



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:43 AM UTC

PDB ID : 6PFB / pdb_00006pfb
Title : Crystal structure of TS-DHFR from *Cryptosporidium hominis* in complex with NADPH, FdUMP and 3-(2-(4-((2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl)benzamido)phenyl)propanoic acid.
Authors : Czyzyk, D.J.; Valhondo, M.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2019-06-21
Resolution : 3.09 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

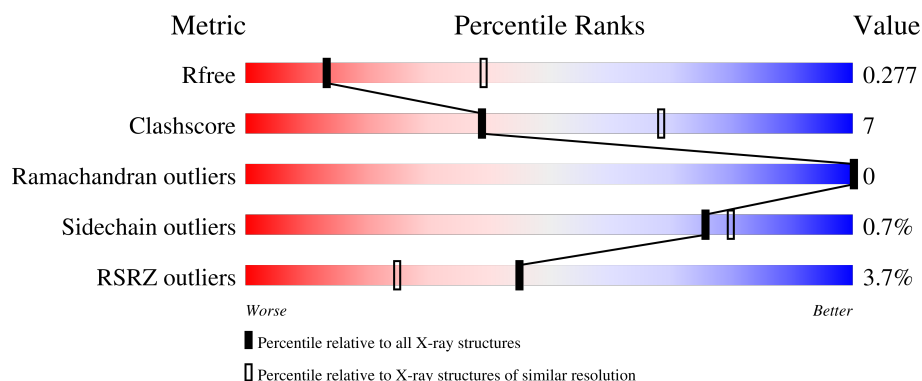
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	3% 78% 19% .
1	B	521	4% 80% 17% .
1	C	521	4% 81% 17% .
1	D	521	2% 80% 17% .

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Mol	Chain	Length	Quality of chain
1	E	521	5% 82% 15%

2 Entry composition ⓘ

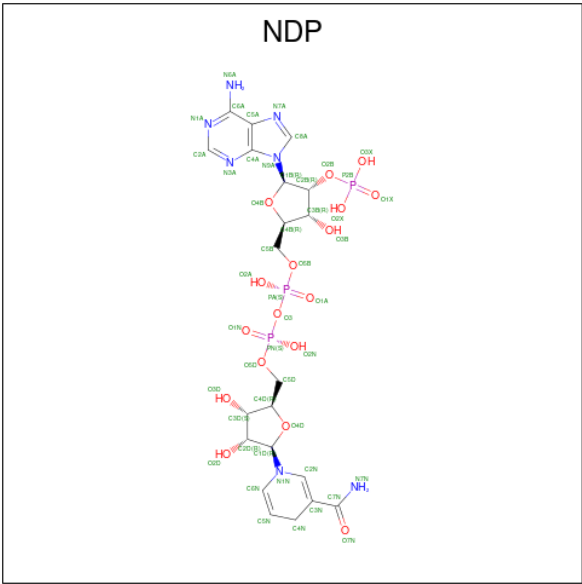
There are 5 unique types of molecules in this entry. The entry contains 20536 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	505	Total	C	N	O	S	0	0	0
			3977	2548	665	743	21			
1	B	505	Total	C	N	O	S	0	0	0
			3996	2557	673	746	20			
1	C	506	Total	C	N	O	S	0	0	0
			3964	2538	667	738	21			
1	D	506	Total	C	N	O	S	0	0	0
			3997	2554	664	758	21			
1	E	505	Total	C	N	O	S	0	0	0
			3932	2516	662	733	21			

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



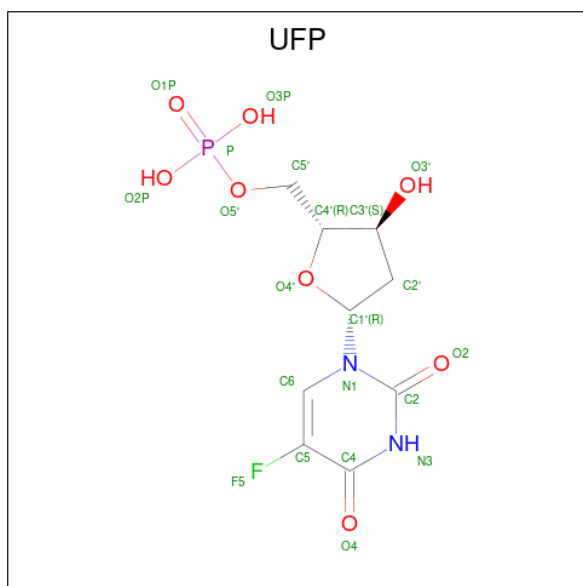
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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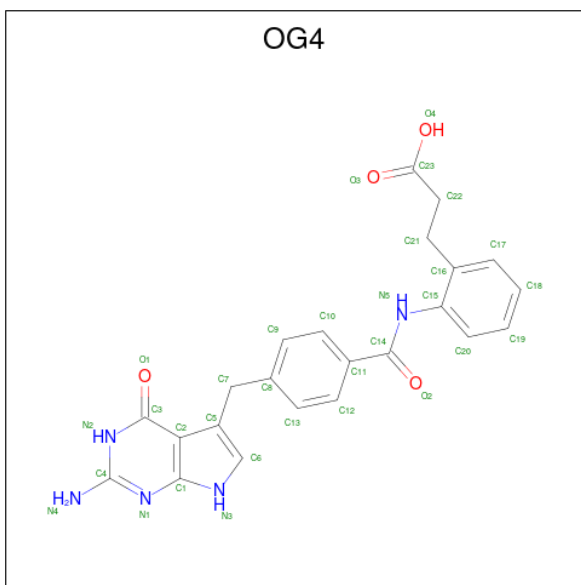
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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



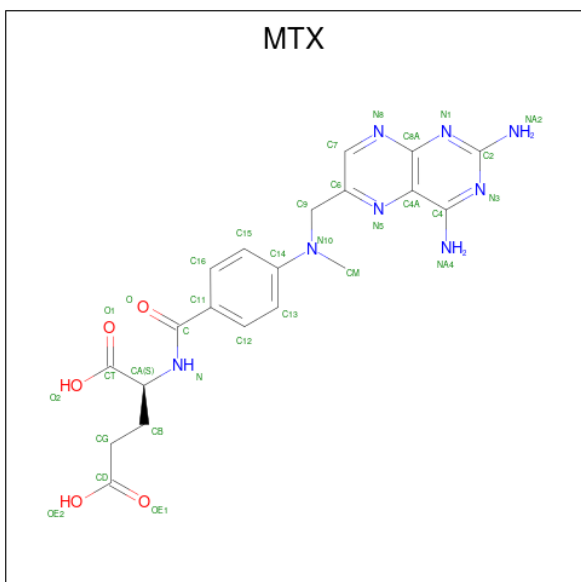
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is 3-[2-({4-[(2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl]benzene-1-carbonyl}amino)phenyl]propanoic acid (CCD ID: OG4) (formula: C₂₃H₂₁N₅O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	23	5	4		
4	B	1	Total	C	N	O	0	0
			32	23	5	4		
4	C	1	Total	C	N	O	0	0
			32	23	5	4		
4	D	1	Total	C	N	O	0	0
			32	23	5	4		
4	E	1	Total	C	N	O	0	0
			32	23	5	4		

- Molecule 5 is METHOTREXATE (CCD ID: MTX) (formula: $C_{20}H_{22}N_8O_5$).

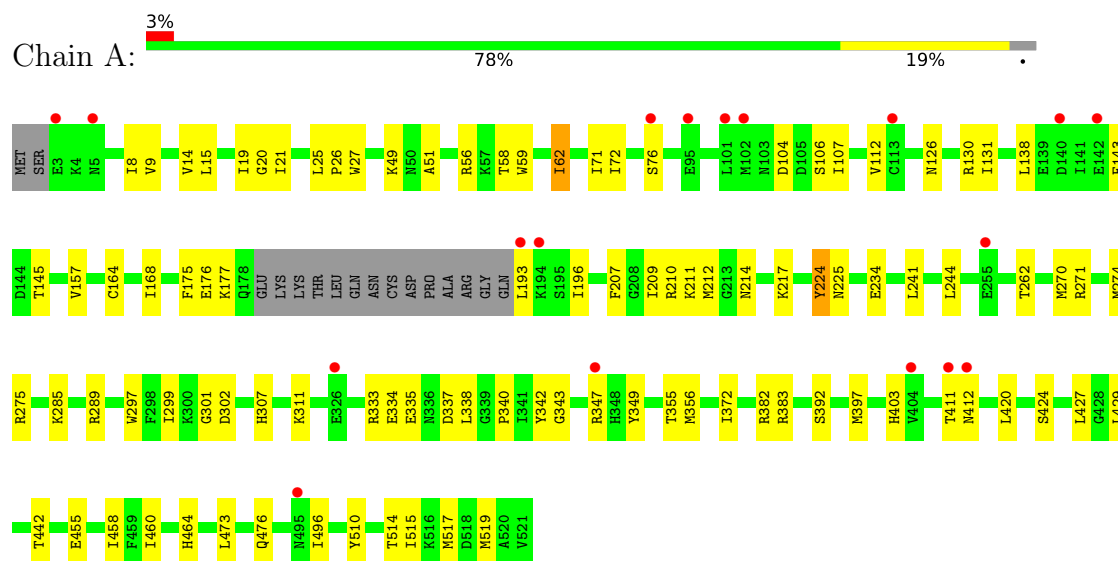


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 33	C 20	N 8	O 5	0	0
5	B	1	Total 33	C 20	N 8	O 5	0	0
5	C	1	Total 33	C 20	N 8	O 5	0	0
5	D	1	Total 33	C 20	N 8	O 5	0	0
5	E	1	Total 33	C 20	N 8	O 5	0	0

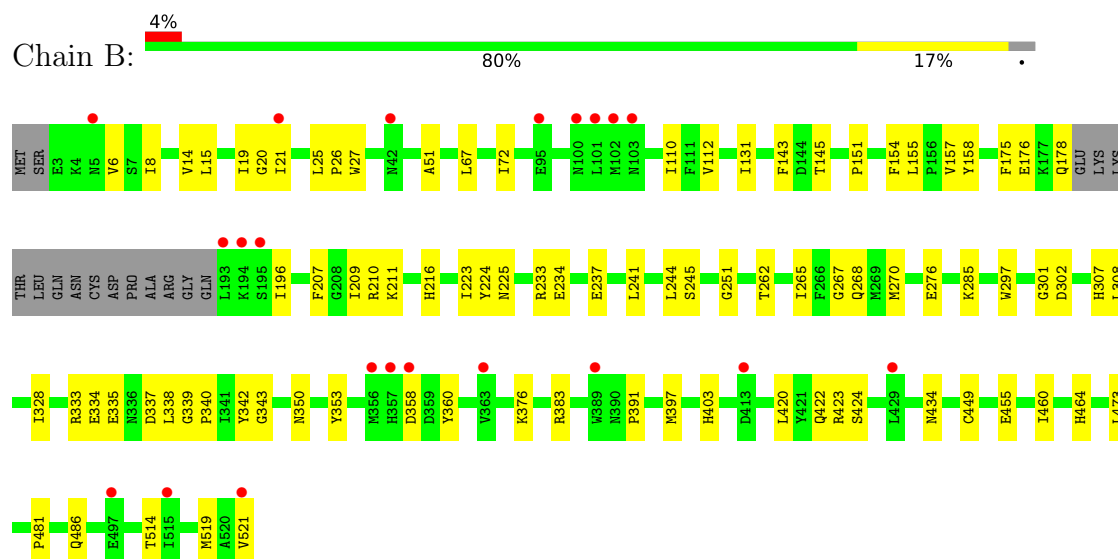
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

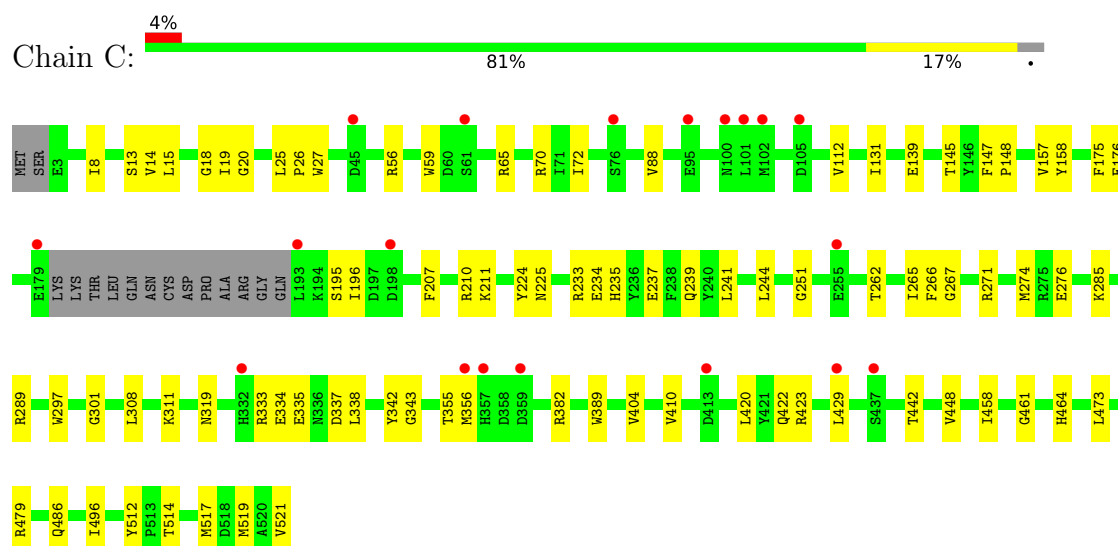
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



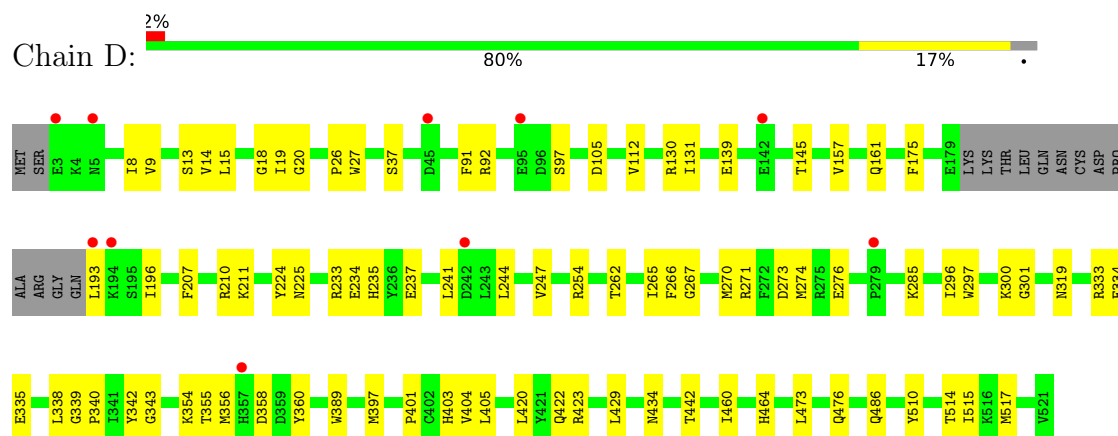
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



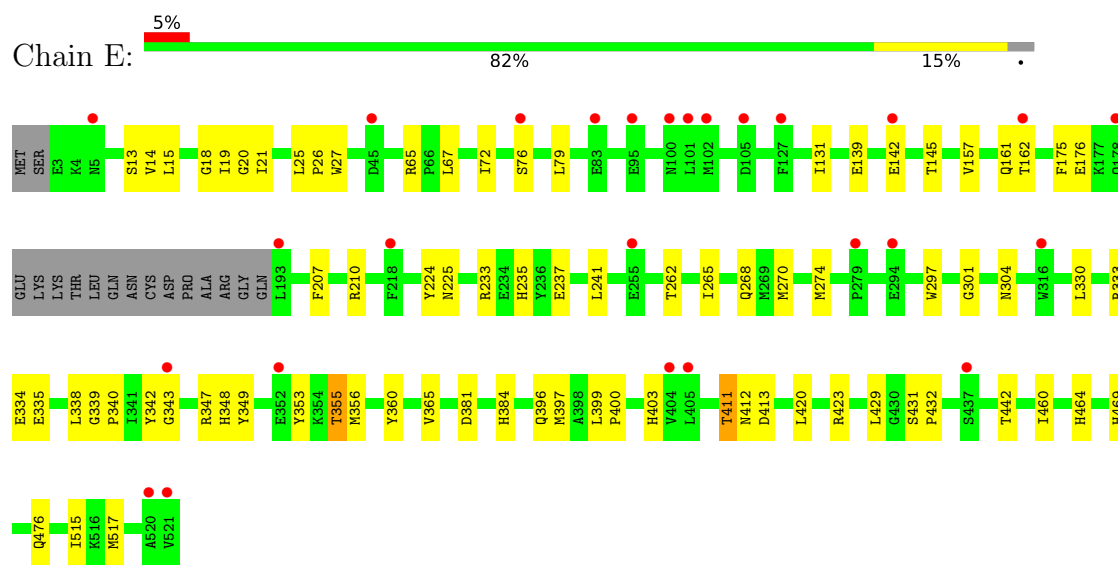
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.99Å 116.24Å 221.67Å 90.00° 94.75° 90.00°	Depositor
Resolution (Å)	49.65 – 3.09 49.65 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.65-3.09) 98.5 (49.65-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.39	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472)	Depositor
R, R_{free}	0.237 , 0.271 0.242 , 0.277	Depositor DCC
R_{free} test set	2008 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	93.5	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20536	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MTX, OG4, UFP, NDP

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	0.10	0/4071	0.30	0/5530
1	B	0.10	0/4091	0.29	0/5556
1	C	0.09	0/4058	0.29	0/5517
1	D	0.09	0/4091	0.28	0/5560
1	E	0.09	0/4027	0.28	0/5485
All	All	0.09	0/20338	0.29	0/27648

