



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 09:11 PM BST

PDB ID : 5X66  
Title : Human thymidylate synthase in complex with dUMP and methotrexate  
Authors : Chen, D.; Jansson, A.; Larsson, A.; Nordlund, P.  
Deposited on : 2017-02-21  
Resolution : 1.99 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

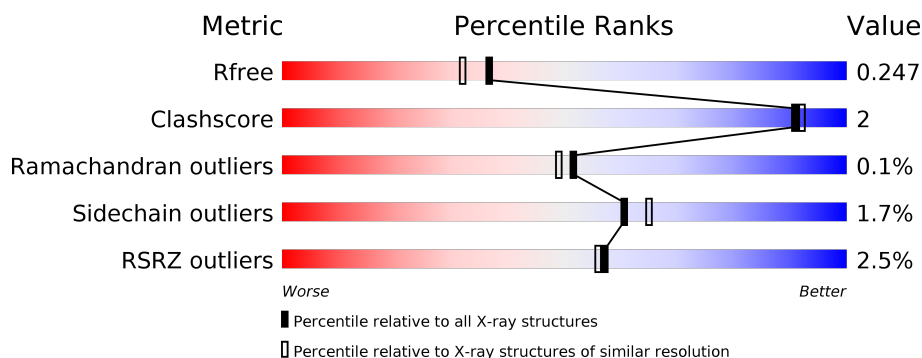
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	290	<div> <div>93%</div> <div>7% .</div> </div>
1	B	290	<div> <div>2%</div> <div>92%</div> <div>7% ..</div> </div>
1	C	290	<div> <div>2%</div> <div>91%</div> <div>7% ..</div> </div>
1	D	290	<div> <div>2%</div> <div>91%</div> <div>8% .</div> </div>
1	E	290	<div> <div>3%</div> <div>90%</div> <div>9% .</div> </div>
1	F	290	<div> <div>7%</div> <div>91%</div> <div>8% ..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15109 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.

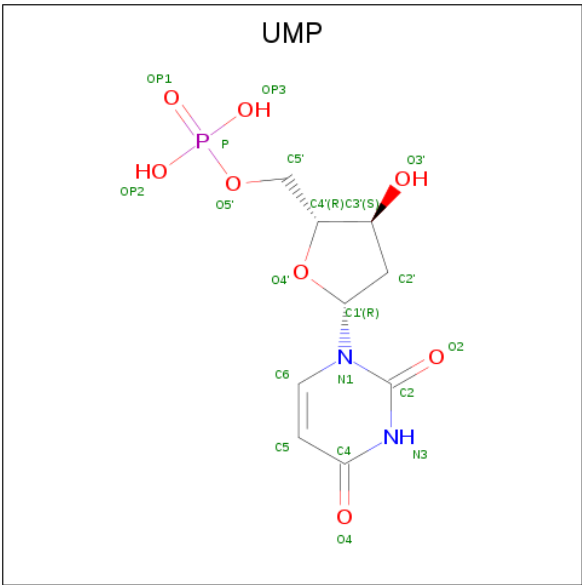
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2314	1480	403	418	13			
1	B	288	Total	C	N	O	S	0	0	0
			2310	1477	402	418	13			
1	C	288	Total	C	N	O	S	0	0	0
			2309	1478	400	418	13			
1	D	288	Total	C	N	O	S	0	0	0
			2312	1479	402	418	13			
1	E	287	Total	C	N	O	S	0	0	0
			2300	1471	399	417	13			
1	F	288	Total	C	N	O	S	0	1	0
			2312	1479	402	418	13			

There are 12 discrepancies between the modelled and reference sequences:

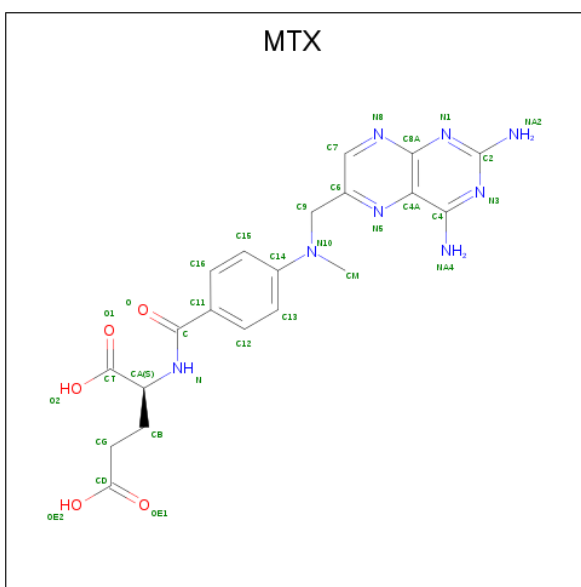
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP P04818
A	25	MET	-	expression tag	UNP P04818
B	24	SER	-	expression tag	UNP P04818
B	25	MET	-	expression tag	UNP P04818
C	24	SER	-	expression tag	UNP P04818
C	25	MET	-	expression tag	UNP P04818
D	24	SER	-	expression tag	UNP P04818
D	25	MET	-	expression tag	UNP P04818
E	24	SER	-	expression tag	UNP P04818
E	25	MET	-	expression tag	UNP P04818
F	24	SER	-	expression tag	UNP P04818
F	25	MET	-	expression tag	UNP P04818

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	F	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	200	Total	O	0	0
			200	200		
4	B	162	Total	O	0	0
			162	162		
4	C	131	Total	O	0	0
			131	131		
4	D	179	Total	O	0	0
			179	179		
4	E	150	Total	O	0	0
			150	150		
4	F	112	Total	O	0	0
			112	112		

### 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: Thymidylate synthase

Chain A: 




- Molecule 1: Thymidylate synthase

Chain B: 




- Molecule 1: Thymidylate synthase

Chain C: 




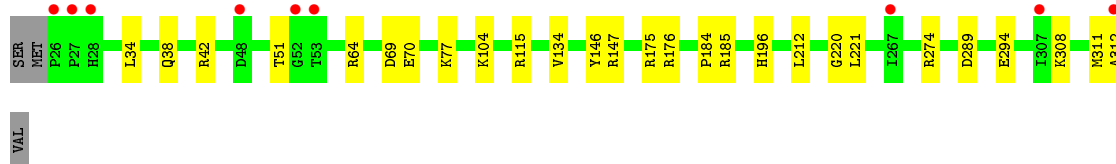
- Molecule 1: Thymidylate synthase

Chain D: 

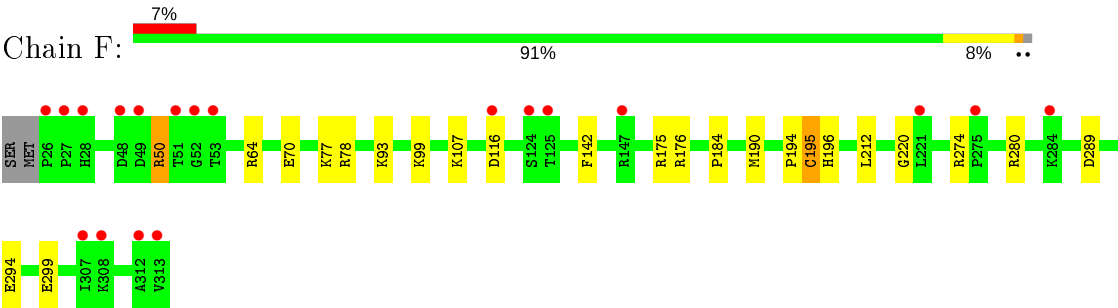


- Molecule 1: Thymidylate synthase

Chain E: 



● Molecule 1: Thymidylate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.20 Å 109.20 Å 317.12 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.18 – 1.99 25.18 – 1.99	Depositor EDS
% Data completeness (in resolution range)	91.3 (25.18-1.99) 91.4 (25.18-1.99)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 1.99 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.201 , 0.238 0.211 , 0.247	Depositor DCC
$R_{free}$ test set	6034 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.58$ , $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4125e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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, UMP

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	0.91	2/2374 (0.1%)	0.99	9/3213 (0.3%)
1	B	0.85	0/2370	0.98	14/3209 (0.4%)
1	C	0.87	1/2369 (0.0%)	0.93	6/3207 (0.2%)
1	D	0.90	0/2372	0.94	10/3211 (0.3%)
1	E	0.86	4/2360 (0.2%)	0.94	8/3195 (0.3%)
1	F	0.85	1/2372 (0.0%)	0.98	12/3212 (0.4%)
All	All	0.87	8/14217 (0.1%)	0.96	59/19247 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	175	ARG	CD-NE	-6.59	1.35	1.46
1	E	146	TYR	C-O	-6.07	1.11	1.23
1	A	175	ARG	CD-NE	-5.90	1.36	1.46
1	E	70	GLU	CD-OE2	-5.65	1.19	1.25
1	F	195	CYS	CB-SG	-5.63	1.72	1.81
1	E	294	GLU	CD-OE2	-5.14	1.20	1.25
1	C	32	GLN	CG-CD	-5.11	1.39	1.51
1	A	145	GLU	CD-OE1	5.08	1.31	1.25

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	115	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	E	175	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	E	115	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	A	115	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	C	175	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	A	175	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	A	115	ARG	NE-CZ-NH1	8.22	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	F	116	ASP	CB-CG-OD1	8.05	125.55	118.30
1	B	115	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	B	175	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	D	50	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	F	175	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	F	116	ASP	OD1-CG-OD2	-6.96	110.07	123.30
1	B	294	GLU	OE1-CD-OE2	6.78	131.44	123.30
1	F	78	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	F	116	ASP	CB-CG-OD2	6.75	124.38	118.30
1	D	78	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	F	70	GLU	OE1-CD-OE2	-6.50	115.50	123.30
1	D	175	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	F	93	LYS	CA-CB-CG	6.43	127.55	113.40
1	B	175	ARG	CB-CG-CD	-6.34	95.12	111.60
1	E	175	ARG	CB-CG-CD	-6.32	95.18	111.60
1	B	294	GLU	CG-CD-OE2	-6.18	105.94	118.30
1	C	294	GLU	CG-CD-OE2	6.12	130.55	118.30
1	C	175	ARG	CB-CG-CD	-6.07	95.83	111.60
1	D	185	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	D	294	GLU	CG-CD-OE2	5.99	130.28	118.30
1	D	274	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	294	GLU	CG-CD-OE2	5.88	130.07	118.30
1	A	50	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	175	ARG	CB-CG-CD	-5.83	96.43	111.60
1	F	175	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	116	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	B	185	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	E	64	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	70	GLU	OE1-CD-OE2	-5.68	116.48	123.30
1	C	176	ARG	CB-CG-CD	5.63	126.25	111.60
1	E	274	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	236	MET	CG-SD-CE	5.62	109.19	100.20
1	D	185	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	F	93	LYS	CB-CA-C	-5.61	99.18	110.40
1	D	64	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	274	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C	64	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	D	192	LEU	CA-CB-CG	5.39	127.69	115.30
1	B	64	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	F	64	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	271	ARG	NE-CZ-NH2	-5.29	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	42	ARG	CG-CD-NE	5.28	122.89	111.80
1	A	126	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	292	LYS	CD-CE-NZ	5.20	123.67	111.70
1	B	32	GLN	CA-CB-CG	5.19	124.82	113.40
1	A	175	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	F	294	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	F	274	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	274	ARG	CA-CB-CG	-5.12	102.13	113.40
1	E	69	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	E	294	GLU	CG-CD-OE2	-5.04	108.21	118.30

