118.89	112.64
3	E	602	UFP	C5-C4-N3	6.80	118.86	112.64
3	B	602	UFP	C5-C4-N3	6.76	118.82	112.64
3	D	602	UFP	C5-C4-N3	6.76	118.82	112.64
3	A	602	UFP	C5-C4-N3	6.67	118.74	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	UFP	O4-C4-C5	-6.20	120.41	125.69
3	E	602	UFP	O4-C4-C5	-6.09	120.50	125.69
3	B	602	UFP	O4-C4-C5	-6.03	120.56	125.69
3	A	602	UFP	O4-C4-C5	-5.92	120.65	125.69
3	C	602	UFP	O4-C4-C5	-5.82	120.73	125.69
3	A	602	UFP	F5-C5-C4	5.74	121.50	116.47
5	A	604	MTX	N1-C2-N3	-5.56	120.15	127.21
2	C	601	NDP	C5A-C4A-N3A	-5.54	119.08	126.72
2	D	601	NDP	C5A-C4A-N3A	-5.53	119.10	126.72
3	C	602	UFP	F5-C5-C4	5.52	121.31	116.47
2	E	601	NDP	C5A-C4A-N3A	-5.52	119.12	126.72
5	B	604	MTX	N1-C2-N3	-5.40	120.35	127.21
2	B	601	NDP	C5A-C4A-N3A	-5.38	119.31	126.72
5	E	604	MTX	N1-C2-N3	-5.35	120.41	127.21
5	C	604	MTX	N1-C2-N3	-5.33	120.43	127.21
2	A	601	NDP	C5A-C4A-N3A	-5.33	119.37	126.72
5	D	604	MTX	N1-C2-N3	-5.32	120.45	127.21
3	E	602	UFP	F5-C5-C4	5.07	120.91	116.47
3	A	602	UFP	C1'-N1-C2	5.03	127.50	117.66
3	B	602	UFP	F5-C5-C4	4.88	120.75	116.47
3	D	602	UFP	F5-C5-C4	4.88	120.74	116.47
3	C	602	UFP	C1'-N1-C2	4.66	126.77	117.66
3	D	602	UFP	C1'-N1-C2	4.61	126.67	117.66
3	C	602	UFP	C4-N3-C2	-4.54	121.39	127.34
3	B	602	UFP	C1'-N1-C2	4.52	126.49	117.66
3	E	602	UFP	C4-N3-C2	-4.50	121.44	127.34
3	E	602	UFP	C1'-N1-C2	4.49	126.44	117.66
3	B	602	UFP	N3-C2-N1	4.49	120.74	114.89
3	B	602	UFP	C4-N3-C2	-4.48	121.46	127.34
3	A	602	UFP	C4-N3-C2	-4.47	121.47	127.34
3	D	602	UFP	C4-N3-C2	-4.44	121.52	127.34
3	E	602	UFP	N3-C2-N1	4.33	120.53	114.89
3	D	602	UFP	N3-C2-N1	4.32	120.52	114.89
3	C	602	UFP	N3-C2-N1	4.27	120.45	114.89
3	A	602	UFP	C1'-N1-C6	-4.26	113.59	120.74
3	A	602	UFP	N3-C2-N1	4.25	120.42	114.89
3	E	602	UFP	C6-C5-C4	-4.21	118.73	122.57
3	A	602	UFP	C6-C5-C4	-4.16	118.77	122.57
3	D	602	UFP	C6-C5-C4	-4.16	118.77	122.57
3	C	602	UFP	C6-C5-C4	-4.14	118.79	122.57
3	B	602	UFP	C6-C5-C4	-4.14	118.80	122.57
4	C	603	OG7	C03-C02-C05	4.01	135.57	129.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	OG7	C03-C02-C05	3.98	135.53	129.16
5	A	604	MTX	C2-N1-C8A	3.91	119.70	115.48
3	C	602	UFP	C1'-N1-C6	-3.91	114.18	120.74
4	A	603	OG7	C15-C16-C21	3.90	126.07	121.72
4	E	603	OG7	C03-C02-C05	3.88	135.37	129.16
2	D	601	NDP	N3A-C2A-N1A	-3.86	122.73	128.58
4	B	603	OG7	C03-C02-C05	3.86	135.34	129.16
2	B	601	NDP	N3A-C2A-N1A	-3.85	122.76	128.58
4	D	603	OG7	C03-C02-C05	3.85	135.31	129.16
5	B	604	MTX	C2-N1-C8A	3.83	119.62	115.48
2	D	601	NDP	N3A-C4A-N9A	3.83	133.68	127.17
2	B	601	NDP	N3A-C4A-N9A	3.83	133.67	127.17
2	E	601	NDP	N3A-C2A-N1A	-3.79	122.84	128.58
2	C	601	NDP	N3A-C4A-N9A	3.79	133.61	127.17
2	C	601	NDP	N3A-C2A-N1A	-3.78	122.85	128.58
2	A	601	NDP	N3A-C2A-N1A	-3.76	122.89	128.58
3	D	602	UFP	C1'-N1-C6	-3.72	114.49	120.74
2	E	601	NDP	N3A-C4A-N9A	3.71	133.48	127.17
4	B	603	OG7	C02-C01-N01	-3.68	120.48	123.46
4	D	603	OG7	C02-C01-N01	-3.62	120.54	123.46
5	E	604	MTX	C2-N1-C8A	3.62	119.38	115.48
3	E	602	UFP	C1'-N1-C6	-3.60	114.69	120.74
5	D	604	MTX	C13-C12-C11	-3.59	116.97	120.80
2	A	601	NDP	N3A-C4A-N9A	3.58	133.26	127.17
5	E	604	MTX	CM-N10-C9	3.58	124.44	115.11
5	D	604	MTX	C2-N1-C8A	3.58	119.34	115.48
5	C	604	MTX	C2-N1-C8A	3.54	119.31	115.48
5	B	604	MTX	CM-N10-C9	3.54	124.31	115.11
5	E	604	MTX	C13-C12-C11	-3.53	117.03	120.80
4	C	603	OG7	C02-C01-N01	-3.49	120.64	123.46
3	B	602	UFP	O4'-C1'-C2'	-3.49	99.73	106.25
4	A	603	OG7	C02-C01-N01	-3.48	120.64	123.46
5	D	604	MTX	C9-C6-C7	3.47	127.70	121.38
3	B	602	UFP	C1'-N1-C6	-3.47	114.91	120.74
2	D	601	NDP	C2A-N3A-C4A	3.45	120.25	111.83
2	C	601	NDP	C2A-N3A-C4A	3.43	120.21	111.83
4	E	603	OG7	C02-C01-N01	-3.43	120.69	123.46
2	E	601	NDP	C2A-N3A-C4A	3.43	120.20	111.83
5	C	604	MTX	C13-C12-C11	-3.41	117.15	120.80
5	C	604	MTX	CM-N10-C9	3.41	123.98	115.11
4	D	603	OG7	C15-C16-C21	3.37	125.48	121.72
2	B	601	NDP	C2A-N3A-C4A	3.37	120.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604	MTX	C13-C12-C11	-3.35	117.22	120.80
2	A	601	NDP	C2A-N3A-C4A	3.34	119.99	111.83
5	A	604	MTX	CM-N10-C9	3.33	123.77	115.11
5	D	604	MTX	CM-N10-C9	3.29	123.68	115.11
4	B	603	OG7	C15-C16-C21	3.29	125.38	121.72
3	B	602	UFP	O2-C2-N3	-3.27	115.45	121.49
4	E	603	OG7	C15-C16-C21	3.23	125.31	121.72
2	B	601	NDP	N9A-C8A-N7A	-3.21	109.38	113.94
4	C	603	OG7	C15-C16-C21	3.19	125.28	121.72
2	A	601	NDP	N9A-C8A-N7A	-3.18	109.43	113.94
5	C	604	MTX	C9-C6-C7	3.16	127.14	121.38
2	D	601	NDP	N9A-C8A-N7A	-3.15	109.46	113.94
5	B	604	MTX	C9-N10-C14	-3.15	116.35	120.17
2	E	601	NDP	C4A-C5A-N7A	-3.15	106.99	110.58
2	C	601	NDP	C4A-C5A-N7A	-3.14	106.99	110.58
5	A	604	MTX	C13-C12-C11	-3.13	117.46	120.80
5	E	604	MTX	C9-N10-C14	-3.12	116.38	120.17
2	A	601	NDP	C4A-C5A-N7A	-3.12	107.02	110.58
2	E	601	NDP	N9A-C8A-N7A	-3.11	109.52	113.94
2	C	601	NDP	N9A-C8A-N7A	-3.11	109.52	113.94
5	C	604	MTX	C12-C13-C14	3.10	124.23	120.30
3	D	602	UFP	O2-C2-N3	-3.10	115.77	121.49
5	B	604	MTX	C9-C6-C7	3.09	127.00	121.38
3	C	602	UFP	O2-C2-N3	-3.06	115.84	121.49
2	C	601	NDP	C5A-N7A-C8A	3.06	108.26	103.45
2	E	601	NDP	C5A-N7A-C8A	3.05	108.25	103.45
3	A	602	UFP	O2-C2-N3	-3.05	115.86	121.49
2	D	601	NDP	C5A-N7A-C8A	3.04	108.22	103.45
2	A	601	NDP	C5A-N7A-C8A	3.03	108.21	103.45
5	E	604	MTX	C12-C13-C14	3.02	124.13	120.30
5	D	604	MTX	C9-C6-N5	-3.02	112.19	117.09
2	D	601	NDP	C4A-C5A-N7A	-3.02	107.13	110.58
5	E	604	MTX	C9-C6-C7	3.00	126.85	121.38
2	B	601	NDP	C5A-N7A-C8A	3.00	108.16	103.45
5	A	604	MTX	C9-C6-C7	2.98	126.80	121.38
5	D	604	MTX	C12-C13-C14	2.98	124.07	120.30
5	A	604	MTX	C12-C13-C14	2.96	124.05	120.30
3	E	602	UFP	O2-C2-N3	-2.92	116.10	121.49
2	B	601	NDP	C4A-C5A-N7A	-2.92	107.25	110.58
4	A	603	OG7	C15-N05-C14	2.85	134.83	126.90
5	B	604	MTX	C12-C13-C14	2.83	123.88	120.30
3	B	602	UFP	C6-N1-C2	-2.72	118.59	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	MTX	C9-N10-C14	-2.72	116.87	120.17
5	C	604	MTX	N8-C8A-N1	2.69	118.69	115.77
5	B	604	MTX	C9-C6-N5	-2.66	112.77	117.09
5	C	604	MTX	C9-N10-C14	-2.65	116.96	120.17
5	C	604	MTX	C9-C6-N5	-2.61	112.86	117.09
2	C	601	NDP	O5D-C5D-C4D	2.56	117.72	108.99
5	D	604	MTX	N8-C8A-N1	2.55	118.54	115.77
5	B	604	MTX	NA2-C2-N3	2.51	120.99	117.22
2	C	601	NDP	O5B-C5B-C4B	2.51	117.53	108.99
5	C	604	MTX	NA4-C4-N3	2.48	123.78	117.11
3	D	602	UFP	C6-N1-C2	-2.47	118.84	121.30
5	D	604	MTX	C11-C-N	-2.47	112.45	117.04
5	A	604	MTX	C9-C6-N5	-2.47	113.09	117.09
2	D	601	NDP	O5B-C5B-C4B	2.47	117.39	108.99
5	E	604	MTX	NA4-C4-N3	2.46	123.73	117.11
5	E	604	MTX	N8-C8A-N1	2.45	118.44	115.77
5	D	604	MTX	C15-C14-N10	-2.45	118.17	121.59
5	E	604	MTX	C11-C-N	-2.45	112.50	117.04
3	E	602	UFP	C6-N1-C2	-2.45	118.87	121.30
4	E	603	OG7	C15-N05-C14	2.44	133.69	126.90
2	A	601	NDP	C2B-C1B-N9A	-2.43	109.75	113.75
5	E	604	MTX	C9-C6-N5	-2.42	113.17	117.09
4	A	603	OG7	C16-C15-N05	2.42	123.06	118.70
2	D	601	NDP	O5D-C5D-C4D	2.41	117.19	108.99
5	E	604	MTX	NA2-C2-N3	2.41	120.83	117.22
5	A	604	MTX	NA2-C2-N3	2.40	120.83	117.22
3	A	602	UFP	C6-N1-C2	-2.40	118.91	121.30
2	B	601	NDP	C2B-C1B-N9A	-2.40	109.81	113.75
5	B	604	MTX	NA4-C4-N3	2.39	123.54	117.11
2	E	601	NDP	O5D-C5D-C4D	2.38	117.10	108.99
5	B	604	MTX	N8-C8A-N1	2.38	118.36	115.77
5	A	604	MTX	N8-C8A-N1	2.38	118.36	115.77
3	C	602	UFP	O4'-C1'-C2'	-2.37	101.82	106.25
5	D	604	MTX	NA4-C4-N3	2.35	123.42	117.11
2	B	601	NDP	C4A-N9A-C8A	2.34	108.20	105.74
2	B	601	NDP	O5D-C5D-C4D	2.33	116.92	108.99
2	A	601	NDP	O5B-C5B-C4B	2.30	116.82	108.99
4	D	603	OG7	C15-N05-C14	2.30	133.29	126.90
4	B	603	OG7	C15-N05-C14	2.30	133.29	126.90
2	E	601	NDP	O5B-C5B-C4B	2.29	116.80	108.99
3	C	602	UFP	C6-N1-C2	-2.26	119.05	121.30
5	D	604	MTX	C13-C14-N10	2.26	124.74	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	604	MTX	NA2-C2-N3	2.24	120.59	117.22
5	A	604	MTX	NA4-C4-N3	2.23	123.11	117.11
5	A	604	MTX	C2-N3-C4	2.23	123.08	116.72
5	C	604	MTX	NA2-C2-N3	2.22	120.55	117.22
2	A	601	NDP	O5D-C5D-C4D	2.22	116.55	108.99
5	D	604	MTX	C4A-C4-N3	-2.19	118.25	120.84
5	D	604	MTX	C2-N3-C4	2.17	122.93	116.72
5	A	604	MTX	C11-C-N	-2.17	113.01	117.04
2	B	601	NDP	O4D-C1D-N1N	2.17	112.22	108.08
5	C	604	MTX	C2-N3-C4	2.16	122.89	116.72
5	B	604	MTX	C2-N3-C4	2.15	122.87	116.72
5	B	604	MTX	C4A-C4-N3	-2.15	118.30	120.84
5	E	604	MTX	C2-N3-C4	2.15	122.84	116.72
4	C	603	OG7	C15-N05-C14	2.15	132.87	126.90
5	E	604	MTX	C4A-C4-N3	-2.14	118.31	120.84
2	A	601	NDP	C4A-N9A-C8A	2.14	107.98	105.74
3	D	602	UFP	O4'-C1'-C2'	-2.13	102.27	106.25
5	C	604	MTX	C4A-C4-N3	-2.12	118.33	120.84
2	D	601	NDP	C4A-N9A-C8A	2.12	107.97	105.74
2	C	601	NDP	C2B-C1B-N9A	-2.12	110.27	113.75
5	B	604	MTX	C11-C-N	-2.12	113.12	117.04
2	B	601	NDP	O4B-C1B-N9A	2.11	112.15	108.09
5	A	604	MTX	C4A-C4-N3	-2.11	118.35	120.84
4	B	603	OG7	C16-C15-N05	2.10	122.49	118.70
2	B	601	NDP	O5B-C5B-C4B	2.09	116.12	108.99
2	C	601	NDP	C3N-C7N-N7N	2.09	121.38	117.67
2	C	601	NDP	C4A-N9A-C8A	2.08	107.92	105.74
5	E	604	MTX	C15-C14-N10	-2.07	118.70	121.59
5	C	604	MTX	C11-C-N	-2.02	113.29	117.04
4	C	603	OG7	C16-C15-N05	2.02	122.33	118.70
2	E	601	NDP	C4A-N9A-C8A	2.01	107.85	105.74
2	E	601	NDP	C3N-C7N-N7N	2.00	121.23	117.67
3	A	602	UFP	O4'-C1'-C2'	-2.00	102.50	106.25