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3977	0	3795	64	0
1	B	3996	0	3816	60	0
1	C	3964	0	3753	57	0
1	D	3997	0	3787	57	0
1	E	3932	0	3685	46	0
2	A	48	0	26	2	0
2	B	48	0	26	2	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	2	0
2	E	48	0	26	1	0
3	A	21	0	10	1	0
3	B	21	0	10	2	0
3	C	21	0	10	1	0
3	D	21	0	10	2	0
3	E	21	0	10	1	0
4	A	32	0	0	0	0
4	B	32	0	0	0	0
4	C	32	0	0	1	0
4	D	32	0	0	1	0
4	E	32	0	0	0	0
5	A	33	0	20	4	0
5	B	33	0	20	3	0
5	C	33	0	20	3	0
5	D	33	0	20	3	0
5	E	33	0	20	1	0
All	All	20536	0	19116	270	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:GLY:HA2	1:D:343:GLY:O	1.85	0.76
1:B:301:GLY:HA2	1:B:343:GLY:O	1.86	0.75
1:A:301:GLY:HA2	1:A:343:GLY:O	1.86	0.74
1:C:355:THR:HG22	1:C:356:MET:H	1.59	0.67
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.78	0.66
1:C:251:GLY:O	1:E:65:ARG:NH1	2.30	0.65
1:E:301:GLY:HA2	1:E:343:GLY:O	1.97	0.65
1:B:21:ILE:HG22	1:B:143:PHE:HA	1.78	0.65
1:B:225:ASN:O	1:B:233:ARG:NH2	2.27	0.64
1:A:355:THR:HG22	1:A:356:MET:H	1.62	0.64
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.80	0.64
1:D:355:THR:HG22	1:D:356:MET:H	1.63	0.64
1:D:429:LEU:HD21	1:D:517:MET:HB2	1.80	0.63
1:D:161:GLN:NE2	1:D:273:ASP:OD2	2.32	0.62
1:A:285:LYS:HB3	1:A:514:THR:HB	1.79	0.62
1:C:285:LYS:HB3	1:C:514:THR:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:GLY:O	1:D:271:ARG:NH2	2.33	0.61
1:E:225:ASN:O	1:E:233:ARG:NH2	2.30	0.61
1:A:71:ILE:HD12	1:A:107:ILE:HD11	1.82	0.61
1:A:271:ARG:NH2	1:B:267:GLY:O	2.34	0.61
1:A:382:ARG:NH1	3:B:602:UFP:O3P	2.34	0.61
1:A:49:LYS:HE2	1:A:71:ILE:HD11	1.82	0.61
1:E:21:ILE:HD12	1:E:142:GLU:O	2.01	0.61
1:C:429:LEU:HD21	1:C:517:MET:HB2	1.83	0.61
1:A:429:LEU:HD21	1:A:517:MET:HB2	1.81	0.60
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.82	0.60
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.82	0.60
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.67	0.59
1:C:207:PHE:HB3	1:C:210:ARG:HB2	1.84	0.59
1:B:67:LEU:HG	1:B:72:ILE:HD11	1.85	0.59
1:D:285:LYS:HB3	1:D:514:THR:HB	1.84	0.59
1:A:289:ARG:NH2	1:A:311:LYS:O	2.36	0.58
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.85	0.58
1:E:349:TYR:HB3	1:E:365:VAL:HB	1.84	0.58
1:A:21:ILE:HG22	1:A:143:PHE:HA	1.85	0.58
1:B:285:LYS:HB3	1:B:514:THR:HB	1.85	0.58
1:C:157:VAL:HG21	1:C:176:GLU:HG3	1.86	0.58
1:D:20:GLY:HA2	1:D:26:PRO:HD3	1.86	0.58
1:A:193:LEU:HD21	1:A:196:ILE:HD13	1.85	0.57
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.84	0.57
1:A:234:GLU:OE2	1:B:211:LYS:NZ	2.37	0.57
1:E:207:PHE:HB3	1:E:210:ARG:HB2	1.86	0.56
1:E:403:HIS:HB2	1:E:420:LEU:HD11	1.87	0.56
1:E:423:ARG:NH1	3:E:602:UFP:O3P	2.39	0.56
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.87	0.56
1:A:476:GLN:HG3	1:A:515:ILE:HD11	1.86	0.56
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.86	0.56
1:D:91:PHE:CD2	1:D:97:SER:HA	2.41	0.55
1:A:207:PHE:HB3	1:A:210:ARG:HB2	1.87	0.55
1:A:334:GLU:HG2	1:A:335:GLU:H	1.71	0.55
2:B:601:NDP:H8A	2:B:601:NDP:H52A	1.88	0.55
1:E:25:LEU:HD11	5:E:604:MTX:H7	1.88	0.55
1:A:157:VAL:HG12	1:B:196:ILE:HD11	1.89	0.54
1:B:207:PHE:HB3	1:B:210:ARG:HB2	1.89	0.54
1:A:214:ASN:HD22	1:A:217:LYS:HE2	1.73	0.54
1:E:265:ILE:HD12	1:E:268:GLN:HE21	1.71	0.54
1:B:422:GLN:NE2	1:B:434:ASN:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:GLY:HA2	1:E:26:PRO:HD3	1.90	0.54
1:A:211:LYS:NZ	1:B:234:GLU:OE2	2.35	0.54
1:E:340:PRO:O	1:E:397:MET:HG2	2.09	0.53
1:D:423:ARG:NH1	3:D:602:UFP:O3P	2.42	0.53
1:B:302:ASP:OD2	1:B:307:HIS:ND1	2.26	0.53
1:B:519:MET:HE3	1:B:521:VAL:HG22	1.91	0.53
1:C:289:ARG:NH2	1:C:311:LYS:O	2.42	0.53
1:A:302:ASP:OD2	1:A:307:HIS:ND1	2.28	0.52
1:C:262:THR:HB	1:C:464:HIS:HB2	1.90	0.52
1:E:270:MET:HE2	1:E:460:ILE:HD11	1.92	0.52
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.90	0.52
1:B:297:TRP:CD2	1:B:308:LEU:HD11	2.45	0.52
1:C:19:ILE:HG13	1:C:145:THR:HG22	1.91	0.52
1:C:225:ASN:ND2	1:C:241:LEU:HD13	2.24	0.52
1:C:20:GLY:HA2	1:C:26:PRO:HD3	1.91	0.52
1:B:157:VAL:HG21	1:B:176:GLU:HG3	1.91	0.52
1:C:234:GLU:OE2	1:D:211:LYS:NZ	2.43	0.51
1:D:262:THR:HB	1:D:464:HIS:HB2	1.92	0.51
1:D:276:GLU:O	1:D:486:GLN:NE2	2.38	0.51
1:D:207:PHE:HB3	1:D:210:ARG:HB2	1.91	0.51
1:D:193:LEU:HD21	1:D:196:ILE:HG12	1.92	0.51
1:A:104:ASP:OD1	1:A:106:SER:OG	2.27	0.51
1:E:297:TRP:HH2	1:E:338:LEU:HD12	1.76	0.51
1:B:358:ASP:HB3	1:B:360:TYR:CE2	2.46	0.51
1:B:265:ILE:HD12	1:B:268:GLN:HE21	1.76	0.51
1:D:355:THR:O	1:D:360:TYR:OH	2.21	0.51
1:B:339:GLY:HA2	1:B:353:TYR:CZ	2.46	0.50
2:C:601:NDP:H8A	2:C:601:NDP:H3B	1.91	0.50
1:D:8:ILE:HG12	1:D:112:VAL:HB	1.93	0.50
1:C:244:LEU:HD21	1:C:473:LEU:HD22	1.94	0.50
1:A:58:THR:O	1:A:62:ILE:HG23	2.12	0.49
1:C:334:GLU:HG2	1:C:335:GLU:H	1.77	0.49
1:B:270:MET:HE2	1:B:460:ILE:HD11	1.94	0.49
1:B:334:GLU:HG2	1:B:335:GLU:H	1.78	0.49
1:C:319:ASN:OD1	4:C:603:OG4:N3	2.44	0.49
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.77	0.49
1:C:271:ARG:NH2	1:D:267:GLY:O	2.45	0.49
1:C:420:LEU:HD22	1:C:458:ILE:HG23	1.94	0.49
1:B:358:ASP:HB3	1:B:360:TYR:CZ	2.48	0.49
1:C:301:GLY:HA2	1:C:343:GLY:O	2.12	0.49
1:D:476:GLN:HG3	1:D:515:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HH12	1:B:209:ILE:HG22	1.78	0.49
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.48	0.49
1:D:15:LEU:HD11	1:D:510:TYR:HB3	1.95	0.49
1:E:76:SER:OG	1:E:79:LEU:HB2	2.13	0.49
1:C:276:GLU:O	1:C:486:GLN:NE2	2.35	0.49
1:E:67:LEU:HG	1:E:72:ILE:HD11	1.95	0.49
1:A:420:LEU:HD22	1:A:458:ILE:HG23	1.94	0.48
1:B:19:ILE:HG13	1:B:145:THR:HG22	1.94	0.48
1:D:333:ARG:HH22	1:D:339:GLY:CA	2.26	0.48
1:E:429:LEU:HD11	1:E:517:MET:HB2	1.96	0.48
1:B:14:VAL:HG13	1:B:15:LEU:HG	1.96	0.48
1:D:92:ARG:O	2:D:601:NDP:H2A	2.13	0.48
1:E:14:VAL:HG13	1:E:15:LEU:HG	1.95	0.48
1:C:355:THR:HG22	1:C:356:MET:N	2.26	0.48
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.48	0.48
1:E:225:ASN:ND2	1:E:241:LEU:HD13	2.29	0.48
1:E:274:MET:HE1	1:E:442:THR:HG21	1.96	0.48
1:B:423:ARG:NH1	3:B:602:UFP:O1P	2.47	0.48
1:A:355:THR:HG22	1:A:356:MET:N	2.29	0.47
2:D:601:NDP:H8A	2:D:601:NDP:H52A	1.95	0.47
1:D:225:ASN:O	1:D:233:ARG:NH2	2.40	0.47
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.49	0.47
1:D:225:ASN:ND2	1:D:241:LEU:HD13	2.29	0.47
1:D:274:MET:HE1	1:D:442:THR:HG21	1.96	0.47
1:D:334:GLU:HG2	1:D:335:GLU:H	1.78	0.47
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.50	0.47
1:A:225:ASN:ND2	1:A:241:LEU:HD13	2.30	0.47
1:A:14:VAL:HG13	1:A:15:LEU:HG	1.96	0.47
3:A:602:UFP:O3P	1:B:383:ARG:NH2	2.47	0.47
1:E:262:THR:HB	1:E:464:HIS:HB2	1.96	0.47
1:B:225:ASN:ND2	1:B:241:LEU:HD13	2.30	0.47
1:A:15:LEU:HD11	1:A:510:TYR:HB3	1.97	0.47
1:C:382:ARG:NH1	3:D:602:UFP:O1P	2.47	0.47
1:B:25:LEU:HD11	5:B:604:MTX:H7	1.97	0.47
1:C:70:ARG:NH1	5:C:604:MTX:O1	2.43	0.47
1:C:72:ILE:HB	1:C:88:VAL:HG22	1.97	0.46
1:D:9:VAL:O	5:D:604:MTX:NA4	2.45	0.46
1:D:247:VAL:HA	1:D:265:ILE:HD11	1.97	0.46
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.98	0.46
1:B:339:GLY:HA2	1:B:353:TYR:CE2	2.51	0.46
1:B:340:PRO:O	1:B:397:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLY:HA2	1:B:26:PRO:HD3	1.97	0.46
1:E:19:ILE:HG13	1:E:145:THR:HG22	1.96	0.46
1:A:8:ILE:HG12	1:A:112:VAL:HB	1.97	0.46
1:B:223:ILE:O	1:B:245:SER:OG	2.30	0.46
1:C:25:LEU:HD11	5:C:604:MTX:H7	1.98	0.46
1:C:479:ARG:HD2	1:C:512:TYR:CD2	2.50	0.46
1:D:105:ASP:OD1	1:D:105:ASP:N	2.48	0.46
1:A:130:ARG:HD3	1:A:176:GLU:OE2	2.16	0.46
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.51	0.46
2:B:601:NDP:H42N	5:B:604:MTX:N5	2.31	0.46
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.81	0.46
1:E:333:ARG:HH22	1:E:396:GLN:HB3	1.80	0.46
1:E:334:GLU:HG2	1:E:335:GLU:H	1.81	0.46
1:A:340:PRO:O	1:A:397:MET:HG2	2.16	0.45
1:A:411:THR:HG22	1:A:412:ASN:H	1.81	0.45
2:A:601:NDP:H8A	2:A:601:NDP:H52A	1.98	0.45
1:E:304:ASN:ND2	1:E:356:MET:SD	2.89	0.45
1:A:333:ARG:CG	1:A:337:ASP:HB3	2.46	0.45
1:D:265:ILE:HG22	1:D:266:PHE:H	1.82	0.45
1:E:400:PRO:HG2	1:E:423:ARG:NH2	2.31	0.45
1:A:299:ILE:O	1:A:347:ARG:HD2	2.17	0.45
1:E:355:THR:O	1:E:360:TYR:OH	2.31	0.45
1:E:399:LEU:HD12	1:E:400:PRO:HD2	1.98	0.45
1:E:411:THR:HG22	1:E:412:ASN:H	1.80	0.45
1:E:429:LEU:HD13	1:E:469:HIS:CE1	2.52	0.45
1:B:151:PRO:HG2	1:B:154:PHE:HD1	1.82	0.45
1:C:14:VAL:HG13	1:C:15:LEU:HG	1.98	0.45
1:D:244:LEU:HD21	1:D:473:LEU:HD22	1.98	0.45
1:C:420:LEU:HD21	1:C:422:GLN:HB2	1.98	0.45
1:A:244:LEU:HD21	1:A:473:LEU:HD22	1.99	0.45
1:C:59:TRP:CZ3	1:C:72:ILE:HG21	2.52	0.45
1:D:14:VAL:HG13	1:D:15:LEU:HG	1.99	0.45
1:B:251:GLY:O	1:C:65:ARG:NH1	2.49	0.44
1:C:297:TRP:HB2	1:C:308:LEU:HD21	1.98	0.44
1:D:355:THR:HG22	1:D:356:MET:N	2.28	0.44
1:D:389:TRP:HB2	1:D:404:VAL:CG1	2.48	0.44
1:E:330:LEU:HD13	1:E:333:ARG:NH1	2.32	0.44
1:C:410:VAL:O	1:D:254:ARG:NH2	2.49	0.44
1:E:476:GLN:HG3	1:E:515:ILE:HD11	1.99	0.44
1:A:262:THR:HB	1:A:464:HIS:HB2	2.00	0.44
1:B:25:LEU:HD11	5:B:604:MTX:C7	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:PHE:HA	1:C:461:GLY:O	2.18	0.44
1:D:13:SER:HB3	1:D:18:GLY:H	1.83	0.44
1:A:270:MET:HE2	1:A:460:ILE:HD11	2.00	0.44
1:C:423:ARG:NH1	3:C:602:UFP:O3P	2.48	0.44
1:C:519:MET:HE3	1:C:521:VAL:HG22	1.99	0.44
1:D:9:VAL:HG12	5:D:604:MTX:N3	2.33	0.44
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.83	0.43
1:A:403:HIS:HB2	1:A:420:LEU:HD11	2.00	0.43
1:C:196:ILE:HD11	1:D:157:VAL:HG12	2.00	0.43
2:E:601:NDP:H52A	2:E:601:NDP:H8A	2.00	0.43
1:A:9:VAL:HG12	5:A:604:MTX:N3	2.33	0.43
1:C:195:SER:OG	1:D:130:ARG:NH1	2.50	0.43
1:C:479:ARG:HD2	1:C:512:TYR:CG	2.52	0.43
1:D:13:SER:OG	1:D:139:GLU:OE2	2.28	0.43
1:A:383:ARG:HA	1:B:423:ARG:HD2	2.00	0.43
1:B:262:THR:HB	1:B:464:HIS:HB2	2.00	0.43
1:D:340:PRO:O	1:D:397:MET:HG2	2.18	0.43
1:E:356:MET:HE2	1:E:356:MET:HB3	1.85	0.43
1:A:59:TRP:CZ3	1:A:72:ILE:HG21	2.53	0.43
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.53	0.43
1:E:13:SER:HB3	1:E:18:GLY:H	1.84	0.43
1:C:158:TYR:HB2	1:D:196:ILE:HD12	2.00	0.43
1:B:6:VAL:HG22	1:B:110:ILE:HB	1.99	0.43
1:B:376:LYS:HE2	1:B:449:CYS:HA	2.00	0.43
1:A:25:LEU:HD21	5:A:604:MTX:C7	2.49	0.43
1:D:37:SER:OG	5:D:604:MTX:HB1	2.19	0.43
1:D:270:MET:HE2	1:D:460:ILE:HD11	2.00	0.43
1:D:397:MET:SD	1:D:401:PRO:HD3	2.59	0.43
1:A:244:LEU:HD12	1:A:427:LEU:HD13	2.00	0.43
1:C:239:GLN:HG3	1:C:271:ARG:O	2.18	0.43
1:B:244:LEU:HD21	1:B:473:LEU:HD22	1.99	0.43
1:D:235:HIS:CD2	1:D:237:GLU:H	2.36	0.43
1:D:296:ILE:HG13	1:D:300:LYS:HE3	2.00	0.43
1:E:411:THR:HB	1:E:413:ASP:OD1	2.19	0.43
1:A:20:GLY:HA2	1:A:25:LEU:HA	2.00	0.42
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.54	0.42
1:B:158:TYR:OH	1:B:234:GLU:OE1	2.35	0.42
1:C:13:SER:OG	1:C:139:GLU:OE2	2.33	0.42
1:E:13:SER:OG	1:E:139:GLU:OE2	2.32	0.42
1:C:56:ARG:HB3	2:C:601:NDP:H4B	2.01	0.42
1:E:235:HIS:CD2	1:E:237:GLU:H	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:VAL:HG21	1:C:496:ILE:HD13	2.01	0.42
1:A:25:LEU:HD21	5:A:604:MTX:H7	2.02	0.42
1:A:51:ALA:HB2	1:A:107:ILE:HD12	2.00	0.42
1:C:274:MET:HE1	1:C:442:THR:HG21	2.01	0.42
1:A:455:GLU:OE2	1:B:216:HIS:NE2	2.52	0.42
1:B:8:ILE:HG12	1:B:112:VAL:HB	2.01	0.42
1:B:276:GLU:O	1:B:486:GLN:NE2	2.39	0.42
1:D:405:LEU:O	1:D:420:LEU:HD12	2.20	0.42
1:B:51:ALA:HB3	1:B:110:ILE:HD13	2.02	0.42
1:E:161:GLN:HG2	1:E:162:THR:N	2.35	0.42
1:C:13:SER:HB3	1:C:18:GLY:H	1.85	0.42
1:A:126:ASN:OD1	1:A:177:LYS:NZ	2.29	0.41
1:D:422:GLN:NE2	1:D:434:ASN:OD1	2.52	0.41
1:E:355:THR:HG22	1:E:356:MET:H	1.85	0.41
1:A:164:CYS:O	1:B:210:ARG:NH2	2.53	0.41
2:A:601:NDP:H42N	5:A:604:MTX:H92	2.01	0.41
1:C:211:LYS:NZ	1:D:234:GLU:OE2	2.33	0.41
1:A:392:SER:OG	1:B:350:ASN:ND2	2.53	0.41
1:B:328:ILE:HD12	1:B:328:ILE:HA	1.95	0.41
1:E:157:VAL:HG21	1:E:176:GLU:HG3	2.02	0.41
1:E:339:GLY:HA2	1:E:353:TYR:CZ	2.56	0.41
1:C:265:ILE:HG22	1:C:266:PHE:H	1.85	0.41
1:D:354:LYS:HB2	1:D:358:ASP:OD2	2.21	0.41
1:A:274:MET:HE1	1:A:442:THR:HG21	2.02	0.41
1:C:25:LEU:HD11	5:C:604:MTX:C7	2.51	0.41
1:D:19:ILE:HG13	1:D:145:THR:HG22	2.02	0.41
1:A:224:TYR:HD1	1:A:224:TYR:HA	1.79	0.41
1:A:372:ILE:HD11	1:A:496:ILE:HD12	2.01	0.41
1:C:8:ILE:HG12	1:C:112:VAL:HB	2.02	0.41
1:E:347:ARG:HG3	1:E:348:HIS:CE1	2.55	0.41
1:B:155:LEU:HD13	1:B:178:GLN:HB2	2.03	0.41
1:A:56:ARG:HB2	1:A:76:SER:OG	2.21	0.41
1:C:265:ILE:HG22	1:C:266:PHE:N	2.35	0.41
1:C:389:TRP:HB2	1:C:404:VAL:CG1	2.51	0.41
1:E:381:ASP:HB3	1:E:384:HIS:NE2	2.36	0.41
1:A:138:LEU:HD11	1:A:168:ILE:HD13	2.02	0.41
1:B:424:SER:HB2	1:B:464:HIS:HE1	1.85	0.41
1:A:424:SER:HB2	1:A:464:HIS:HE1	1.86	0.41
1:C:147:PHE:CD1	1:C:148:PRO:HD2	2.56	0.41
1:B:225:ASN:HD22	1:B:241:LEU:HD13	1.87	0.40
1:A:212:MET:HE3	1:B:455:GLU:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:HIS:CD2	1:C:237:GLU:H	2.39	0.40
1:E:431:SER:HB3	1:E:432:PRO:HD3	2.04	0.40
1:A:20:GLY:HA2	1:A:26:PRO:HD3	2.04	0.40
1:A:519:MET:HE2	1:A:519:MET:HB3	1.99	0.40
1:A:19:ILE:HG13	1:A:145:THR:HG22	2.04	0.40
1:B:237:GLU:OE1	1:B:481:PRO:HB3	2.21	0.40
1:B:297:TRP:CE2	1:B:308:LEU:HD11	2.56	0.40
1:D:319:ASN:OD1	4:D:603:OG4:N3	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/521 (96%)	464 (93%)	37 (7%)	0	100	100
1	B	501/521 (96%)	469 (94%)	32 (6%)	0	100	100
1	C	502/521 (96%)	464 (92%)	38 (8%)	0	100	100
1	D	502/521 (96%)	467 (93%)	35 (7%)	0	100	100
1	E	501/521 (96%)	466 (93%)	35 (7%)	0	100	100
All	All	2507/2605 (96%)	2330 (93%)	177 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/470 (90%)	418 (99%)	4 (1%)	70	78
1	B	425/470 (90%)	423 (100%)	2 (0%)	81	83
1	C	415/470 (88%)	412 (99%)	3 (1%)	76	80
1	D	426/470 (91%)	424 (100%)	2 (0%)	81	83
1	E	409/470 (87%)	405 (99%)	4 (1%)	68	77
All	All	2097/2350 (89%)	2082 (99%)	15 (1%)	76	80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	209	ILE
1	A	224	TYR
1	A	342	TYR
1	B	224	TYR
1	B	342	TYR
1	C	224	TYR
1	C	233	ARG
1	C	342	TYR
1	D	224	TYR
1	D	342	TYR
1	E	224	TYR
1	E	342	TYR
1	E	355	THR
1	E	411	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	396	GLN
1	B	109	ASN
1	B	390	ASN
1	C	41	ASN
1	C	214	ASN
1	C	306	ASN
1	C	336	ASN
1	C	390	ASN

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Mol	Chain	Res	Type
1	C	396	GLN
1	D	109	ASN
1	D	126	ASN
1	D	306	ASN
1	D	336	ASN
1	D	447	GLN
1	E	69	ASN
1	E	306	ASN
1	E	336	ASN
1	E	345	GLN
1	E	390	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDP	A	601	-	51,52,52	1.96	11 (21%)	71,80,80	1.51	11 (15%)
2	NDP	B	601	-	51,52,52	1.96	11 (21%)	71,80,80	1.52	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UFP	B	602	-	22,22,22	1.29	3 (13%)	32,33,33	2.71	11 (34%)
4	OG4	C	603	-	35,35,35	1.44	5 (14%)	45,49,49	1.58	5 (11%)
5	MTX	B	604	-	35,35,35	1.60	5 (14%)	47,49,49	1.75	7 (14%)
5	MTX	A	604	-	35,35,35	1.61	5 (14%)	47,49,49	1.75	8 (17%)
4	OG4	D	603	-	35,35,35	1.45	5 (14%)	45,49,49	1.70	6 (13%)
5	MTX	C	604	-	35,35,35	1.62	5 (14%)	47,49,49	1.74	7 (14%)
2	NDP	D	601	-	51,52,52	1.96	11 (21%)	71,80,80	1.51	11 (15%)
3	UFP	D	602	-	22,22,22	1.05	0	32,33,33	2.68	10 (31%)
2	NDP	C	601	-	51,52,52	1.95	11 (21%)	71,80,80	1.53	11 (15%)
4	OG4	E	603	-	35,35,35	1.45	5 (14%)	45,49,49	1.58	6 (13%)
5	MTX	D	604	-	35,35,35	1.61	5 (14%)	47,49,49	1.78	8 (17%)
3	UFP	C	602	-	22,22,22	1.29	2 (9%)	32,33,33	2.68	11 (34%)
4	OG4	B	603	-	35,35,35	1.45	5 (14%)	45,49,49	1.55	6 (13%)
3	UFP	A	602	-	22,22,22	1.28	1 (4%)	32,33,33	2.66	10 (31%)
4	OG4	A	603	-	35,35,35	1.44	5 (14%)	45,49,49	1.54	5 (11%)
2	NDP	E	601	-	51,52,52	1.97	11 (21%)	71,80,80	1.52	11 (15%)
3	UFP	E	602	-	22,22,22	1.28	1 (4%)	32,33,33	2.67	11 (34%)
5	MTX	E	604	-	35,35,35	1.62	5 (14%)	47,49,49	1.76	7 (14%)