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	2314	0	2275	5	0
1	B	2310	0	2264	5	0
1	C	2309	0	2266	11	0
1	D	2312	0	2268	7	0
1	E	2300	0	2253	11	0
1	F	2312	0	2261	11	0
2	A	20	0	10	0	0
2	B	20	0	11	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	3	0
3	A	33	0	19	0	0
3	B	33	0	21	0	0
3	C	33	0	20	2	0
3	D	33	0	20	1	0
3	E	33	0	20	2	0
3	F	33	0	21	0	0
4	A	200	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	162	0	0	0	0
4	C	131	0	0	2	0
4	D	179	0	0	0	0
4	E	150	0	0	4	0
4	F	112	0	0	3	0
All	All	15109	0	13769	48	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 2.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:THR:HG21	1:E:312:ALA:HB1	1.57	0.87
1:C:176:ARG:NH1	2:F:401:UMP:OP1	2.13	0.80
1:C:196:HIS:HB3	1:C:212:LEU:HD11	1.64	0.78
1:D:80:PHE:CD2	3:D:402:MTX:HA	2.30	0.67
1:F:99:LYS:HE2	4:F:512:HOH:O	1.95	0.65
1:E:196:HIS:HB3	1:E:212:LEU:HD11	1.78	0.65
3:E:402:MTX:HG2	3:E:402:MTX:O1	1.98	0.64
1:A:107:LYS:CD	4:A:582:HOH:O	2.45	0.64
1:B:196:HIS:HB3	1:B:212:LEU:HD11	1.84	0.60
1:F:196:HIS:HB3	1:F:212:LEU:HD11	1.84	0.58
1:F:50:ARG:NH1	2:F:401:UMP:OP2	2.35	0.58
1:C:104:LYS:HE2	4:C:502:HOH:O	2.04	0.57
1:A:196:HIS:HB3	1:A:212:LEU:HD11	1.87	0.57
1:D:196:HIS:HB3	1:D:212:LEU:HD11	1.85	0.56
1:E:185:ARG:NH2	4:E:502:HOH:O	2.40	0.54
1:E:308:LYS:O	4:E:501:HOH:O	2.19	0.53
1:F:99:LYS:NZ	4:F:502:HOH:O	2.44	0.51
1:E:221:LEU:CD2	1:E:311:MET:HG3	2.41	0.50
1:C:142:PHE:CZ	1:F:184:PRO:HD2	2.47	0.50
1:C:107:LYS:CD	4:C:549:HOH:O	2.58	0.50
1:C:184:PRO:HD2	1:F:142:PHE:CZ	2.47	0.49
1:C:51:THR:HB	1:C:313:VAL:HG22	1.94	0.49
1:C:77:LYS:NZ	1:C:220:GLY:O	2.47	0.48
1:F:77:LYS:NZ	1:F:220:GLY:O	2.47	0.48
1:F:280:ARG:NH2	1:F:299:GLU:CB	2.77	0.47
1:D:77:LYS:NZ	1:D:220:GLY:O	2.48	0.47
1:E:77:LYS:NZ	1:E:220:GLY:O	2.48	0.47
1:C:221:LEU:HD12	1:C:261:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HD2	1:D:142:PHE:CZ	2.51	0.46
1:B:221:LEU:HD11	1:B:309:MET:O	2.15	0.46
1:A:142:PHE:CZ	1:D:184:PRO:HD2	2.50	0.46
3:C:402:MTX:N	3:C:402:MTX:OE2	2.49	0.46
1:E:42:ARG:NH2	4:E:503:HOH:O	2.47	0.46
1:A:221:LEU:HD11	1:A:309:MET:O	2.16	0.46
1:E:104:LYS:HE2	4:E:512:HOH:O	2.16	0.45
1:E:312:ALA:HB2	3:E:402:MTX:HN22	1.80	0.45
1:D:221:LEU:HD11	1:D:309:MET:O	2.16	0.44
1:F:190:MET:SD	1:F:194:PRO:HD3	2.57	0.44
1:C:28:HIS:NE2	1:C:274:ARG:O	2.48	0.44
1:B:28:HIS:NE2	1:B:274:ARG:O	2.48	0.43
1:F:107:LYS:CD	4:F:520:HOH:O	2.65	0.42
1:E:34:LEU:O	1:E:38:GLN:HG3	2.19	0.42
1:B:77:LYS:NZ	1:B:220:GLY:O	2.52	0.41
1:D:190:MET:SD	1:D:194:PRO:HD3	2.60	0.41
1:F:50:ARG:HH12	2:F:401:UMP:P	2.42	0.41
3:C:402:MTX:HM1	3:C:402:MTX:H13	1.67	0.41
1:C:126:ARG:HG2	1:C:130:ASP:HB3	2.02	0.40
1:B:142:PHE:CZ	1:E:184:PRO:HD2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/290 (99%)	277 (97%)	9 (3%)	0	100	100
1	B	286/290 (99%)	277 (97%)	8 (3%)	1 (0%)	41	37
1	C	286/290 (99%)	277 (97%)	9 (3%)	0	100	100
1	D	286/290 (99%)	277 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	285/290 (98%)	276 (97%)	8 (3%)	1 (0%)	34	30
1	F	287/290 (99%)	278 (97%)	9 (3%)	0	100	100
All	All	1716/1740 (99%)	1662 (97%)	52 (3%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	134	VAL
1	B	134	VAL

### 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	248/253 (98%)	243 (98%)	5 (2%)	55	58
1	B	247/253 (98%)	244 (99%)	3 (1%)	71	76
1	C	247/253 (98%)	241 (98%)	6 (2%)	49	51
1	D	247/253 (98%)	243 (98%)	4 (2%)	62	67
1	E	246/253 (97%)	243 (99%)	3 (1%)	71	76
1	F	246/253 (97%)	242 (98%)	4 (2%)	62	67
All	All	1481/1518 (98%)	1456 (98%)	25 (2%)	60	65

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	147	ARG
1	A	176	ARG
1	A	289	ASP
1	A	313	VAL
1	B	147	ARG
1	B	289	ASP
1	B	294	GLU

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Mol	Chain	Res	Type
1	C	50	ARG
1	C	69	ASP
1	C	77	LYS
1	C	176	ARG
1	C	221	LEU
1	C	313	VAL
1	D	176	ARG
1	D	270	GLN
1	D	289	ASP
1	D	313	VAL
1	E	147	ARG
1	E	176	ARG
1	E	289	ASP
1	F	50	ARG
1	F	176	ARG
1	F	195	CYS
1	F	289	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	UMP	D	401	-	18,21,21	2.88	5 (27%)	21,31,31	2.37	4 (19%)
2	UMP	A	401	-	18,21,21	2.72	6 (33%)	21,31,31	1.78	2 (9%)
3	MTX	D	402	-	29,35,35	2.23	4 (13%)	38,49,49	4.61	15 (39%)
2	UMP	C	401	-	18,21,21	3.22	5 (27%)	21,31,31	2.36	3 (14%)
3	MTX	F	402	-	29,35,35	2.48	10 (34%)	38,49,49	2.23	11 (28%)
3	MTX	B	402	-	29,35,35	2.52	10 (34%)	38,49,49	2.26	11 (28%)
3	MTX	E	402	-	29,35,35	2.42	9 (31%)	38,49,49	2.70	16 (42%)
2	UMP	F	401	-	18,21,21	2.94	6 (33%)	21,31,31	2.30	3 (14%)
3	MTX	C	402	-	29,35,35	2.37	9 (31%)	38,49,49	2.82	17 (44%)
3	MTX	A	402	-	29,35,35	2.29	7 (24%)	38,49,49	2.71	7 (18%)
2	UMP	E	401	-	18,21,21	2.87	5 (27%)	21,31,31	2.23	5 (23%)
2	UMP	B	401	-	18,21,21	2.84	7 (38%)	21,31,31	1.55	3 (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	UMP	D	401	-	-	1/7/22/22	0/2/2/2
2	UMP	A	401	-	-	1/7/22/22	0/2/2/2
3	MTX	D	402	-	-	8/19/25/25	0/3/3/3
2	UMP	C	401	-	-	1/7/22/22	0/2/2/2
3	MTX	F	402	-	-	4/19/25/25	0/3/3/3
3	MTX	B	402	-	-	6/19/25/25	0/3/3/3
3	MTX	E	402	-	-	3/19/25/25	0/3/3/3
2	UMP	F	401	-	-	2/7/22/22	0/2/2/2
3	MTX	C	402	-	-	2/19/25/25	0/3/3/3
3	MTX	A	402	-	-	3/19/25/25	0/3/3/3
2	UMP	E	401	-	-	4/7/22/22	0/2/2/2
2	UMP	B	401	-	-	1/7/22/22	0/2/2/2