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	UFP	C5'-O5'-P-O2P
3	A	602	UFP	C5'-O5'-P-O3P
3	B	602	UFP	C5'-O5'-P-O3P
3	C	602	UFP	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
3	C	602	UFP	C5'-O5'-P-O3P
3	D	602	UFP	C5'-O5'-P-O2P
3	D	602	UFP	C5'-O5'-P-O3P
3	E	602	UFP	C5'-O5'-P-O2P
3	E	602	UFP	C5'-O5'-P-O3P
5	C	604	MTX	N-CA-CB-CG
5	D	604	MTX	N-CA-CB-CG
5	E	604	MTX	N-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-CB-CG
5	E	604	MTX	CT-CA-CB-CG
3	E	602	UFP	O4'-C4'-C5'-O5'
3	B	602	UFP	C2'-C1'-N1-C2
3	A	602	UFP	C2'-C1'-N1-C2
3	D	602	UFP	C2'-C1'-N1-C2
5	C	604	MTX	CT-CA-CB-CG
2	D	601	NDP	C3D-C4D-C5D-O5D
3	A	602	UFP	O4'-C4'-C5'-O5'
3	A	602	UFP	C2'-C1'-N1-C6
3	B	602	UFP	C2'-C1'-N1-C6
3	D	602	UFP	O4'-C4'-C5'-O5'
3	C	602	UFP	C2'-C1'-N1-C2
3	E	602	UFP	C2'-C1'-N1-C2
3	D	602	UFP	C2'-C1'-N1-C6
2	E	601	NDP	C3D-C4D-C5D-O5D
3	C	602	UFP	O4'-C4'-C5'-O5'
3	B	602	UFP	C5'-O5'-P-O1P
2	D	601	NDP	O4D-C4D-C5D-O5D
3	E	602	UFP	C3'-C4'-C5'-O5'
3	C	602	UFP	C2'-C1'-N1-C6
3	E	602	UFP	C2'-C1'-N1-C6
3	B	602	UFP	C5'-O5'-P-O2P
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	C6-C9-N10-CM
2	E	601	NDP	O4D-C4D-C5D-O5D
3	C	602	UFP	C3'-C4'-C5'-O5'
4	C	603	OG7	C20-C15-N05-C14
4	D	603	OG7	C20-C15-N05-C14

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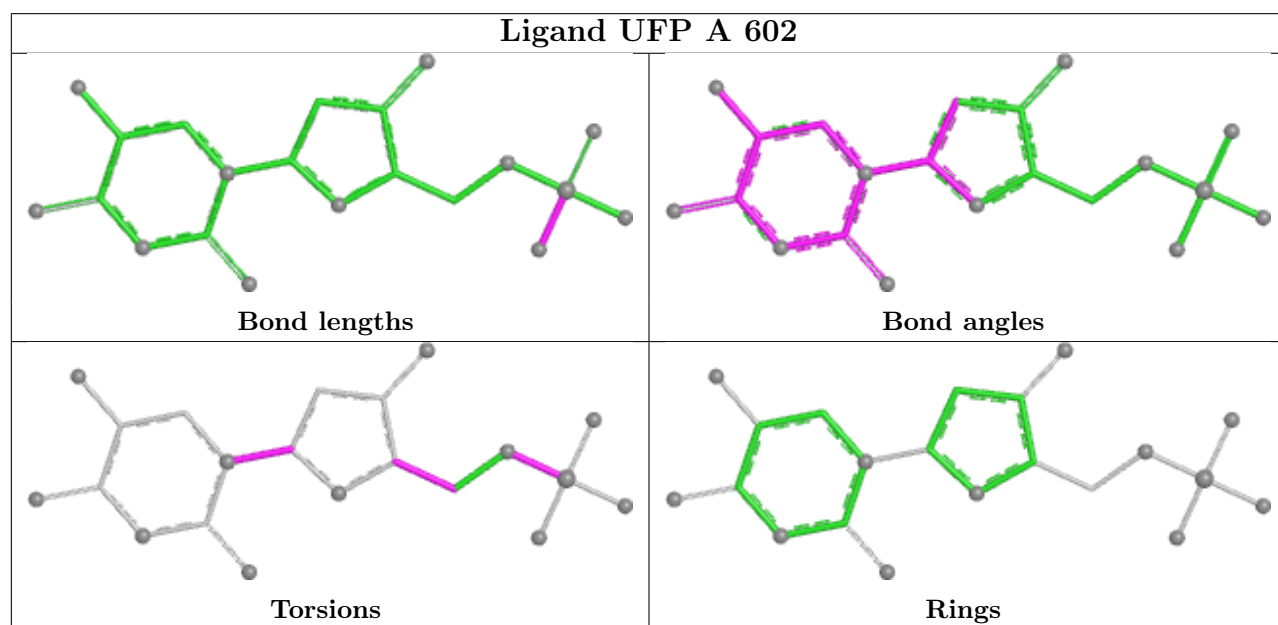
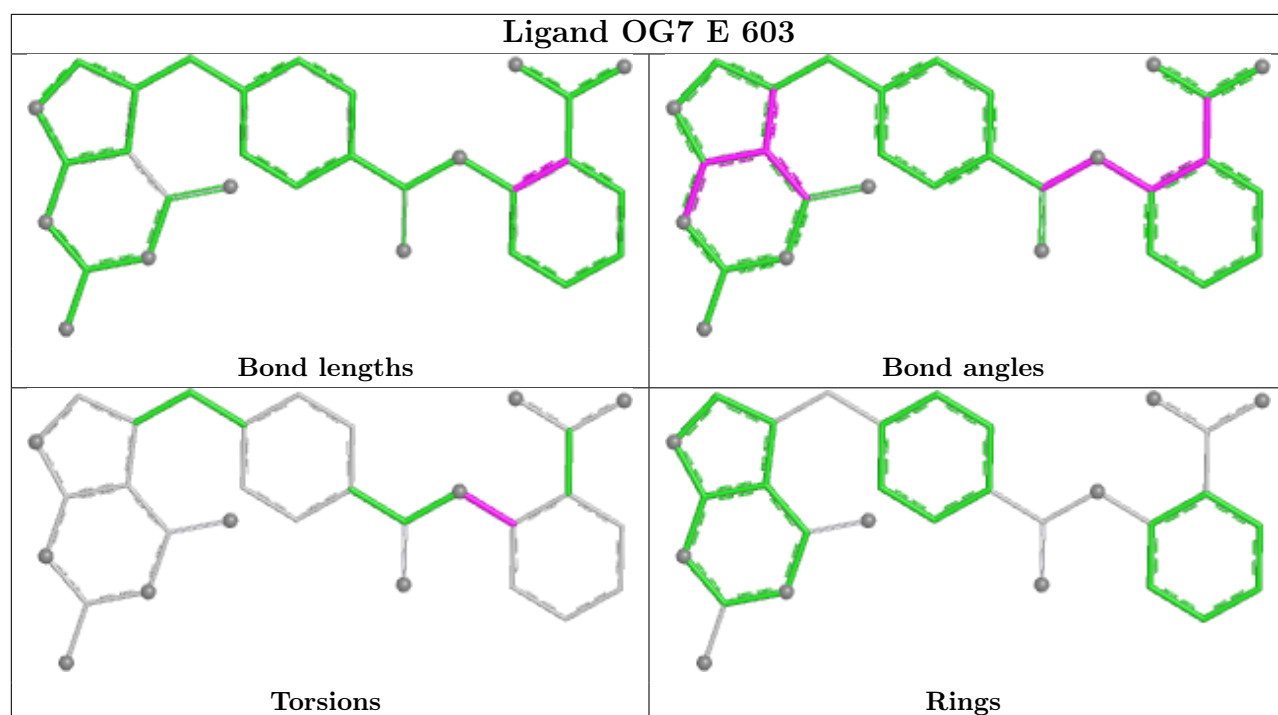
Mol	Chain	Res	Type	Atoms
4	B	603	OG7	C20-C15-N05-C14
5	D	604	MTX	C15-C14-N10-CM
4	E	603	OG7	C20-C15-N05-C14
4	A	603	OG7	C20-C15-N05-C14
5	D	604	MTX	C13-C14-N10-CM
5	E	604	MTX	C15-C14-N10-CM
2	C	601	NDP	O4D-C1D-N1N-C2N
2	E	601	NDP	O4D-C1D-N1N-C2N
4	A	603	OG7	C16-C15-N05-C14
2	A	601	NDP	O4D-C1D-N1N-C2N
2	B	601	NDP	O4D-C1D-N1N-C2N
2	D	601	NDP	O4D-C1D-N1N-C2N
4	B	603	OG7	C16-C15-N05-C14
4	E	603	OG7	C16-C15-N05-C14
4	C	603	OG7	C16-C15-N05-C14
4	D	603	OG7	C16-C15-N05-C14
5	A	604	MTX	C13-C14-N10-CM
5	B	604	MTX	C13-C14-N10-CM
5	C	604	MTX	C13-C14-N10-CM
5	E	604	MTX	C13-C14-N10-CM
5	A	604	MTX	C15-C14-N10-CM
5	C	604	MTX	C15-C14-N10-CM
2	D	601	NDP	C2D-C1D-N1N-C2N
2	C	601	NDP	C4D-C5D-O5D-PN
2	D	601	NDP	C4D-C5D-O5D-PN
2	E	601	NDP	C4D-C5D-O5D-PN
5	E	604	MTX	OE1-CD-CG-CB
5	C	604	MTX	OE1-CD-CG-CB
5	D	604	MTX	OE2-CD-CG-CB
5	D	604	MTX	OE1-CD-CG-CB
5	B	604	MTX	C15-C14-N10-CM
5	C	604	MTX	OE2-CD-CG-CB
2	A	601	NDP	C2D-C1D-N1N-C2N
2	B	601	NDP	C2D-C1D-N1N-C2N
2	C	601	NDP	C2D-C1D-N1N-C2N
5	E	604	MTX	OE2-CD-CG-CB
2	A	601	NDP	C4D-C5D-O5D-PN
5	B	604	MTX	OE2-CD-CG-CB
5	B	604	MTX	OE1-CD-CG-CB
2	B	601	NDP	C4D-C5D-O5D-PN
2	E	601	NDP	C3B-C4B-C5B-O5B

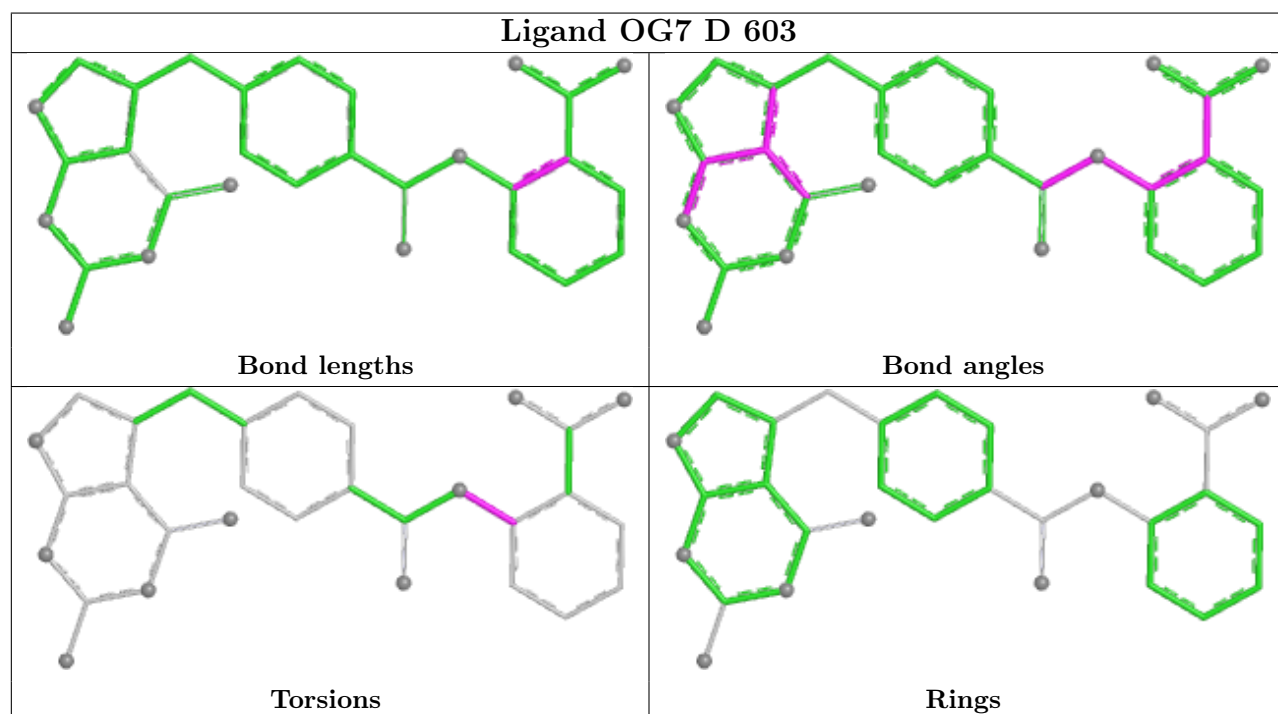
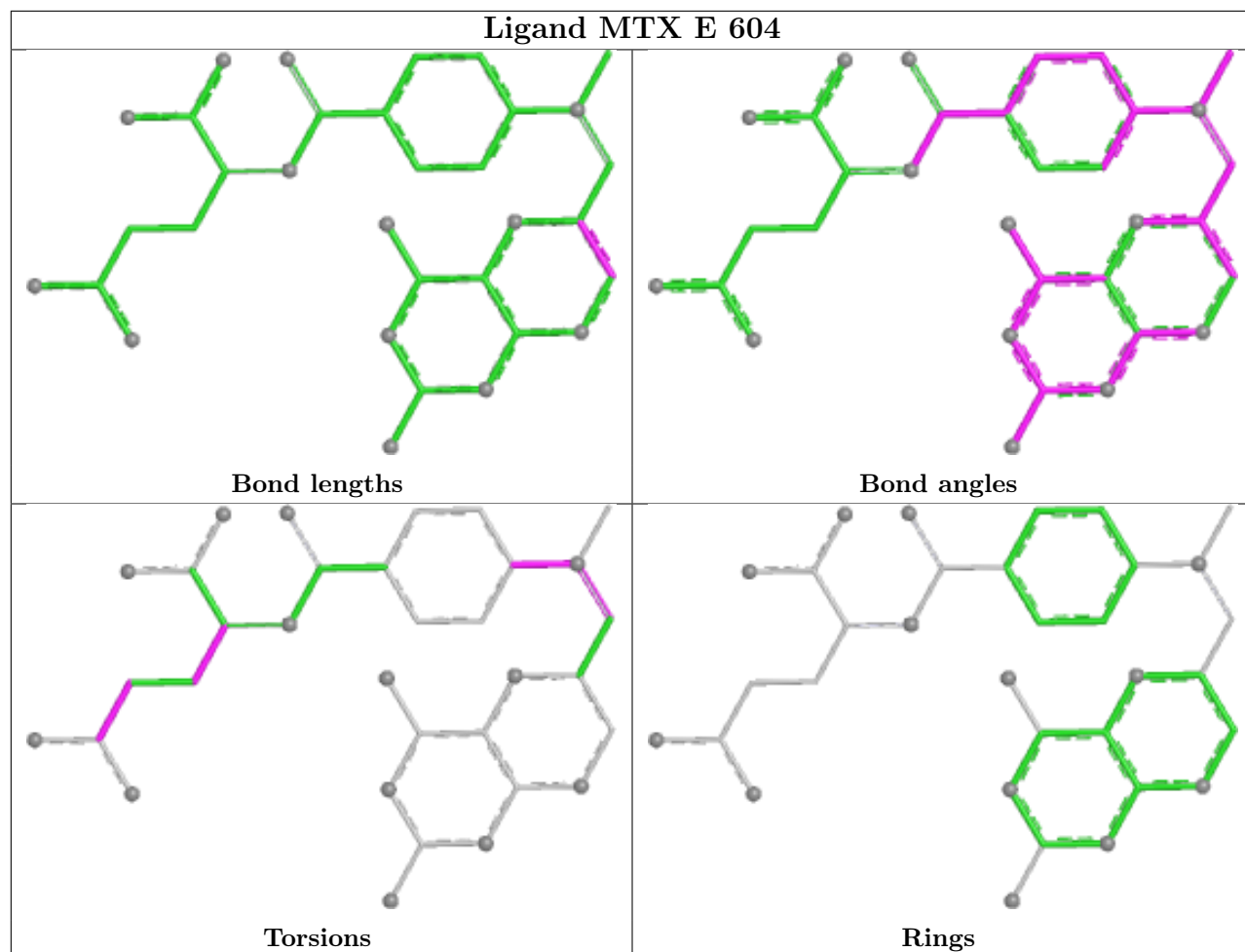
There are no ring outliers.