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	A	601	-	-	5/34/77/77	0/5/5/5
2	NDP	B	601	-	-	9/34/77/77	0/5/5/5
3	UFP	B	602	-	-	7/10/22/22	0/2/2/2
4	OG4	C	603	-	-	2/17/17/17	0/4/4/4
5	MTX	B	604	-	-	8/25/25/25	0/3/3/3
5	MTX	A	604	-	-	8/25/25/25	0/3/3/3
4	OG4	D	603	-	-	3/17/17/17	0/4/4/4
5	MTX	C	604	-	-	8/25/25/25	0/3/3/3
2	NDP	D	601	-	-	10/34/77/77	0/5/5/5
3	UFP	D	602	-	-	7/10/22/22	0/2/2/2
2	NDP	C	601	-	-	11/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OG4	E	603	-	-	4/17/17/17	0/4/4/4
5	MTX	D	604	-	-	8/25/25/25	0/3/3/3
3	UFP	C	602	-	-	7/10/22/22	0/2/2/2
4	OG4	B	603	-	-	2/17/17/17	0/4/4/4
3	UFP	A	602	-	-	3/10/22/22	0/2/2/2
4	OG4	A	603	-	-	4/17/17/17	0/4/4/4
2	NDP	E	601	-	-	8/34/77/77	0/5/5/5
3	UFP	E	602	-	-	2/10/22/22	0/2/2/2
5	MTX	E	604	-	-	8/25/25/25	0/3/3/3

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NDP	C6A-N6A	5.79	1.49	1.34
2	D	601	NDP	C6A-N6A	5.79	1.49	1.34
2	A	601	NDP	C6A-N6A	5.78	1.49	1.34
2	C	601	NDP	C6A-N6A	5.77	1.48	1.34
2	B	601	NDP	C6A-N6A	5.75	1.48	1.34
5	C	604	MTX	C2-NA2	5.34	1.44	1.33
5	D	604	MTX	C2-NA2	5.33	1.44	1.33
5	A	604	MTX	C2-NA2	5.31	1.44	1.33
5	B	604	MTX	C2-NA2	5.30	1.44	1.33
5	E	604	MTX	C2-NA2	5.28	1.44	1.33
4	B	603	OG4	C4-N4	5.27	1.46	1.34
4	D	603	OG4	C4-N4	5.24	1.46	1.34
4	E	603	OG4	C4-N4	5.24	1.46	1.34
4	C	603	OG4	C4-N4	5.23	1.46	1.34
4	A	603	OG4	C4-N4	5.20	1.46	1.34
5	C	604	MTX	C-N	4.75	1.45	1.34
5	E	604	MTX	C-N	4.75	1.45	1.34
5	D	604	MTX	C-N	4.71	1.45	1.34
5	A	604	MTX	C-N	4.70	1.45	1.34
2	D	601	NDP	C4N-C3N	-4.70	1.41	1.50
2	A	601	NDP	C4N-C3N	-4.69	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
5	B	604	MTX	C-N	4.68	1.45	1.34
2	C	601	NDP	C4N-C3N	-4.63	1.41	1.50
4	B	603	OG4	O3-C23	4.31	1.36	1.22
4	E	603	OG4	O3-C23	4.29	1.36	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	OG4	O3-C23	4.29	1.36	1.22
4	A	603	OG4	O3-C23	4.29	1.36	1.22
4	D	603	OG4	O3-C23	4.26	1.36	1.22
2	B	601	NDP	C2D-C3D	-4.02	1.42	1.53
2	E	601	NDP	C2D-C3D	-3.98	1.42	1.53
2	A	601	NDP	C3B-C2B	-3.97	1.44	1.53
2	A	601	NDP	C2D-C3D	-3.94	1.42	1.53
2	C	601	NDP	C2D-C3D	-3.94	1.42	1.53
2	E	601	NDP	C3B-C2B	-3.93	1.44	1.53
2	D	601	NDP	C2D-C3D	-3.93	1.42	1.53
2	D	601	NDP	C3B-C2B	-3.86	1.44	1.53
2	C	601	NDP	C3B-C2B	-3.85	1.44	1.53
2	B	601	NDP	C3B-C2B	-3.81	1.44	1.53
2	B	601	NDP	C7N-N7N	3.71	1.44	1.33
2	A	601	NDP	C7N-N7N	3.70	1.44	1.33
2	C	601	NDP	C7N-N7N	3.70	1.44	1.33
2	E	601	NDP	C7N-N7N	3.69	1.44	1.33
2	D	601	NDP	C7N-N7N	3.69	1.44	1.33
3	C	602	UFP	P-O1P	3.46	1.61	1.50
3	A	602	UFP	P-O1P	3.45	1.61	1.50
3	E	602	UFP	P-O1P	3.42	1.61	1.50
3	B	602	UFP	P-O1P	3.41	1.61	1.50
2	E	601	NDP	C4N-C5N	-3.28	1.40	1.49
2	A	601	NDP	C4N-C5N	-3.26	1.40	1.49
2	D	601	NDP	C4N-C5N	-3.25	1.40	1.49
2	C	601	NDP	C4N-C5N	-3.24	1.40	1.49
2	B	601	NDP	C4N-C5N	-3.22	1.40	1.49
2	B	601	NDP	C2B-C1B	-3.20	1.45	1.53
2	E	601	NDP	C2B-C1B	-3.16	1.45	1.53
2	A	601	NDP	C2B-C1B	-3.15	1.45	1.53
2	D	601	NDP	C2B-C1B	-3.11	1.45	1.53
2	C	601	NDP	C2B-C1B	-3.00	1.45	1.53
4	C	603	OG4	C15-N5	2.63	1.46	1.41
4	A	603	OG4	C2-C1	-2.61	1.39	1.45
5	E	604	MTX	C4-NA4	2.61	1.43	1.34
4	E	603	OG4	C2-C1	-2.60	1.39	1.45
4	D	603	OG4	C2-C1	-2.60	1.39	1.45
5	C	604	MTX	C4-NA4	2.59	1.43	1.34
5	A	604	MTX	C4-NA4	2.59	1.43	1.34
4	B	603	OG4	C2-C1	-2.59	1.39	1.45
5	E	604	MTX	C14-N10	2.57	1.46	1.38
4	A	603	OG4	C15-N5	2.56	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	MTX	C4-NA4	2.56	1.43	1.34
5	D	604	MTX	C4-NA4	2.55	1.43	1.34
4	E	603	OG4	C15-N5	2.55	1.46	1.41
4	D	603	OG4	C15-N5	2.53	1.46	1.41
4	B	603	OG4	C15-N5	2.53	1.46	1.41
5	C	604	MTX	C14-N10	2.52	1.46	1.38
4	C	603	OG4	C2-C1	-2.49	1.39	1.45
5	B	604	MTX	C14-N10	2.47	1.45	1.38
5	D	604	MTX	C14-N10	2.46	1.45	1.38
5	A	604	MTX	C14-N10	2.43	1.45	1.38
2	C	601	NDP	C3B-C4B	-2.43	1.46	1.53
2	A	601	NDP	C3B-C4B	-2.41	1.46	1.53
2	C	601	NDP	C4A-N3A	2.40	1.38	1.34
2	D	601	NDP	C3B-C4B	-2.40	1.46	1.53
4	D	603	OG4	O4-C23	-2.40	1.22	1.30
2	E	601	NDP	C3B-C4B	-2.40	1.46	1.53
4	A	603	OG4	O4-C23	-2.39	1.22	1.30
2	E	601	NDP	C4A-N3A	2.38	1.38	1.34
2	B	601	NDP	C4A-N3A	2.34	1.38	1.34
2	D	601	NDP	C4A-N3A	2.34	1.38	1.34
2	B	601	NDP	C3B-C4B	-2.32	1.47	1.53
4	E	603	OG4	O4-C23	-2.32	1.23	1.30
2	A	601	NDP	C4A-N3A	2.31	1.38	1.34
4	C	603	OG4	O4-C23	-2.31	1.23	1.30
4	B	603	OG4	O4-C23	-2.30	1.23	1.30
2	B	601	NDP	C3D-C4D	-2.28	1.47	1.53
2	E	601	NDP	C3D-C4D	-2.28	1.47	1.53
5	C	604	MTX	C7-N8	2.27	1.35	1.31
2	A	601	NDP	C3D-C4D	-2.25	1.47	1.53
5	A	604	MTX	C7-N8	2.23	1.35	1.31
5	E	604	MTX	C7-N8	2.23	1.35	1.31
2	E	601	NDP	C6N-C5N	2.22	1.39	1.33
2	A	601	NDP	C6N-C5N	2.22	1.39	1.33
2	D	601	NDP	C6N-C5N	2.22	1.39	1.33
5	D	604	MTX	C7-N8	2.21	1.35	1.31
2	C	601	NDP	C6N-C5N	2.21	1.39	1.33
2	C	601	NDP	C3D-C4D	-2.20	1.47	1.53
5	B	604	MTX	C7-N8	2.19	1.35	1.31
2	B	601	NDP	C6N-C5N	2.19	1.39	1.33
2	D	601	NDP	C3D-C4D	-2.18	1.47	1.53
3	B	602	UFP	C4-N3	-2.03	1.35	1.38
3	B	602	UFP	C4-C5	-2.01	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	UFP	C4-N3	-2.01	1.35	1.38

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	UFP	C5-C4-N3	6.82	118.88	112.64
3	E	602	UFP	C5-C4-N3	6.79	118.85	112.64
3	C	602	UFP	C5-C4-N3	6.75	118.81	112.64
3	A	602	UFP	C5-C4-N3	6.70	118.77	112.64
3	B	602	UFP	C5-C4-N3	6.65	118.72	112.64
3	D	602	UFP	O4-C4-C5	-6.16	120.44	125.69
3	A	602	UFP	O4-C4-C5	-6.15	120.45	125.69
3	E	602	UFP	O4-C4-C5	-6.15	120.45	125.69
3	B	602	UFP	O4-C4-C5	-6.12	120.48	125.69
3	C	602	UFP	O4-C4-C5	-6.12	120.48	125.69
2	C	601	NDP	C5A-C4A-N3A	-5.57	119.05	126.72
2	A	601	NDP	C5A-C4A-N3A	-5.47	119.19	126.72
2	D	601	NDP	C5A-C4A-N3A	-5.44	119.23	126.72
2	E	601	NDP	C5A-C4A-N3A	-5.43	119.24	126.72
2	B	601	NDP	C5A-C4A-N3A	-5.36	119.34	126.72
5	E	604	MTX	C6-C7-N8	-5.07	118.28	123.14
5	D	604	MTX	C6-C7-N8	-5.06	118.28	123.14
3	D	602	UFP	F5-C5-C4	5.02	120.87	116.47
5	C	604	MTX	C6-C7-N8	-5.00	118.34	123.14
5	A	604	MTX	C6-C7-N8	-4.96	118.38	123.14
4	C	603	OG4	C5-C2-C1	-4.95	107.00	112.68
3	B	602	UFP	C1'-N1-C2	4.90	127.24	117.66
5	B	604	MTX	C6-C7-N8	-4.90	118.44	123.14
3	A	602	UFP	F5-C5-C4	4.88	120.75	116.47
3	E	602	UFP	F5-C5-C4	4.85	120.72	116.47
4	A	603	OG4	C5-C2-C1	-4.84	107.14	112.68
4	B	603	OG4	C5-C2-C1	-4.79	107.18	112.68
3	C	602	UFP	F5-C5-C4	4.78	120.66	116.47
4	E	603	OG4	C5-C2-C1	-4.77	107.21	112.68
4	D	603	OG4	C5-C2-C1	-4.74	107.24	112.68
3	C	602	UFP	C1'-N1-C2	4.73	126.91	117.66
3	B	602	UFP	F5-C5-C4	4.69	120.58	116.47
3	A	602	UFP	C1'-N1-C2	4.62	126.70	117.66
3	D	602	UFP	C1'-N1-C2	4.62	126.69	117.66
4	D	603	OG4	O3-C23-C22	-4.50	108.83	123.09
3	D	602	UFP	C4-N3-C2	-4.49	121.46	127.34
3	E	602	UFP	C1'-N1-C2	4.46	126.38	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	602	UFP	C4-N3-C2	-4.45	121.51	127.34
4	D	603	OG4	O4-C23-C22	4.45	128.05	114.00
4	E	603	OG4	O3-C23-C22	-4.43	109.03	123.09
4	E	603	OG4	O4-C23-C22	4.40	127.89	114.00
3	A	602	UFP	C4-N3-C2	-4.40	121.58	127.34
3	C	602	UFP	C4-N3-C2	-4.35	121.63	127.34
3	E	602	UFP	N3-C2-N1	4.32	120.52	114.89
3	A	602	UFP	N3-C2-N1	4.31	120.50	114.89
3	B	602	UFP	N3-C2-N1	4.31	120.50	114.89
3	C	602	UFP	N3-C2-N1	4.28	120.46	114.89
3	B	602	UFP	C4-N3-C2	-4.27	121.75	127.34
4	B	603	OG4	O3-C23-C22	-4.26	109.59	123.09
3	D	602	UFP	N3-C2-N1	4.24	120.41	114.89
3	D	602	UFP	C6-C5-C4	-4.22	118.72	122.57
3	E	602	UFP	C6-C5-C4	-4.22	118.72	122.57
4	B	603	OG4	O4-C23-C22	4.21	127.30	114.00
3	A	602	UFP	C6-C5-C4	-4.21	118.73	122.57
3	C	602	UFP	C6-C5-C4	-4.18	118.75	122.57
3	B	602	UFP	C6-C5-C4	-4.18	118.75	122.57
4	C	603	OG4	O3-C23-C22	-4.18	109.85	123.09
4	A	603	OG4	O3-C23-C22	-4.13	109.98	123.09
4	C	603	OG4	O4-C23-C22	4.13	127.05	114.00
4	A	603	OG4	O4-C23-C22	4.08	126.90	114.00
5	E	604	MTX	N8-C8A-N1	3.98	120.11	115.77
5	C	604	MTX	N8-C8A-N1	3.96	120.08	115.77
5	E	604	MTX	CG-CB-CA	3.96	120.46	113.16
5	B	604	MTX	CG-CB-CA	3.96	120.46	113.16
5	D	604	MTX	N1-C2-N3	-3.95	122.18	127.21
5	B	604	MTX	N1-C2-N3	-3.94	122.20	127.21
5	A	604	MTX	N1-C2-N3	-3.94	122.21	127.21
3	B	602	UFP	C1'-N1-C6	-3.90	114.19	120.74
4	D	603	OG4	C21-C22-C23	-3.88	103.38	113.83
2	E	601	NDP	N3A-C2A-N1A	-3.88	122.71	128.58
5	B	604	MTX	N8-C8A-N1	3.88	120.00	115.77
5	C	604	MTX	N1-C2-N3	-3.88	122.28	127.21
2	B	601	NDP	N3A-C2A-N1A	-3.87	122.72	128.58
5	A	604	MTX	N8-C8A-N1	3.86	119.98	115.77
5	E	604	MTX	N1-C2-N3	-3.86	122.30	127.21
5	D	604	MTX	N8-C8A-N1	3.82	119.93	115.77
5	C	604	MTX	CG-CB-CA	3.81	120.19	113.16
5	D	604	MTX	CG-CB-CA	3.81	120.18	113.16
3	D	602	UFP	C1'-N1-C6	-3.80	114.35	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NDP	N3A-C2A-N1A	-3.80	122.82	128.58
3	C	602	UFP	C1'-N1-C6	-3.80	114.36	120.74
2	C	601	NDP	N3A-C2A-N1A	-3.80	122.83	128.58
2	D	601	NDP	N3A-C2A-N1A	-3.77	122.87	128.58
2	C	601	NDP	N3A-C4A-N9A	3.76	133.56	127.17
2	A	601	NDP	N3A-C4A-N9A	3.73	133.50	127.17
3	A	602	UFP	C1'-N1-C6	-3.71	114.51	120.74
2	E	601	NDP	N3A-C4A-N9A	3.71	133.47	127.17
5	A	604	MTX	CG-CB-CA	3.70	119.98	113.16
5	A	604	MTX	C2-N1-C8A	3.69	119.47	115.48
2	B	601	NDP	N3A-C4A-N9A	3.67	133.41	127.17
5	C	604	MTX	C2-N1-C8A	3.66	119.43	115.48
5	B	604	MTX	C2-N1-C8A	3.65	119.42	115.48
2	D	601	NDP	N3A-C4A-N9A	3.64	133.35	127.17
5	E	604	MTX	C2-N1-C8A	3.63	119.40	115.48
5	D	604	MTX	C2-N1-C8A	3.58	119.34	115.48
3	E	602	UFP	C1'-N1-C6	-3.55	114.79	120.74
2	C	601	NDP	C2A-N3A-C4A	3.42	120.19	111.83
2	E	601	NDP	C2A-N3A-C4A	3.41	120.17	111.83
2	A	601	NDP	C2A-N3A-C4A	3.41	120.16	111.83
2	B	601	NDP	C2A-N3A-C4A	3.40	120.12	111.83
2	D	601	NDP	C2A-N3A-C4A	3.38	120.10	111.83
3	B	602	UFP	O2-C2-N3	-3.30	115.40	121.49
2	B	601	NDP	N9A-C8A-N7A	-3.22	109.37	113.94
3	C	602	UFP	O2-C2-N3	-3.21	115.57	121.49
2	A	601	NDP	C4A-C5A-N7A	-3.19	106.94	110.58
2	A	601	NDP	N9A-C8A-N7A	-3.17	109.44	113.94
2	E	601	NDP	C4A-C5A-N7A	-3.15	106.98	110.58
2	E	601	NDP	N9A-C8A-N7A	-3.14	109.48	113.94
2	D	601	NDP	C4A-C5A-N7A	-3.14	106.99	110.58
2	B	601	NDP	C4A-C5A-N7A	-3.14	106.99	110.58
2	C	601	NDP	C4A-C5A-N7A	-3.13	107.00	110.58
4	D	603	OG4	C8-C7-C5	-3.09	107.58	114.10
2	A	601	NDP	C5A-N7A-C8A	3.08	108.28	103.45
2	B	601	NDP	C5A-N7A-C8A	3.05	108.24	103.45
2	D	601	NDP	N9A-C8A-N7A	-3.05	109.61	113.94
2	E	601	NDP	C5A-N7A-C8A	3.04	108.23	103.45
3	A	602	UFP	O2-C2-N3	-3.02	115.92	121.49
3	E	602	UFP	O2-C2-N3	-3.01	115.93	121.49
2	D	601	NDP	C5A-N7A-C8A	3.00	108.16	103.45
2	C	601	NDP	C5A-N7A-C8A	3.00	108.16	103.45
2	C	601	NDP	N9A-C8A-N7A	-2.97	109.73	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	UFP	O2-C2-N3	-2.96	116.02	121.49
3	B	602	UFP	C6-N1-C2	-2.75	118.56	121.30
4	C	603	OG4	C16-C15-N5	2.72	124.02	119.35
2	D	601	NDP	O5B-C5B-C4B	2.59	117.80	108.99
2	E	601	NDP	O5B-C5B-C4B	2.59	117.80	108.99
3	C	602	UFP	C6-N1-C2	-2.58	118.73	121.30
2	C	601	NDP	O5B-C5B-C4B	2.56	117.72	108.99
2	E	601	NDP	O5D-C5D-C4D	2.54	117.64	108.99
2	B	601	NDP	O5D-C5D-C4D	2.53	117.62	108.99
5	D	604	MTX	C7-N8-C8A	2.52	120.72	117.20
3	A	602	UFP	C6-N1-C2	-2.52	118.79	121.30
5	C	604	MTX	C7-N8-C8A	2.51	120.69	117.20
5	E	604	MTX	C7-N8-C8A	2.51	120.69	117.20
2	C	601	NDP	O5D-C5D-C4D	2.51	117.53	108.99
3	E	602	UFP	C6-N1-C2	-2.48	118.83	121.30
5	B	604	MTX	C7-N8-C8A	2.46	120.63	117.20
2	D	601	NDP	O5D-C5D-C4D	2.44	117.30	108.99
5	A	604	MTX	C7-N8-C8A	2.44	120.59	117.20
2	A	601	NDP	O5D-C5D-C4D	2.43	117.28	108.99
3	E	602	UFP	O4'-C1'-C2'	-2.43	101.70	106.25
2	A	601	NDP	O5B-C5B-C4B	2.41	117.19	108.99
2	B	601	NDP	O5B-C5B-C4B	2.38	117.09	108.99
5	D	604	MTX	C11-C-N	2.37	121.44	117.04
3	D	602	UFP	C6-N1-C2	-2.35	118.96	121.30
4	A	603	OG4	C16-C15-N5	2.30	123.31	119.35
2	B	601	NDP	C4A-N9A-C8A	2.29	108.14	105.74
2	B	601	NDP	O4D-C1D-N1N	2.25	112.38	108.08
4	E	603	OG4	C8-C7-C5	-2.23	109.39	114.10
4	E	603	OG4	C16-C15-N5	2.22	123.17	119.35
4	B	603	OG4	C8-C7-C5	-2.20	109.45	114.10
2	C	601	NDP	O4D-C1D-N1N	2.20	112.29	108.08
2	A	601	NDP	C4A-N9A-C8A	2.18	108.03	105.74
4	E	603	OG4	O2-C14-C11	2.17	125.20	120.90
4	C	603	OG4	C20-C15-N5	-2.17	116.79	121.82
2	E	601	NDP	C4A-N9A-C8A	2.17	108.02	105.74
3	B	602	UFP	O4'-C1'-C2'	-2.17	102.19	106.25
4	D	603	OG4	O2-C14-C11	2.16	125.17	120.90
4	B	603	OG4	O2-C14-C11	2.12	125.11	120.90
3	C	602	UFP	O4'-C1'-C2'	-2.10	102.32	106.25
5	C	604	MTX	O2-CT-CA	2.09	120.58	113.51
5	B	604	MTX	O2-CT-CA	2.08	120.56	113.51
5	D	604	MTX	CM-N10-C9	2.08	120.53	115.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	MTX	O2-CT-CA	2.07	120.52	113.51
2	C	601	NDP	C2B-C1B-N9A	-2.05	110.38	113.75
5	E	604	MTX	O2-CT-CA	2.04	120.41	113.51
4	B	603	OG4	C16-C15-N5	2.04	122.85	119.35
2	A	601	NDP	C3N-C7N-N7N	2.04	121.28	117.67
2	E	601	NDP	C3N-C7N-N7N	2.03	121.27	117.67
2	D	601	NDP	C3N-C7N-N7N	2.02	121.26	117.67
4	A	603	OG4	O2-C14-C11	2.01	124.89	120.90
5	A	604	MTX	CM-N10-C9	2.01	120.34	115.11
2	D	601	NDP	O4D-C1D-N1N	2.00	111.90	108.08