All (83) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	MTX	C-N	10.26	1.56	1.34
2	C	401	UMP	C6-N1	9.80	1.47	1.35
3	F	402	MTX	C-N	9.24	1.54	1.34
2	E	401	UMP	C6-N1	8.90	1.46	1.35
3	D	402	MTX	C-N	8.71	1.53	1.34
2	B	401	UMP	C6-N1	8.50	1.46	1.35
3	E	402	MTX	C-N	8.45	1.52	1.34
3	A	402	MTX	C-N	8.42	1.52	1.34
2	A	401	UMP	C6-N1	8.38	1.46	1.35
3	C	402	MTX	C-N	7.51	1.50	1.34
2	D	401	UMP	C6-N1	7.47	1.45	1.35
2	F	401	UMP	C6-N1	7.41	1.45	1.35
2	C	401	UMP	C4-N3	6.94	1.45	1.33
2	D	401	UMP	C4-N3	6.19	1.43	1.33
2	F	401	UMP	C4-N3	5.80	1.43	1.33
3	F	402	MTX	C2-NA2	5.50	1.44	1.33
3	D	402	MTX	C2-NA2	5.33	1.44	1.33
2	E	401	UMP	C4-N3	5.16	1.42	1.33
2	F	401	UMP	C6-C5	5.12	1.49	1.38
2	D	401	UMP	C2-N3	4.77	1.47	1.38
3	E	402	MTX	C2-NA2	4.57	1.43	1.33
3	E	402	MTX	CB-CA	-4.51	1.47	1.53
2	A	401	UMP	C4-N3	4.37	1.40	1.33
2	F	401	UMP	C2-N3	4.24	1.46	1.38
3	C	402	MTX	C2-NA2	4.13	1.42	1.33
2	B	401	UMP	C4-N3	4.11	1.40	1.33
2	D	401	UMP	C6-C5	3.97	1.46	1.38
3	A	402	MTX	C2-NA2	3.97	1.41	1.33
3	C	402	MTX	CB-CA	-3.82	1.48	1.53
2	C	401	UMP	C6-C5	3.74	1.46	1.38
2	E	401	UMP	C6-C5	3.69	1.46	1.38
3	B	402	MTX	C7-N8	3.64	1.37	1.31
2	B	401	UMP	C2-N3	3.62	1.45	1.38
2	A	401	UMP	C2'-C3'	-3.48	1.43	1.52
2	B	401	UMP	C1'-N1	-3.37	1.39	1.49
3	F	402	MTX	C7-C6	3.36	1.45	1.39
3	A	402	MTX	C7-C6	3.27	1.45	1.39
3	C	402	MTX	C12-C11	-3.24	1.33	1.39
3	E	402	MTX	C12-C11	-3.22	1.33	1.39
3	A	402	MTX	C7-N8	3.17	1.36	1.31
3	C	402	MTX	C4A-N5	-3.17	1.30	1.37
3	C	402	MTX	C8A-N1	-3.04	1.30	1.36
2	E	401	UMP	C2-N3	2.99	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	UMP	C2-N3	2.96	1.44	1.38
2	B	401	UMP	C2'-C3'	-2.96	1.45	1.52
3	B	402	MTX	CB-CA	-2.90	1.49	1.53
3	A	402	MTX	C6-N5	2.89	1.37	1.32
2	C	401	UMP	C2-N3	2.87	1.43	1.38
3	E	402	MTX	C4A-N5	-2.86	1.31	1.37
3	C	402	MTX	C13-C14	-2.85	1.33	1.39
3	B	402	MTX	C7-C6	2.85	1.44	1.39
3	E	402	MTX	C8A-N1	-2.84	1.31	1.36
2	F	401	UMP	C2'-C3'	-2.78	1.45	1.52
2	B	401	UMP	C6-C5	2.75	1.44	1.38
3	B	402	MTX	C2-NA2	2.71	1.39	1.33
3	A	402	MTX	C8A-N1	-2.62	1.31	1.36
3	F	402	MTX	C2-N3	2.59	1.40	1.35
3	B	402	MTX	C13-C12	2.55	1.43	1.38
2	A	401	UMP	C1'-N1	-2.49	1.42	1.49
3	F	402	MTX	C6-N5	2.47	1.36	1.32
3	F	402	MTX	C14-N10	2.45	1.46	1.39
3	B	402	MTX	C12-C11	-2.42	1.35	1.39
3	A	402	MTX	CA-N	2.41	1.49	1.46
3	E	402	MTX	CM-N10	-2.35	1.42	1.46
2	F	401	UMP	C1'-N1	-2.33	1.42	1.49
3	F	402	MTX	C8A-N8	2.31	1.40	1.37
2	C	401	UMP	C2'-C3'	-2.25	1.46	1.52
3	D	402	MTX	C6-N5	2.24	1.36	1.32
3	B	402	MTX	CA-N	2.24	1.49	1.46
3	B	402	MTX	C6-N5	2.20	1.36	1.32
2	D	401	UMP	C2'-C3'	-2.19	1.47	1.52
2	A	401	UMP	C6-C5	2.19	1.42	1.38
3	F	402	MTX	CA-N	2.19	1.49	1.46
3	C	402	MTX	CM-N10	-2.17	1.42	1.46
3	B	402	MTX	C4A-C8A	2.10	1.44	1.40
3	E	402	MTX	C13-C14	-2.09	1.35	1.39
3	C	402	MTX	C11-C	-2.07	1.45	1.50
3	F	402	MTX	C4-NA4	2.06	1.41	1.34
3	F	402	MTX	C15-C14	2.06	1.43	1.39
3	E	402	MTX	C16-C15	-2.05	1.35	1.38
2	B	401	UMP	O4'-C4'	-2.02	1.40	1.45
3	D	402	MTX	C12-C11	-2.02	1.35	1.39
2	E	401	UMP	C2'-C3'	-2.02	1.47	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	MTX	C11-C-N	16.96	149.58	117.06
3	D	402	MTX	CA-N-C	12.27	138.16	122.34
3	D	402	MTX	O-C-C11	-9.81	103.45	120.94
3	A	402	MTX	CB-CA-N	9.37	123.84	110.19
2	C	401	UMP	C2'-C1'-N1	8.99	135.00	114.27
3	C	402	MTX	C2-N1-C8A	8.98	125.61	115.36
3	D	402	MTX	O-C-N	-8.77	106.32	122.45
3	B	402	MTX	CA-N-C	8.44	133.22	122.34
3	A	402	MTX	CA-N-C	8.38	133.14	122.34
2	D	401	UMP	C2'-C1'-N1	8.35	133.52	114.27
2	F	401	UMP	C2'-C1'-N1	8.27	133.35	114.27
2	E	401	UMP	C2'-C1'-N1	7.56	131.71	114.27
3	E	402	MTX	C2-N1-C8A	7.28	123.67	115.36
3	A	402	MTX	CB-CG-CD	6.86	128.33	113.59
3	D	402	MTX	N8-C8A-N1	6.61	123.37	115.82
3	F	402	MTX	CA-N-C	6.26	130.41	122.34
3	D	402	MTX	CG-CB-CA	6.17	125.51	113.04
2	A	401	UMP	C2'-C1'-N1	5.99	128.08	114.27
3	C	402	MTX	C4A-C4-N3	-5.65	117.30	121.01
3	C	402	MTX	N1-C2-N3	-5.56	119.80	127.22
3	E	402	MTX	C11-C-N	5.30	127.23	117.06
3	F	402	MTX	CB-CG-CD	5.20	124.77	113.59
3	E	402	MTX	CG-CB-CA	5.13	123.40	113.04
3	B	402	MTX	C7-C6-N5	-5.05	117.55	120.85
3	A	402	MTX	C2-N1-C8A	5.05	121.12	115.36
3	E	402	MTX	N1-C2-N3	-4.95	120.62	127.22
3	F	402	MTX	N8-C8A-N1	4.84	121.35	115.82
2	B	401	UMP	C2'-C1'-N1	4.77	125.26	114.27
3	C	402	MTX	CA-N-C	-4.76	116.20	122.34
3	C	402	MTX	N8-C8A-N1	4.49	120.95	115.82
2	D	401	UMP	O5'-P-OP1	4.20	118.27	106.47
3	D	402	MTX	C7-C6-N5	-4.19	118.11	120.85
3	E	402	MTX	N8-C8A-N1	4.16	120.57	115.82
3	E	402	MTX	CB-CG-CD	4.15	122.50	113.59
2	E	401	UMP	O5'-P-OP1	4.14	118.09	106.47
3	E	402	MTX	NA2-C2-N3	4.11	123.64	117.25
3	D	402	MTX	C7-N8-C8A	4.02	120.73	116.69
2	C	401	UMP	P-O5'-C5'	3.99	129.27	118.30
3	F	402	MTX	C7-C6-N5	-3.59	118.50	120.85
3	B	402	MTX	N8-C8A-N1	3.57	119.90	115.82
2	F	401	UMP	P-O5'-C5'	3.33	127.48	118.30
3	F	402	MTX	CG-CB-CA	3.33	119.76	113.04
3	F	402	MTX	C4A-C4-N3	-3.31	118.84	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	MTX	O-C-N	-3.27	116.43	122.45
3	B	402	MTX	CG-CB-CA	3.27	119.64	113.04
3	E	402	MTX	C7-C6-N5	-3.20	118.76	120.85
3	C	402	MTX	CB-CG-CD	3.15	120.36	113.59
3	C	402	MTX	C4A-C8A-N1	-3.14	116.62	121.71
3	B	402	MTX	C2-N1-C8A	3.12	118.92	115.36
3	C	402	MTX	C4A-C4-NA4	3.07	125.02	120.35
3	A	402	MTX	N1-C2-N3	-3.07	123.13	127.22
3	C	402	MTX	C8A-C4A-N5	-3.06	118.71	122.41
3	C	402	MTX	NA2-C2-N3	3.02	121.95	117.25
3	D	402	MTX	CM-N10-C14	2.96	124.69	119.57
3	C	402	MTX	C4-C4A-N5	2.89	122.55	120.33
3	C	402	MTX	C11-C-N	2.88	122.59	117.06
3	D	402	MTX	CB-CG-CD	2.87	119.76	113.59
3	E	402	MTX	C4A-C4-N3	-2.82	119.16	121.01
2	F	401	UMP	OP2-P-OP1	2.81	121.70	110.68
3	D	402	MTX	C4-C4A-N5	-2.81	118.16	120.33
3	B	402	MTX	C7-N8-C8A	-2.80	113.88	116.69
2	E	401	UMP	O5'-C5'-C4'	2.69	118.25	108.99
3	E	402	MTX	C6-C7-N8	-2.66	120.52	123.13
2	E	401	UMP	P-O5'-C5'	2.65	125.60	118.30
2	D	401	UMP	P-O5'-C5'	2.62	125.51	118.30
3	E	402	MTX	C8A-C4A-N5	-2.61	119.26	122.41
3	A	402	MTX	C15-C14-N10	-2.61	117.87	121.62
3	E	402	MTX	O-C-C11	-2.60	116.30	120.94
2	B	401	UMP	P-O5'-C5'	2.57	125.38	118.30
3	F	402	MTX	C6-C9-N10	2.54	117.95	113.60
3	B	402	MTX	C6-C7-N8	2.48	125.56	123.13
2	C	401	UMP	C5-C4-N3	-2.46	117.90	123.31
3	F	402	MTX	C2-N1-C8A	2.45	118.15	115.36
3	C	402	MTX	CM-N10-C9	2.42	121.28	114.84
3	F	402	MTX	N1-C2-N3	-2.41	124.01	127.22
3	D	402	MTX	NA2-C2-N1	2.40	121.71	117.79
3	B	402	MTX	C15-C14-N10	-2.39	118.18	121.62
3	C	402	MTX	CG-CB-CA	2.35	117.79	113.04
3	C	402	MTX	O-C-N	-2.32	118.18	122.45
3	C	402	MTX	C6-C7-N8	-2.32	120.86	123.13
3	D	402	MTX	C6-C7-N8	-2.30	120.87	123.13
3	D	402	MTX	N1-C2-N3	-2.28	124.18	127.22
2	D	401	UMP	C6-N1-C2	2.27	124.80	121.20
3	E	402	MTX	C4A-C8A-N1	-2.22	118.12	121.71
3	B	402	MTX	O-C-N	2.21	126.52	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	MTX	C13-C14-N10	2.20	124.78	121.62
2	E	401	UMP	OP3-P-O5'	-2.16	100.98	106.73
3	E	402	MTX	C6-N5-C4A	2.16	121.53	118.04
3	C	402	MTX	C6-N5-C4A	2.15	121.52	118.04
3	F	402	MTX	C13-C12-C11	2.15	123.28	120.78
3	A	402	MTX	N8-C8A-N1	2.13	118.25	115.82
3	B	402	MTX	C15-C16-C11	2.10	123.22	120.78
2	B	401	UMP	C5-C4-N3	-2.09	118.71	123.31
3	F	402	MTX	C7-N8-C8A	2.07	118.78	116.69
3	E	402	MTX	CA-N-C	2.07	125.01	122.34
3	D	402	MTX	NA2-C2-N3	-2.05	114.06	117.25
2	A	401	UMP	P-O5'-C5'	2.01	123.82	118.30

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	402	MTX	CB-CA-N-C
3	B	402	MTX	CT-CA-N-C
3	B	402	MTX	CB-CA-N-C
3	E	402	MTX	CB-CA-N-C
3	A	402	MTX	CT-CA-N-C
3	A	402	MTX	CA-CB-CG-CD
3	D	402	MTX	O-C-N-CA
3	D	402	MTX	C11-C-N-CA
3	D	402	MTX	O-C-C11-C12
3	D	402	MTX	N-C-C11-C12
3	D	402	MTX	O-C-C11-C16
3	C	402	MTX	CA-CB-CG-CD
3	F	402	MTX	CA-CB-CG-CD
3	B	402	MTX	CA-CB-CG-CD
2	E	401	UMP	C3'-C4'-C5'-O5'
2	E	401	UMP	O4'-C4'-C5'-O5'
3	E	402	MTX	CT-CA-N-C
2	F	401	UMP	C5'-O5'-P-OP2
3	D	402	MTX	C6-C9-N10-CM
3	F	402	MTX	C6-C9-N10-CM
3	E	402	MTX	C6-C9-N10-CM
3	C	402	MTX	C6-C9-N10-CM
2	E	401	UMP	C5'-O5'-P-OP1
2	F	401	UMP	O4'-C4'-C5'-O5'
3	D	402	MTX	N-CA-CB-CG

