



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:54 PM UTC

PDB ID : 6PFA / pdb_00006pfa
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)methyl)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

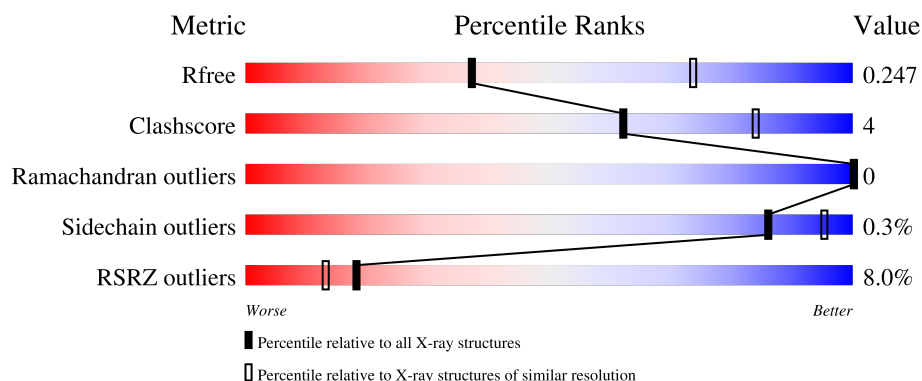
1 Overall quality at a glance

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	5% 86% 11%
1	B	521	4% 86% 11%
1	C	521	6% 87% 10%
1	D	521	7% 86% 11%

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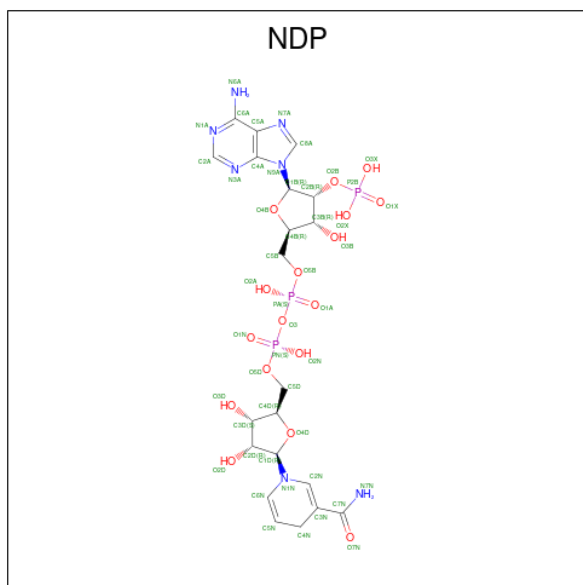
Mol	Chain	Length	Quality of chain
1	E	521	17% 89% 8%

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	506	Total 4076	C 2605	N 686	O 764	S 21	0	0	0
1	B	506	Total 4080	C 2608	N 687	O 764	S 21	0	0	0
1	C	505	Total 4037	C 2582	N 678	O 756	S 21	0	0	0
1	D	506	Total 4058	C 2595	N 681	O 761	S 21	0	0	0
1	E	506	Total 4003	C 2561	N 664	O 757	S 21	0	0	0

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



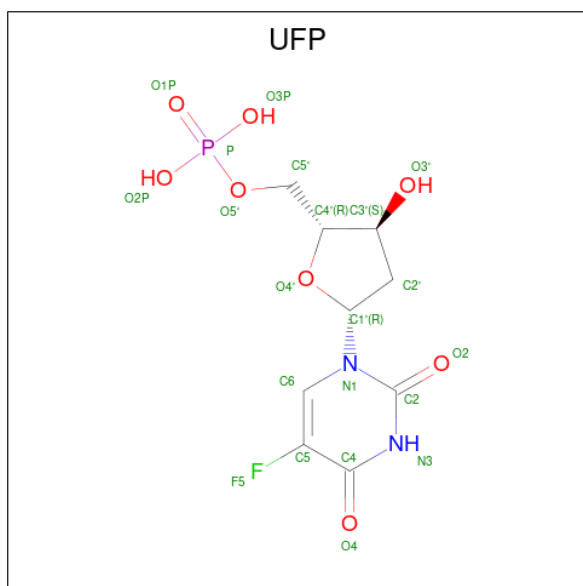
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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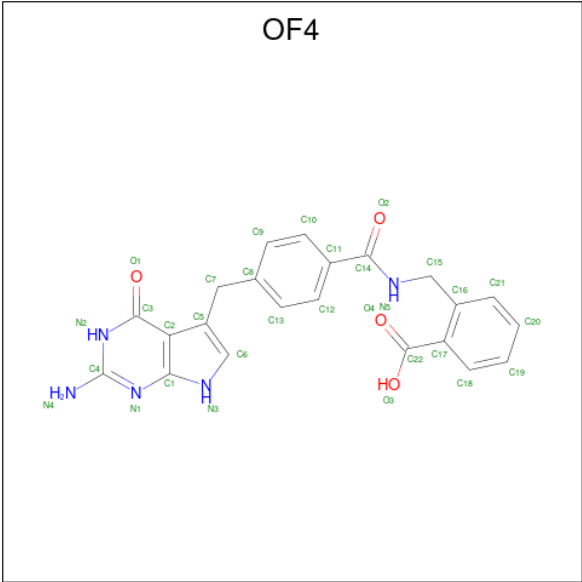
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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



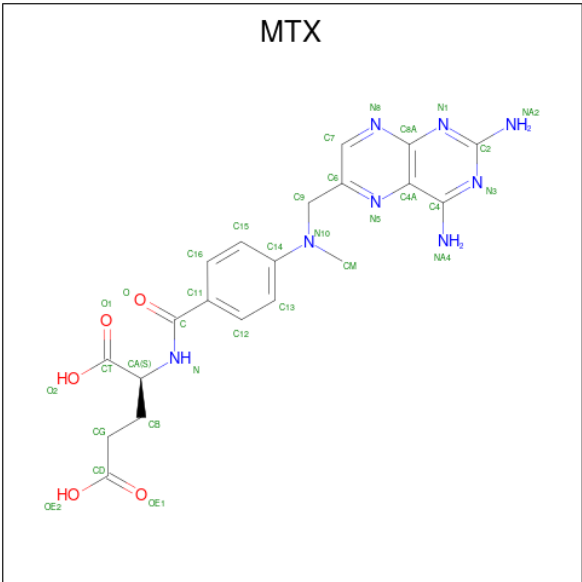
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is 2-[(4-[(2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl]benzene-1-carbonyl)amino)methyl]benzoic acid (CCD ID: OF4) (formula: C₂₂H₁₉N₅O₄) (labeled as "Ligand of Interest" by depositor).



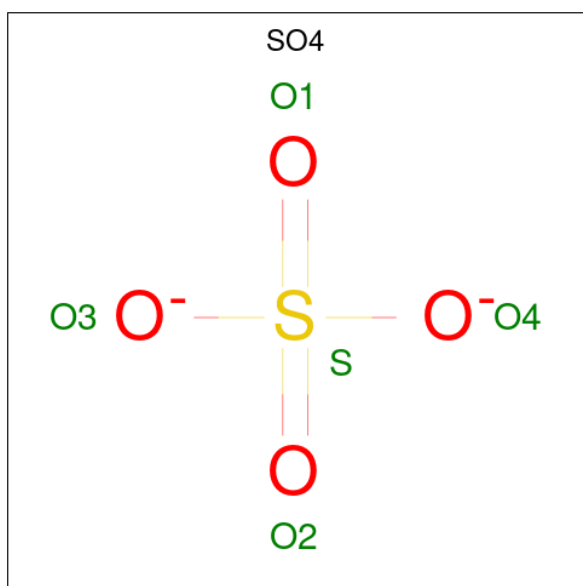
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			31	22	5	4		
4	B	1	Total	C	N	O	0	0
			31	22	5	4		
4	C	1	Total	C	N	O	0	0
			31	22	5	4		
4	D	1	Total	C	N	O	0	0
			31	22	5	4		
4	E	1	Total	C	N	O	0	0
			31	22	5	4		

- 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		
6	E	1	Total	O	S	0	0
			5	4	1		

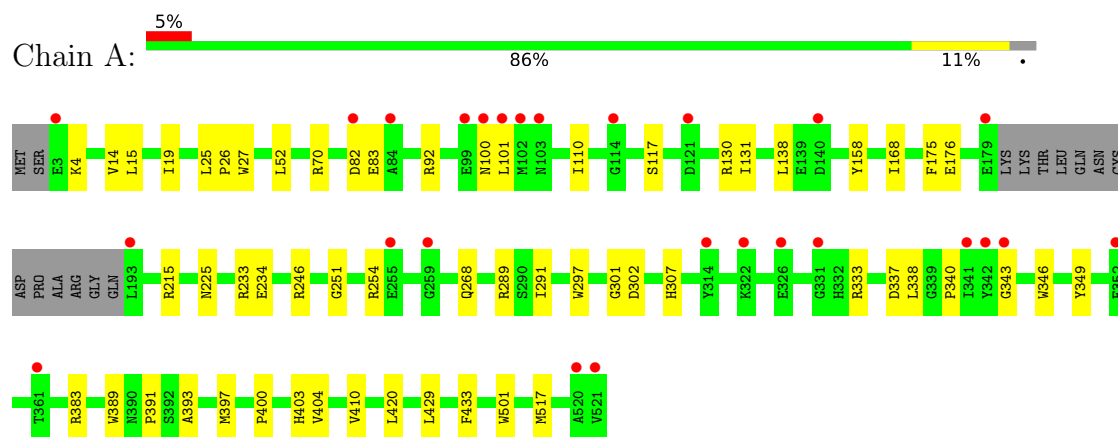
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total 24	O 24	0	0
7	B	37	Total 37	O 37	0	0
7	C	15	Total 15	O 15	0	0
7	D	18	Total 18	O 18	0	0
7	E	7	Total 7	O 7	0	0

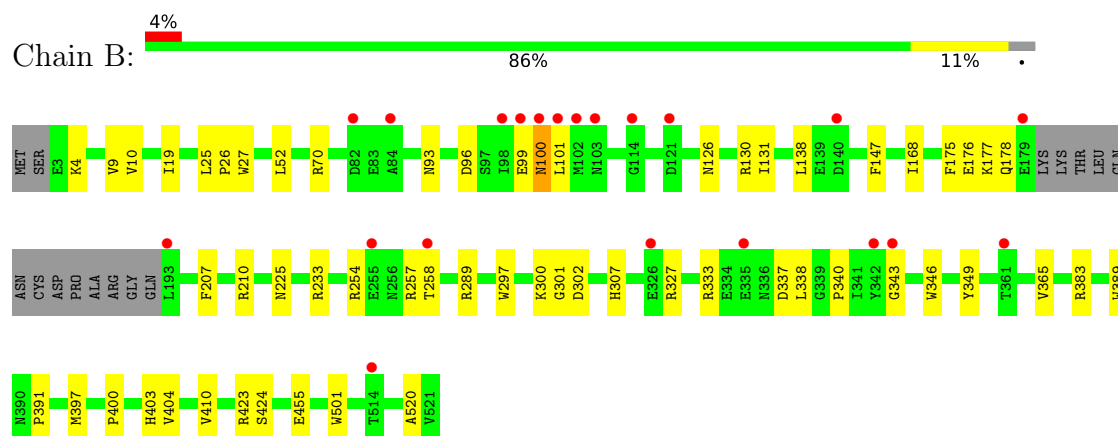
3 Residue-property plots

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.

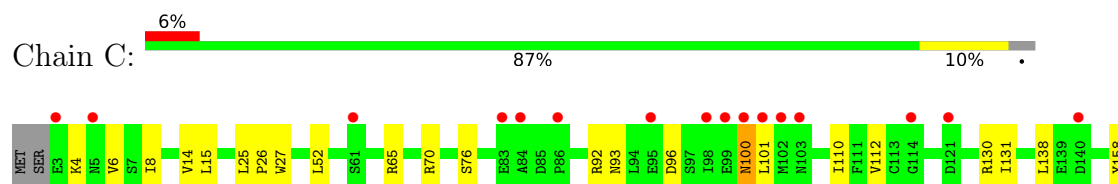
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

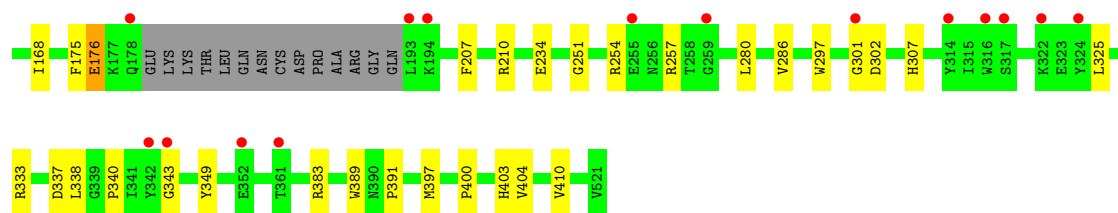


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

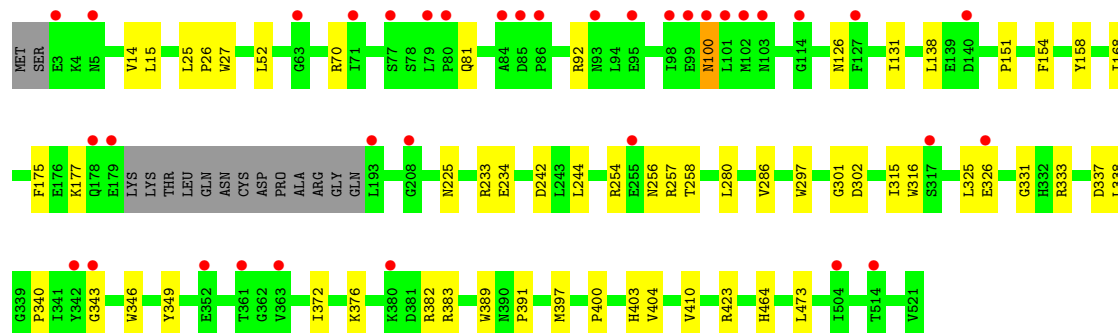
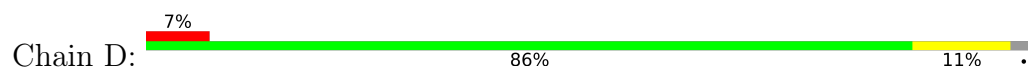


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

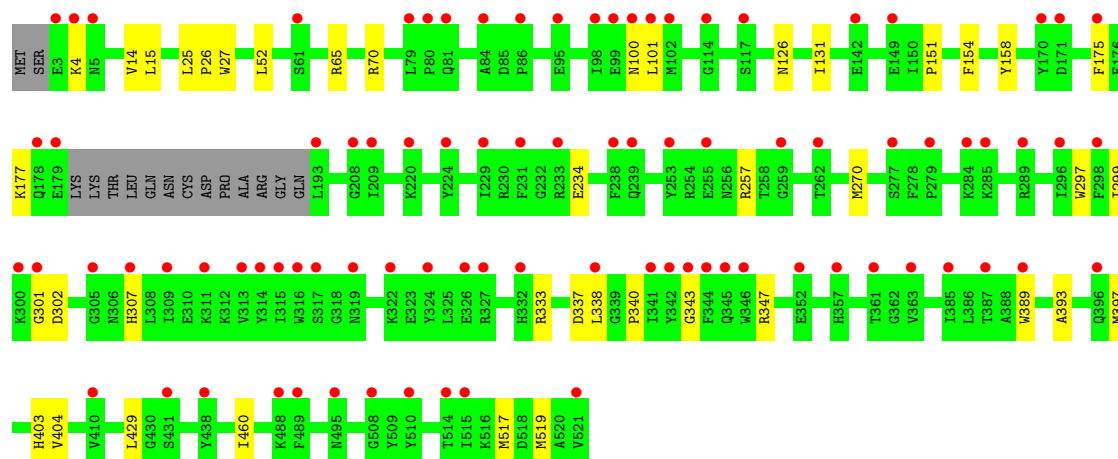
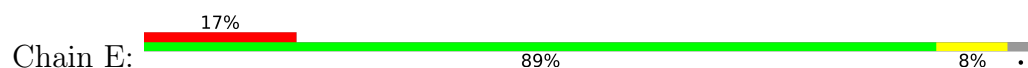




● Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



● 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	213.21Å 117.29Å 222.82Å 90.00° 95.72° 90.00°	Depositor
Resolution (Å)	48.93 – 2.79 48.93 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.93-2.79) 99.5 (48.93-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: 000)	Depositor
R, R_{free}	0.221 , 0.249 0.223 , 0.247	Depositor DCC
R_{free} test set	6780 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21045	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: NDP, OF4, MTX, SO4, 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	0/4171	0.31	0/5648
1	B	0.11	0/4175	0.32	0/5652
1	C	0.10	0/4132	0.30	0/5602
1	D	0.10	0/4153	0.29	0/5627
1	E	0.09	0/4097	0.28	0/5564
All	All	0.10	0/20728	0.30	0/28093

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	4076	0	3962	41	0
1	B	4080	0	3973	41	0
1	C	4037	0	3898	36	0
1	D	4058	0	3926	40	0
1	E	4003	0	3814	24	0
2	A	48	0	26	2	0
2	B	48	0	26	1	0
2	C	48	0	26	2	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	0	0
3	A	21	0	10	0	0
3	B	21	0	10	3	0
3	C	21	0	10	2	0
3	D	21	0	10	3	0
3	E	21	0	10	1	0
4	A	31	0	0	0	0
4	B	31	0	0	1	0
4	C	31	0	0	0	0
4	D	31	0	0	0	0
4	E	31	0	0	0	0
5	A	33	0	20	1	0
5	B	33	0	20	2	0
5	C	33	0	20	2	0
5	D	33	0	20	1	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
6	E	5	0	0	0	0
7	A	24	0	0	0	0
7	B	37	0	0	2	0
7	C	15	0	0	0	0
7	D	18	0	0	0	0
7	E	7	0	0	0	0
All	All	21045	0	19853	168	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 4.

