



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:23 AM UTC

PDB ID : 4KY8 / pdb_00004ky8
Title : Crystal structure of TS-DHFR from *Cryptosporidium hominis* in complex with NADPH, methotrexate, FdUMP and 4-((2-amino-6-methyl-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)thio)-2-chlorophenyl)-L-glutamic acid
Authors : Kumar, V.P.; Anderson, K.S.
Deposited on : 2013-05-28
Resolution : 3.08 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

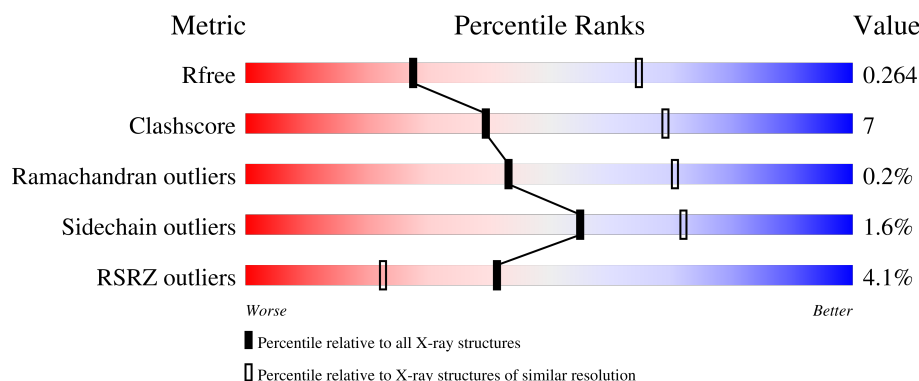
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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% 76% 20% ..
1	B	521	5% 77% 19% .
1	C	521	3% 78% 19% .
1	D	521	3% 80% 16% ..

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Mol	Chain	Length	Quality of chain
1	E	521	5% 82% 14% ••

2 Entry composition ⓘ

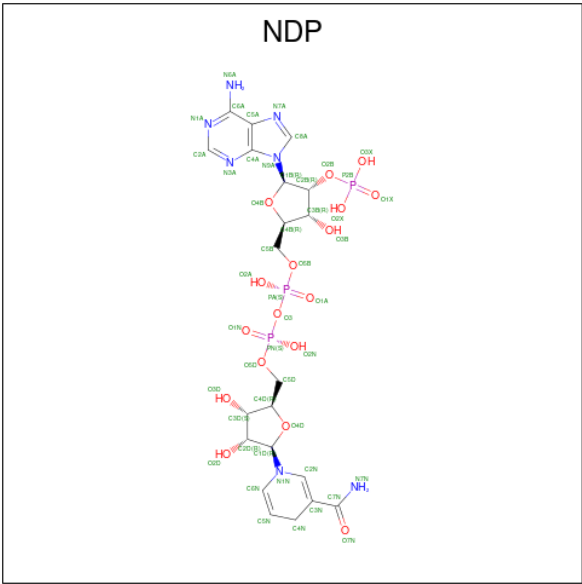
There are 5 unique types of molecules in this entry. The entry contains 21240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 thymidylate synthase-dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			
1	B	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			
1	C	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			
1	D	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			
1	E	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			

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



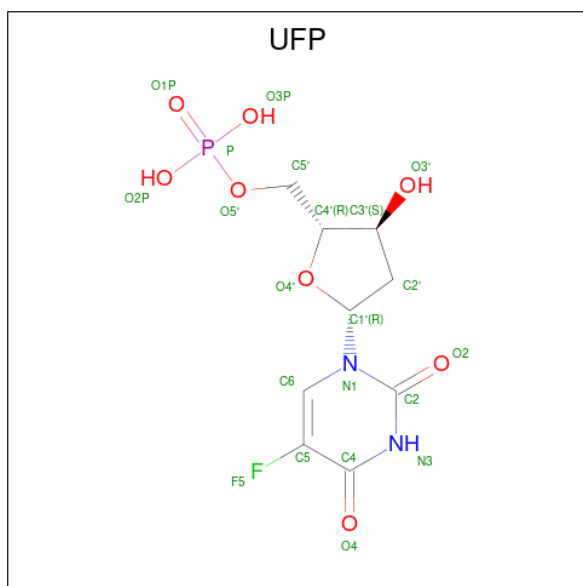
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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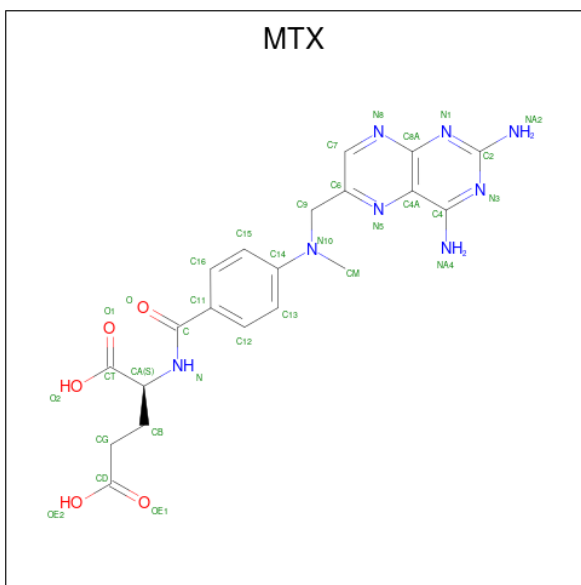
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: UFP) (formula: $C_9H_{12}FN_2O_8P$).



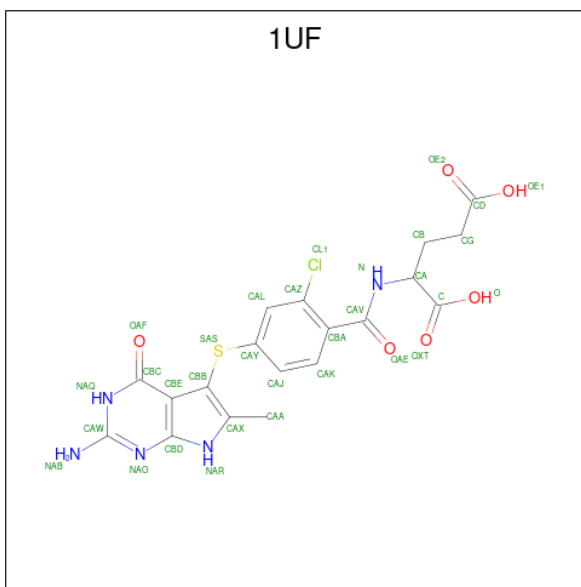
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is METHOTREXATE (CCD ID: MTX) (formula: $C_{20}H_{22}N_8O_5$).



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

- Molecule 5 is N-{4-[(2-amino-6-methyl-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)sulfanyl]-2-chlorobenzoyl}-L-glutamic acid (CCD ID: 1UF) (formula: C₁₉H₁₈ClN₅O₆S).

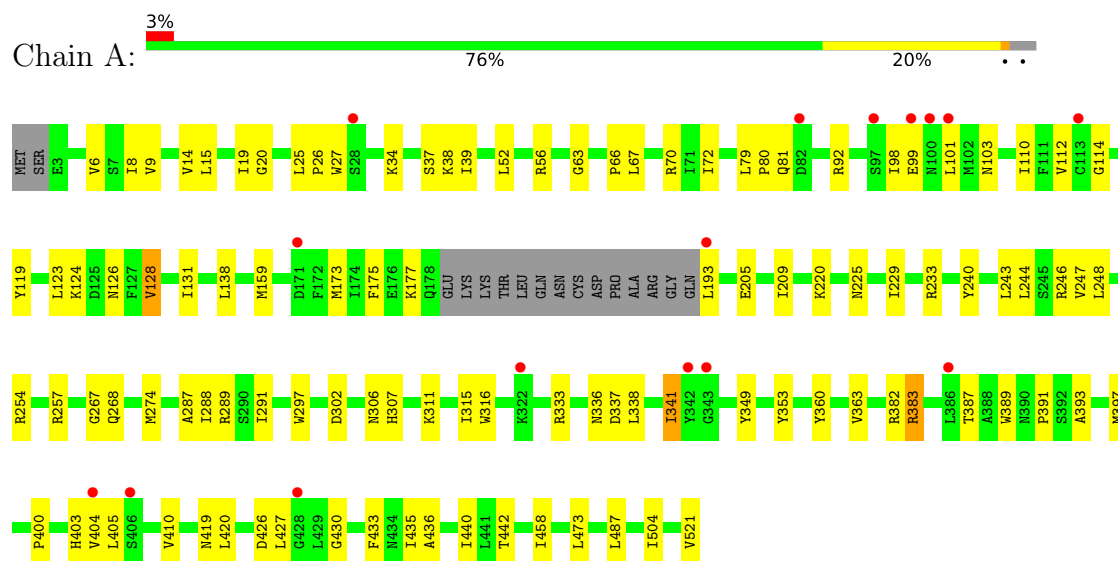


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0
5	B	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0
5	C	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0
5	D	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0
5	E	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0

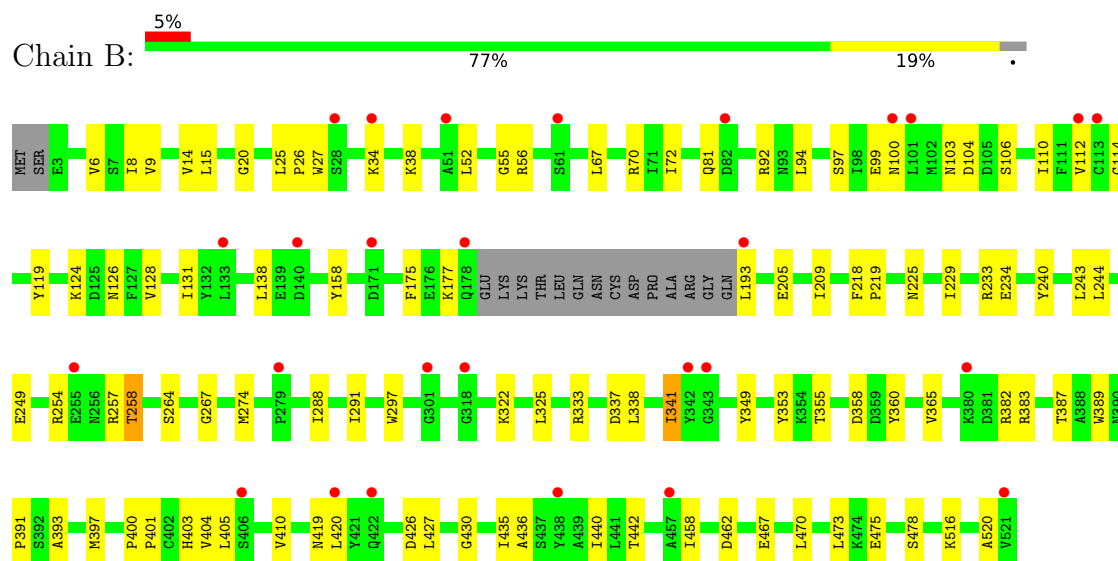
3 Residue-property plots

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.

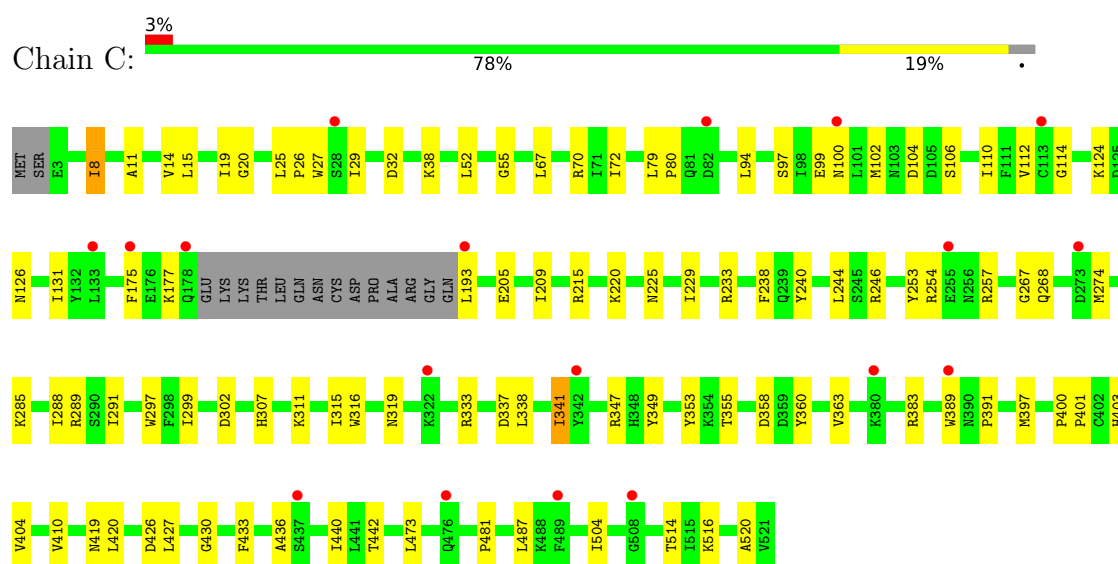
- Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase



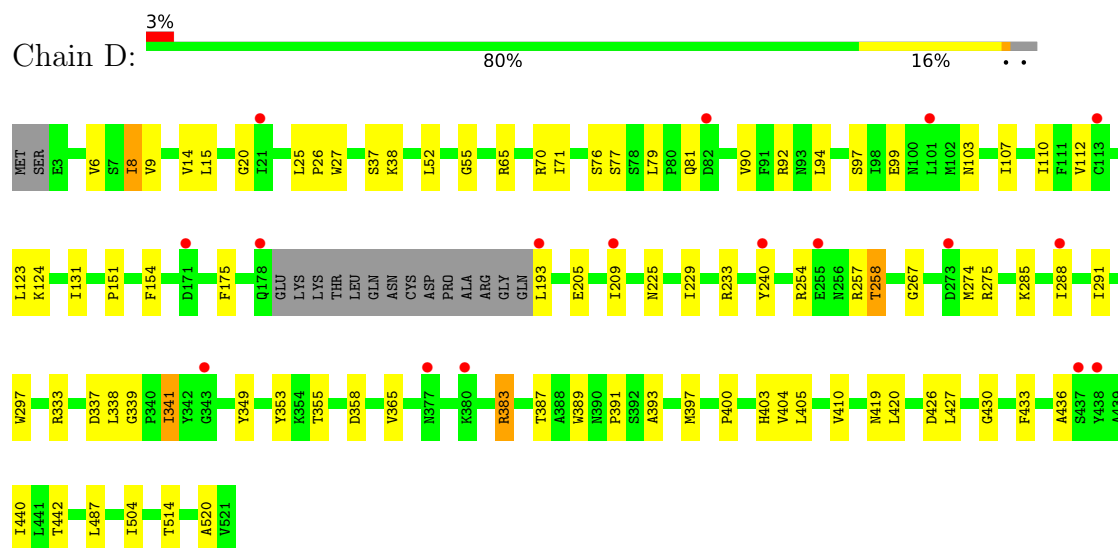
- Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase



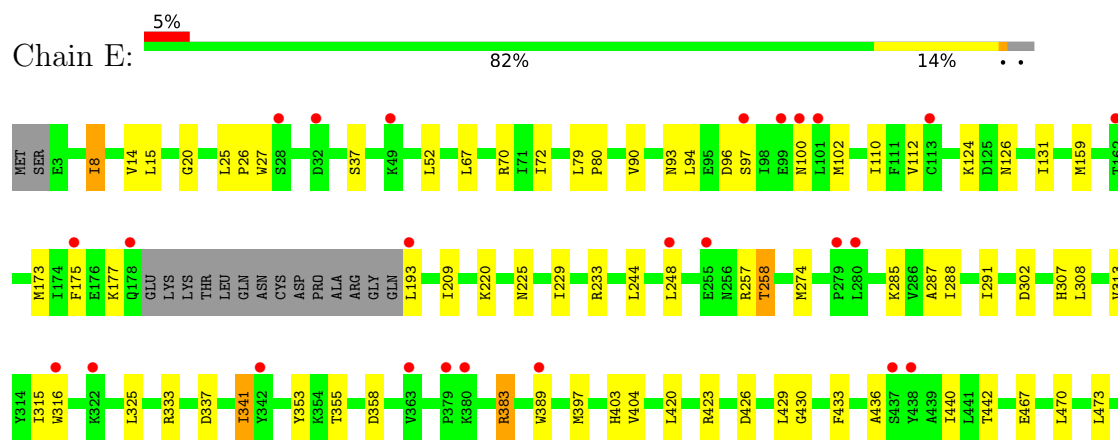
- Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase



- Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase



- Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.16Å 115.67Å 218.77Å 90.00° 94.36° 90.00°	Depositor
Resolution (Å)	48.12 – 3.08 48.12 – 3.08	Depositor EDS
% Data completeness (in resolution range)	71.2 (48.12-3.08) 71.2 (48.12-3.08)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.232 , 0.266 0.234 , 0.264	Depositor DCC
R_{free} test set	1961 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21240	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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, UFP, NDP, 1UF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/4209	0.70	0/5688
1	B	0.25	0/4209	0.69	0/5688
1	C	0.25	0/4209	0.69	0/5688
1	D	0.25	0/4209	0.69	0/5688
1	E	0.25	0/4209	0.69	0/5688
All	All	0.25	0/21045	0.69	0/28440