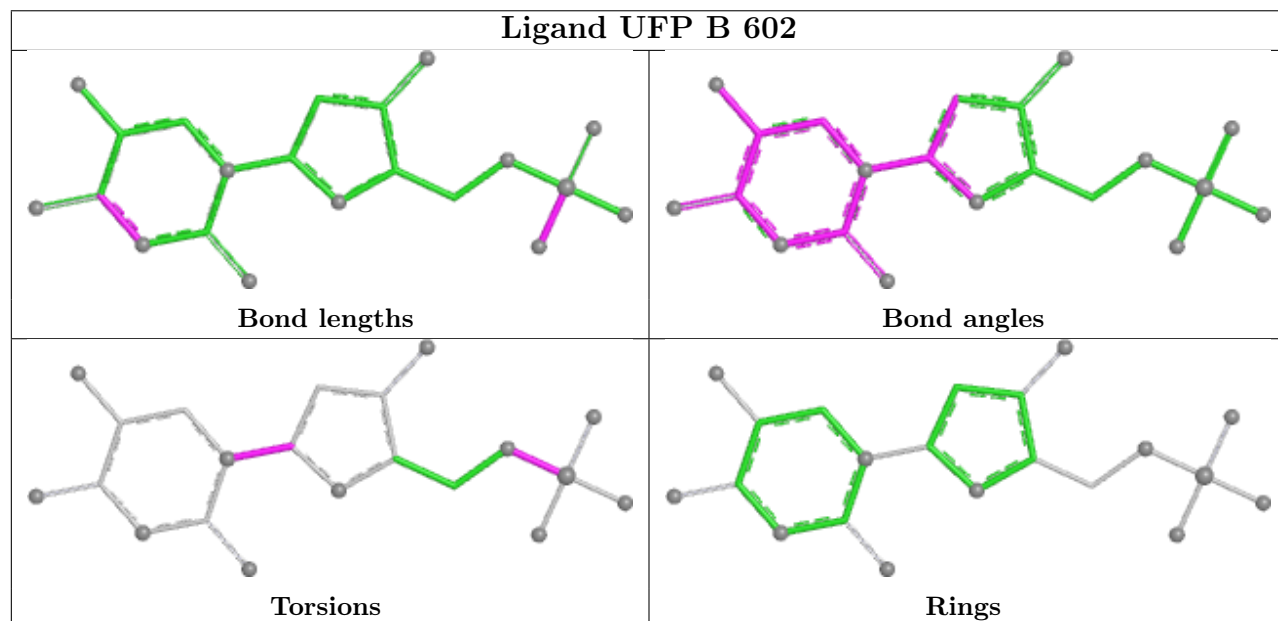
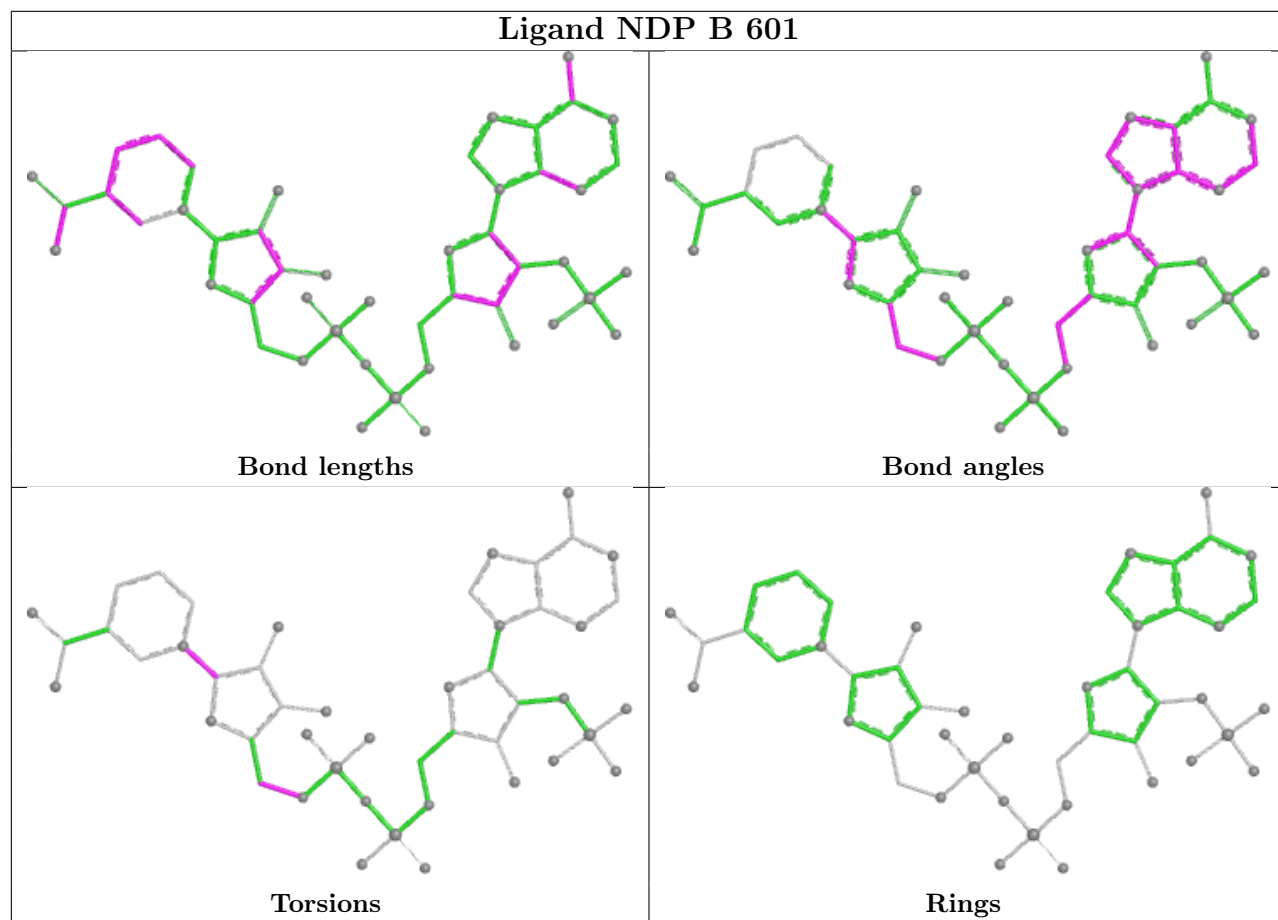
14 monomers are involved in 19 short contacts:

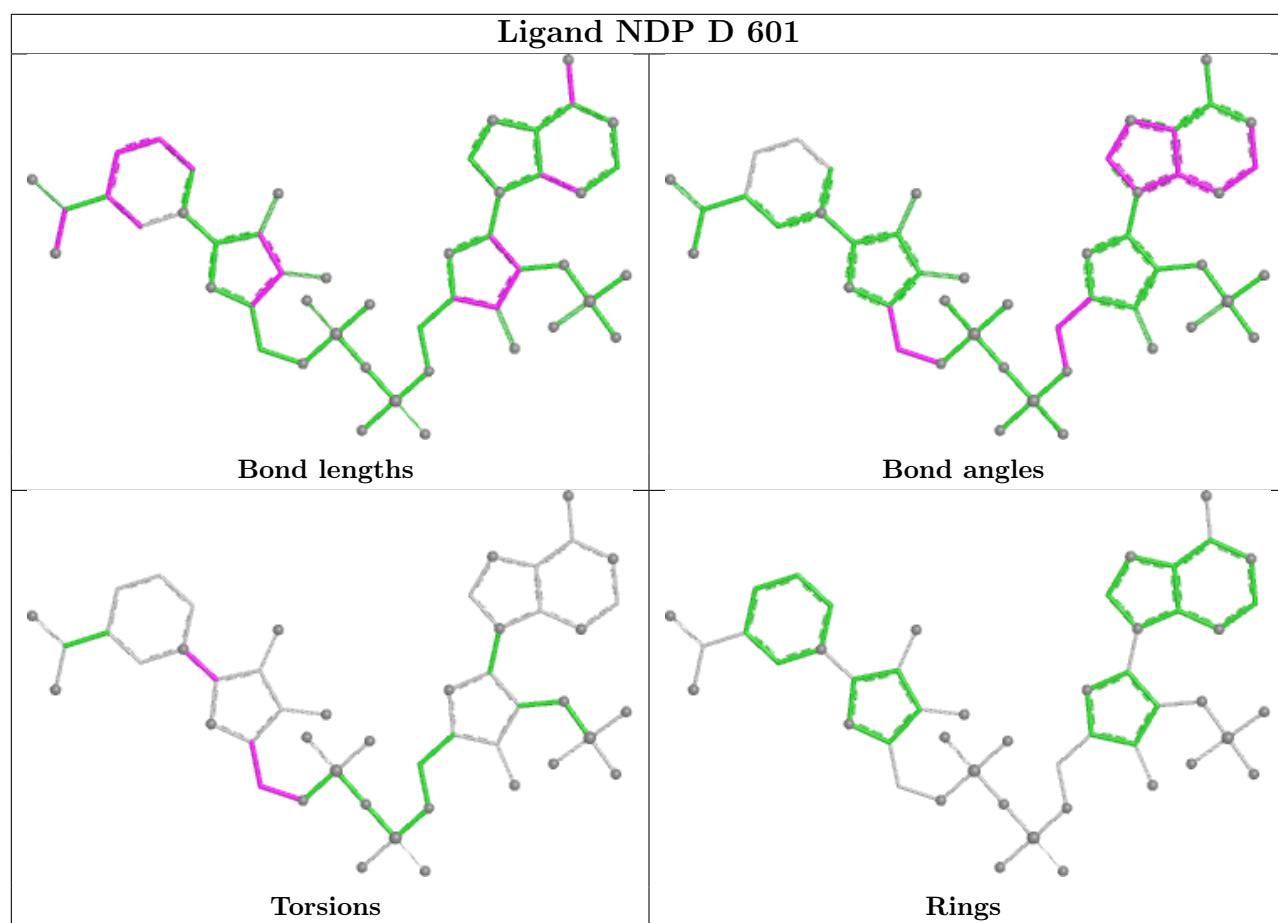
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	UFP	2	0
5	E	604	MTX	1	0
2	B	601	NDP	1	0
3	B	602	UFP	2	0
2	A	601	NDP	1	0
2	E	601	NDP	2	0
5	D	604	MTX	2	0
3	D	602	UFP	1	0
2	C	601	NDP	3	0
4	B	603	OG7	1	0
3	E	602	UFP	1	0
5	C	604	MTX	2	0
3	C	602	UFP	1	0
5	B	604	MTX	1	0

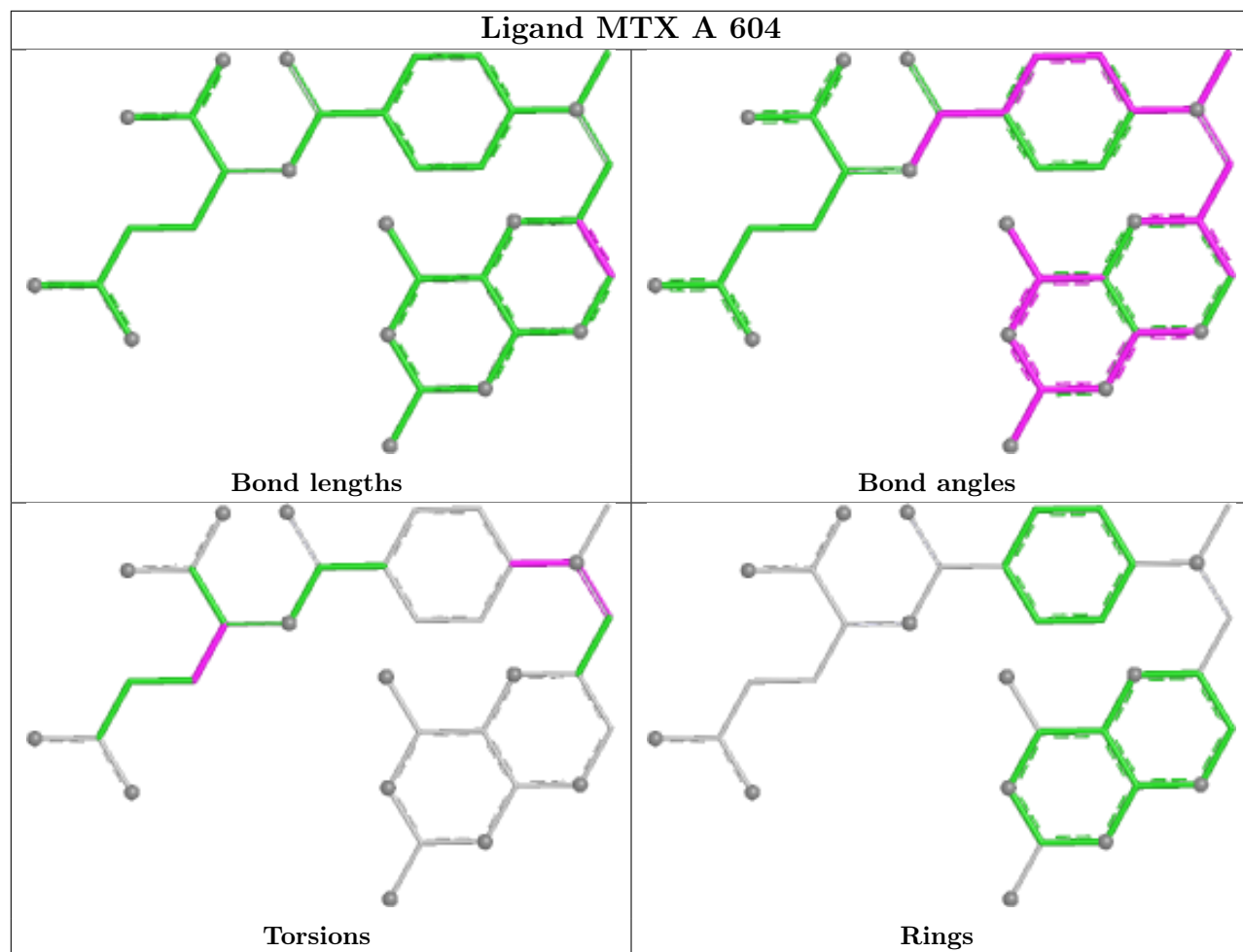
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