All (168) 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:B:258:THR:HG21	1:B:520:ALA:HB1	1.68	0.75
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.75	0.66
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.78	0.64
1:E:126:ASN:OD1	1:E:177:LYS:NZ	2.30	0.64
1:B:52:LEU:HD11	1:B:70:ARG:HD2	1.81	0.63
1:B:126:ASN:OD1	1:B:177:LYS:NZ	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ASN:OD1	1:D:177:LYS:NZ	2.31	0.62
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.81	0.62
1:A:225:ASN:O	1:A:233:ARG:NH2	2.31	0.62
1:B:257:ARG:HH21	3:B:602:UFP:H5'2	1.66	0.61
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.84	0.60
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.82	0.60
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.83	0.59
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.84	0.59
1:A:349:TYR:HH	1:B:349:TYR:HH	1.48	0.59
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.83	0.59
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.84	0.59
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.83	0.58
1:B:225:ASN:O	1:B:233:ARG:NH2	2.28	0.58
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.85	0.58
1:B:301:GLY:HA2	1:B:343:GLY:O	2.04	0.57
1:A:52:LEU:HD11	1:A:70:ARG:HD2	1.86	0.57
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.85	0.57
1:D:225:ASN:O	1:D:233:ARG:NH2	2.37	0.57
1:B:327:ARG:NH2	7:B:703:HOH:O	2.38	0.56
1:E:302:ASP:OD2	1:E:307:HIS:ND1	2.33	0.56
1:A:301:GLY:HA2	1:A:343:GLY:O	2.05	0.56
1:B:4:LYS:HG2	1:B:101:LEU:HD23	1.86	0.56
1:B:300:LYS:NZ	7:B:704:HOH:O	2.39	0.56
1:C:254:ARG:NH2	1:D:410:VAL:O	2.38	0.56
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.89	0.55
1:C:130:ARG:NH1	1:C:176:GLU:OE2	2.40	0.55
1:E:52:LEU:HD11	1:E:70:ARG:HD2	1.88	0.55
1:C:52:LEU:HD11	1:C:70:ARG:HD2	1.88	0.55
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.88	0.54
1:A:4:LYS:HG2	1:A:101:LEU:HD23	1.87	0.54
1:C:301:GLY:HA2	1:C:343:GLY:O	2.06	0.54
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.73	0.54
1:B:130:ARG:NH1	1:B:176:GLU:OE2	2.41	0.53
1:C:410:VAL:O	1:D:254:ARG:NH2	2.41	0.53
1:D:301:GLY:HA2	1:D:343:GLY:O	2.08	0.53
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.45	0.52
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.45	0.52
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.46	0.51
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.45	0.51
1:A:254:ARG:NH2	1:B:410:VAL:O	2.44	0.51
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:VAL:HG13	1:E:15:LEU:HG	1.92	0.51
1:C:302:ASP:OD2	1:C:307:HIS:ND1	2.33	0.51
1:E:403:HIS:H	1:E:403:HIS:CD2	2.28	0.51
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.46	0.50
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.47	0.50
1:A:410:VAL:O	1:B:254:ARG:NH2	2.44	0.50
1:A:302:ASP:OD2	1:A:307:HIS:ND1	2.37	0.50
1:C:25:LEU:HD11	5:C:604:MTX:H7	1.95	0.49
1:B:138:LEU:HD11	1:B:168:ILE:HD13	1.93	0.49
1:B:349:TYR:HB3	1:B:365:VAL:HB	1.94	0.49
1:B:93:ASN:ND2	1:B:96:ASP:OD2	2.31	0.49
1:E:25:LEU:HD11	5:E:604:MTX:H7	1.95	0.49
1:A:383:ARG:NE	1:B:400:PRO:HG2	2.28	0.49
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.48	0.49
1:D:256:ASN:OD1	1:D:258:THR:OG1	2.25	0.49
1:A:429:LEU:HD21	1:A:517:MET:HB2	1.94	0.49
1:E:158:TYR:OH	1:E:234:GLU:OE1	2.28	0.49
1:A:26:PRO:HG2	1:A:27:TRP:CZ3	2.48	0.48
1:B:343:GLY:HA2	1:B:346:TRP:HB2	1.95	0.48
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.48	0.48
1:D:372:ILE:HG22	1:D:376:LYS:HE2	1.96	0.48
1:E:297:TRP:HH2	1:E:338:LEU:HD12	1.78	0.48
1:D:326:GLU:HG2	1:D:331:GLY:HA2	1.95	0.48
1:C:4:LYS:HG2	1:C:101:LEU:HD23	1.95	0.48
1:B:26:PRO:HG2	1:B:27:TRP:CZ3	2.49	0.48
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.95	0.48
1:E:4:LYS:H	1:E:101:LEU:HD22	1.78	0.48
1:E:299:ILE:O	1:E:347:ARG:NH1	2.45	0.48
1:E:301:GLY:HA2	1:E:343:GLY:O	2.13	0.48
1:A:215:ARG:NH1	1:B:455:GLU:OE2	2.46	0.48
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.79	0.48
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.49	0.48
1:C:403:HIS:H	1:C:403:HIS:CD2	2.31	0.48
1:D:14:VAL:HG13	1:D:15:LEU:HG	1.96	0.48
1:B:403:HIS:H	1:B:403:HIS:CD2	2.32	0.47
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.78	0.47
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.97	0.47
1:A:138:LEU:HD11	1:A:168:ILE:HD13	1.96	0.47
3:C:602:UFP:O1P	1:D:382:ARG:NE	2.47	0.47
1:D:343:GLY:HA2	1:D:346:TRP:HB2	1.97	0.47
1:A:130:ARG:HG3	1:A:176:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TRP:CD1	1:C:302:ASP:HB3	2.49	0.47
1:C:158:TYR:OH	1:C:234:GLU:OE1	2.32	0.46
1:B:302:ASP:OD2	1:B:307:HIS:ND1	2.33	0.46
1:C:14:VAL:HG13	1:C:15:LEU:HG	1.97	0.46
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.96	0.46
1:C:251:GLY:O	1:E:65:ARG:NH1	2.46	0.46
1:D:244:LEU:HD22	1:D:473:LEU:HD13	1.98	0.46
1:C:100:ASN:N	1:C:100:ASN:OD1	2.49	0.45
1:C:340:PRO:O	1:C:397:MET:HG2	2.16	0.45
1:D:158:TYR:OH	1:D:234:GLU:OE1	2.33	0.45
1:D:100:ASN:OD1	1:D:100:ASN:N	2.48	0.45
1:A:25:LEU:HD11	5:A:604:MTX:H7	1.98	0.45
1:A:400:PRO:HG2	1:B:383:ARG:NE	2.31	0.45
1:B:423:ARG:NH2	3:B:602:UFP:O3P	2.49	0.45
1:E:340:PRO:O	1:E:397:MET:HG2	2.16	0.45
1:A:100:ASN:HB2	1:A:110:ILE:HD11	1.99	0.45
1:D:257:ARG:HH21	3:D:602:UFP:H5'2	1.81	0.45
1:C:325:LEU:HD23	1:C:333:ARG:HB3	1.99	0.45
1:C:383:ARG:NE	1:D:400:PRO:HG2	2.32	0.44
1:A:158:TYR:OH	1:A:234:GLU:OE1	2.30	0.44
1:A:403:HIS:CD2	1:A:403:HIS:H	2.34	0.44
1:D:81:GLN:HG3	1:D:92:ARG:NH2	2.32	0.44
1:A:340:PRO:O	1:A:397:MET:HG2	2.18	0.44
1:D:26:PRO:HG2	1:D:27:TRP:CZ3	2.53	0.44
1:B:25:LEU:HD11	5:B:604:MTX:H7	1.98	0.44
1:A:251:GLY:O	1:C:65:ARG:NH1	2.49	0.44
1:D:151:PRO:HG2	1:D:154:PHE:HD1	1.83	0.44
1:D:403:HIS:H	1:D:403:HIS:CD2	2.34	0.44
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.53	0.43
1:A:291:ILE:HG12	1:A:433:PHE:CD2	2.53	0.43
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.82	0.43
1:E:151:PRO:HG2	1:E:154:PHE:HD1	1.84	0.43
1:C:138:LEU:HD11	1:C:168:ILE:HD13	1.99	0.43
1:A:4:LYS:HG2	1:A:101:LEU:CD2	2.49	0.43
1:B:207:PHE:HB3	1:B:210:ARG:HB2	2.01	0.43
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.54	0.43
1:C:76:SER:OG	2:C:601:NDP:O2X	2.37	0.43
1:C:6:VAL:HG22	1:C:110:ILE:HB	2.00	0.43
1:A:92:ARG:HA	1:A:92:ARG:HD3	1.89	0.42
1:C:207:PHE:HB3	1:C:210:ARG:HB2	2.01	0.42
1:B:100:ASN:OD1	1:B:100:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:393:ALA:O	1:E:397:MET:HG3	2.19	0.42
1:C:257:ARG:NE	3:C:602:UFP:O2P	2.49	0.42
1:A:246:ARG:NH2	1:A:268:GLN:OE1	2.30	0.42
1:B:19:ILE:O	2:B:601:NDP:H2N	2.19	0.42
1:E:519:MET:HE2	1:E:519:MET:HB3	1.96	0.42
1:C:400:PRO:HG2	1:D:383:ARG:NE	2.35	0.42
1:A:19:ILE:O	2:A:601:NDP:H2N	2.20	0.42
1:B:9:VAL:O	5:B:604:MTX:NA4	2.50	0.42
3:B:602:UFP:H4'	4:B:603:OF4:N4	2.35	0.42
1:C:26:PRO:HG2	1:C:27:TRP:CZ3	2.54	0.42
1:D:138:LEU:HD11	1:D:168:ILE:HD13	2.02	0.41
1:A:403:HIS:HB2	1:A:420:LEU:HD11	2.01	0.41
2:C:601:NDP:H42N	5:C:604:MTX:N5	2.34	0.41
1:A:393:ALA:O	1:A:397:MET:HG3	2.20	0.41
1:E:26:PRO:HG2	1:E:27:TRP:CZ3	2.54	0.41
1:C:280:LEU:HD11	1:C:286:VAL:HB	2.01	0.41
1:A:14:VAL:HG13	1:A:15:LEU:HG	2.03	0.41
1:A:343:GLY:HA2	1:A:346:TRP:HB2	2.03	0.41
1:D:233:ARG:NH1	1:D:242:ASP:OD1	2.53	0.41
1:D:340:PRO:O	1:D:397:MET:HG2	2.20	0.41
1:B:10:VAL:HG21	1:B:147:PHE:CD1	2.56	0.41
1:E:429:LEU:HD21	1:E:517:MET:HB2	2.03	0.41
1:B:340:PRO:O	1:B:397:MET:HG2	2.21	0.41
1:D:325:LEU:HD23	1:D:333:ARG:HB3	2.02	0.41
1:A:117:SER:OG	2:A:601:NDP:O1A	2.39	0.41
1:B:423:ARG:HG3	1:B:424:SER:N	2.36	0.41
1:C:93:ASN:ND2	1:C:96:ASP:OD2	2.39	0.41
1:D:280:LEU:HD11	1:D:286:VAL:HB	2.02	0.41
1:D:315:ILE:HG13	1:D:316:TRP:CD1	2.56	0.41
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.56	0.41
1:B:297:TRP:CD1	1:B:302:ASP:HB3	2.56	0.40
1:C:92:ARG:HD3	1:C:92:ARG:HA	1.89	0.40
1:D:464:HIS:NE2	3:D:602:UFP:O3'	2.45	0.40
1:E:257:ARG:HH21	3:E:602:UFP:H5'1	1.86	0.40
1:D:423:ARG:NH2	3:D:602:UFP:O3P	2.49	0.40
1:E:270:MET:HE2	1:E:460:ILE:HD11	2.02	0.40
1:A:82:ASP:OD1	1:A:83:GLU:N	2.55	0.40
1:D:25:LEU:HD11	5:D:604:MTX:H7	2.03	0.40
1:D:151:PRO:HG2	1:D:154:PHE:CD1	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	502/521 (96%)	473 (94%)	29 (6%)	0	100	100
1	B	502/521 (96%)	473 (94%)	29 (6%)	0	100	100
1	C	501/521 (96%)	472 (94%)	29 (6%)	0	100	100
1	D	502/521 (96%)	474 (94%)	28 (6%)	0	100	100
1	E	502/521 (96%)	474 (94%)	28 (6%)	0	100	100
All	All	2509/2605 (96%)	2366 (94%)	143 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/470 (95%)	445 (100%)	0	100	100
1	B	446/470 (95%)	443 (99%)	3 (1%)	76	91
1	C	437/470 (93%)	435 (100%)	2 (0%)	81	93
1	D	440/470 (94%)	439 (100%)	1 (0%)	87	96
1	E	428/470 (91%)	427 (100%)	1 (0%)	87	96
All	All	2196/2350 (93%)	2189 (100%)	7 (0%)	86	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	99	GLU
1	B	100	ASN
1	B	178	GLN
1	C	100	ASN
1	C	176	GLU
1	D	100	ASN
1	E	100	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	B	178	GLN
1	B	336	ASN
1	B	345	GLN
1	B	390	ASN
1	C	306	ASN
1	C	319	ASN
1	C	336	ASN
1	C	345	GLN
1	C	350	ASN
1	C	390	ASN
1	C	414	ASN
1	D	41	ASN
1	D	336	ASN
1	D	345	GLN
1	D	350	ASN
1	D	390	ASN
1	D	414	ASN
1	D	486	GLN
1	E	396	GLN
1	E	414	ASN
1	E	486	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 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	E	601	-	51,52,52	1.94	12 (23%)	71,80,80	1.52	11 (15%)
5	MTX	A	604	-	35,35,35	1.61	5 (14%)	47,49,49	1.80	8 (17%)
5	MTX	C	604	-	35,35,35	1.61	5 (14%)	47,49,49	1.81	8 (17%)
2	NDP	A	601	-	51,52,52	1.96	12 (23%)	71,80,80	1.49	12 (16%)
4	OF4	C	603	-	34,34,34	1.39	4 (11%)	44,48,48	1.26	4 (9%)
6	SO4	D	605	-	4,4,4	0.26	0	6,6,6	0.07	0
2	NDP	D	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.52	12 (16%)
5	MTX	D	604	-	35,35,35	1.62	5 (14%)	47,49,49	1.80	9 (19%)
4	OF4	A	603	-	34,34,34	1.39	3 (8%)	44,48,48	1.18	4 (9%)
5	MTX	E	604	-	35,35,35	1.61	5 (14%)	47,49,49	1.76	8 (17%)
2	NDP	C	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.52	11 (15%)
4	OF4	E	603	-	34,34,34	1.40	5 (14%)	44,48,48	1.31	7 (15%)
4	OF4	B	603	-	34,34,34	1.38	3 (8%)	44,48,48	1.28	4 (9%)
3	UFP	B	602	-	22,22,22	1.07	0	32,33,33	2.73	11 (34%)
6	SO4	E	605	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	C	605	-	4,4,4	0.25	0	6,6,6	0.09	0
3	UFP	C	602	-	22,22,22	1.06	0	32,33,33	2.67	11 (34%)
4	OF4	D	603	-	34,34,34	1.38	4 (11%)	44,48,48	1.28	5 (11%)
3	UFP	A	602	-	22,22,22	1.03	0	32,33,33	2.71	11 (34%)
6	SO4	B	605	-	4,4,4	0.25	0	6,6,6	0.04	0
5	MTX	B	604	-	35,35,35	1.62	5 (14%)	47,49,49	1.79	8 (17%)
3	UFP	E	602	-	22,22,22	1.28	1 (4%)	32,33,33	2.63	11 (34%)
2	NDP	B	601	-	51,52,52	1.95	11 (21%)	71,80,80	1.48	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UFP	D	602	-	22,22,22	1.04	0	32,33,33	2.68	11 (34%)
6	SO4	A	605	-	4,4,4	0.24	0	6,6,6	0.09	0

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	E	601	-	-	6/34/77/77	0/5/5/5
5	MTX	A	604	-	-	6/25/25/25	0/3/3/3
5	MTX	C	604	-	-	6/25/25/25	0/3/3/3
2	NDP	A	601	-	-	3/34/77/77	0/5/5/5
4	OF4	C	603	-	-	1/17/17/17	0/4/4/4
2	NDP	D	601	-	-	5/34/77/77	0/5/5/5
5	MTX	D	604	-	-	6/25/25/25	0/3/3/3
4	OF4	A	603	-	-	3/17/17/17	0/4/4/4
5	MTX	E	604	-	-	6/25/25/25	0/3/3/3
2	NDP	C	601	-	-	4/34/77/77	0/5/5/5
4	OF4	E	603	-	-	1/17/17/17	0/4/4/4
4	OF4	B	603	-	-	5/17/17/17	0/4/4/4
3	UFP	B	602	-	-	5/10/22/22	0/2/2/2
3	UFP	C	602	-	-	5/10/22/22	0/2/2/2
4	OF4	D	603	-	-	5/17/17/17	0/4/4/4
3	UFP	A	602	-	-	3/10/22/22	0/2/2/2
5	MTX	B	604	-	-	6/25/25/25	0/3/3/3
3	UFP	E	602	-	-	4/10/22/22	0/2/2/2
2	NDP	B	601	-	-	2/34/77/77	0/5/5/5
3	UFP	D	602	-	-	5/10/22/22	0/2/2/2

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NDP	C6A-N6A	5.82	1.49	1.34
2	E	601	NDP	C6A-N6A	5.81	1.49	1.34
2	A	601	NDP	C6A-N6A	5.80	1.49	1.34
2	B	601	NDP	C6A-N6A	5.79	1.49	1.34
2	D	601	NDP	C6A-N6A	5.77	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	604	MTX	C2-NA2	5.34	1.44	1.33
5	B	604	MTX	C2-NA2	5.34	1.44	1.33
5	E	604	MTX	C2-NA2	5.27	1.44	1.33
5	C	604	MTX	C2-NA2	5.27	1.44	1.33
5	A	604	MTX	C2-NA2	5.22	1.44	1.33
5	B	604	MTX	C-N	4.74	1.45	1.34
5	E	604	MTX	C-N	4.73	1.45	1.34
5	D	604	MTX	C-N	4.71	1.45	1.34
2	C	601	NDP	C4N-C3N	-4.69	1.41	1.50
5	A	604	MTX	C-N	4.67	1.45	1.34
2	B	601	NDP	C4N-C3N	-4.67	1.41	1.50
2	A	601	NDP	C4N-C3N	-4.67	1.41	1.50
2	D	601	NDP	C4N-C3N	-4.63	1.41	1.50
2	E	601	NDP	C4N-C3N	-4.63	1.41	1.50
5	C	604	MTX	C-N	4.62	1.44	1.34
2	A	601	NDP	C2D-C3D	-3.99	1.42	1.53
2	D	601	NDP	C2D-C3D	-3.94	1.42	1.53
2	B	601	NDP	C2D-C3D	-3.93	1.42	1.53
2	D	601	NDP	C3B-C2B	-3.89	1.44	1.53
2	E	601	NDP	C2D-C3D	-3.89	1.42	1.53
2	C	601	NDP	C2D-C3D	-3.87	1.42	1.53
2	B	601	NDP	C3B-C2B	-3.82	1.44	1.53
2	E	601	NDP	C3B-C2B	-3.81	1.44	1.53
2	C	601	NDP	C3B-C2B	-3.80	1.44	1.53
2	A	601	NDP	C3B-C2B	-3.80	1.44	1.53
2	D	601	NDP	C7N-N7N	3.72	1.44	1.33
2	B	601	NDP	C7N-N7N	3.70	1.44	1.33
2	E	601	NDP	C7N-N7N	3.68	1.44	1.33
2	C	601	NDP	C7N-N7N	3.68	1.44	1.33
2	A	601	NDP	C7N-N7N	3.67	1.44	1.33
4	D	603	OF4	C2-C1	-3.56	1.37	1.45
4	B	603	OF4	C2-C1	-3.51	1.37	1.45
4	A	603	OF4	C2-C1	-3.48	1.37	1.45
4	C	603	OF4	C2-C1	-3.48	1.37	1.45
4	E	603	OF4	C2-C1	-3.47	1.37	1.45
3	E	602	UFP	P-O1P	3.42	1.61	1.50
2	A	601	NDP	C4N-C5N	-3.27	1.40	1.49
2	D	601	NDP	C4N-C5N	-3.27	1.40	1.49
2	C	601	NDP	C4N-C5N	-3.26	1.40	1.49
2	E	601	NDP	C4N-C5N	-3.24	1.40	1.49
2	B	601	NDP	C4N-C5N	-3.24	1.40	1.49
2	C	601	NDP	C2B-C1B	-3.10	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NDP	C2B-C1B	-3.05	1.45	1.53
2	A	601	NDP	C2B-C1B	-3.03	1.45	1.53
2	D	601	NDP	C2B-C1B	-3.01	1.45	1.53
2	B	601	NDP	C2B-C1B	-2.97	1.45	1.53
5	D	604	MTX	C14-N10	2.70	1.46	1.38
5	E	604	MTX	C14-N10	2.67	1.46	1.38
5	B	604	MTX	C14-N10	2.65	1.46	1.38
5	C	604	MTX	C14-N10	2.64	1.46	1.38
5	D	604	MTX	C4-NA4	2.62	1.43	1.34
5	A	604	MTX	C14-N10	2.62	1.46	1.38
5	C	604	MTX	C4-NA4	2.61	1.43	1.34
5	E	604	MTX	C4-NA4	2.60	1.43	1.34
5	B	604	MTX	C4-NA4	2.59	1.43	1.34
5	A	604	MTX	C4-NA4	2.59	1.43	1.34
2	D	601	NDP	C3B-C4B	-2.43	1.46	1.53
2	D	601	NDP	C4A-N3A	2.41	1.38	1.34
2	C	601	NDP	C3B-C4B	-2.40	1.46	1.53
2	A	601	NDP	C3B-C4B	-2.40	1.46	1.53
2	E	601	NDP	C4A-N3A	2.38	1.38	1.34
2	A	601	NDP	C4A-N3A	2.38	1.38	1.34
2	E	601	NDP	C3B-C4B	-2.37	1.47	1.53
2	B	601	NDP	C3B-C4B	-2.36	1.47	1.53
2	A	601	NDP	C3D-C4D	-2.36	1.47	1.53
2	C	601	NDP	C4A-N3A	2.34	1.38	1.34
2	B	601	NDP	C3D-C4D	-2.31	1.47	1.53
2	C	601	NDP	C3D-C4D	-2.30	1.47	1.53
5	A	604	MTX	C7-N8	2.29	1.35	1.31
2	D	601	NDP	C3D-C4D	-2.29	1.47	1.53
2	E	601	NDP	C3D-C4D	-2.29	1.47	1.53
2	B	601	NDP	C4A-N3A	2.28	1.38	1.34
5	C	604	MTX	C7-N8	2.25	1.35	1.31
4	E	603	OF4	C17-C16	2.25	1.43	1.40
5	B	604	MTX	C7-N8	2.24	1.35	1.31
5	D	604	MTX	C7-N8	2.23	1.35	1.31
2	A	601	NDP	C6N-C5N	2.23	1.39	1.33
2	D	601	NDP	C6N-C5N	2.23	1.39	1.33
4	A	603	OF4	O3-C22	2.22	1.37	1.30
2	E	601	NDP	C6N-C5N	2.21	1.39	1.33
2	B	601	NDP	C6N-C5N	2.20	1.39	1.33
2	C	601	NDP	C6N-C5N	2.20	1.39	1.33
4	C	603	OF4	O3-C22	2.20	1.37	1.30
5	E	604	MTX	C7-N8	2.17	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	OF4	C17-C16	2.17	1.43	1.40
4	E	603	OF4	O3-C22	2.15	1.36	1.30
4	D	603	OF4	O3-C22	2.15	1.36	1.30
4	B	603	OF4	O3-C22	2.13	1.36	1.30
2	C	601	NDP	C2N-C3N	2.05	1.40	1.35
4	E	603	OF4	C10-C11	2.04	1.42	1.39
4	D	603	OF4	C3-N2	-2.04	1.35	1.38
2	D	601	NDP	C2N-C3N	2.03	1.40	1.35
4	C	603	OF4	C1-N1	2.02	1.39	1.36
4	E	603	OF4	C2-C3	2.01	1.48	1.44
4	A	603	OF4	C2-C3	2.01	1.48	1.44
4	B	603	OF4	C2-C3	2.01	1.48	1.44
2	A	601	NDP	C2N-C3N	2.01	1.40	1.35
2	E	601	NDP	C2N-C3N	2.01	1.40	1.35
4	D	603	OF4	C10-C11	2.01	1.42	1.39