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	4114	0	4049	71	0
1	B	4114	0	4049	66	0
1	C	4114	0	4049	62	0
1	D	4114	0	4049	57	0
1	E	4114	0	4049	44	1
2	A	48	0	26	4	0
2	B	48	0	26	4	0
2	C	48	0	26	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	26	4	0
2	E	48	0	26	1	0
3	A	21	0	10	2	0
3	B	21	0	10	3	0
3	C	21	0	10	2	0
3	D	21	0	10	1	0
3	E	21	0	10	2	1
4	A	33	0	20	5	0
4	B	33	0	20	3	0
4	C	33	0	20	2	0
4	D	33	0	20	3	0
4	E	33	0	20	2	0
5	A	32	0	16	4	0
5	B	32	0	16	0	0
5	C	32	0	16	3	0
5	D	32	0	16	1	0
5	E	32	0	16	6	0
All	All	21240	0	20605	281	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:NH1	3:B:602:UFP:O3P	2.05	0.89
1:A:341:ILE:HA	1:A:397:MET:HE3	1.64	0.78
1:D:341:ILE:HA	1:D:397:MET:HE3	1.66	0.77
1:B:341:ILE:HA	1:B:397:MET:HE3	1.67	0.76
1:C:341:ILE:HA	1:C:397:MET:HE3	1.67	0.75
3:C:602:UFP:O3P	1:D:383:ARG:NH1	2.21	0.73
1:C:244:LEU:HD11	1:C:473:LEU:HD13	1.72	0.71
1:E:257:ARG:NE	3:E:602:UFP:O2P	2.19	0.71
1:C:383:ARG:HE	1:D:400:PRO:HG2	1.54	0.71
1:E:341:ILE:HA	1:E:397:MET:HE3	1.73	0.70
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.72	0.69
1:C:52:LEU:HD11	1:C:70:ARG:HD2	1.75	0.68
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.75	0.68
1:B:8:ILE:HG12	1:B:112:VAL:HB	1.76	0.68
1:E:25:LEU:HD11	4:E:603:MTX:H7	1.76	0.68
1:B:52:LEU:HD11	1:B:70:ARG:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:LEU:HD11	1:E:70:ARG:HD2	1.76	0.67
1:D:8:ILE:HG12	1:D:112:VAL:HB	1.75	0.67
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.77	0.67
1:E:37:SER:HB2	4:E:603:MTX:HB1	1.75	0.67
1:A:52:LEU:HD11	1:A:70:ARG:HD2	1.76	0.66
1:A:400:PRO:HG2	1:B:383:ARG:HE	1.60	0.66
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.78	0.66
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.78	0.65
1:A:244:LEU:HD11	1:A:473:LEU:HD13	1.78	0.65
1:A:289:ARG:NH2	1:A:311:LYS:O	2.31	0.64
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.80	0.64
1:C:410:VAL:O	1:D:254:ARG:NH2	2.25	0.64
1:C:257:ARG:NE	3:C:602:UFP:O2P	2.26	0.64
1:B:244:LEU:HD11	1:B:473:LEU:HD13	1.77	0.64
1:C:349:TYR:HH	1:D:349:TYR:HH	1.44	0.64
1:D:79:LEU:HD22	1:D:90:VAL:HG21	1.80	0.64
1:D:288:ILE:HD11	1:D:440:ILE:HD11	1.80	0.63
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.81	0.63
1:C:289:ARG:NH2	1:C:311:LYS:O	2.32	0.63
1:D:257:ARG:NE	3:D:602:UFP:O2P	2.29	0.62
1:E:244:LEU:HD11	1:E:473:LEU:HD13	1.81	0.62
1:A:225:ASN:O	1:A:233:ARG:NH2	2.33	0.62
1:C:285:LYS:HB3	1:C:514:THR:HG22	1.83	0.61
1:A:99:GLU:HB3	1:A:103:ASN:HD21	1.63	0.61
1:A:229:ILE:HG22	1:A:233:ARG:HG2	1.80	0.61
1:B:229:ILE:HG22	1:B:233:ARG:HG2	1.82	0.61
1:D:285:LYS:HB3	1:D:514:THR:HG22	1.82	0.61
1:B:258:THR:HG21	1:B:520:ALA:HB1	1.83	0.60
1:A:8:ILE:HG12	1:A:112:VAL:HB	1.83	0.60
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.82	0.60
1:A:419:ASN:HD21	1:B:267:GLY:HA2	1.67	0.59
1:D:225:ASN:O	1:D:233:ARG:NH2	2.35	0.59
1:E:229:ILE:HG22	1:E:233:ARG:HG2	1.83	0.59
1:B:225:ASN:O	1:B:233:ARG:NH2	2.35	0.59
1:E:225:ASN:O	1:E:233:ARG:NH2	2.35	0.59
1:C:520:ALA:O	5:C:604:1UF:NAB	2.36	0.59
1:E:288:ILE:HD11	1:E:440:ILE:HD11	1.83	0.59
1:C:229:ILE:HG22	1:C:233:ARG:HG2	1.84	0.58
1:C:225:ASN:O	1:C:233:ARG:NH2	2.37	0.58
1:D:25:LEU:HD11	4:D:603:MTX:H7	1.86	0.58
1:B:349:TYR:HB3	1:B:365:VAL:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.85	0.57
1:C:246:ARG:NH1	1:C:268:GLN:OE1	2.36	0.57
1:E:258:THR:HG21	1:E:520:ALA:HB1	1.87	0.57
1:C:419:ASN:HD21	1:D:267:GLY:HA2	1.68	0.57
1:D:81:GLN:OE1	1:D:92:ARG:NH2	2.37	0.57
1:C:267:GLY:HA2	1:D:419:ASN:HD21	1.69	0.57
1:E:285:LYS:HB3	1:E:514:THR:HG22	1.86	0.56
1:D:229:ILE:HG22	1:D:233:ARG:HG2	1.86	0.56
1:A:126:ASN:OD1	1:A:177:LYS:NZ	2.37	0.56
1:E:79:LEU:HD22	1:E:90:VAL:HG21	1.88	0.56
1:B:322:LYS:NZ	1:B:333:ARG:O	2.38	0.55
1:A:274:MET:HE1	1:A:442:THR:HG21	1.89	0.55
1:C:205:GLU:OE1	1:D:38:LYS:NZ	2.32	0.54
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.89	0.54
1:D:349:TYR:HB3	1:D:365:VAL:HB	1.89	0.54
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.89	0.54
1:B:288:ILE:HD11	1:B:440:ILE:HD11	1.89	0.54
1:A:37:SER:HB2	4:A:603:MTX:HB1	1.88	0.54
1:A:81:GLN:OE1	1:A:92:ARG:NH2	2.40	0.54
1:A:123:LEU:HD23	1:A:128:VAL:HG11	1.90	0.53
1:C:25:LEU:HD11	4:C:603:MTX:H7	1.90	0.53
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.89	0.53
1:A:38:LYS:NZ	1:B:205:GLU:OE1	2.32	0.53
1:B:325:LEU:HD23	1:B:333:ARG:HB3	1.89	0.53
1:A:288:ILE:HD11	1:A:440:ILE:HD11	1.89	0.53
1:B:6:VAL:HG22	1:B:110:ILE:HB	1.91	0.53
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.90	0.53
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.90	0.53
1:D:99:GLU:O	1:D:103:ASN:ND2	2.41	0.53
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.44	0.53
1:A:240:TYR:OH	1:A:427:LEU:O	2.25	0.53
1:C:38:LYS:NZ	1:D:205:GLU:OE1	2.32	0.52
1:B:99:GLU:HB2	1:B:103:ASN:HD21	1.75	0.52
1:D:426:ASP:HB3	1:D:430:GLY:H	1.74	0.52
1:A:25:LEU:HD11	4:A:603:MTX:H7	1.90	0.52
1:C:240:TYR:OH	1:C:427:LEU:O	2.24	0.52
1:E:429:LEU:HD13	5:E:604:1UF:CL1	2.47	0.52
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.92	0.52
1:C:288:ILE:HD11	1:C:440:ILE:HD11	1.91	0.51
1:B:114:GLY:HA3	2:B:601:NDP:H5N	1.92	0.51
1:C:254:ARG:NH2	1:D:410:VAL:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ASP:OD1	1:C:106:SER:OG	2.24	0.51
1:B:126:ASN:OD1	1:B:177:LYS:NZ	2.43	0.51
1:A:6:VAL:HG22	1:A:110:ILE:HB	1.93	0.51
1:B:467:GLU:HA	1:B:470:LEU:HD23	1.91	0.51
1:B:81:GLN:OE1	1:B:92:ARG:NH2	2.42	0.50
1:B:355:THR:O	1:B:360:TYR:OH	2.25	0.50
1:E:433:PHE:CZ	5:E:604:1UF:H10	2.46	0.50
1:B:104:ASP:OD1	1:B:106:SER:OG	2.21	0.50
1:D:274:MET:HE1	1:D:442:THR:HG21	1.93	0.50
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.92	0.50
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.47	0.50
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.47	0.50
1:A:67:LEU:HG	1:A:72:ILE:HD11	1.93	0.49
1:A:246:ARG:NH1	1:A:268:GLN:OE1	2.37	0.49
1:A:302:ASP:OD2	1:A:307:HIS:ND1	2.44	0.49
1:B:55:GLY:HA3	2:B:601:NDP:H52A	1.93	0.49
1:D:355:THR:OG1	1:D:358:ASP:OD2	2.24	0.49
1:D:76:SER:HA	2:D:601:NDP:H1B	1.95	0.49
5:E:604:1UF:H2	5:E:604:1UF:CAV	2.43	0.49
1:A:433:PHE:CE1	5:A:604:1UF:H10	2.47	0.49
1:B:274:MET:HE1	1:B:442:THR:HG21	1.94	0.49
1:D:71:ILE:HD12	1:D:107:ILE:HD11	1.92	0.49
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.46	0.49
1:B:25:LEU:HD11	4:B:603:MTX:H7	1.94	0.49
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.94	0.49
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.95	0.48
1:E:467:GLU:HA	1:E:470:LEU:HD23	1.95	0.48
1:C:20:GLY:HA2	1:C:26:PRO:HD3	1.94	0.48
1:A:114:GLY:HA3	2:A:601:NDP:H5N	1.94	0.48
1:A:267:GLY:HA2	1:B:419:ASN:HD21	1.78	0.48
1:D:240:TYR:OH	1:D:427:LEU:O	2.29	0.48
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.48	0.48
1:A:254:ARG:NH2	1:B:410:VAL:O	2.27	0.48
1:B:158:TYR:OH	1:B:234:GLU:OE2	2.28	0.48
1:A:287:ALA:HB3	5:A:604:1UF:H3	1.96	0.48
1:C:11:ALA:O	2:C:601:NDP:N7N	2.46	0.48
1:C:114:GLY:HA3	2:C:601:NDP:H5N	1.96	0.48
1:C:14:VAL:HG13	1:C:15:LEU:HG	1.96	0.48
1:C:274:MET:HE1	1:C:442:THR:HG21	1.96	0.48
1:B:240:TYR:OH	1:B:427:LEU:O	2.28	0.47
1:E:433:PHE:CE2	5:E:604:1UF:H10	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:SER:OG	1:B:462:ASP:OD1	2.28	0.47
1:C:319:ASN:OD1	5:C:604:1UF:NAR	2.45	0.47
1:E:274:MET:HE1	1:E:442:THR:HG21	1.97	0.47
1:D:37:SER:HB2	4:D:603:MTX:HB1	1.97	0.47
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.80	0.47
1:A:403:HIS:HB2	1:A:420:LEU:HD11	1.96	0.47
2:A:601:NDP:H42N	4:A:603:MTX:C6	2.44	0.47
1:C:383:ARG:HH22	1:D:257:ARG:HD3	1.80	0.47
1:C:19:ILE:O	2:C:601:NDP:H2N	2.15	0.47
1:D:20:GLY:HA2	1:D:26:PRO:HD3	1.97	0.47
1:D:258:THR:HG21	1:D:520:ALA:HB1	1.97	0.47
1:A:257:ARG:HD3	1:B:383:ARG:HH22	1.80	0.46
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.80	0.46
1:E:14:VAL:HG13	1:E:15:LEU:HG	1.97	0.46
2:B:601:NDP:H8A	2:B:601:NDP:H51A	1.97	0.46
1:E:423:ARG:NH2	3:E:602:UFP:O3P	2.49	0.46
1:E:519:MET:HB2	5:E:604:1UF:CL1	2.52	0.46
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.97	0.46
1:A:14:VAL:HG13	1:A:15:LEU:HG	1.98	0.46
1:D:77:SER:HB3	2:D:601:NDP:H2A	1.97	0.46
1:C:299:ILE:O	1:C:347:ARG:NH1	2.45	0.46
1:A:337:ASP:OD1	1:A:353:TYR:OH	2.23	0.46
1:A:410:VAL:O	1:B:254:ARG:NH2	2.29	0.46
1:B:100:ASN:HB2	1:B:110:ILE:HD11	1.98	0.46
1:C:55:GLY:HA3	2:C:601:NDP:H52A	1.97	0.46
1:E:126:ASN:OD1	1:E:177:LYS:NZ	2.49	0.46
1:D:387:THR:HB	1:D:405:LEU:HD12	1.98	0.45
3:A:602:UFP:O1P	1:B:382:ARG:NE	2.50	0.45
1:C:433:PHE:CZ	5:C:604:1UF:H10	2.51	0.45
5:A:604:1UF:CAV	5:A:604:1UF:H2	2.46	0.45
1:C:383:ARG:NE	1:D:400:PRO:HG2	2.27	0.45
1:C:426:ASP:HB3	1:C:430:GLY:H	1.82	0.45
1:E:93:ASN:ND2	1:E:96:ASP:H	2.14	0.45
1:A:257:ARG:NE	3:A:602:UFP:O2P	2.44	0.45
1:C:126:ASN:OD1	1:C:177:LYS:NZ	2.50	0.44
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.98	0.44
1:E:426:ASP:HB3	1:E:430:GLY:H	1.82	0.44
1:E:100:ASN:HB2	1:E:110:ILE:HD11	1.99	0.44
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.98	0.44
1:E:308:LEU:HG	1:E:313:VAL:HB	1.99	0.44
1:C:100:ASN:HB2	1:C:110:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.98	0.44
1:E:20:GLY:HA2	1:E:26:PRO:HD3	2.00	0.44
1:C:67:LEU:HG	1:C:72:ILE:HD11	2.00	0.44
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.99	0.44
2:D:601:NDP:H52N	2:D:601:NDP:H6N	2.00	0.44
1:A:79:LEU:HA	1:A:80:PRO:HD3	1.86	0.44
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.98	0.44
1:B:14:VAL:HG13	1:B:15:LEU:HG	2.00	0.44
1:B:243:LEU:HG	1:B:427:LEU:HD21	2.00	0.44
1:B:355:THR:OG1	1:B:358:ASP:OD2	2.27	0.44
1:C:79:LEU:HA	1:C:80:PRO:HD3	1.89	0.44
1:C:102:MET:HE3	1:C:102:MET:HA	2.00	0.44
1:A:244:LEU:O	1:A:248:LEU:HB2	2.18	0.44
1:B:393:ALA:O	1:B:397:MET:HG3	2.18	0.44
1:D:487:LEU:HD11	1:D:504:ILE:HG23	2.00	0.44
2:E:601:NDP:H52N	2:E:601:NDP:H6N	1.98	0.44
1:A:114:GLY:HA2	1:A:119:TYR:CZ	2.53	0.43
1:A:159:MET:HA	1:A:173:MET:HG2	2.00	0.43
1:B:9:VAL:O	4:B:603:MTX:NA4	2.51	0.43
1:D:94:LEU:O	1:D:97:SER:OG	2.30	0.43
1:A:487:LEU:HD11	1:A:504:ILE:HG23	2.00	0.43
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.83	0.43
1:E:287:ALA:HB3	5:E:604:1UF:H3	1.99	0.43
1:B:400:PRO:HA	1:B:401:PRO:HD3	1.90	0.43
1:A:9:VAL:HG12	4:A:603:MTX:N3	2.33	0.43
1:D:337:ASP:OD1	1:D:353:TYR:OH	2.24	0.43
1:E:302:ASP:OD2	1:E:307:HIS:ND1	2.48	0.43
1:A:387:THR:HB	1:A:405:LEU:HD12	2.00	0.43
1:B:475:GLU:O	1:B:478:SER:OG	2.35	0.43
1:C:94:LEU:O	1:C:97:SER:OG	2.30	0.43
1:A:205:GLU:OE1	1:B:38:LYS:NZ	2.29	0.43
1:E:291:ILE:HD13	1:E:436:ALA:HB3	1.99	0.43
1:A:243:LEU:O	1:A:247:VAL:HG12	2.19	0.43
1:B:9:VAL:HG12	4:B:603:MTX:N3	2.34	0.43
1:A:56:ARG:NH1	2:A:601:NDP:O1X	2.52	0.43
1:B:67:LEU:HG	1:B:72:ILE:HD11	2.00	0.43
1:B:94:LEU:O	1:B:97:SER:OG	2.30	0.42
1:B:291:ILE:HD13	1:B:436:ALA:HB3	2.01	0.42
1:E:315:ILE:HG13	1:E:316:TRP:CD1	2.55	0.42
1:D:6:VAL:HG22	1:D:110:ILE:HB	2.01	0.42
1:E:355:THR:OG1	1:E:358:ASP:OD2	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ILE:HG12	1:A:458:ILE:HD12	2.00	0.42
1:B:337:ASP:OD1	1:B:353:TYR:OH	2.31	0.42
1:D:14:VAL:HG13	1:D:15:LEU:HG	2.01	0.42
1:E:79:LEU:HA	1:E:80:PRO:HD3	1.92	0.42
1:A:34:LYS:O	1:A:38:LYS:HG3	2.20	0.42
1:A:393:ALA:O	1:A:397:MET:HG3	2.19	0.42
1:B:20:GLY:HA2	1:B:26:PRO:HD3	2.00	0.42
1:B:249:GLU:O	1:D:65:ARG:NH2	2.53	0.42
1:A:400:PRO:HG2	1:B:383:ARG:NE	2.29	0.42
1:B:218:PHE:CD1	1:B:219:PRO:HD2	2.55	0.42
1:C:215:ARG:NH1	1:D:275:ARG:HD2	2.34	0.42
1:A:433:PHE:CZ	5:A:604:1UF:H10	2.54	0.42
1:D:151:PRO:HG2	1:D:154:PHE:HD2	1.85	0.42
1:A:19:ILE:O	2:A:601:NDP:H2N	2.20	0.42
1:E:159:MET:HA	1:E:173:MET:HG2	2.01	0.42
1:A:9:VAL:O	4:A:603:MTX:NA4	2.53	0.41
1:B:426:ASP:HB3	1:B:430:GLY:H	1.84	0.41
1:C:131:ILE:HB	1:C:175:PHE:HB2	2.01	0.41
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.55	0.41
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.55	0.41
1:C:337:ASP:OD1	1:C:353:TYR:OH	2.26	0.41
1:E:67:LEU:HG	1:E:72:ILE:HD11	2.03	0.41
1:E:337:ASP:OD1	1:E:353:TYR:OH	2.26	0.41
1:C:360:TYR:O	1:C:363:VAL:HG22	2.21	0.41
1:D:55:GLY:HA3	2:D:601:NDP:H52A	2.03	0.41
1:A:426:ASP:HB3	1:A:430:GLY:H	1.86	0.41
1:C:355:THR:OG1	1:C:358:ASP:OD2	2.33	0.41
1:D:393:ALA:O	1:D:397:MET:HG3	2.21	0.41
1:A:315:ILE:HG13	1:A:316:TRP:CD1	2.55	0.41
1:B:34:LYS:O	1:B:38:LYS:HG3	2.20	0.41
1:D:433:PHE:CZ	5:D:604:1UF:H10	2.56	0.41
1:C:302:ASP:OD2	1:C:307:HIS:ND1	2.49	0.41
1:C:487:LEU:HD11	1:C:504:ILE:HG23	2.03	0.41
1:E:94:LEU:O	1:E:97:SER:OG	2.34	0.41
1:A:66:PRO:HA	1:A:72:ILE:HD12	2.03	0.41
1:A:98:ILE:HG22	1:A:101:LEU:HG	2.03	0.41
1:B:387:THR:HB	1:B:405:LEU:HD12	2.02	0.41
1:C:238:PHE:CE1	1:C:481:PRO:HG2	2.56	0.41
1:C:315:ILE:HG13	1:C:316:TRP:CD1	2.56	0.41
1:A:257:ARG:NH2	1:A:521:VAL:OXT	2.43	0.41
2:C:601:NDP:H42N	4:C:603:MTX:C6	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:LEU:O	1:E:248:LEU:HB2	2.20	0.41
1:D:9:VAL:HG12	4:D:603:MTX:N3	2.35	0.40
1:E:325:LEU:HD12	1:E:325:LEU:HA	1.90	0.40
1:A:360:TYR:O	1:A:363:VAL:HG22	2.21	0.40
1:B:435:ILE:HG12	1:B:458:ILE:HD12	2.04	0.40
1:C:29:ILE:HG22	1:C:32:ASP:H	1.85	0.40
1:C:400:PRO:HA	1:C:401:PRO:HD3	1.91	0.40
1:A:39:ILE:HD12	1:A:39:ILE:HA	1.99	0.40
1:A:63:GLY:HA2	1:C:253:TYR:HB3	2.03	0.40
1:B:56:ARG:H	2:B:601:NDP:C4B	2.34	0.40
1:B:114:GLY:HA2	1:B:119:TYR:CZ	2.56	0.40
1:E:403:HIS:HB2	1:E:420:LEU:HD11	2.02	0.40
1:A:306:ASN:ND2	1:A:336:ASN:HB2	2.37	0.40
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.86	0.40
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.56	0.40
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.57	0.40
1:A:382:ARG:NE	3:B:602:UFP:O1P	2.54	0.40
1:B:257:ARG:NE	3:B:602:UFP:O2P	2.45	0.40
1:D:339:GLY:HA2	1:D:353:TYR:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:ARG:NH1	3:E:602:UFP:O3P[2_859]	2.06	0.14

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%)	472 (94%)	28 (6%)	1 (0%)	43 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	501/521 (96%)	471 (94%)	29 (6%)	1 (0%)	43	71
1	C	501/521 (96%)	472 (94%)	28 (6%)	1 (0%)	43	71
1	D	501/521 (96%)	472 (94%)	28 (6%)	1 (0%)	43	71
1	E	501/521 (96%)	474 (95%)	26 (5%)	1 (0%)	43	71
All	All	2505/2605 (96%)	2361 (94%)	139 (6%)	5 (0%)	43	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	341	ILE
1	C	341	ILE
1	D	341	ILE
1	A	341	ILE
1	E	341	ILE

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	456/470 (97%)	449 (98%)	7 (2%)	57	73
1	B	456/470 (97%)	449 (98%)	7 (2%)	57	73
1	C	456/470 (97%)	449 (98%)	7 (2%)	57	73
1	D	456/470 (97%)	449 (98%)	7 (2%)	57	73
1	E	456/470 (97%)	448 (98%)	8 (2%)	51	70
All	All	2280/2350 (97%)	2244 (98%)	36 (2%)	55	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LYS
1	A	128	VAL
1	A	138	LEU

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	209	ILE
1	A	220	LYS
1	A	383	ARG
1	B	124	LYS
1	B	128	VAL
1	B	138	LEU
1	B	193	LEU
1	B	209	ILE
1	B	258	THR
1	B	516	LYS
1	C	8	ILE
1	C	99	GLU
1	C	124	LYS
1	C	193	LEU
1	C	209	ILE
1	C	220	LYS
1	C	516	LYS
1	D	8	ILE
1	D	123	LEU
1	D	124	LYS
1	D	193	LEU
1	D	209	ILE
1	D	258	THR
1	D	383	ARG
1	E	8	ILE
1	E	102	MET
1	E	124	LYS
1	E	193	LEU
1	E	209	ILE
1	E	220	LYS
1	E	258	THR
1	E	383	ARG

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	5	ASN
1	A	24	GLN
1	A	103	ASN
1	A	486	GLN
1	B	5	ASN

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Mol	Chain	Res	Type
1	B	24	GLN
1	B	103	ASN
1	B	486	GLN
1	C	5	ASN
1	C	24	GLN
1	C	486	GLN
1	D	5	ASN
1	D	24	GLN
1	D	103	ASN
1	D	178	GLN
1	D	486	GLN
1	E	5	ASN
1	E	24	GLN
1	E	93	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UFP	D	602	-	22,22,22	1.11	0	32,33,33	2.55	10 (31%)
2	NDP	E	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.55	12 (16%)
5	1UF	B	604	-	34,34,34	2.05	7 (20%)	43,49,49	1.99	11 (25%)
4	MTX	B	603	-	35,35,35	1.61	5 (14%)	47,49,49	1.75	8 (17%)
3	UFP	E	602	-	22,22,22	1.10	0	32,33,33	2.55	9 (28%)
3	UFP	C	602	-	22,22,22	1.09	0	32,33,33	2.52	9 (28%)
2	NDP	B	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.52	11 (15%)
2	NDP	D	601	-	51,52,52	1.96	12 (23%)	71,80,80	1.53	11 (15%)
5	1UF	D	604	-	34,34,34	2.04	7 (20%)	43,49,49	1.97	11 (25%)
3	UFP	B	602	-	22,22,22	1.09	0	32,33,33	2.57	9 (28%)
4	MTX	D	603	-	35,35,35	1.61	5 (14%)	47,49,49	1.75	8 (17%)
5	1UF	C	604	-	34,34,34	2.04	7 (20%)	43,49,49	1.89	11 (25%)
4	MTX	C	603	-	35,35,35	1.61	6 (17%)	47,49,49	1.76	10 (21%)
5	1UF	E	604	-	34,34,34	2.04	7 (20%)	43,49,49	1.98	10 (23%)
2	NDP	C	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.53	12 (16%)
4	MTX	E	603	-	35,35,35	1.61	5 (14%)	47,49,49	1.74	10 (21%)
3	UFP	A	602	-	22,22,22	1.09	0	32,33,33	2.56	9 (28%)
5	1UF	A	604	-	34,34,34	2.04	7 (20%)	43,49,49	1.96	11 (25%)
4	MTX	A	603	-	35,35,35	1.61	5 (14%)	47,49,49	1.73	8 (17%)
2	NDP	A	601	-	51,52,52	1.95	12 (23%)	71,80,80	1.51	12 (16%)