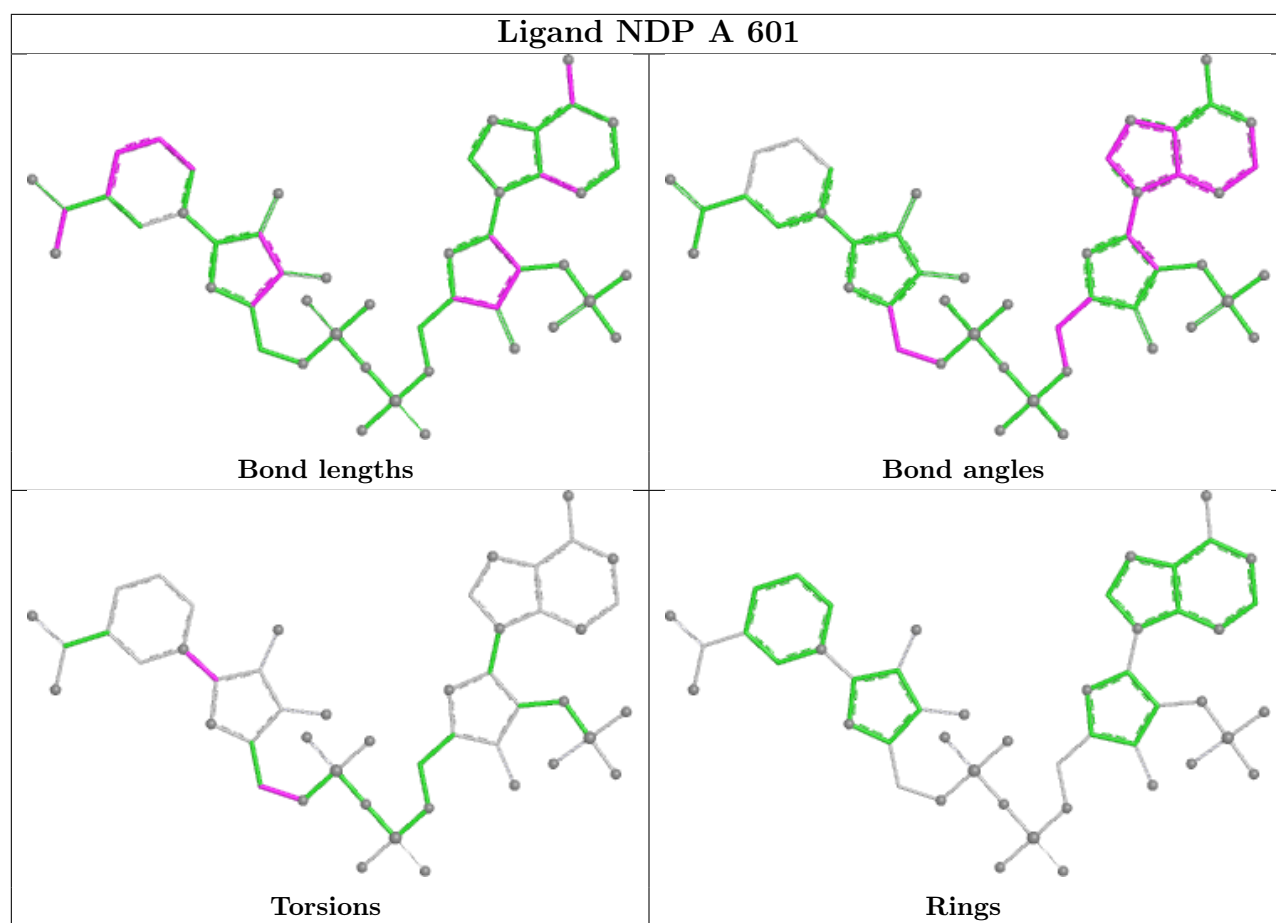


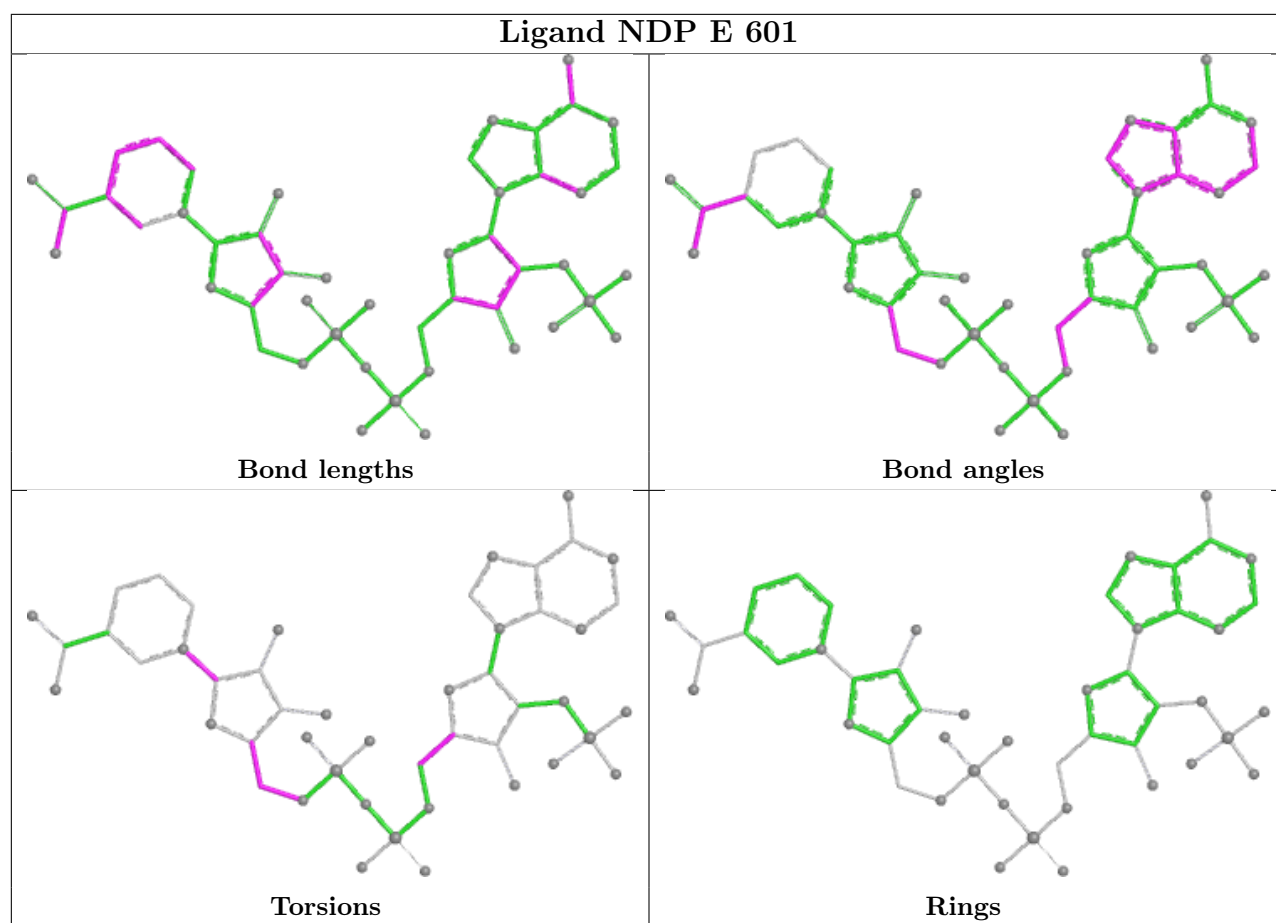


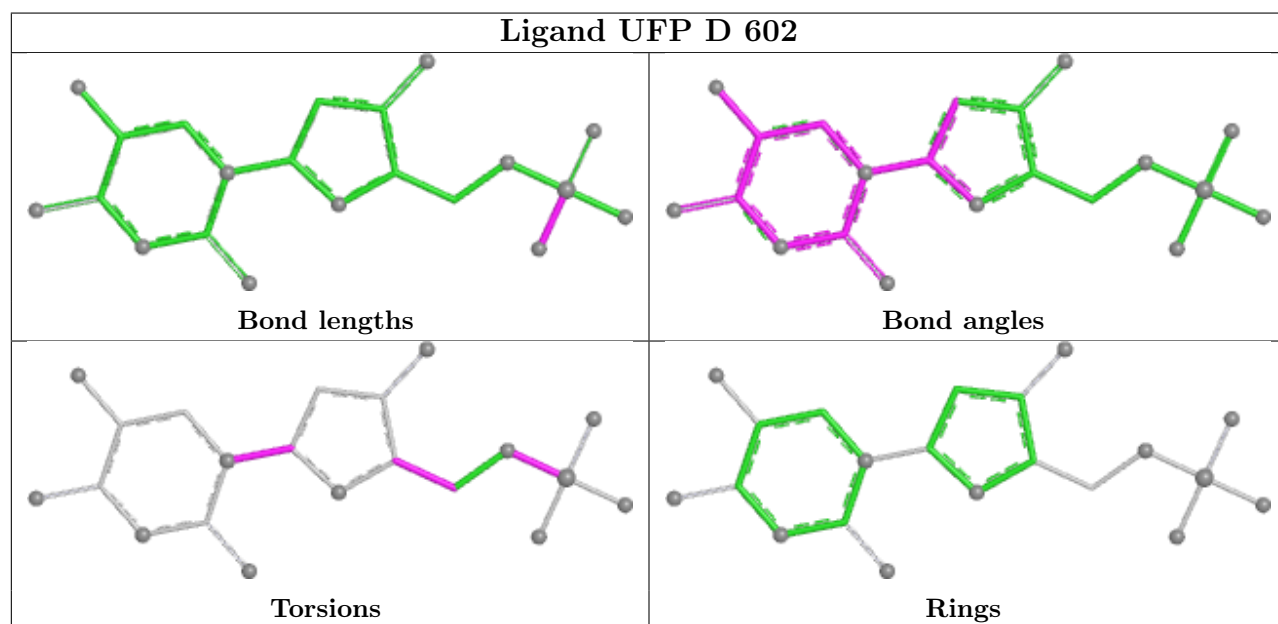
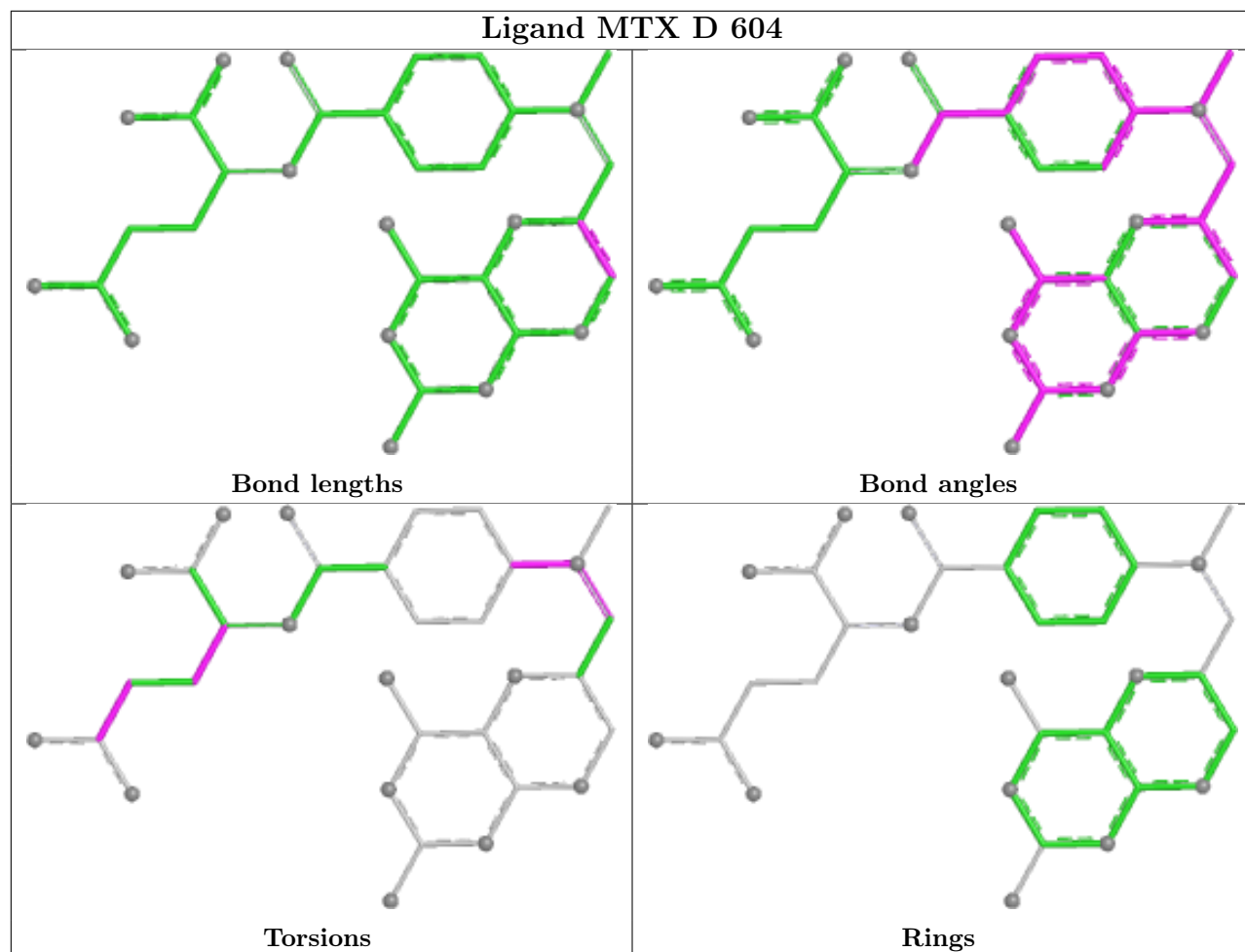


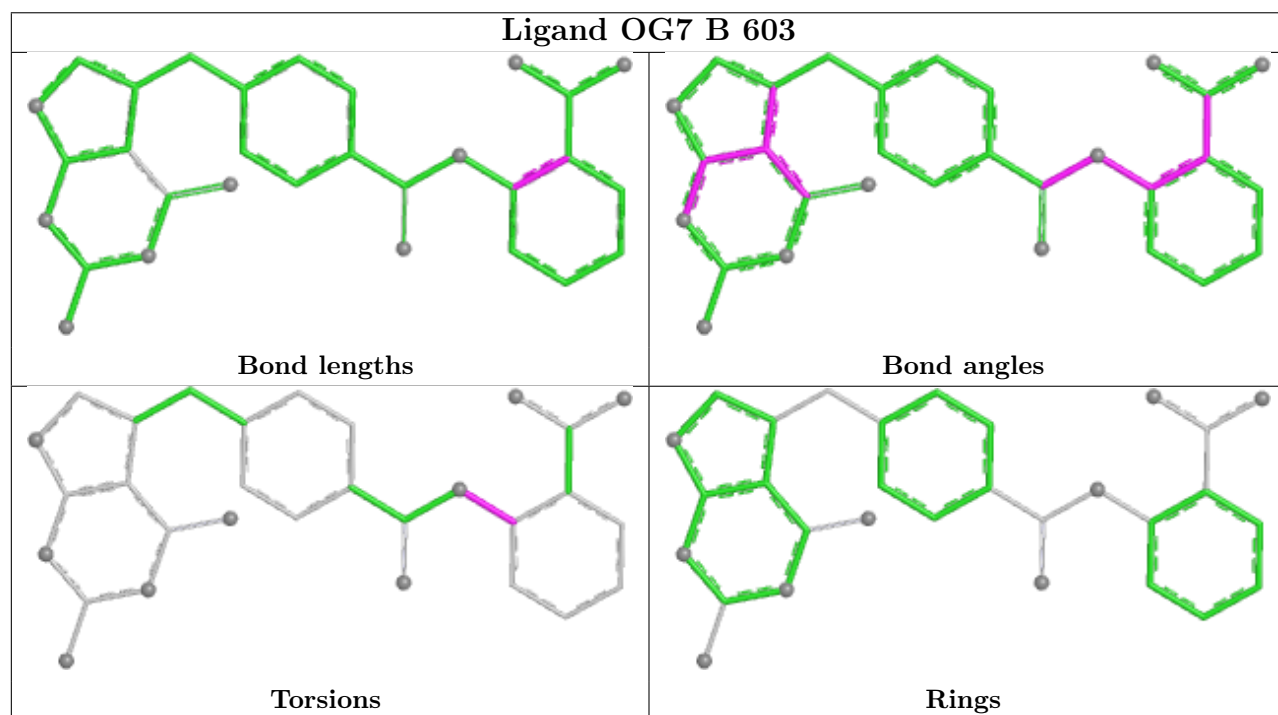
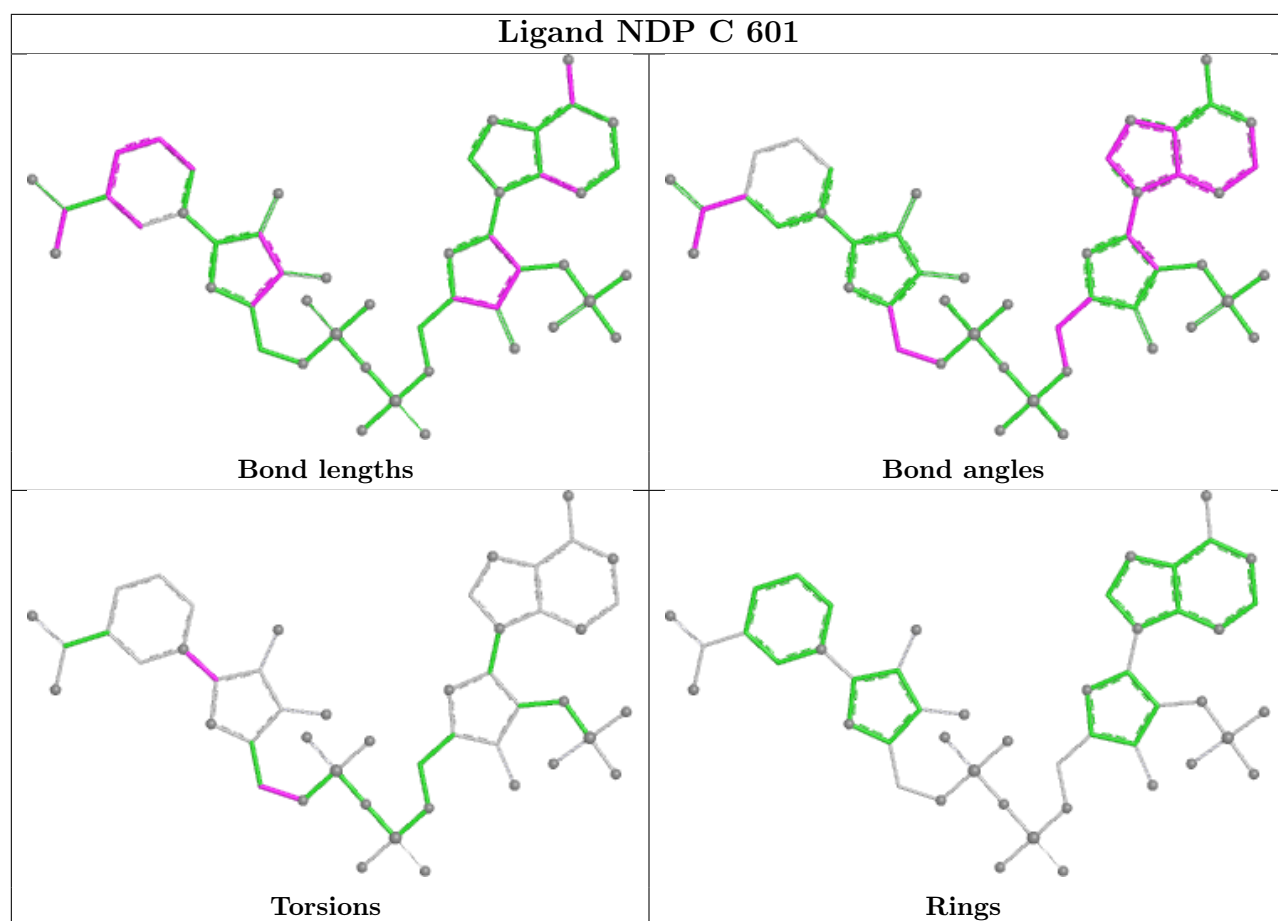




