



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:23 PM EDT

PDB ID : 7F3Y / pdb_00007f3y
Title : Wild-type Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with methotrexate (MTX), NADPH and dUMP
Authors : Vanichtanankul, J.; Tanramluk, D.; Yuvaniyama, J.; Yuthavong, Y.
Deposited on : 2021-06-17
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

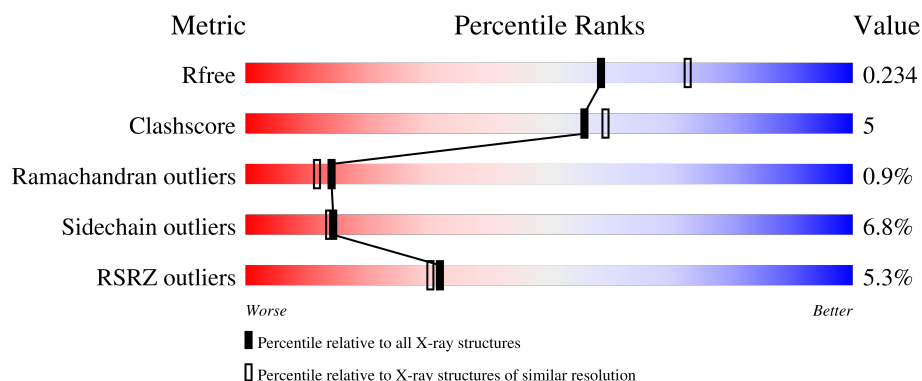
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	608	3% 75% 13% 10%
1	B	608	6% 74% 14% 10%

2 Entry composition [i](#)

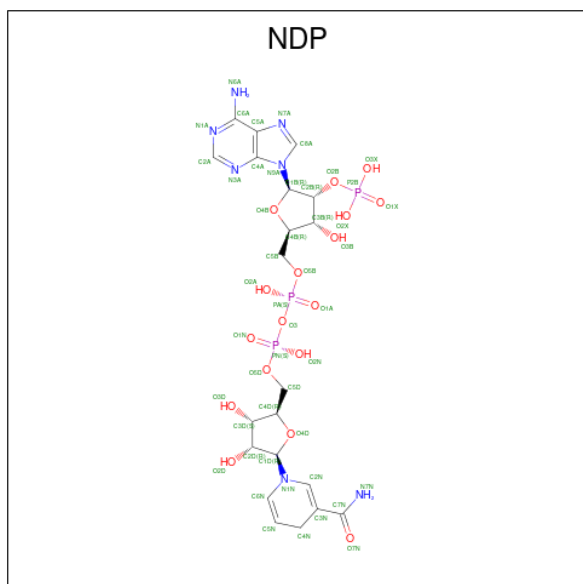
There are 6 unique types of molecules in this entry. The entry contains 9868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bifunctional dihydrofolate reductase-thymidylate synthase.

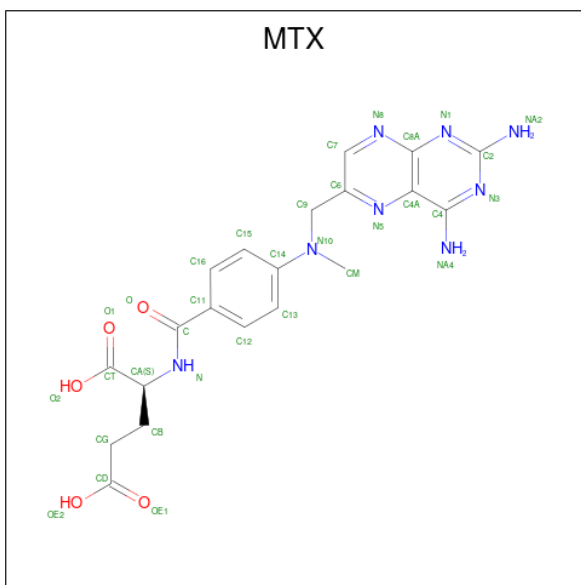
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4543	2931	750	834	28			
1	B	546	Total	C	N	O	S	0	0	0
			4532	2926	749	829	28			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



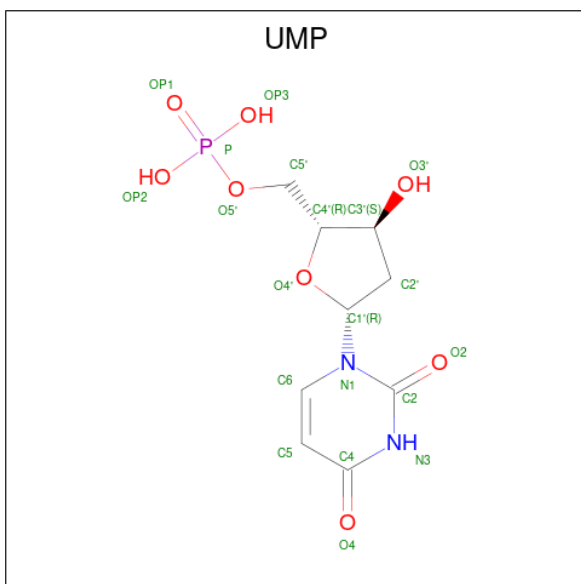
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is METHOTREXATE (CCD ID: MTX) (formula: $C_{20}H_{22}N_8O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

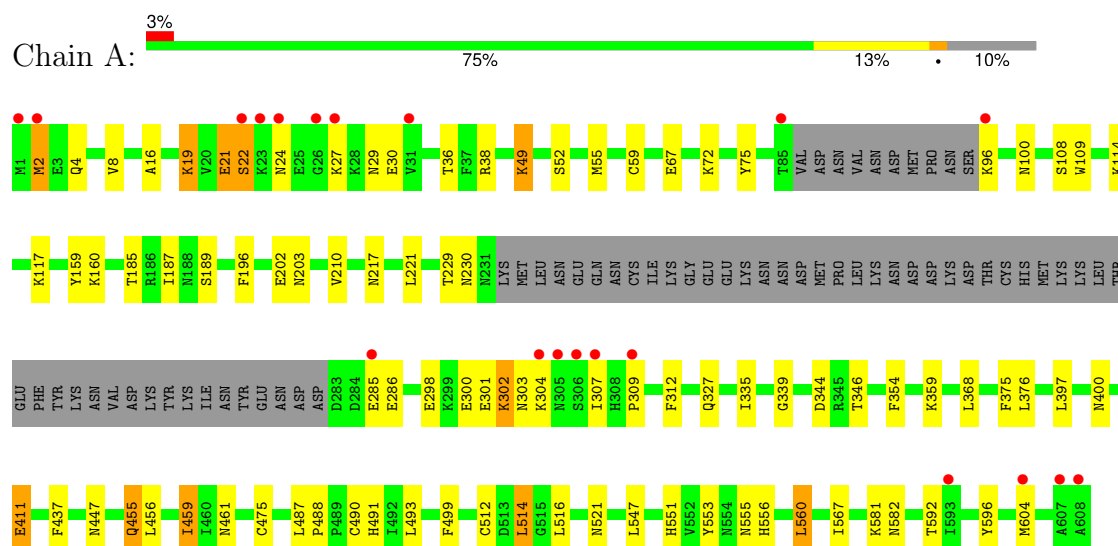
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	293	Total	O	0	0
			293	293		
6	B	253	Total	O	0	0
			253	253		