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	NDP	C5D-O5D-PN-O3
2	C	601	NDP	C5D-O5D-PN-O1N
2	D	601	NDP	C5D-O5D-PN-O3
2	D	601	NDP	C5D-O5D-PN-O1N
3	B	602	UFP	C3'-C4'-C5'-O5'
3	B	602	UFP	O4'-C4'-C5'-O5'
3	B	602	UFP	C5'-O5'-P-O1P
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	D	602	UFP	C5'-O5'-P-O2P
4	B	603	OG4	C16-C21-C22-C23
4	C	603	OG4	C16-C21-C22-C23
4	D	603	OG4	C16-C21-C22-C23
4	E	603	OG4	C16-C21-C22-C23
5	B	604	MTX	N-CA-CB-CG
5	C	604	MTX	N-CA-CB-CG
5	E	604	MTX	N-CA-CB-CG
5	D	604	MTX	N-CA-CB-CG
2	C	601	NDP	C3B-C4B-C5B-O5B
2	C	601	NDP	O4D-C4D-C5D-O5D
2	D	601	NDP	O4D-C4D-C5D-O5D
2	D	601	NDP	C3D-C4D-C5D-O5D
5	C	604	MTX	C13-C14-N10-CM
3	C	602	UFP	C2'-C1'-N1-C2
4	A	603	OG4	C16-C21-C22-C23
5	B	604	MTX	CT-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	C	601	NDP	C3D-C4D-C5D-O5D
5	A	604	MTX	C13-C14-N10-CM
5	B	604	MTX	C13-C14-N10-CM
5	D	604	MTX	C13-C14-N10-CM
5	E	604	MTX	C13-C14-N10-CM
5	A	604	MTX	N-CA-CB-CG
3	B	602	UFP	C2'-C1'-N1-C2
3	C	602	UFP	C3'-C4'-C5'-O5'
3	C	602	UFP	O4'-C4'-C5'-O5'
3	B	602	UFP	C2'-C1'-N1-C6
5	A	604	MTX	C15-C14-N10-CM
5	B	604	MTX	C15-C14-N10-CM
5	C	604	MTX	C15-C14-N10-CM
5	D	604	MTX	C15-C14-N10-CM
5	E	604	MTX	C15-C14-N10-CM
5	A	604	MTX	CT-CA-CB-CG
5	C	604	MTX	CT-CA-CB-CG
5	D	604	MTX	CT-CA-CB-CG
5	E	604	MTX	CT-CA-CB-CG
3	D	602	UFP	C3'-C4'-C5'-O5'
3	D	602	UFP	O4'-C4'-C5'-O5'
3	C	602	UFP	C2'-C1'-N1-C6
3	D	602	UFP	C2'-C1'-N1-C2
2	C	601	NDP	O4B-C4B-C5B-O5B
3	A	602	UFP	C2'-C1'-N1-C2
3	E	602	UFP	C2'-C1'-N1-C2
3	C	602	UFP	C5'-O5'-P-O1P
2	B	601	NDP	C3B-C4B-C5B-O5B
3	D	602	UFP	C2'-C1'-N1-C6
3	A	602	UFP	C2'-C1'-N1-C6
3	E	602	UFP	C2'-C1'-N1-C6
2	A	601	NDP	PA-O3-PN-O5D
2	B	601	NDP	PA-O3-PN-O5D
2	C	601	NDP	PA-O3-PN-O5D
2	D	601	NDP	PA-O3-PN-O5D
2	E	601	NDP	PA-O3-PN-O5D
3	C	602	UFP	C5'-O5'-P-O3P
3	D	602	UFP	C5'-O5'-P-O3P
5	A	604	MTX	C6-C9-N10-CM
5	B	604	MTX	C6-C9-N10-CM
5	C	604	MTX	C6-C9-N10-CM
5	E	604	MTX	C6-C9-N10-CM

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Mol	Chain	Res	Type	Atoms
2	B	601	NDP	C3D-C4D-C5D-O5D
2	E	601	NDP	C3D-C4D-C5D-O5D
2	C	601	NDP	C5D-O5D-PN-O2N
2	D	601	NDP	C5D-O5D-PN-O2N
2	C	601	NDP	O4D-C1D-N1N-C2N
3	D	602	UFP	C5'-O5'-P-O1P
5	A	604	MTX	OE2-CD-CG-CB
5	E	604	MTX	OE2-CD-CG-CB
2	D	601	NDP	O4D-C1D-N1N-C2N
2	E	601	NDP	C4D-C5D-O5D-PN
5	D	604	MTX	OE2-CD-CG-CB
3	A	602	UFP	O4'-C4'-C5'-O5'
5	D	604	MTX	OE1-CD-CG-CB
2	B	601	NDP	O4D-C1D-N1N-C2N
5	A	604	MTX	OE1-CD-CG-CB
5	B	604	MTX	OE1-CD-CG-CB
5	C	604	MTX	OE1-CD-CG-CB
5	E	604	MTX	OE1-CD-CG-CB
2	A	601	NDP	C4D-C5D-O5D-PN
2	B	601	NDP	C4D-C5D-O5D-PN
2	C	601	NDP	C4D-C5D-O5D-PN
2	D	601	NDP	C4D-C5D-O5D-PN
5	C	604	MTX	OE2-CD-CG-CB
2	A	601	NDP	O4D-C1D-N1N-C2N
2	E	601	NDP	O4D-C1D-N1N-C2N
5	B	604	MTX	OE2-CD-CG-CB
4	D	603	OG4	C21-C22-C23-O4
4	D	603	OG4	C21-C22-C23-O3
5	C	604	MTX	C15-C14-N10-C9
2	E	601	NDP	C2D-C1D-N1N-C2N
2	E	601	NDP	C3B-C4B-C5B-O5B
5	D	604	MTX	C6-C9-N10-CM
4	A	603	OG4	C21-C22-C23-O4
2	A	601	NDP	C2D-C1D-N1N-C2N
5	B	604	MTX	C15-C14-N10-C9
5	E	604	MTX	C15-C14-N10-C9
2	D	601	NDP	C3B-C4B-C5B-O5B
2	E	601	NDP	O4D-C4D-C5D-O5D
4	A	603	OG4	C21-C22-C23-O3
2	B	601	NDP	C2D-C1D-N1N-C2N
2	B	601	NDP	C2B-O2B-P2B-O3X
4	E	603	OG4	C21-C22-C23-O3

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Mol	Chain	Res	Type	Atoms
5	A	604	MTX	C15-C14-N10-C9
4	C	603	OG4	C16-C15-N5-C14
4	E	603	OG4	C21-C22-C23-O4
2	B	601	NDP	O4D-C4D-C5D-O5D
4	A	603	OG4	C16-C15-N5-C14
2	A	601	NDP	C2B-O2B-P2B-O1X
2	C	601	NDP	C2B-O2B-P2B-O1X
2	D	601	NDP	C2B-O2B-P2B-O1X
2	E	601	NDP	C2B-O2B-P2B-O1X
4	B	603	OG4	C16-C15-N5-C14
5	D	604	MTX	C15-C14-N10-C9
4	E	603	OG4	C16-C15-N5-C14
2	B	601	NDP	O4B-C4B-C5B-O5B

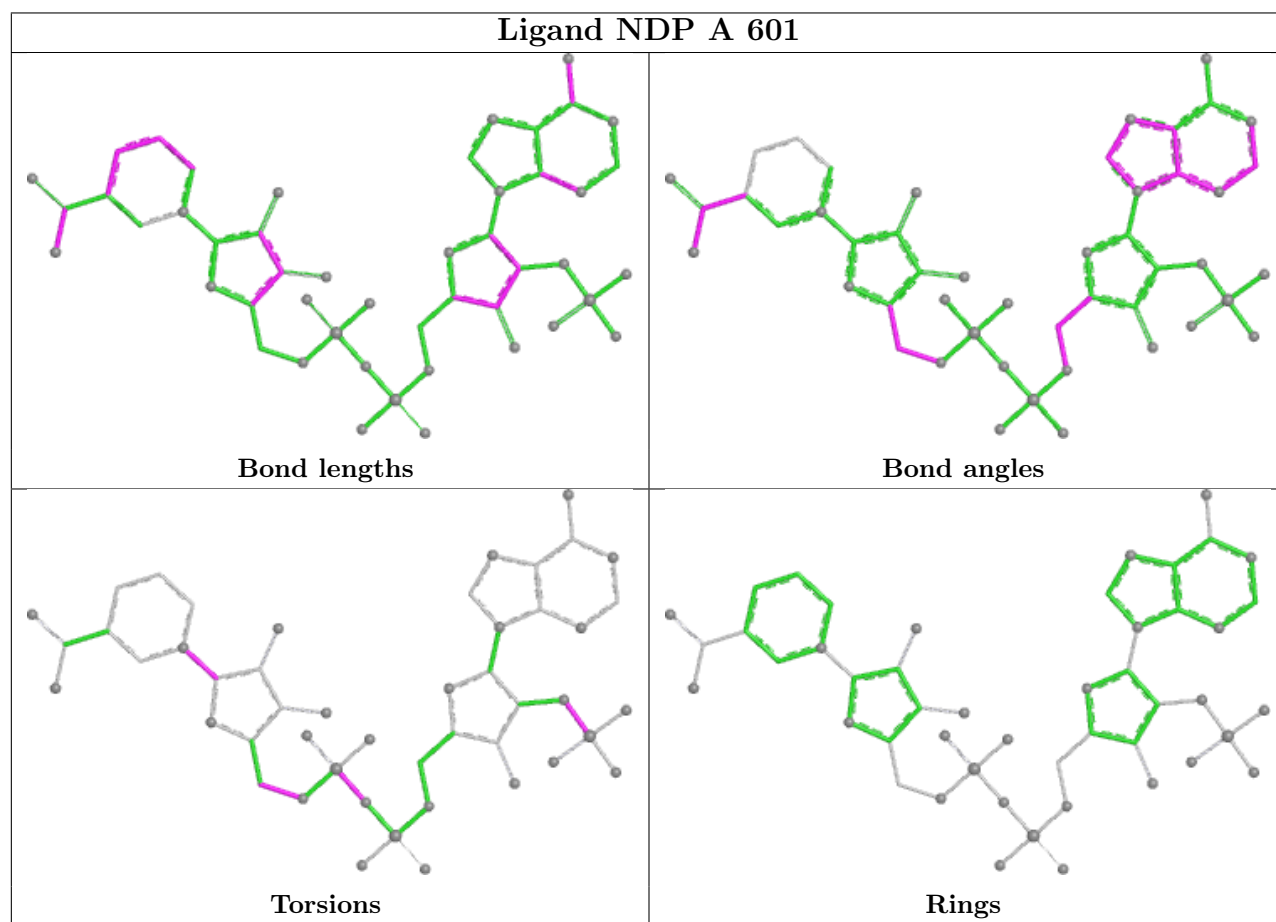
There are no ring outliers.

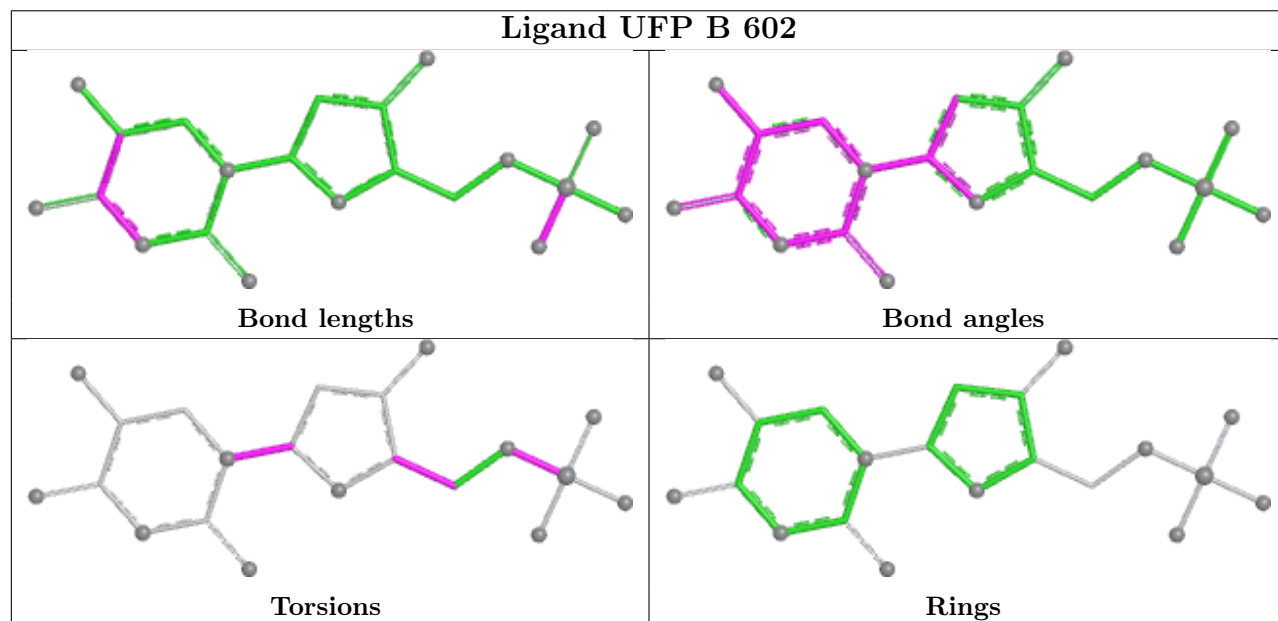
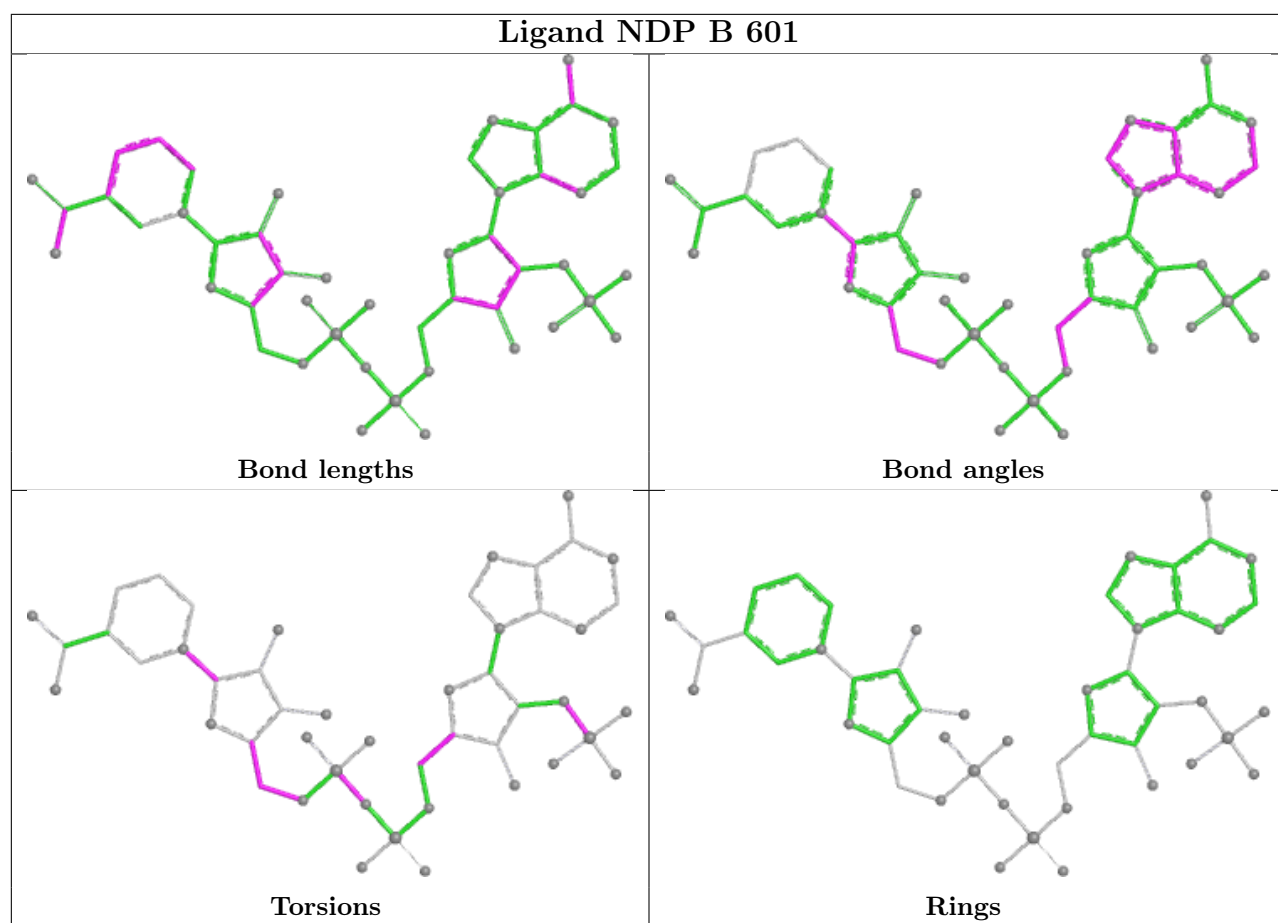
17 monomers are involved in 30 short contacts:

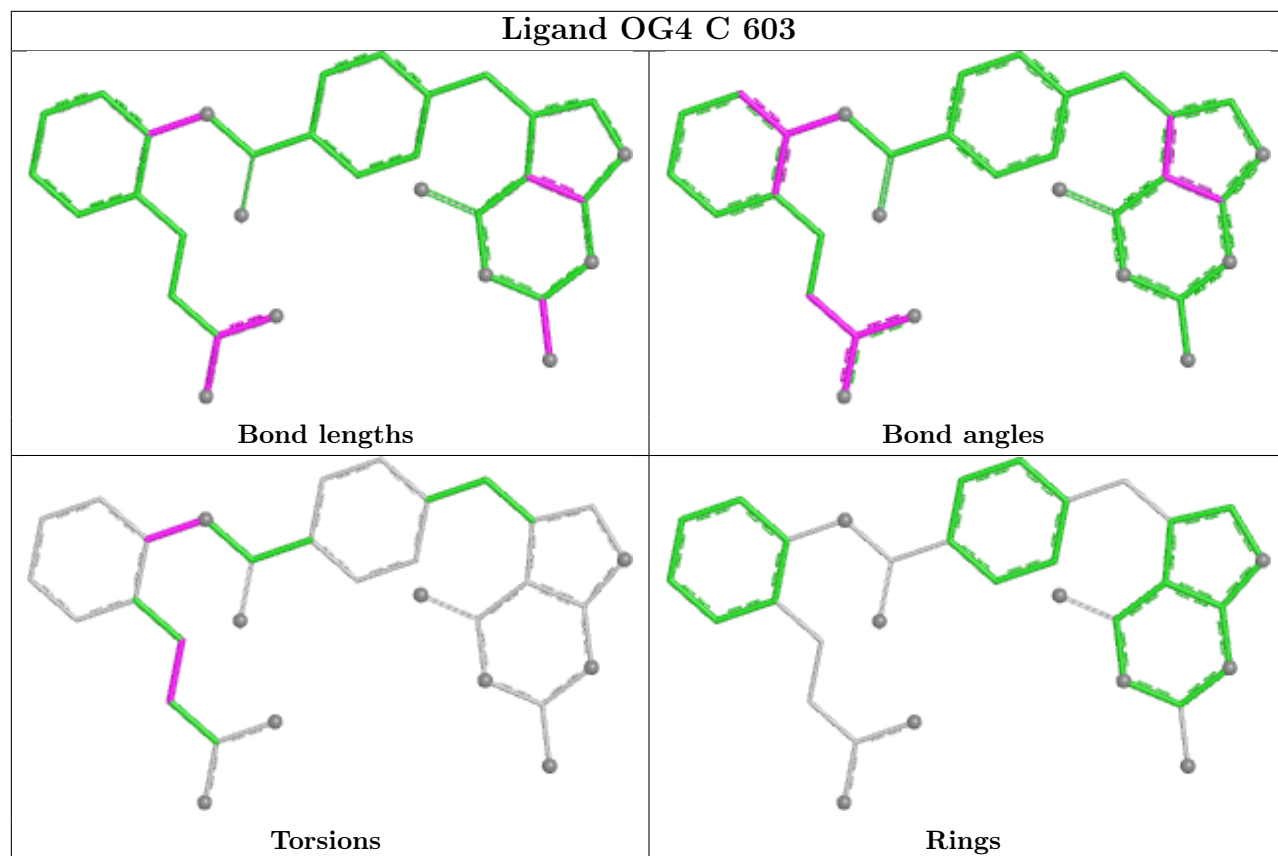
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NDP	2	0
2	B	601	NDP	2	0
3	B	602	UFP	2	0
4	C	603	OG4	1	0
5	B	604	MTX	3	0
5	A	604	MTX	4	0
4	D	603	OG4	1	0
5	C	604	MTX	3	0
2	D	601	NDP	2	0
3	D	602	UFP	2	0
2	C	601	NDP	2	0
5	D	604	MTX	3	0
3	C	602	UFP	1	0
3	A	602	UFP	1	0
2	E	601	NDP	1	0
3	E	602	UFP	1	0
5	E	604	MTX	1	0