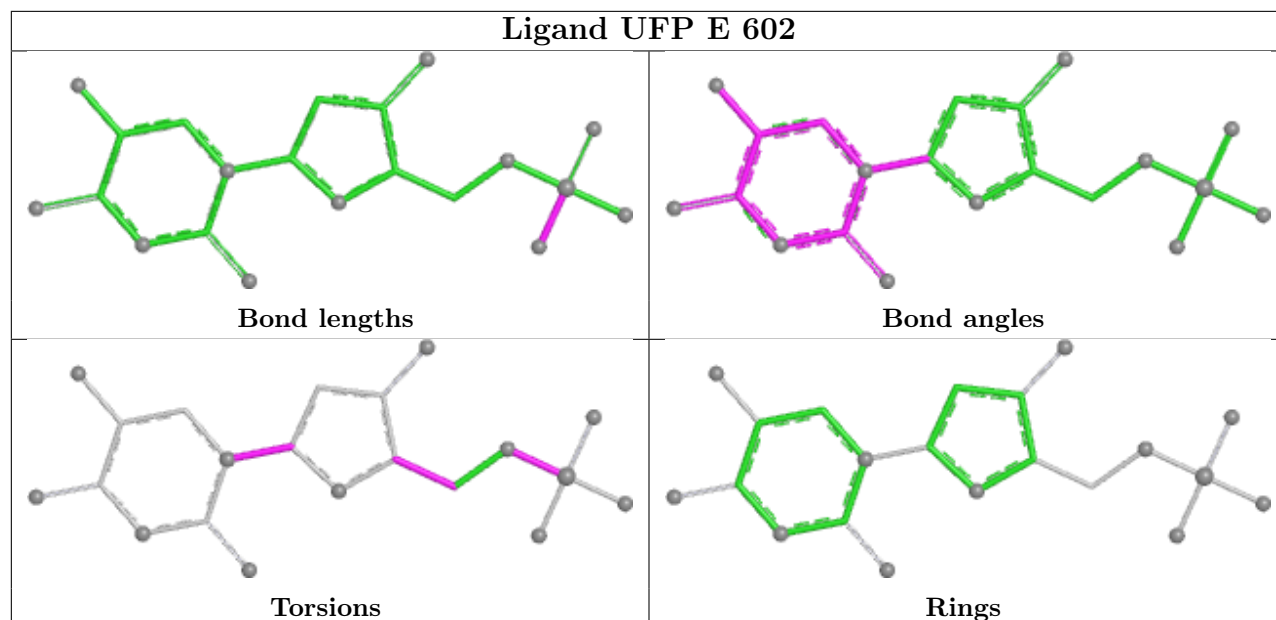




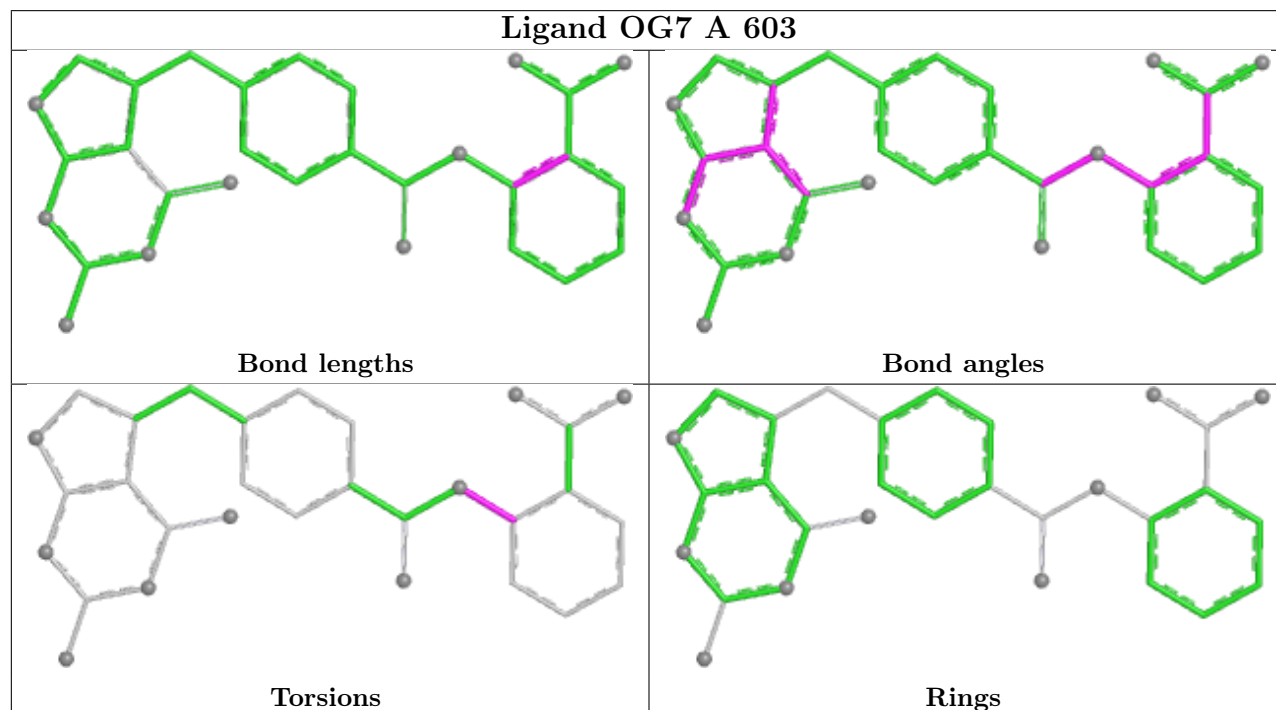


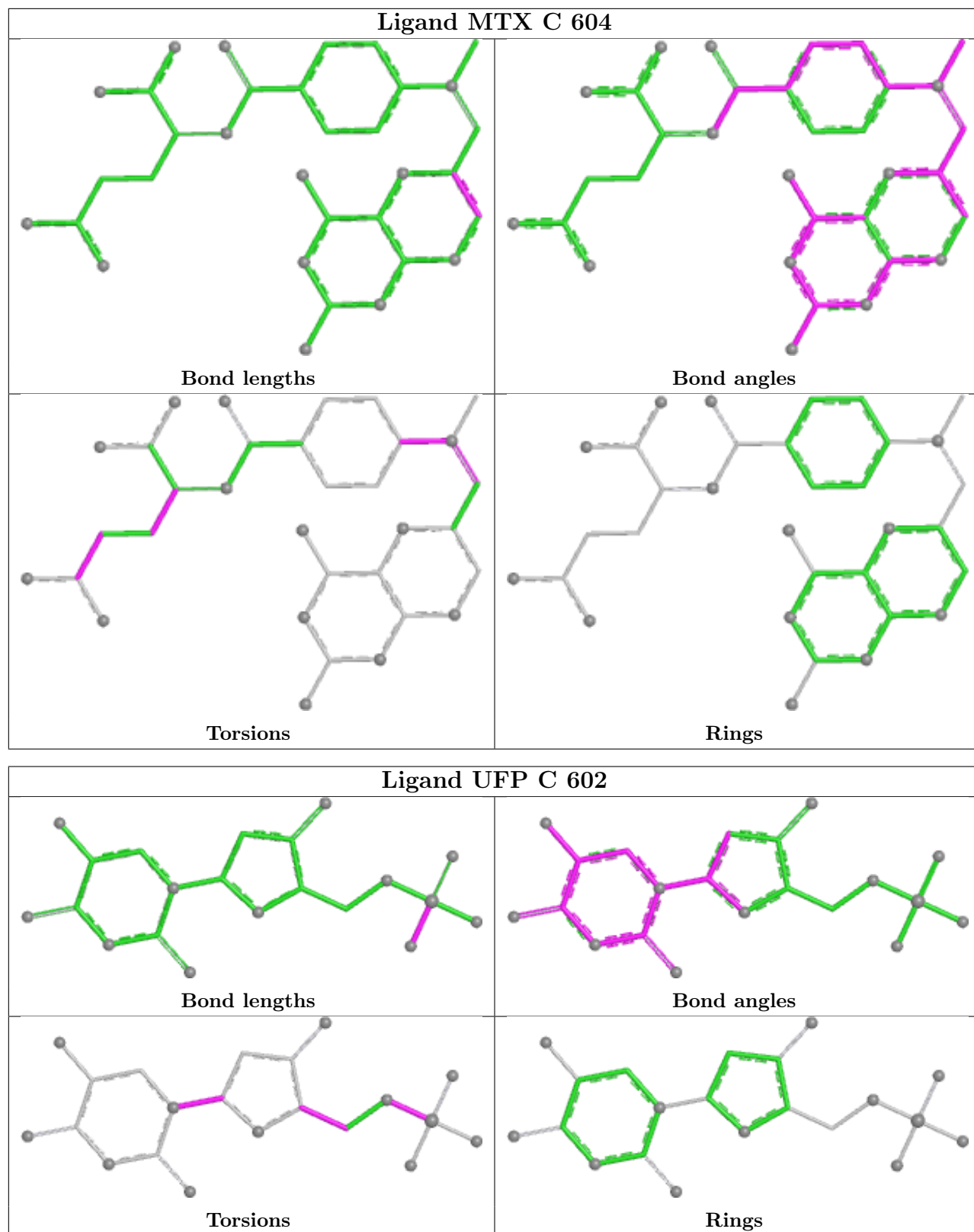


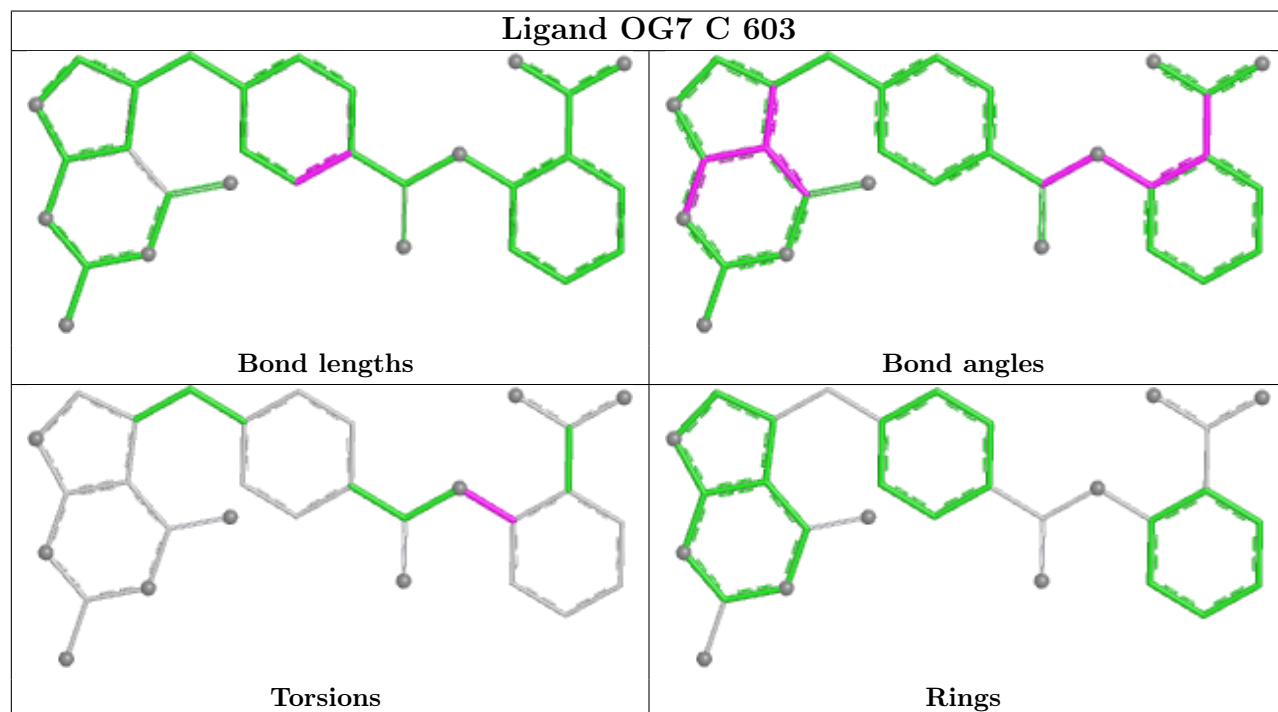
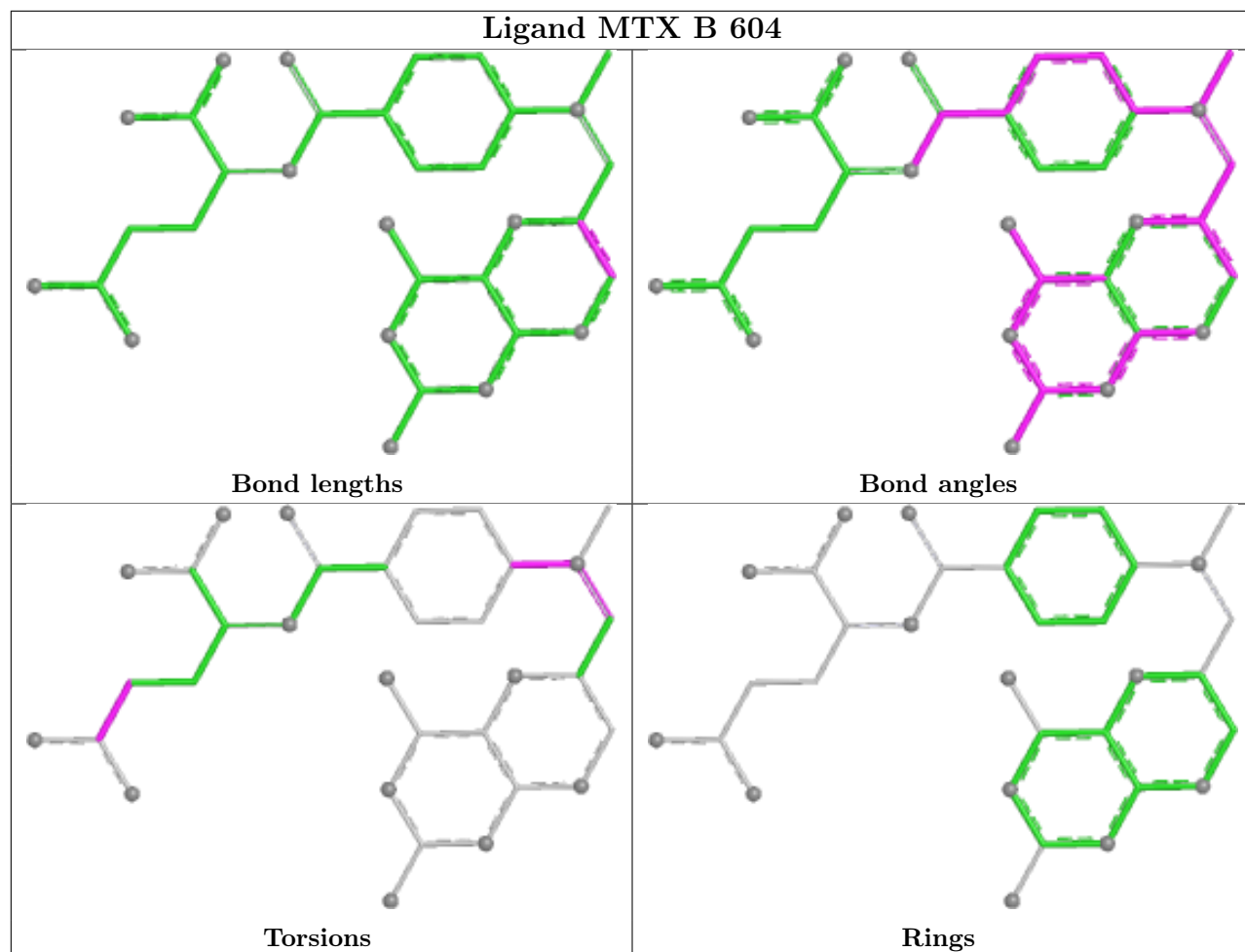
Ligand UFP E 602