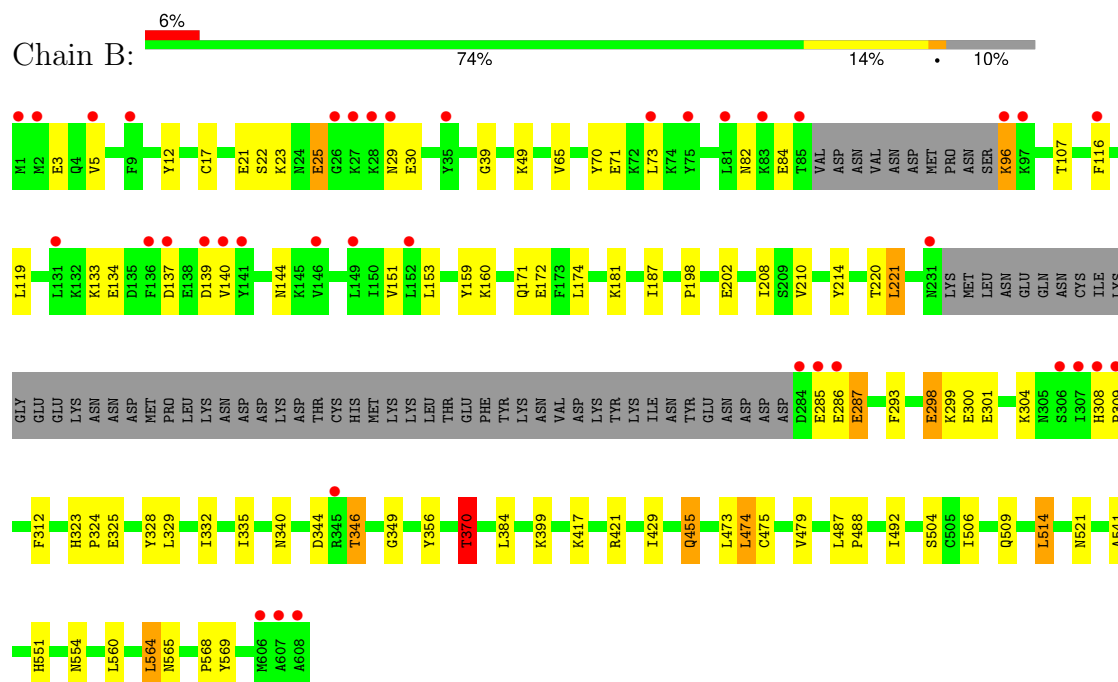
3 Residue-property plots [i](#)

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

- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.68Å 154.40Å 164.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.58 – 2.25 27.58 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.9 (27.58-2.25) 93.9 (27.58-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.233 0.189 , 0.234	Depositor DCC
R_{free} test set	3247 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9868	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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, NDP, GOL, 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	1.04	1/4648 (0.0%)	1.34	4/6272 (0.1%)
1	B	1.08	2/4637 (0.0%)	1.39	8/6257 (0.1%)
All	All	1.06	3/9285 (0.0%)	1.37	12/12529 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	LEU	C-O	5.63	1.30	1.24
1	A	19	LYS	C-O	5.22	1.30	1.23
1	B	504	SER	C-O	5.19	1.30	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	THR	N-CA-CB	-7.30	101.19	110.90
1	B	370	THR	CB-CA-C	5.84	118.82	109.02
1	B	488	PRO	N-CA-CB	5.66	106.16	103.22
1	A	567	ILE	CA-C-O	5.55	122.42	119.15
1	B	474	LEU	CA-C-O	-5.19	114.91	120.46
1	B	541	ALA	CA-C-O	-5.16	116.40	119.55
1	B	293	PHE	CB-CA-C	5.12	121.01	110.31
1	A	75	TYR	CA-C-N	5.08	127.40	120.54
1	A	75	TYR	C-N-CA	5.08	127.40	120.54
1	B	370	THR	N-CA-C	-5.05	107.79	114.31
1	B	356	TYR	CA-C-O	-5.04	115.70	121.40
1	A	488	PRO	O-C-N	-5.01	119.01	121.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4543	0	4497	46	0
1	B	4532	0	4491	42	0
2	A	48	0	26	1	0
2	B	48	0	26	3	0
3	A	66	0	40	2	0
3	B	33	0	20	2	0
4	A	20	0	11	5	0
4	B	20	0	11	1	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	293	0	0	8	0
6	B	253	0	0	5	0
All	All	9868	0	9138	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:THR:HG21	1:B:569:TYR:H	1.30	0.93
1:B:210:VAL:HG12	6:B:822:HOH:O	1.70	0.90
1:B:370:THR:CG2	1:B:569:TYR:H	1.86	0.88
1:A:327:GLN:HE22	1:A:359:LYS:H	1.22	0.86
1:A:461:ASN:HB2	6:A:804:HOH:O	1.80	0.82
1:B:370:THR:HG21	1:B:569:TYR:N	2.03	0.74
1:A:521:ASN:HD21	4:A:703:UMP:HN3	1.36	0.72
1:A:59:CYS:SG	6:A:1059:HOH:O	2.49	0.69
1:A:560:LEU:HD13	1:A:604:MET:HE1	1.73	0.69
1:A:100:ASN:HD22	1:A:160:LYS:H	1.45	0.64
1:A:455:GLN:HE22	1:A:475:CYS:H	1.44	0.64
1:B:328:TYR:CZ	1:B:332:ILE:HD11	2.33	0.64
1:B:421:ARG:NH1	6:B:801:HOH:O	2.26	0.60
1:B:335:ILE:CD1	1:B:514:LEU:HD13	2.33	0.58
1:B:455:GLN:HE22	1:B:475:CYS:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:GLN:HE22	1:B:521:ASN:ND2	2.05	0.55
1:A:491:HIS:ND1	6:A:803:HOH:O	2.34	0.54
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.42	0.54
1:A:493:LEU:HD22	1:B:492:ILE:HG21	1.90	0.54
1:A:461:ASN:CB	6:A:804:HOH:O	2.45	0.54
1:A:19:LYS:HG2	1:A:36:THR:HG22	1.89	0.53
1:B:22:SER:HB2	1:B:25:GLU:HB3	1.90	0.53
1:A:327:GLN:NE2	1:A:359:LYS:H	2.01	0.53
1:B:399:LYS:HE2	6:B:816:HOH:O	2.09	0.53
1:A:491:HIS:CE1	4:A:703:UMP:O4	2.64	0.51
1:B:325:GLU:OE1	1:B:370:THR:HB	2.09	0.51
1:B:332:ILE:HD13	1:B:560:LEU:HD22	1.91	0.51
1:A:210:VAL:HB	6:A:985:HOH:O	2.11	0.50
1:B:349:GLY:HA3	1:B:554:ASN:ND2	2.27	0.50
1:A:344:ASP:OD2	1:A:346:THR:OG1	2.27	0.49
1:B:160:LYS:HE3	6:B:874:HOH:O	2.12	0.49
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.47	0.49
1:A:411:GLU:OE2	6:A:801:HOH:O	2.20	0.49
1:A:302:LYS:HE3	1:A:339:GLY:O	2.12	0.49
1:A:437:PHE:CD1	1:B:479:VAL:HB	2.47	0.49
1:B:312:PHE:HA	1:B:565:ASN:HD21	1.77	0.49
1:B:329:LEU:HD22	1:B:564:LEU:HD12	1.95	0.48
1:A:491:HIS:HE1	4:A:703:UMP:O4	1.96	0.48
2:B:701:NDP:H42N	3:B:702:MTX:N5	2.28	0.48
1:B:172:GLU:OE2	2:B:701:NDP:N7A	2.47	0.48
3:A:704:MTX:H13	3:A:704:MTX:C6	2.45	0.47
1:A:553:TYR:HB3	1:A:555:ASN:OD1	2.15	0.47
1:B:214:TYR:O	1:B:220:THR:HA	2.14	0.47
1:A:490:CYS:SG	4:A:703:UMP:C6	3.08	0.46
1:A:108:SER:OG	2:A:701:NDP:H6N	2.15	0.46
1:B:17:CYS:HA	1:B:39:GLY:O	2.17	0.45
1:A:516:LEU:HD21	3:A:704:MTX:HB2	1.98	0.45
1:A:335:ILE:HD12	1:A:514:LEU:HD13	1.99	0.44
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.52	0.44
1:B:301:GLU:O	1:B:304:LYS:HB2	2.17	0.44
1:A:38:ARG:O	1:A:196:PHE:HA	2.17	0.44
1:B:96:LYS:HA	1:B:96:LYS:HE2	1.98	0.44
1:B:221:LEU:HD12	1:B:221:LEU:N	2.32	0.44
1:A:512:CYS:SG	1:A:547:LEU:HD22	2.58	0.43
1:B:309:PRO:HA	1:B:312:PHE:HD2	1.82	0.43
1:B:344:ASP:O	1:B:346:THR:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD12	1:B:198:PRO:HG2	2.00	0.43
1:B:116:PHE:CD1	3:B:702:MTX:HB1	2.54	0.43
1:A:301:GLU:O	1:A:304:LYS:HB3	2.19	0.43
1:A:335:ILE:CD1	1:A:514:LEU:HD13	2.49	0.43
1:A:582:ASN:HB3	6:A:893:HOH:O	2.17	0.43
1:B:335:ILE:HD12	1:B:514:LEU:HD13	2.00	0.43
1:B:551:HIS:HE1	4:B:703:UMP:O3'	2.02	0.43
1:B:370:THR:HG22	1:B:568:PRO:HA	2.01	0.43
1:B:70:TYR:O	1:B:71:GLU:C	2.61	0.43
1:A:203:ASN:O	1:A:229:THR:OG1	2.32	0.42
1:A:556:HIS:HB3	1:A:560:LEU:HD22	2.02	0.42
1:A:456:LEU:O	1:A:459:ILE:HG13	2.19	0.42
1:A:309:PRO:HA	1:A:312:PHE:HD2	1.83	0.42
1:B:65:VAL:HG12	1:B:159:TYR:CB	2.50	0.42
1:A:560:LEU:HD12	1:A:560:LEU:HA	1.93	0.42
1:A:16:ALA:HA	1:A:185:THR:HB	2.02	0.42
1:B:298:GLU:HB2	1:B:300:GLU:O	2.19	0.42
1:A:21:GLU:O	1:A:22:SER:CB	2.67	0.41
1:A:52:SER:H	1:A:217:ASN:ND2	2.19	0.41
1:A:286:GLU:HG2	6:B:973:HOH:O	2.19	0.41
1:A:4:GLN:O	1:A:8:VAL:HG23	2.21	0.41
1:A:55:MET:CE	6:A:950:HOH:O	2.69	0.41
1:B:285:GLU:C	1:B:287:GLU:N	2.79	0.41
1:A:368:LEU:HD23	1:A:596:TYR:CE1	2.55	0.41
1:B:323:HIS:HA	1:B:324:PRO:HD3	1.98	0.41
1:A:100:ASN:HD21	1:A:159:TYR:HD2	1.69	0.40
1:B:144:ASN:O	2:B:701:NDP:H2A	2.21	0.40
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.56	0.40
1:A:551:HIS:HE1	4:A:703:UMP:O3'	2.04	0.40
1:B:214:TYR:HB2	1:B:221:LEU:HD13	2.04	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	541/608 (89%)	508 (94%)	29 (5%)	4 (1%)	18	17
1	B	540/608 (89%)	495 (92%)	39 (7%)	6 (1%)	11	8
All	All	1081/1216 (89%)	1003 (93%)	68 (6%)	10 (1%)	14	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	B	23	LYS
1	A	2	MET
1	B	151	VAL
1	A	21	GLU
1	A	49	LYS
1	B	49	LYS
1	B	25	GLU
1	B	308	HIS
1	B	429	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	510/570 (90%)	476 (93%)	34 (7%)	15	14
1	B	508/570 (89%)	473 (93%)	35 (7%)	14	13
All	All	1018/1140 (89%)	949 (93%)	69 (7%)	14	14