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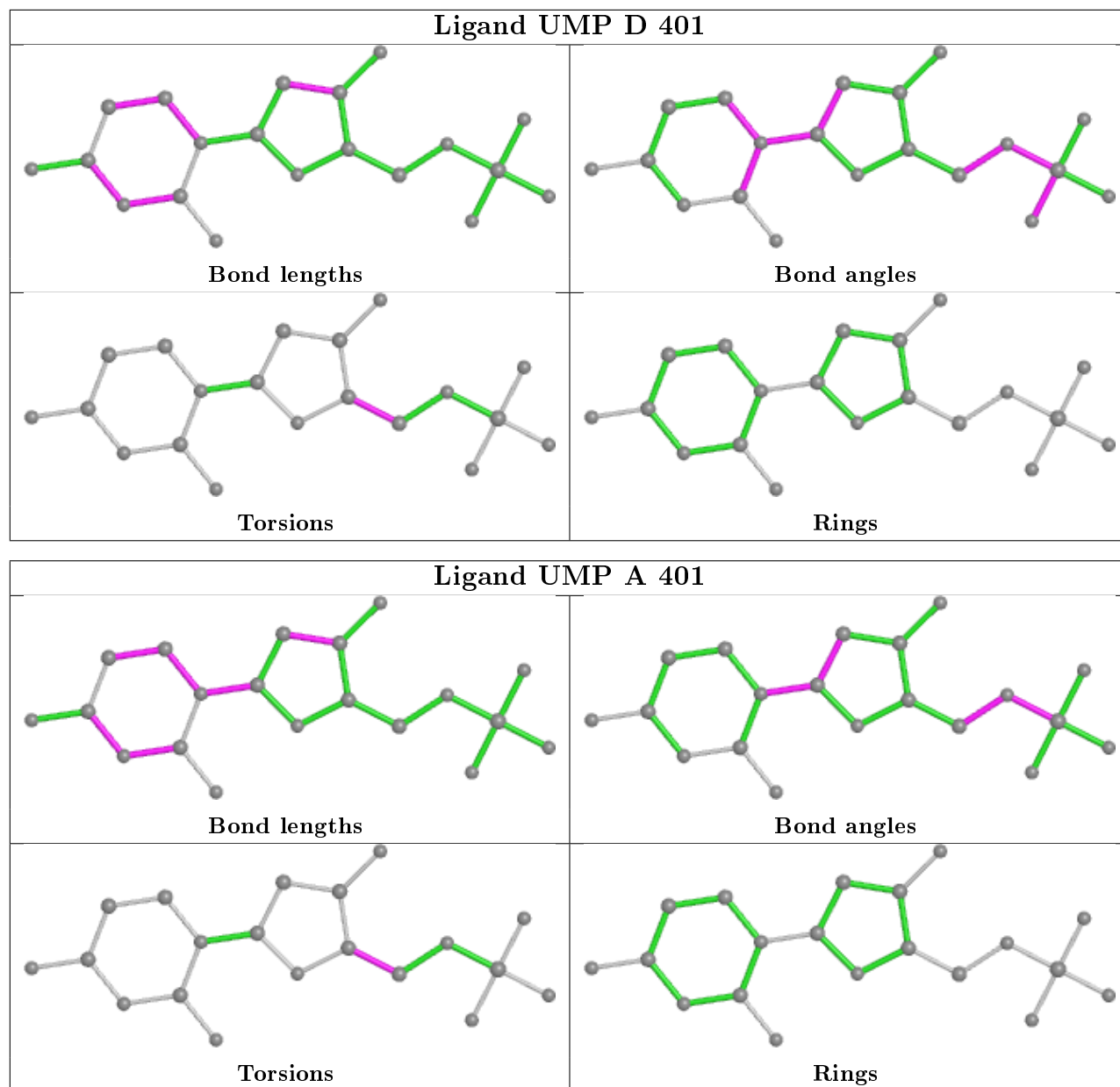
Mol	Chain	Res	Type	Atoms
3	A	402	MTX	N-CA-CB-CG
2	D	401	UMP	O4'-C4'-C5'-O5'
3	B	402	MTX	O-C-C11-C12
3	B	402	MTX	N-CA-CB-CG
2	E	401	UMP	C5'-O5'-P-OP2
3	D	402	MTX	N-C-C11-C16
2	C	401	UMP	O4'-C4'-C5'-O5'
3	F	402	MTX	C6-C9-N10-C14
3	B	402	MTX	N-C-C11-C12
2	A	401	UMP	O4'-C4'-C5'-O5'
2	B	401	UMP	O4'-C4'-C5'-O5'

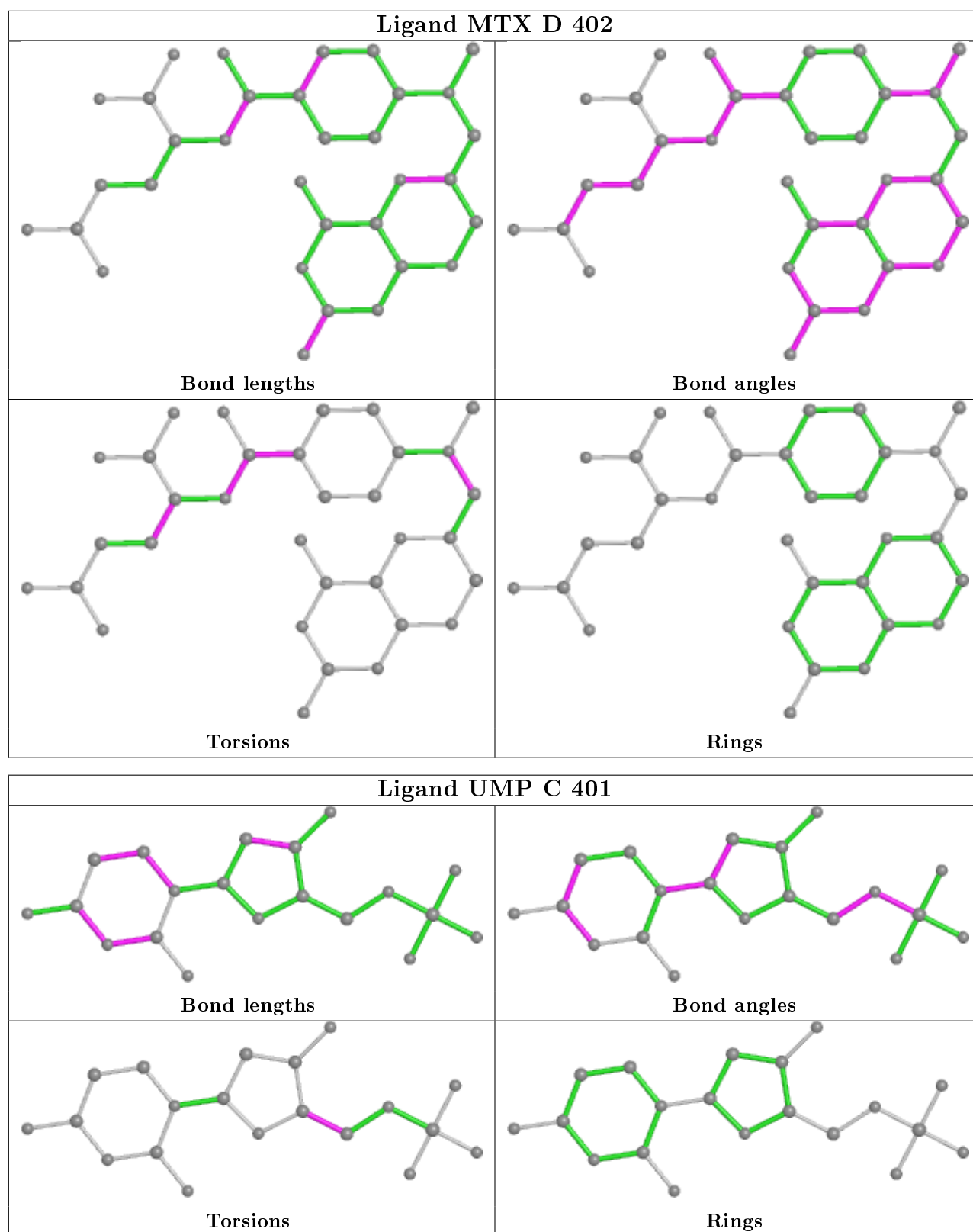
There are no ring outliers.

4 monomers are involved in 8 short contacts:

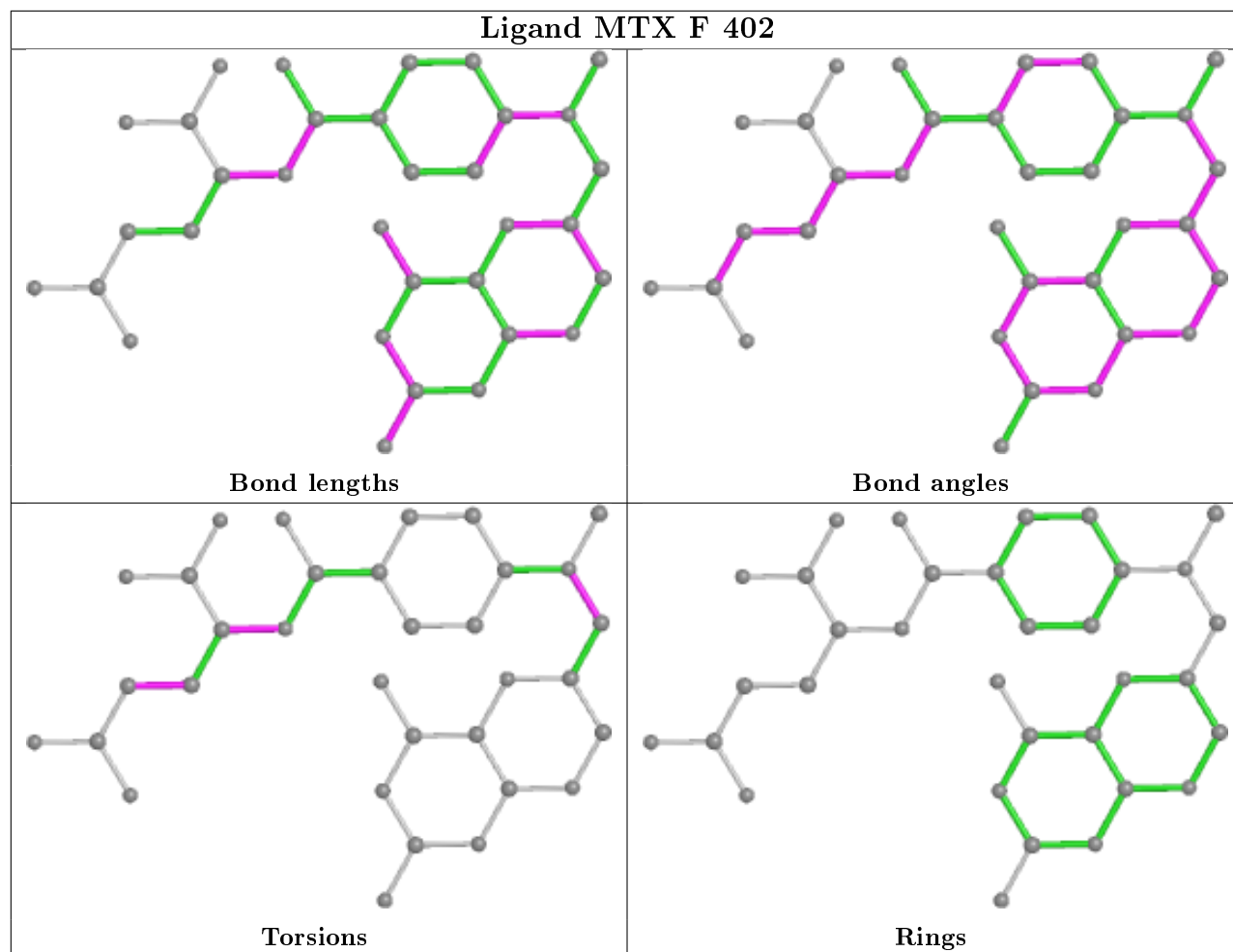
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	MTX	1	0
3	E	402	MTX	2	0
2	F	401	UMP	3	0
3	C	402	MTX	2	0