Ligand OG7 A 603







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

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	507/521 (97%)	0.25	20 (3%)	43	34	42, 57, 85, 128	0
1	B	507/521 (97%)	0.43	28 (5%)	30	23	43, 61, 94, 141	0
1	C	508/521 (97%)	0.65	32 (6%)	26	19	46, 70, 111, 158	0
1	D	507/521 (97%)	0.64	28 (5%)	30	23	50, 72, 104, 137	0
1	E	508/521 (97%)	1.18	68 (13%)	7	5	74, 94, 129, 143	0
All	All	2537/2605 (97%)	0.63	176 (6%)	23	16	42, 70, 117, 158	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	MET	6.9
1	E	193	LEU	5.9
1	C	193	LEU	5.8
1	C	102	MET	5.7
1	A	193	LEU	5.6
1	D	193	LEU	5.6
1	D	194	LYS	5.4
1	D	3	GLU	5.3
1	A	104	ASP	5.2
1	A	194	LYS	4.9
1	C	194	LYS	4.8
1	A	102	MET	4.8
1	B	194	LYS	4.7
1	B	103	ASN	4.7
1	C	101	LEU	4.7
1	D	102	MET	4.7
1	E	102	MET	4.6
1	E	352	GLU	4.5
1	E	194	LYS	4.5
1	A	103	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	180	LYS	4.4
1	D	343	GLY	4.3
1	B	180	LYS	4.2
1	E	342	TYR	4.2
1	B	193	LEU	4.1
1	E	343	GLY	4.1
1	D	100	ASN	4.1
1	B	3	GLU	4.0
1	E	100	ASN	3.8
1	E	3	GLU	3.8
1	E	101	LEU	3.7
1	B	343	GLY	3.7
1	C	343	GLY	3.5
1	A	99	GLU	3.5
1	D	101	LEU	3.4
1	D	84	ALA	3.4
1	E	327	ARG	3.3
1	E	363	VAL	3.3
1	E	181	LYS	3.2
1	C	140	ASP	3.2
1	C	142	GLU	3.2
1	C	171	ASP	3.1
1	E	309	ILE	3.1
1	E	98	ILE	3.1
1	D	103	ASN	3.1
1	E	308	LEU	3.1
1	A	179	GLU	3.1
1	E	208	GLY	3.1
1	E	5	ASN	3.1
1	C	99	GLU	3.1
1	D	95	GLU	3.1
1	E	514	THR	3.0
1	C	342	TYR	3.0
1	C	363	VAL	3.0
1	E	326	GLU	3.0
1	B	101	LEU	3.0
1	C	95	GLU	3.0
1	B	5	ASN	3.0
1	A	101	LEU	2.9
1	B	326	GLU	2.9
1	C	3	GLU	2.8
1	E	316	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	175	PHE	2.8
1	E	179	GLU	2.8
1	E	84	ALA	2.8
1	D	363	VAL	2.8
1	E	209	ILE	2.8
1	B	140	ASP	2.8
1	B	99	GLU	2.8
1	E	521	VAL	2.8
1	D	171	ASP	2.8
1	E	287	ALA	2.8
1	C	181	LYS	2.7
1	E	103	ASN	2.7
1	C	83	GLU	2.7
1	D	83	GLU	2.7
1	D	326	GLU	2.7
1	E	323	GLU	2.7
1	A	343	GLY	2.7
1	C	208	GLY	2.7
1	A	342	TYR	2.6
1	A	83	GLU	2.6
1	E	300	LYS	2.6
1	C	49	LYS	2.6
1	A	84	ALA	2.6
1	B	521	VAL	2.6
1	B	314	TYR	2.6
1	E	319	ASN	2.6
1	A	140	ASP	2.6
1	C	98	ILE	2.6
1	C	179	GLU	2.6
1	A	114	GLY	2.6
1	B	114	GLY	2.6
1	A	100	ASN	2.6
1	C	84	ALA	2.6
1	B	179	GLU	2.5
1	E	279	PRO	2.5
1	E	346	TRP	2.5
1	E	257	ARG	2.5
1	B	342	TYR	2.5
1	B	208	GLY	2.5
1	A	180	LYS	2.5
1	E	288	ILE	2.5
1	E	519	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	98	ILE	2.5
1	E	338	LEU	2.5
1	E	490	LYS	2.4
1	D	514	THR	2.4
1	E	50	ASN	2.4
1	D	98	ILE	2.4
1	D	179	GLU	2.4
1	A	113	CYS	2.4
1	E	373	GLU	2.4
1	E	437	SER	2.4
1	D	361	THR	2.4
1	C	86	PRO	2.4
1	A	208	GLY	2.3
1	E	25	LEU	2.3
1	E	520	ALA	2.3
1	E	361	THR	2.3
1	E	149	GLU	2.3
1	E	502	GLU	2.3
1	B	113	CYS	2.3
1	E	260	ILE	2.3
1	E	324	TYR	2.3
1	C	112	VAL	2.3
1	E	231	PHE	2.3
1	E	322	LYS	2.3
1	E	224	TYR	2.3
1	B	340	PRO	2.3
1	B	520	ALA	2.2
1	E	290	SER	2.2
1	E	431	SER	2.2
1	B	331	GLY	2.2
1	E	89	VAL	2.2
1	B	84	ALA	2.2
1	D	342	TYR	2.2
1	D	42	ASN	2.2
1	E	360	TYR	2.2
1	E	396	GLN	2.2
1	A	115	GLY	2.2
1	D	208	GLY	2.2
1	E	267	GLY	2.2
1	E	429	LEU	2.2
1	C	149	GLU	2.2
1	C	4	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	79	LEU	2.2
1	E	259	GLY	2.2
1	D	209	ILE	2.2
1	C	452	GLU	2.1
1	E	171	ASP	2.1
1	C	127	PHE	2.1
1	E	314	TYR	2.1
1	C	63	GLY	2.1
1	E	318	GLY	2.1
1	C	35	PHE	2.1
1	E	344	PHE	2.1
1	D	255	GLU	2.1
1	C	514	THR	2.1
1	E	391	PRO	2.1
1	B	100	ASN	2.1
1	B	259	GLY	2.1
1	D	114	GLY	2.1
1	C	53	ILE	2.1
1	C	75	ILE	2.1
1	D	521	VAL	2.1
1	D	149	GLU	2.1
1	E	255	GLU	2.1
1	E	389	TRP	2.1
1	E	95	GLU	2.0
1	B	361	THR	2.0
1	A	171	ASP	2.0
1	E	99	GLU	2.0
1	B	46	SER	2.0
1	D	86	PRO	2.0
1	E	63	GLY	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 ⓘ

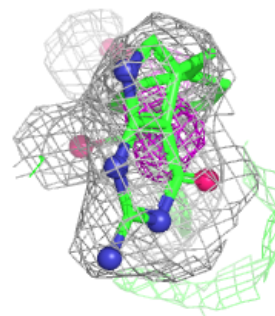
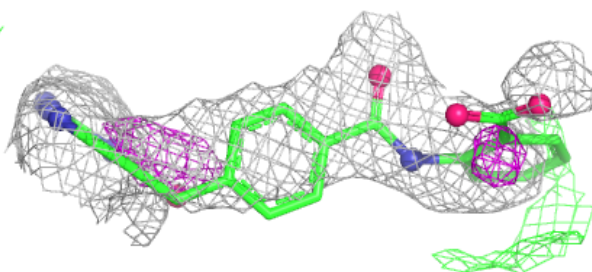
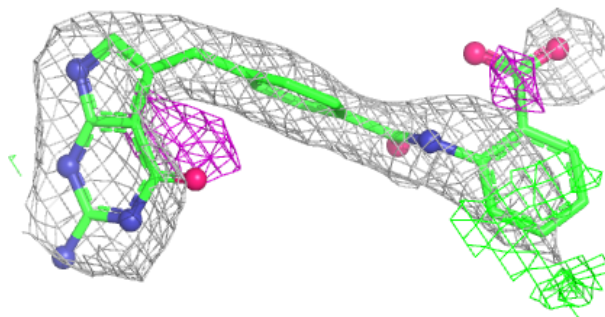
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	OG7	E	603	30/30	0.75	0.27	100,121,137,139	0
4	OG7	B	603	30/30	0.77	0.26	65,85,111,115	0
4	OG7	D	603	30/30	0.79	0.23	83,102,118,128	0
4	OG7	A	603	30/30	0.82	0.21	56,70,101,108	0
4	OG7	C	603	30/30	0.84	0.21	58,77,101,104	0
3	UFP	E	602	21/21	0.89	0.12	85,113,122,123	0
6	SO4	D	605	5/5	0.90	0.18	93,97,117,120	0
6	SO4	C	605	5/5	0.91	0.14	74,96,103,117	0
5	MTX	C	604	33/33	0.91	0.13	66,82,90,98	0
2	NDP	C	601	48/48	0.92	0.11	75,96,116,118	0
6	SO4	B	605	5/5	0.92	0.18	68,86,98,101	0
3	UFP	B	602	21/21	0.93	0.12	54,77,98,100	0
5	MTX	E	604	33/33	0.93	0.12	75,86,98,102	0
6	SO4	A	605	5/5	0.93	0.15	54,102,111,117	0
3	UFP	D	602	21/21	0.93	0.10	67,87,102,105	0
2	NDP	E	601	48/48	0.93	0.10	74,92,111,115	0
3	UFP	A	602	21/21	0.93	0.11	53,63,78,79	0
5	MTX	D	604	33/33	0.94	0.12	55,70,81,84	0
5	MTX	A	604	33/33	0.94	0.10	40,55,65,76	0
2	NDP	D	601	48/48	0.94	0.10	60,75,99,115	0
3	UFP	C	602	21/21	0.95	0.10	46,66,84,87	0
2	NDP	B	601	48/48	0.96	0.08	46,59,68,75	0
5	MTX	B	604	33/33	0.96	0.08	44,56,79,87	0
2	NDP	A	601	48/48	0.96	0.08	48,59,73,79	0

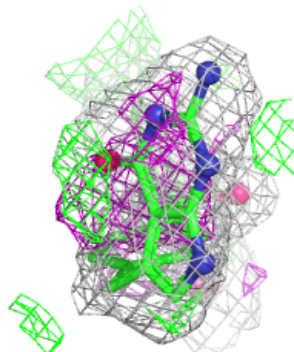
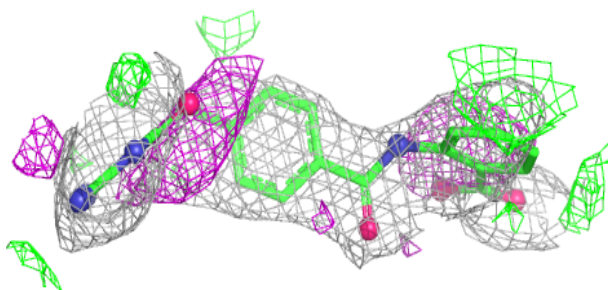
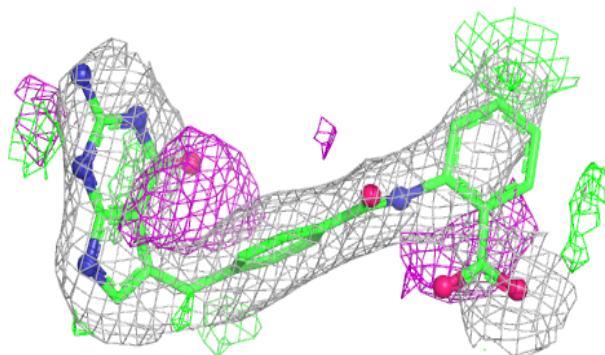
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OG7 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)

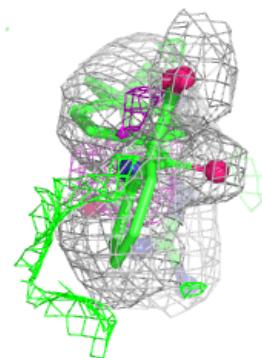
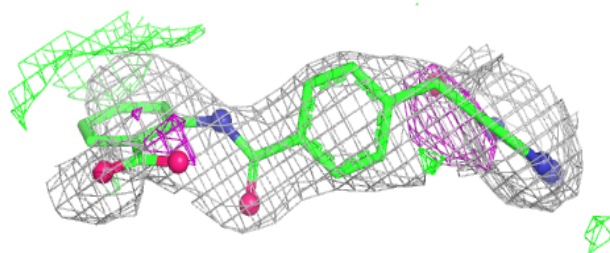
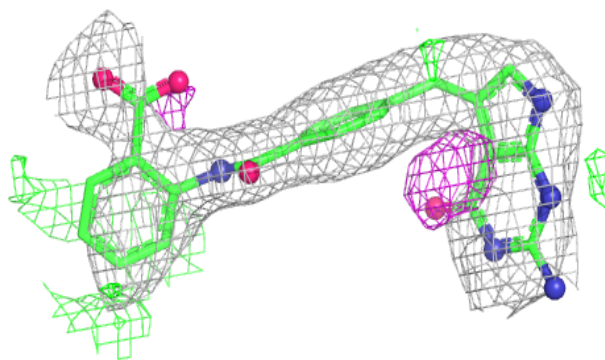
**Electron density around OG7 B 603:**

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

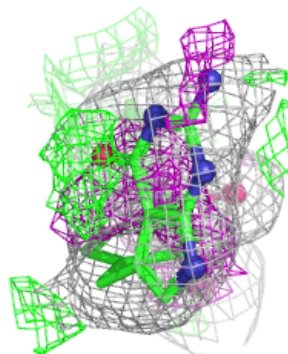
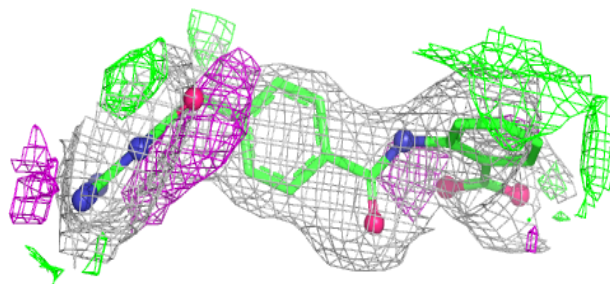
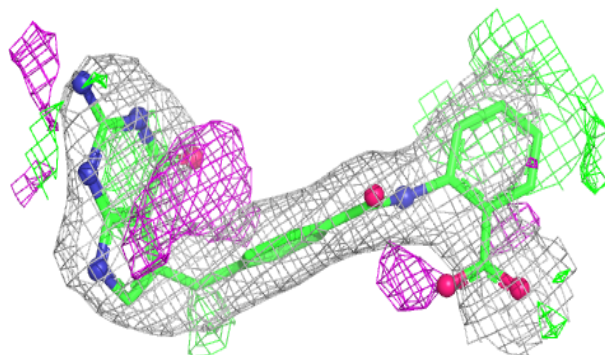