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	24	ASN
1	A	27	LYS

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Mol	Chain	Res	Type
1	A	29	ASN
1	A	30	GLU
1	A	49	LYS
1	A	67	GLU
1	A	72	LYS
1	A	96	LYS
1	A	114	LYS
1	A	187	ILE
1	A	189	SER
1	A	202	GLU
1	A	221	LEU
1	A	230	ASN
1	A	285	GLU
1	A	298	GLU
1	A	300	GLU
1	A	302	LYS
1	A	303	ASN
1	A	307	ILE
1	A	375	PHE
1	A	376	LEU
1	A	397	LEU
1	A	400	ASN
1	A	411	GLU
1	A	447	ASN
1	A	455	GLN
1	A	459	ILE
1	A	487	LEU
1	A	514	LEU
1	A	560	LEU
1	A	581	LYS
1	A	592	THR
1	B	3	GLU
1	B	5	VAL
1	B	21	GLU
1	B	29	ASN
1	B	30	GLU
1	B	73	LEU
1	B	82	ASN
1	B	84	GLU
1	B	96	LYS
1	B	107	THR
1	B	119	LEU

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Mol	Chain	Res	Type
1	B	133	LYS
1	B	134	GLU
1	B	137	ASP
1	B	139	ASP
1	B	140	VAL
1	B	153	LEU
1	B	171	GLN
1	B	187	ILE
1	B	202	GLU
1	B	208	ILE
1	B	221	LEU
1	B	286	GLU
1	B	287	GLU
1	B	298	GLU
1	B	299	LYS
1	B	346	THR
1	B	370	THR
1	B	417	LYS
1	B	455	GLN
1	B	473	LEU
1	B	474	LEU
1	B	487	LEU
1	B	514	LEU
1	B	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	100	ASN
1	A	203	ASN
1	A	217	ASN
1	A	327	GLN
1	A	340	ASN
1	A	364	GLN
1	A	394	ASN
1	A	424	ASN
1	A	447	ASN
1	A	450	ASN
1	A	455	GLN
1	A	465	ASN
1	A	521	ASN

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Mol	Chain	Res	Type
1	A	530	HIS
1	A	551	HIS
1	B	121	ASN
1	B	171	GLN
1	B	316	ASN
1	B	364	GLN
1	B	394	ASN
1	B	407	ASN
1	B	424	ASN
1	B	455	GLN
1	B	521	ASN
1	B	542	GLN
1	B	551	HIS
1	B	554	ASN
1	B	565	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UMP	A	703	-	21,21,21	0.54	0	30,31,31	0.90	1 (3%)
5	GOL	A	705	-	5,5,5	0.13	0	5,5,5	0.36	0
3	MTX	A	702	-	35,35,35	0.58	0	47,49,49	1.11	3 (6%)
4	UMP	B	703	-	21,21,21	0.76	0	30,31,31	1.11	2 (6%)
5	GOL	B	704	-	5,5,5	0.16	0	5,5,5	0.51	0
3	MTX	A	704	-	35,35,35	0.75	0	47,49,49	1.01	1 (2%)
2	NDP	A	701	-	51,52,52	0.61	0	71,80,80	0.75	0
3	MTX	B	702	-	35,35,35	0.74	0	47,49,49	1.00	2 (4%)
2	NDP	B	701	-	51,52,52	0.57	0	71,80,80	0.75	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UMP	A	703	-	-	1/10/22/22	0/2/2/2
5	GOL	A	705	-	-	0/4/4/4	-
3	MTX	A	702	-	-	8/25/25/25	0/3/3/3
4	UMP	B	703	-	-	3/10/22/22	0/2/2/2
5	GOL	B	704	-	-	4/4/4/4	-
3	MTX	A	704	-	-	7/25/25/25	0/3/3/3
2	NDP	A	701	-	-	3/34/77/77	0/5/5/5
3	MTX	B	702	-	-	8/25/25/25	0/3/3/3
2	NDP	B	701	-	-	3/34/77/77	0/5/5/5

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	MTX	N8-C8A-N1	3.23	119.28	115.77
4	B	703	UMP	O2-C2-N1	3.01	126.72	122.80
3	B	702	MTX	C6-C9-N10	-2.63	108.45	112.95
3	A	702	MTX	N8-C8A-N1	2.49	118.48	115.77
2	B	701	NDP	O2A-PA-O1A	2.47	123.95	112.44
4	A	703	UMP	C2'-C1'-N1	2.28	119.50	113.81
3	B	702	MTX	N8-C8A-N1	2.23	118.19	115.77
3	A	702	MTX	CM-N10-C14	2.22	123.28	119.59
4	B	703	UMP	C1'-N1-C6	-2.05	117.49	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	MTX	C6-C9-N10	-2.04	109.46	112.95