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
3	UFP	D	602	-	-	3/10/22/22	0/2/2/2
2	NDP	E	601	-	-	5/34/77/77	0/5/5/5
5	1UF	B	604	-	-	3/21/21/21	0/3/3/3
4	MTX	B	603	-	-	6/25/25/25	0/3/3/3
3	UFP	E	602	-	-	4/10/22/22	0/2/2/2
3	UFP	C	602	-	-	3/10/22/22	0/2/2/2
2	NDP	B	601	-	-	5/34/77/77	0/5/5/5
2	NDP	D	601	-	-	5/34/77/77	0/5/5/5
5	1UF	D	604	-	-	5/21/21/21	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UFP	B	602	-	-	3/10/22/22	0/2/2/2
4	MTX	D	603	-	-	5/25/25/25	0/3/3/3
5	1UF	C	604	-	-	0/21/21/21	0/3/3/3
4	MTX	C	603	-	-	7/25/25/25	0/3/3/3
5	1UF	E	604	-	-	2/21/21/21	0/3/3/3
2	NDP	C	601	-	-	6/34/77/77	0/5/5/5
4	MTX	E	603	-	-	9/25/25/25	0/3/3/3
3	UFP	A	602	-	-	5/10/22/22	0/2/2/2
5	1UF	A	604	-	-	2/21/21/21	0/3/3/3
4	MTX	A	603	-	-	7/25/25/25	0/3/3/3
2	NDP	A	601	-	-	6/34/77/77	0/5/5/5

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	604	1UF	OAF-CBC	7.56	1.37	1.23
5	D	604	1UF	OAF-CBC	7.56	1.37	1.23
5	B	604	1UF	OAF-CBC	7.54	1.37	1.23
5	A	604	1UF	OAF-CBC	7.53	1.37	1.23
5	C	604	1UF	OAF-CBC	7.53	1.37	1.23
2	D	601	NDP	C6A-N6A	5.80	1.49	1.34
2	E	601	NDP	C6A-N6A	5.79	1.49	1.34
2	C	601	NDP	C6A-N6A	5.75	1.48	1.34
2	B	601	NDP	C6A-N6A	5.74	1.48	1.34
2	A	601	NDP	C6A-N6A	5.74	1.48	1.34
4	D	603	MTX	C2-NA2	5.19	1.44	1.33
4	A	603	MTX	C2-NA2	5.19	1.44	1.33
4	C	603	MTX	C2-NA2	5.17	1.44	1.33
4	E	603	MTX	C2-NA2	5.17	1.44	1.33
4	B	603	MTX	C2-NA2	5.16	1.44	1.33
4	C	603	MTX	C-N	4.82	1.45	1.34
4	E	603	MTX	C-N	4.81	1.45	1.34
4	A	603	MTX	C-N	4.78	1.45	1.34
4	B	603	MTX	C-N	4.78	1.45	1.34
2	D	601	NDP	C4N-C3N	-4.70	1.41	1.50
4	D	603	MTX	C-N	4.70	1.45	1.34
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	C	601	NDP	C4N-C3N	-4.68	1.41	1.50
2	E	601	NDP	C4N-C3N	-4.65	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	1UF	CAV-N	4.34	1.44	1.34
5	D	604	1UF	CAV-N	4.23	1.44	1.34
5	C	604	1UF	CAV-N	4.16	1.43	1.34
5	A	604	1UF	CAV-N	4.10	1.43	1.34
5	E	604	1UF	CAV-N	4.07	1.43	1.34
5	A	604	1UF	CAW-NAB	3.98	1.43	1.34
5	C	604	1UF	CAW-NAB	3.97	1.43	1.34
5	E	604	1UF	CAW-NAB	3.95	1.43	1.34
5	B	604	1UF	CAW-NAB	3.94	1.43	1.34
5	D	604	1UF	CAW-NAB	3.92	1.43	1.34
2	D	601	NDP	C3B-C2B	-3.89	1.44	1.53
2	A	601	NDP	C3B-C2B	-3.87	1.44	1.53
2	C	601	NDP	C3B-C2B	-3.84	1.44	1.53
2	B	601	NDP	C2D-C3D	-3.84	1.43	1.53
2	B	601	NDP	C3B-C2B	-3.84	1.44	1.53
2	A	601	NDP	C2D-C3D	-3.83	1.43	1.53
2	E	601	NDP	C2D-C3D	-3.83	1.43	1.53
2	C	601	NDP	C2D-C3D	-3.82	1.43	1.53
2	D	601	NDP	C2D-C3D	-3.80	1.43	1.53
2	E	601	NDP	C3B-C2B	-3.75	1.44	1.53
2	B	601	NDP	C7N-N7N	3.71	1.44	1.33
2	E	601	NDP	C7N-N7N	3.71	1.44	1.33
2	D	601	NDP	C7N-N7N	3.70	1.44	1.33
2	C	601	NDP	C7N-N7N	3.70	1.44	1.33
2	A	601	NDP	C7N-N7N	3.67	1.44	1.33
5	E	604	1UF	CAW-NAQ	3.41	1.45	1.37
5	C	604	1UF	CAW-NAQ	3.39	1.45	1.37
5	A	604	1UF	CAW-NAQ	3.38	1.45	1.37
5	D	604	1UF	CAW-NAQ	3.37	1.45	1.37
5	B	604	1UF	CAW-NAQ	3.35	1.45	1.37
2	B	601	NDP	C4N-C5N	-3.26	1.40	1.49
2	E	601	NDP	C4N-C5N	-3.24	1.40	1.49
2	C	601	NDP	C4N-C5N	-3.23	1.40	1.49
2	A	601	NDP	C4N-C5N	-3.22	1.40	1.49
2	D	601	NDP	C4N-C5N	-3.22	1.40	1.49
5	B	604	1UF	CAW-NAO	3.16	1.40	1.33
5	D	604	1UF	CAW-NAO	3.16	1.40	1.33
5	E	604	1UF	CAW-NAO	3.13	1.40	1.33
5	C	604	1UF	CAW-NAO	3.11	1.40	1.33
5	A	604	1UF	CAW-NAO	3.10	1.40	1.33
2	A	601	NDP	C2B-C1B	-3.00	1.45	1.53
2	D	601	NDP	C2B-C1B	-3.00	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NDP	C2B-C1B	-2.96	1.45	1.53
2	B	601	NDP	C2B-C1B	-2.96	1.45	1.53
2	E	601	NDP	C2B-C1B	-2.88	1.46	1.53
5	C	604	1UF	CBE-CBD	-2.68	1.39	1.45
5	E	604	1UF	CBE-CBD	-2.66	1.39	1.45
5	D	604	1UF	CBE-CBD	-2.65	1.39	1.45
5	B	604	1UF	CBE-CBD	-2.65	1.39	1.45
5	A	604	1UF	CBE-CBD	-2.65	1.39	1.45
4	B	603	MTX	C4-NA4	2.59	1.43	1.34
4	C	603	MTX	C4-NA4	2.58	1.43	1.34
4	E	603	MTX	C4-NA4	2.58	1.43	1.34
4	A	603	MTX	C4-NA4	2.57	1.43	1.34
4	D	603	MTX	C4-NA4	2.55	1.43	1.34
4	E	603	MTX	C14-N10	2.54	1.46	1.38
2	E	601	NDP	C4A-N3A	2.54	1.39	1.34
4	D	603	MTX	C14-N10	2.54	1.46	1.38
4	B	603	MTX	C14-N10	2.53	1.46	1.38
4	A	603	MTX	C14-N10	2.52	1.45	1.38
2	C	601	NDP	C4A-N3A	2.50	1.39	1.34
4	C	603	MTX	C14-N10	2.50	1.45	1.38
2	E	601	NDP	C3B-C4B	-2.49	1.46	1.53
2	D	601	NDP	C4A-N3A	2.48	1.39	1.34
2	B	601	NDP	C4A-N3A	2.47	1.39	1.34
2	A	601	NDP	C3B-C4B	-2.46	1.46	1.53
2	B	601	NDP	C3B-C4B	-2.45	1.46	1.53
2	C	601	NDP	C3B-C4B	-2.45	1.46	1.53
2	A	601	NDP	C4A-N3A	2.44	1.39	1.34
2	D	601	NDP	C3B-C4B	-2.41	1.46	1.53
2	B	601	NDP	C3D-C4D	-2.38	1.46	1.53
2	C	601	NDP	C3D-C4D	-2.35	1.47	1.53
4	D	603	MTX	C7-N8	2.35	1.35	1.31
2	D	601	NDP	C3D-C4D	-2.35	1.47	1.53
4	B	603	MTX	C7-N8	2.33	1.35	1.31
5	C	604	1UF	CBD-NAR	2.33	1.41	1.37
4	A	603	MTX	C7-N8	2.32	1.35	1.31
4	C	603	MTX	C7-N8	2.32	1.35	1.31
2	E	601	NDP	C3D-C4D	-2.29	1.47	1.53
5	B	604	1UF	CBD-NAR	2.29	1.41	1.37
4	E	603	MTX	C7-N8	2.27	1.35	1.31
5	D	604	1UF	CBD-NAR	2.25	1.41	1.37
2	A	601	NDP	C3D-C4D	-2.25	1.47	1.53
5	A	604	1UF	CBD-NAR	2.24	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	604	1UF	CBD-NAR	2.23	1.41	1.37
2	E	601	NDP	C6N-C5N	2.17	1.39	1.33
2	C	601	NDP	C6N-C5N	2.16	1.39	1.33
2	D	601	NDP	C6N-C5N	2.14	1.39	1.33
2	B	601	NDP	C6N-C5N	2.13	1.39	1.33
2	A	601	NDP	C6N-C5N	2.12	1.39	1.33
2	E	601	NDP	C2N-C3N	2.06	1.40	1.35
2	D	601	NDP	C2N-C3N	2.05	1.40	1.35
2	A	601	NDP	C2N-C3N	2.05	1.40	1.35
2	B	601	NDP	C2N-C3N	2.05	1.40	1.35
2	C	601	NDP	C2N-C3N	2.05	1.40	1.35
4	C	603	MTX	C6-N5	2.02	1.35	1.32

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	UFP	C5-C4-N3	7.12	119.15	112.64
3	B	602	UFP	C5-C4-N3	7.12	119.15	112.64
3	E	602	UFP	C5-C4-N3	7.10	119.13	112.64
3	A	602	UFP	C5-C4-N3	7.09	119.12	112.64
3	C	602	UFP	C5-C4-N3	7.03	119.07	112.64
3	D	602	UFP	O4-C4-C5	-6.36	120.28	125.69
3	E	602	UFP	O4-C4-C5	-6.23	120.39	125.69
3	A	602	UFP	O4-C4-C5	-6.23	120.39	125.69
3	B	602	UFP	O4-C4-C5	-6.22	120.40	125.69
3	C	602	UFP	O4-C4-C5	-6.06	120.53	125.69
2	B	601	NDP	C5A-C4A-N3A	-5.51	119.14	126.72
2	C	601	NDP	C5A-C4A-N3A	-5.49	119.15	126.72
2	D	601	NDP	C5A-C4A-N3A	-5.48	119.18	126.72
2	E	601	NDP	C5A-C4A-N3A	-5.46	119.19	126.72
2	A	601	NDP	C5A-C4A-N3A	-5.35	119.36	126.72
4	B	603	MTX	C6-C7-N8	-5.03	118.31	123.14
4	C	603	MTX	C6-C7-N8	-4.98	118.36	123.14
5	D	604	1UF	CG-CB-CA	4.96	122.31	113.16
4	A	603	MTX	C6-C7-N8	-4.95	118.39	123.14
3	D	602	UFP	C4-N3-C2	-4.91	120.90	127.34
3	C	602	UFP	C4-N3-C2	-4.91	120.91	127.34
3	A	602	UFP	C4-N3-C2	-4.90	120.91	127.34
3	B	602	UFP	C4-N3-C2	-4.90	120.91	127.34
4	D	603	MTX	C6-C7-N8	-4.87	118.46	123.14
3	E	602	UFP	C4-N3-C2	-4.84	120.99	127.34
4	E	603	MTX	C6-C7-N8	-4.82	118.52	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	UFP	F5-C5-C4	4.74	120.62	116.47
5	B	604	1UF	CAW-NAO-CBD	4.71	121.67	113.36
5	E	604	1UF	CAW-NAO-CBD	4.69	121.64	113.36
3	A	602	UFP	F5-C5-C4	4.69	120.58	116.47
5	D	604	1UF	CAW-NAO-CBD	4.69	121.64	113.36
5	C	604	1UF	CAW-NAO-CBD	4.66	121.59	113.36
5	A	604	1UF	CAW-NAO-CBD	4.66	121.58	113.36
3	C	602	UFP	F5-C5-C4	4.64	120.53	116.47
3	E	602	UFP	F5-C5-C4	4.55	120.46	116.47
3	C	602	UFP	N3-C2-N1	4.51	120.76	114.89
3	A	602	UFP	N3-C2-N1	4.50	120.75	114.89
3	D	602	UFP	N3-C2-N1	4.50	120.75	114.89
5	E	604	1UF	CG-CB-CA	4.49	121.43	113.16
3	E	602	UFP	N3-C2-N1	4.49	120.73	114.89
5	A	604	1UF	CG-CB-CA	4.47	121.41	113.16
3	B	602	UFP	N3-C2-N1	4.47	120.72	114.89
3	D	602	UFP	F5-C5-C4	4.43	120.35	116.47
5	B	604	1UF	CG-CB-CA	4.18	120.87	113.16
5	C	604	1UF	CAA-CAX-CBB	-4.13	125.96	130.98
2	D	601	NDP	N3A-C2A-N1A	-4.11	122.36	128.58
2	C	601	NDP	N3A-C2A-N1A	-4.11	122.37	128.58
2	E	601	NDP	N3A-C2A-N1A	-4.09	122.39	128.58
2	B	601	NDP	N3A-C2A-N1A	-4.06	122.44	128.58
5	A	604	1UF	CAA-CAX-CBB	-4.04	126.07	130.98
5	B	604	1UF	CAA-CAX-CBB	-4.03	126.08	130.98
2	A	601	NDP	N3A-C2A-N1A	-4.03	122.48	128.58
5	E	604	1UF	CAA-CAX-CBB	-4.03	126.09	130.98
3	E	602	UFP	C6-C5-C4	-4.01	118.91	122.57
4	A	603	MTX	N8-C8A-N1	4.01	120.14	115.77
5	D	604	1UF	CAA-CAX-CBB	-4.00	126.13	130.98
4	B	603	MTX	N8-C8A-N1	3.96	120.08	115.77
3	B	602	UFP	C6-C5-C4	-3.95	118.96	122.57
3	A	602	UFP	C6-C5-C4	-3.93	118.98	122.57
5	B	604	1UF	NAR-CBD-NAO	3.90	130.79	125.80
4	D	603	MTX	N8-C8A-N1	3.87	119.98	115.77
3	D	602	UFP	C6-C5-C4	-3.87	119.04	122.57
3	C	602	UFP	C6-C5-C4	-3.86	119.04	122.57
2	C	601	NDP	N3A-C4A-N9A	3.85	133.71	127.17
4	C	603	MTX	N8-C8A-N1	3.85	119.96	115.77
5	C	604	1UF	NAR-CBD-NAO	3.84	130.71	125.80
5	E	604	1UF	NAR-CBD-NAO	3.84	130.71	125.80
2	B	601	NDP	N3A-C4A-N9A	3.83	133.68	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	MTX	N1-C2-N3	-3.82	122.35	127.21
4	A	603	MTX	N1-C2-N3	-3.82	122.35	127.21
5	D	604	1UF	NAR-CBD-NAO	3.82	130.69	125.80
2	D	601	NDP	N3A-C4A-N9A	3.81	133.65	127.17
2	E	601	NDP	N3A-C4A-N9A	3.81	133.65	127.17
4	E	603	MTX	N1-C2-N3	-3.80	122.38	127.21
4	B	603	MTX	N1-C2-N3	-3.78	122.41	127.21
4	C	603	MTX	N1-C2-N3	-3.77	122.42	127.21
5	E	604	1UF	CAY-SAS-CBB	3.70	110.36	103.63
5	A	604	1UF	NAR-CBD-NAO	3.69	130.52	125.80
4	E	603	MTX	N8-C8A-N1	3.69	119.79	115.77
2	A	601	NDP	N3A-C4A-N9A	3.68	133.43	127.17
5	A	604	1UF	CAY-SAS-CBB	3.68	110.32	103.63
4	D	603	MTX	C2-N1-C8A	3.65	119.42	115.48
5	C	604	1UF	CG-CB-CA	3.62	119.84	113.16
4	B	603	MTX	C2-N1-C8A	3.62	119.39	115.48
4	A	603	MTX	C2-N1-C8A	3.62	119.38	115.48
4	C	603	MTX	C2-N1-C8A	3.61	119.38	115.48
4	E	603	MTX	C2-N1-C8A	3.61	119.38	115.48
2	D	601	NDP	C2A-N3A-C4A	3.52	120.43	111.83
2	C	601	NDP	C2A-N3A-C4A	3.52	120.42	111.83
2	B	601	NDP	C2A-N3A-C4A	3.51	120.40	111.83
2	E	601	NDP	C2A-N3A-C4A	3.50	120.39	111.83
2	A	601	NDP	C2A-N3A-C4A	3.46	120.28	111.83
5	C	604	1UF	CAY-SAS-CBB	3.26	109.57	103.63
2	E	601	NDP	N9A-C8A-N7A	-3.25	109.32	113.94
2	A	601	NDP	N9A-C8A-N7A	-3.25	109.33	113.94
5	B	604	1UF	CAY-SAS-CBB	3.21	109.47	103.63
2	B	601	NDP	N9A-C8A-N7A	-3.18	109.42	113.94
2	D	601	NDP	N9A-C8A-N7A	-3.18	109.43	113.94
2	A	601	NDP	C4A-C5A-N7A	-3.16	106.97	110.58
4	E	603	MTX	C6-C9-N10	3.15	118.34	112.95
2	E	601	NDP	C4A-C5A-N7A	-3.14	106.99	110.58
2	C	601	NDP	N9A-C8A-N7A	-3.14	109.49	113.94
3	E	602	UFP	C1'-N1-C2	3.13	123.79	117.66
5	A	604	1UF	CB-CG-CD	3.13	120.84	112.49
5	D	604	1UF	CAY-SAS-CBB	3.13	109.32	103.63
2	E	601	NDP	C5A-N7A-C8A	3.13	108.36	103.45
2	A	601	NDP	C5A-N7A-C8A	3.11	108.34	103.45
2	B	601	NDP	C4A-C5A-N7A	-3.11	107.03	110.58
3	A	602	UFP	C1'-N1-C2	3.09	123.70	117.66
2	D	601	NDP	C4A-C5A-N7A	-3.08	107.06	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	NDP	C4A-C5A-N7A	-3.08	107.06	110.58
2	D	601	NDP	C5A-N7A-C8A	3.08	108.29	103.45
2	B	601	NDP	C5A-N7A-C8A	3.07	108.28	103.45
2	C	601	NDP	C5A-N7A-C8A	3.06	108.25	103.45
3	B	602	UFP	C1'-N1-C2	2.99	123.52	117.66
5	C	604	1UF	CAW-NAQ-CBC	-2.98	119.71	125.11
3	C	602	UFP	C1'-N1-C2	2.98	123.48	117.66
5	E	604	1UF	CAW-NAQ-CBC	-2.97	119.72	125.11
4	C	603	MTX	C6-C9-N10	2.97	118.04	112.95
5	D	604	1UF	CAW-NAQ-CBC	-2.97	119.73	125.11
5	E	604	1UF	CB-CG-CD	2.96	120.39	112.49
5	B	604	1UF	CAW-NAQ-CBC	-2.96	119.75	125.11
5	A	604	1UF	CAW-NAQ-CBC	-2.93	119.80	125.11
3	D	602	UFP	C1'-N1-C2	2.92	123.36	117.66
4	B	603	MTX	CG-CB-CA	2.84	118.40	113.16
4	D	603	MTX	C6-C9-N10	2.81	117.77	112.95
5	D	604	1UF	NAQ-CAW-NAO	-2.80	118.20	123.32
5	B	604	1UF	NAQ-CAW-NAO	-2.79	118.21	123.32
5	E	604	1UF	NAQ-CAW-NAO	-2.79	118.22	123.32
5	A	604	1UF	NAQ-CAW-NAO	-2.78	118.24	123.32
4	D	603	MTX	CG-CB-CA	2.76	118.24	113.16
5	C	604	1UF	NAQ-CAW-NAO	-2.76	118.28	123.32
4	C	603	MTX	C7-N8-C8A	2.74	121.01	117.20
5	C	604	1UF	CB-CG-CD	2.72	119.74	112.49
5	B	604	1UF	CB-CG-CD	2.71	119.72	112.49
4	A	603	MTX	C7-N8-C8A	2.69	120.94	117.20
4	B	603	MTX	C7-N8-C8A	2.68	120.93	117.20
4	D	603	MTX	C7-N8-C8A	2.65	120.88	117.20
4	E	603	MTX	C7-N8-C8A	2.63	120.86	117.20
4	B	603	MTX	C11-C-N	2.62	121.90	117.04
4	A	603	MTX	C6-C9-N10	2.58	117.36	112.95
5	C	604	1UF	CAX-NAR-CBD	-2.55	107.78	109.21
4	A	603	MTX	CG-CB-CA	2.53	117.83	113.16
5	A	604	1UF	CAX-NAR-CBD	-2.52	107.80	109.21
4	E	603	MTX	CG-CB-CA	2.50	117.77	113.16
4	A	603	MTX	C11-C-N	2.48	121.64	117.04
4	C	603	MTX	C11-C-N	2.47	121.61	117.04
2	E	601	NDP	O5D-C5D-C4D	2.46	117.36	108.99
4	E	603	MTX	C11-C-N	2.44	121.57	117.04
4	C	603	MTX	CG-CB-CA	2.44	117.66	113.16
4	D	603	MTX	C11-C-N	2.44	121.56	117.04
5	E	604	1UF	CAX-NAR-CBD	-2.44	107.84	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	604	1UF	CAX-NAR-CBD	-2.43	107.85	109.21
2	D	601	NDP	O5D-C5D-C4D	2.42	117.25	108.99
3	A	602	UFP	C1'-N1-C6	-2.41	116.69	120.74
5	B	604	1UF	CAK-CBA-CAZ	2.40	120.59	117.79
3	E	602	UFP	C1'-N1-C6	-2.40	116.72	120.74
2	C	601	NDP	O5D-C5D-C4D	2.39	117.13	108.99
2	E	601	NDP	C3N-C7N-N7N	2.37	121.87	117.67
4	B	603	MTX	C6-C9-N10	2.35	116.97	112.95
3	B	602	UFP	C1'-N1-C6	-2.34	116.81	120.74
2	E	601	NDP	O5B-C5B-C4B	2.34	116.96	108.99
2	C	601	NDP	C3N-C7N-N7N	2.34	121.82	117.67
2	B	601	NDP	O5D-C5D-C4D	2.34	116.95	108.99
5	B	604	1UF	CA-N-CAV	2.33	127.16	121.56
3	A	602	UFP	O2-C2-N3	-2.33	117.19	121.49
3	E	602	UFP	O2-C2-N3	-2.33	117.19	121.49
2	A	601	NDP	C3N-C7N-N7N	2.33	121.80	117.67
3	D	602	UFP	O2-C2-N3	-2.32	117.21	121.49
5	B	604	1UF	CAX-NAR-CBD	-2.32	107.91	109.21
2	B	601	NDP	O5B-C5B-C4B	2.32	116.88	108.99
3	C	602	UFP	C1'-N1-C6	-2.31	116.86	120.74
2	E	601	NDP	C4A-N9A-C8A	2.31	108.17	105.74
3	C	602	UFP	O2-C2-N3	-2.29	117.27	121.49
2	A	601	NDP	O5D-C5D-C4D	2.28	116.77	108.99
2	A	601	NDP	C4A-N9A-C8A	2.28	108.13	105.74
3	B	602	UFP	O2-C2-N3	-2.26	117.32	121.49
2	D	601	NDP	C3N-C7N-N7N	2.25	121.66	117.67
3	D	602	UFP	C1'-N1-C6	-2.24	116.99	120.74
2	B	601	NDP	C4A-N9A-C8A	2.23	108.08	105.74
2	A	601	NDP	C2B-C1B-N9A	-2.23	110.08	113.75
2	C	601	NDP	C4A-N9A-C8A	2.21	108.06	105.74
5	D	604	1UF	CB-CG-CD	2.21	118.38	112.49
2	D	601	NDP	C4A-N9A-C8A	2.20	108.05	105.74
2	B	601	NDP	C3N-C7N-N7N	2.19	121.56	117.67
2	D	601	NDP	O5B-C5B-C4B	2.17	116.38	108.99
4	E	603	MTX	C4-C4A-N5	2.17	122.00	120.33
5	E	604	1UF	CAK-CBA-CAZ	2.17	120.32	117.79
5	D	604	1UF	CAK-CBA-CAZ	2.16	120.32	117.79
4	C	603	MTX	C4-C4A-N5	2.13	121.97	120.33
4	C	603	MTX	C8A-C4A-N5	-2.13	119.97	122.35
4	E	603	MTX	C8A-C4A-N5	-2.13	119.97	122.35
2	A	601	NDP	O5B-C5B-C4B	2.12	116.20	108.99
2	E	601	NDP	C2B-C1B-N9A	-2.07	110.34	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	UFP	O4'-C1'-N1	2.07	111.53	107.86
2	C	601	NDP	O5B-C5B-C4B	2.07	116.03	108.99
2	C	601	NDP	C2B-C1B-N9A	-2.07	110.35	113.75
5	C	604	1UF	CBB-CAX-NAR	2.04	108.79	105.70
5	A	604	1UF	CBB-CAX-NAR	2.04	108.78	105.70
5	C	604	1UF	CAK-CBA-CAZ	2.02	120.15	117.79
5	D	604	1UF	CBB-CAX-NAR	2.02	108.75	105.70
5	A	604	1UF	CAK-CBA-CAZ	2.01	120.14	117.79