Electron density around OG7 D 603:

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

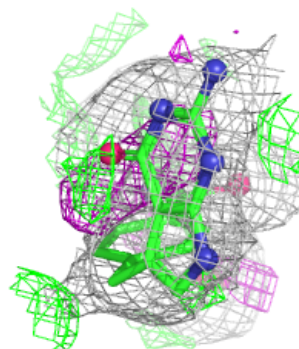
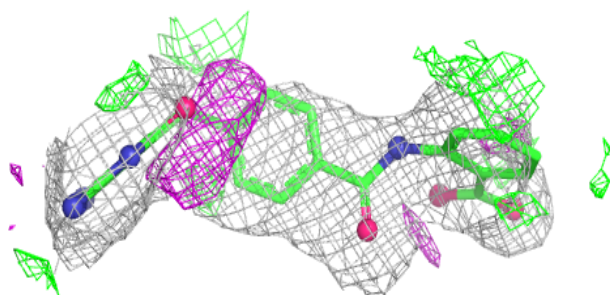
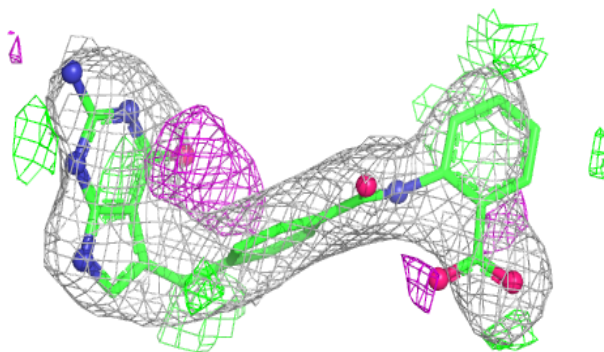
**Electron density around OG7 A 603:**

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

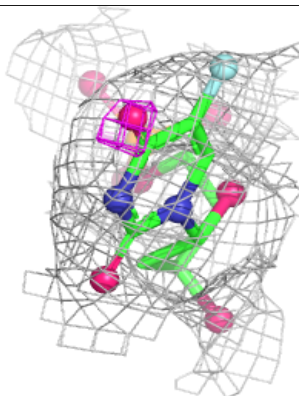
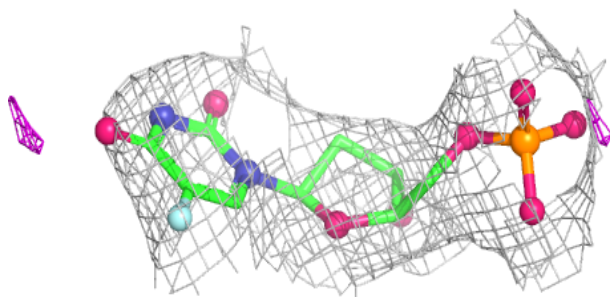
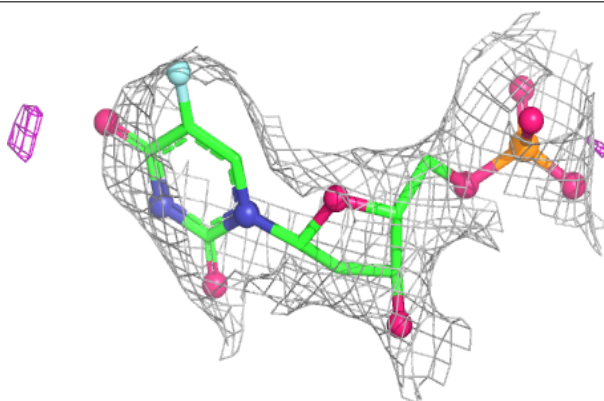


Electron density around OG7 C 603:

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

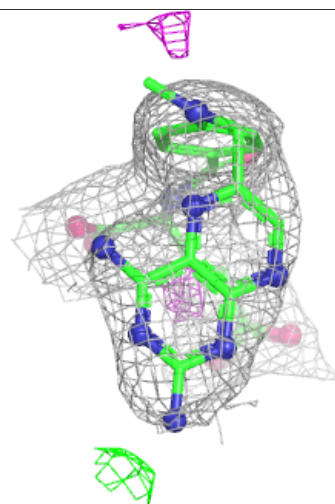
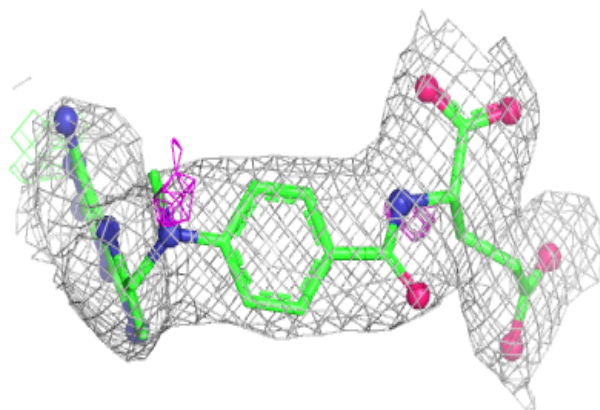
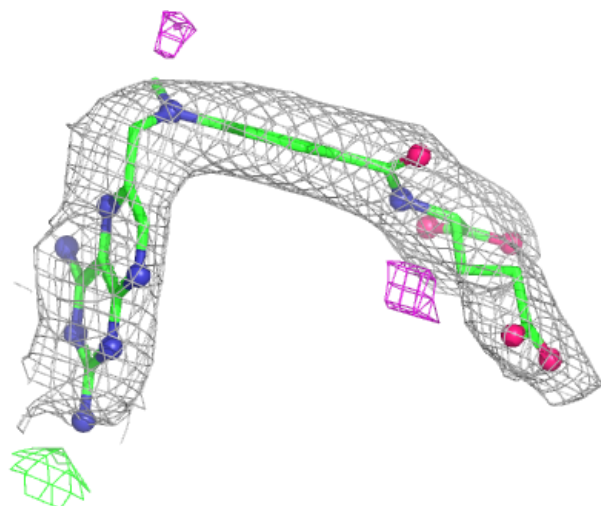
**Electron density around UFP E 602:**

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



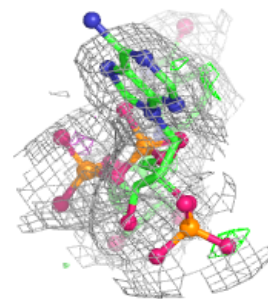
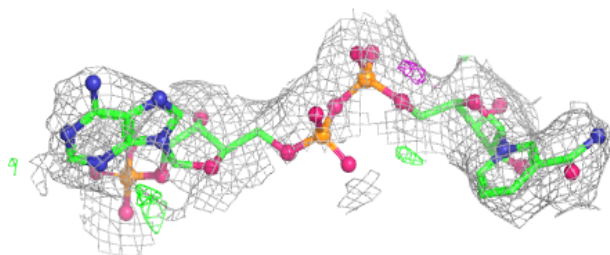
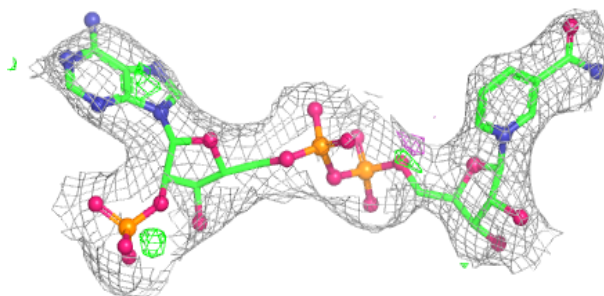
Electron density around MTX C 604:

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

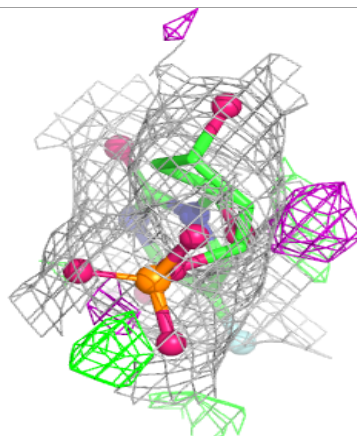
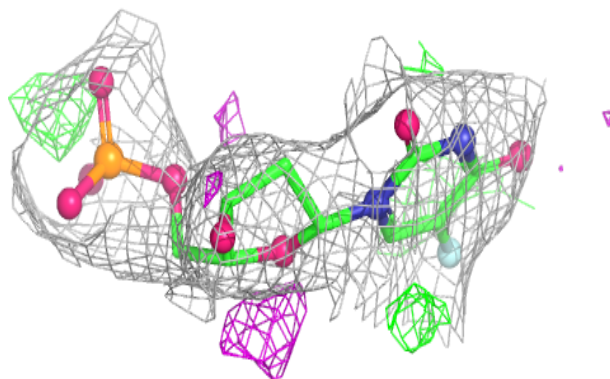
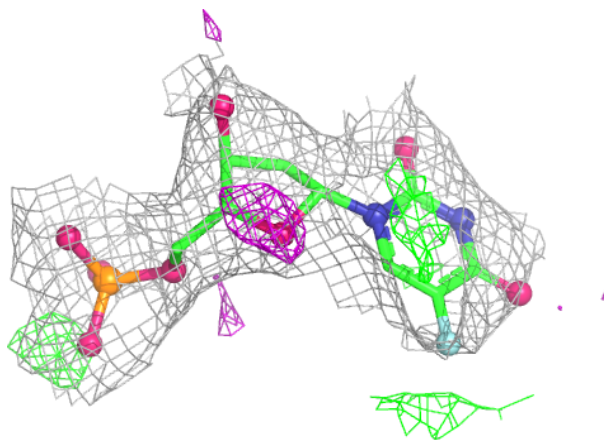


Electron density around NDP C 601:

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

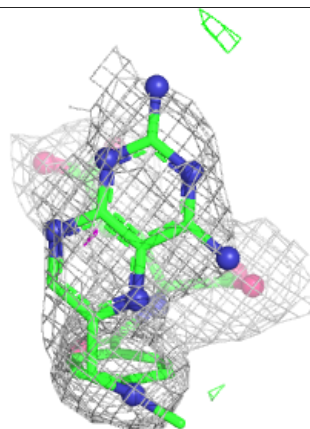
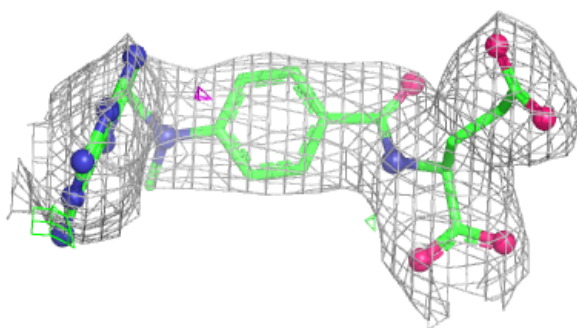
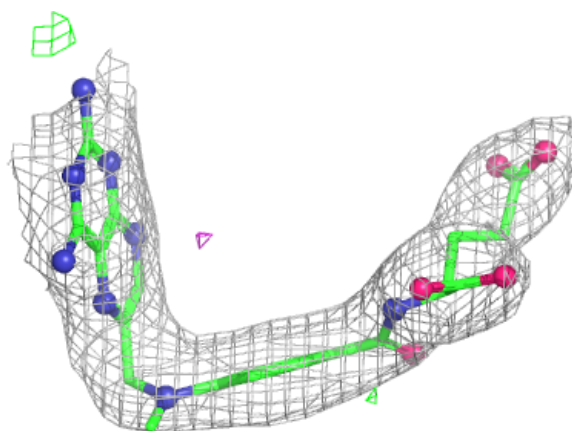
**Electron density around UFP B 602:**

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

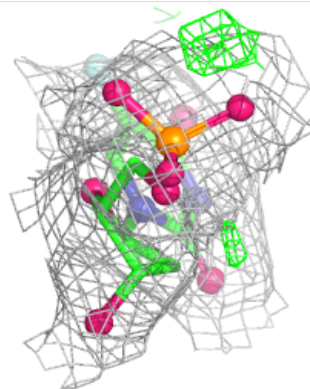
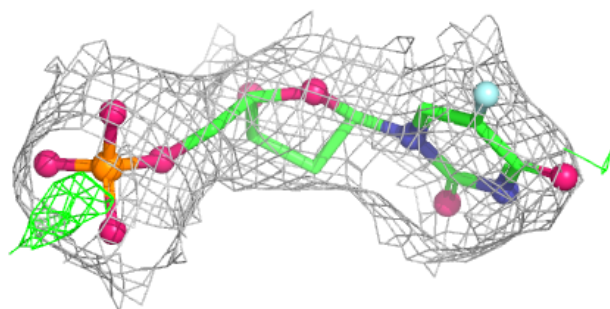
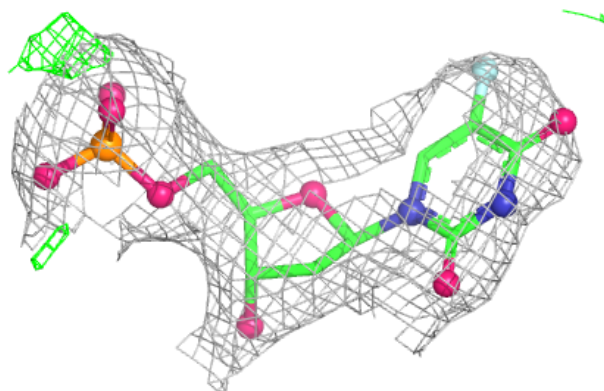


Electron density around MTX E 604:

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

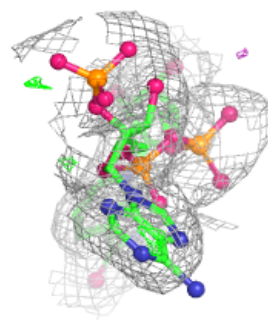
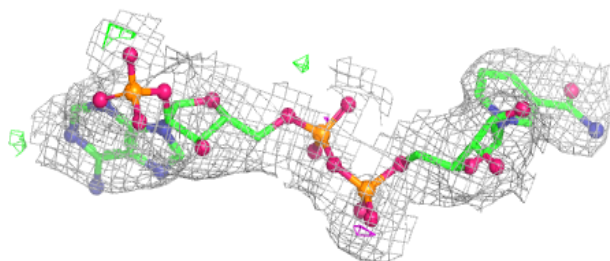
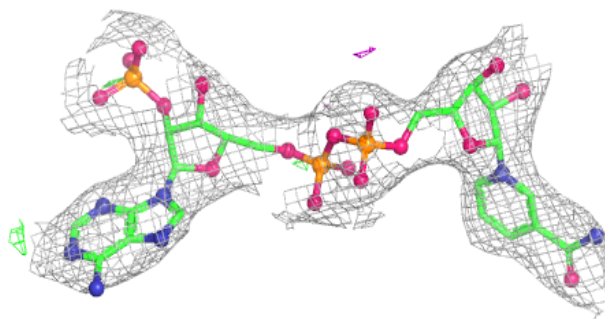
**Electron density around UFP D 602:**