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	MTX	N-CA-CB-CG
5	B	704	GOL	O1-C1-C2-C3
3	A	702	MTX	N-CA-CB-CG
3	A	702	MTX	C13-C14-N10-CM
3	A	702	MTX	C15-C14-N10-CM
3	B	702	MTX	C13-C14-N10-CM
3	B	702	MTX	C15-C14-N10-CM
3	A	702	MTX	C13-C14-N10-C9
3	A	702	MTX	CT-CA-CB-CG
3	B	702	MTX	C13-C14-N10-C9
5	B	704	GOL	C1-C2-C3-O3
5	B	704	GOL	O2-C2-C3-O3
3	B	702	MTX	CT-CA-CB-CG
5	B	704	GOL	O1-C1-C2-O2
4	B	703	UMP	O4'-C4'-C5'-O5'
4	B	703	UMP	C3'-C4'-C5'-O5'
3	B	702	MTX	C11-C-N-CA
3	B	702	MTX	O-C-N-CA
3	A	702	MTX	C15-C14-N10-C9
3	B	702	MTX	C15-C14-N10-C9
2	B	701	NDP	O4D-C1D-N1N-C2N
4	B	703	UMP	C5'-O5'-P-OP1
3	A	704	MTX	N-C-C11-C12
2	A	701	NDP	C2B-O2B-P2B-O2X
2	B	701	NDP	C2B-O2B-P2B-O3X
3	A	702	MTX	OE2-CD-CG-CB
2	A	701	NDP	O4D-C1D-N1N-C2N
3	A	704	MTX	OE1-CD-CG-CB
3	A	702	MTX	OE1-CD-CG-CB
3	A	704	MTX	N-C-C11-C16
3	A	704	MTX	OE2-CD-CG-CB
3	A	704	MTX	O-C-C11-C12
2	B	701	NDP	C4D-C5D-O5D-PN
3	A	704	MTX	C6-C9-N10-CM
4	A	703	UMP	O4'-C4'-C5'-O5'
2	A	701	NDP	C2D-C1D-N1N-C2N

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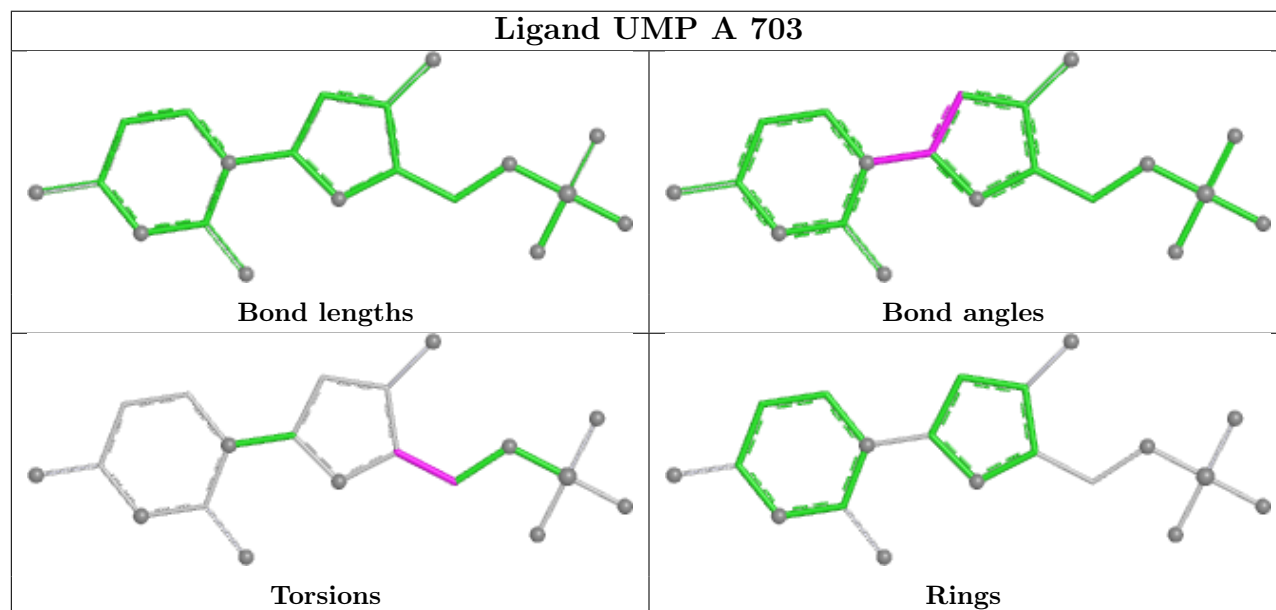
Mol	Chain	Res	Type	Atoms
3	A	704	MTX	O-C-C11-C16

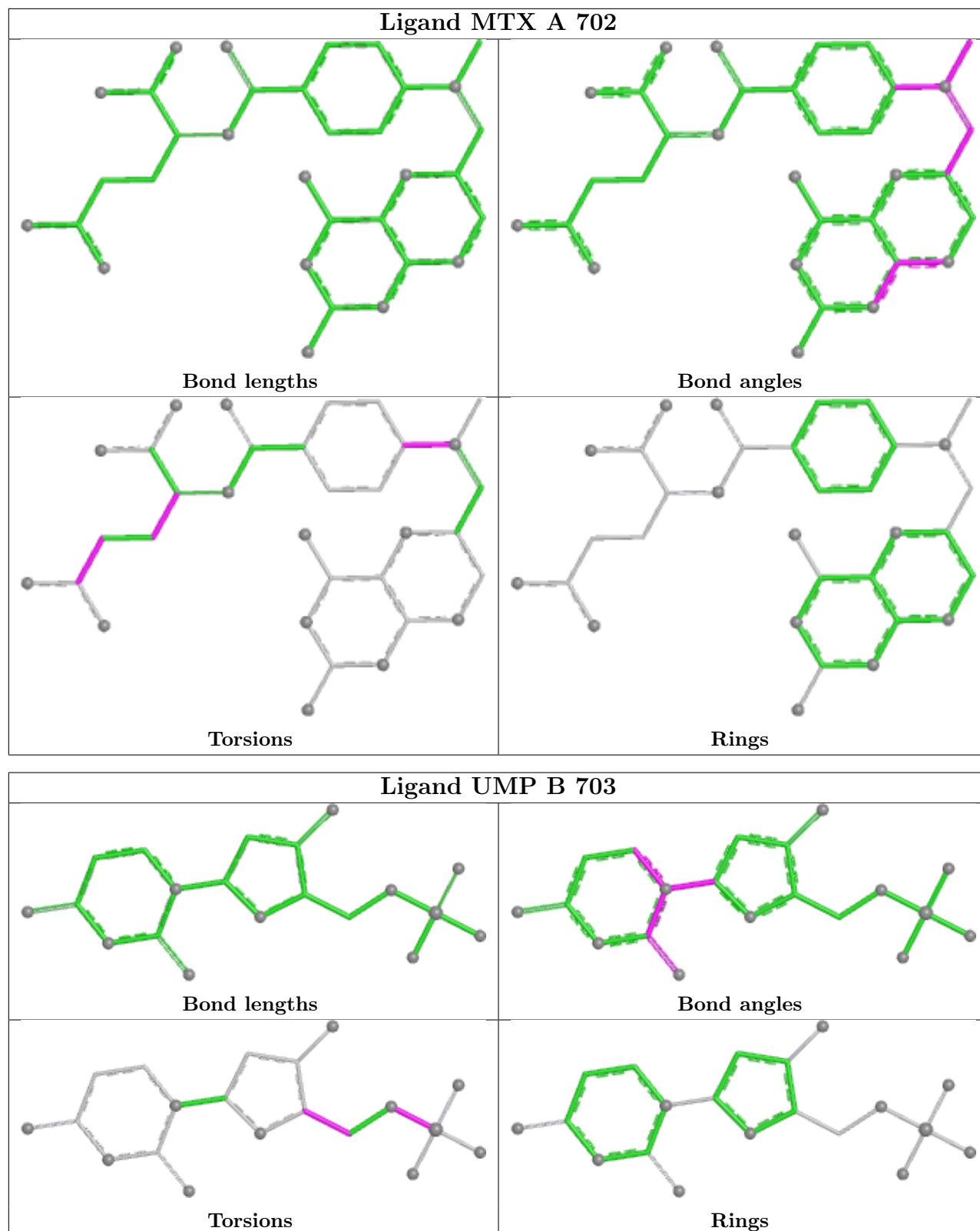
There are no ring outliers.