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	UFP	C5'-O5'-P-O1P
3	A	602	UFP	C5'-O5'-P-O2P
3	A	602	UFP	C5'-O5'-P-O3P
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
3	E	602	UFP	C5'-O5'-P-O1P
3	E	602	UFP	C5'-O5'-P-O3P
4	C	603	MTX	N-CA-CB-CG
4	E	603	MTX	N-CA-CB-CG
5	B	604	1UF	CB-CA-N-CAV
5	D	604	1UF	CB-CA-N-CAV
2	E	601	NDP	C3B-C4B-C5B-O5B
2	E	601	NDP	O4B-C4B-C5B-O5B
4	A	603	MTX	N-CA-CB-CG
4	A	603	MTX	CT-CA-CB-CG
4	C	603	MTX	CT-CA-CB-CG
4	E	603	MTX	CT-CA-CB-CG
4	E	603	MTX	C15-C14-N10-CM
2	A	601	NDP	C3B-C4B-C5B-O5B
4	E	603	MTX	C13-C14-N10-CM
3	B	602	UFP	C5'-O5'-P-O1P
3	C	602	UFP	C5'-O5'-P-O1P
3	D	602	UFP	C5'-O5'-P-O1P
4	A	603	MTX	C13-C14-N10-CM
4	A	603	MTX	C15-C14-N10-CM

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Mol	Chain	Res	Type	Atoms
4	D	603	MTX	N-CA-CB-CG
4	C	603	MTX	C13-C14-N10-CM
2	A	601	NDP	PA-O3-PN-O5D
4	D	603	MTX	CT-CA-CB-CG
5	D	604	1UF	C-CA-CB-CG
4	C	603	MTX	C15-C14-N10-CM
5	D	604	1UF	N-CA-CB-CG
2	B	601	NDP	C4D-C5D-O5D-PN
2	C	601	NDP	C4D-C5D-O5D-PN
2	D	601	NDP	C4D-C5D-O5D-PN
2	E	601	NDP	C4D-C5D-O5D-PN
2	D	601	NDP	C2D-C1D-N1N-C2N
5	A	604	1UF	OE1-CD-CG-CB
5	E	604	1UF	OE1-CD-CG-CB
2	D	601	NDP	O4D-C1D-N1N-C2N
4	B	603	MTX	CT-CA-CB-CG
2	B	601	NDP	C2D-C1D-N1N-C2N
5	A	604	1UF	OE2-CD-CG-CB
2	A	601	NDP	O4D-C1D-N1N-C2N
5	E	604	1UF	OE2-CD-CG-CB
2	B	601	NDP	O4D-C1D-N1N-C2N
2	C	601	NDP	O4D-C1D-N1N-C2N
2	E	601	NDP	O4D-C1D-N1N-C2N
2	C	601	NDP	C2D-C1D-N1N-C2N
5	D	604	1UF	OE2-CD-CG-CB
2	C	601	NDP	C2N-C3N-C7N-N7N
5	D	604	1UF	OE1-CD-CG-CB
5	B	604	1UF	OE1-CD-CG-CB
2	A	601	NDP	C2D-C1D-N1N-C2N
4	D	603	MTX	OE2-CD-CG-CB
4	B	603	MTX	OE2-CD-CG-CB
4	C	603	MTX	OE2-CD-CG-CB
2	D	601	NDP	O4D-C1D-N1N-C6N
4	A	603	MTX	OE2-CD-CG-CB
2	A	601	NDP	C4D-C5D-O5D-PN
5	B	604	1UF	OE2-CD-CG-CB
3	E	602	UFP	C5'-O5'-P-O2P
4	A	603	MTX	C6-C9-N10-CM
4	B	603	MTX	C6-C9-N10-CM
4	C	603	MTX	C6-C9-N10-CM
4	D	603	MTX	C6-C9-N10-CM
4	E	603	MTX	C6-C9-N10-CM

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Mol	Chain	Res	Type	Atoms
4	E	603	MTX	OE2-CD-CG-CB
4	C	603	MTX	OE1-CD-CG-CB
4	E	603	MTX	CA-CB-CG-CD
4	B	603	MTX	OE1-CD-CG-CB
4	D	603	MTX	OE1-CD-CG-CB
2	D	601	NDP	C2D-C1D-N1N-C6N
4	E	603	MTX	C6-C9-N10-C14
4	E	603	MTX	OE1-CD-CG-CB
4	B	603	MTX	C13-C14-N10-CM
2	E	601	NDP	C2D-C1D-N1N-C2N
4	A	603	MTX	OE1-CD-CG-CB
2	B	601	NDP	O4D-C1D-N1N-C6N
2	C	601	NDP	O4D-C1D-N1N-C6N
2	A	601	NDP	O4B-C4B-C5B-O5B
3	A	602	UFP	C3'-C4'-C5'-O5'
2	B	601	NDP	C2D-C1D-N1N-C6N
4	B	603	MTX	C15-C14-N10-CM
3	A	602	UFP	O4'-C4'-C5'-O5'
2	C	601	NDP	C2D-C1D-N1N-C6N
3	E	602	UFP	C2'-C1'-N1-C2

There are no ring outliers.

19 monomers are involved in 56 short contacts:

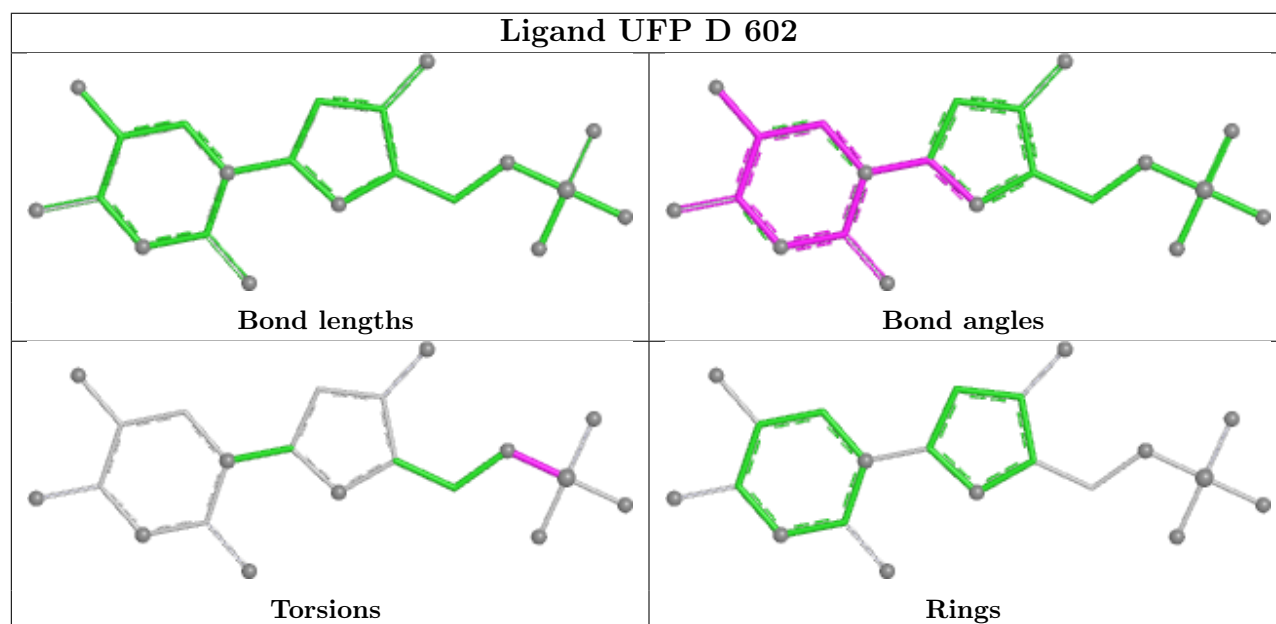
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	UFP	1	0
2	E	601	NDP	1	0
4	B	603	MTX	3	0
3	E	602	UFP	2	1
3	C	602	UFP	2	0
2	B	601	NDP	4	0
2	D	601	NDP	4	0
5	D	604	1UF	1	0
3	B	602	UFP	3	0
4	D	603	MTX	3	0
5	C	604	1UF	3	0
4	C	603	MTX	2	0
5	E	604	1UF	6	0
2	C	601	NDP	5	0
4	E	603	MTX	2	0
3	A	602	UFP	2	0
5	A	604	1UF	4	0