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	602	UFP	C5-C4-N3	6.84	118.90	112.64
3	A	602	UFP	C5-C4-N3	6.75	118.81	112.64
3	D	602	UFP	C5-C4-N3	6.75	118.81	112.64
3	C	602	UFP	C5-C4-N3	6.72	118.79	112.64
3	B	602	UFP	C5-C4-N3	6.50	118.58	112.64
3	E	602	UFP	O4-C4-C5	-6.13	120.47	125.69
3	A	602	UFP	O4-C4-C5	-6.13	120.47	125.69
3	C	602	UFP	O4-C4-C5	-5.89	120.67	125.69
3	D	602	UFP	O4-C4-C5	-5.85	120.71	125.69
3	B	602	UFP	F5-C5-C4	5.63	121.40	116.47
2	C	601	NDP	C5A-C4A-N3A	-5.60	119.01	126.72
2	D	601	NDP	C5A-C4A-N3A	-5.55	119.07	126.72
2	E	601	NDP	C5A-C4A-N3A	-5.48	119.17	126.72
3	D	602	UFP	F5-C5-C4	5.37	121.17	116.47
2	B	601	NDP	C5A-C4A-N3A	-5.36	119.34	126.72
3	A	602	UFP	F5-C5-C4	5.35	121.16	116.47
2	A	601	NDP	C5A-C4A-N3A	-5.35	119.35	126.72
3	B	602	UFP	O4-C4-C5	-5.34	121.14	125.69
3	C	602	UFP	F5-C5-C4	5.18	121.01	116.47
3	E	602	UFP	F5-C5-C4	5.05	120.89	116.47
5	C	604	MTX	C6-C7-N8	-4.92	118.42	123.14
5	B	604	MTX	C6-C7-N8	-4.87	118.46	123.14
5	D	604	MTX	C6-C7-N8	-4.83	118.50	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	MTX	C6-C7-N8	-4.78	118.55	123.14
3	A	602	UFP	C1'-N1-C2	4.78	127.00	117.66
3	B	602	UFP	C1'-N1-C2	4.75	126.95	117.66
5	E	604	MTX	C6-C7-N8	-4.67	118.66	123.14
3	D	602	UFP	C4-N3-C2	-4.56	121.36	127.34
3	E	602	UFP	C4-N3-C2	-4.50	121.44	127.34
3	C	602	UFP	C4-N3-C2	-4.47	121.48	127.34
3	B	602	UFP	N3-C2-N1	4.44	120.67	114.89
3	B	602	UFP	C4-N3-C2	-4.42	121.54	127.34
3	A	602	UFP	C6-C5-C4	-4.38	118.57	122.57
3	C	602	UFP	N3-C2-N1	4.37	120.58	114.89
4	A	603	OF4	C5-C2-C1	-4.37	107.67	112.68
3	A	602	UFP	C4-N3-C2	-4.35	121.63	127.34
3	C	602	UFP	C1'-N1-C2	4.35	126.17	117.66
4	C	603	OF4	C5-C2-C1	-4.33	107.71	112.68
3	D	602	UFP	C1'-N1-C2	4.33	126.12	117.66
4	D	603	OF4	C5-C2-C1	-4.31	107.73	112.68
3	D	602	UFP	N3-C2-N1	4.29	120.48	114.89
4	E	603	OF4	C5-C2-C1	-4.28	107.77	112.68
4	B	603	OF4	C5-C2-C1	-4.28	107.77	112.68
3	E	602	UFP	N3-C2-N1	4.25	120.43	114.89
3	C	602	UFP	C6-C5-C4	-4.22	118.72	122.57
3	E	602	UFP	C6-C5-C4	-4.20	118.74	122.57
5	C	604	MTX	CG-CB-CA	4.17	120.84	113.16
3	D	602	UFP	C6-C5-C4	-4.15	118.78	122.57
3	E	602	UFP	C1'-N1-C2	4.13	125.73	117.66
5	A	604	MTX	N8-C8A-N1	4.13	120.27	115.77
3	B	602	UFP	C6-C5-C4	-4.13	118.80	122.57
3	A	602	UFP	N3-C2-N1	4.12	120.26	114.89
5	D	604	MTX	N8-C8A-N1	4.08	120.21	115.77
5	A	604	MTX	CG-CB-CA	4.04	120.60	113.16
5	B	604	MTX	N8-C8A-N1	4.00	120.12	115.77
3	A	602	UFP	C1'-N1-C6	-4.00	114.03	120.74
4	B	603	OF4	C8-C7-C5	-3.95	105.75	114.10
5	D	604	MTX	CG-CB-CA	3.94	120.43	113.16
5	E	604	MTX	N1-C2-N3	-3.93	122.21	127.21
5	C	604	MTX	N8-C8A-N1	3.91	120.03	115.77
5	D	604	MTX	N1-C2-N3	-3.89	122.26	127.21
5	C	604	MTX	N1-C2-N3	-3.88	122.28	127.21
5	B	604	MTX	N1-C2-N3	-3.87	122.29	127.21
2	E	601	NDP	N3A-C2A-N1A	-3.87	122.73	128.58
2	C	601	NDP	N3A-C2A-N1A	-3.84	122.77	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	NDP	N3A-C4A-N9A	3.81	133.65	127.17
5	E	604	MTX	CG-CB-CA	3.80	120.17	113.16
3	B	602	UFP	C1'-N1-C6	-3.80	114.36	120.74
2	E	601	NDP	N3A-C4A-N9A	3.80	133.63	127.17
2	D	601	NDP	N3A-C4A-N9A	3.80	133.62	127.17
5	A	604	MTX	N1-C2-N3	-3.79	122.39	127.21
2	B	601	NDP	N3A-C2A-N1A	-3.77	122.87	128.58
2	D	601	NDP	N3A-C2A-N1A	-3.75	122.91	128.58
5	E	604	MTX	N8-C8A-N1	3.74	119.84	115.77
5	B	604	MTX	CG-CB-CA	3.72	120.02	113.16
2	A	601	NDP	N3A-C4A-N9A	3.71	133.48	127.17
2	A	601	NDP	N3A-C2A-N1A	-3.70	122.98	128.58
5	A	604	MTX	C2-N1-C8A	3.64	119.41	115.48
2	B	601	NDP	N3A-C4A-N9A	3.61	133.31	127.17
4	D	603	OF4	C8-C7-C5	-3.61	106.48	114.10
5	B	604	MTX	C2-N1-C8A	3.58	119.34	115.48
3	D	602	UFP	C1'-N1-C6	-3.55	114.78	120.74
5	C	604	MTX	C2-N1-C8A	3.55	119.31	115.48
5	E	604	MTX	C2-N1-C8A	3.53	119.29	115.48
5	D	604	MTX	C2-N1-C8A	3.53	119.28	115.48
2	C	601	NDP	C2A-N3A-C4A	3.50	120.37	111.83
2	E	601	NDP	C2A-N3A-C4A	3.45	120.25	111.83
3	C	602	UFP	C1'-N1-C6	-3.41	115.01	120.74
2	D	601	NDP	C2A-N3A-C4A	3.41	120.15	111.83
2	B	601	NDP	C2A-N3A-C4A	3.36	120.03	111.83
3	E	602	UFP	C1'-N1-C6	-3.33	115.15	120.74
2	A	601	NDP	C2A-N3A-C4A	3.32	119.94	111.83
2	B	601	NDP	N9A-C8A-N7A	-3.23	109.35	113.94
3	B	602	UFP	O2-C2-N3	-3.22	115.55	121.49
2	A	601	NDP	N9A-C8A-N7A	-3.21	109.38	113.94
2	C	601	NDP	C4A-C5A-N7A	-3.20	106.93	110.58
2	E	601	NDP	N9A-C8A-N7A	-3.19	109.40	113.94
2	C	601	NDP	N9A-C8A-N7A	-3.16	109.45	113.94
2	D	601	NDP	C4A-C5A-N7A	-3.15	106.98	110.58
2	B	601	NDP	C4A-C5A-N7A	-3.13	107.01	110.58
2	D	601	NDP	N9A-C8A-N7A	-3.13	109.50	113.94
2	C	601	NDP	C5A-N7A-C8A	3.10	108.33	103.45
5	D	604	MTX	C11-C-N	3.10	122.79	117.04
5	B	604	MTX	C11-C-N	3.08	122.75	117.04
2	A	601	NDP	C4A-C5A-N7A	-3.08	107.06	110.58
2	E	601	NDP	C4A-C5A-N7A	-3.07	107.07	110.58
2	D	601	NDP	C5A-N7A-C8A	3.05	108.25	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	NDP	C5A-N7A-C8A	3.04	108.23	103.45
2	B	601	NDP	C5A-N7A-C8A	3.03	108.20	103.45
2	A	601	NDP	C5A-N7A-C8A	3.02	108.20	103.45
4	C	603	OF4	C8-C7-C5	-3.02	107.73	114.10
3	B	602	UFP	O4'-C1'-C2'	-2.99	100.65	106.25
3	A	602	UFP	O2-C2-N3	-2.91	116.12	121.49
3	D	602	UFP	O2-C2-N3	-2.91	116.13	121.49
3	C	602	UFP	O2-C2-N3	-2.89	116.16	121.49
5	C	604	MTX	C11-C-N	2.86	122.34	117.04
4	E	603	OF4	C8-C7-C5	-2.84	108.10	114.10
5	E	604	MTX	C11-C-N	2.80	122.22	117.04
3	C	602	UFP	O4'-C1'-C2'	-2.76	101.08	106.25
3	D	602	UFP	O4'-C1'-C2'	-2.76	101.09	106.25
5	A	604	MTX	C11-C-N	2.76	122.15	117.04
3	E	602	UFP	O2-C2-N3	-2.70	116.51	121.49
2	D	601	NDP	O5B-C5B-C4B	2.68	118.12	108.99
3	B	602	UFP	C6-N1-C2	-2.63	118.69	121.30
4	C	603	OF4	N4-C4-N2	-2.61	111.26	116.76
5	A	604	MTX	C13-C14-N10	-2.59	117.98	121.59
4	B	603	OF4	N4-C4-N2	-2.57	111.34	116.76
4	D	603	OF4	N4-C4-N2	-2.54	111.39	116.76
4	A	603	OF4	C8-C7-C5	-2.53	108.76	114.10
3	C	602	UFP	C6-N1-C2	-2.49	118.82	121.30
4	E	603	OF4	N4-C4-N2	-2.48	111.52	116.76
4	A	603	OF4	N4-C4-N2	-2.48	111.53	116.76
2	D	601	NDP	O5D-C5D-C4D	2.46	117.37	108.99
2	E	601	NDP	O5B-C5B-C4B	2.44	117.31	108.99
3	E	602	UFP	O4'-C1'-C2'	-2.42	101.72	106.25
5	D	604	MTX	C7-N8-C8A	2.41	120.56	117.20
5	C	604	MTX	C7-N8-C8A	2.40	120.54	117.20
4	C	603	OF4	N4-C4-N1	2.39	124.34	119.67
2	E	601	NDP	O5D-C5D-C4D	2.37	117.06	108.99
5	E	604	MTX	C7-N8-C8A	2.36	120.48	117.20
5	B	604	MTX	C13-C14-N10	-2.35	118.31	121.59
3	A	602	UFP	C6-N1-C2	-2.35	118.97	121.30
4	A	603	OF4	N4-C4-N1	2.34	124.24	119.67
4	D	603	OF4	N4-C4-N1	2.34	124.23	119.67
3	A	602	UFP	O4'-C1'-C2'	-2.33	101.89	106.25
2	A	601	NDP	C4A-N9A-C8A	2.33	108.18	105.74
4	B	603	OF4	N4-C4-N1	2.30	124.16	119.67
2	C	601	NDP	O5B-C5B-C4B	2.27	116.72	108.99
2	A	601	NDP	O5B-C5B-C4B	2.27	116.72	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	603	OF4	N4-C4-N1	2.27	124.10	119.67
2	E	601	NDP	C4A-N9A-C8A	2.24	108.09	105.74
5	A	604	MTX	C7-N8-C8A	2.24	120.32	117.20
2	C	601	NDP	O5D-C5D-C4D	2.24	116.62	108.99
2	B	601	NDP	C4A-N9A-C8A	2.23	108.08	105.74
3	D	602	UFP	C6-N1-C2	-2.22	119.10	121.30
3	E	602	UFP	C6-N1-C2	-2.20	119.11	121.30
5	B	604	MTX	C7-N8-C8A	2.19	120.24	117.20
2	B	601	NDP	C3N-C7N-N7N	2.18	121.54	117.67
5	D	604	MTX	C13-C14-N10	-2.17	118.56	121.59
2	A	601	NDP	O5D-C5D-C4D	2.13	116.26	108.99
2	E	601	NDP	C3N-C7N-N7N	2.13	121.44	117.67
2	A	601	NDP	O4D-C1D-N1N	2.13	112.14	108.08
2	D	601	NDP	C4A-N9A-C8A	2.12	107.96	105.74
5	C	604	MTX	C13-C14-N10	-2.12	118.64	121.59
2	C	601	NDP	C4A-N9A-C8A	2.11	107.96	105.74
4	E	603	OF4	C15-C16-C17	2.08	124.09	121.99
2	D	601	NDP	C2B-C1B-N9A	-2.08	110.33	113.75
4	E	603	OF4	C7-C8-C13	-2.08	117.83	120.89
4	E	603	OF4	C15-C16-C21	-2.07	116.40	120.98
5	E	604	MTX	C13-C14-N10	-2.07	118.70	121.59
2	B	601	NDP	O5B-C5B-C4B	2.06	116.01	108.99
2	C	601	NDP	C3N-C7N-N7N	2.05	121.31	117.67
4	D	603	OF4	C7-C8-C13	-2.04	117.90	120.89
5	D	604	MTX	O-C-N	-2.03	118.61	122.47
2	A	601	NDP	C3N-C7N-N7N	2.01	121.24	117.67
2	D	601	NDP	O4D-C1D-N1N	2.01	111.91	108.08
2	B	601	NDP	O5D-C5D-C4D	2.00	115.80	108.99

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	UFP	C5'-O5'-P-O2P
3	B	602	UFP	C5'-O5'-P-O3P
3	C	602	UFP	C5'-O5'-P-O2P
3	C	602	UFP	C5'-O5'-P-O3P
3	D	602	UFP	C5'-O5'-P-O2P
3	D	602	UFP	C5'-O5'-P-O3P
5	C	604	MTX	N-CA-CB-CG
5	A	604	MTX	N-CA-CB-CG
5	B	604	MTX	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	D	601	NDP	C3D-C4D-C5D-O5D
5	B	604	MTX	CT-CA-CB-CG
2	D	601	NDP	O4D-C4D-C5D-O5D
3	E	602	UFP	C3'-C4'-C5'-O5'
5	A	604	MTX	CT-CA-CB-CG
5	C	604	MTX	CT-CA-CB-CG
2	E	601	NDP	C3D-C4D-C5D-O5D
3	E	602	UFP	O4'-C4'-C5'-O5'
3	B	602	UFP	C2'-C1'-N1-C2
5	D	604	MTX	N-CA-CB-CG
3	A	602	UFP	C2'-C1'-N1-C2
5	D	604	MTX	CT-CA-CB-CG
3	B	602	UFP	C5'-O5'-P-O1P
3	C	602	UFP	C5'-O5'-P-O1P
3	D	602	UFP	C5'-O5'-P-O1P
5	E	604	MTX	CT-CA-CB-CG
2	E	601	NDP	O4D-C4D-C5D-O5D
3	A	602	UFP	C2'-C1'-N1-C6
3	B	602	UFP	C2'-C1'-N1-C6
5	E	604	MTX	N-CA-CB-CG
4	D	603	OF4	C18-C17-C22-O4
3	C	602	UFP	C2'-C1'-N1-C2
3	D	602	UFP	C2'-C1'-N1-C2
3	E	602	UFP	C2'-C1'-N1-C2
4	D	603	OF4	C18-C17-C22-O3
4	B	603	OF4	C18-C17-C22-O4
2	D	601	NDP	C5D-O5D-PN-O2N
4	D	603	OF4	C16-C17-C22-O4
4	B	603	OF4	C18-C17-C22-O3
5	E	604	MTX	C13-C14-N10-CM
4	D	603	OF4	C16-C17-C22-O3
3	C	602	UFP	C2'-C1'-N1-C6
3	E	602	UFP	C2'-C1'-N1-C6
4	B	603	OF4	N5-C15-C16-C21
4	D	603	OF4	N5-C15-C16-C21
5	E	604	MTX	C15-C14-N10-CM
4	C	603	OF4	N5-C15-C16-C21
4	E	603	OF4	N5-C15-C16-C21
4	A	603	OF4	N5-C15-C16-C21
2	B	601	NDP	O4D-C1D-N1N-C2N
2	D	601	NDP	O4D-C1D-N1N-C2N
2	E	601	NDP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	B	603	OF4	C16-C17-C22-O4
5	A	604	MTX	C15-C14-N10-CM
5	D	604	MTX	C15-C14-N10-CM
4	B	603	OF4	C16-C17-C22-O3
2	A	601	NDP	O4D-C1D-N1N-C2N
2	C	601	NDP	O4D-C1D-N1N-C2N
2	E	601	NDP	C2N-C3N-C7N-N7N
3	D	602	UFP	C2'-C1'-N1-C6
5	B	604	MTX	C15-C14-N10-CM
5	C	604	MTX	C15-C14-N10-CM
4	A	603	OF4	C18-C17-C22-O4
4	A	603	OF4	C18-C17-C22-O3
5	E	604	MTX	OE2-CD-CG-CB
5	D	604	MTX	OE2-CD-CG-CB
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	D	604	MTX	C13-C14-N10-CM
5	B	604	MTX	OE2-CD-CG-CB
2	C	601	NDP	C2D-C1D-N1N-C2N
5	A	604	MTX	OE2-CD-CG-CB
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
5	C	604	MTX	OE2-CD-CG-CB
2	A	601	NDP	C2D-C1D-N1N-C2N
2	E	601	NDP	C2D-C1D-N1N-C2N
3	A	602	UFP	O4'-C4'-C5'-O5'
2	D	601	NDP	C4D-C5D-O5D-PN
2	C	601	NDP	C4D-C5D-O5D-PN
2	E	601	NDP	C4D-C5D-O5D-PN
2	A	601	NDP	C4D-C5D-O5D-PN
2	B	601	NDP	C4D-C5D-O5D-PN
2	C	601	NDP	C3B-C4B-C5B-O5B

There are no ring outliers.

13 monomers are involved in 20 short contacts:

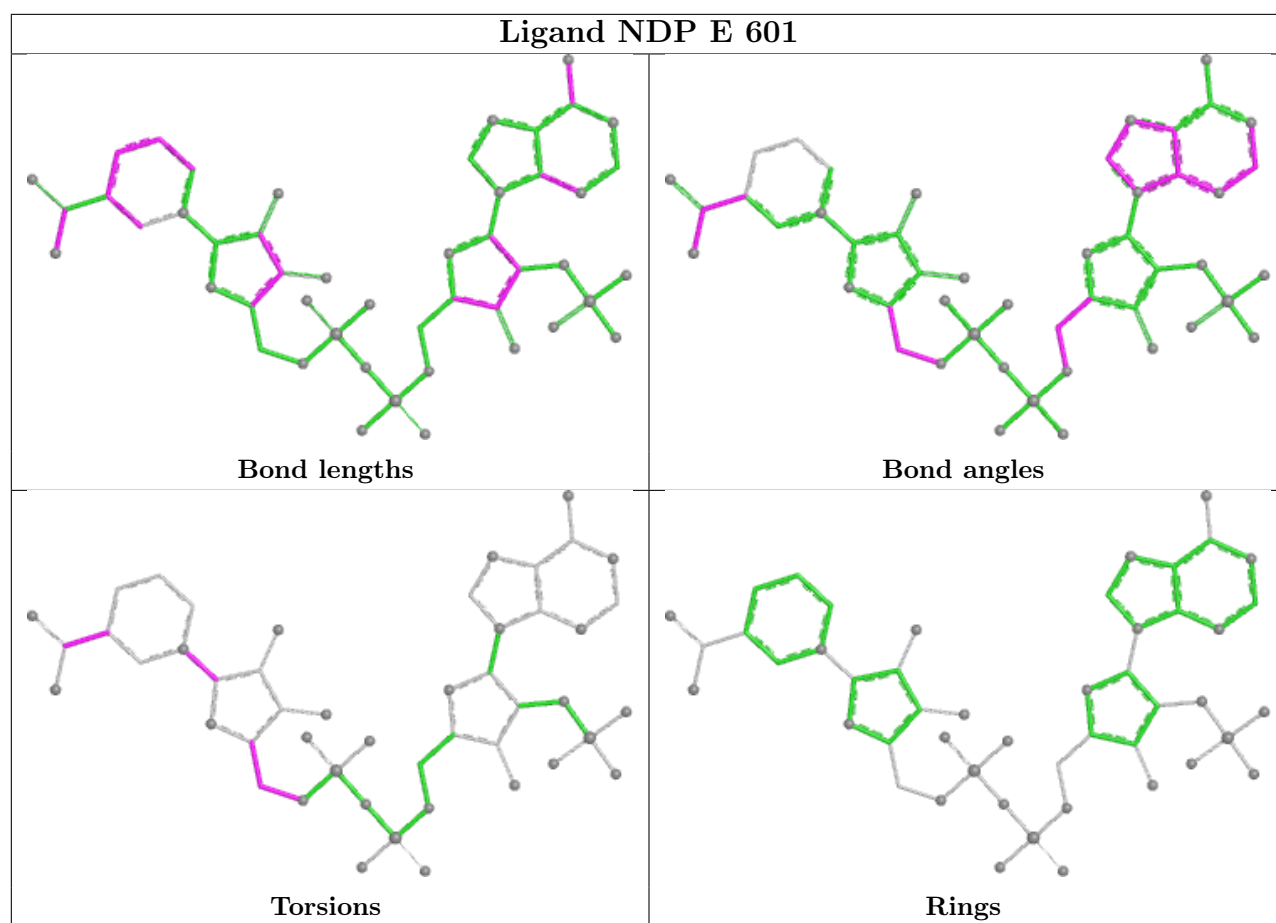
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	MTX	1	0