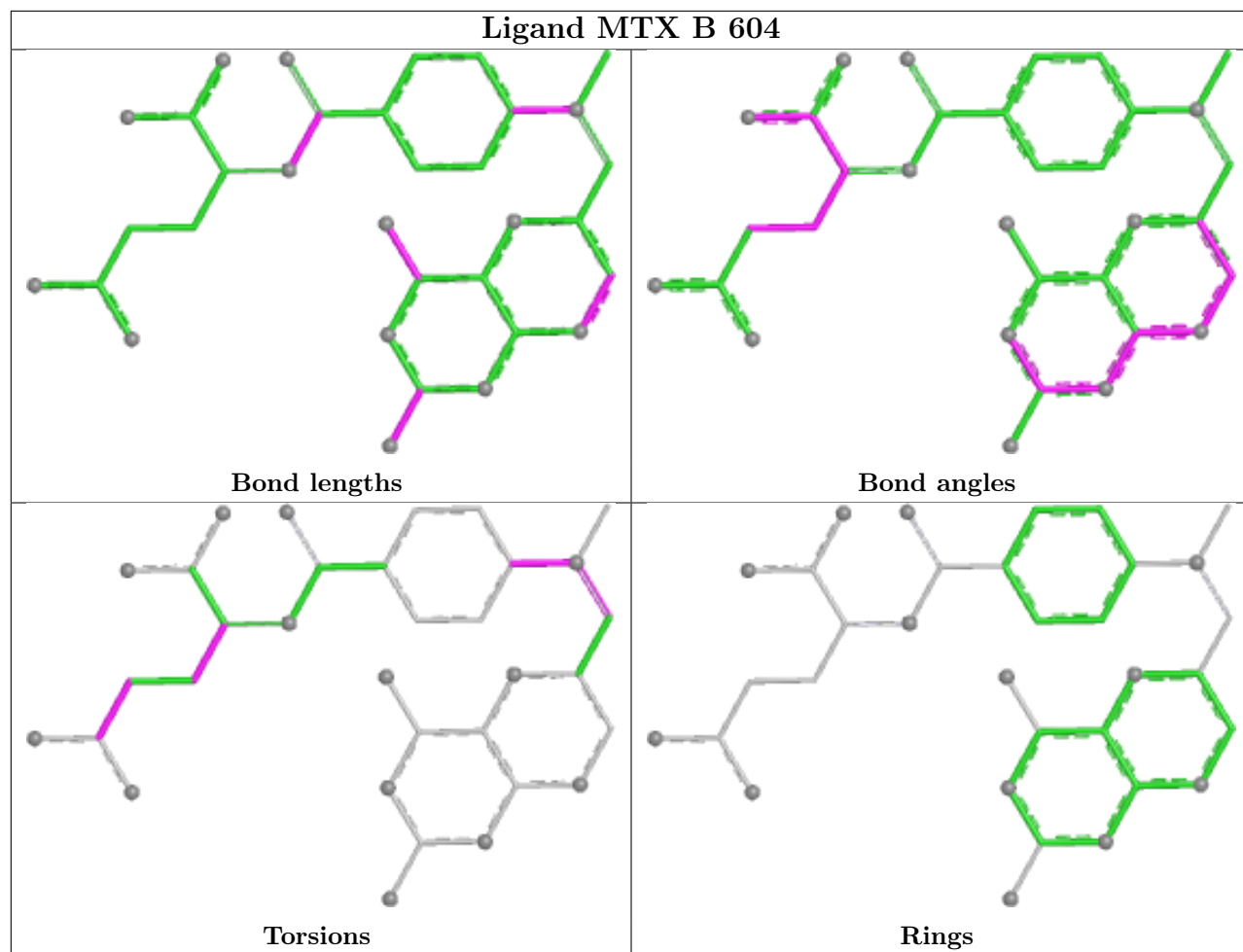
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

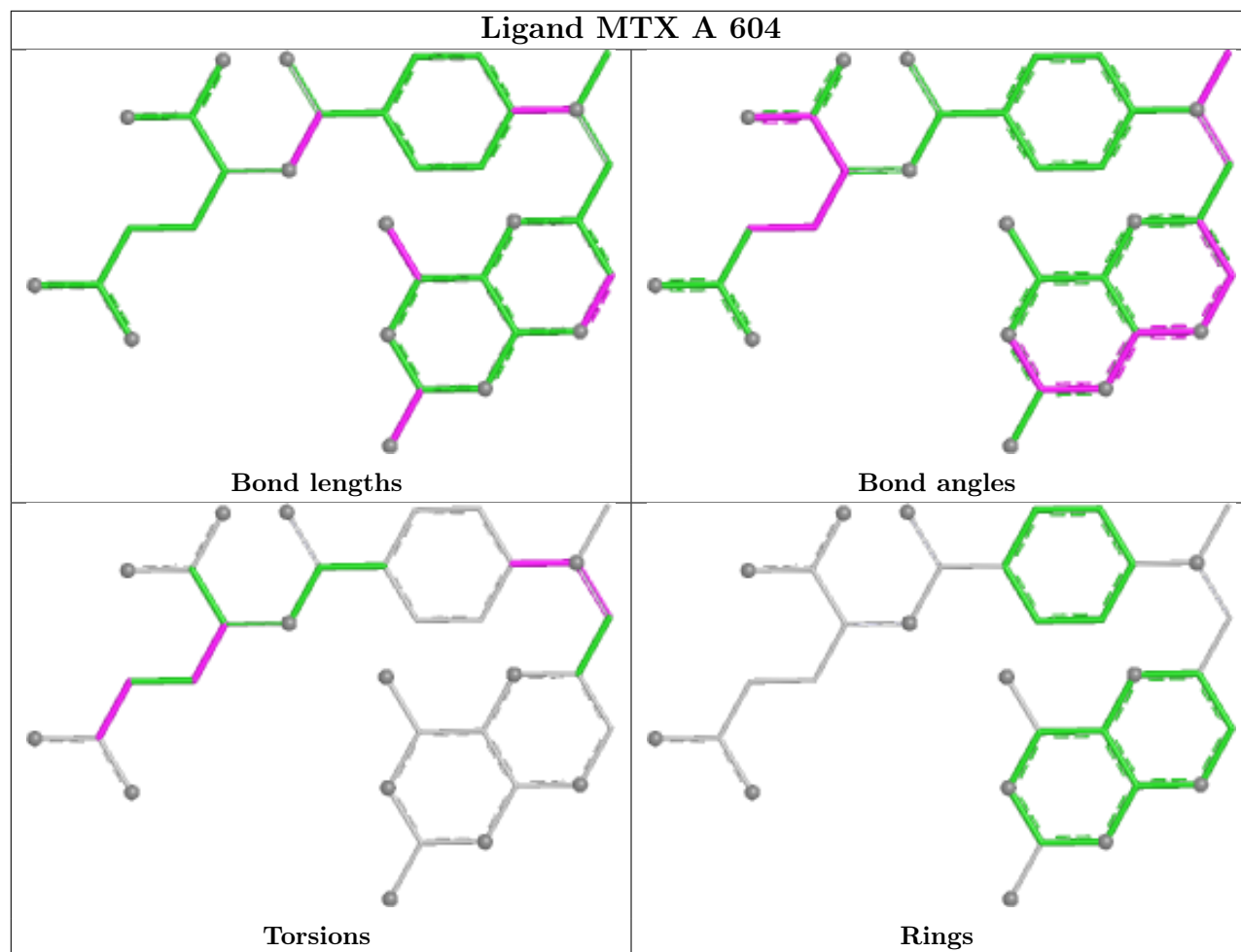
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

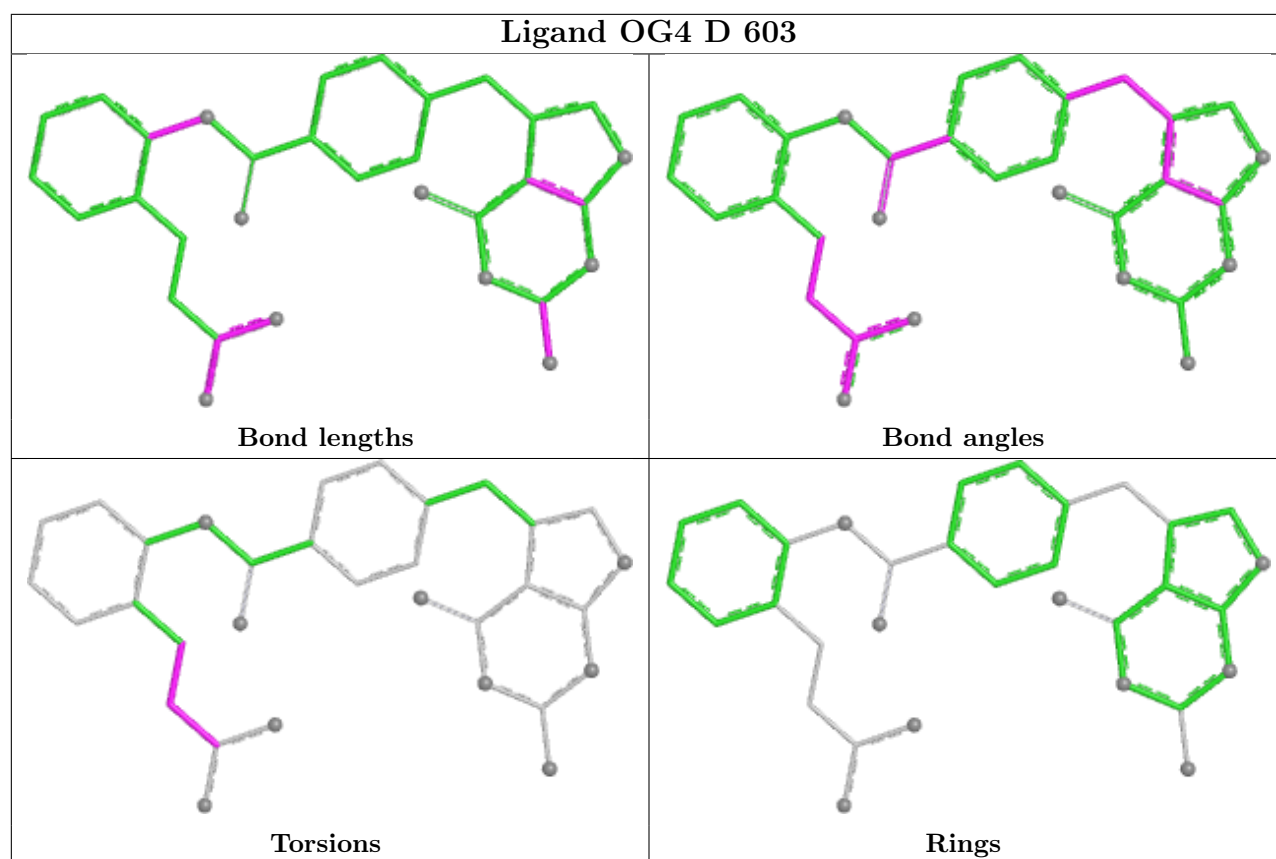


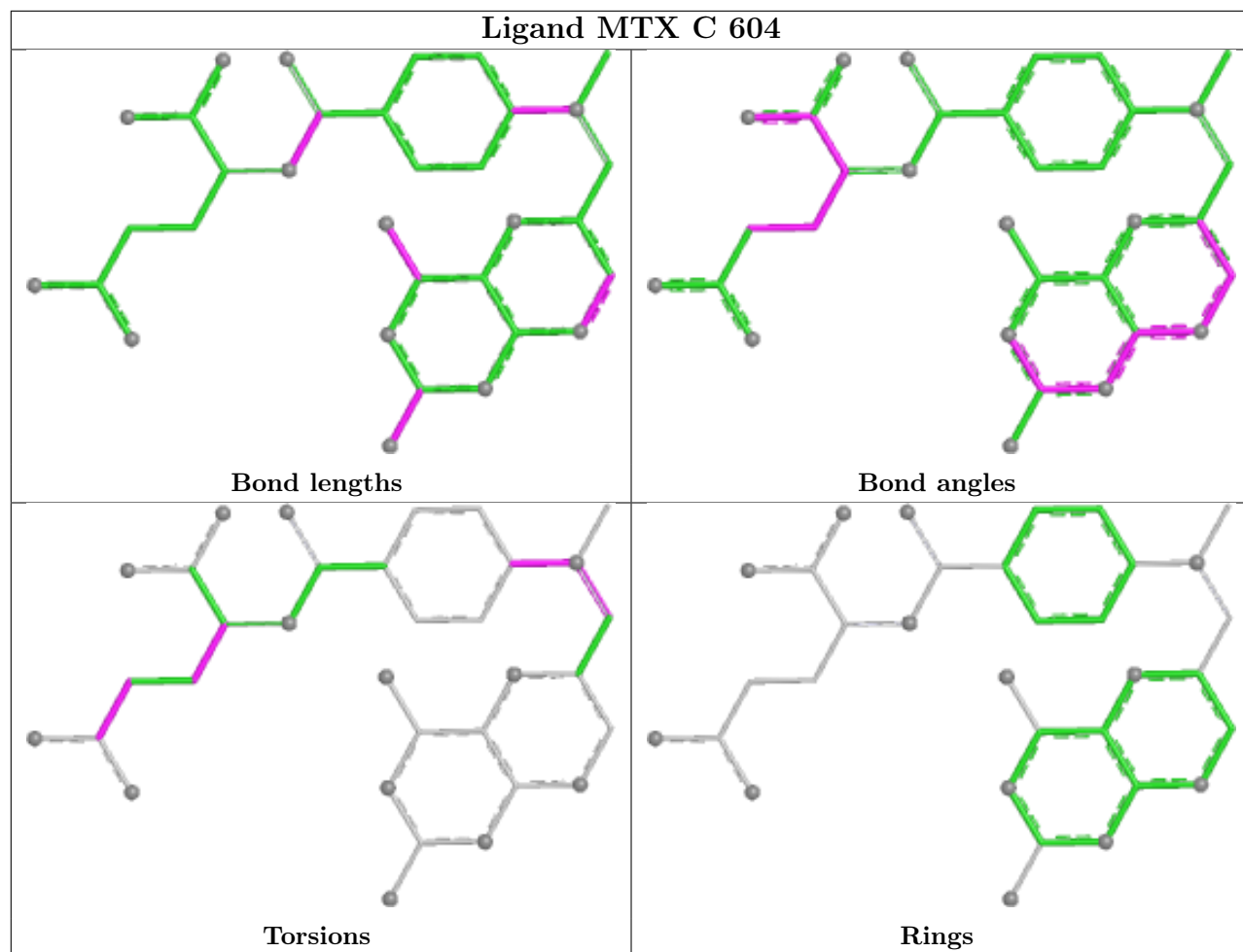


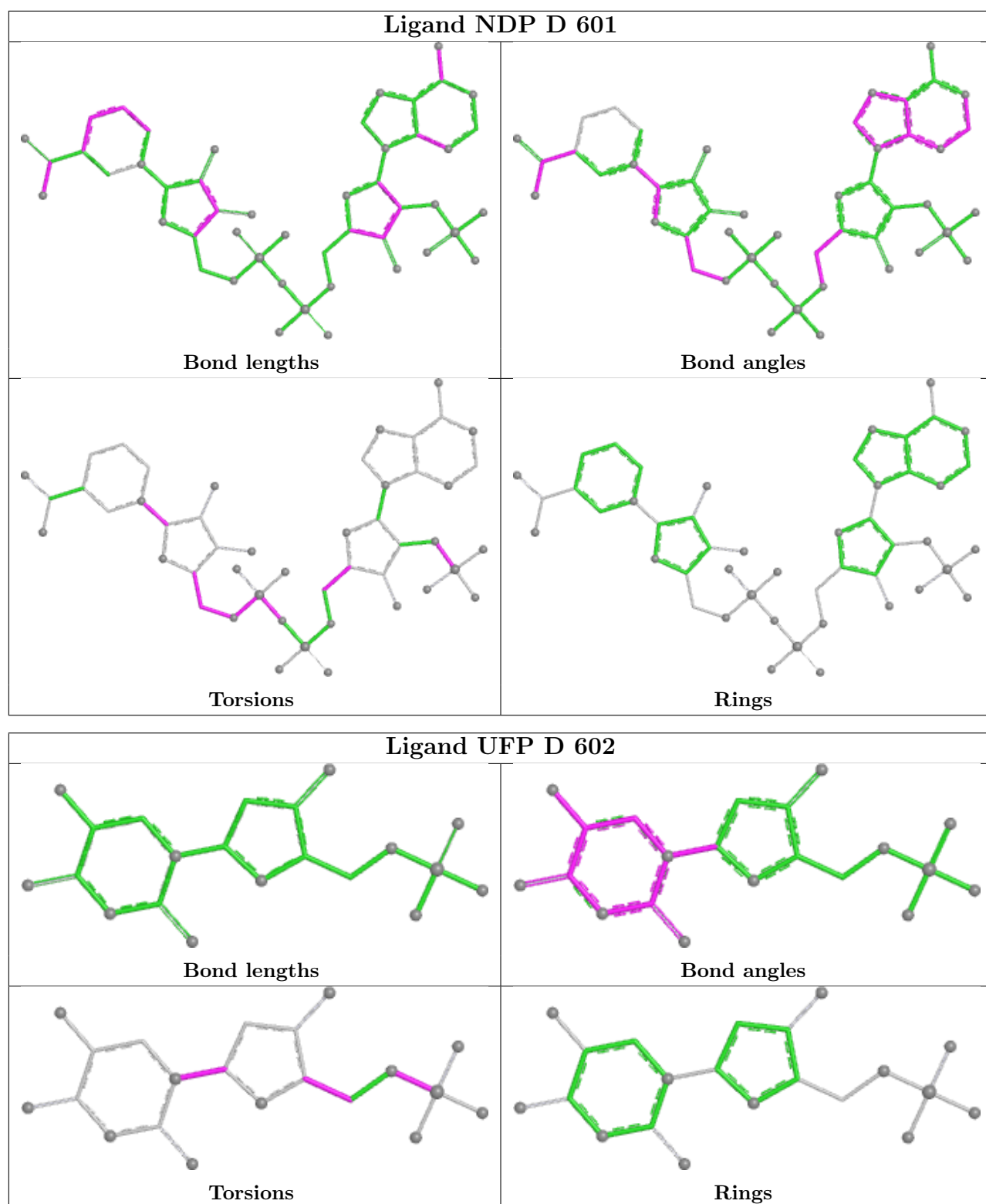


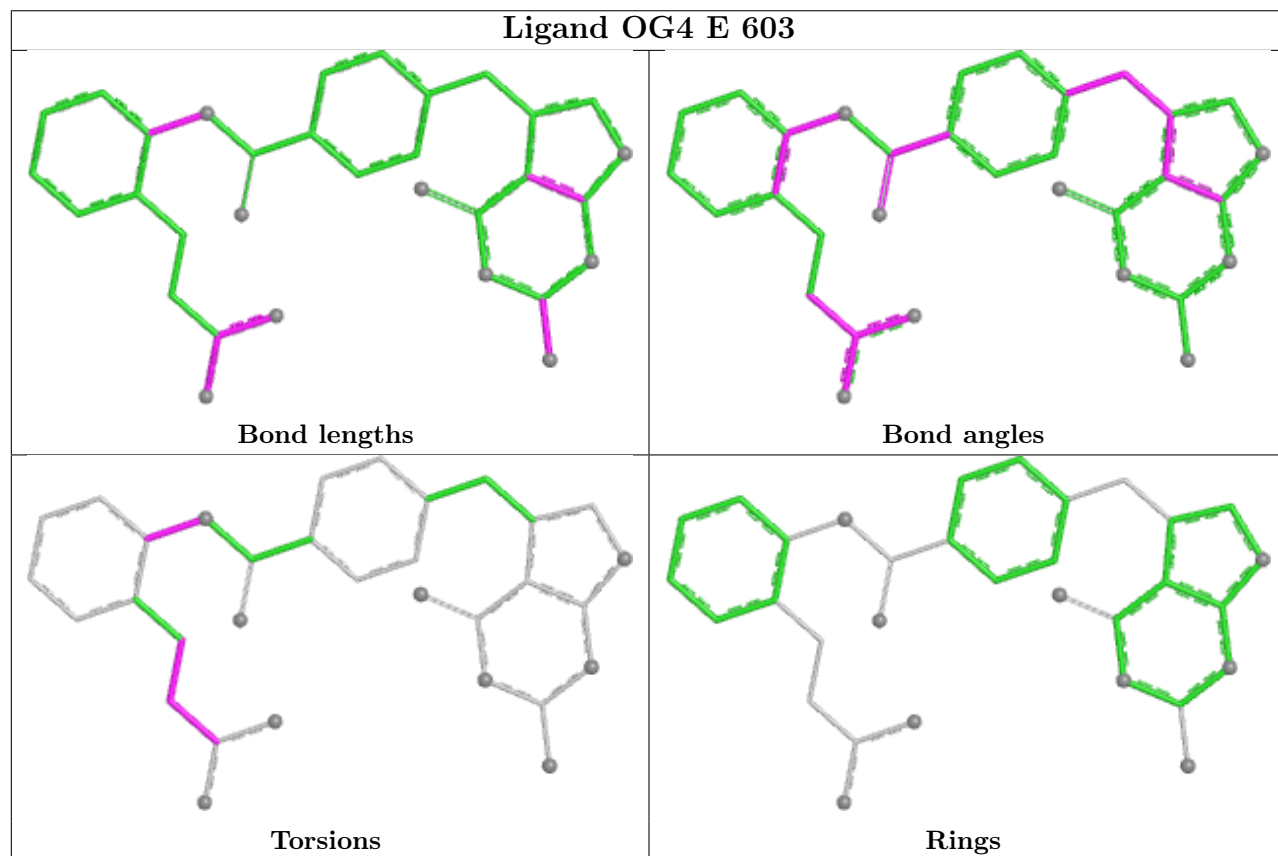
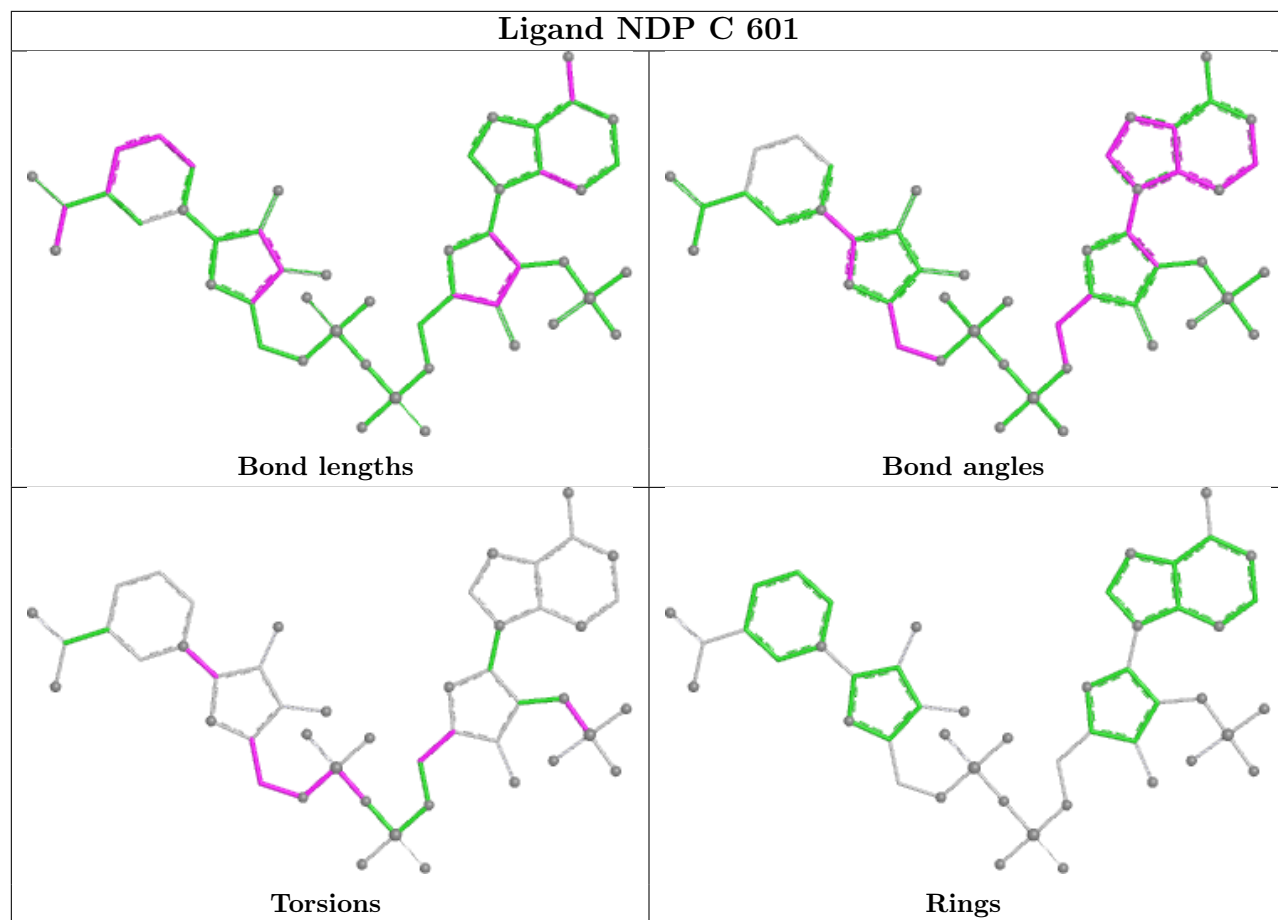