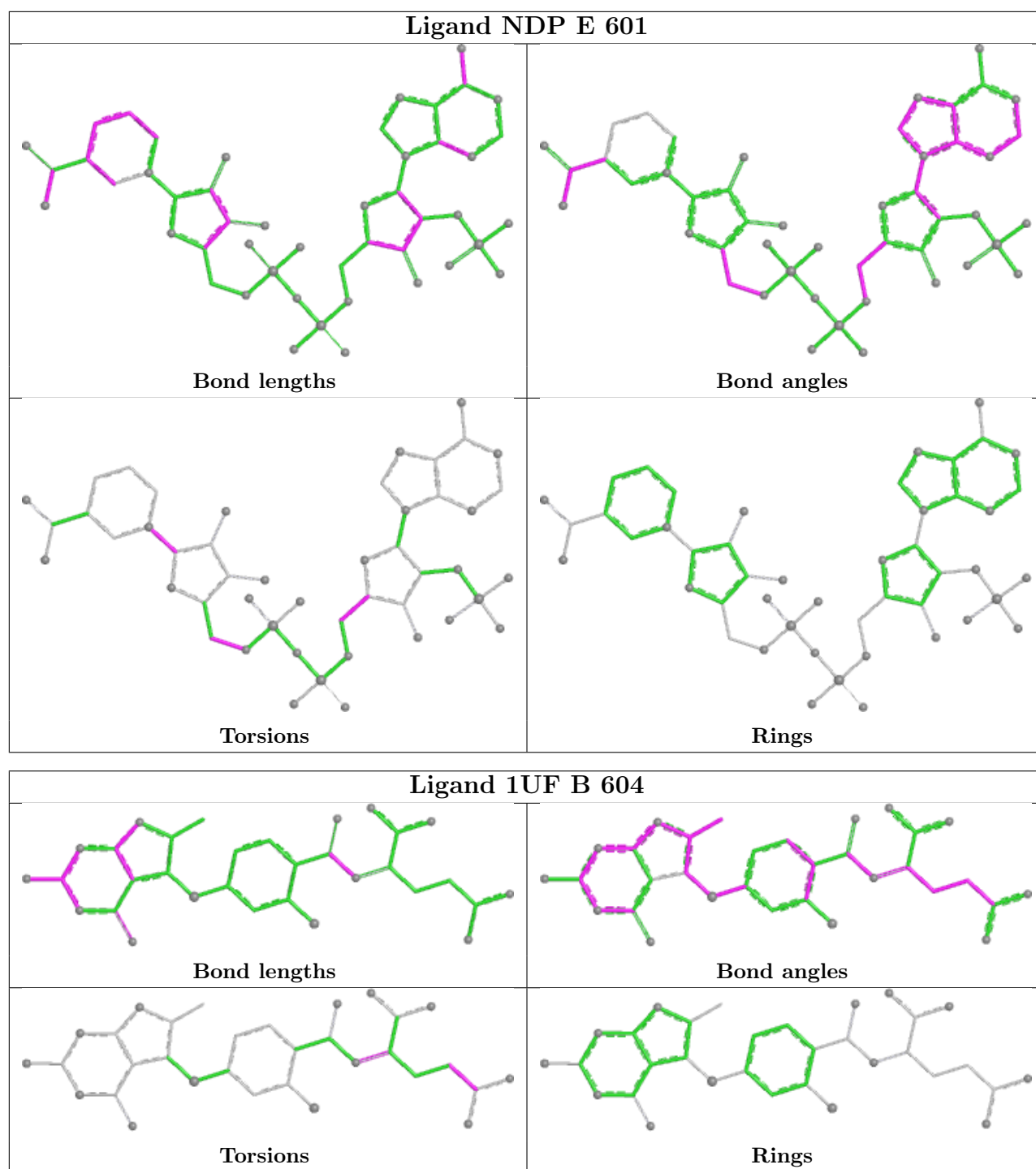
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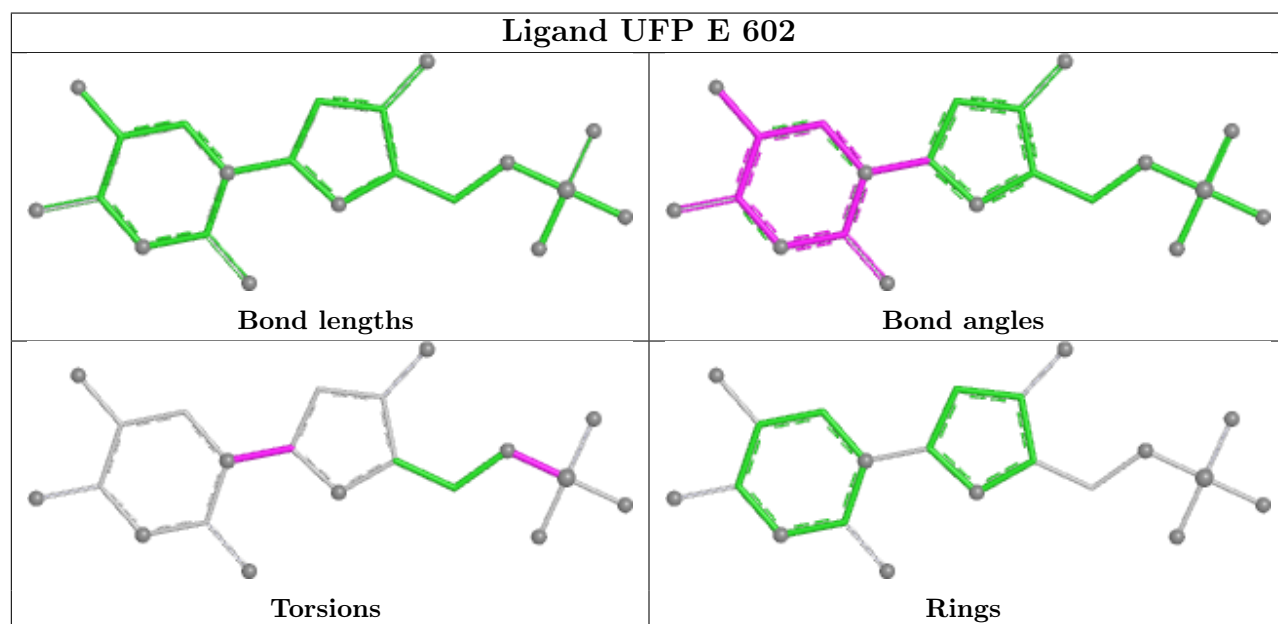
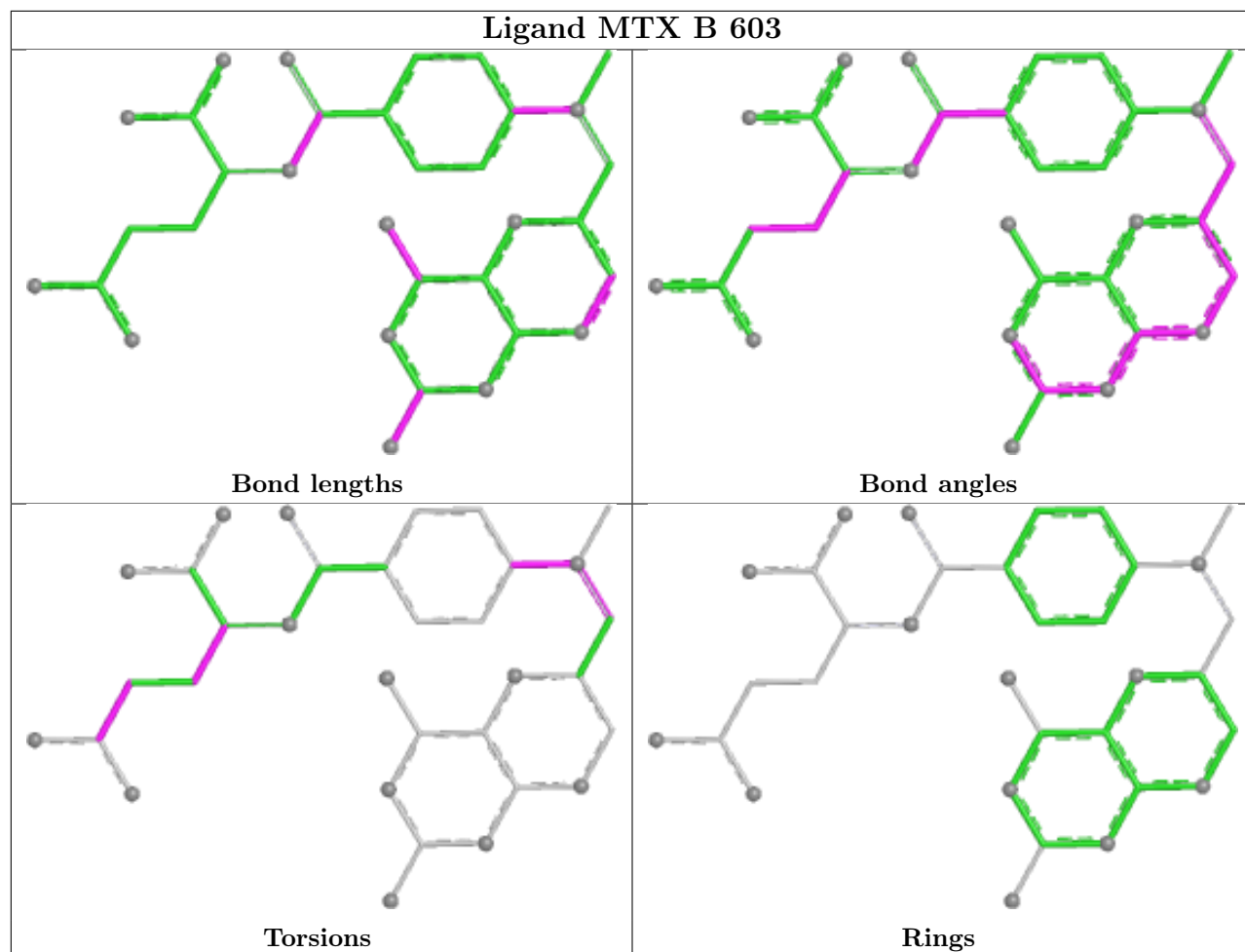
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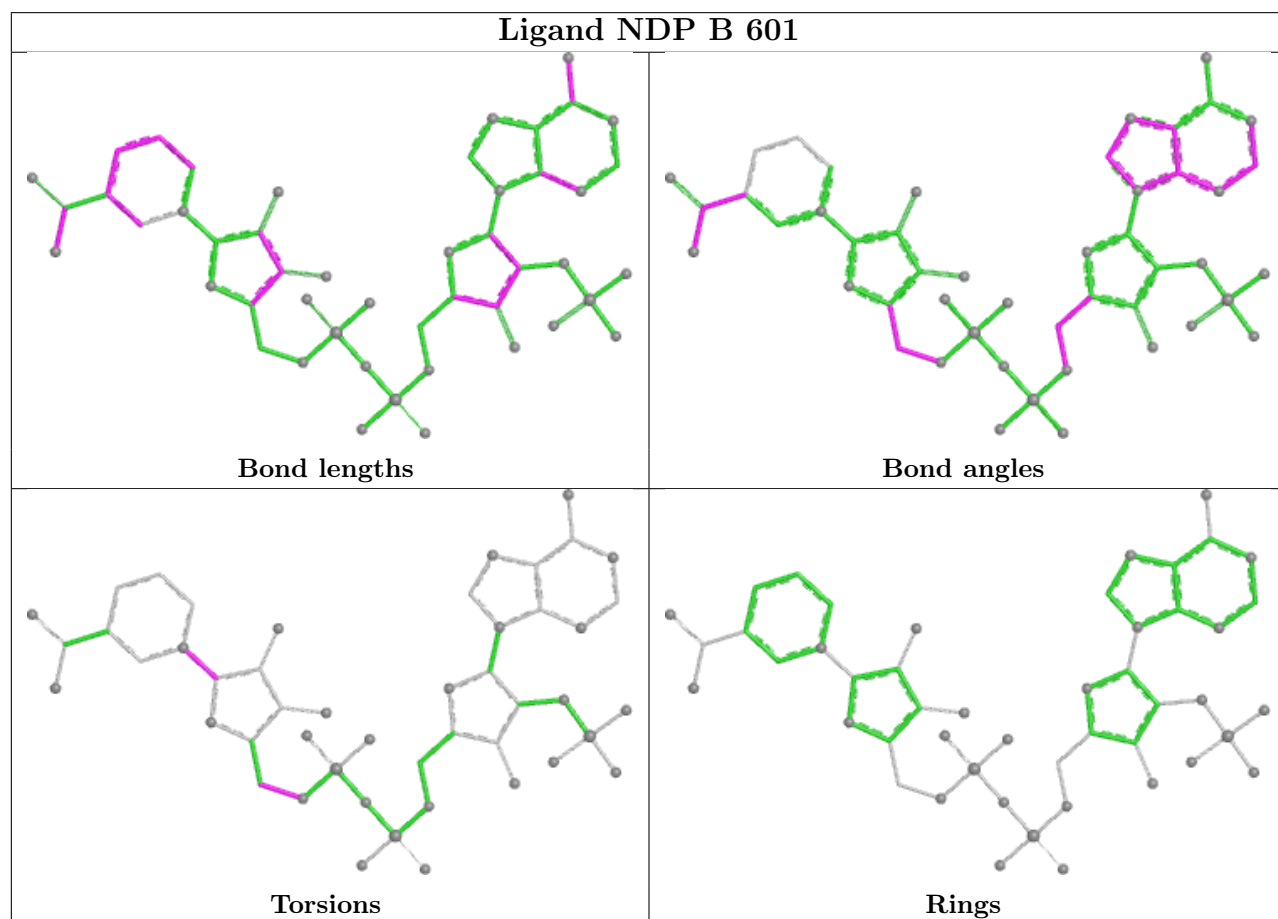
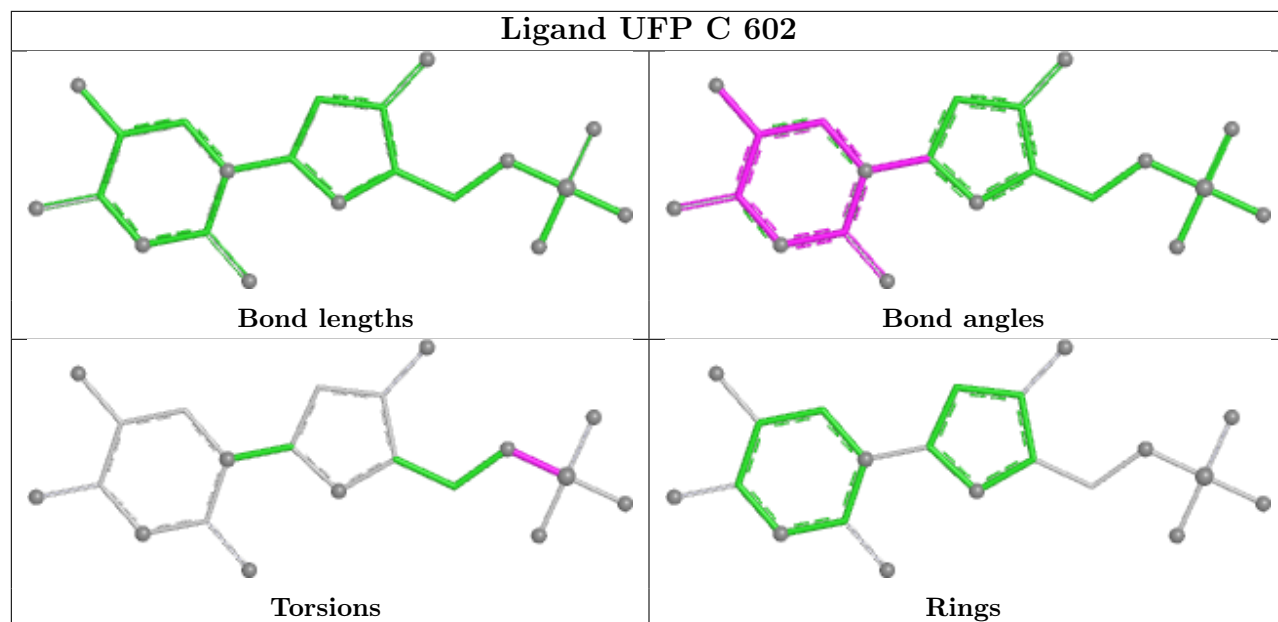
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	MTX	5	0
2	A	601	NDP	4	0

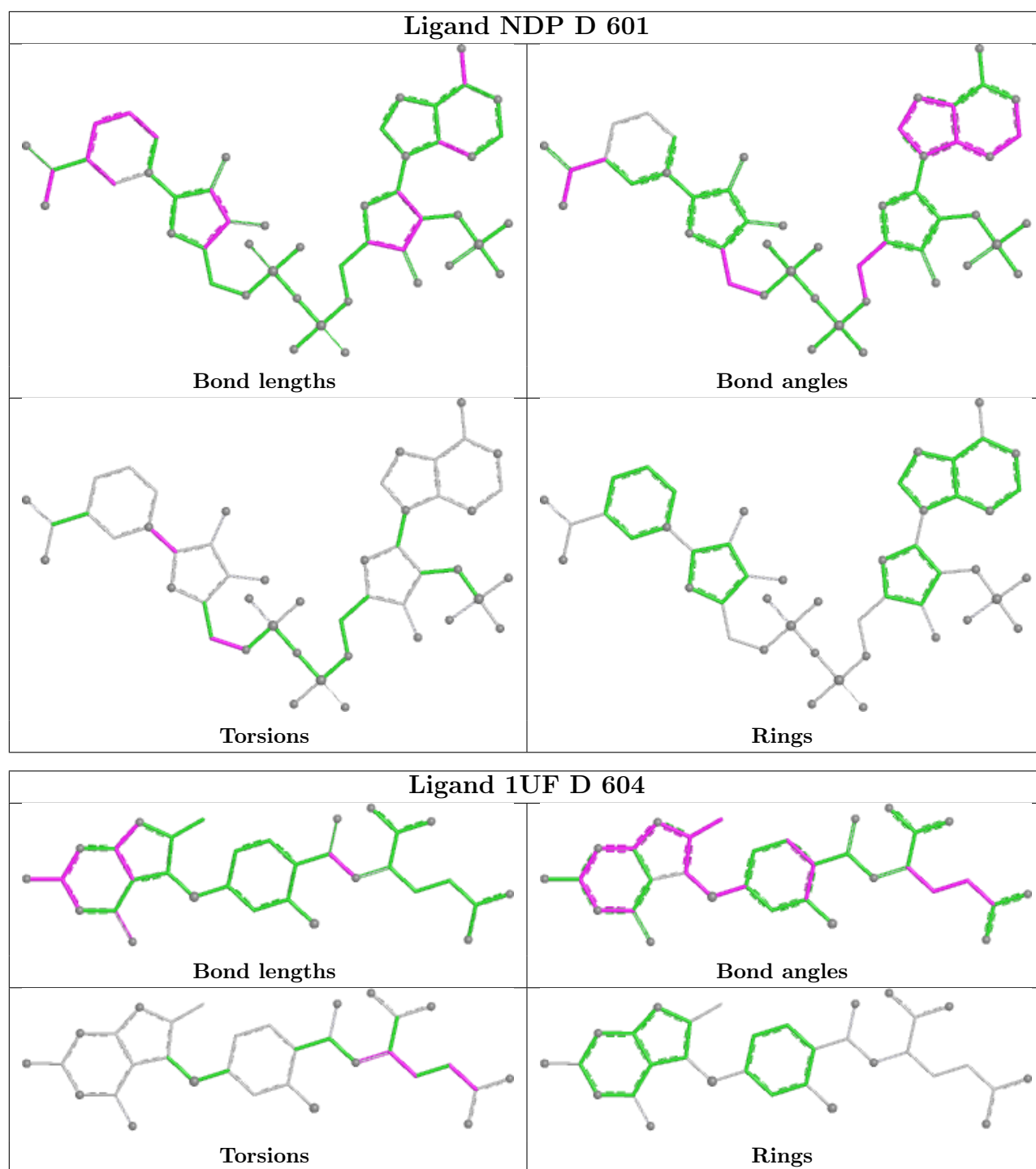
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

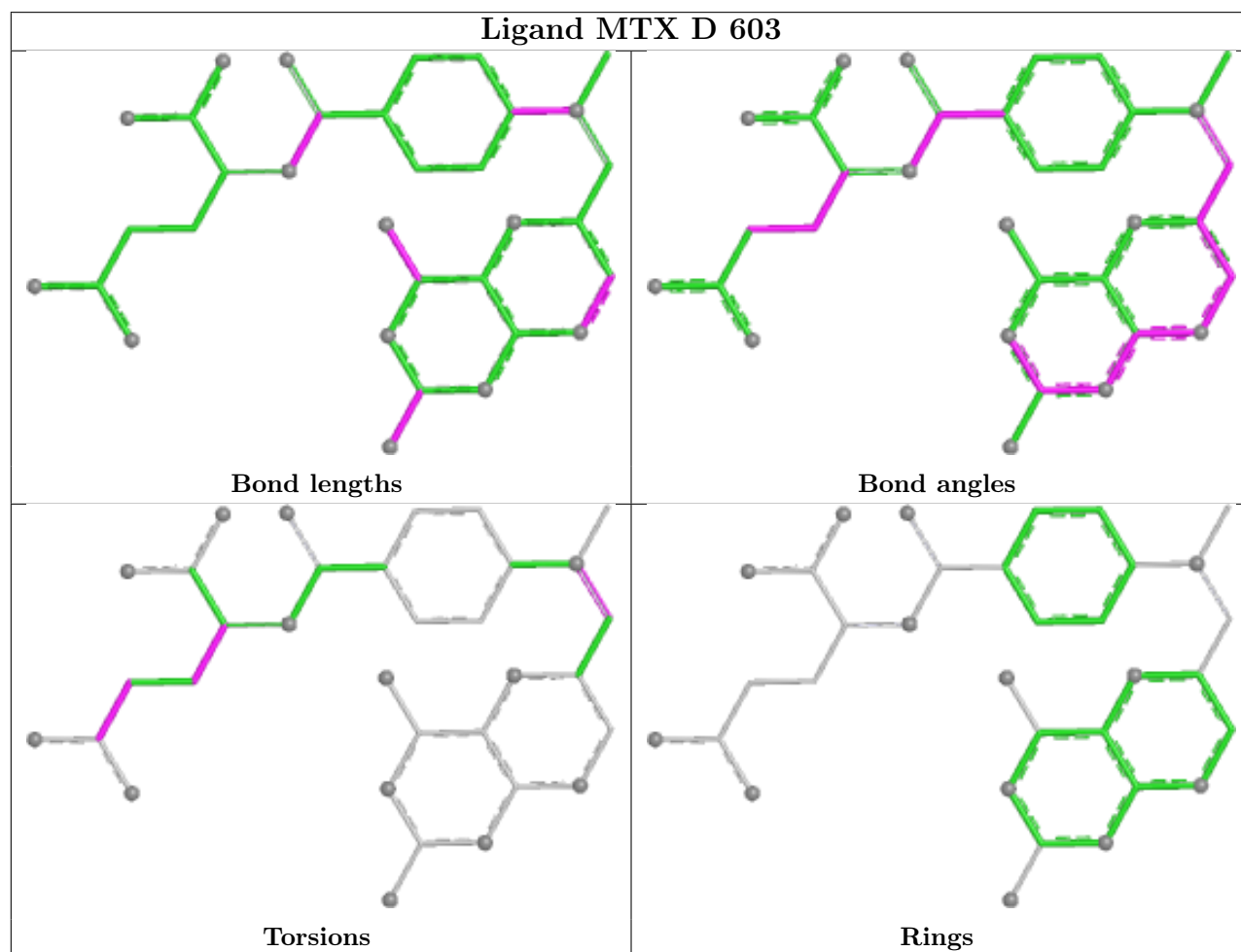
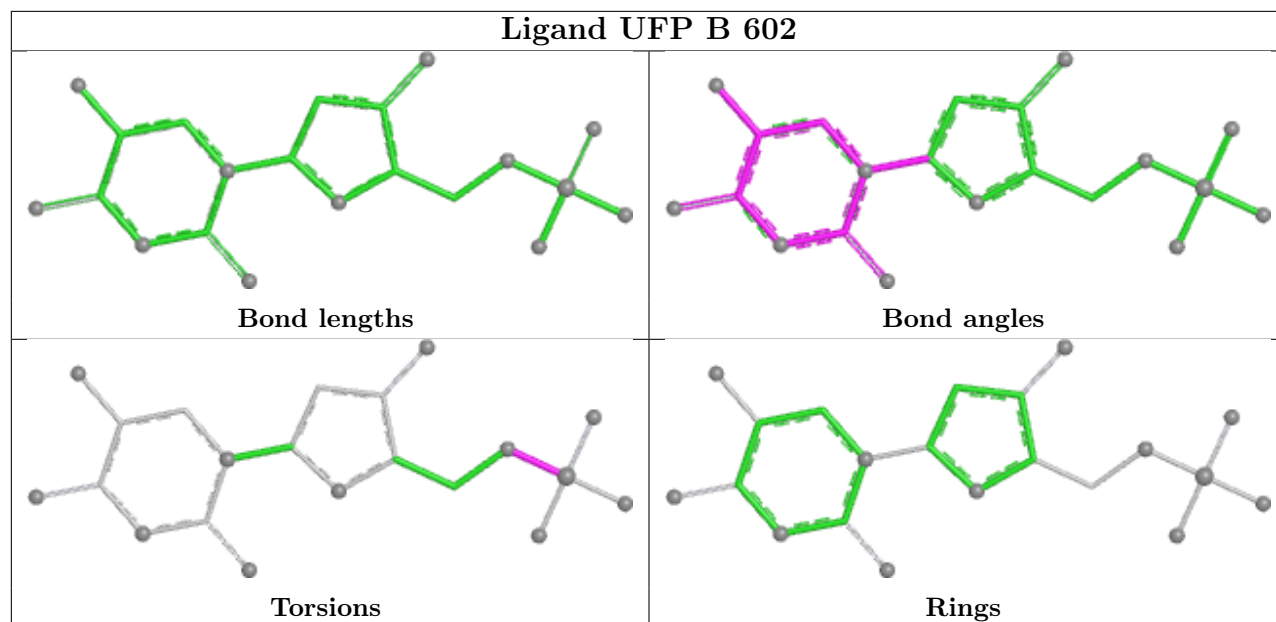