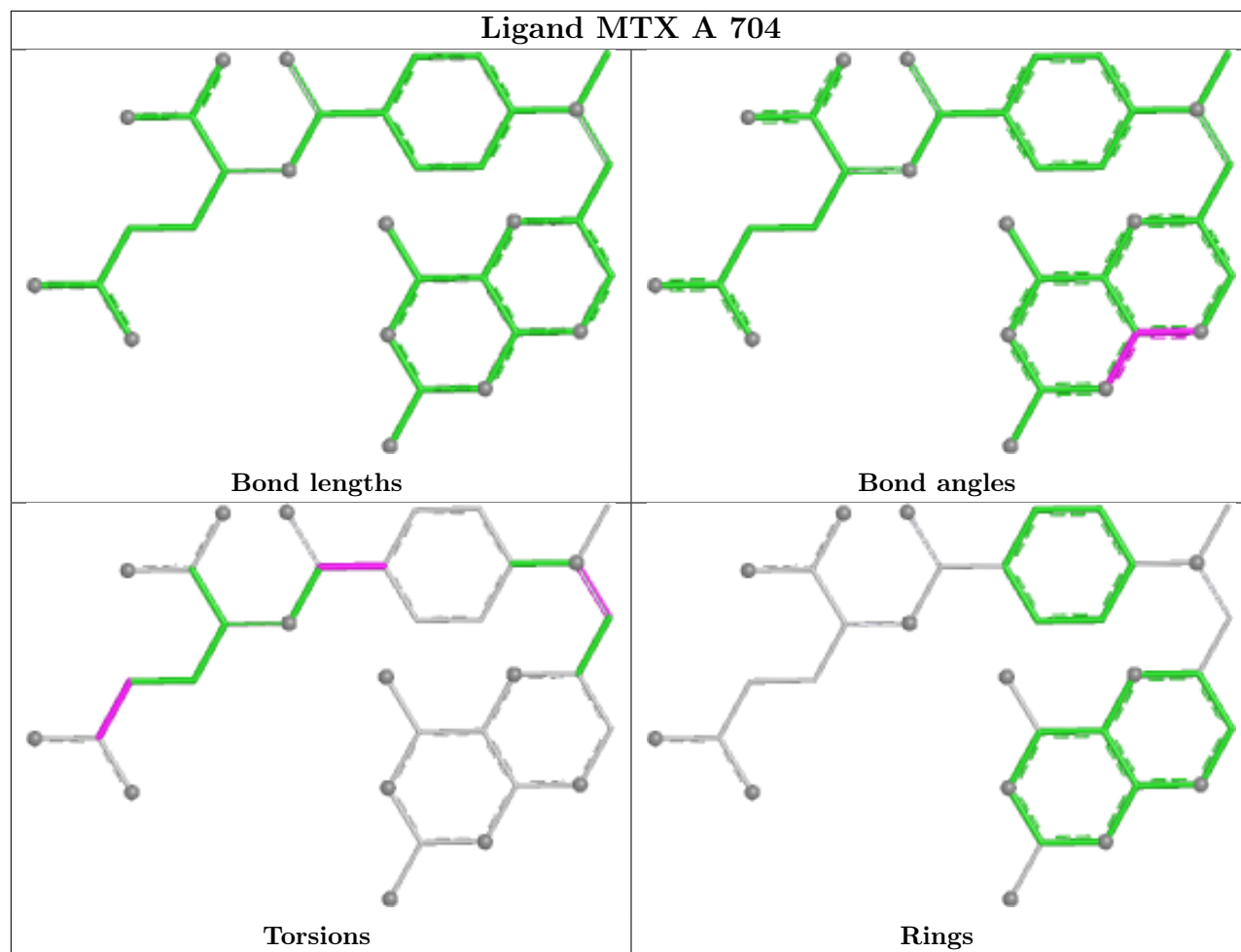
6 monomers are involved in 13 short contacts:

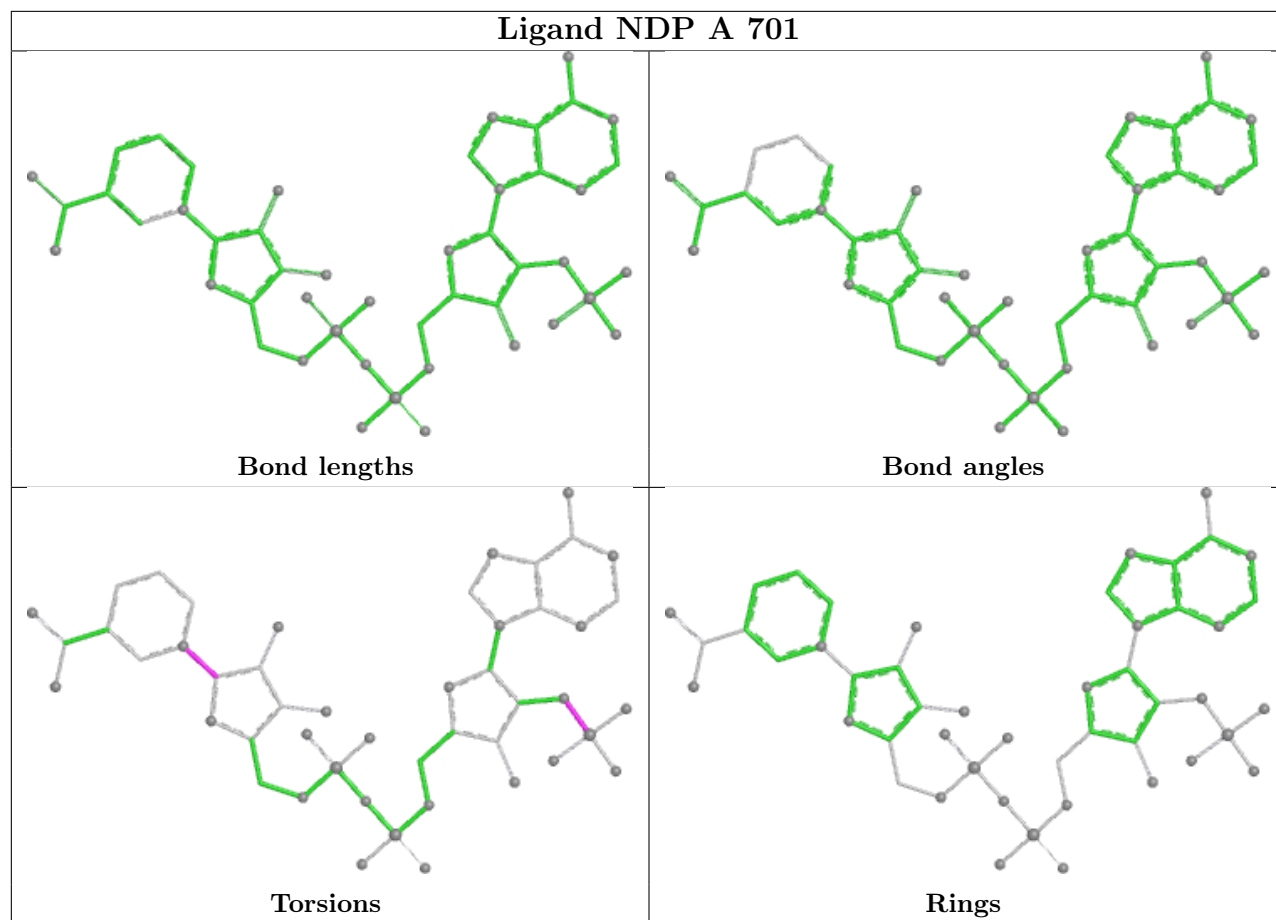
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	UMP	5	0
4	B	703	UMP	1	0
3	A	704	MTX	2	0
2	A	701	NDP	1	0
3	B	702	MTX	2	0
2	B	701	NDP	3	0