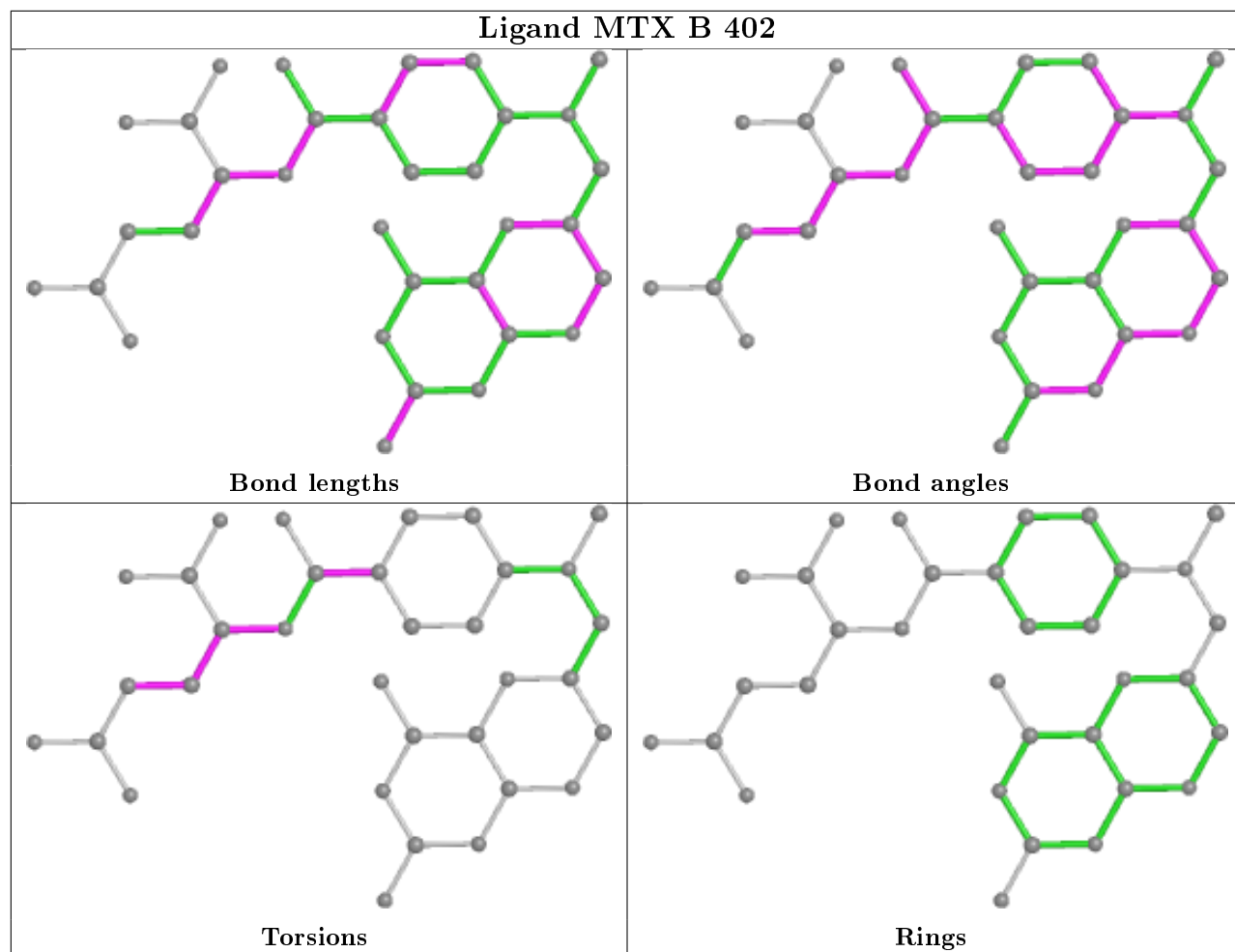
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

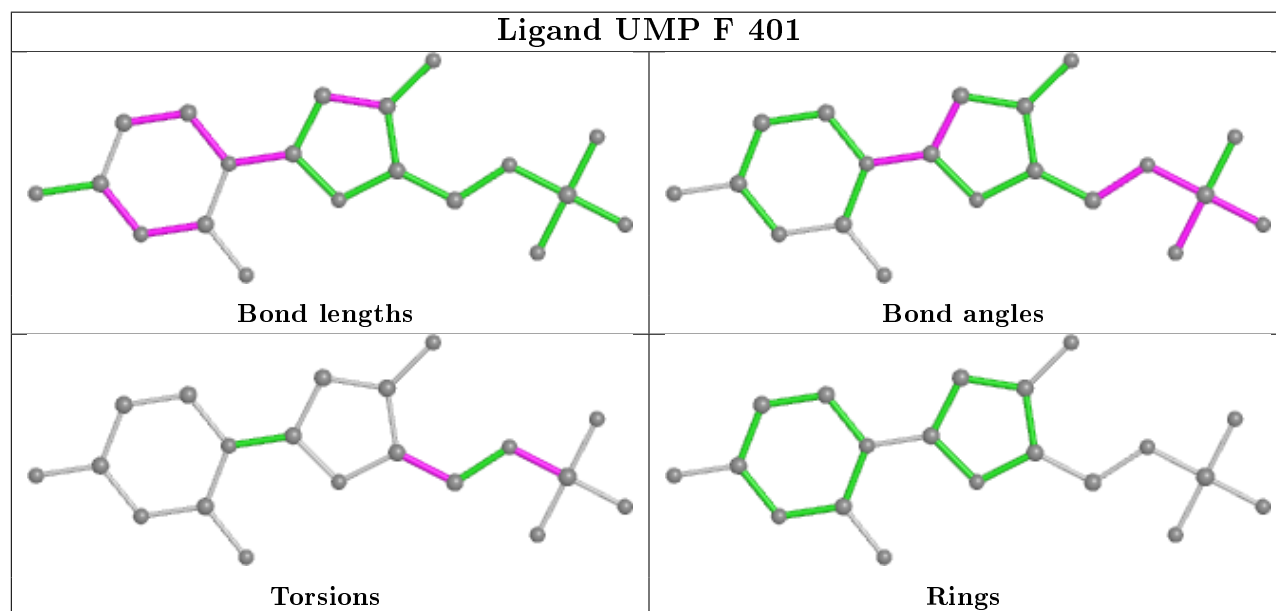
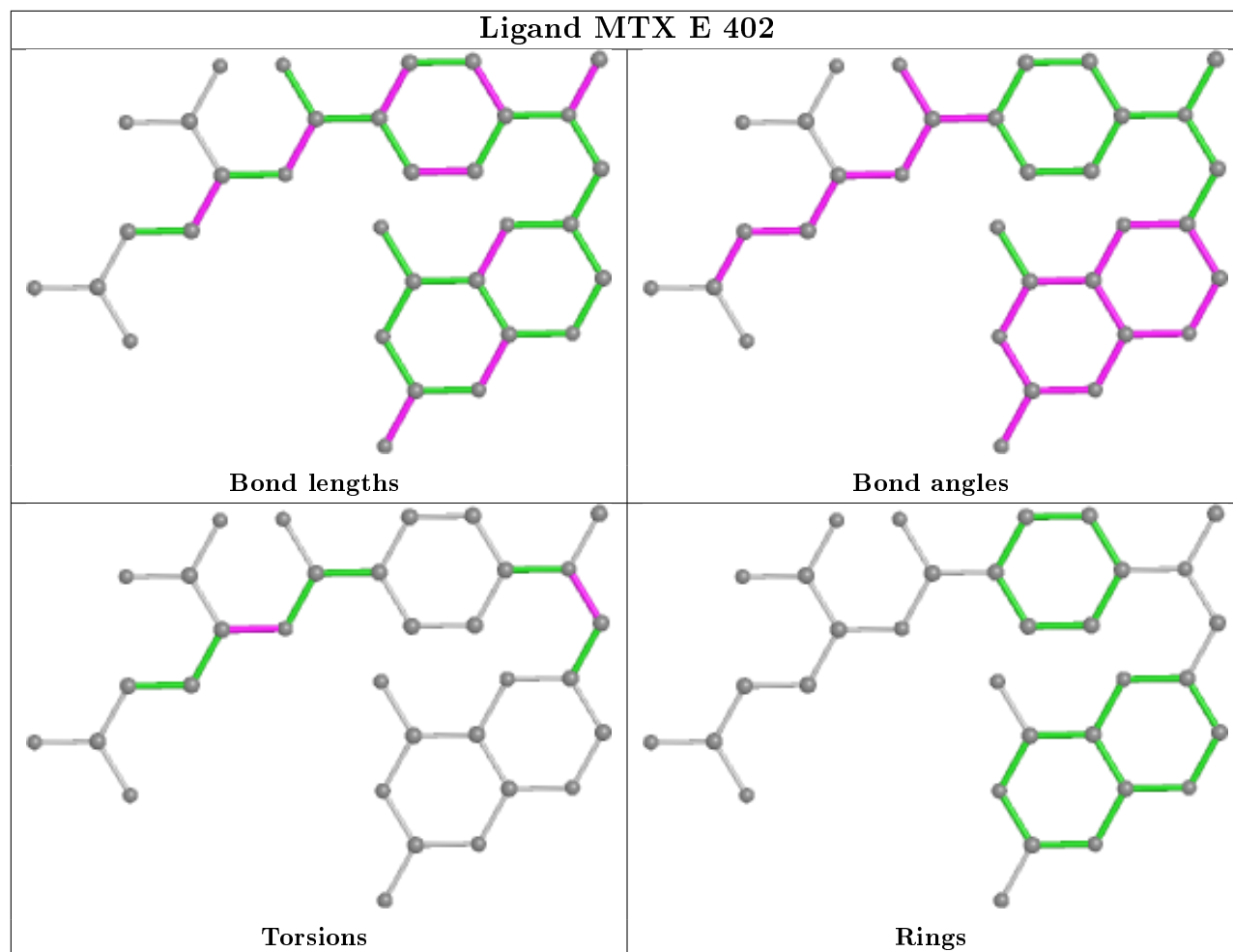