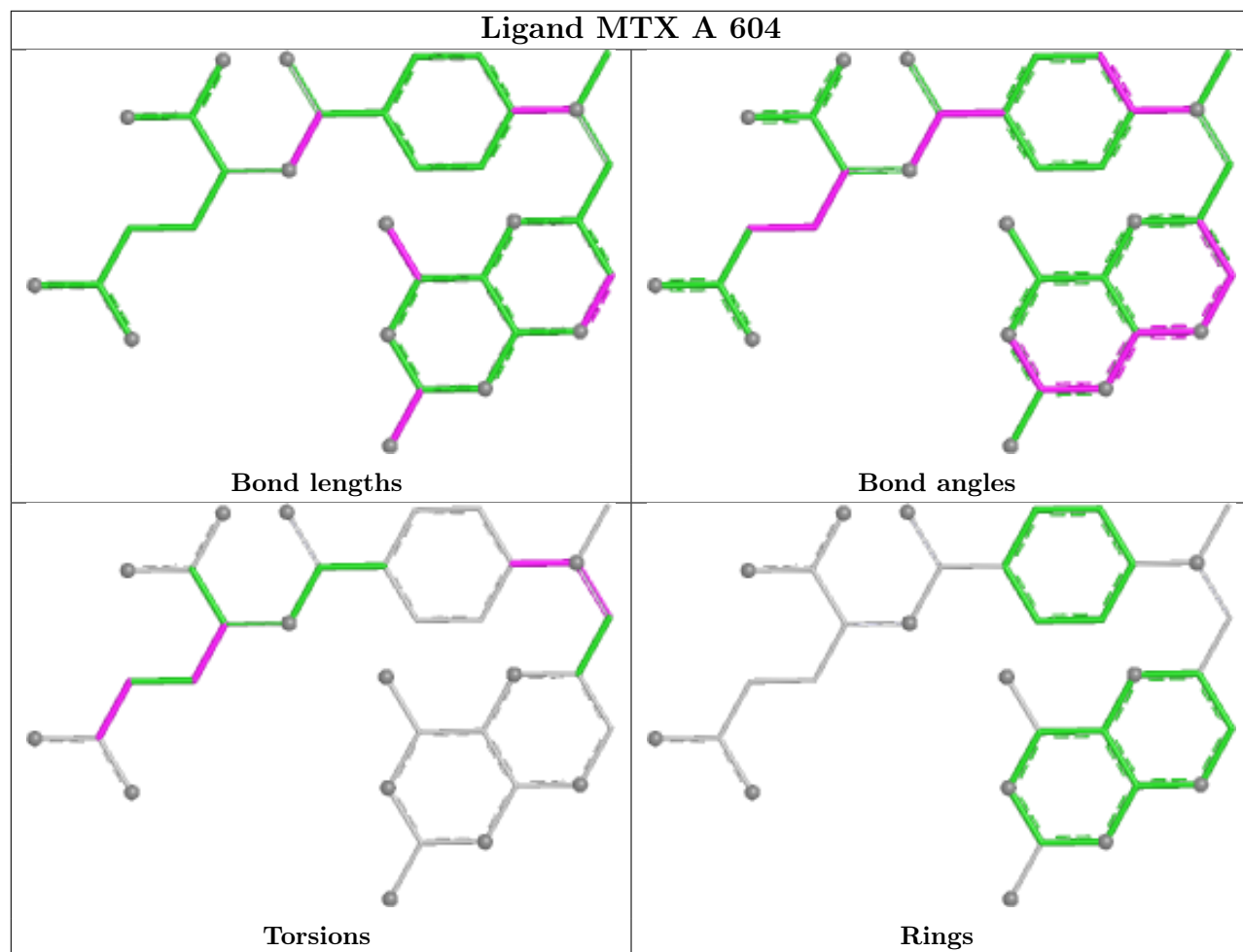
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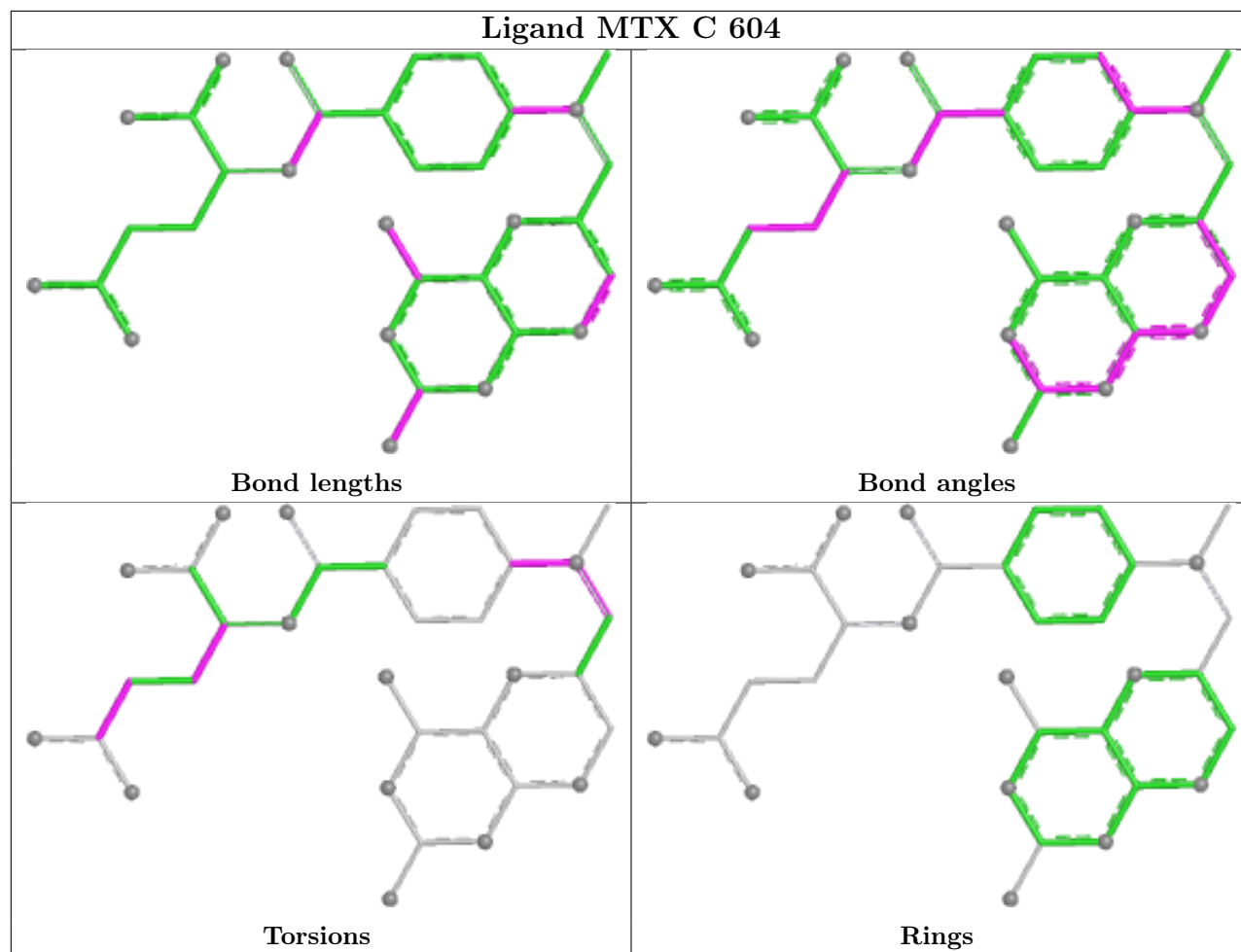
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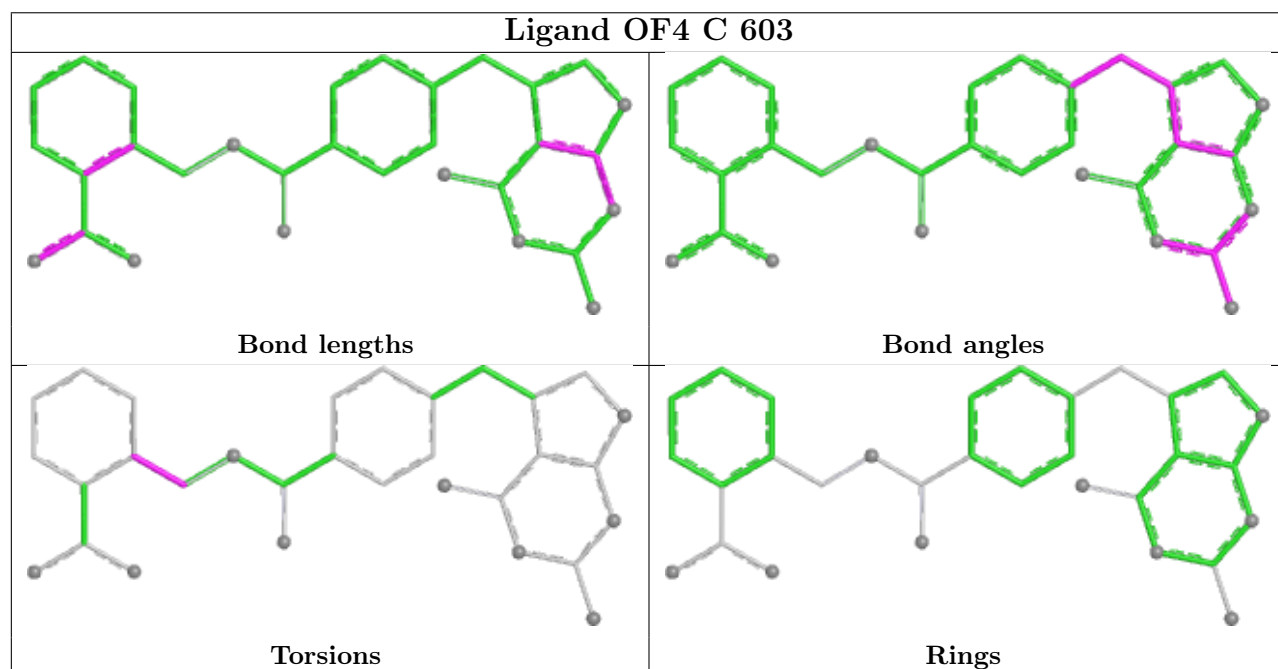
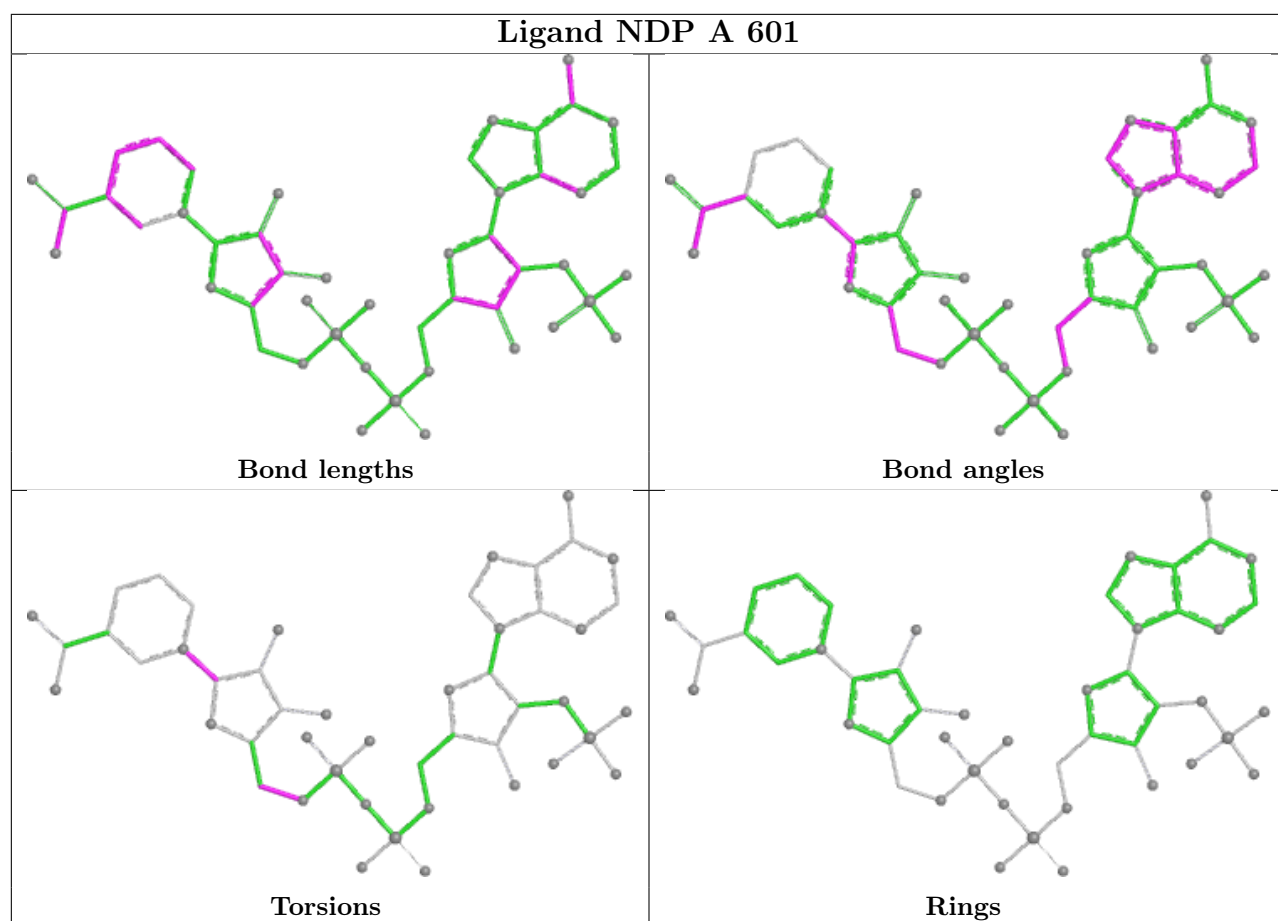
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	604	MTX	2	0
2	A	601	NDP	2	0
5	D	604	MTX	1	0
5	E	604	MTX	1	0
2	C	601	NDP	2	0
4	B	603	OF4	1	0
3	B	602	UFP	3	0
3	C	602	UFP	2	0
5	B	604	MTX	2	0
3	E	602	UFP	1	0
2	B	601	NDP	1	0
3	D	602	UFP	3	0

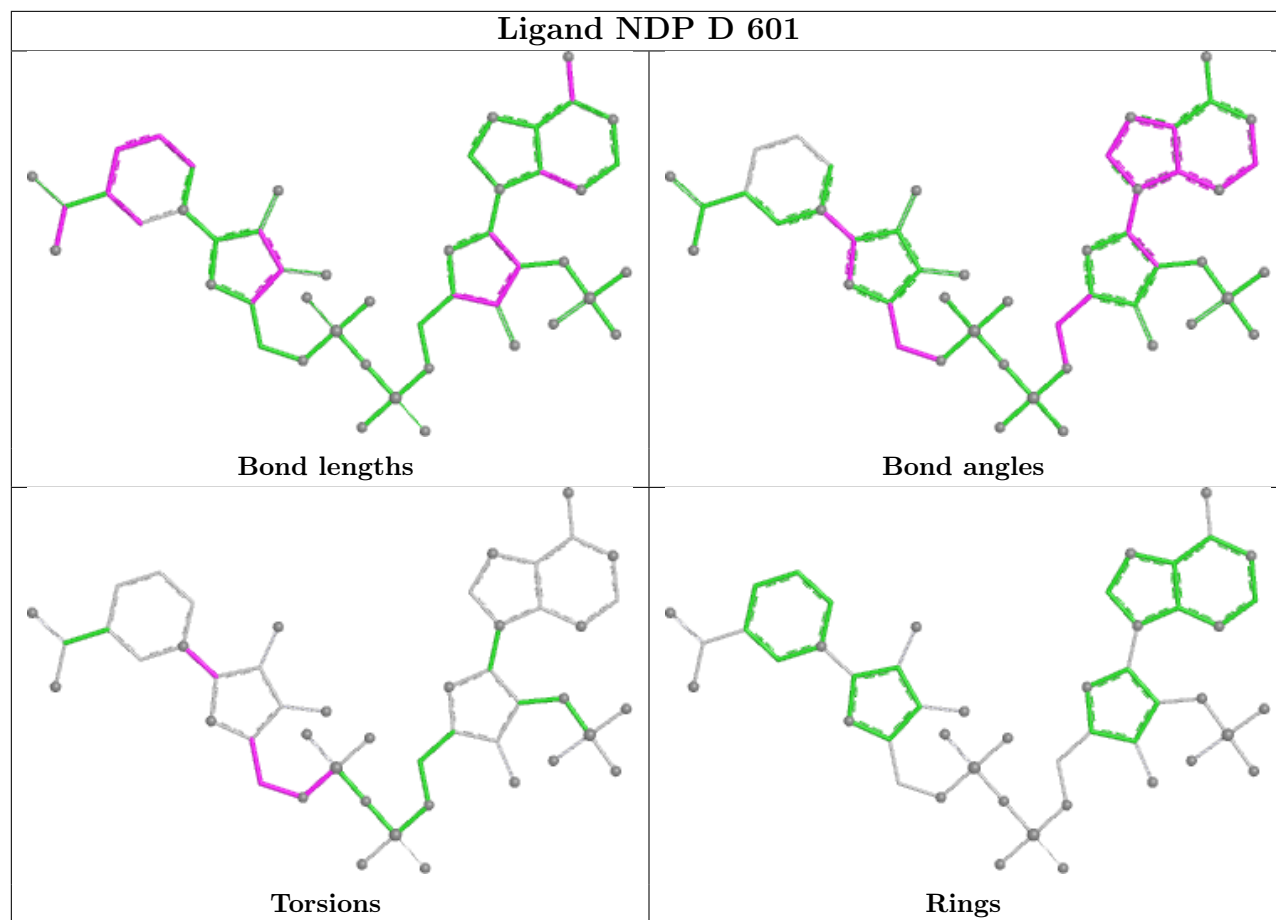
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

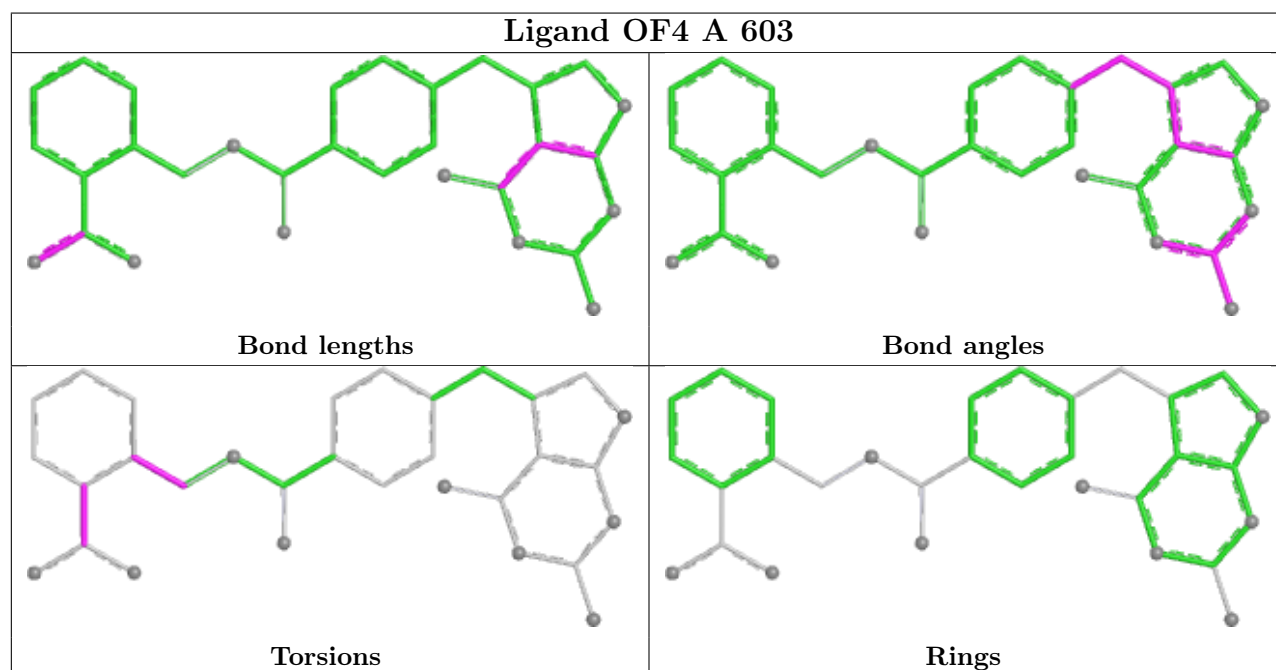
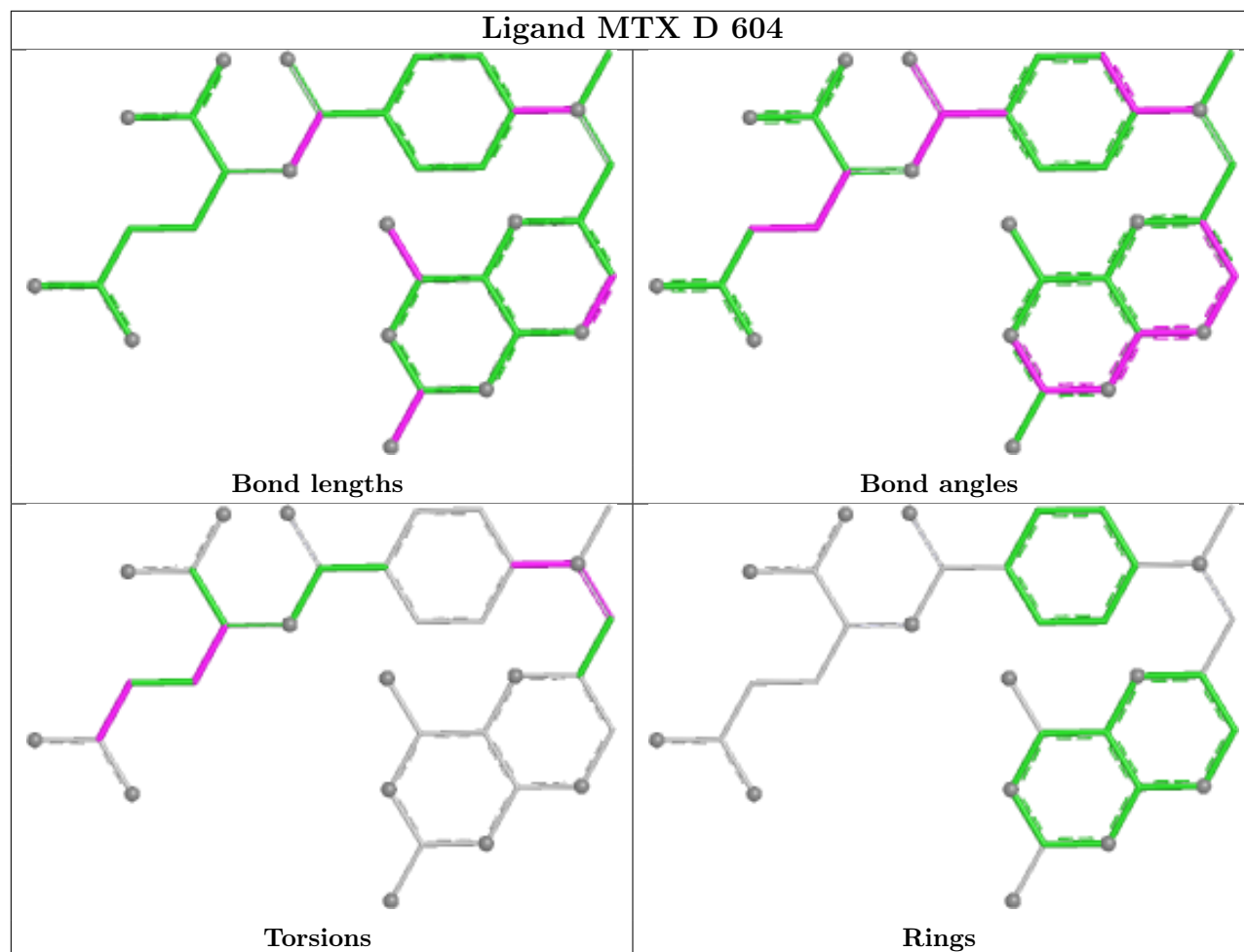