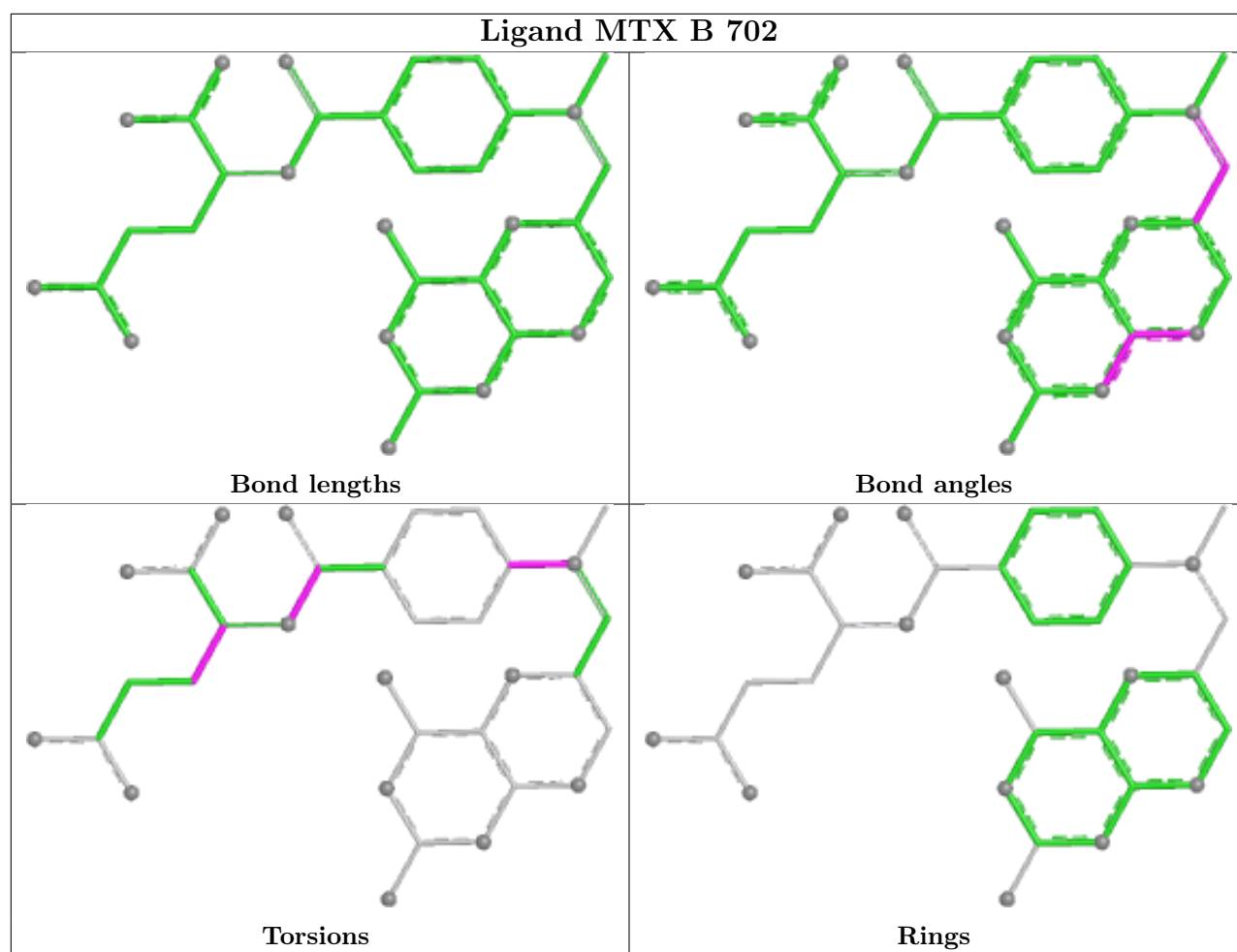
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

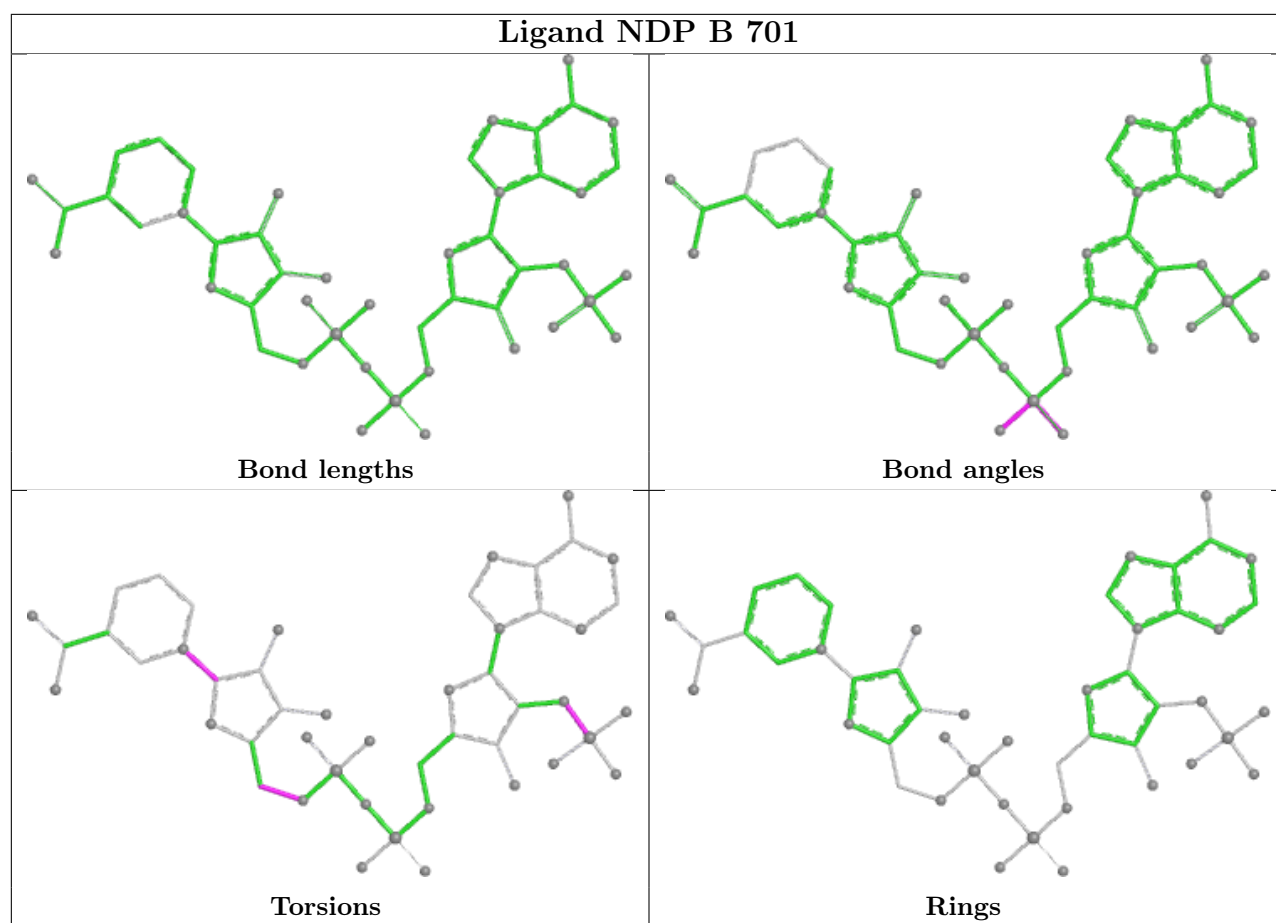












5.7 Other polymers [i](#)

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	547/608 (89%)	-0.06	20 (3%)	45 45	19, 32, 100, 162	0
1	B	546/608 (89%)	0.24	38 (6%)	22 21	19, 37, 107, 164	0
All	All	1093/1216 (89%)	0.09	58 (5%)	32 30	19, 34, 106, 164	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	ASP	6.1
1	B	85	THR	5.4
1	B	608	ALA	4.6
1	B	136	PHE	4.4
1	B	309	PRO	4.3
1	A	85	THR	4.2
1	B	140	VAL	4.0
1	A	608	ALA	4.0
1	B	1	MET	3.8
1	A	26	GLY	3.8
1	A	96	LYS	3.7
1	B	83	LYS	3.6
1	A	607	ALA	3.5
1	B	607	ALA	3.5
1	B	307	ILE	3.4
1	B	5	VAL	3.4
1	B	9	PHE	3.3
1	B	75	TYR	3.2
1	B	139	ASP	3.2
1	B	285	GLU	3.2
1	A	31	VAL	3.2
1	A	1	MET	3.1
1	B	116	PHE	3.1
1	A	307	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	285	GLU	3.1
1	B	73	LEU	3.1
1	B	28	LYS	3.0
1	B	26	GLY	3.0
1	B	81	LEU	3.0
1	A	27	LYS	2.9
1	A	2	MET	2.9
1	B	29	ASN	2.7
1	B	2	MET	2.7
1	B	606	MET	2.7
1	A	23	LYS	2.6
1	A	306	SER	2.6
1	B	137	ASP	2.6
1	B	345	ARG	2.5
1	A	309	PRO	2.5
1	B	141	TYR	2.4
1	A	24	ASN	2.4
1	B	96	LYS	2.4
1	A	604	MET	2.4
1	B	149	LEU	2.3
1	B	152	LEU	2.3
1	B	27	LYS	2.2
1	A	305	ASN	2.2
1	B	286	GLU	2.2
1	A	304	LYS	2.2
1	B	35	TYR	2.2
1	B	131	LEU	2.1
1	B	146	VAL	2.1
1	B	308	HIS	2.1
1	A	22	SER	2.1
1	B	306	SER	2.1
1	B	97	LYS	2.1
1	B	231	ASN	2.0
1	A	593	ILE	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