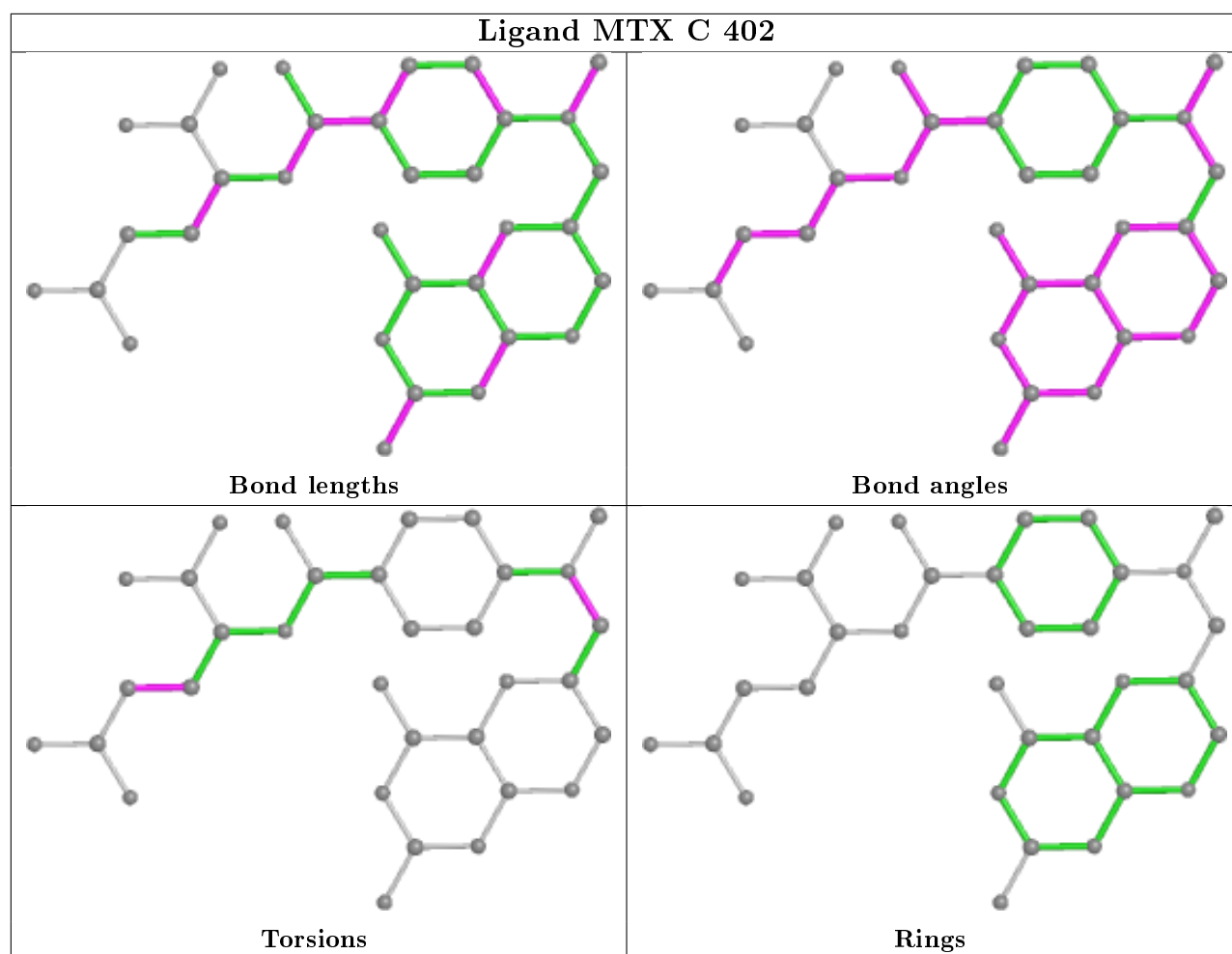


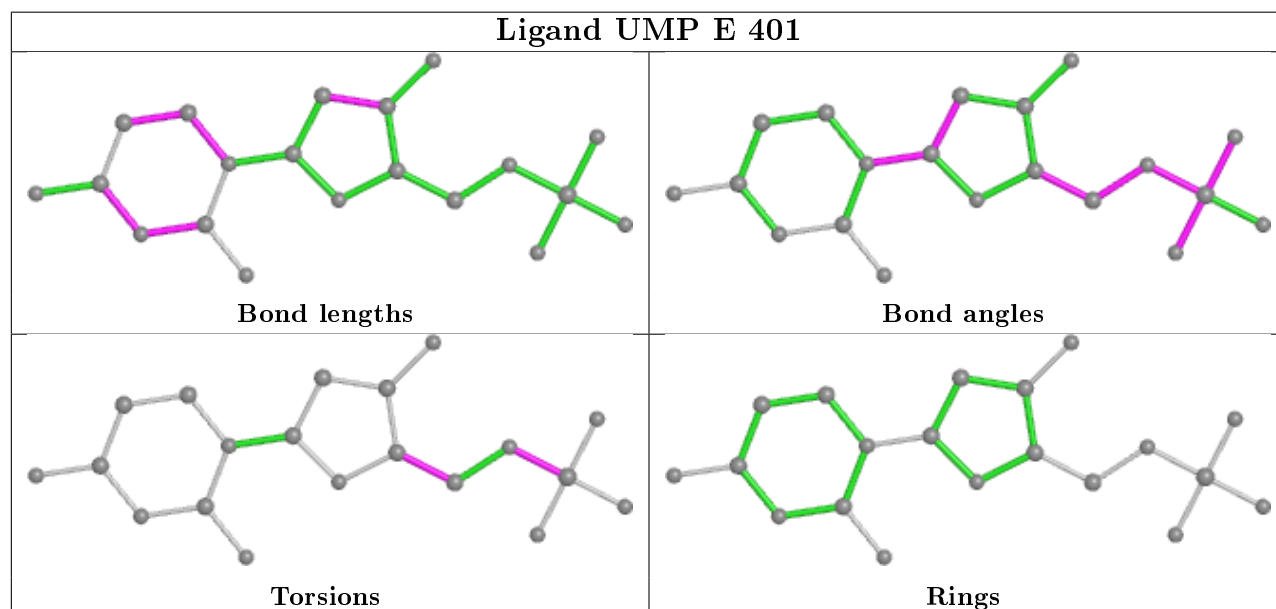
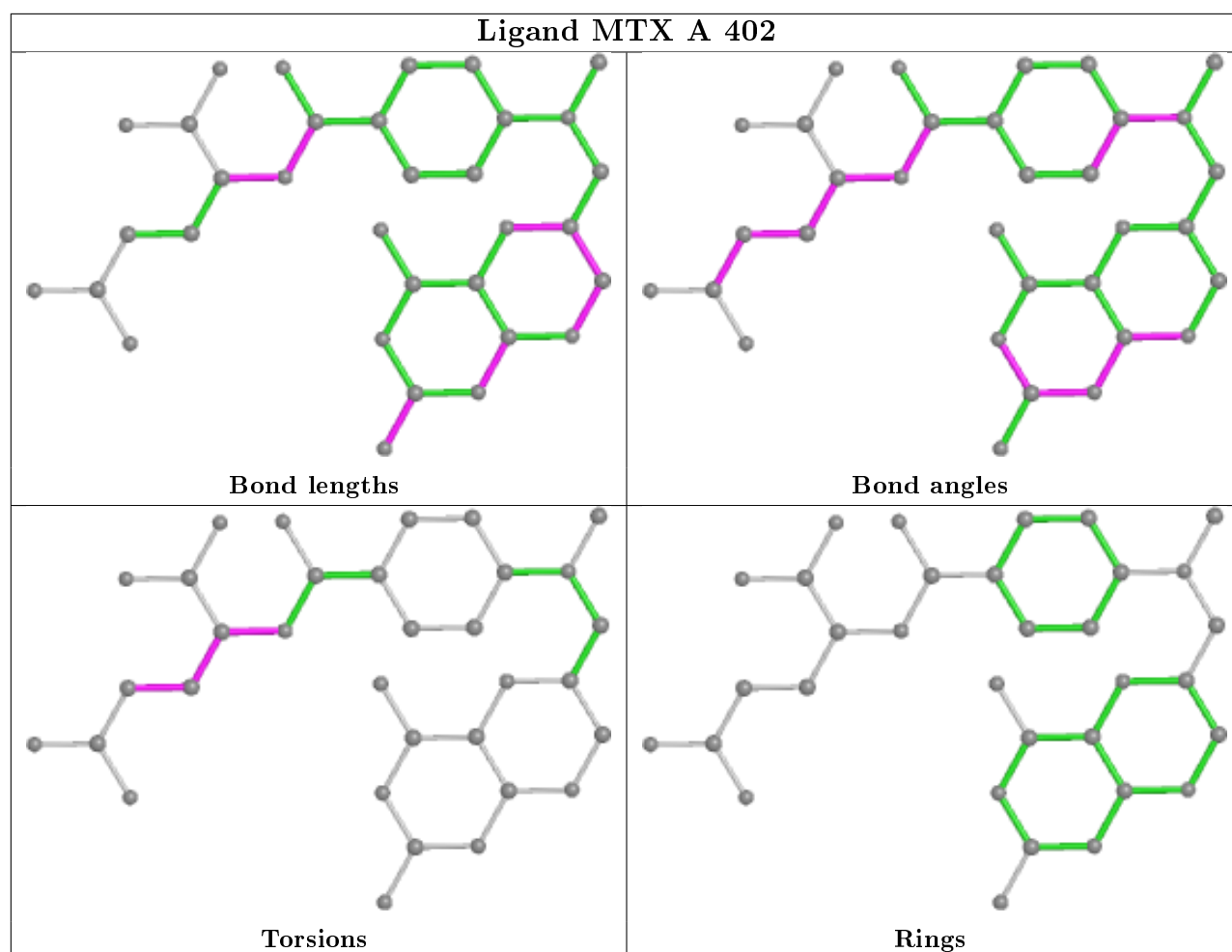


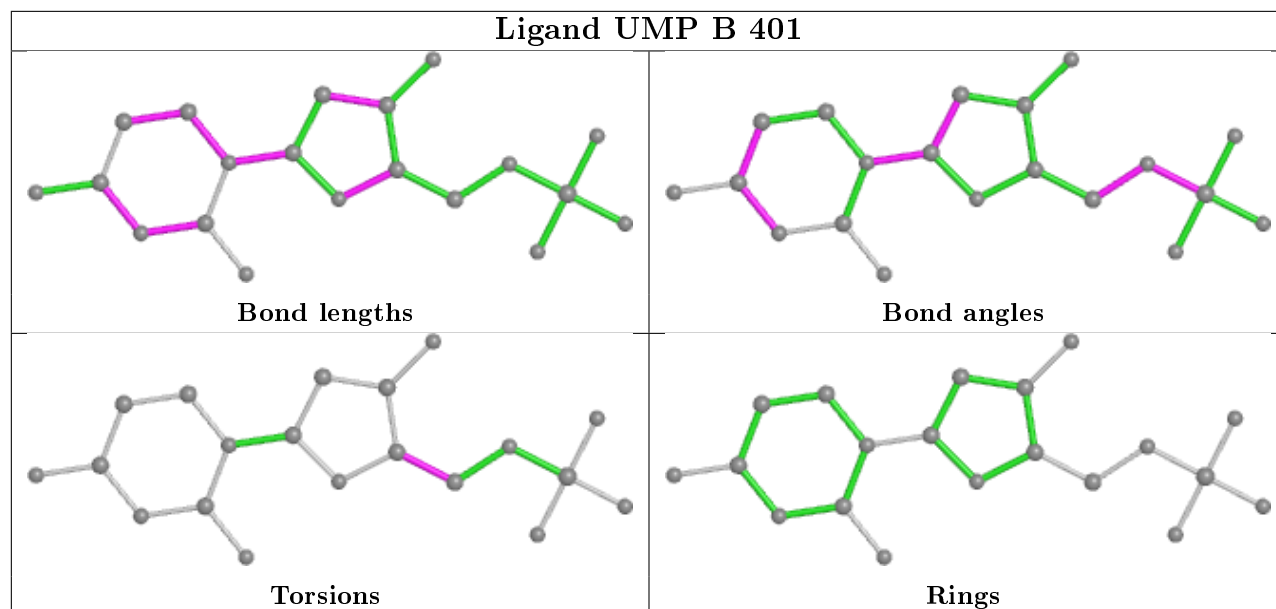












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	288/290 (99%)	-0.16	1 (0%) 94 93	12, 21, 35, 59	0
1	B	288/290 (99%)	-0.07	2 (0%) 87 87	15, 25, 38, 56	0
1	C	288/290 (99%)	0.22	7 (2%) 59 57	17, 28, 49, 62	0
1	D	288/290 (99%)	-0.02	6 (2%) 63 62	13, 22, 42, 68	0
1	E	287/290 (98%)	0.08	9 (3%) 49 48	17, 26, 47, 60	0
1	F	288/290 (99%)	0.35	19 (6%) 18 17	19, 30, 53, 69	0
All	All	1727/1740 (99%)	0.07	44 (2%) 57 56	12, 26, 45, 69	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	313	VAL	10.4
1	D	313	VAL	8.2
1	A	313	VAL	6.5
1	F	313	VAL	5.9
1	F	27	PRO	4.1
1	F	312	ALA	4.1
1	E	26	PRO	4.0
1	D	26	PRO	3.8
1	C	51	THR	3.5
1	F	28	HIS	3.5
1	F	124	SER	3.5
1	B	313	VAL	3.5
1	F	26	PRO	3.4
1	E	28	HIS	3.4
1	E	27	PRO	3.3
1	C	125	THR	3.1
1	D	28	HIS	3.1
1	C	307	ILE	3.0
1	F	307	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	52	GLY	3.0
1	E	312	ALA	2.9
1	E	307	ILE	2.9
1	D	27	PRO	2.8
1	F	49	ASP	2.8
1	F	125	THR	2.8
1	F	52	GLY	2.7
1	F	51	THR	2.6
1	F	308	LYS	2.6
1	C	267	ILE	2.5
1	D	53	THR	2.4
1	F	275	PRO	2.4
1	D	52	GLY	2.3
1	E	267	ILE	2.3
1	F	147	ARG	2.3
1	F	221	LEU	2.2
1	C	170	THR	2.2
1	B	26	PRO	2.1
1	F	116	ASP	2.1
1	F	284	LYS	2.1
1	E	53	THR	2.1
1	C	116	ASP	2.1
1	E	48	ASP	2.1
1	F	48	ASP	2.0
1	F	53	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