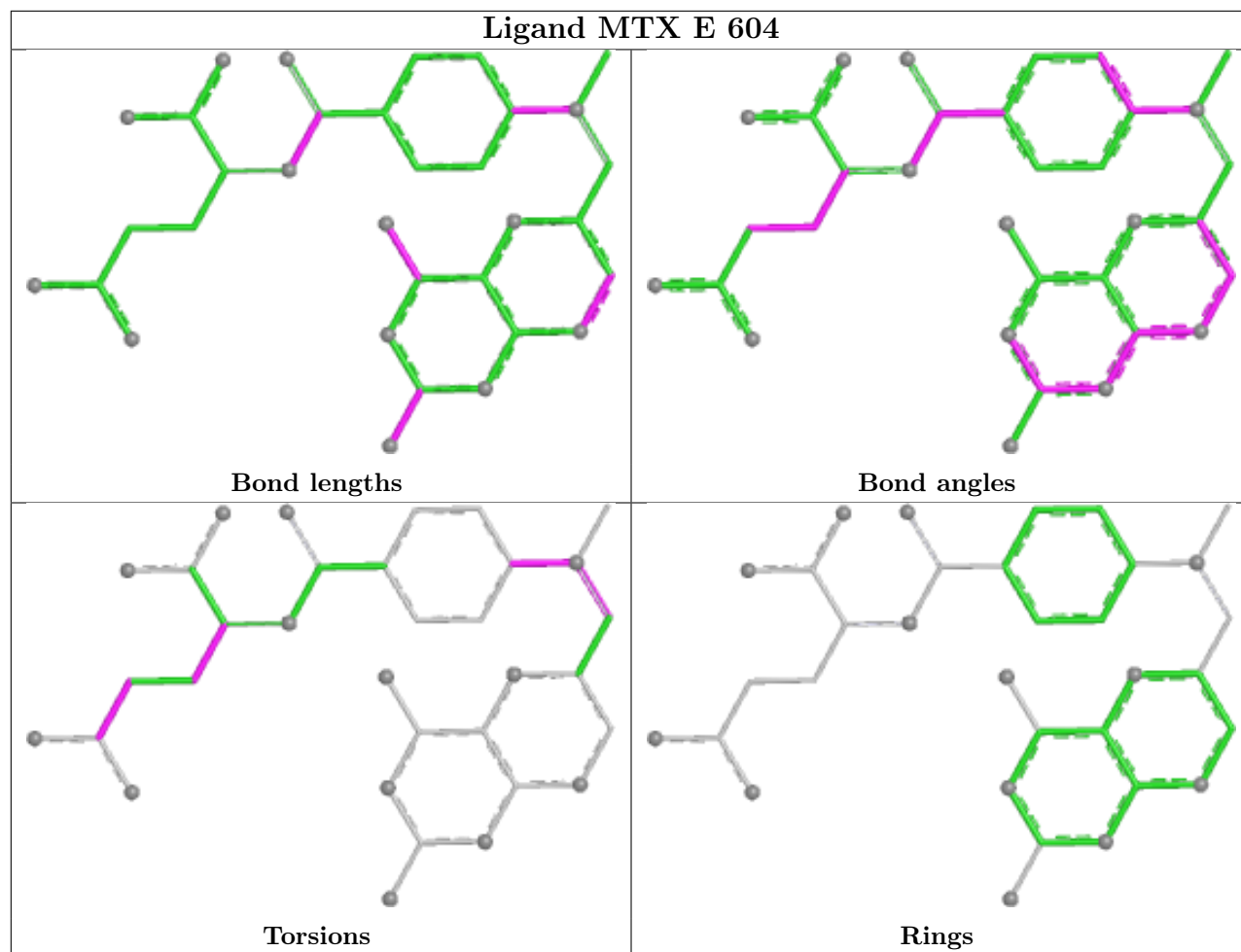


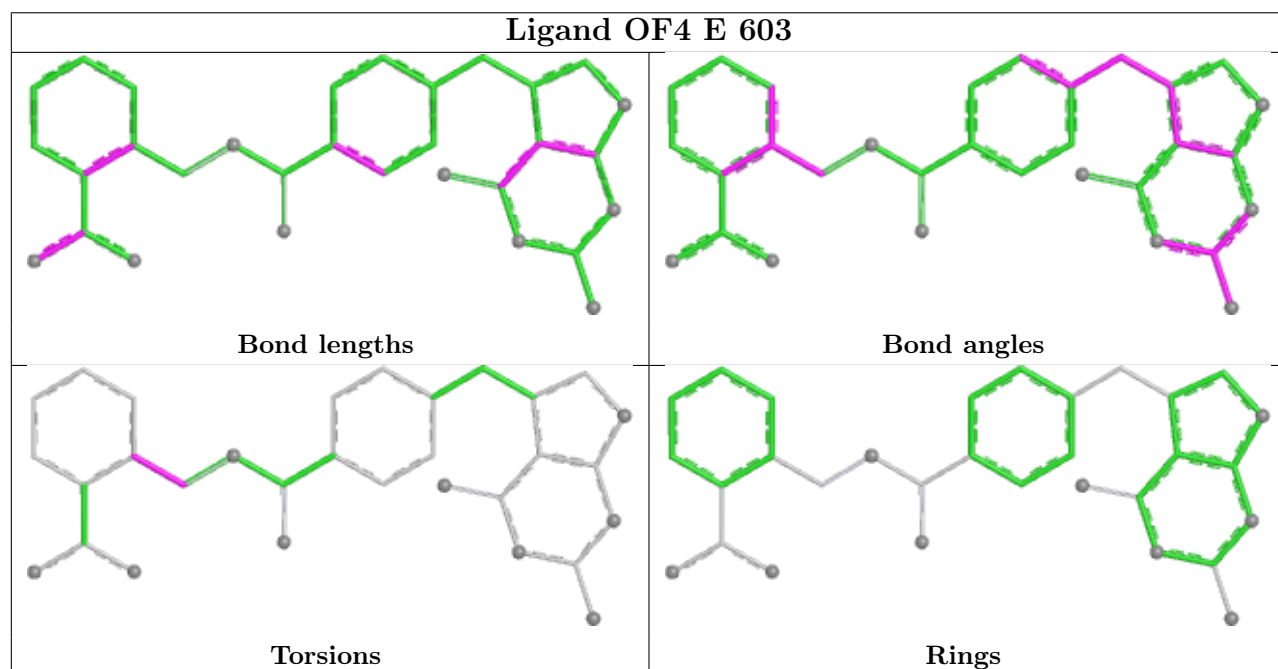
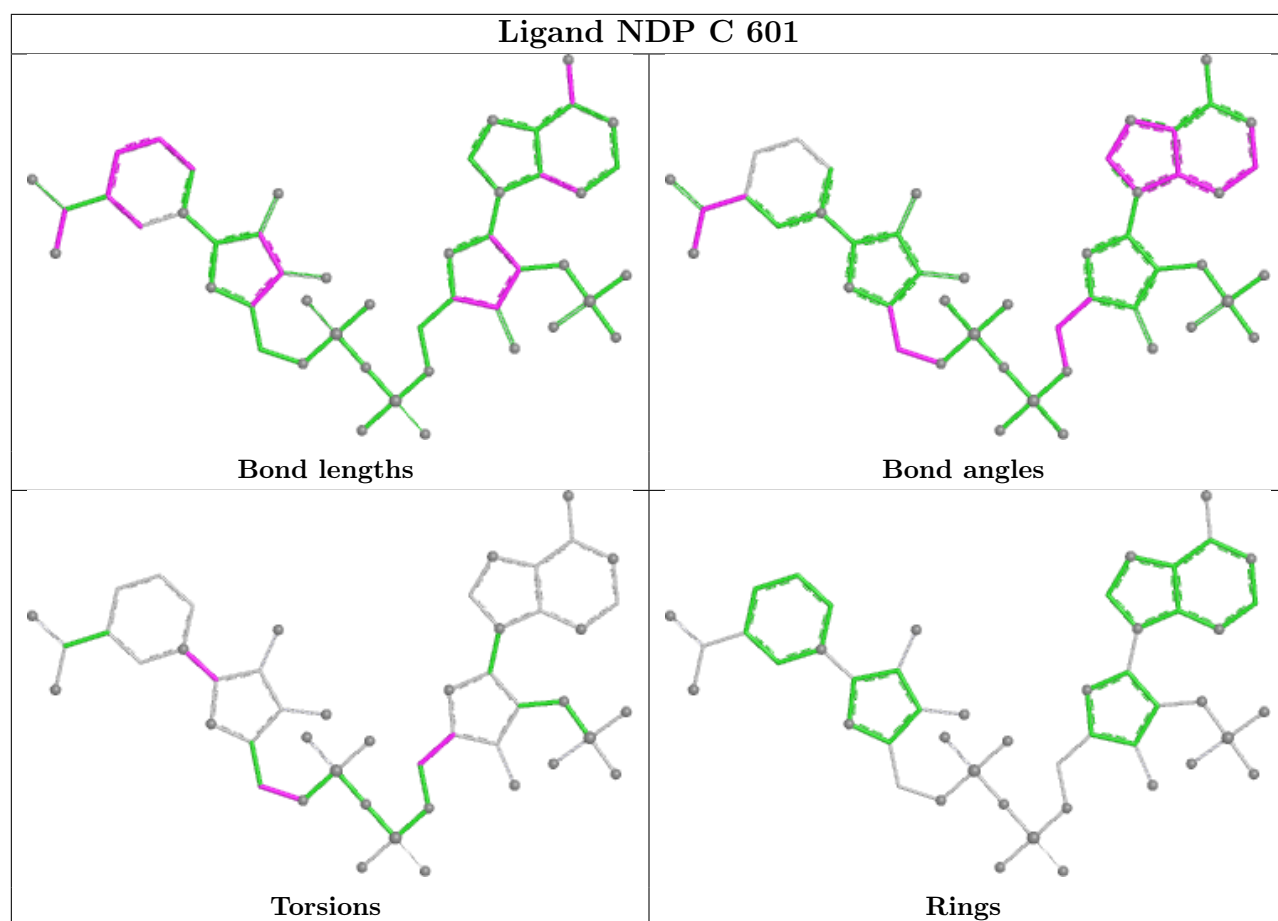


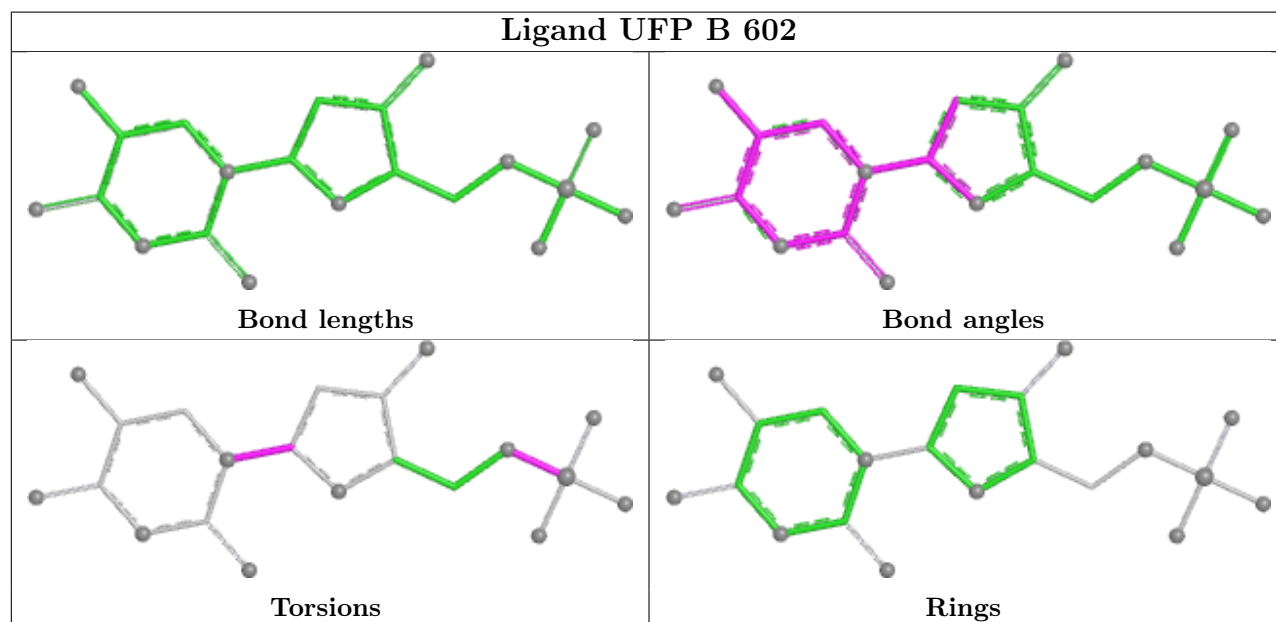
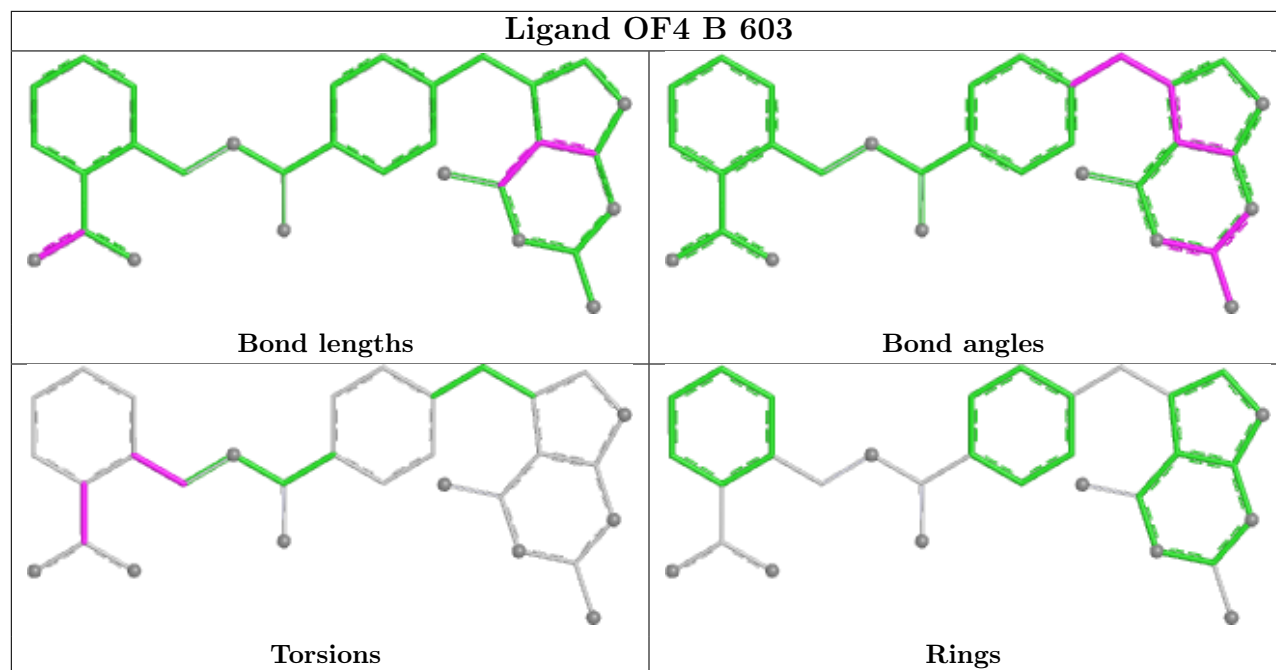


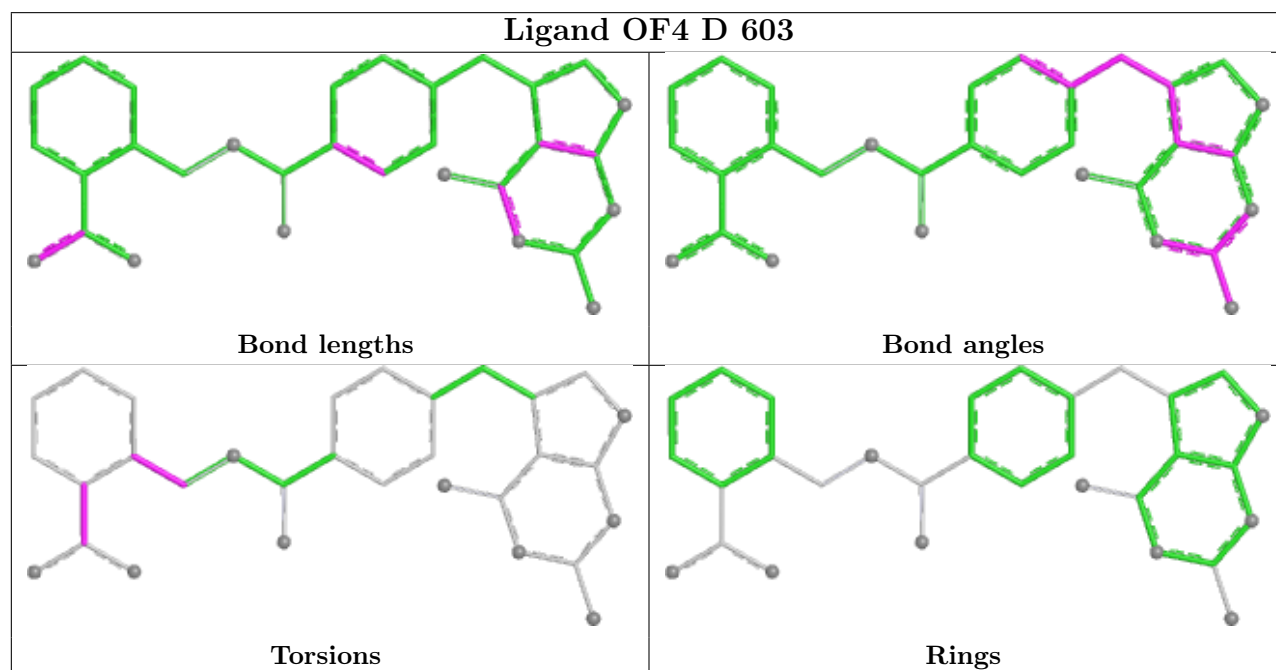
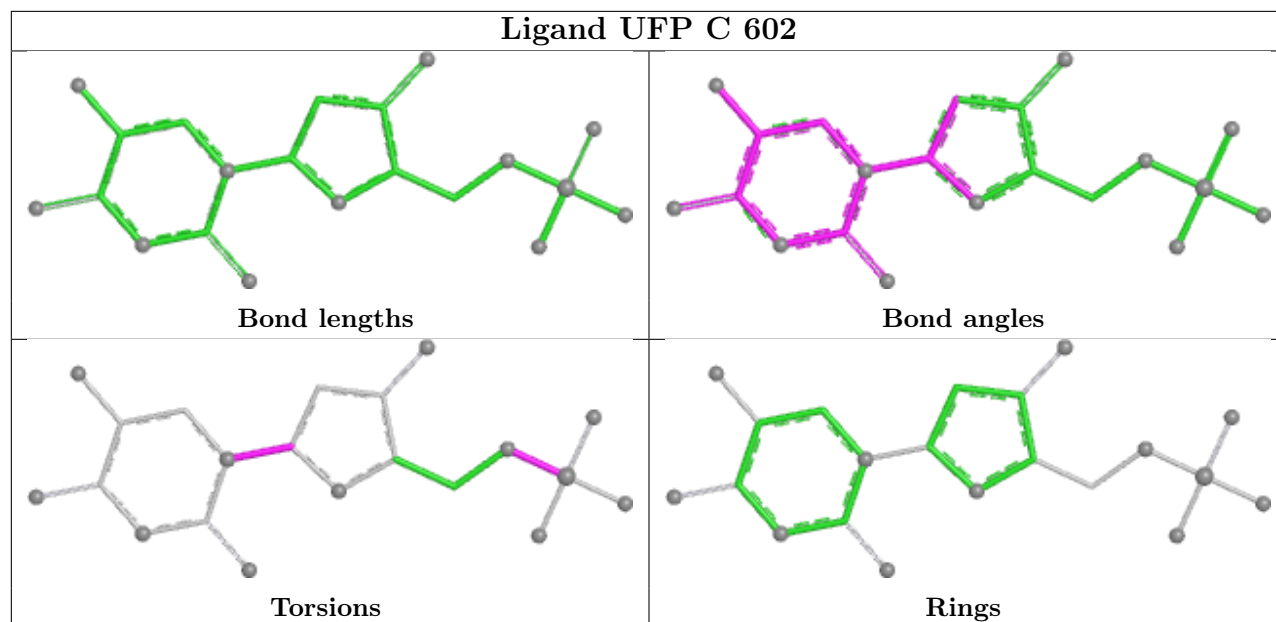