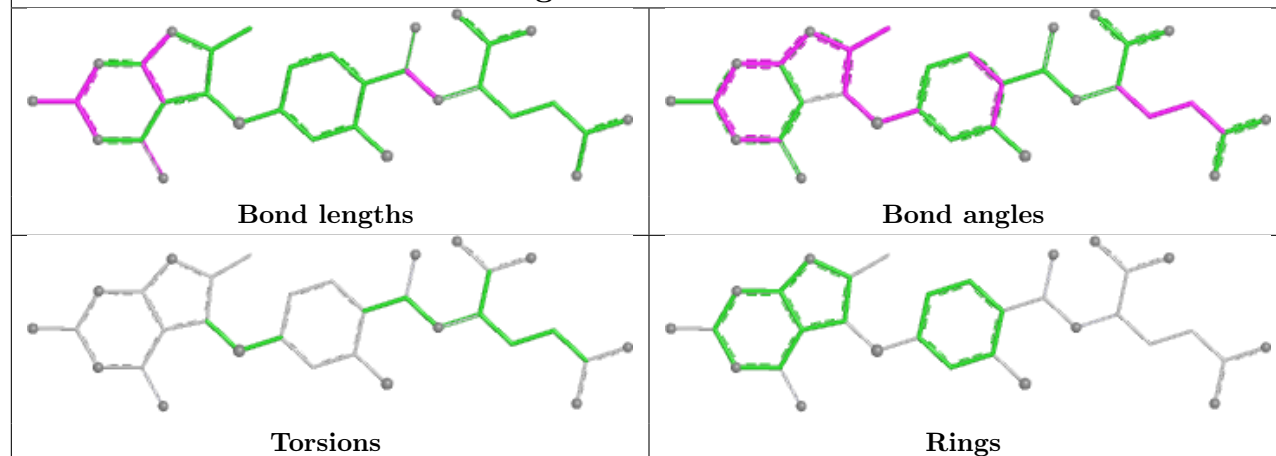




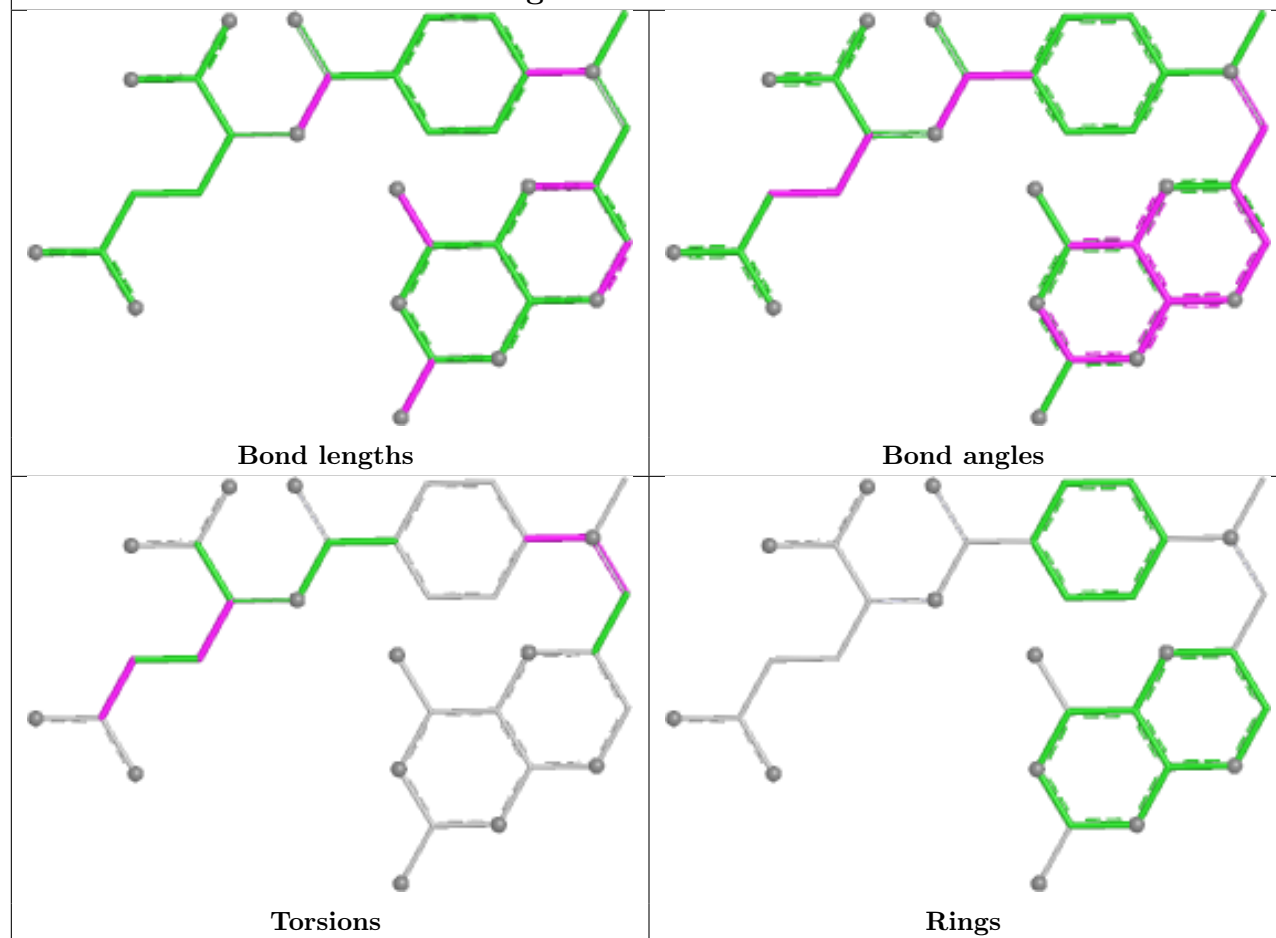




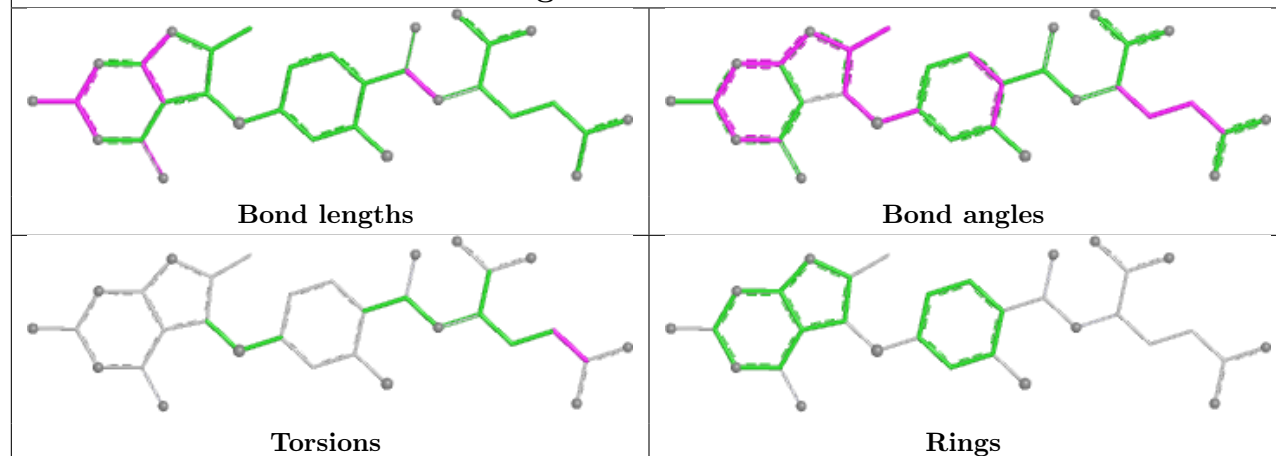
Ligand 1UF C 604



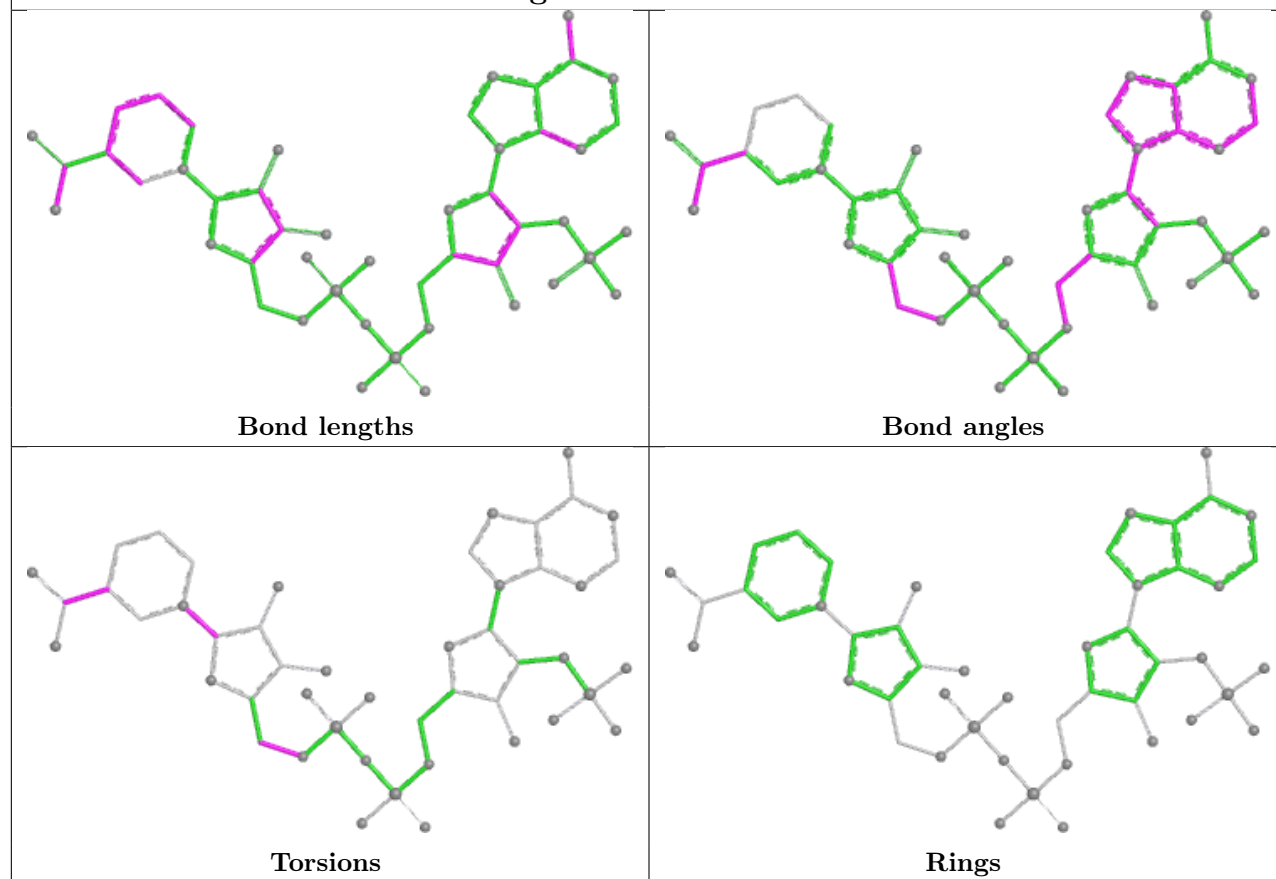
Ligand MTX C 603

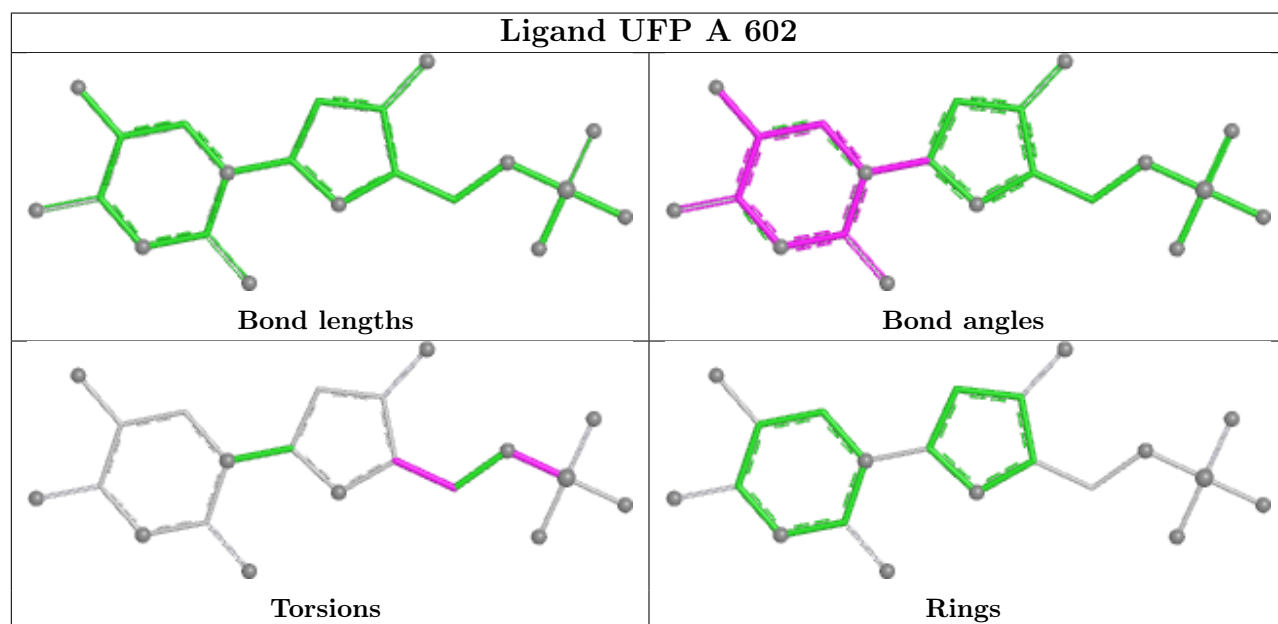
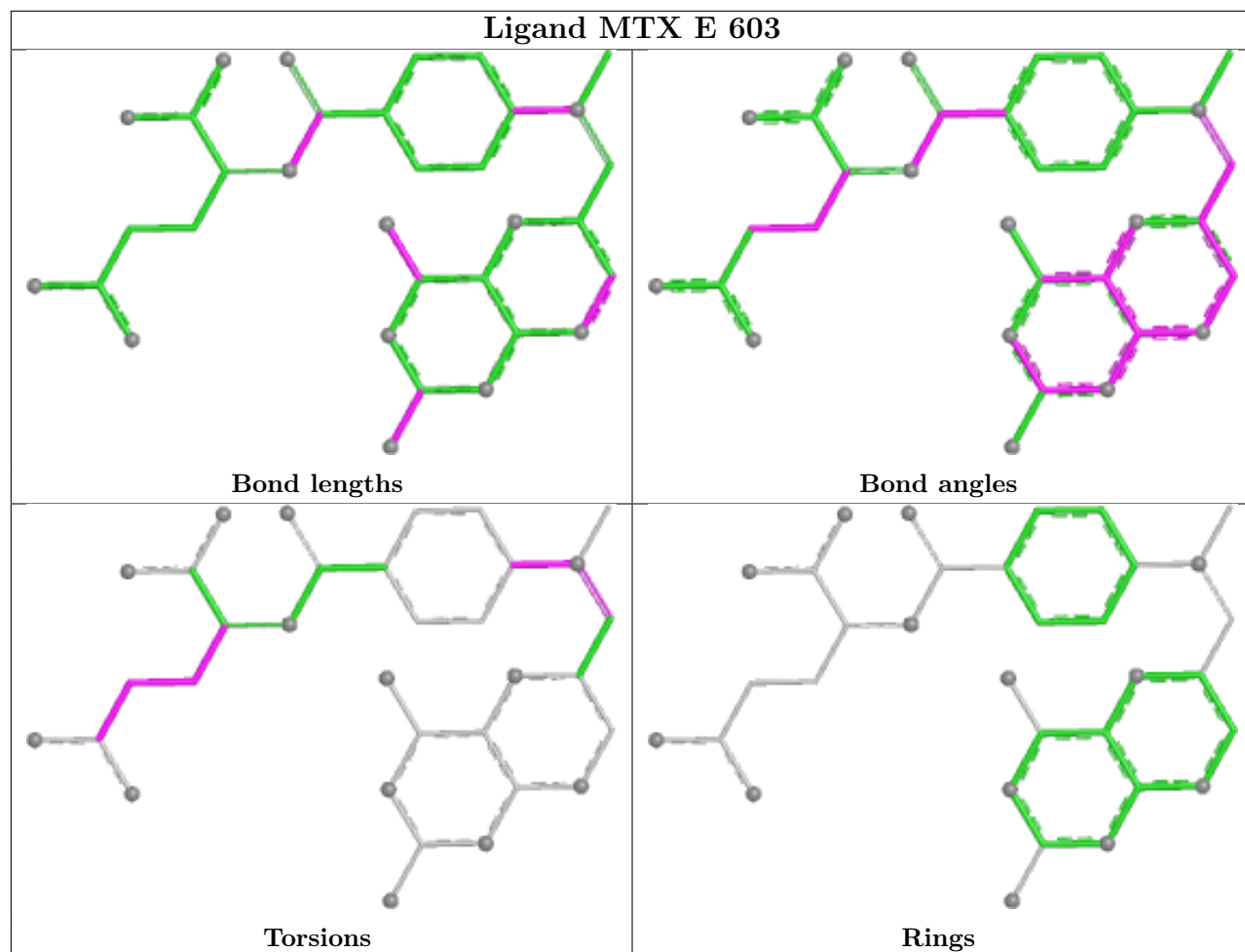