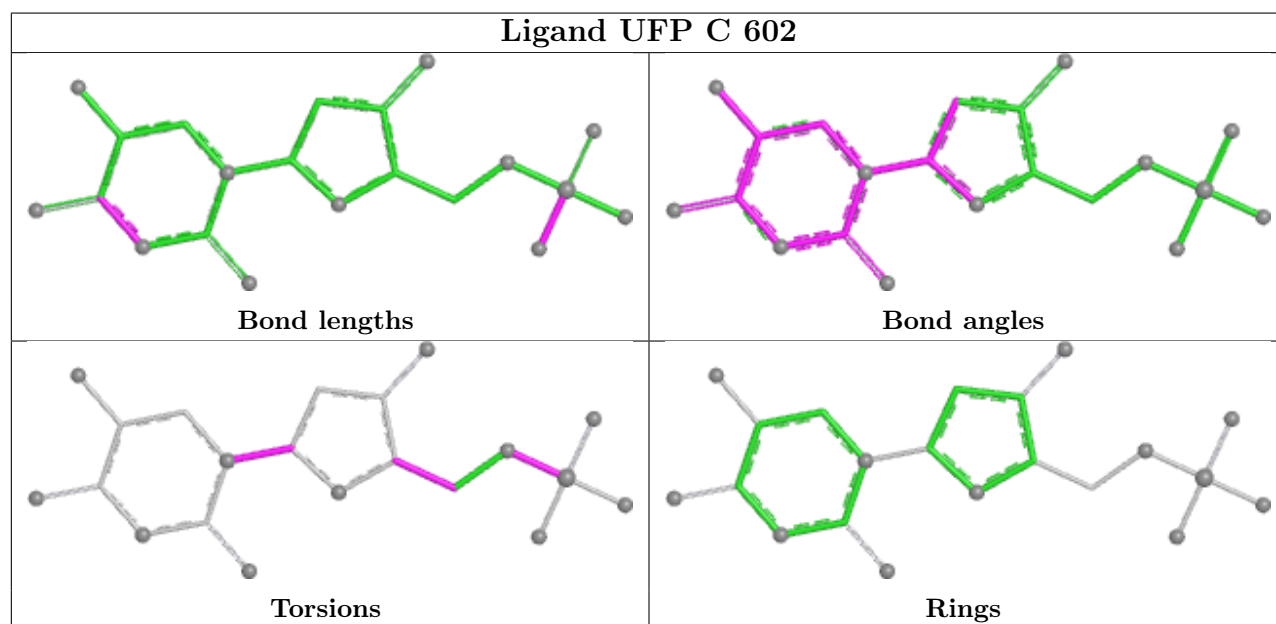
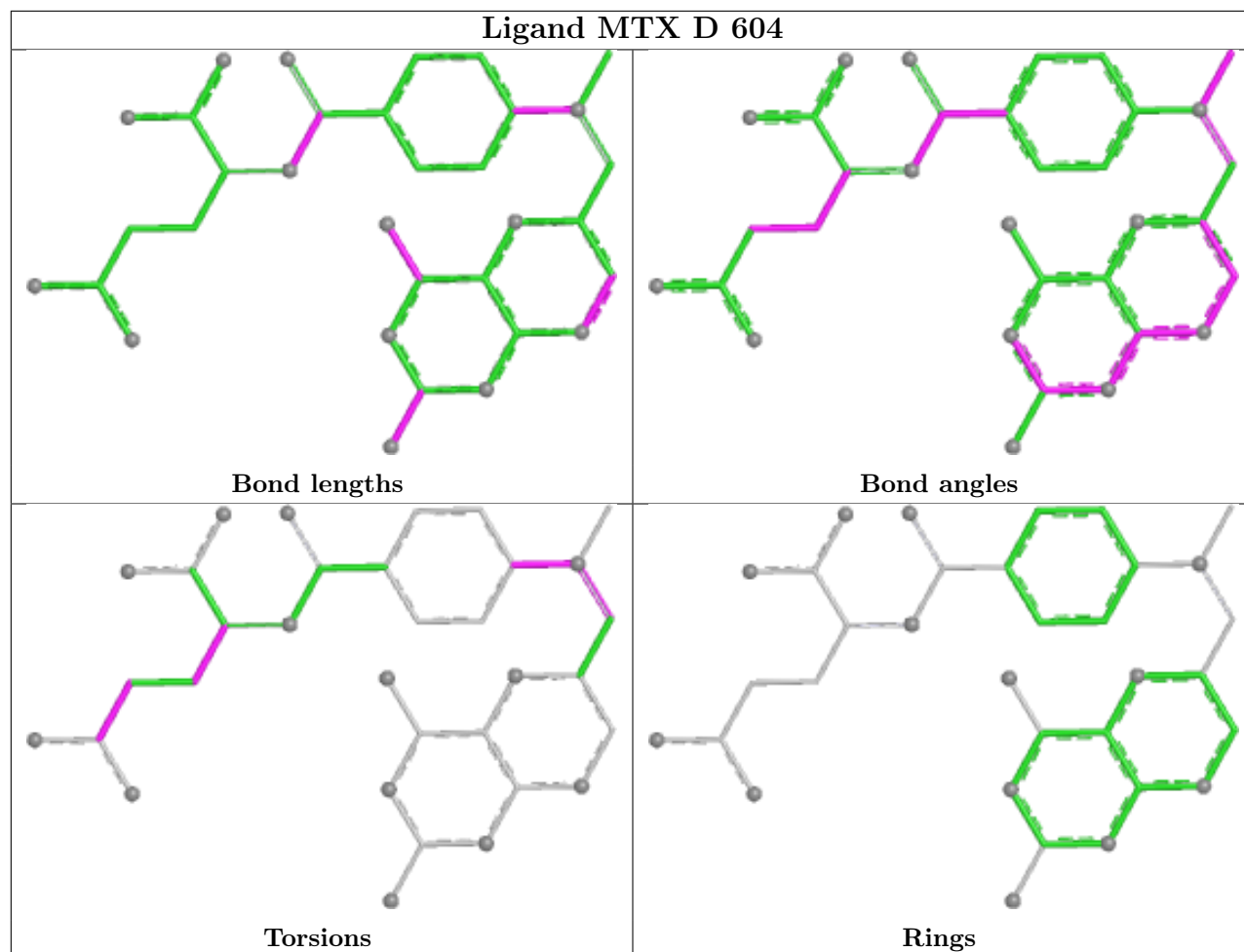