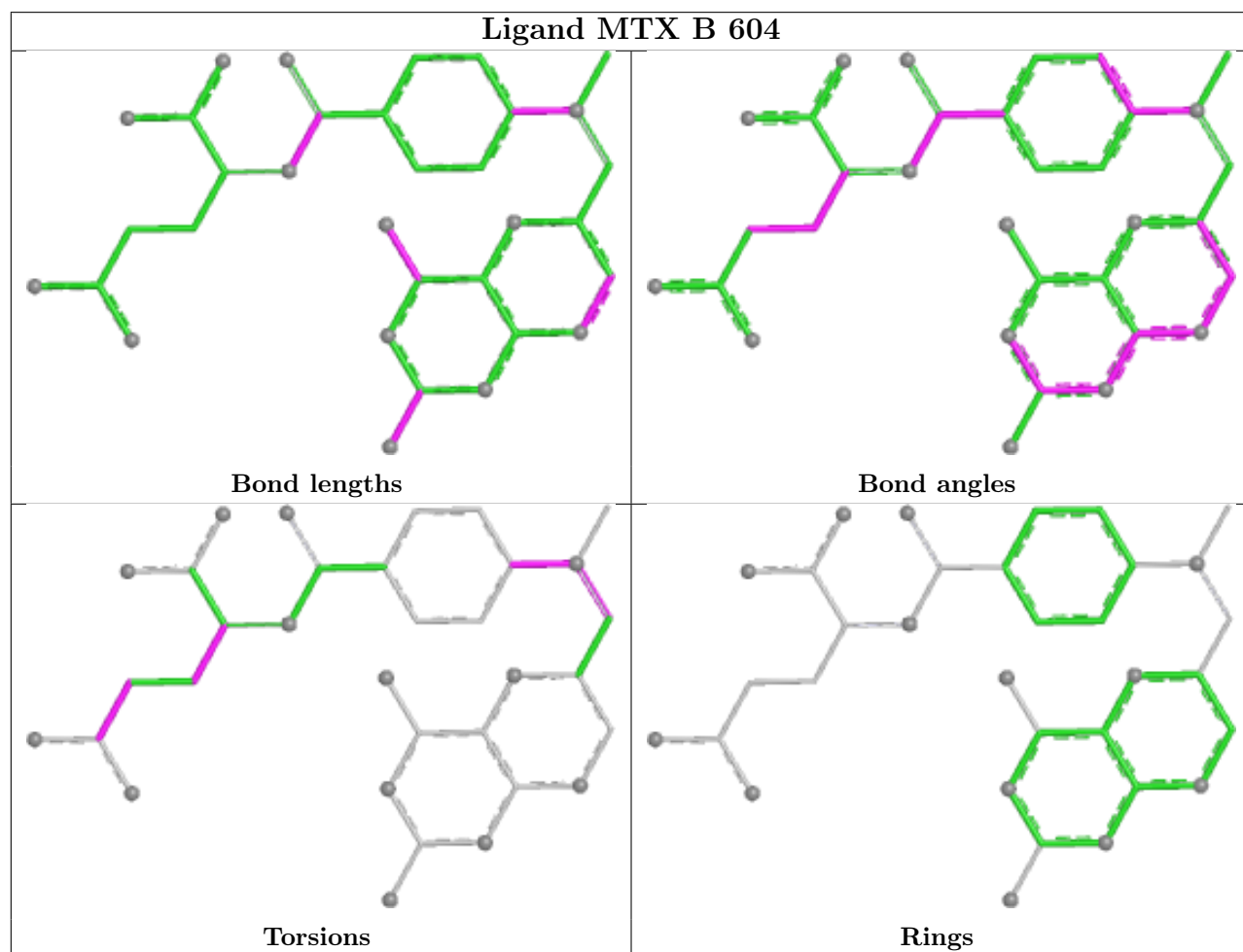
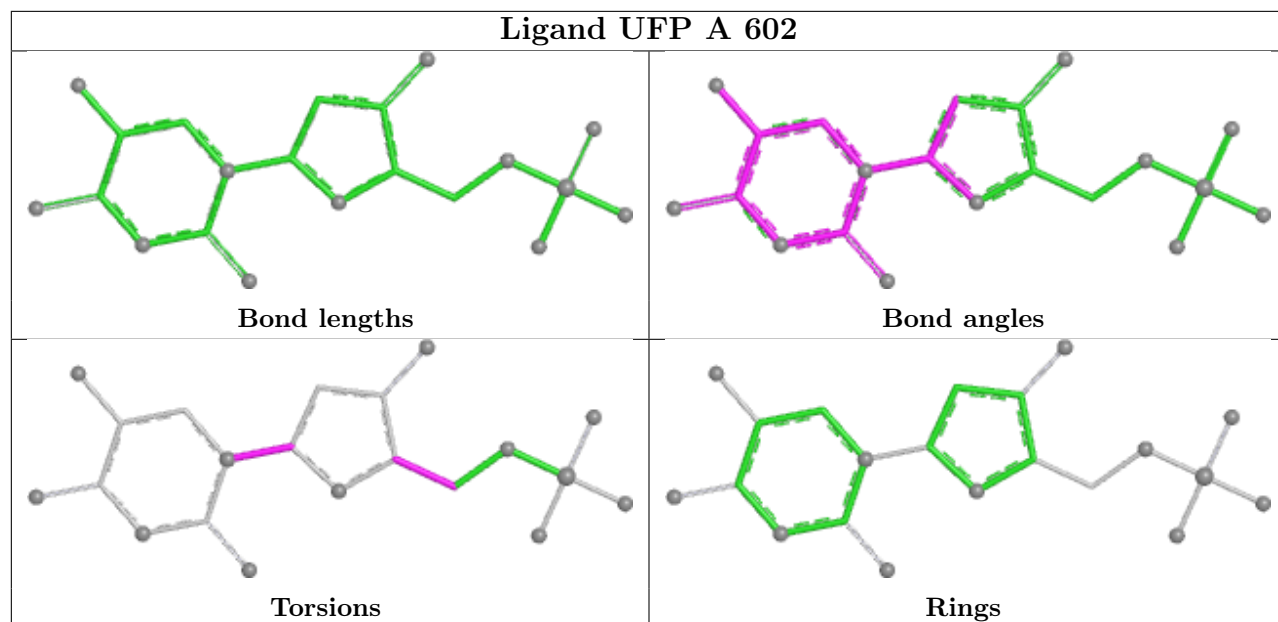




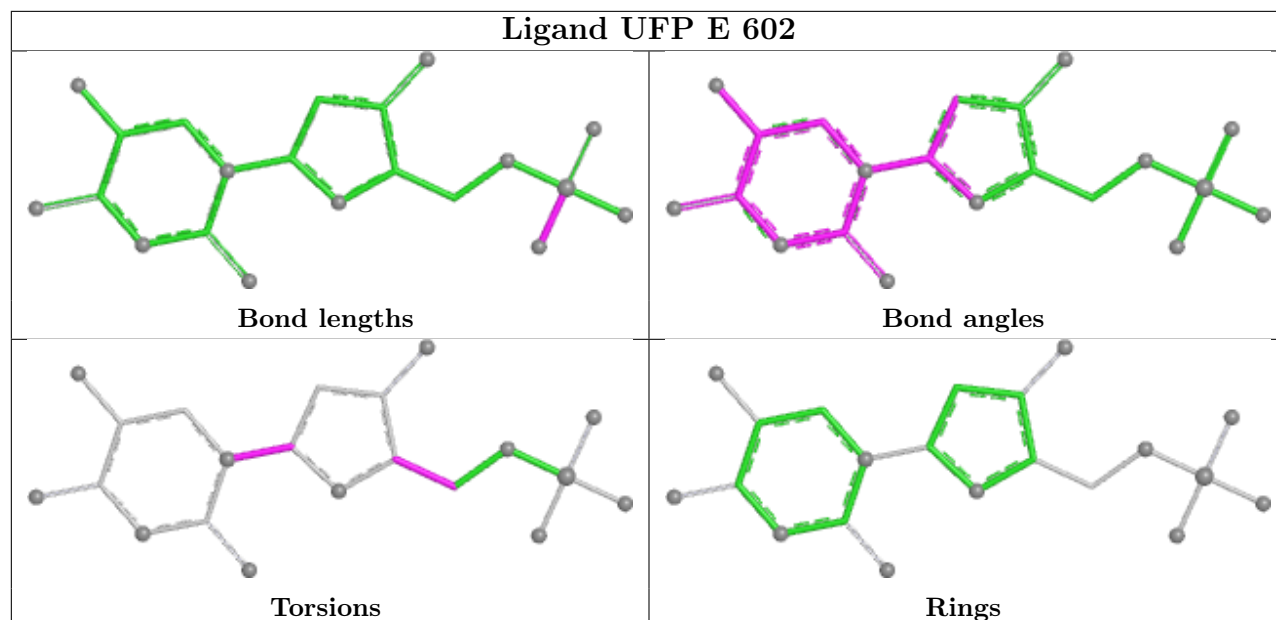




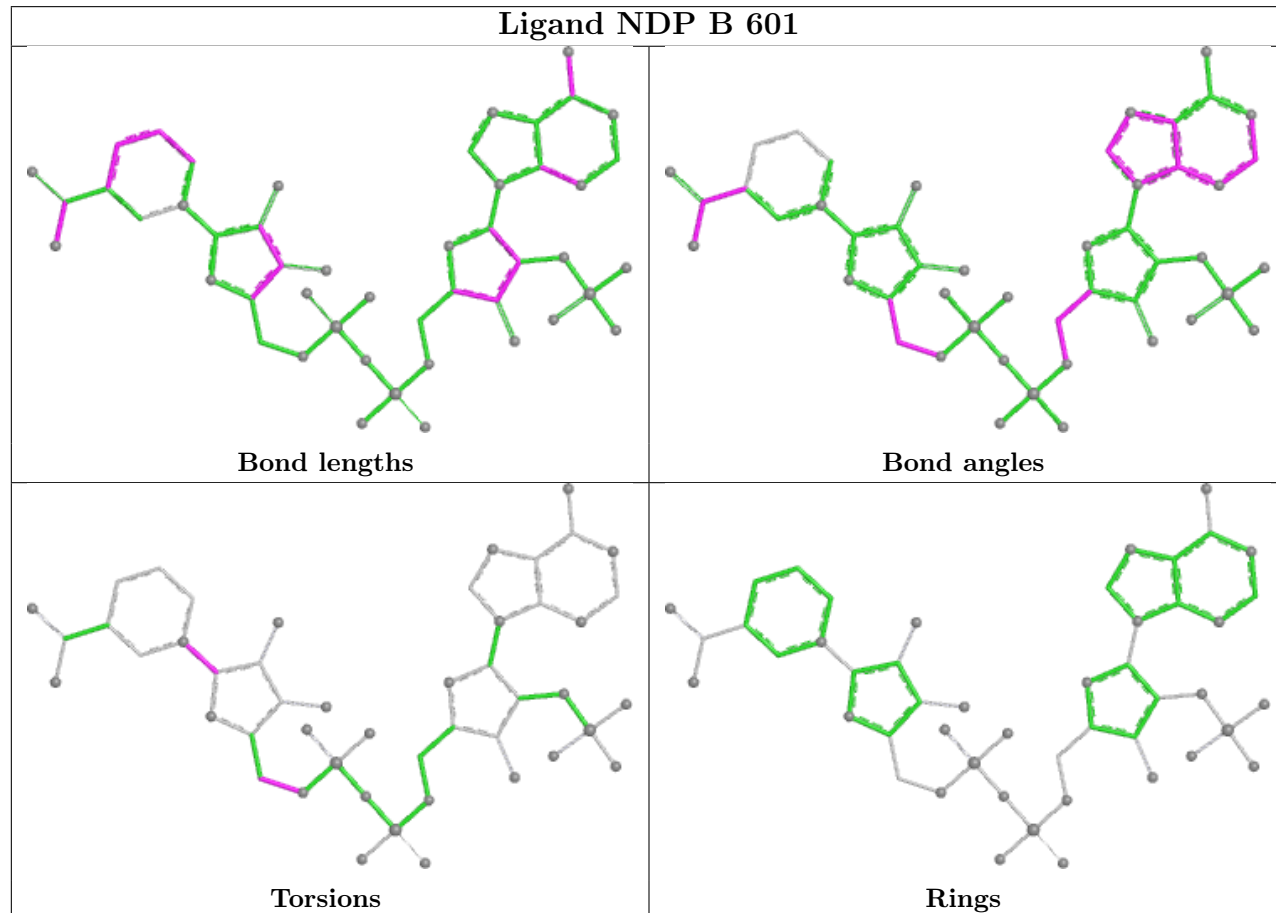


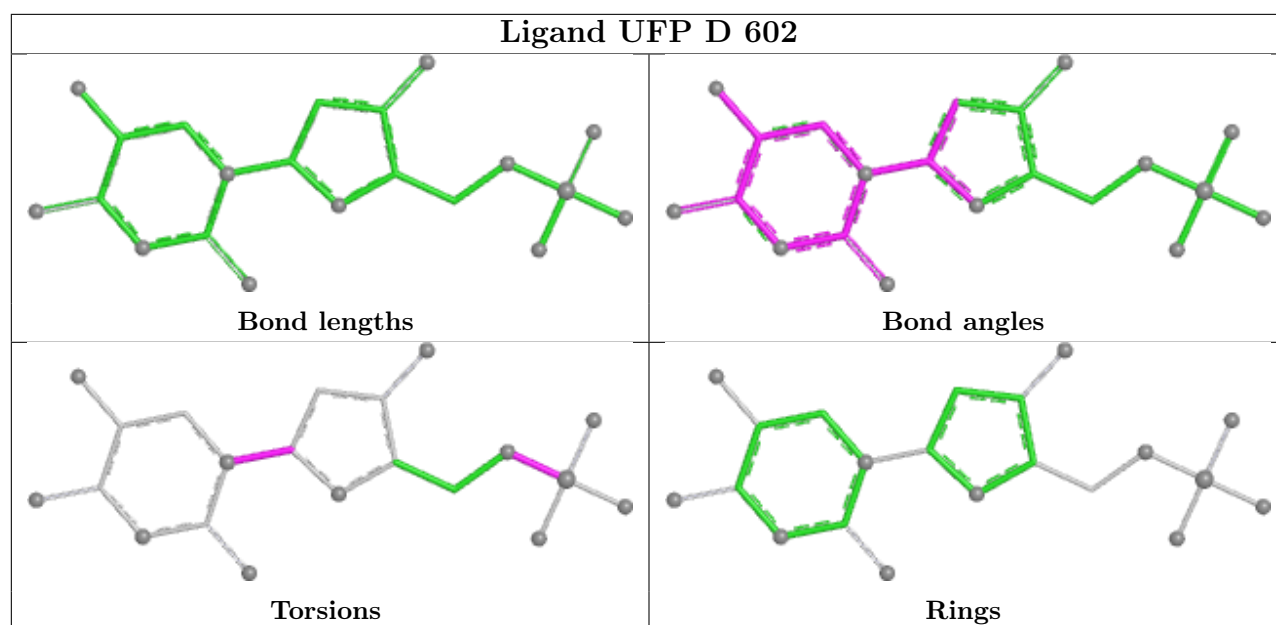


Ligand UFP E 602



Ligand NDP B 601





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	506/521 (97%)	0.58	26 (5%)	33	25	42, 60, 91, 120	0
1	B	506/521 (97%)	0.40	21 (4%)	40	32	40, 56, 82, 124	0
1	C	505/521 (96%)	0.75	31 (6%)	27	20	52, 73, 102, 140	0
1	D	506/521 (97%)	0.73	36 (7%)	22	16	48, 70, 108, 150	0
1	E	506/521 (97%)	1.30	88 (17%)	4	3	69, 90, 125, 143	0
All	All	2529/2605 (97%)	0.75	202 (7%)	18	13	40, 70, 113, 150	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	LEU	7.2
1	E	193	LEU	6.6
1	B	102	MET	6.1
1	B	193	LEU	6.0
1	A	102	MET	6.0
1	D	193	LEU	5.6
1	E	102	MET	5.0
1	D	102	MET	4.9
1	A	114	GLY	4.9
1	C	102	MET	4.8
1	A	193	LEU	4.7
1	B	114	GLY	4.5
1	B	101	LEU	4.4
1	C	84	ALA	4.4
1	E	84	ALA	4.4
1	C	178	GLN	4.3
1	E	101	LEU	4.3
1	C	255	GLU	4.3
1	E	3	GLU	4.3
1	E	343	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	101	LEU	4.1
1	A	179	GLU	4.1
1	E	255	GLU	4.1
1	A	255	GLU	4.0
1	D	103	ASN	4.0
1	D	101	LEU	4.0
1	B	255	GLU	4.0
1	D	84	ALA	4.0
1	E	327	ARG	3.9
1	E	352	GLU	3.9
1	D	255	GLU	3.8
1	A	84	ALA	3.8
1	B	179	GLU	3.7
1	D	3	GLU	3.7
1	E	5	ASN	3.7
1	E	95	GLU	3.7
1	B	343	GLY	3.6
1	A	342	TYR	3.6
1	E	342	TYR	3.6
1	E	179	GLU	3.5
1	D	179	GLU	3.5
1	E	363	VAL	3.5
1	E	322	LYS	3.5
1	C	114	GLY	3.4
1	E	300	LYS	3.4
1	B	84	ALA	3.4
1	D	342	TYR	3.3
1	C	343	GLY	3.3
1	D	352	GLU	3.2
1	D	343	GLY	3.2
1	E	361	THR	3.2
1	D	114	GLY	3.2
1	C	314	TYR	3.1
1	D	5	ASN	3.1
1	A	343	GLY	3.1
1	B	103	ASN	3.1
1	A	99	GLU	3.1
1	D	95	GLU	3.1
1	C	61	SER	3.1
1	A	101	LEU	3.0
1	E	178	GLN	3.0
1	B	82	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	361	THR	3.0
1	C	83	GLU	2.9
1	E	316	TRP	2.9
1	E	332	HIS	2.9
1	B	99	GLU	2.9
1	D	99	GLU	2.9
1	E	208	GLY	2.9
1	E	99	GLU	2.9
1	E	61	SER	2.8
1	E	514	THR	2.8
1	C	342	TYR	2.8
1	E	307	HIS	2.8
1	E	209	ILE	2.8
1	E	346	TRP	2.8
1	E	319	ASN	2.8
1	E	326	GLU	2.8
1	D	86	PRO	2.7
1	D	208	GLY	2.7
1	D	363	VAL	2.7
1	C	103	ASN	2.7
1	B	514	THR	2.7
1	C	121	ASP	2.7
1	E	324	TYR	2.7
1	E	495	ASN	2.7
1	D	100	ASN	2.7
1	E	98	ILE	2.6
1	A	121	ASP	2.6
1	E	296	ILE	2.6
1	A	326	GLU	2.6
1	E	80	PRO	2.6
1	E	86	PRO	2.6
1	E	171	ASP	2.6
1	E	314	TYR	2.6
1	C	259	GLY	2.6
1	E	521	VAL	2.6
1	A	103	ASN	2.6
1	E	298	PHE	2.6
1	A	140	ASP	2.5
1	C	98	ILE	2.5
1	E	315	ILE	2.5
1	C	95	GLU	2.5
1	B	121	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	289	ARG	2.5
1	E	81	GLN	2.5
1	E	231	PHE	2.5
1	E	385	ILE	2.5
1	A	82	ASP	2.5
1	D	326	GLU	2.5
1	E	142	GLU	2.5
1	E	220	LYS	2.4
1	C	86	PRO	2.4
1	E	301	GLY	2.4
1	E	253	TYR	2.4
1	D	98	ILE	2.4
1	E	100	ASN	2.4
1	C	140	ASP	2.4
1	E	389	TRP	2.4
1	A	352	GLU	2.4
1	E	311	LYS	2.4
1	E	488	LYS	2.4
1	E	309	ILE	2.4
1	E	515	ILE	2.4
1	A	100	ASN	2.4
1	E	262	THR	2.4
1	C	317	SER	2.4
1	D	77	SER	2.4
1	E	259	GLY	2.4
1	E	305	GLY	2.4
1	B	98	ILE	2.3
1	D	514	THR	2.3
1	E	357	HIS	2.3
1	B	140	ASP	2.3
1	D	85	ASP	2.3
1	E	114	GLY	2.3
1	E	510	TYR	2.3
1	C	3	GLU	2.3
1	C	352	GLU	2.3
1	E	149	GLU	2.3
1	E	277	SER	2.3
1	E	233	ARG	2.3
1	D	127	PHE	2.3
1	D	361	THR	2.3
1	C	99	GLU	2.3
1	C	5	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	520	ALA	2.2
1	E	229	ILE	2.2
1	C	322	LYS	2.2
1	E	285	LYS	2.2
1	B	258	THR	2.2
1	C	301	GLY	2.2
1	B	335	GLU	2.2
1	E	345	GLN	2.2
1	D	63	GLY	2.2
1	E	4	LYS	2.2
1	A	314	TYR	2.2
1	B	342	TYR	2.2
1	C	324	TYR	2.2
1	E	438	TYR	2.2
1	E	239	GLN	2.2
1	D	71	ILE	2.2
1	D	93	ASN	2.2
1	E	396	GLN	2.2
1	D	504	ILE	2.2
1	E	489	PHE	2.2
1	C	194	LYS	2.1
1	E	284	LYS	2.1
1	E	338	LEU	2.1
1	D	140	ASP	2.1
1	B	326	GLU	2.1
1	E	387	THR	2.1
1	B	100	ASN	2.1
1	C	100	ASN	2.1
1	A	341	ILE	2.1
1	A	521	VAL	2.1
1	D	380	LYS	2.1
1	D	79	LEU	2.1
1	E	170	TYR	2.1
1	E	175	PHE	2.1
1	E	344	PHE	2.1
1	E	431	SER	2.1
1	E	508	GLY	2.1
1	E	313	VAL	2.1
1	A	3	GLU	2.0
1	D	317	SER	2.0
1	E	317	SER	2.0
1	A	322	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	316	TRP	2.0
1	A	361	THR	2.0
1	C	361	THR	2.0
1	D	80	PRO	2.0
1	E	79	LEU	2.0
1	A	259	GLY	2.0
1	A	331	GLY	2.0
1	E	238	PHE	2.0
1	E	117	SER	2.0
1	E	279	PRO	2.0
1	D	178	GLN	2.0
1	E	341	ILE	2.0
1	E	410	VAL	2.0
1	E	224	TYR	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	OF4	E	603	31/31	0.71	0.28	102,118,136,145	0
4	OF4	A	603	31/31	0.76	0.26	70,84,118,132	0
4	OF4	C	603	31/31	0.81	0.25	80,98,129,134	0
4	OF4	B	603	31/31	0.82	0.22	48,66,103,115	0
4	OF4	D	603	31/31	0.84	0.21	58,75,107,120	0
3	UFP	E	602	21/21	0.89	0.14	87,113,123,127	0
5	MTX	C	604	33/33	0.89	0.14	58,72,86,86	0
5	MTX	E	604	33/33	0.89	0.15	75,88,93,97	0
6	SO4	E	605	5/5	0.90	0.10	78,95,111,117	0