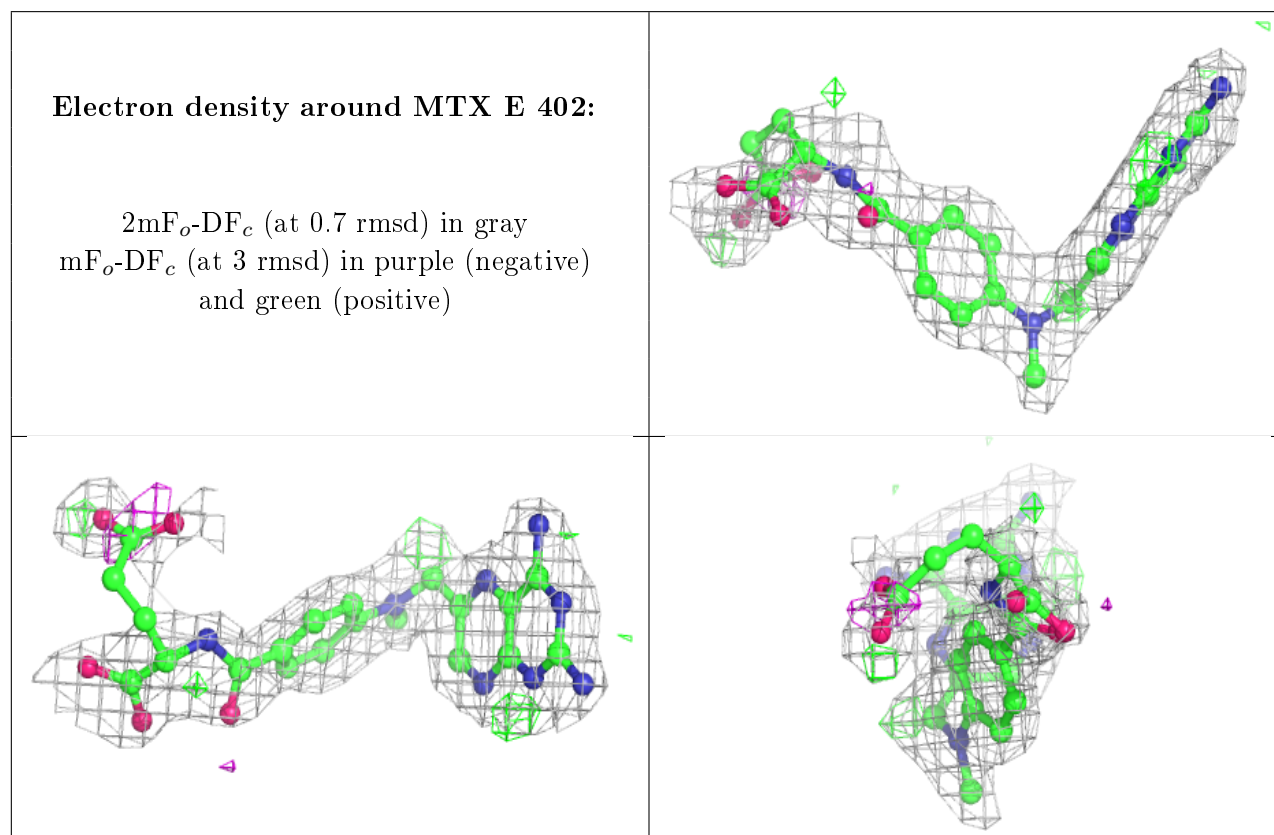
## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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.



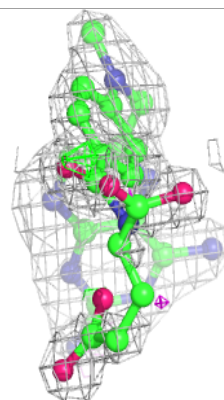
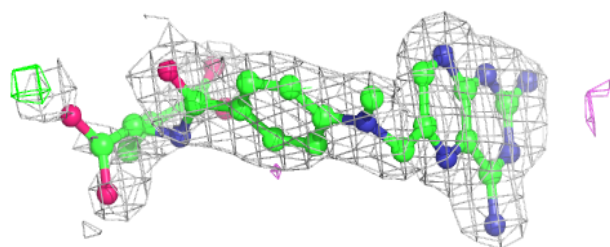
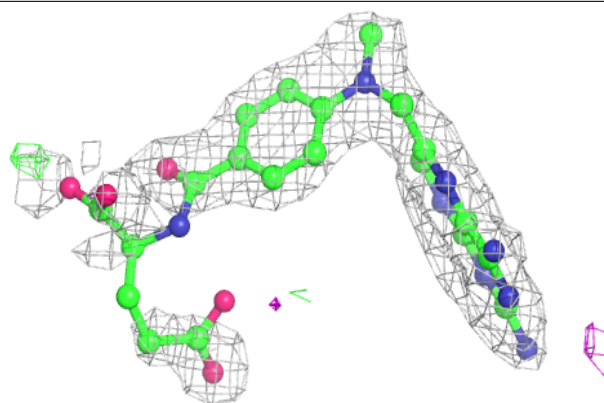
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MTX	E	402	33/33	0.81	0.19	33,38,69,72	0
3	MTX	C	402	33/33	0.82	0.19	32,38,73,83	0
3	MTX	F	402	33/33	0.89	0.17	36,43,93,99	0
3	MTX	D	402	33/33	0.91	0.14	27,31,65,67	0
3	MTX	A	402	33/33	0.91	0.14	22,29,58,63	0
3	MTX	B	402	33/33	0.92	0.14	20,29,92,96	0
2	UMP	F	401	20/20	0.96	0.08	25,34,37,37	0
2	UMP	E	401	20/20	0.96	0.08	27,32,35,36	0
2	UMP	C	401	20/20	0.98	0.07	22,27,29,31	0
2	UMP	D	401	20/20	0.98	0.07	22,26,29,29	0
2	UMP	B	401	20/20	0.98	0.08	18,20,22,22	0
2	UMP	A	401	20/20	0.99	0.08	17,18,21,21	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.

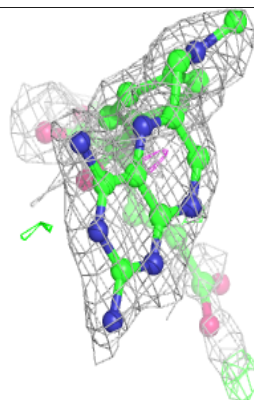
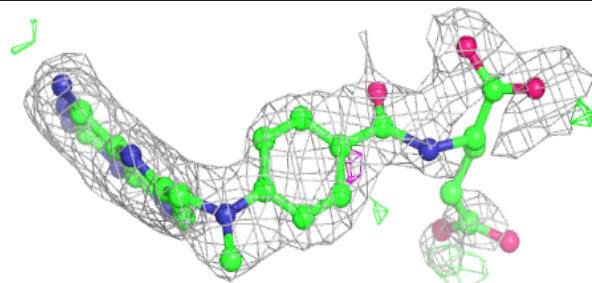
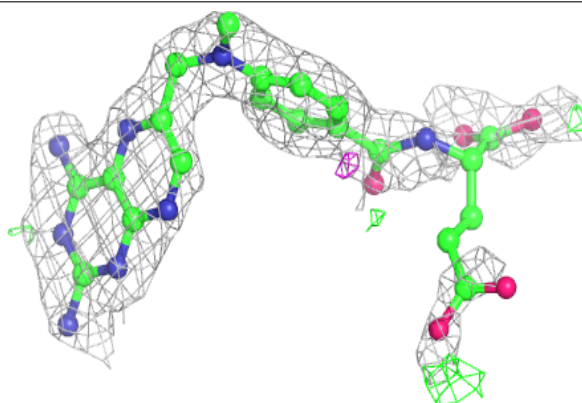


**Electron density around MTX C 402:**

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

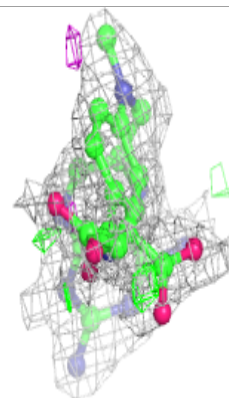
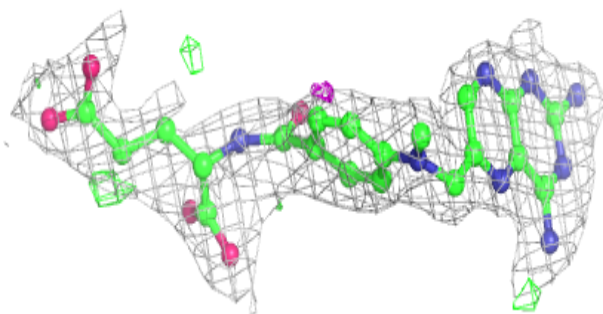
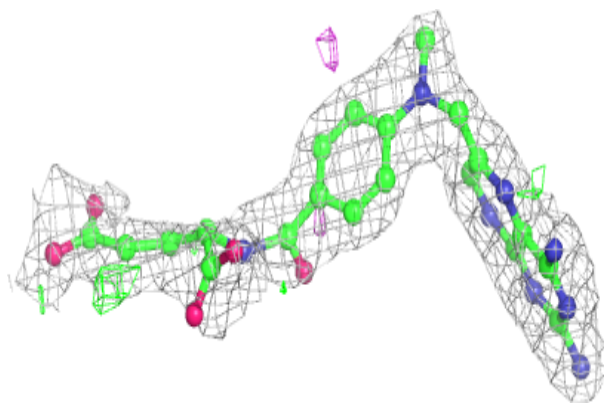
**Electron density around MTX F 402:**

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

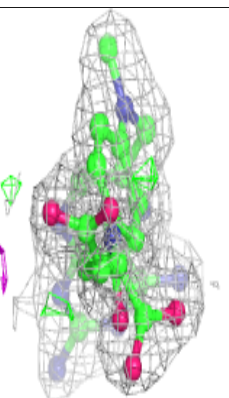
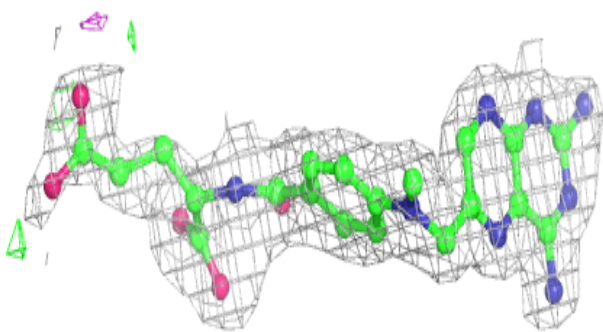
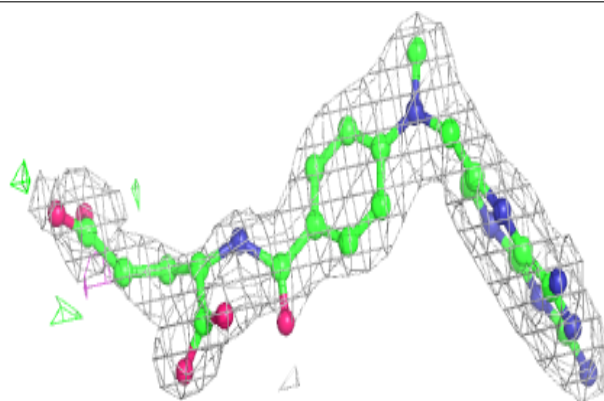


**Electron density around MTX D 402:**

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

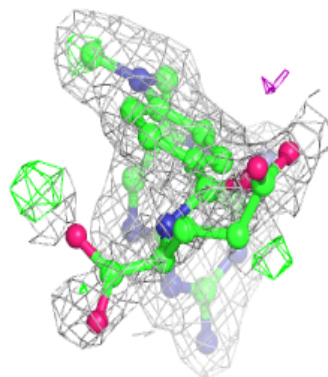
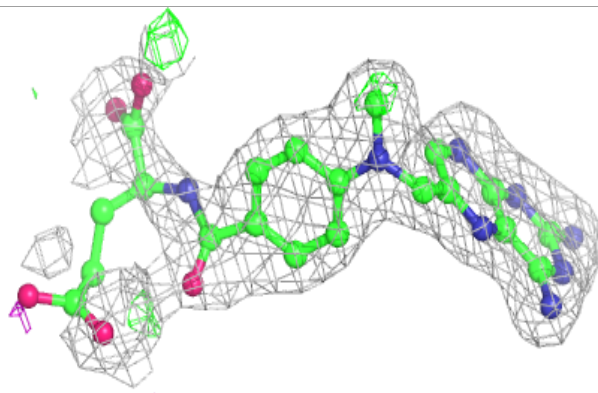
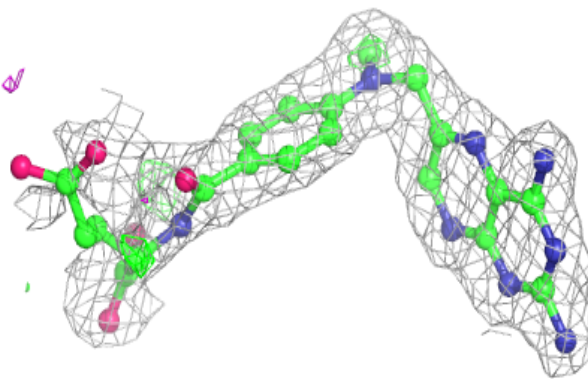
**Electron density around MTX A 402:**