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

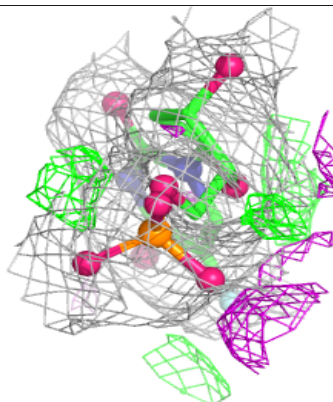
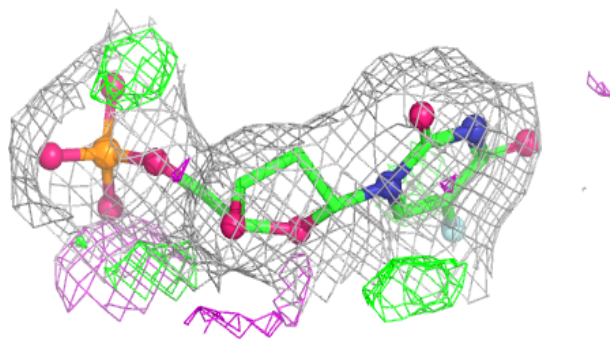
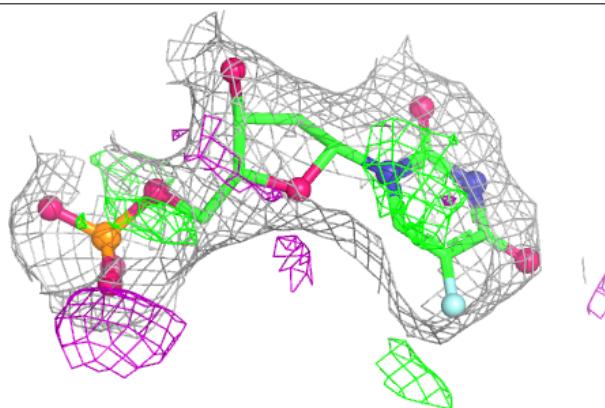


Electron density around NDP E 601:

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

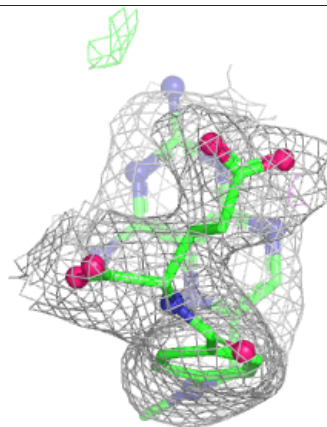
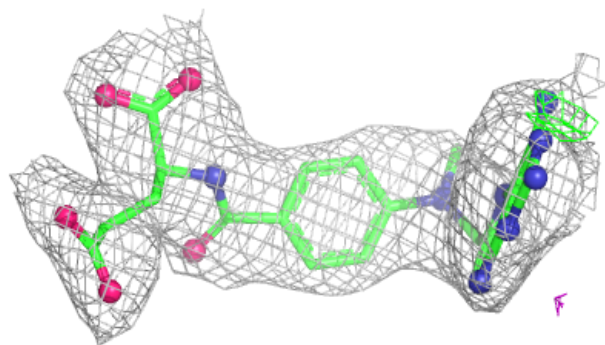
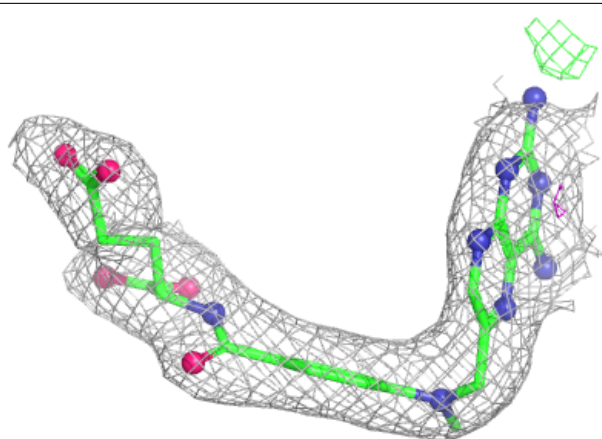
**Electron density around UFP A 602:**

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



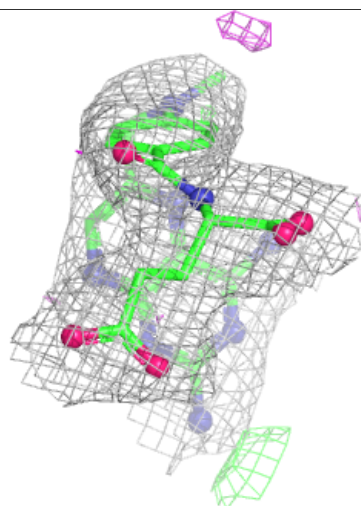
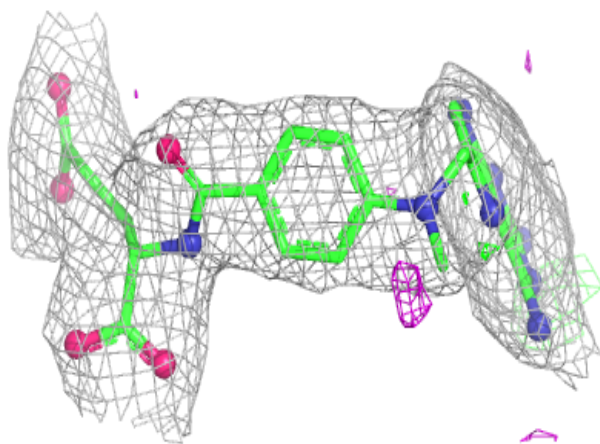
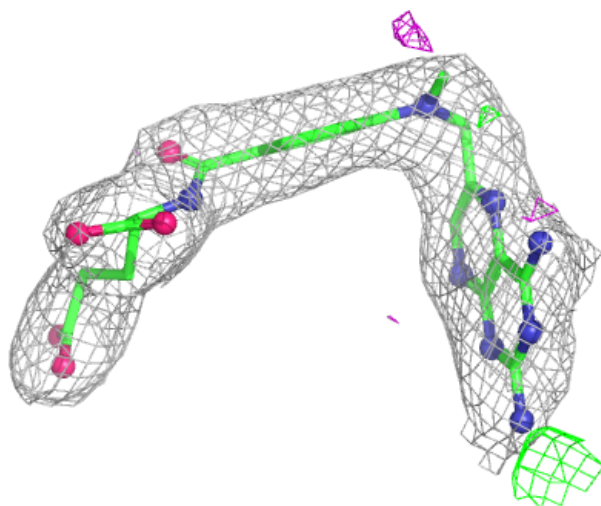
Electron density around MTX D 604:

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



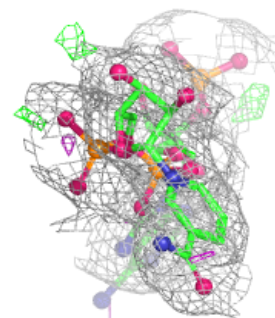
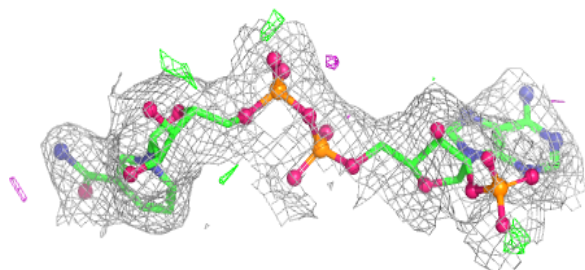
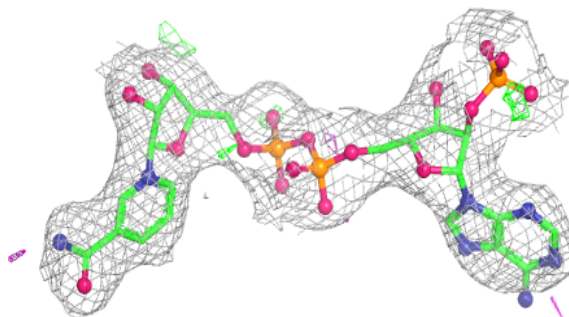
Electron density around MTX A 604:

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

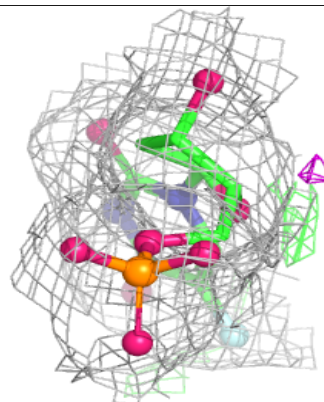
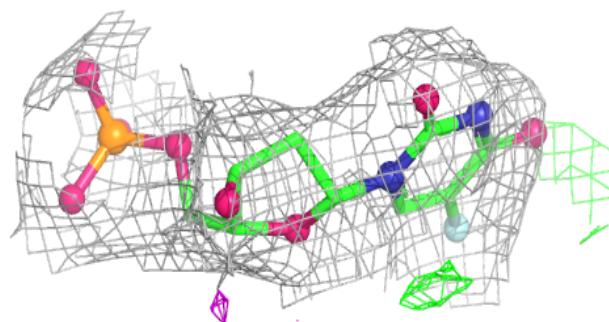
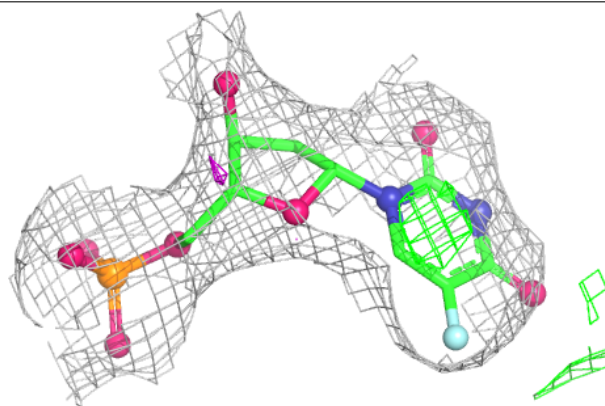


Electron density around NDP D 601:

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

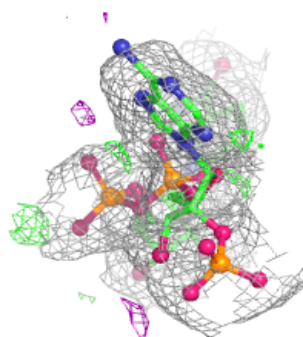
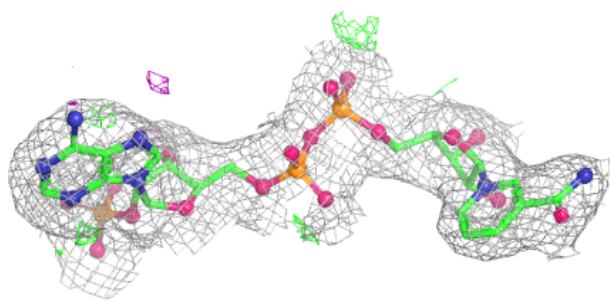
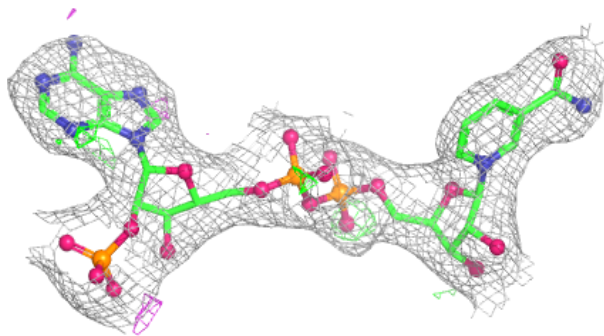
**Electron density around UFP C 602:**

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

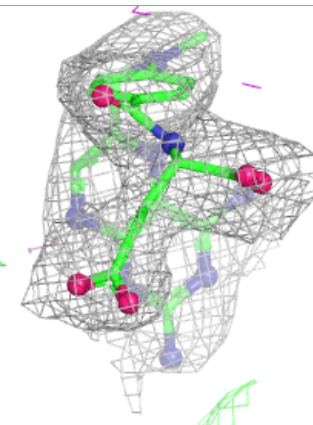
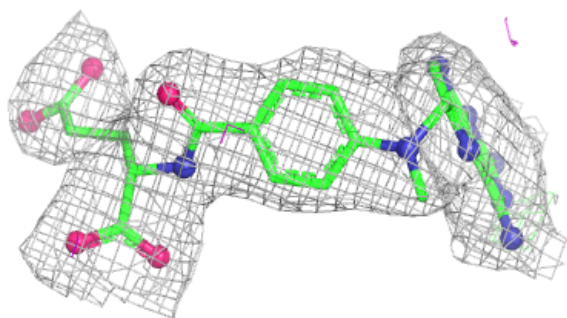
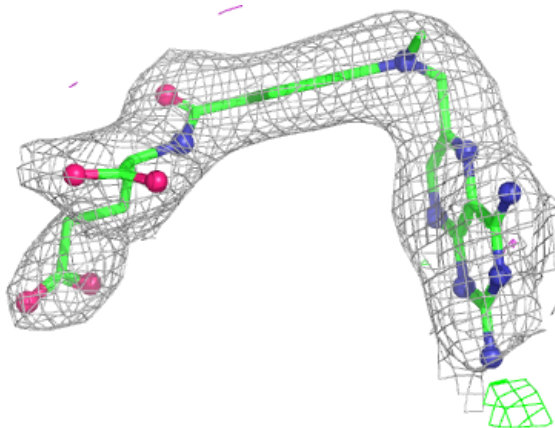


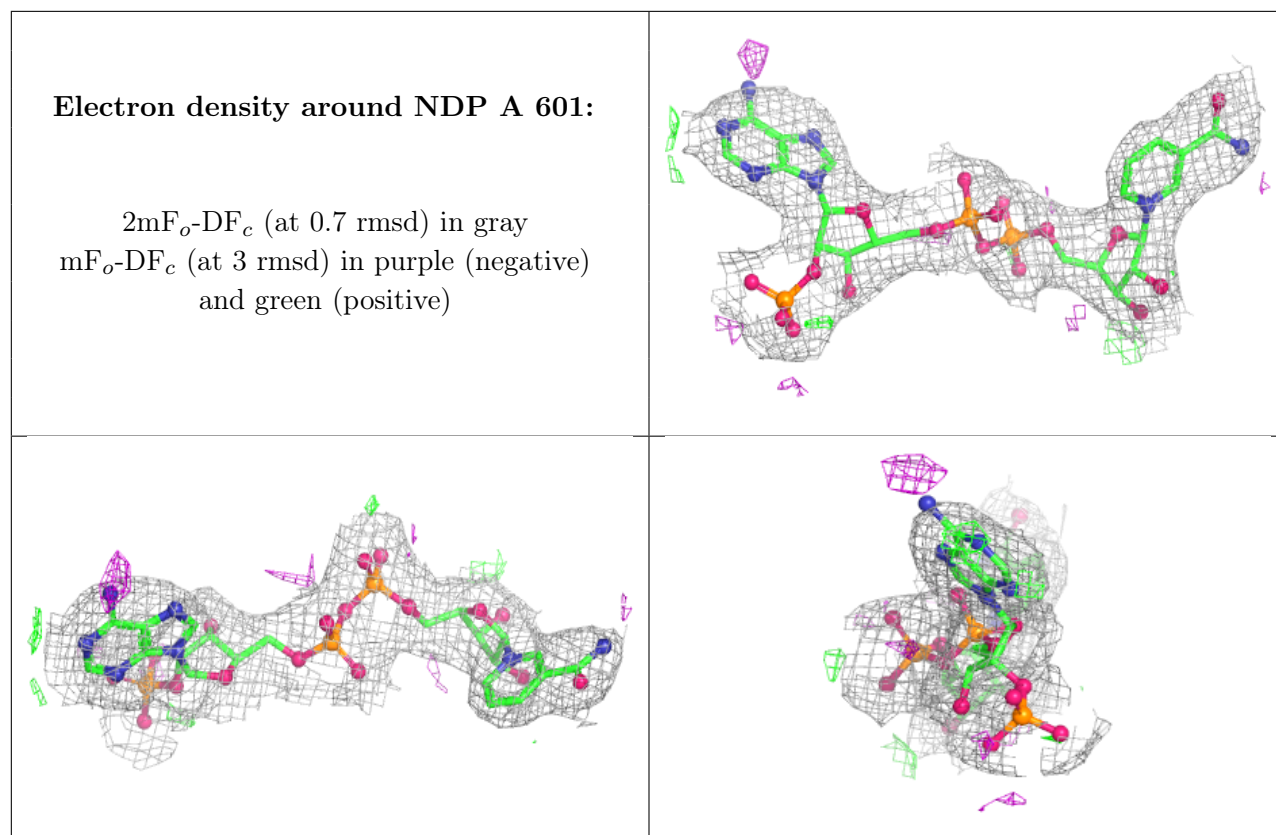
Electron density around NDP B 601:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.