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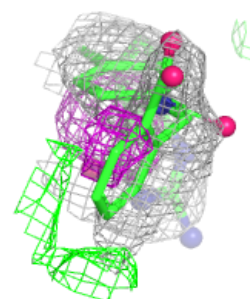
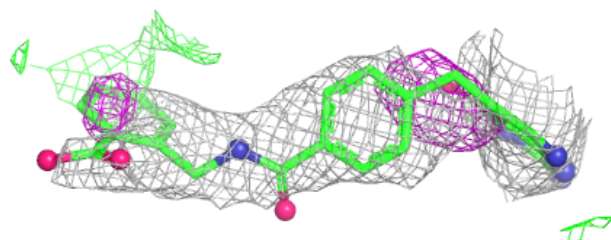
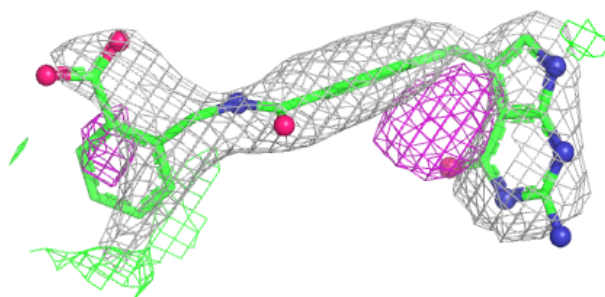
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UFP	C	602	21/21	0.91	0.12	70,85,98,98	0
3	UFP	A	602	21/21	0.92	0.13	55,69,85,92	0
6	SO4	A	605	5/5	0.92	0.12	54,61,79,84	0
5	MTX	D	604	33/33	0.92	0.13	69,81,87,92	0
2	NDP	E	601	48/48	0.93	0.10	78,93,115,117	0
5	MTX	A	604	33/33	0.93	0.11	43,58,76,83	0
5	MTX	B	604	33/33	0.93	0.12	47,60,78,86	0
6	SO4	D	605	5/5	0.93	0.10	74,81,98,102	0
2	NDP	D	601	48/48	0.93	0.11	67,97,118,120	0
2	NDP	C	601	48/48	0.94	0.10	56,81,102,115	0
6	SO4	C	605	5/5	0.94	0.09	68,83,89,90	0
3	UFP	D	602	21/21	0.95	0.10	45,67,75,77	0
3	UFP	B	602	21/21	0.95	0.10	34,60,69,75	0
2	NDP	B	601	48/48	0.96	0.08	47,60,71,87	0
2	NDP	A	601	48/48	0.96	0.09	46,61,76,96	0
6	SO4	B	605	5/5	0.96	0.12	74,75,81,86	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.

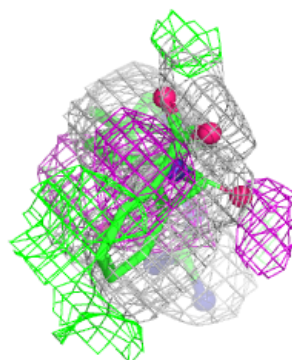
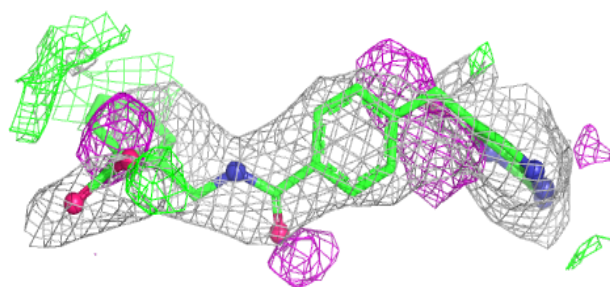
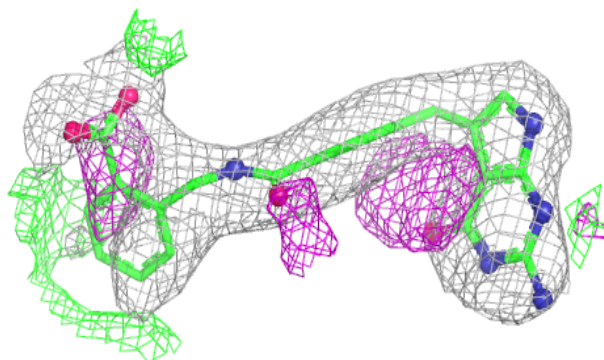
Electron density around OF4 E 603:

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

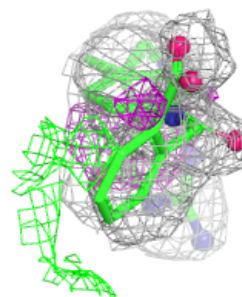
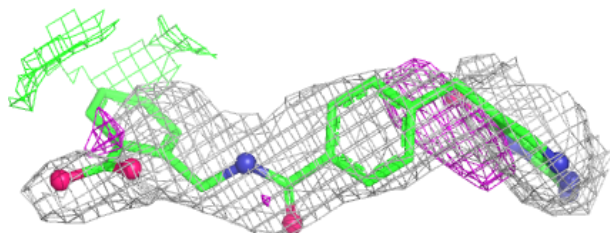
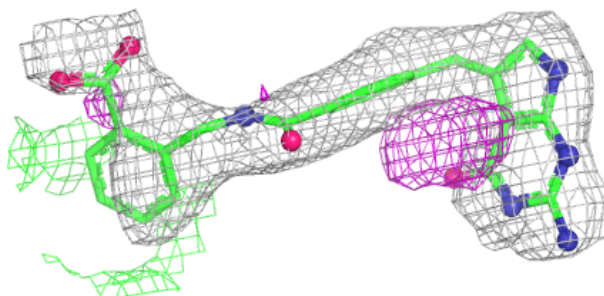


Electron density around OF4 A 603:

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

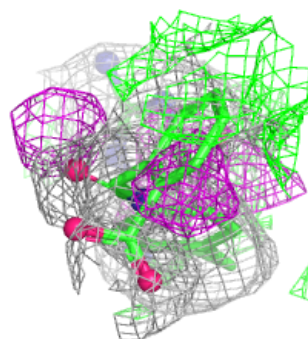
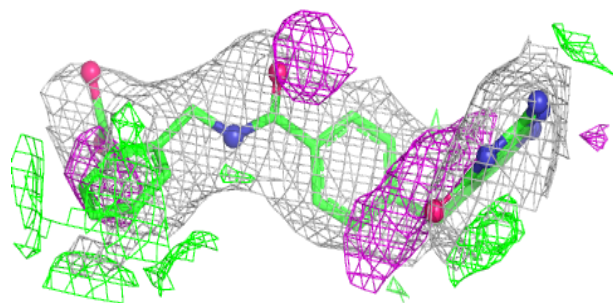
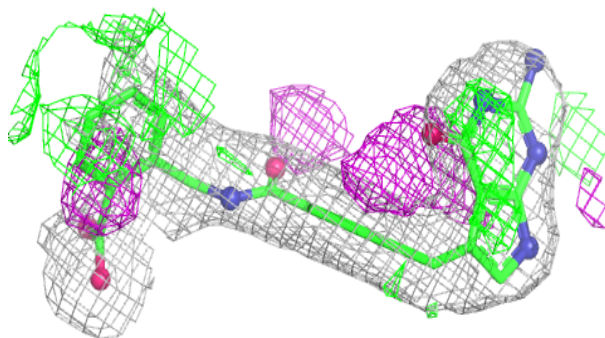
**Electron density around OF4 C 603:**

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

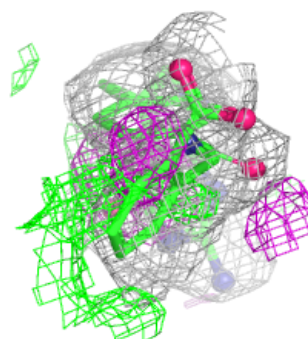
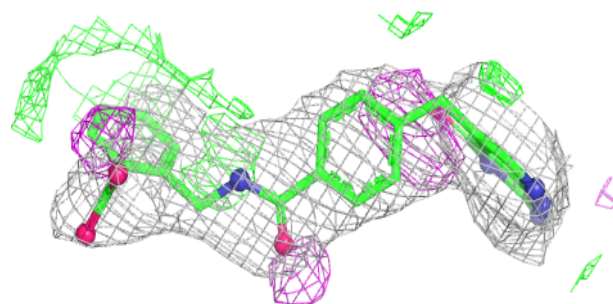
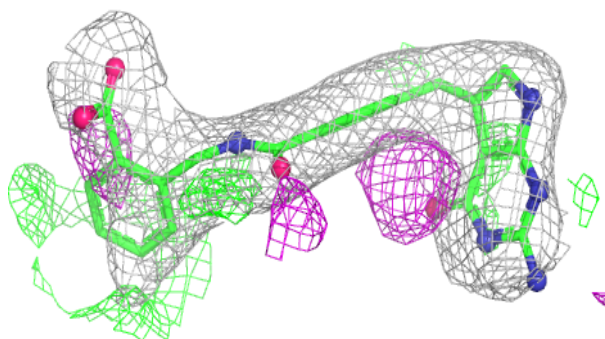


Electron density around OF4 B 603:

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

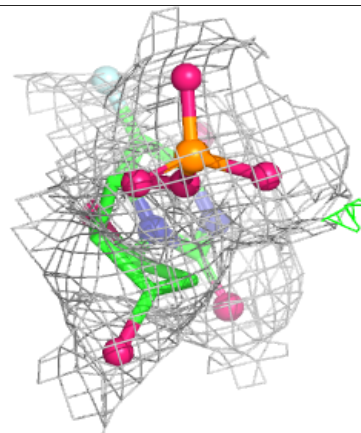
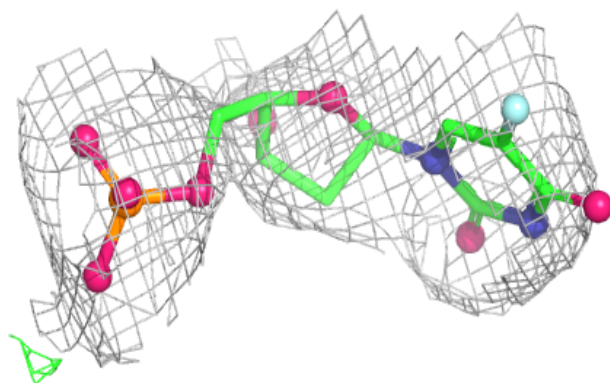
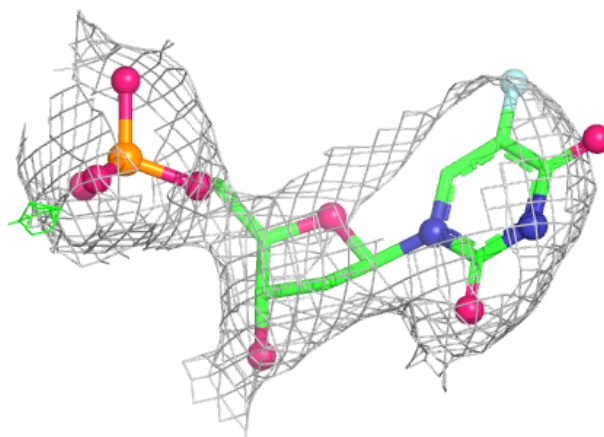
**Electron density around OF4 D 603:**

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



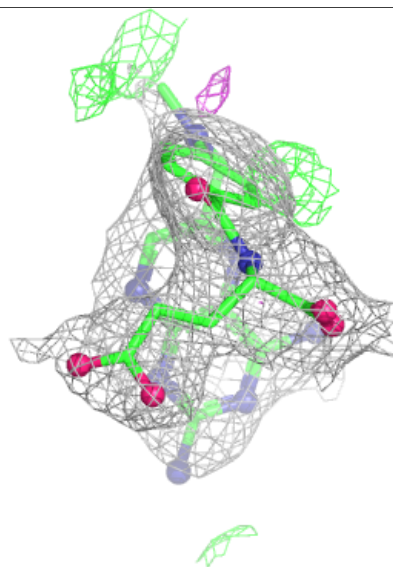
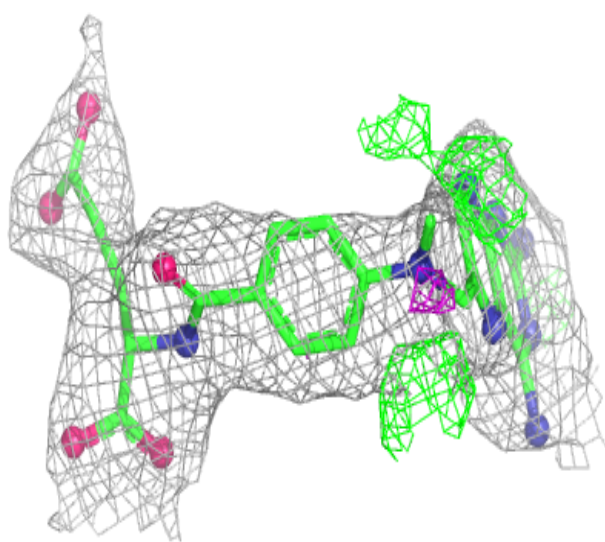
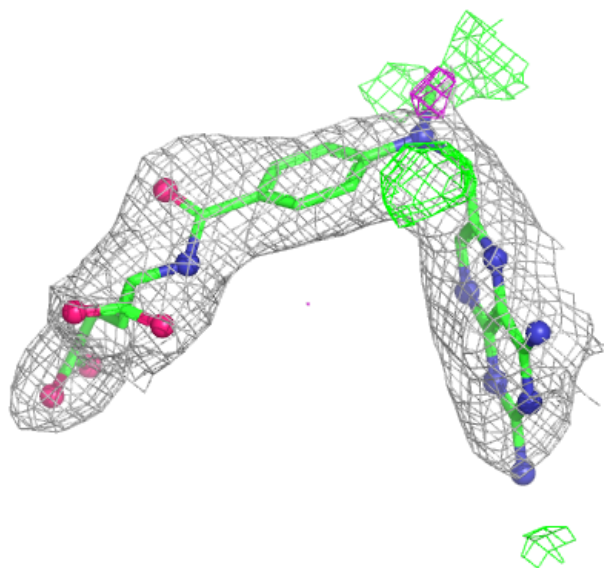
Electron density around UFP E 602:

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



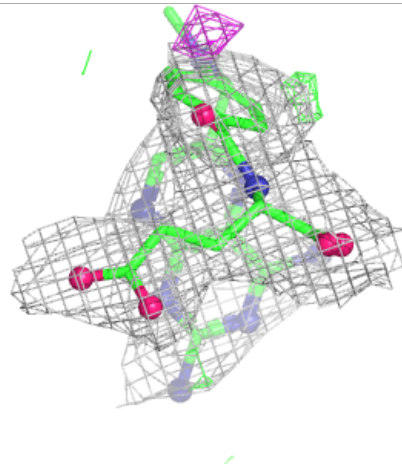
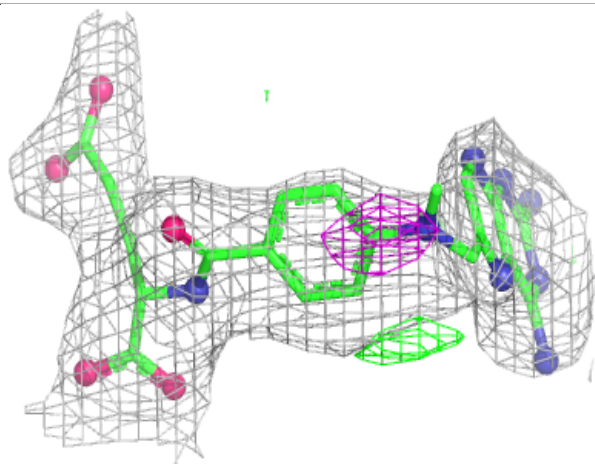
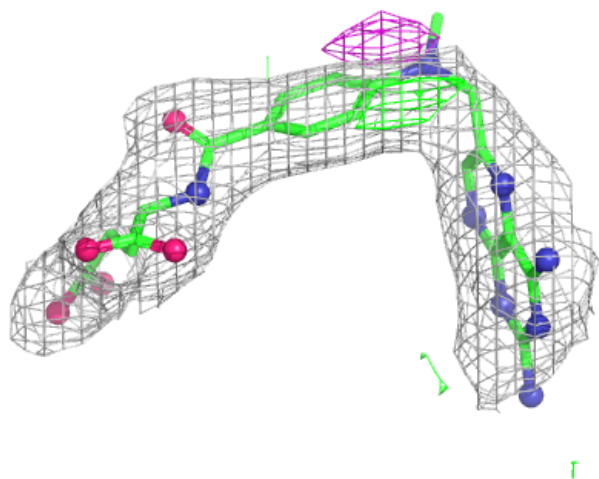
Electron density around MTX C 604:

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



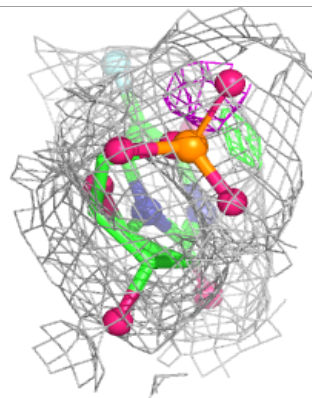
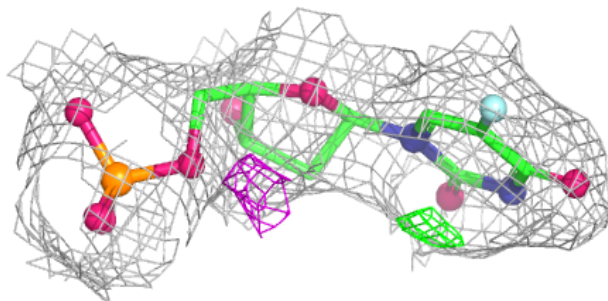
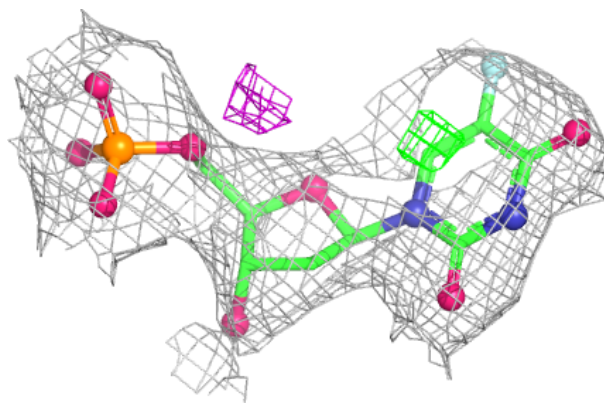
Electron density around MTX E 604:

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



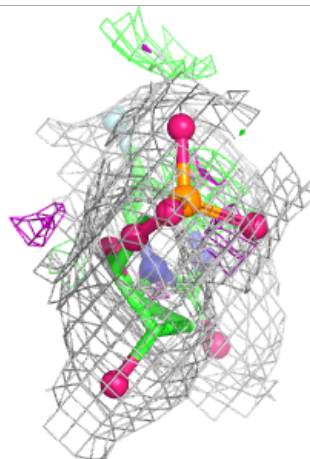
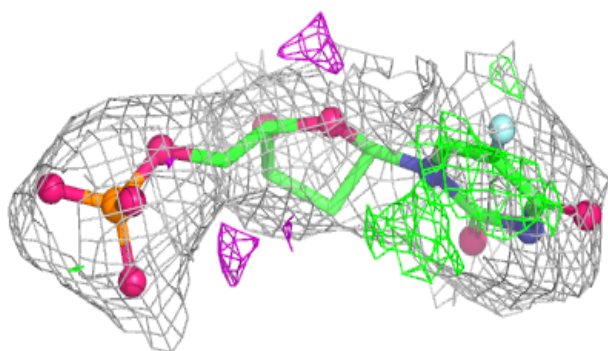
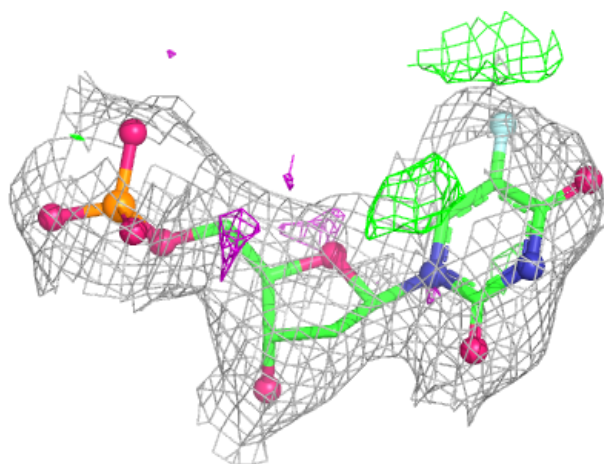
Electron density around UFP C 602:

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



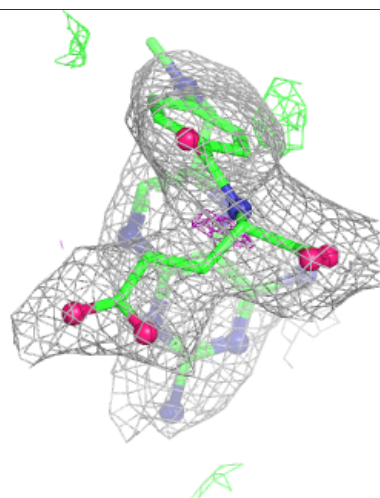
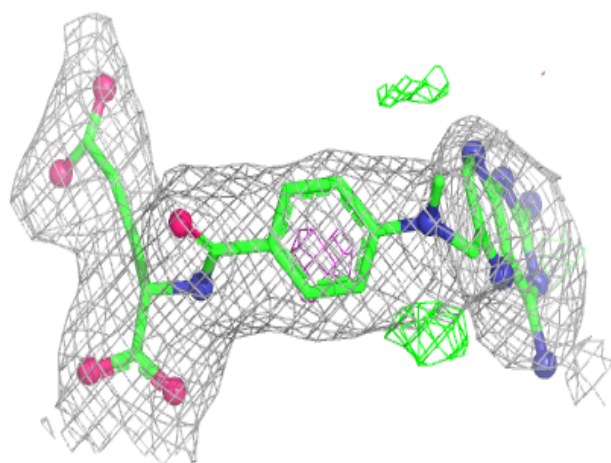
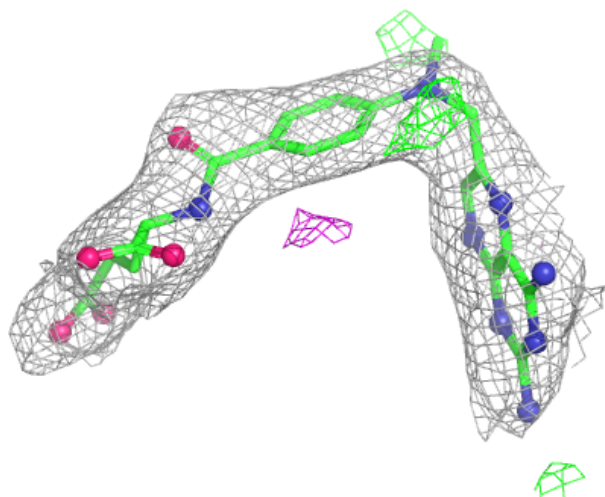
Electron density around UFP A 602:

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



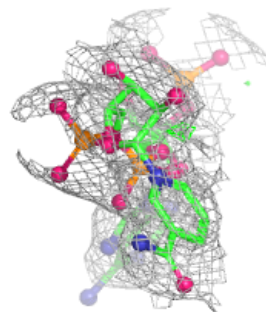
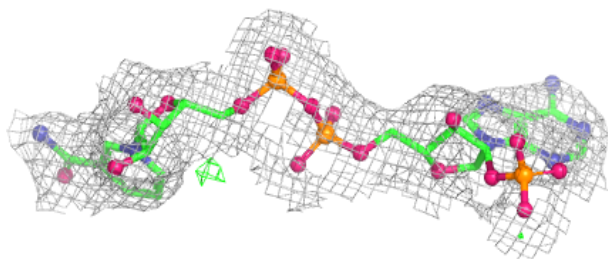
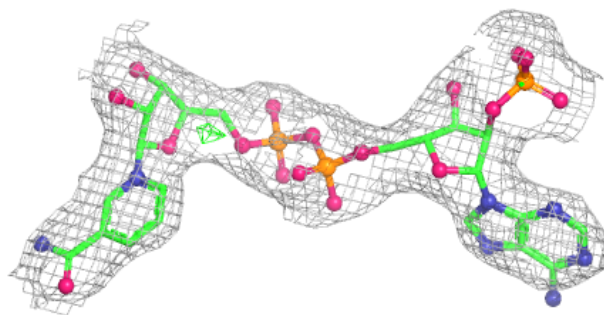
Electron density around MTX D 604:

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



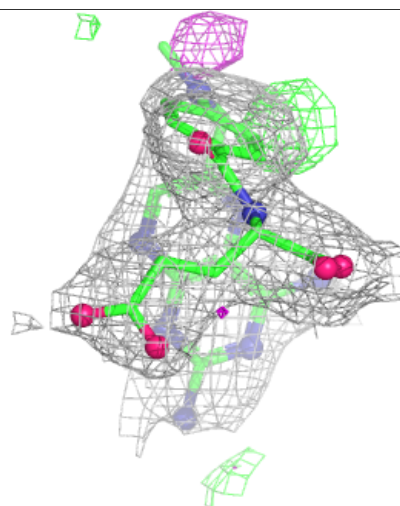
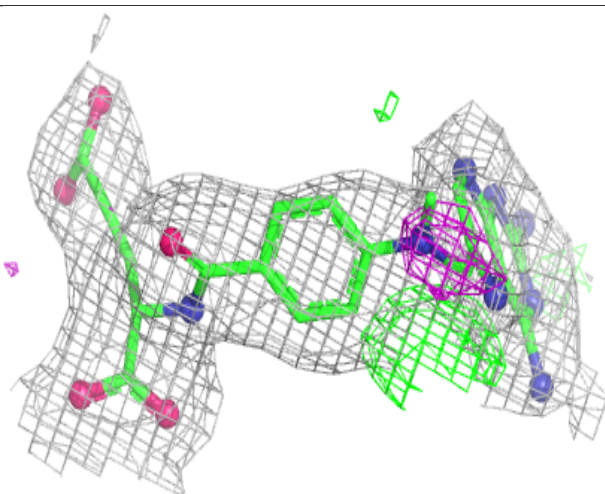
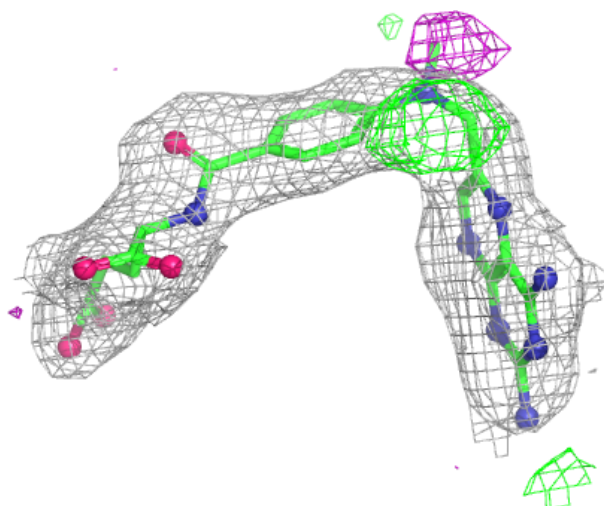
Electron density around NDP E 601:

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



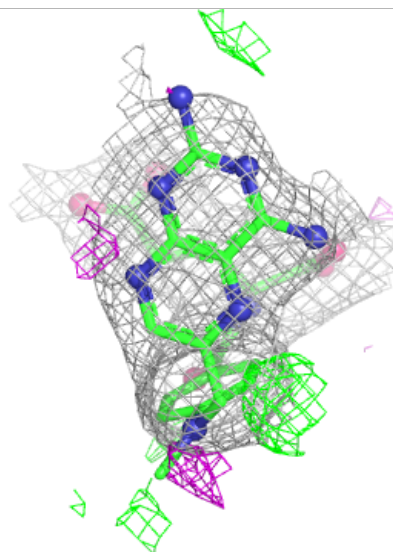
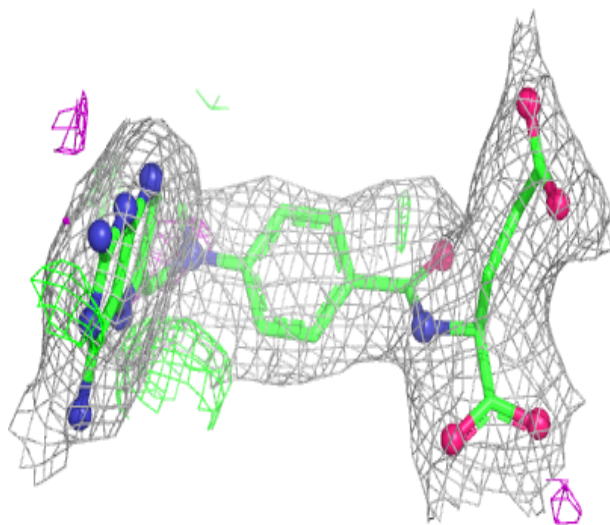
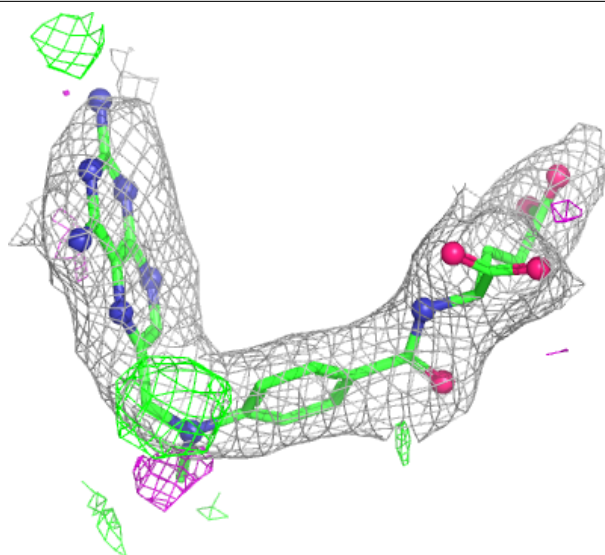
Electron density around MTX A 604:

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



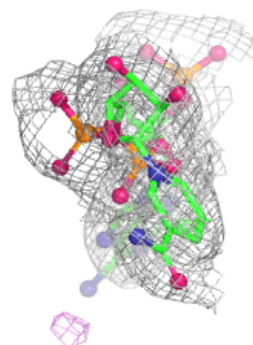
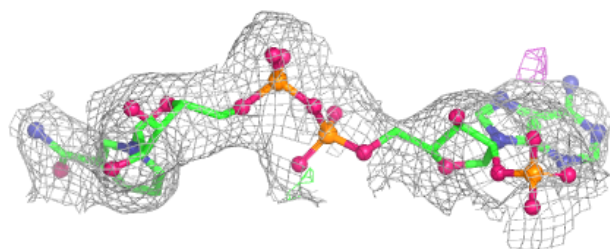
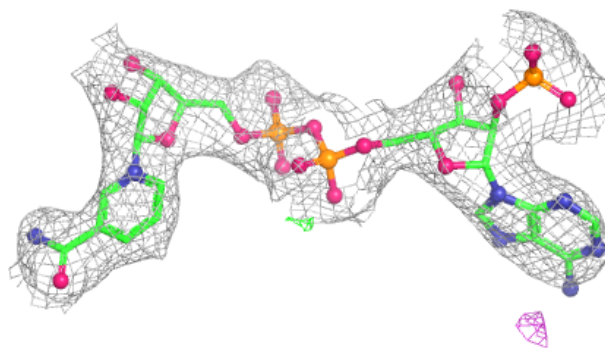
Electron density around MTX B 604:

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

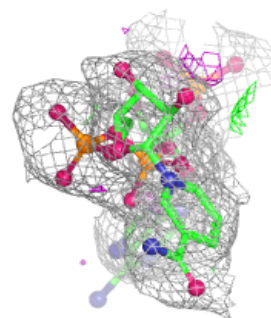
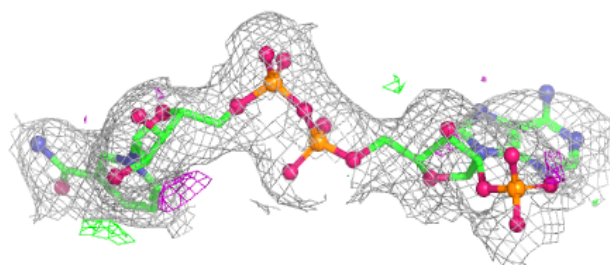
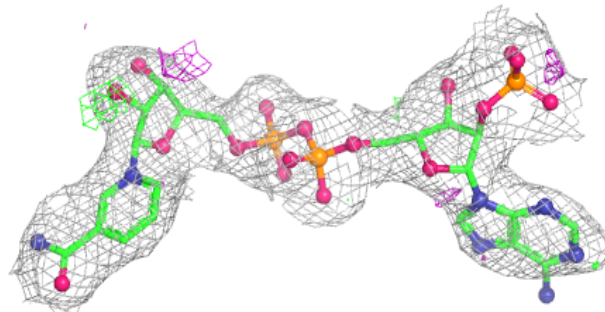


Electron density around NDP D 601:

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

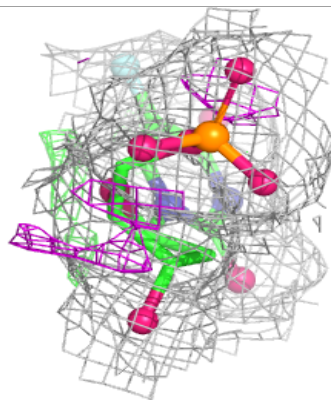
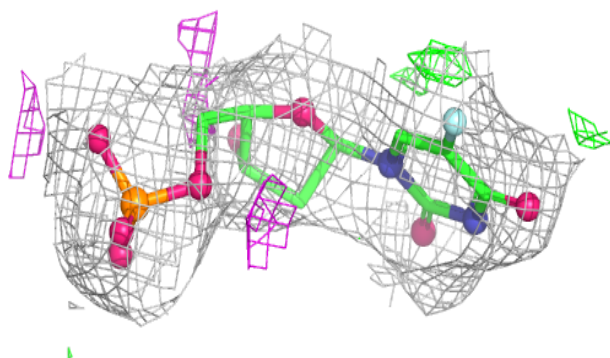
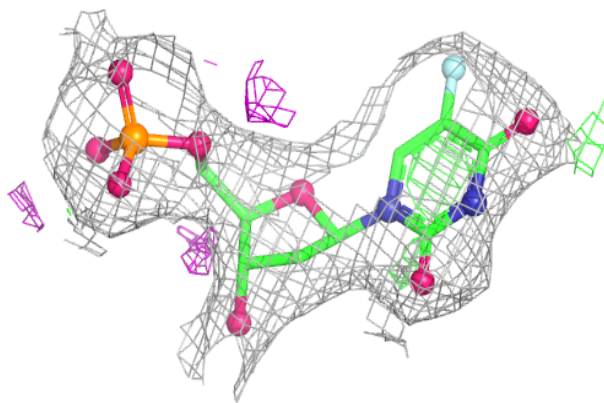
**Electron density around NDP C 601:**

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

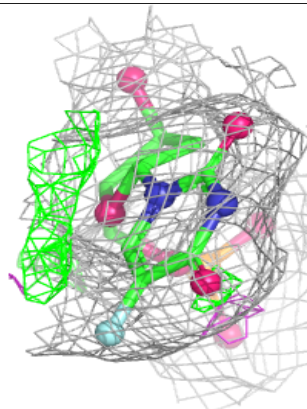
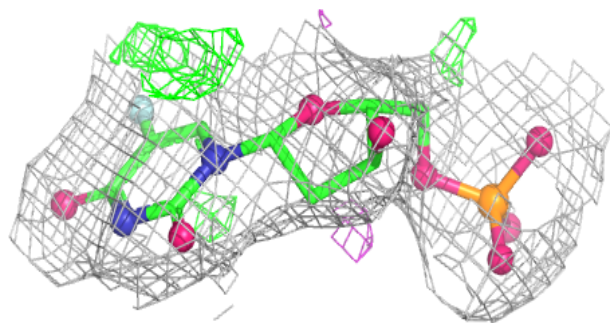
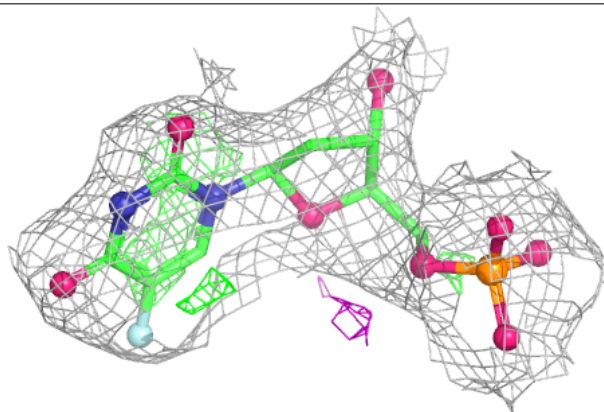


Electron density around UFP D 602:

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

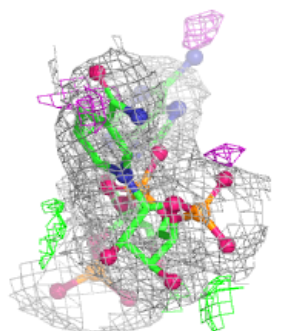
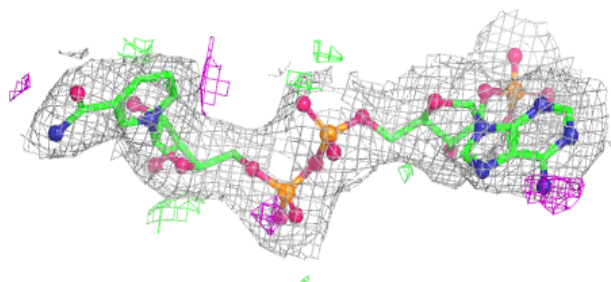
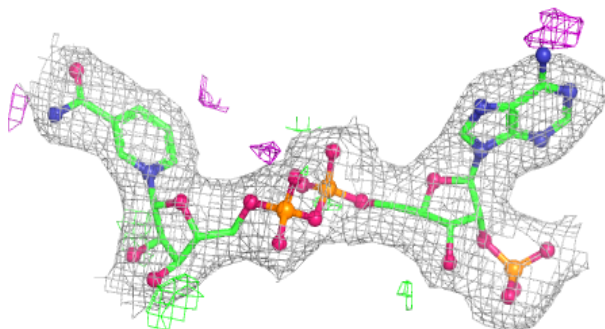
**Electron density around UFP B 602:**

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

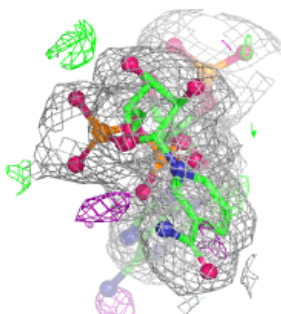
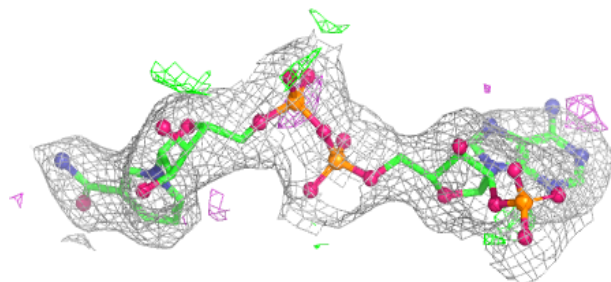
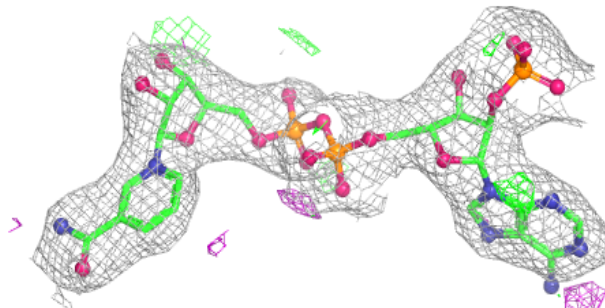


Electron density around NDP B 601:

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

**Electron density around NDP A 601:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.