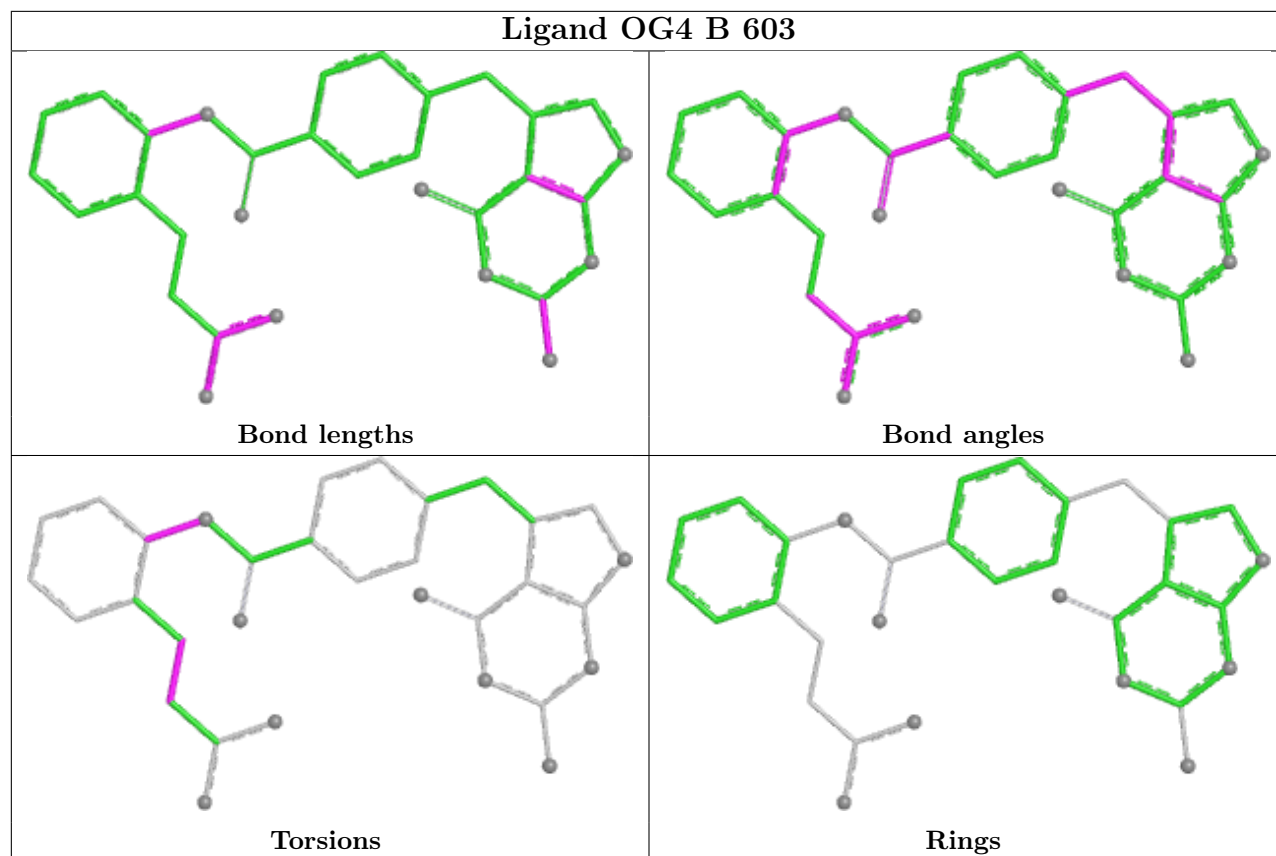




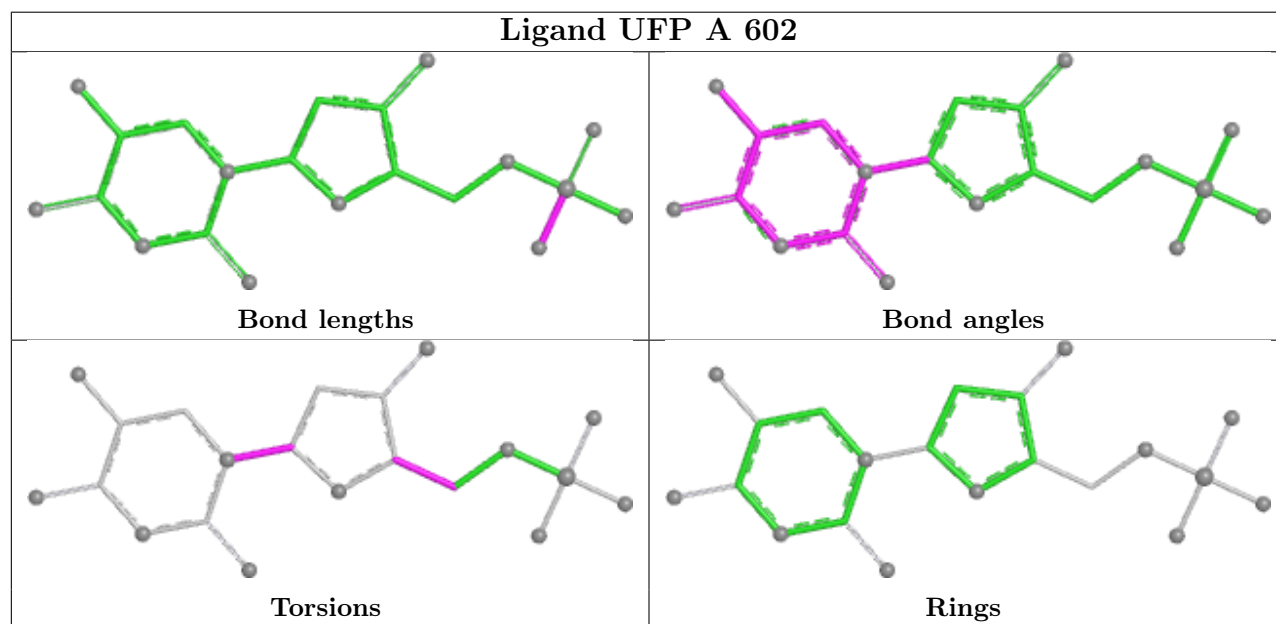




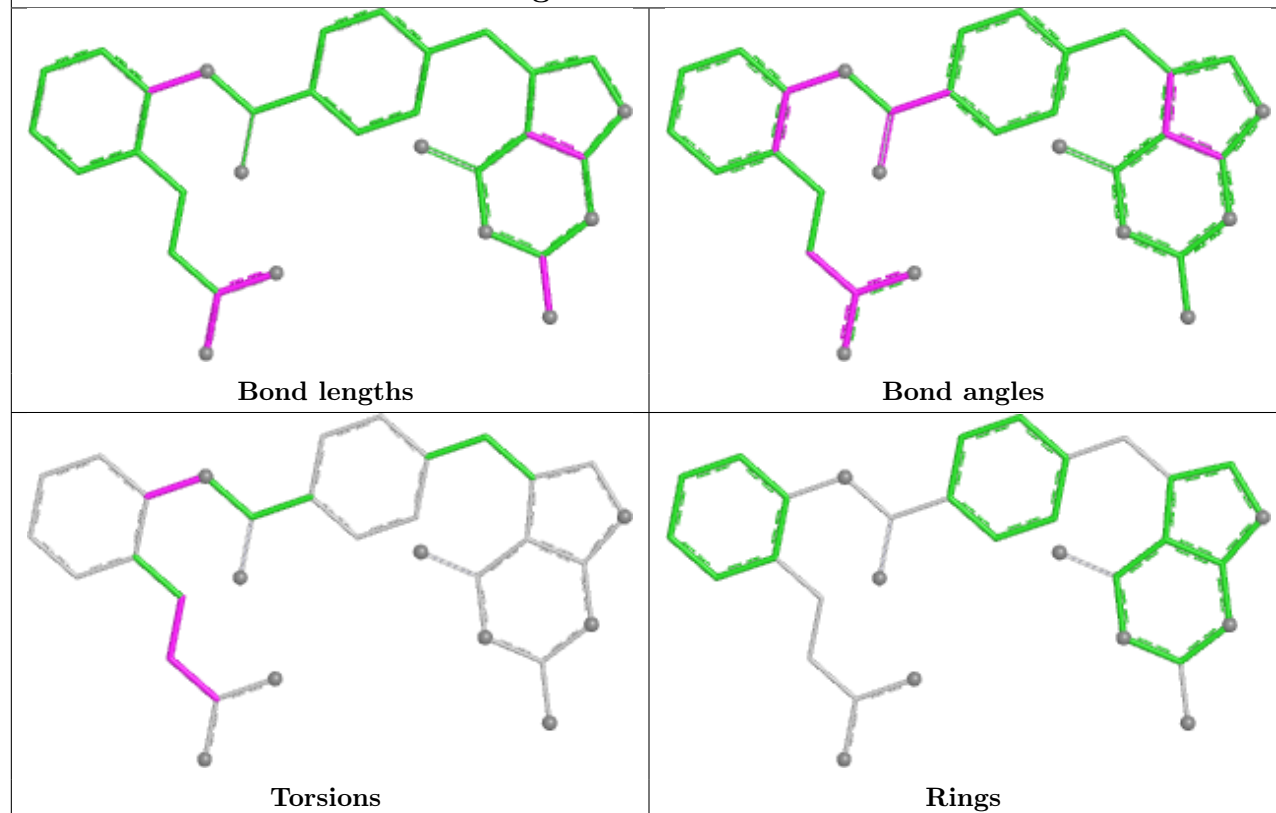
Ligand OG4 B 603



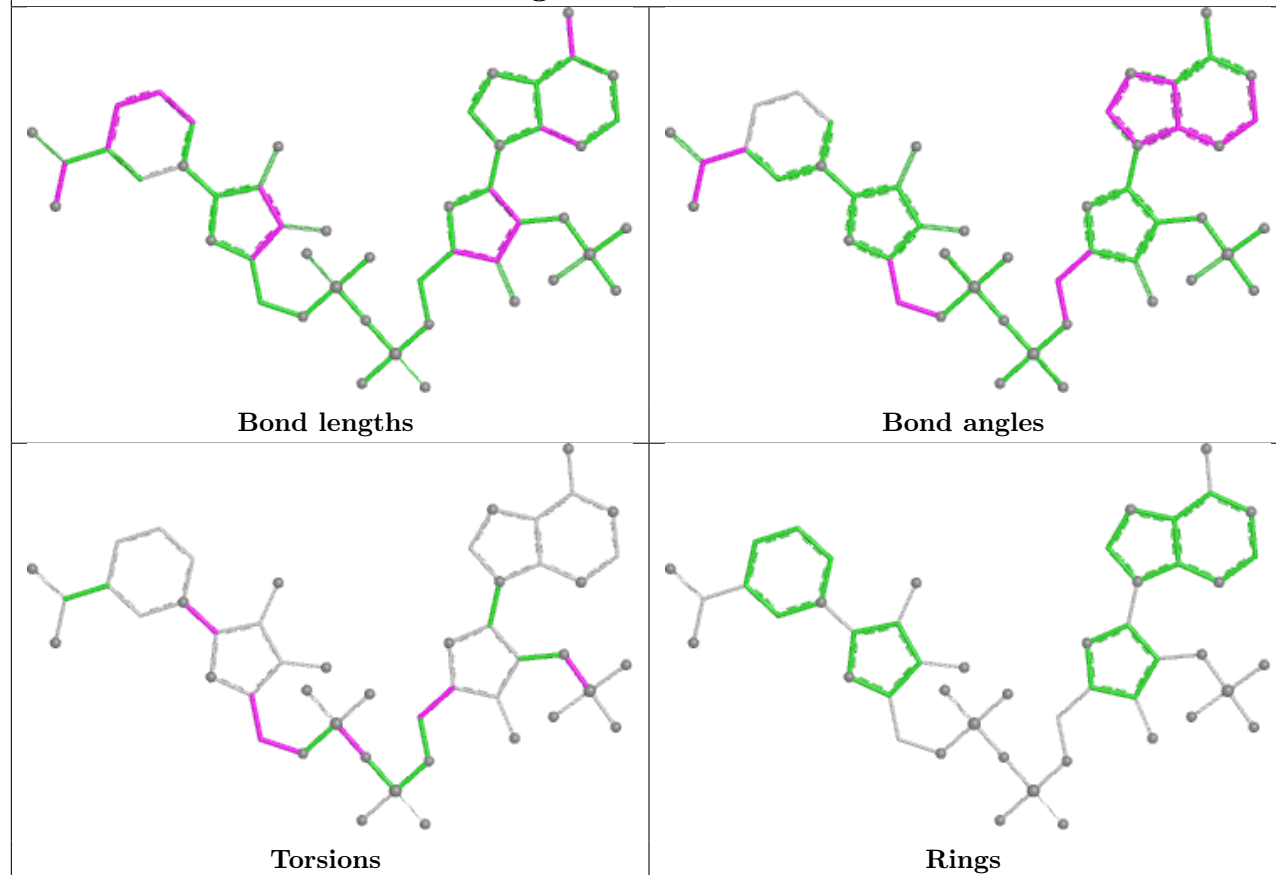
Ligand UFP A 602

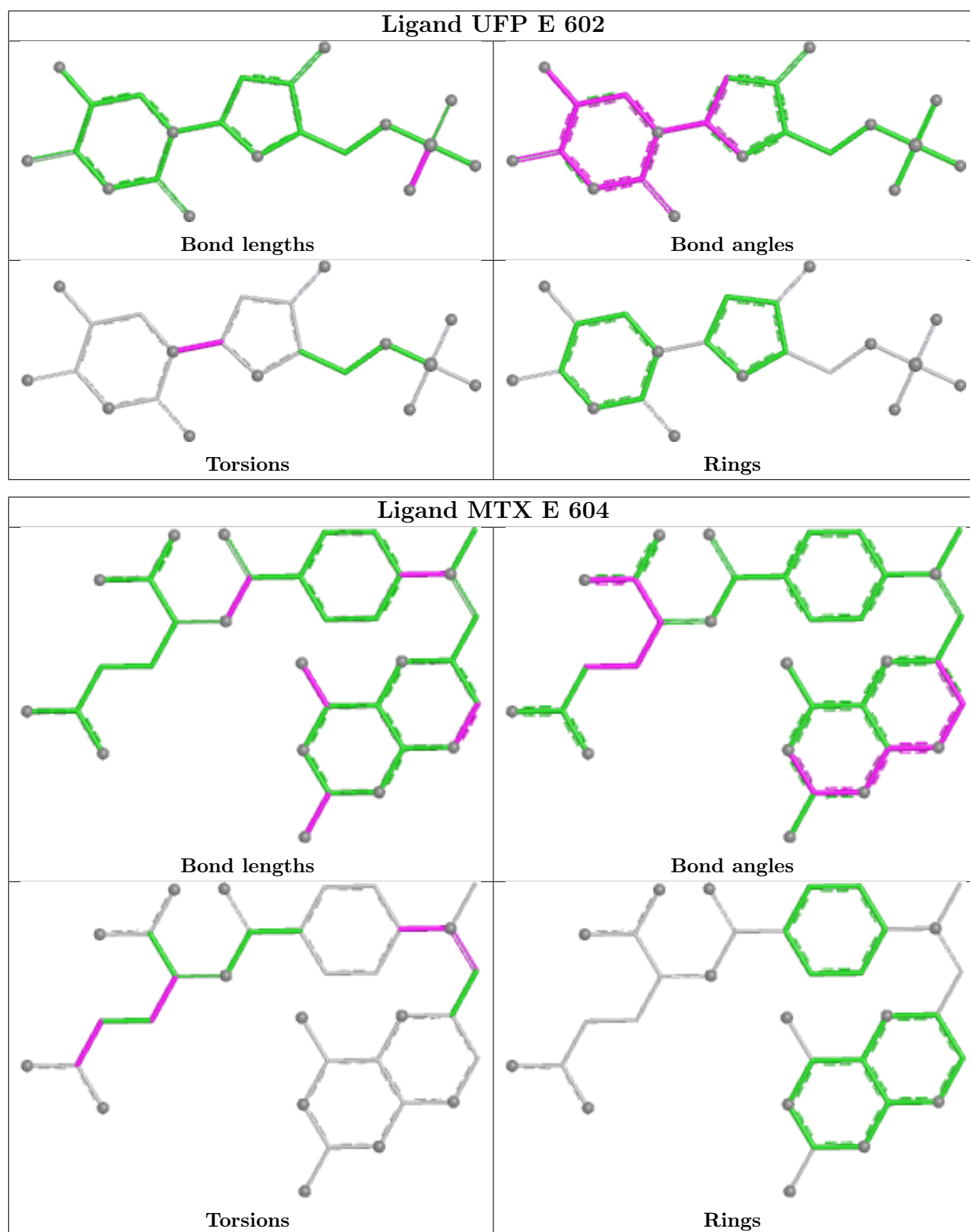


Ligand OG4 A 603



Ligand NDP E 601





5.7 Other polymers [i](#)

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	505/521 (96%)	0.37	18 (3%)	46 26	63, 85, 112, 161	0
1	B	505/521 (96%)	0.45	21 (4%)	40 22	64, 89, 120, 182	0
1	C	506/521 (97%)	0.50	19 (3%)	44 24	71, 95, 125, 180	0
1	D	506/521 (97%)	0.42	10 (1%)	65 42	68, 92, 127, 163	0
1	E	505/521 (96%)	0.61	26 (5%)	33 17	82, 104, 135, 216	0
All	All	2527/2605 (97%)	0.47	94 (3%)	45 25	63, 93, 128, 216	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	LEU	4.7
1	B	102	MET	4.1
1	E	178	GLN	4.1
1	B	101	LEU	3.6
1	C	101	LEU	3.6
1	C	437	SER	3.6
1	B	100	ASN	3.4
1	B	429	LEU	3.4
1	E	142	GLU	3.3
1	A	495	ASN	3.3
1	B	193	LEU	3.2
1	E	45	ASP	3.2
1	D	357	HIS	3.2
1	E	404	VAL	3.2
1	E	101	LEU	3.1
1	E	102	MET	3.1
1	E	521	VAL	3.1
1	D	45	ASP	3.0
1	B	357	HIS	3.0
1	B	356	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	45	ASP	2.9
1	D	193	LEU	2.8
1	E	437	SER	2.8
1	C	413	ASP	2.8
1	E	95	GLU	2.7
1	A	101	LEU	2.7
1	E	76	SER	2.7
1	B	389	TRP	2.7
1	D	279	PRO	2.6
1	A	193	LEU	2.6
1	E	279	PRO	2.6
1	E	193	LEU	2.6
1	C	359	ASP	2.6
1	C	429	LEU	2.6
1	A	76	SER	2.6
1	C	76	SER	2.5
1	E	343	GLY	2.5
1	B	413	ASP	2.5
1	A	3	GLU	2.5
1	B	194	LYS	2.5
1	C	356	MET	2.5
1	D	194	LYS	2.5
1	C	179	GLU	2.5
1	C	255	GLU	2.5
1	E	255	GLU	2.5
1	B	5	ASN	2.5
1	C	100	ASN	2.5
1	A	347	ARG	2.5
1	C	357	HIS	2.5
1	B	515	ILE	2.4
1	B	521	VAL	2.4
1	C	102	MET	2.4
1	D	3	GLU	2.4
1	A	411	THR	2.4
1	A	102	MET	2.4
1	E	294	GLU	2.4
1	A	5	ASN	2.3
1	E	352	GLU	2.3
1	C	105	ASP	2.3
1	D	142	GLU	2.3
1	A	194	LYS	2.3
1	A	142	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	95	GLU	2.3
1	A	404	VAL	2.2
1	B	42	ASN	2.2
1	A	113	CYS	2.2
1	E	83	GLU	2.2
1	E	127	PHE	2.2
1	E	5	ASN	2.2
1	E	100	ASN	2.2
1	A	140	ASP	2.2
1	B	358	ASP	2.2
1	B	21	ILE	2.2
1	B	195	SER	2.2
1	C	61	SER	2.2
1	C	198	ASP	2.1
1	C	95	GLU	2.1
1	A	412	ASN	2.1
1	A	95	GLU	2.1
1	B	497	GLU	2.1
1	E	316	TRP	2.1
1	E	405	LEU	2.1
1	E	105	ASP	2.1
1	E	218	PHE	2.1
1	B	103	ASN	2.0
1	D	5	ASN	2.0
1	C	332	HIS	2.0
1	E	162	THR	2.0
1	E	520	ALA	2.0
1	D	242	ASP	2.0
1	A	255	GLU	2.0
1	A	326	GLU	2.0
1	B	95	GLU	2.0
1	B	363	VAL	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

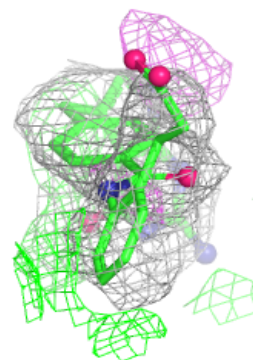
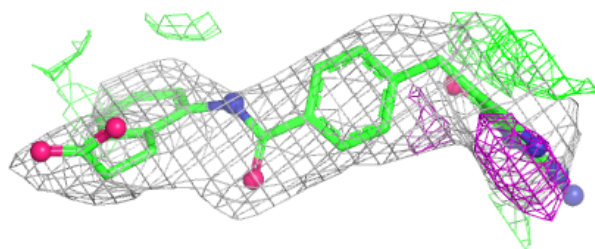
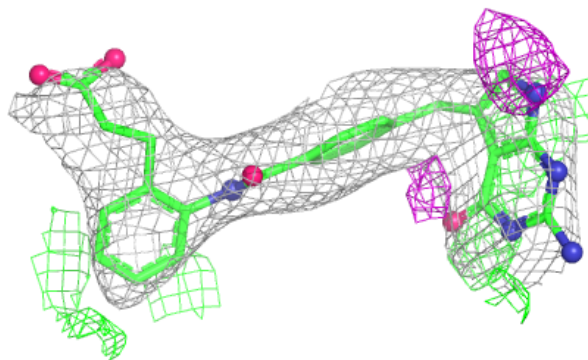
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	OG4	C	603	32/32	0.83	0.21	86,113,129,132	0
4	OG4	B	603	32/32	0.84	0.20	95,109,132,133	0
4	OG4	E	603	32/32	0.84	0.18	92,115,139,144	0
4	OG4	D	603	32/32	0.86	0.20	83,103,121,139	0
4	OG4	A	603	32/32	0.86	0.18	78,101,114,123	0
3	UFP	E	602	21/21	0.90	0.12	89,114,127,140	0
3	UFP	C	602	21/21	0.90	0.14	69,106,115,125	0
5	MTX	D	604	33/33	0.90	0.15	78,102,119,121	0
5	MTX	C	604	33/33	0.91	0.16	88,108,122,132	0
2	NDP	C	601	48/48	0.92	0.11	86,107,126,135	0
2	NDP	D	601	48/48	0.92	0.10	83,108,125,128	0
2	NDP	E	601	48/48	0.92	0.11	92,113,128,137	0
5	MTX	E	604	33/33	0.92	0.14	98,112,129,133	0
3	UFP	B	602	21/21	0.93	0.11	74,103,113,122	0
2	NDP	B	601	48/48	0.93	0.10	71,92,104,111	0
5	MTX	A	604	33/33	0.93	0.11	71,88,108,121	0
3	UFP	D	602	21/21	0.94	0.12	61,95,111,113	0
2	NDP	A	601	48/48	0.94	0.09	72,89,101,107	0
5	MTX	B	604	33/33	0.94	0.12	68,88,112,117	0
3	UFP	A	602	21/21	0.95	0.11	76,92,111,118	0

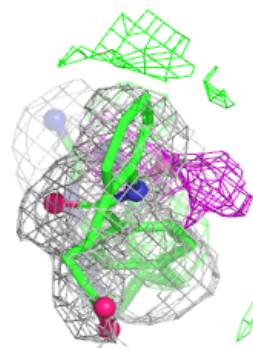
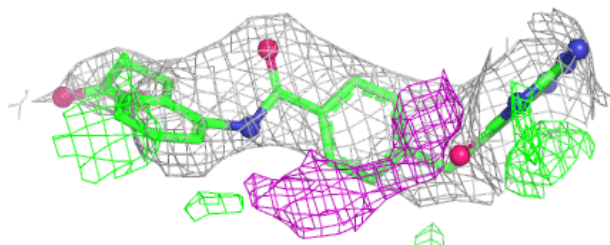
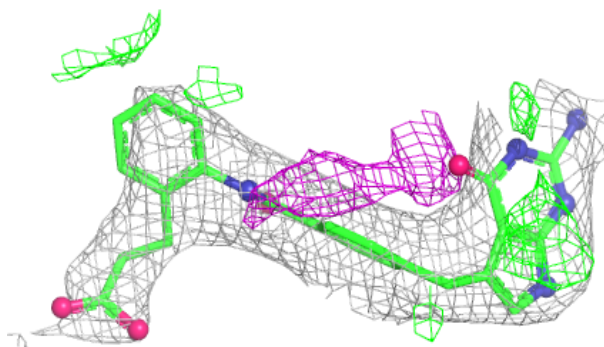
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OG4 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)

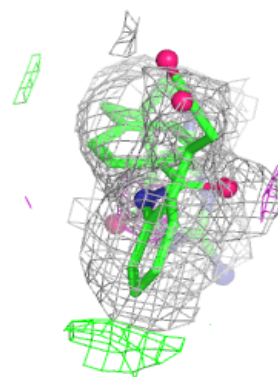
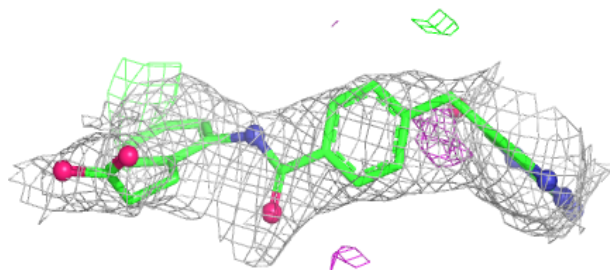
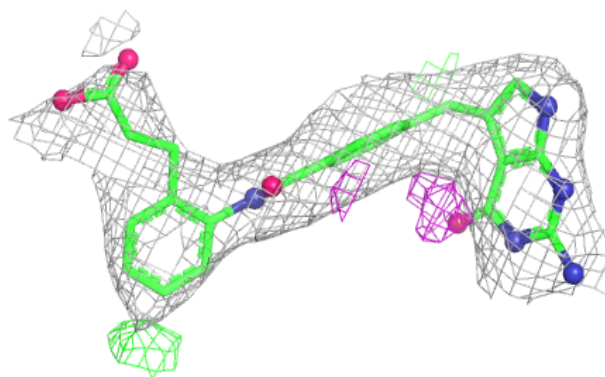
**Electron density around OG4 B 603:**

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

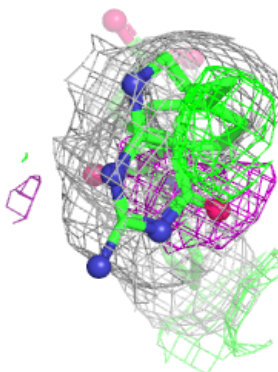
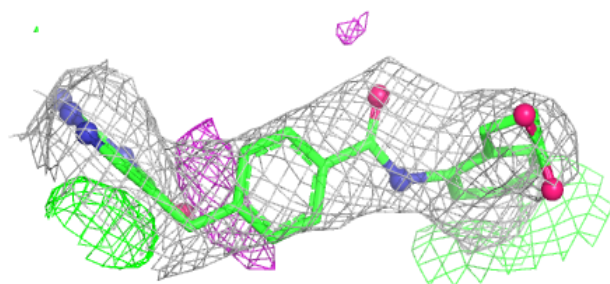
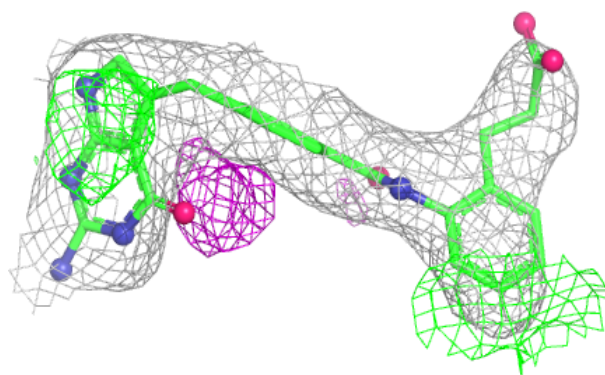


Electron density around OG4 E 603:

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

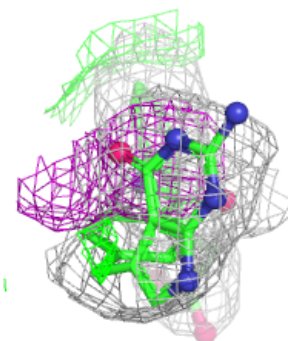
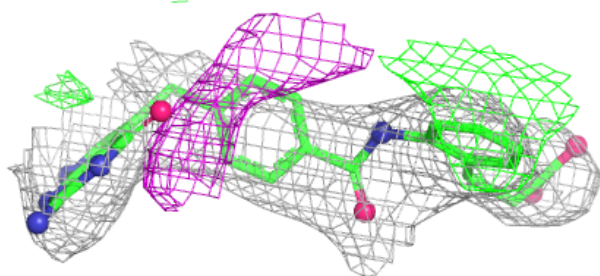
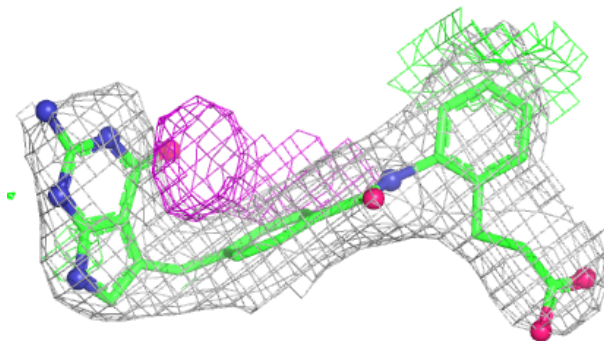
**Electron density around OG4 D 603:**

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

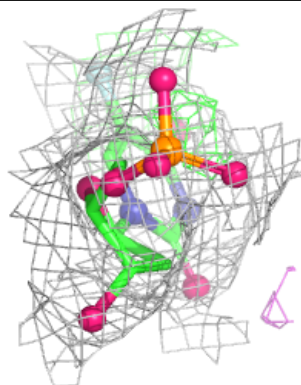
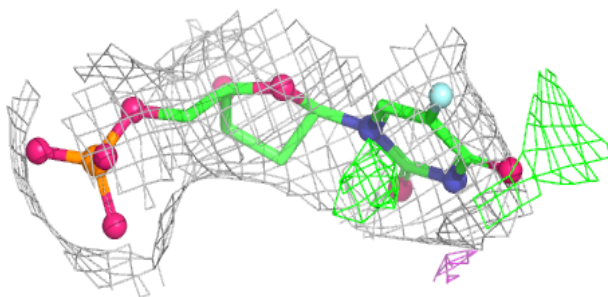
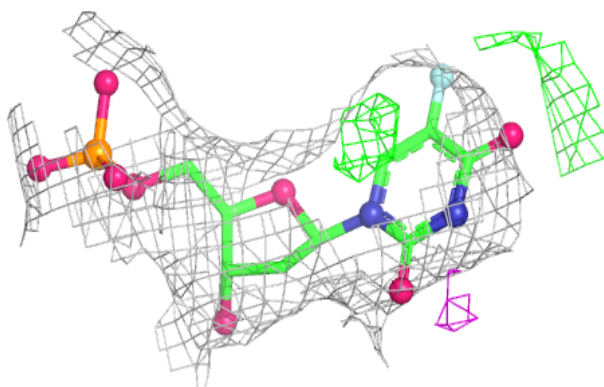


Electron density around OG4 A 603:

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

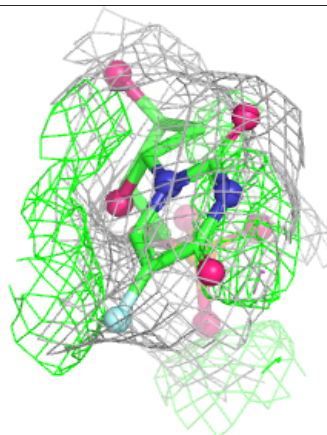
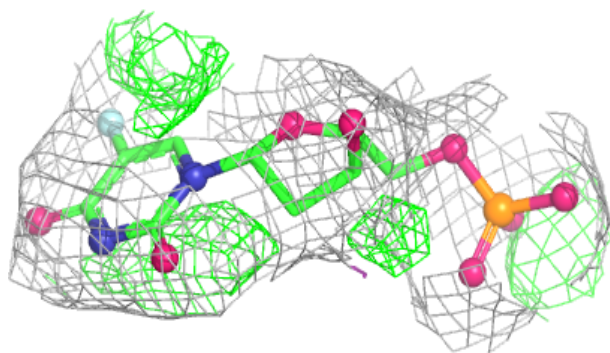
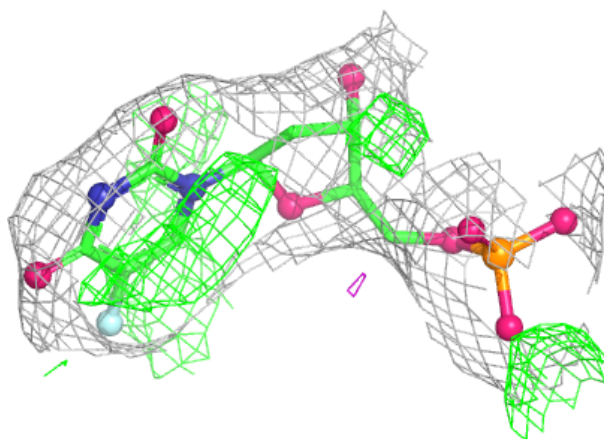
**Electron density around UFP E 602:**

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



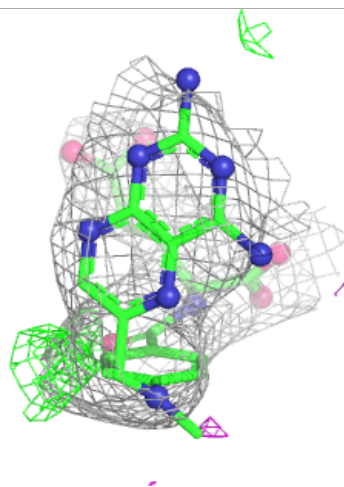
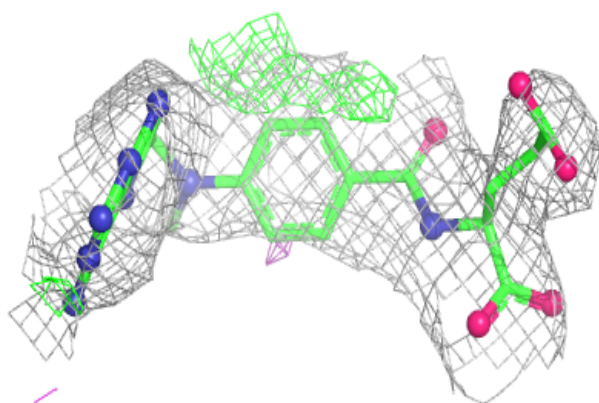
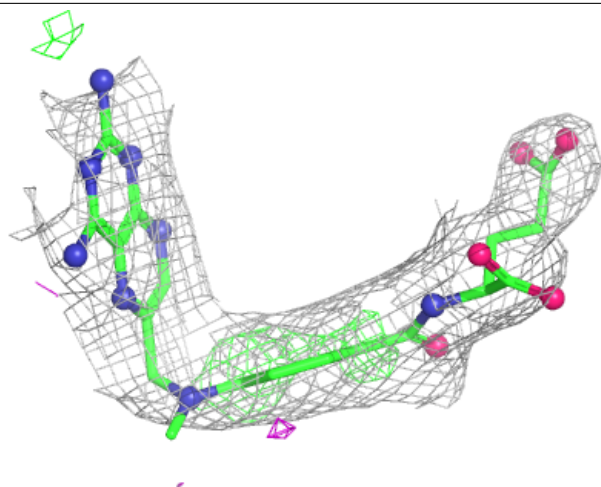
Electron density around UFP C 602:

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



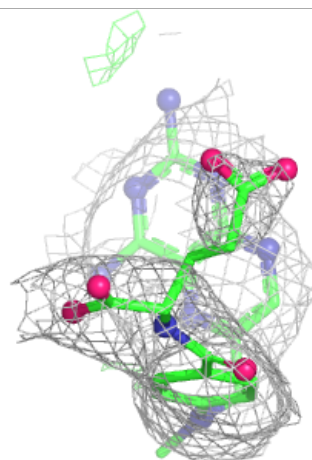
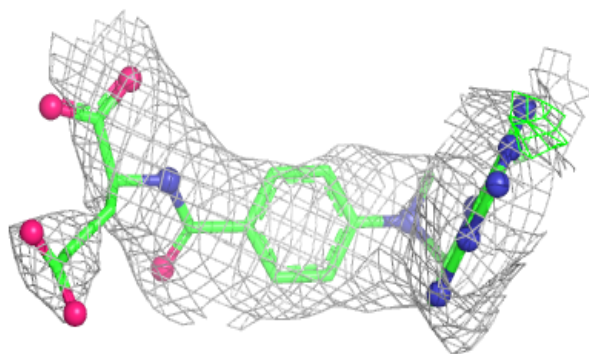
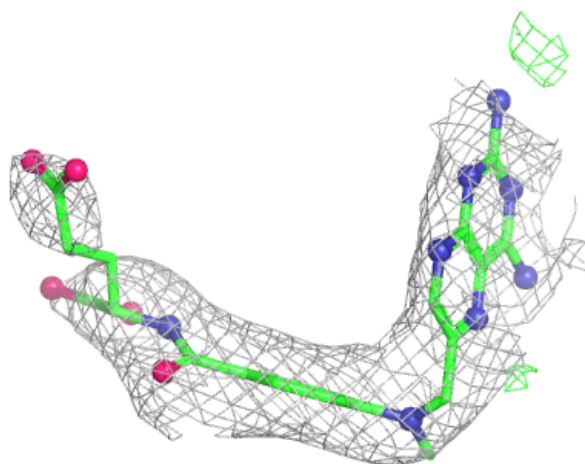
Electron density around MTX D 604:

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



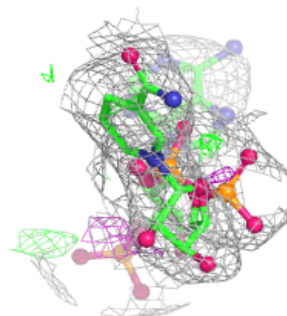
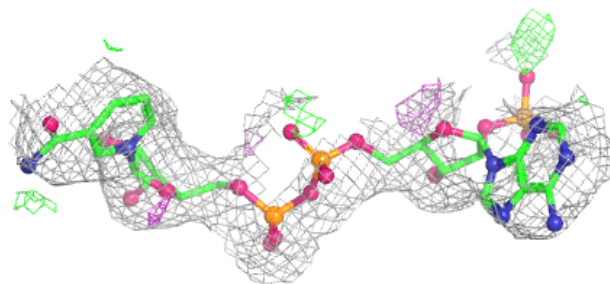
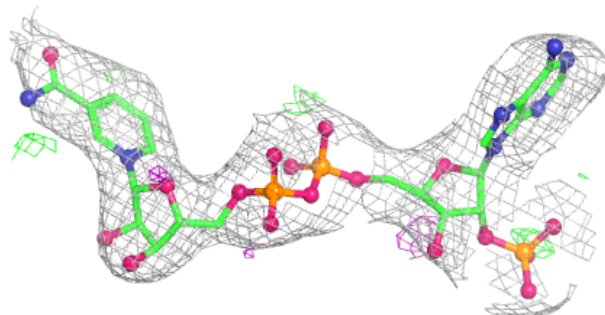
Electron density around MTX C 604:

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

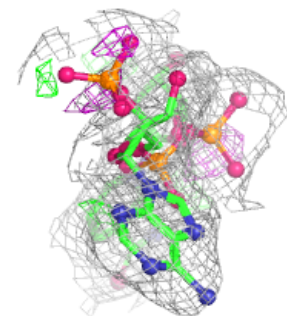
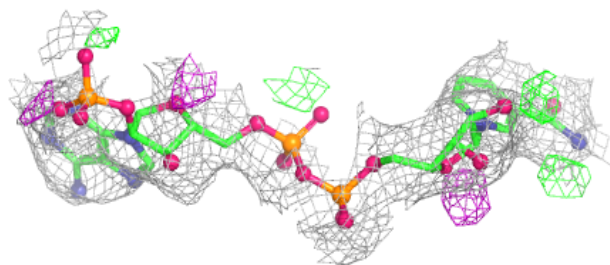
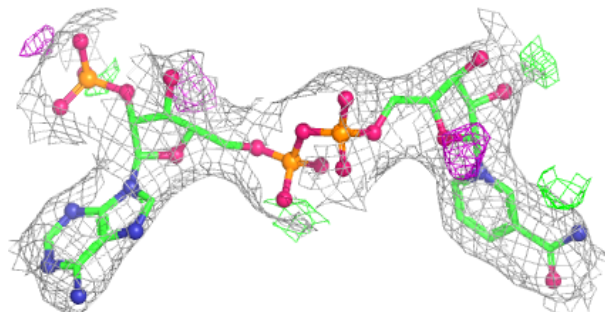


Electron density around NDP C 601:

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

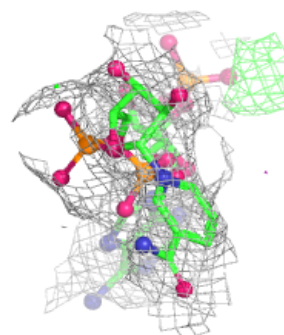
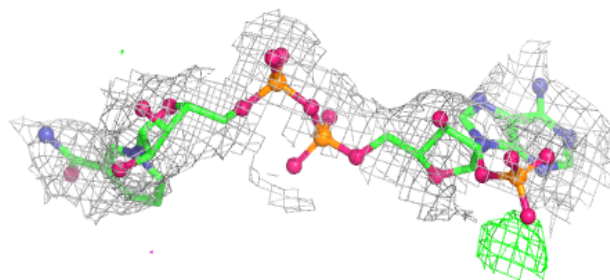
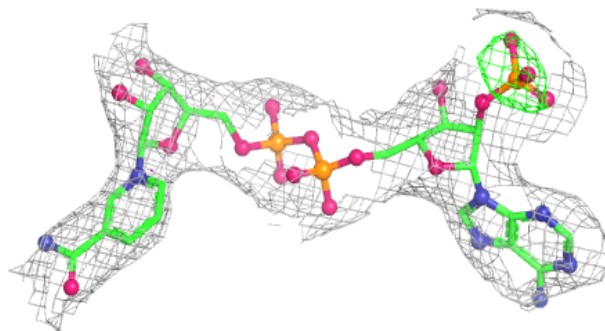
**Electron density around NDP D 601:**

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



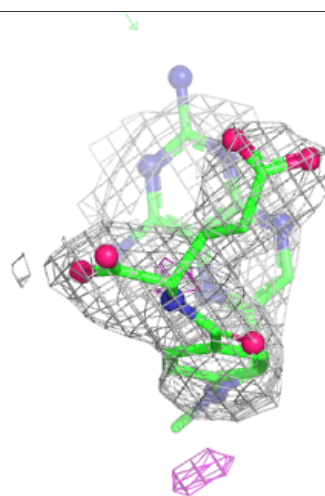
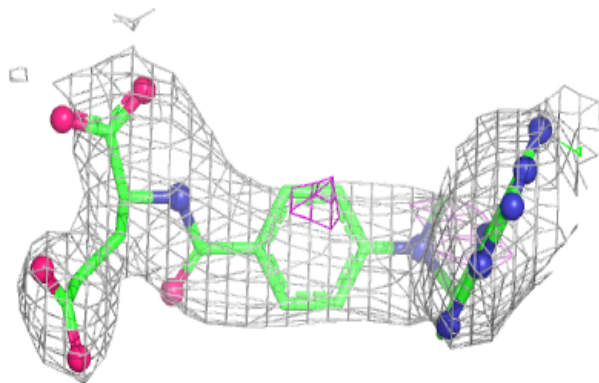
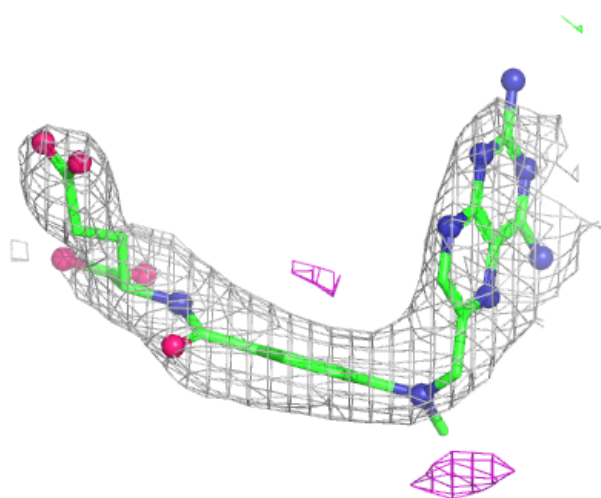
Electron density around NDP E 601:

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and green (positive)



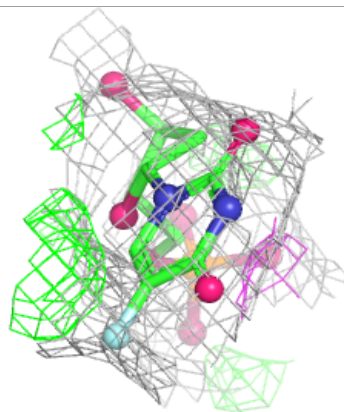
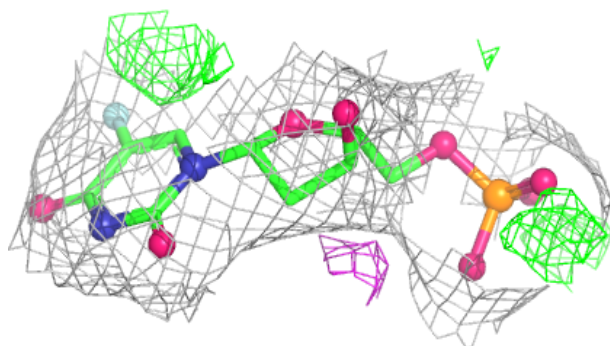
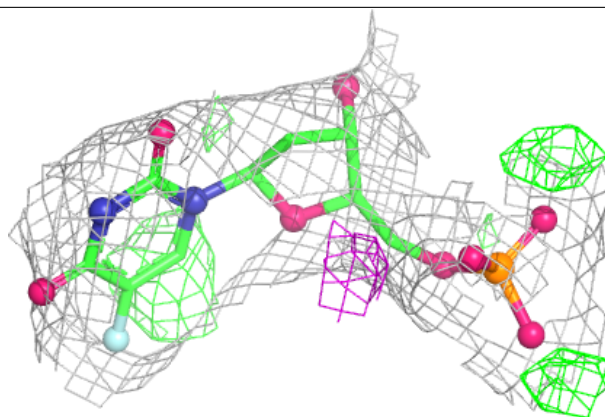
Electron density around MTX E 604:

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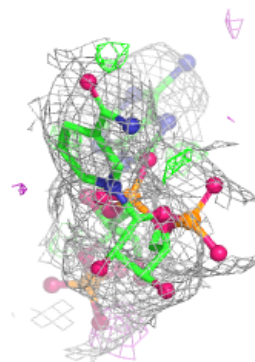
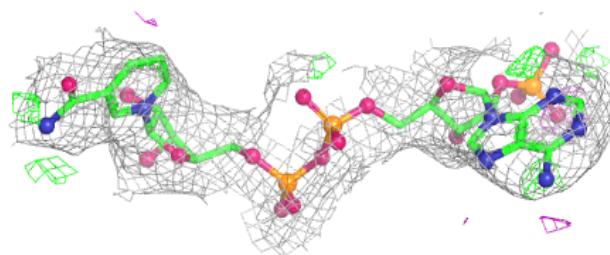
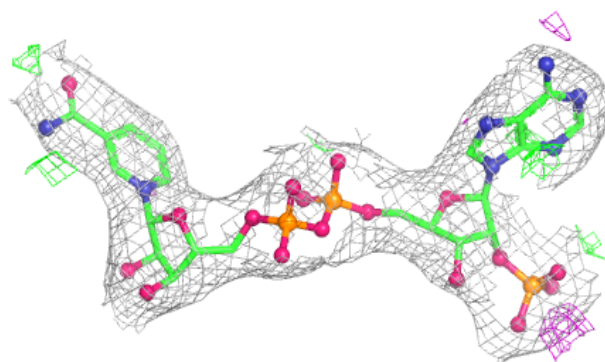


Electron density around UFP B 602:

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

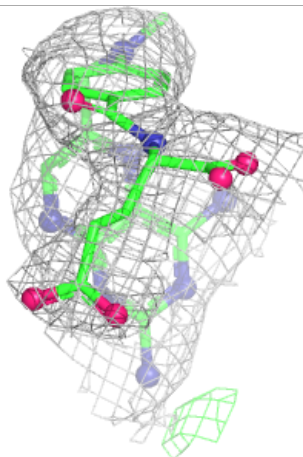
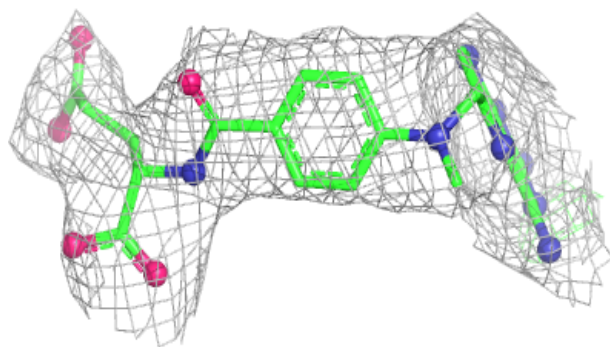
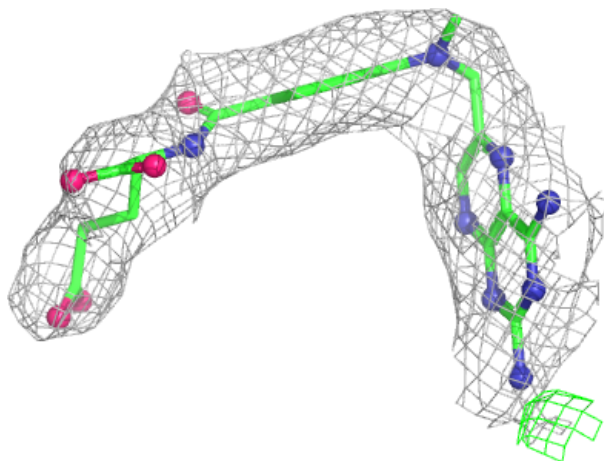
**Electron density around NDP B 601:**

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



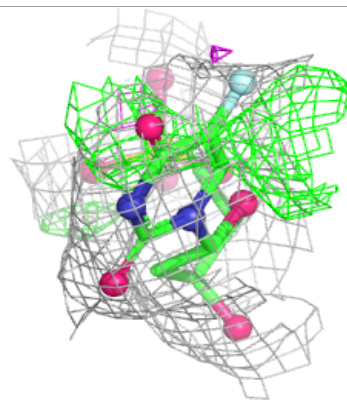
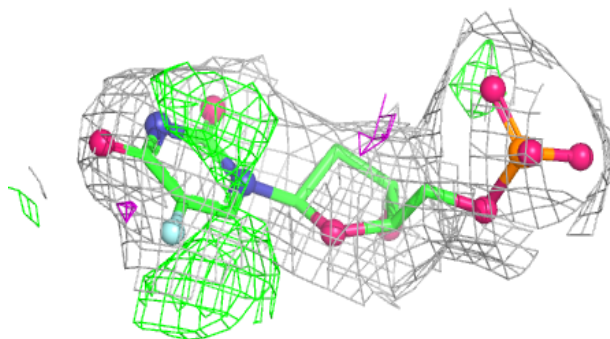
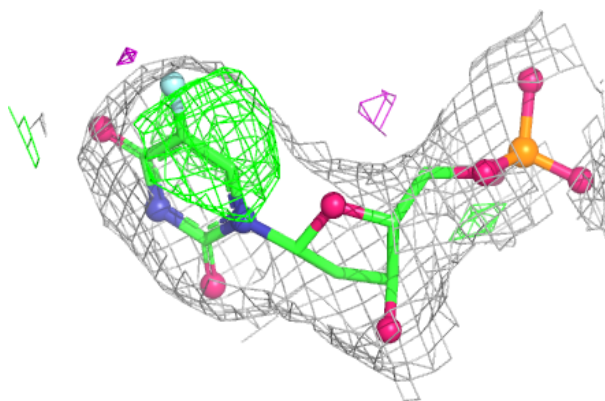
Electron density around MTX A 604:

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

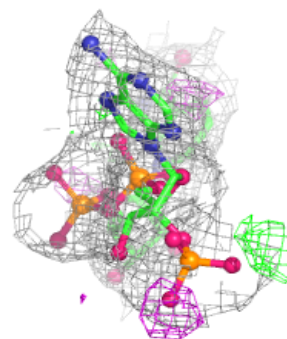
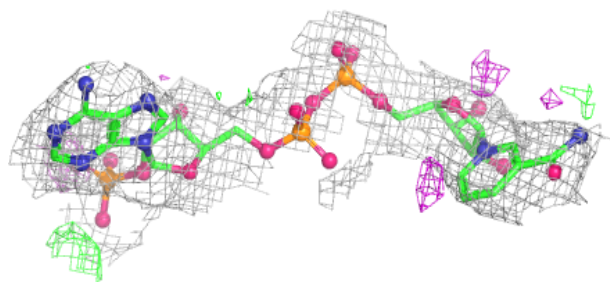
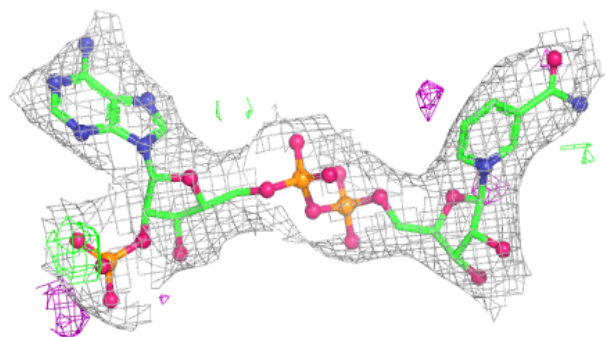


Electron density around UFP D 602:

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

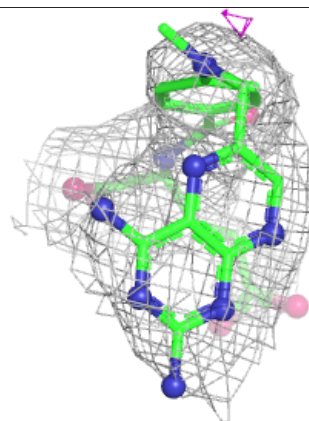
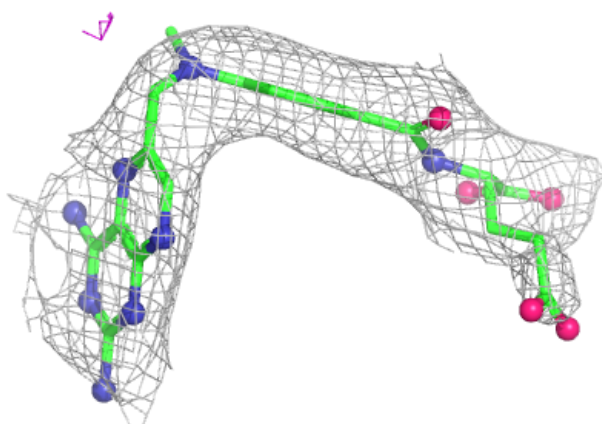
**Electron density around NDP A 601:**

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

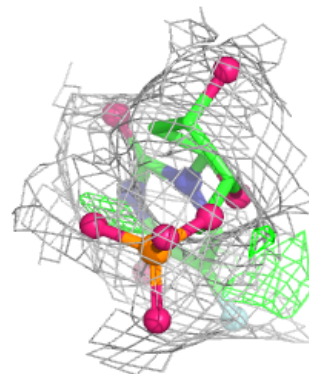
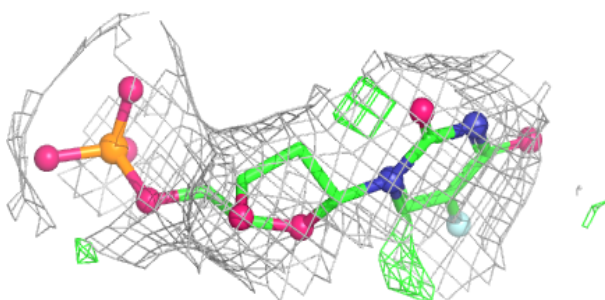
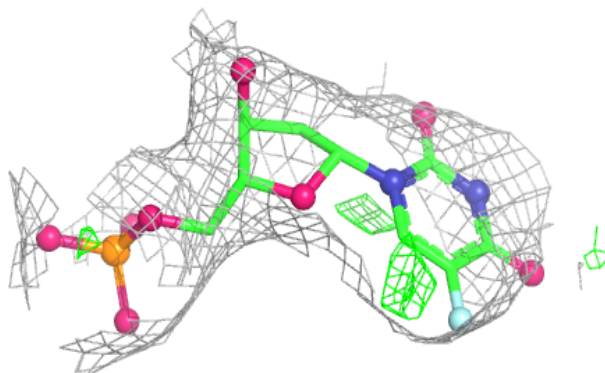


Electron density around MTX B 604:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.