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

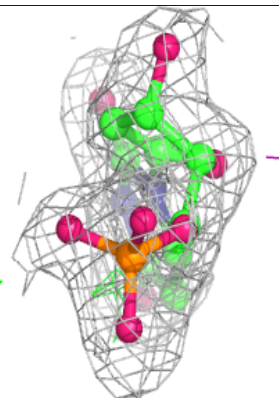
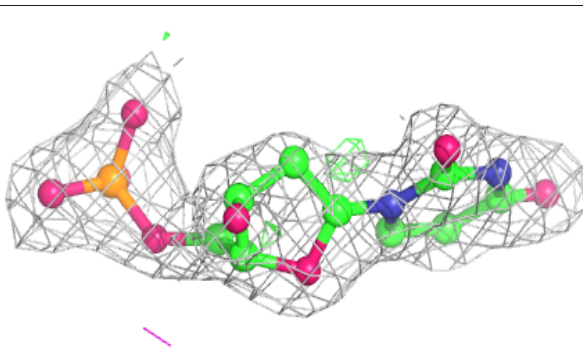
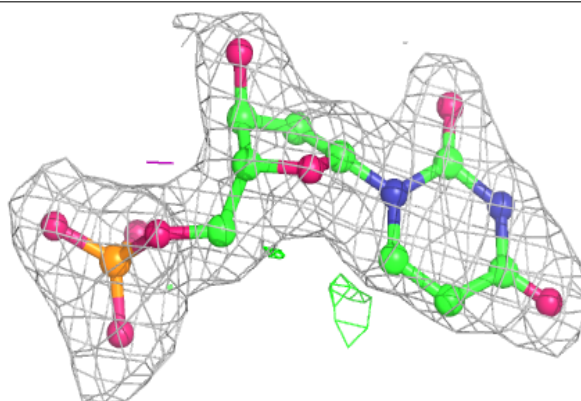


**Electron density around MTX B 402:**

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

**Electron density around UMP F 401:**

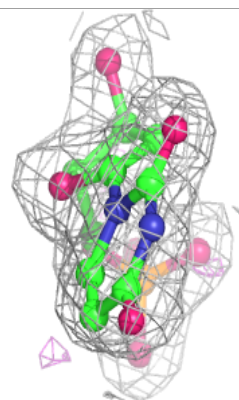
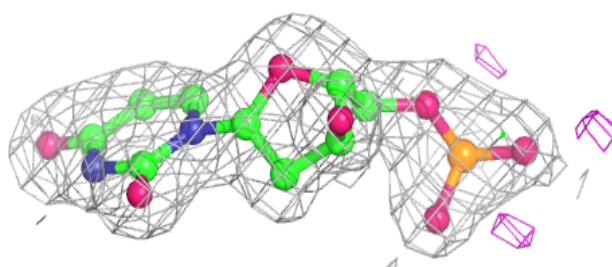
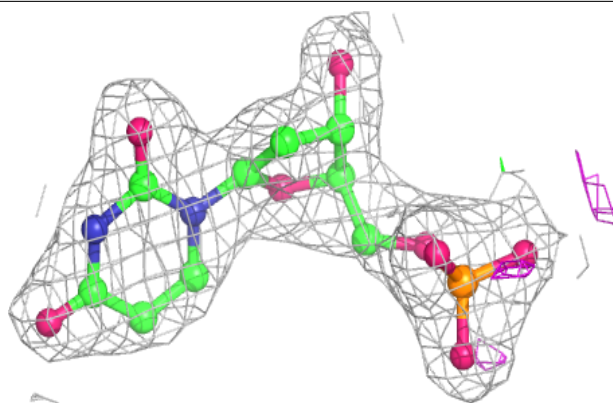
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



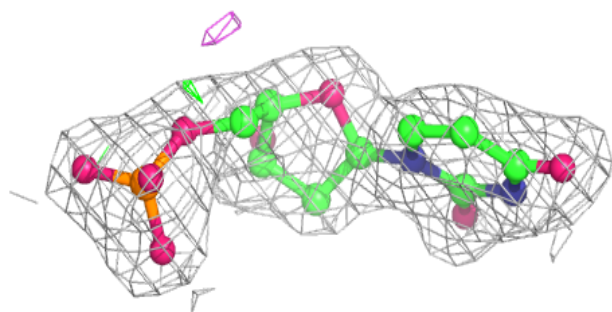
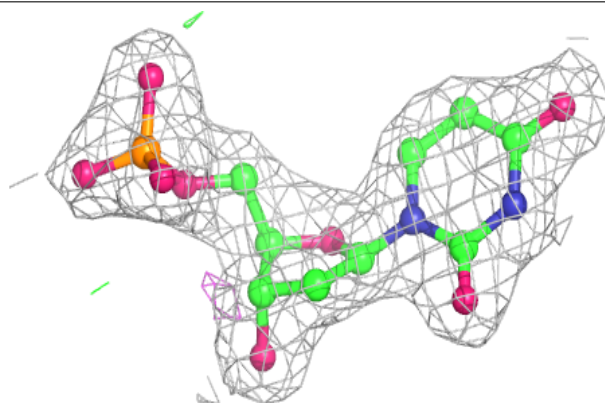


**Electron density around UMP E 401:**

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

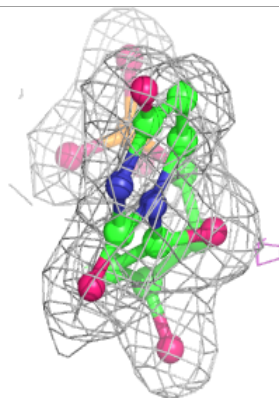
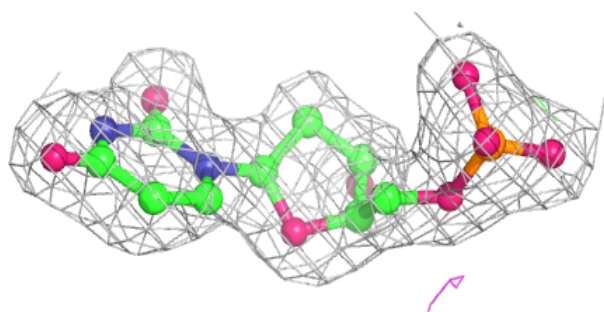
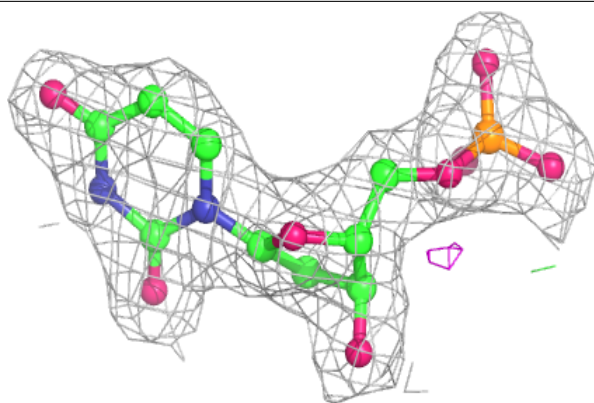
**Electron density around UMP C 401:**

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

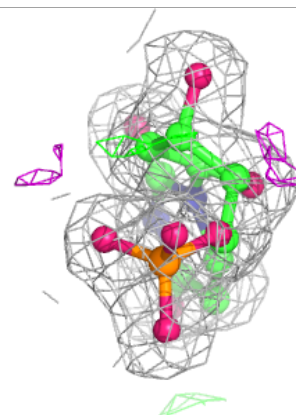
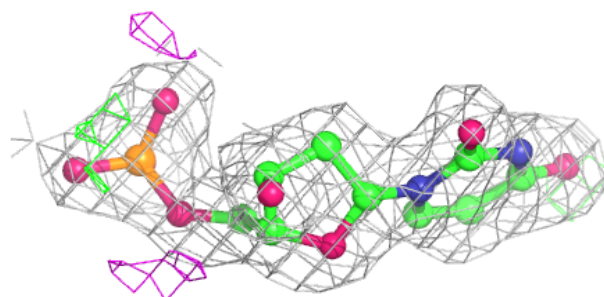
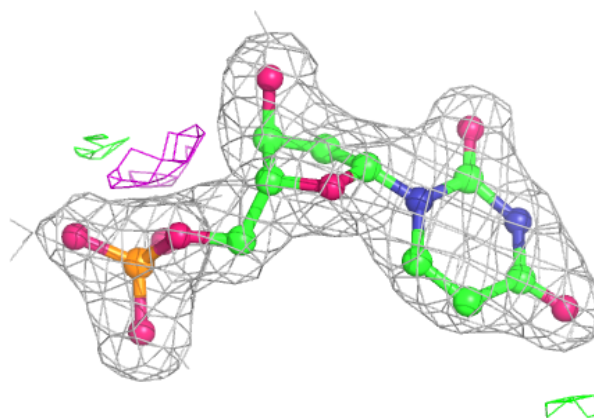


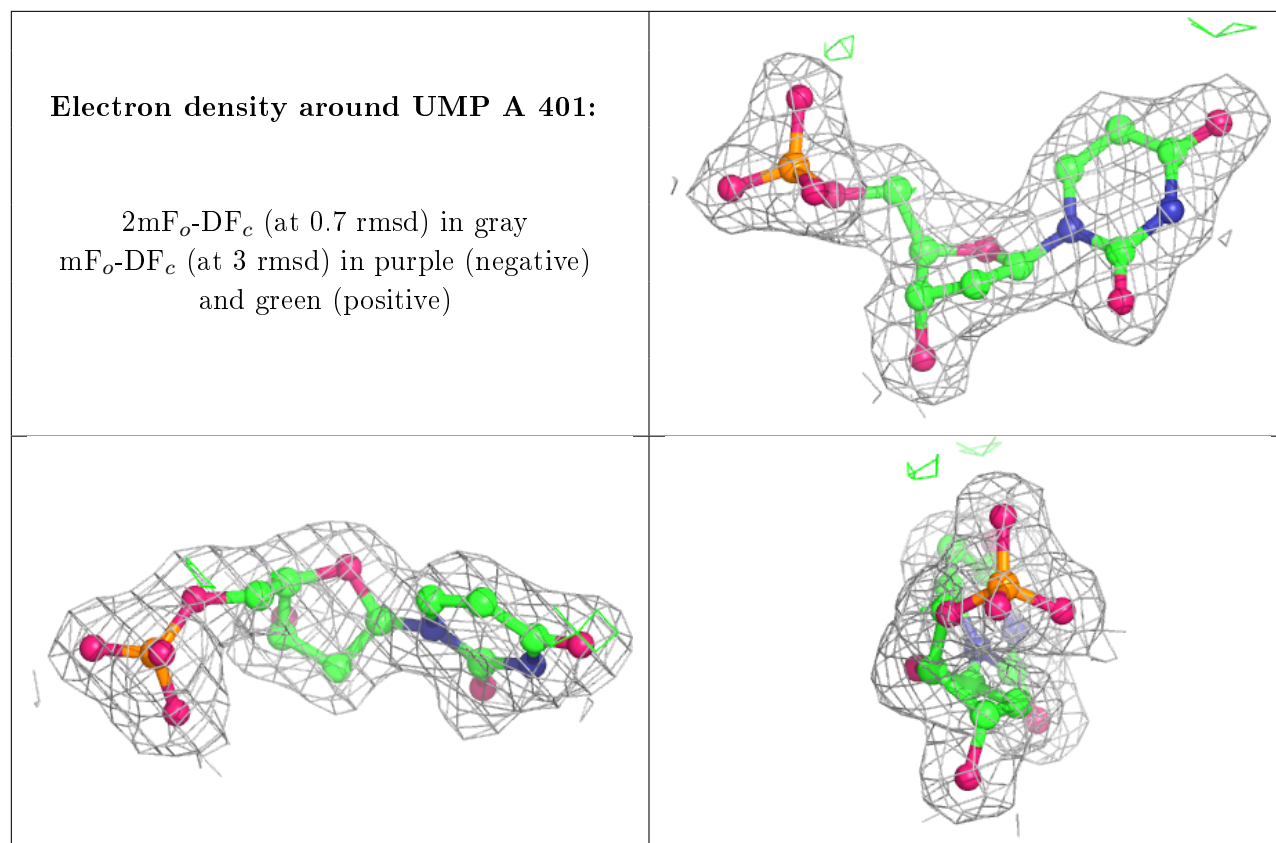
**Electron density around UMP D 401:**

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

**Electron density around UMP B 401:**

$2mF_o-DF_c$  (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.