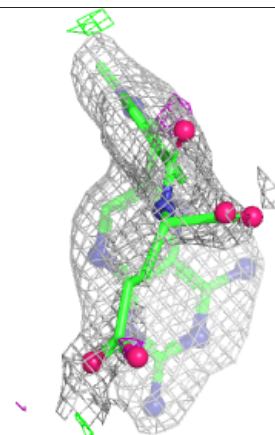
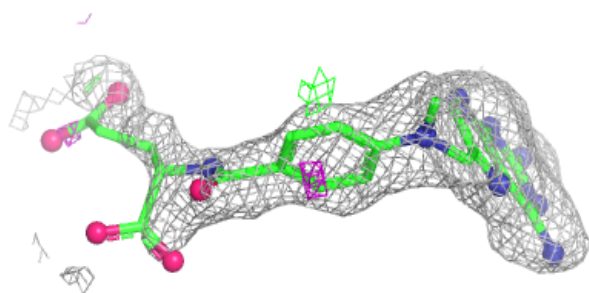
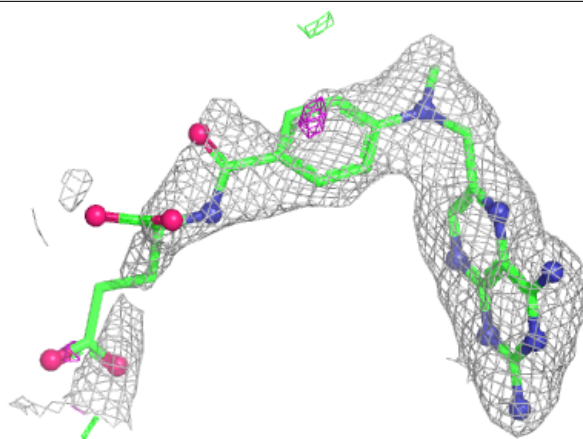
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MTX	A	704	33/33	0.85	0.13	45,57,109,120	0
3	MTX	B	702	33/33	0.85	0.12	45,55,72,85	0
2	NDP	B	701	48/48	0.90	0.10	42,60,88,95	0
5	GOL	B	704	6/6	0.90	0.13	35,41,46,53	0
4	UMP	B	703	20/20	0.93	0.11	35,52,64,64	0
5	GOL	A	705	6/6	0.94	0.08	36,46,47,48	0
3	MTX	A	702	33/33	0.94	0.08	21,27,55,75	0
4	UMP	A	703	20/20	0.97	0.07	26,35,43,43	0
2	NDP	A	701	48/48	0.97	0.05	22,29,33,34	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.

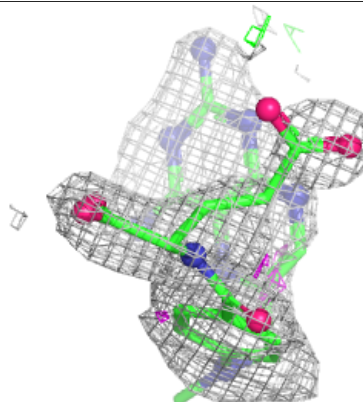
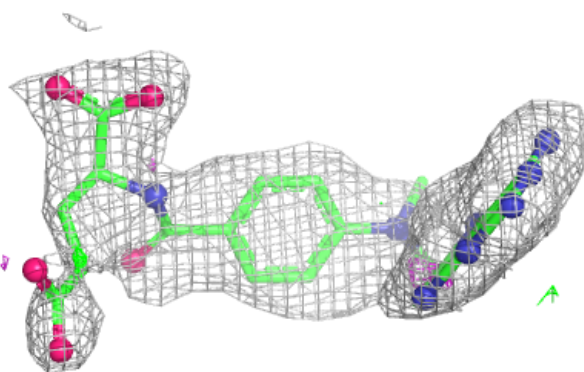
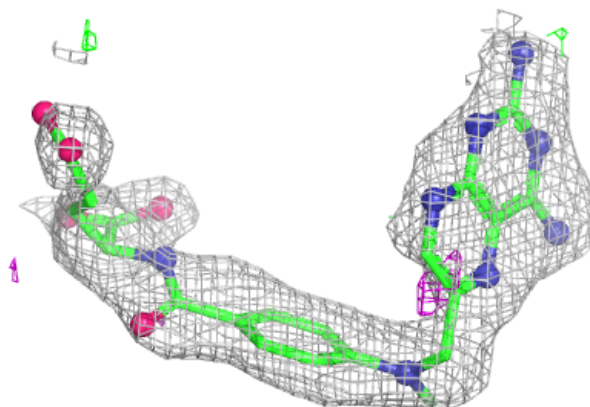
Electron density around MTX A 704:

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

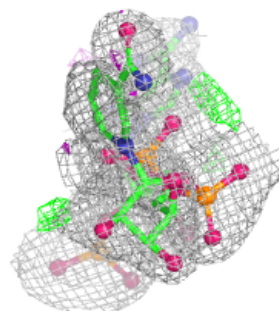
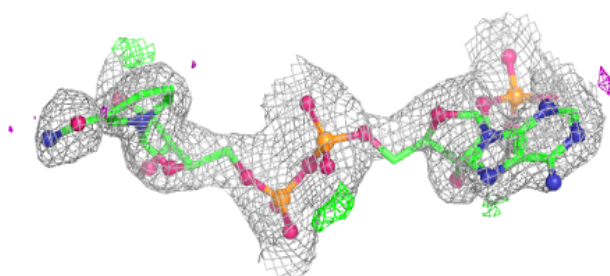
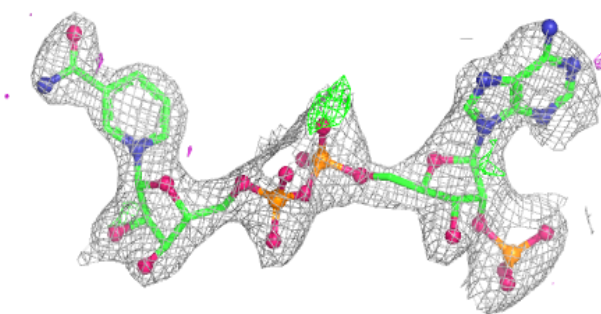


Electron density around MTX B 702:

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

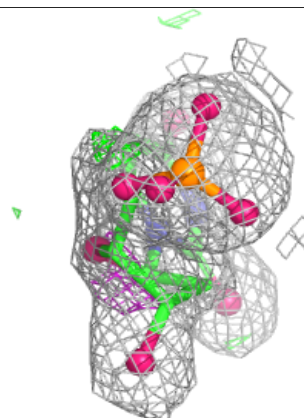
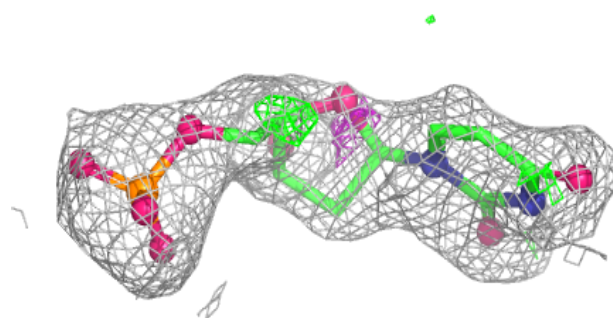
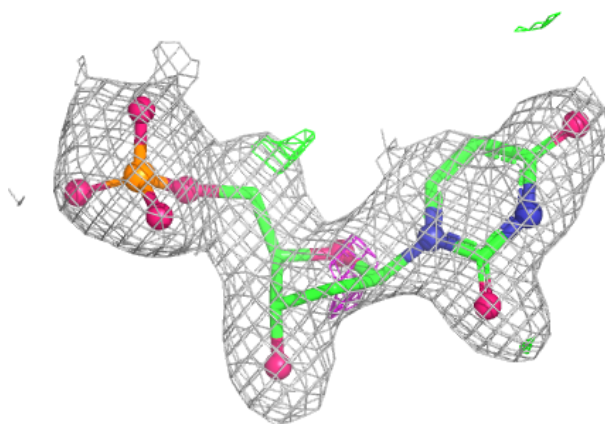
**Electron density around NDP B 701:**