Ligand 1UF E 604

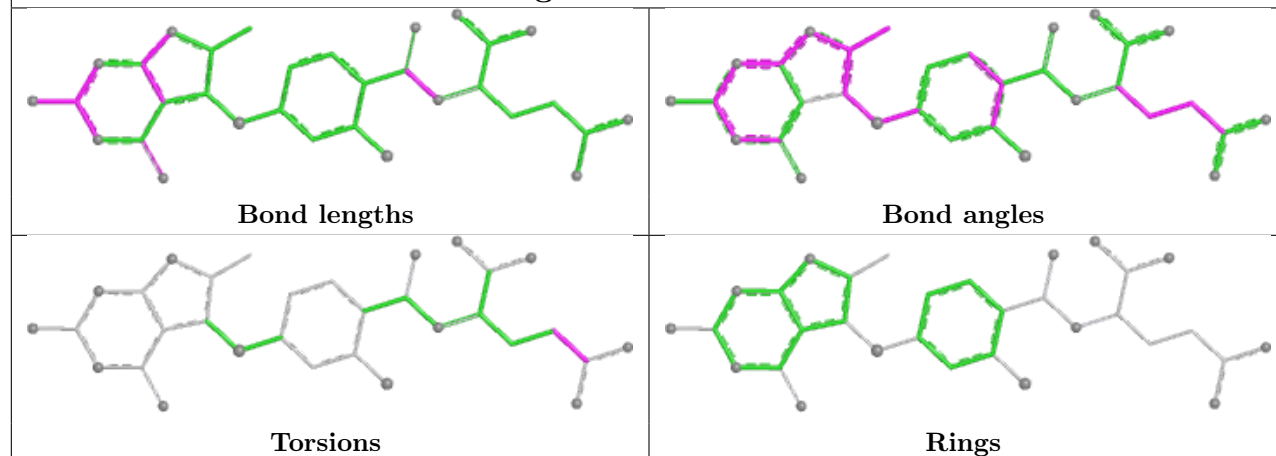


Ligand NDP C 601

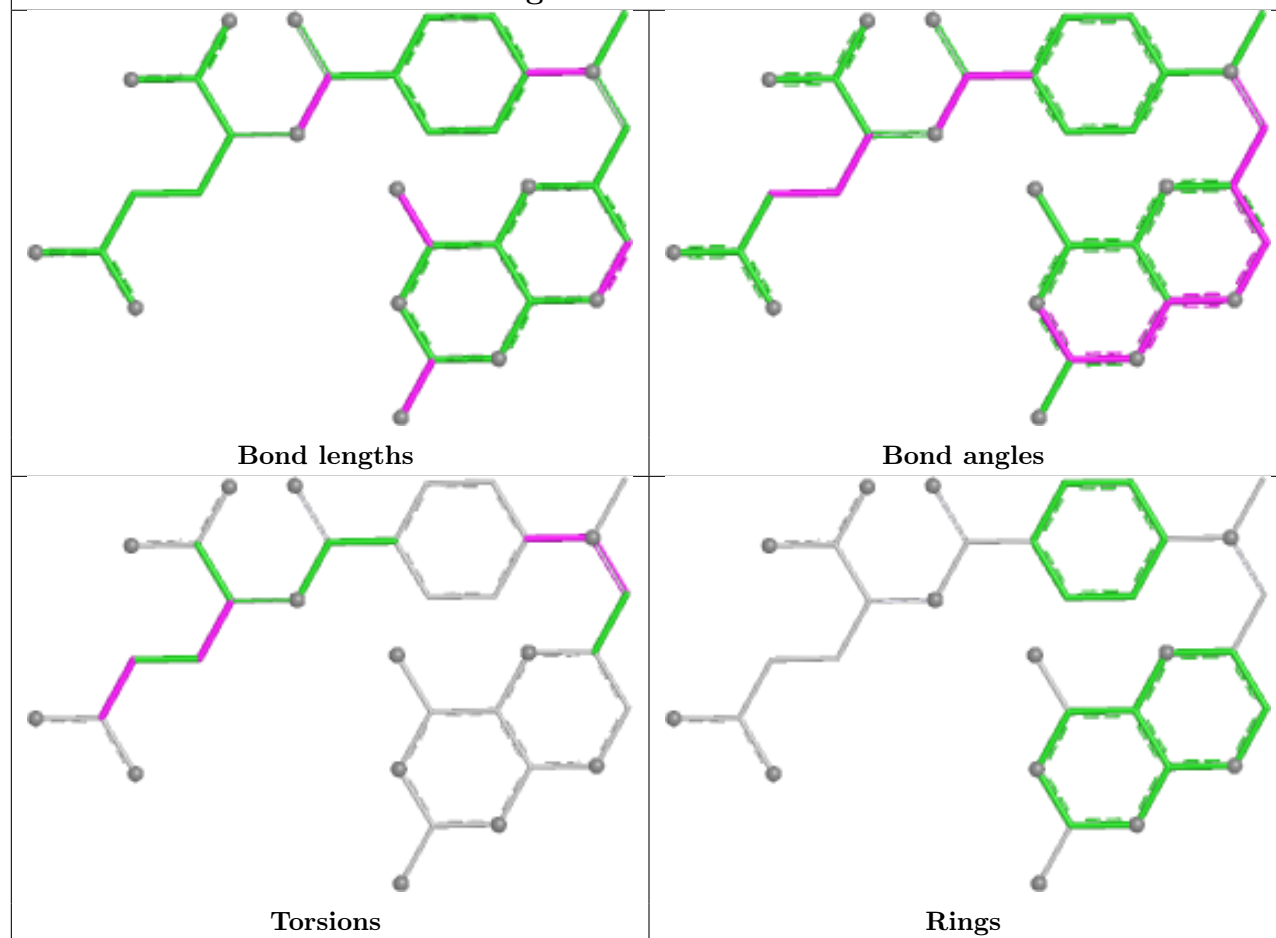


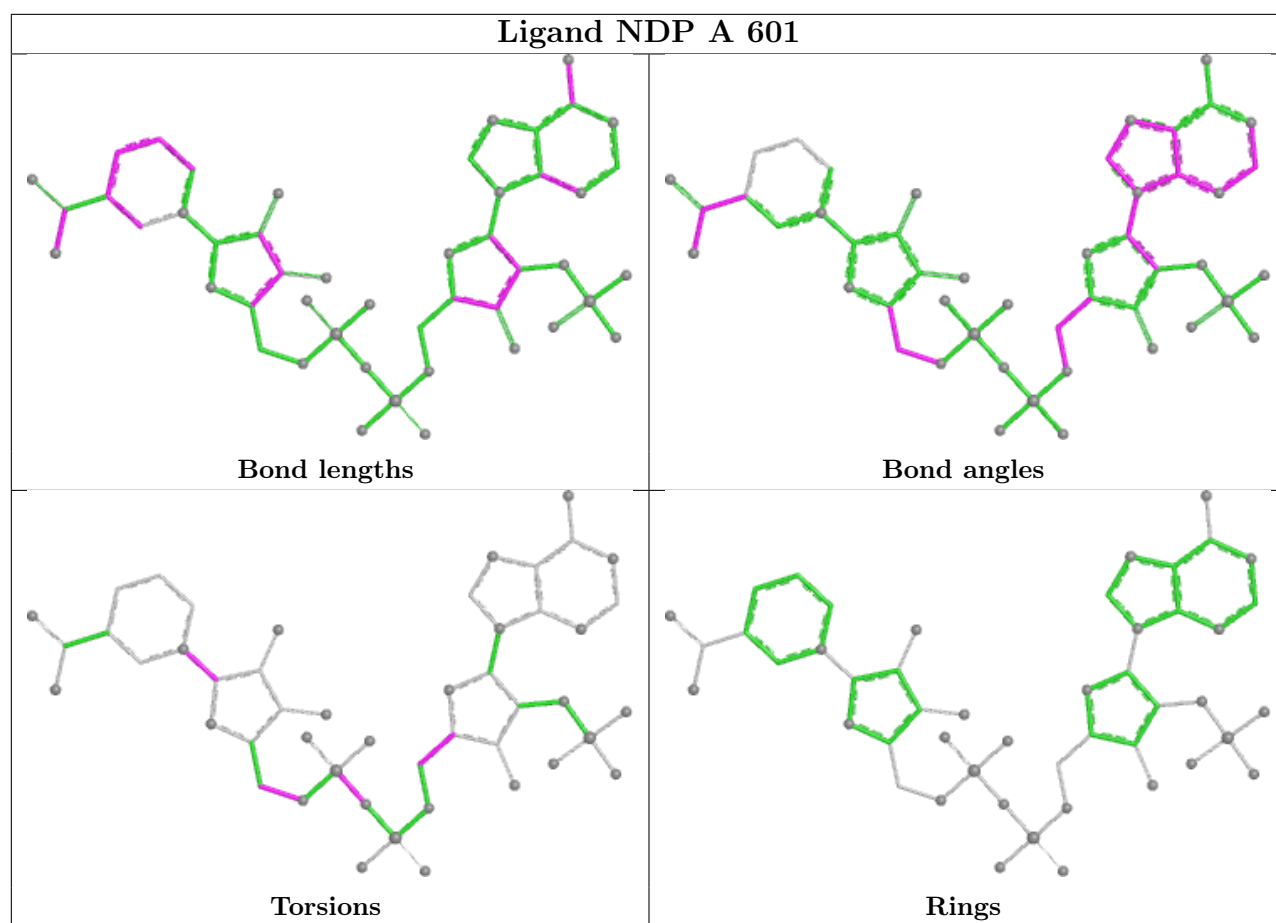


Ligand 1UF A 604



Ligand MTX A 603





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	505/521 (96%)	0.23	16 (3%)	50	28	43, 70, 109, 201	0
1	B	505/521 (96%)	0.35	27 (5%)	32	16	45, 75, 112, 188	0
1	C	505/521 (96%)	0.28	18 (3%)	46	26	40, 83, 124, 205	0
1	D	505/521 (96%)	0.33	17 (3%)	48	27	52, 85, 127, 194	0
1	E	505/521 (96%)	0.44	26 (5%)	33	17	62, 105, 146, 186	0
All	All	2525/2605 (96%)	0.33	104 (4%)	41	22	40, 83, 132, 205	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	6.7
1	B	193	LEU	5.2
1	A	343	GLY	4.9
1	B	113	CYS	4.7
1	B	438	TYR	4.4
1	E	437	SER	4.3
1	C	113	CYS	4.2
1	B	51	ALA	4.1
1	D	437	SER	4.0
1	E	113	CYS	4.0
1	C	193	LEU	4.0
1	E	380	LYS	3.7
1	E	255	GLU	3.7
1	E	162	THR	3.6
1	E	193	LEU	3.6
1	D	113	CYS	3.5
1	D	380	LYS	3.5
1	B	343	GLY	3.5
1	D	193	LEU	3.4
1	B	380	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	437	SER	3.3
1	D	101	LEU	3.2
1	C	175	PHE	3.2
1	D	438	TYR	3.1
1	E	279	PRO	3.1
1	E	342	TYR	3.1
1	E	248	LEU	3.0
1	E	49	LYS	3.0
1	C	342	TYR	3.0
1	E	32	ASP	3.0
1	E	178	GLN	3.0
1	E	175	PHE	2.9
1	C	100	ASN	2.9
1	B	422	GLN	2.9
1	C	82	ASP	2.8
1	B	255	GLU	2.8
1	A	82	ASP	2.8
1	D	255	GLU	2.8
1	B	171	ASP	2.7
1	B	178	GLN	2.7
1	E	322	LYS	2.7
1	B	140	ASP	2.7
1	D	377	ASN	2.7
1	C	178	GLN	2.7
1	C	133	LEU	2.7
1	A	99	GLU	2.6
1	E	438	TYR	2.6
1	B	28	SER	2.6
1	B	318	GLY	2.5
1	E	97	SER	2.5
1	C	476	GLN	2.5
1	A	97	SER	2.5
1	C	322	LYS	2.5
1	E	363	VAL	2.5
1	B	406	SER	2.4
1	A	100	ASN	2.4
1	B	100	ASN	2.4
1	A	322	LYS	2.4
1	D	343	GLY	2.4
1	E	101	LEU	2.4
1	A	428	GLY	2.4
1	B	457	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	521	VAL	2.4
1	E	514	THR	2.3
1	D	82	ASP	2.3
1	D	178	GLN	2.3
1	B	61	SER	2.3
1	C	28	SER	2.3
1	C	389	TRP	2.3
1	C	489	PHE	2.3
1	A	386	LEU	2.2
1	E	316	TRP	2.2
1	B	112	VAL	2.2
1	B	101	LEU	2.2
1	A	404	VAL	2.2
1	D	21	ILE	2.2
1	B	133	LEU	2.2
1	A	113	CYS	2.2
1	C	273	ASP	2.2
1	A	342	TYR	2.2
1	E	379	PRO	2.2
1	D	273	ASP	2.2
1	E	280	LEU	2.1
1	B	82	ASP	2.1
1	A	101	LEU	2.1
1	B	301	GLY	2.1
1	A	171	ASP	2.1
1	D	171	ASP	2.1
1	C	255	GLU	2.1
1	C	508	GLY	2.1
1	E	389	TRP	2.1
1	D	240	TYR	2.1
1	B	34	LYS	2.0
1	A	28	SER	2.0
1	A	406	SER	2.0
1	E	28	SER	2.0
1	C	380	LYS	2.0
1	E	99	GLU	2.0
1	D	288	ILE	2.0
1	E	100	ASN	2.0
1	B	342	TYR	2.0
1	B	279	PRO	2.0
1	B	420	LEU	2.0
1	D	209	ILE	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](#)

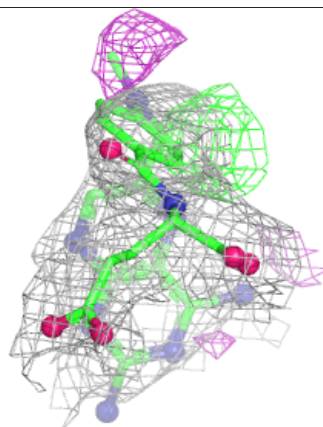
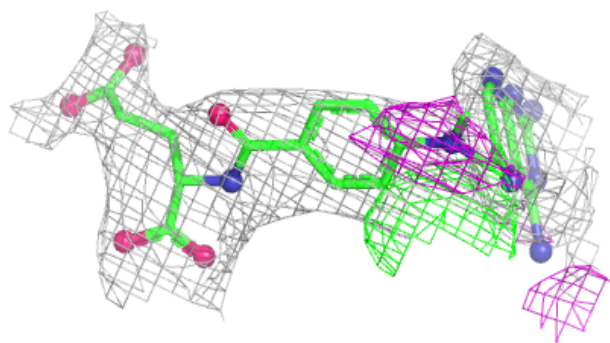
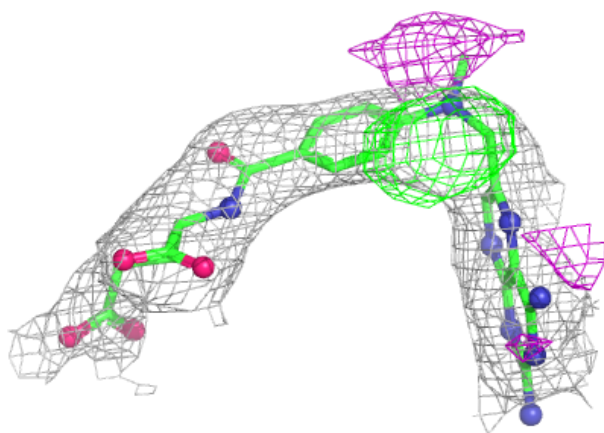
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MTX	B	603	33/33	0.79	0.15	62,69,89,91	0
5	1UF	E	604	32/32	0.79	0.12	135,143,160,170	0
5	1UF	B	604	32/32	0.80	0.12	86,94,111,121	0
5	1UF	D	604	32/32	0.82	0.13	109,117,135,145	0
4	MTX	D	603	33/33	0.84	0.16	78,85,106,108	0
4	MTX	C	603	33/33	0.85	0.18	88,95,115,118	0
3	UFP	B	602	21/21	0.85	0.12	73,82,90,108	0
4	MTX	E	603	33/33	0.85	0.16	93,101,121,123	0
4	MTX	A	603	33/33	0.88	0.13	64,71,91,94	0
5	1UF	C	604	32/32	0.89	0.11	84,92,109,119	0
5	1UF	A	604	32/32	0.89	0.10	77,85,102,112	0
3	UFP	D	602	21/21	0.89	0.10	84,94,102,120	0
3	UFP	A	602	21/21	0.90	0.11	69,79,87,105	0
3	UFP	E	602	21/21	0.90	0.11	112,122,129,147	0
2	NDP	C	601	48/48	0.90	0.09	88,100,104,109	0
3	UFP	C	602	21/21	0.90	0.12	72,82,90,108	0
2	NDP	D	601	48/48	0.92	0.09	80,91,95,100	0
2	NDP	E	601	48/48	0.93	0.08	92,103,107,113	0
2	NDP	B	601	48/48	0.93	0.08	57,69,73,78	0
2	NDP	A	601	48/48	0.94	0.08	62,74,78,83	0

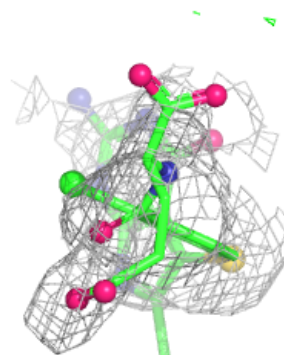
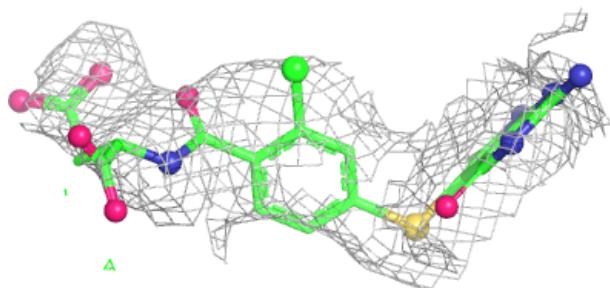
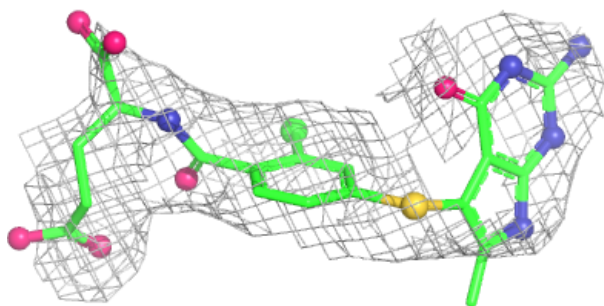
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MTX 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)

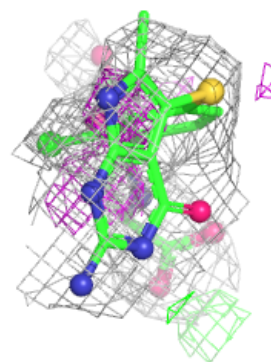
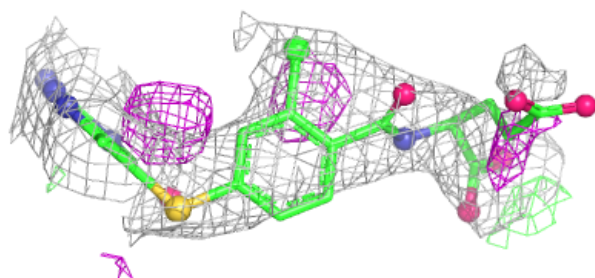
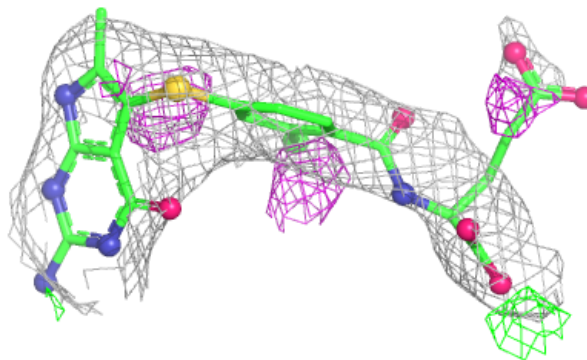
**Electron density around 1UF E 604:**

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

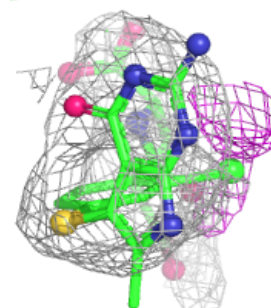
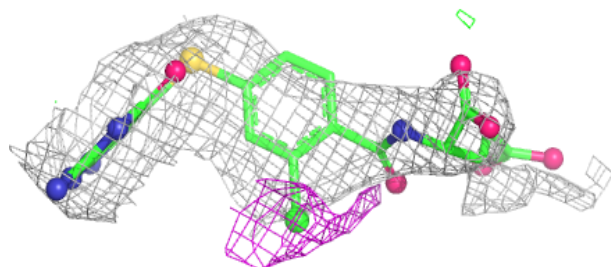
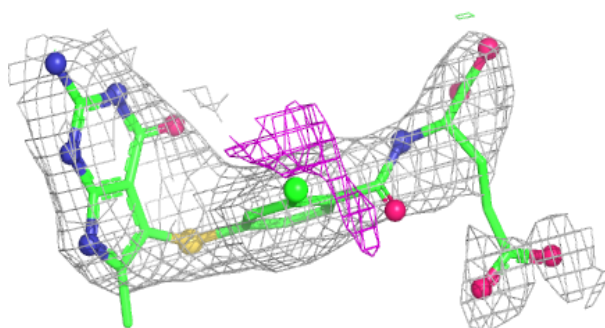


Electron density around 1UF B 604:

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

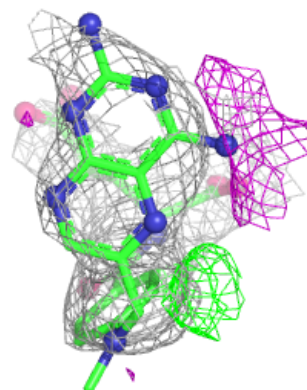
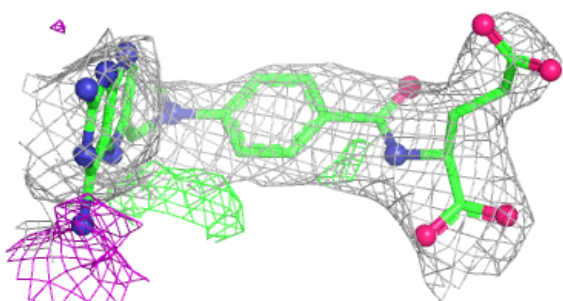
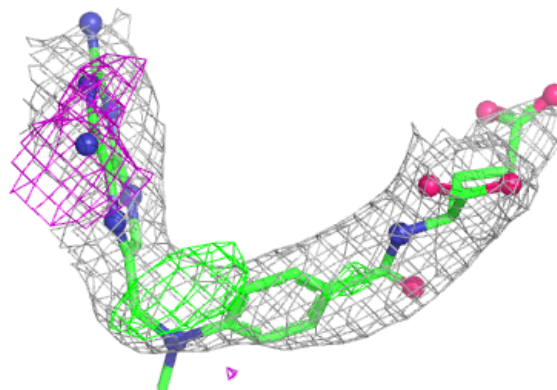
**Electron density around 1UF D 604:**

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

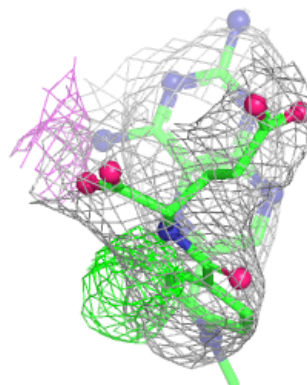
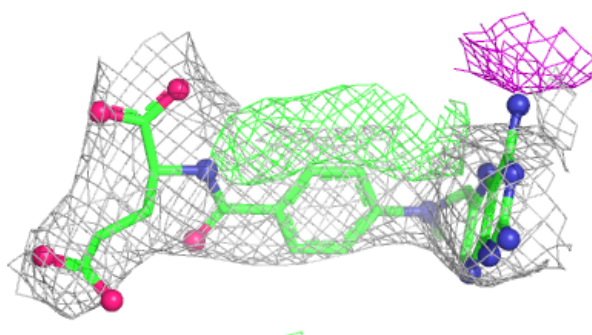
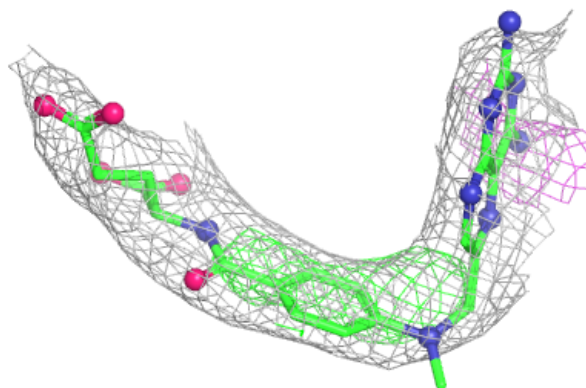


Electron density around MTX D 603:

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

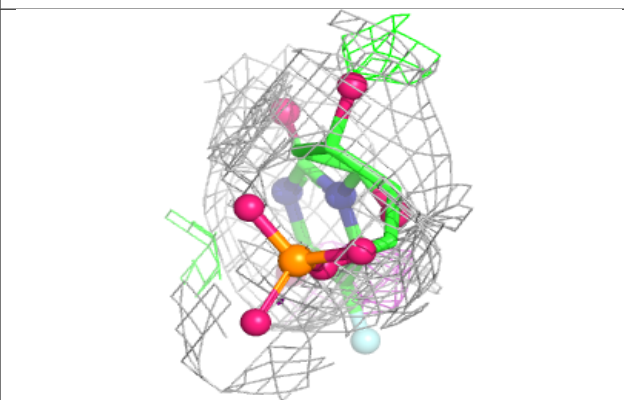
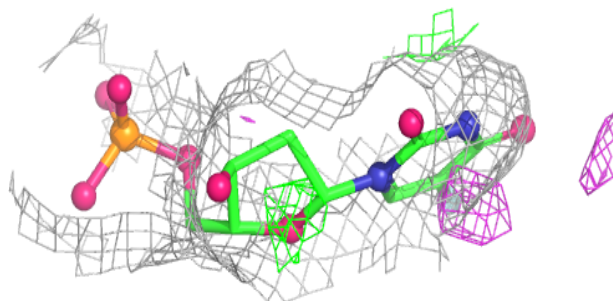
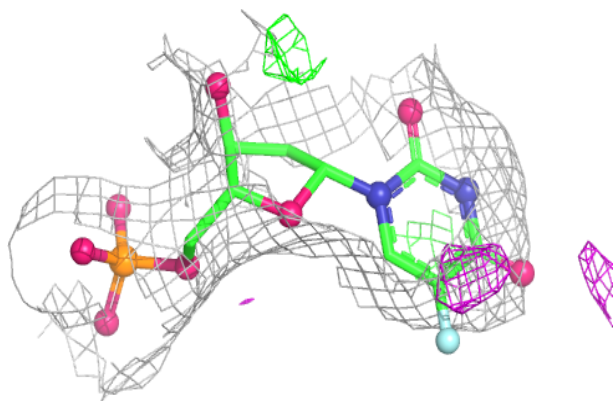
**Electron density around MTX C 603:**

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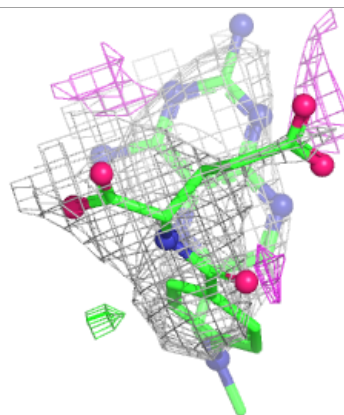
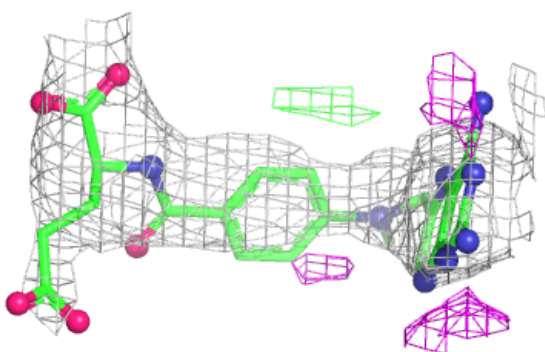
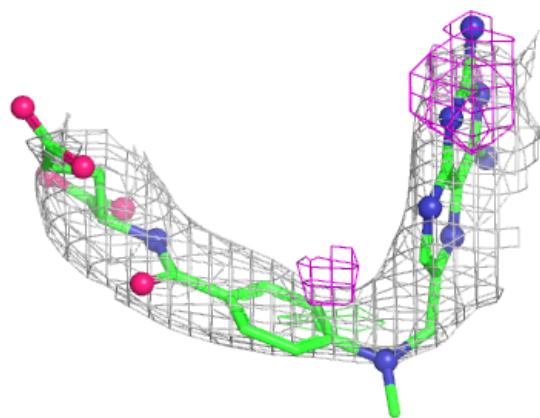