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



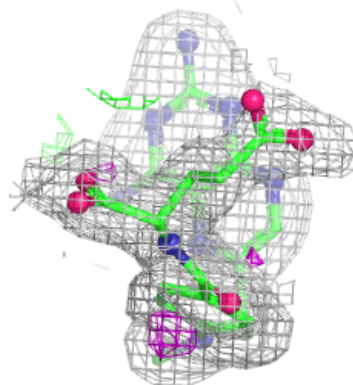
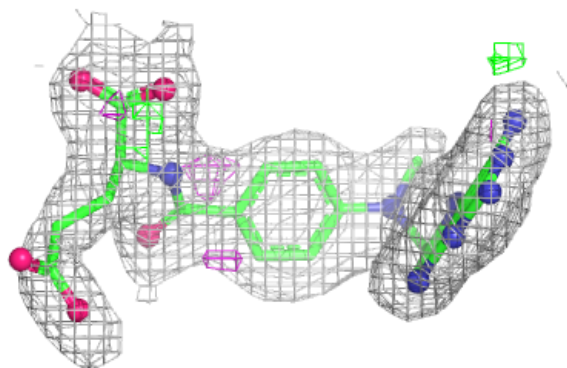
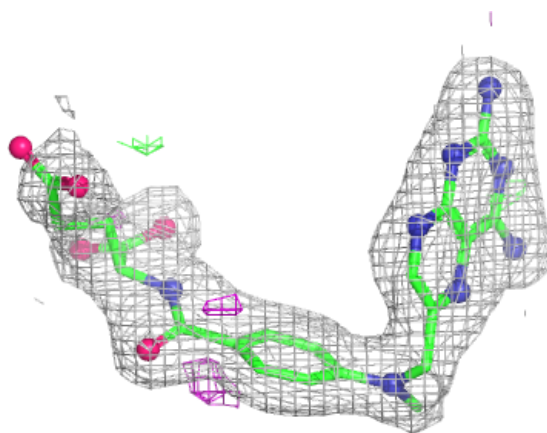
Electron density around UMP B 703:

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

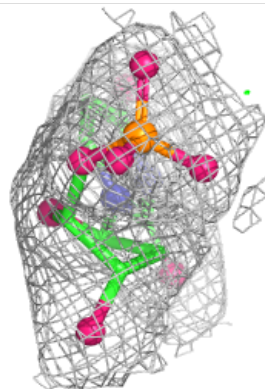
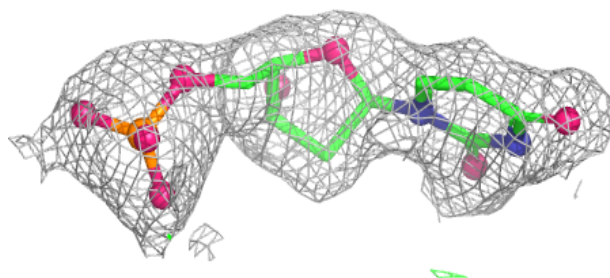
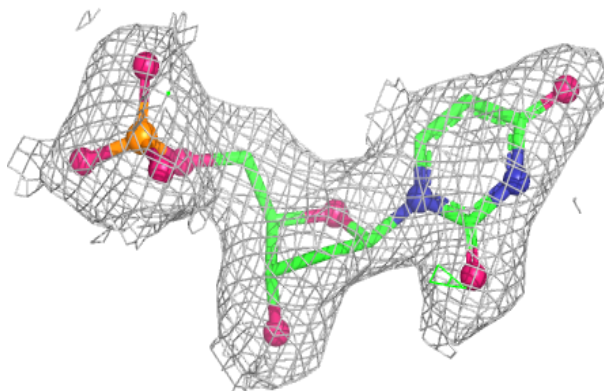


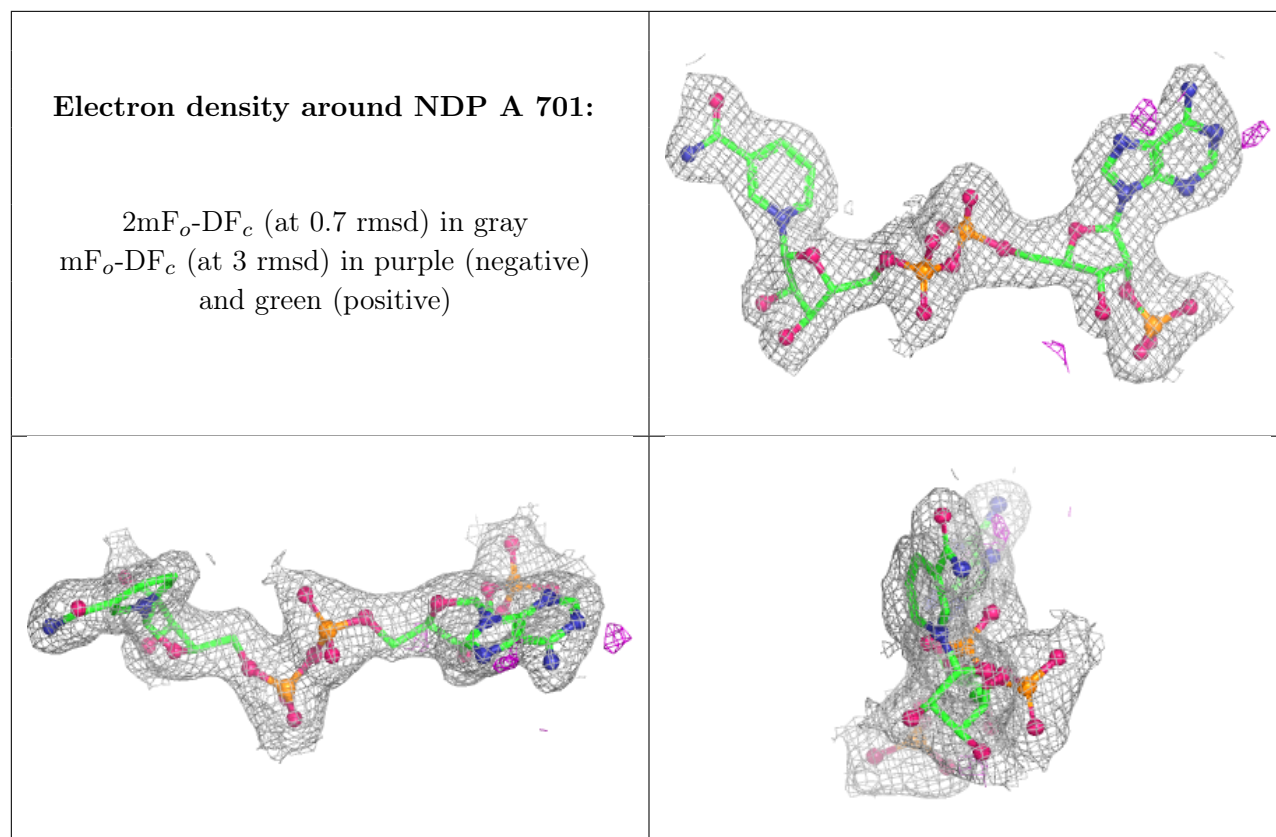
Electron density around MTX A 702:

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

**Electron density around UMP A 703:**

$2mF_o-DF_c$ (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.