Electron density around UFP B 602:

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

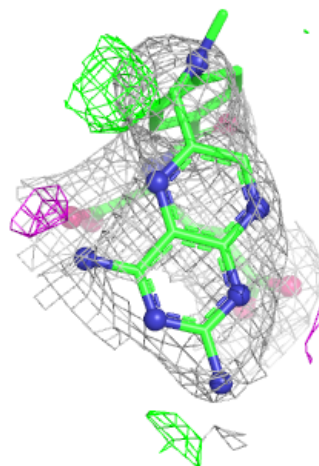
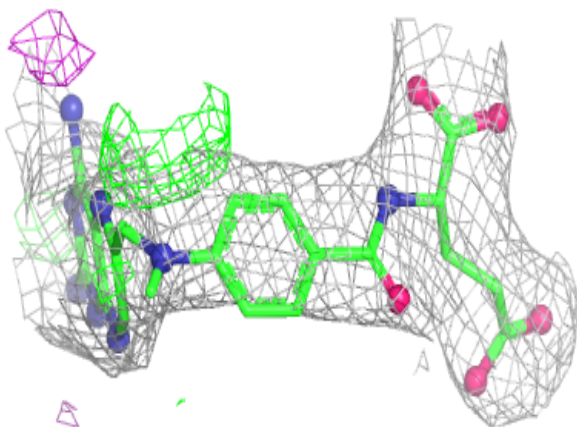
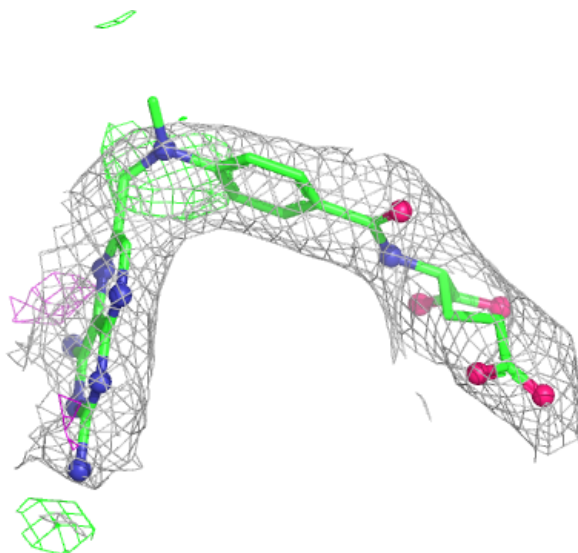
**Electron density around MTX E 603:**

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and green (positive)



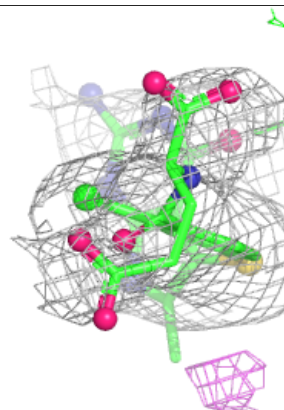
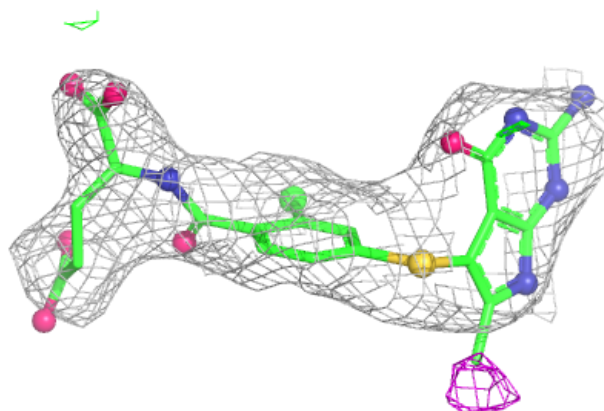
Electron density around MTX A 603:

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and green (positive)



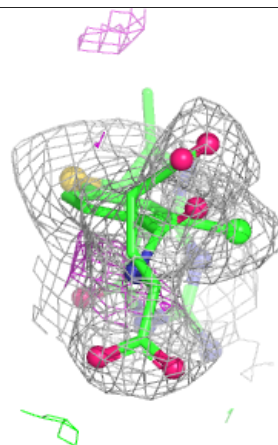
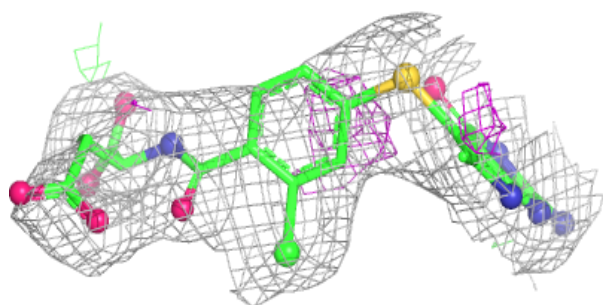
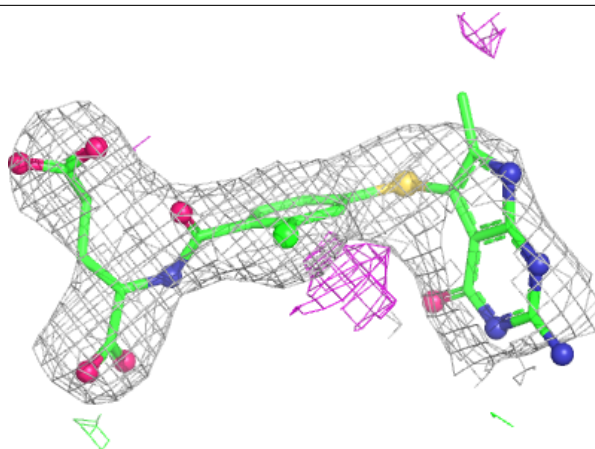
Electron density around 1UF C 604:

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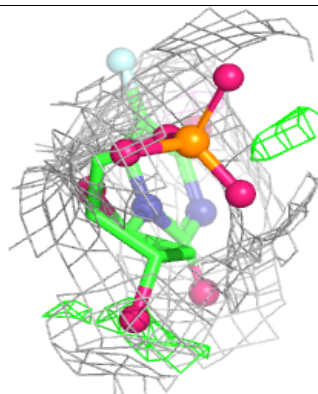
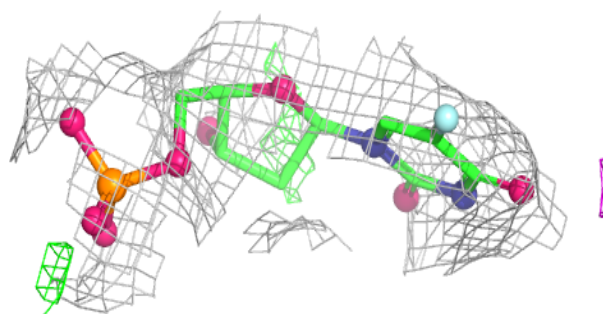
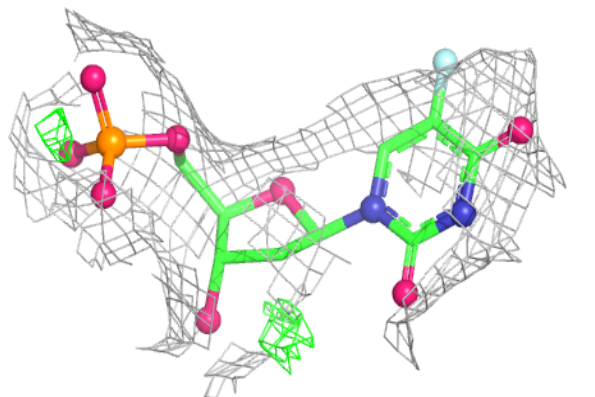


Electron density around 1UF A 604:

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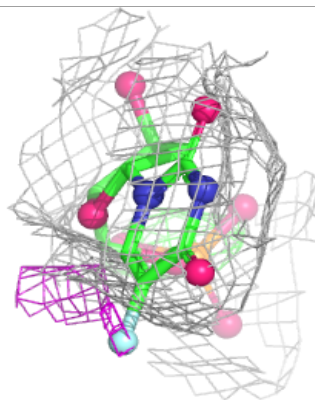
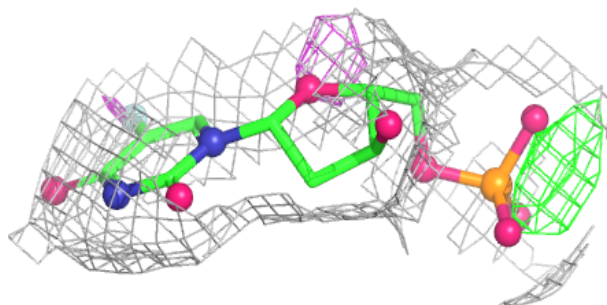
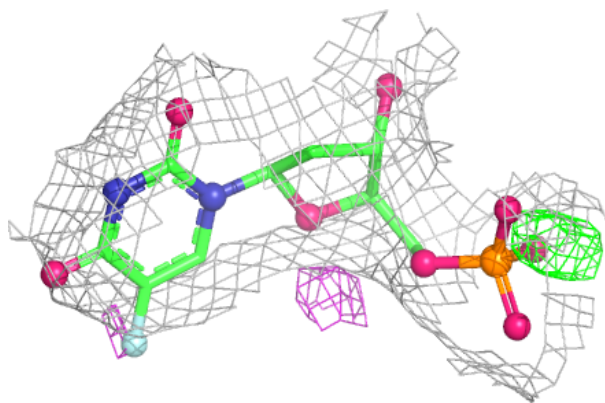
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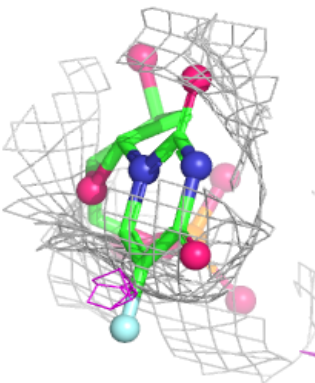
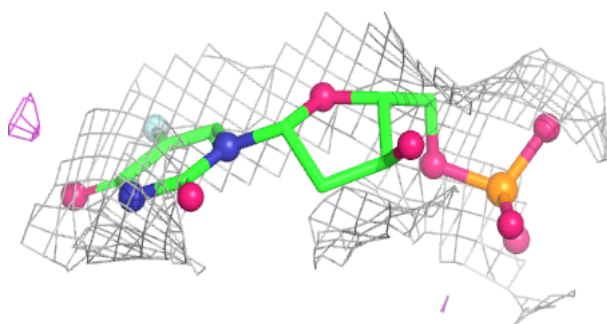
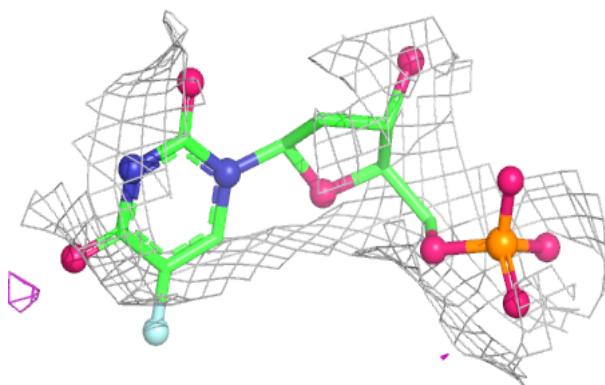


Electron density around UFP A 602:

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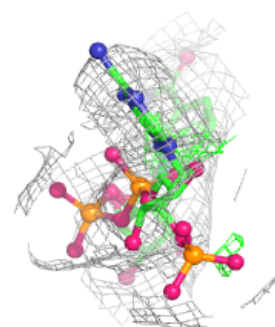
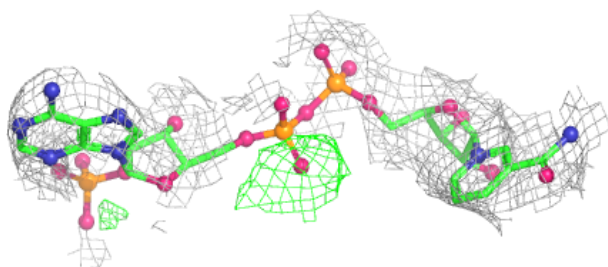
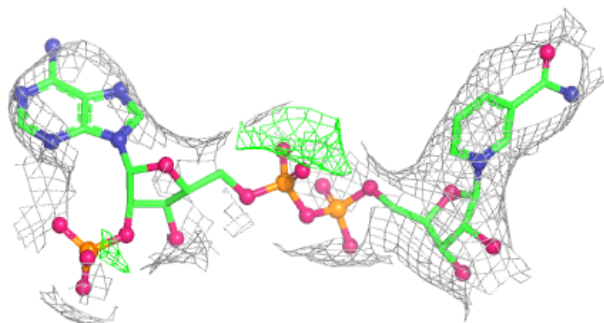
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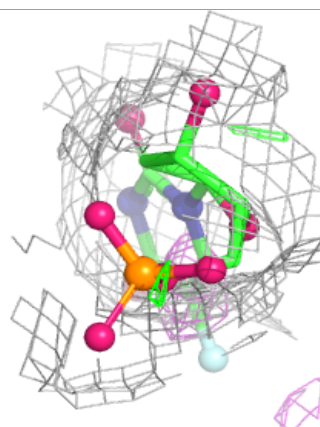
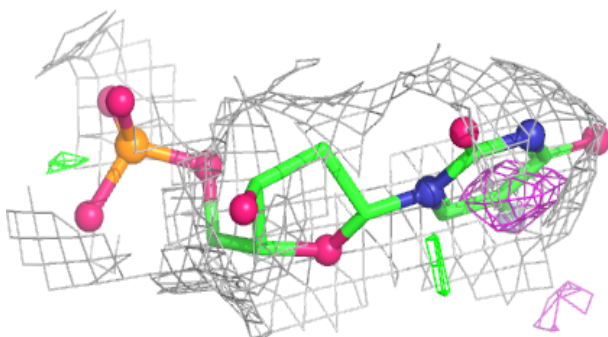
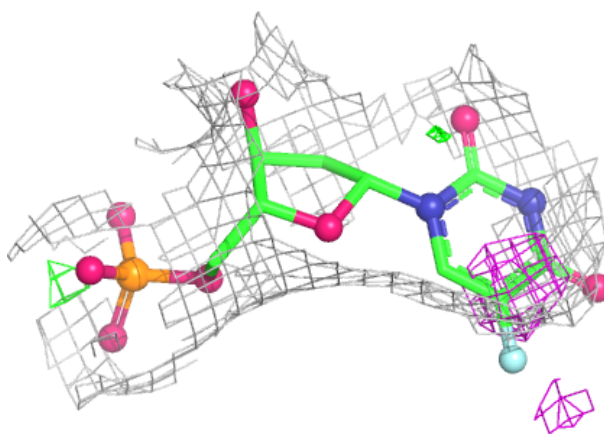


Electron density around NDP C 601:

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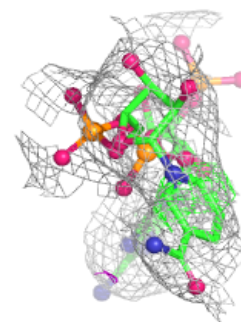
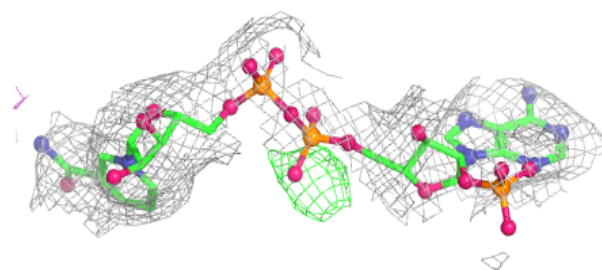
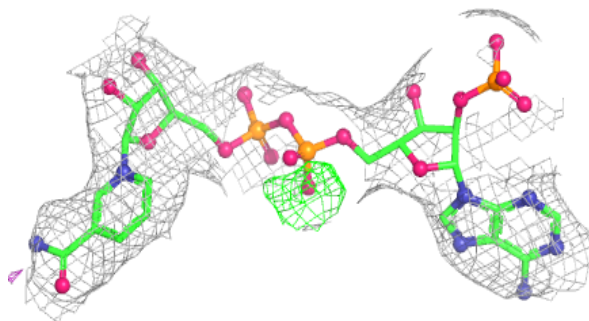
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and green (positive)

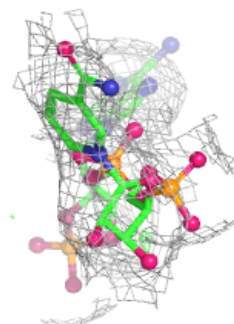
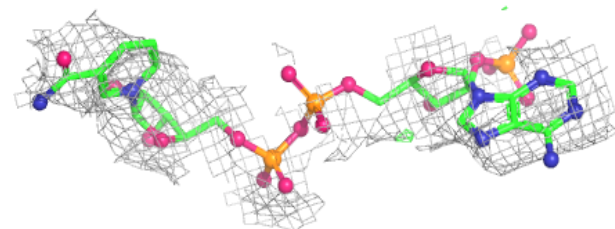
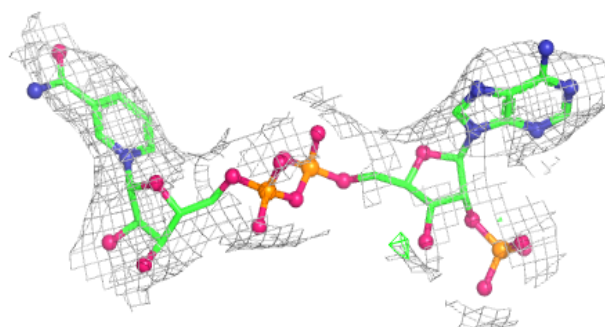


Electron density around NDP D 601:

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

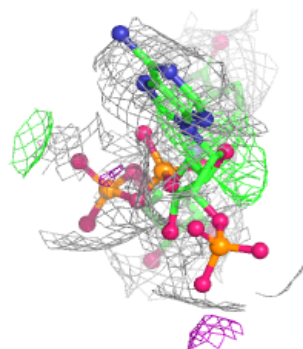
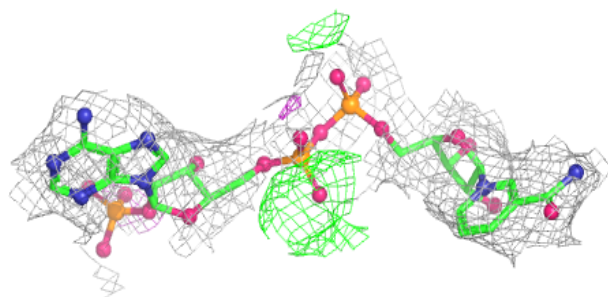
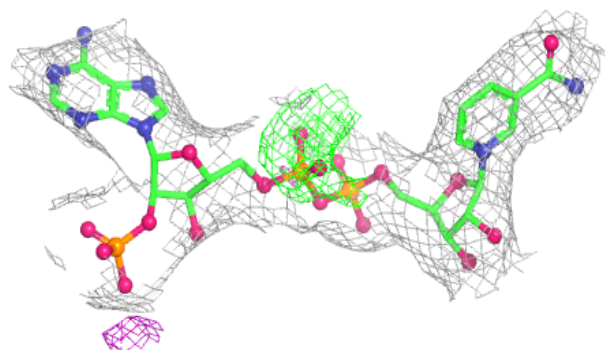
**Electron density around NDP E 601:**

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

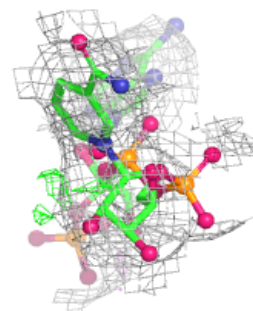
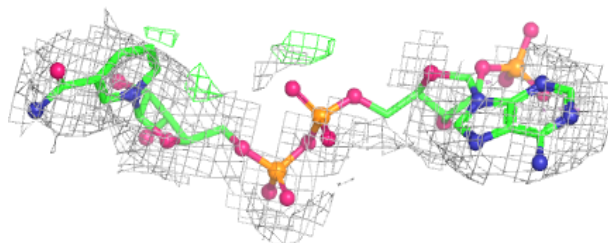
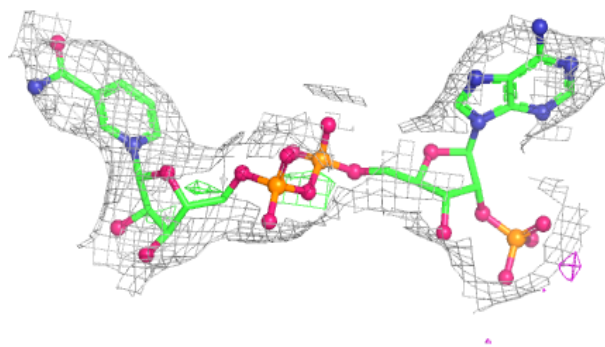


Electron density around NDP B 601:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.