



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2019 – 09:39 AM EDT

PDB ID : 6PF4
Title : Crystal structure of human thymidylate synthase Delta (7-29) in complex with dUMP and 2-(2-(4-((2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl)benzamido)phenyl)acetic acid
Authors : Czyzyk, D.J.; Valhondo, M.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2019-06-21
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

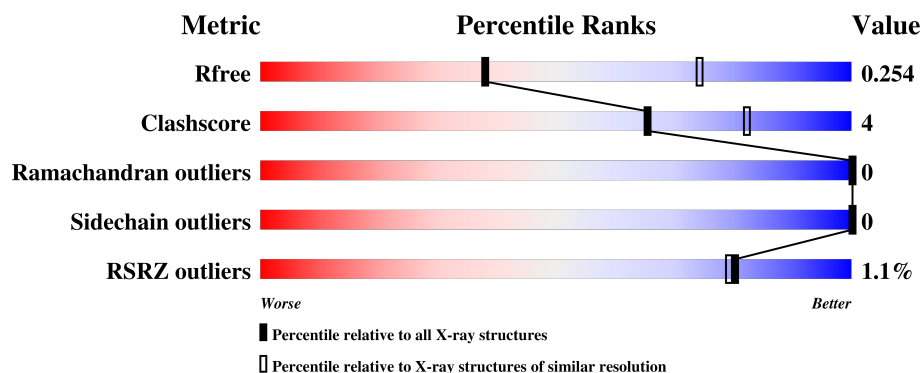
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	111664	2715 (2.90-2.82)
Clashscore	122126	2976 (2.90-2.82)
Ramachandran outliers	120053	2913 (2.90-2.82)
Sidechain outliers	120020	2916 (2.90-2.82)
RSRZ outliers	108989	2654 (2.90-2.82)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>%</div> <div>88% 10% .</div> </div>
1	B	290	<div> <div>2%</div> <div>86% 12% .</div> </div>
1	C	290	<div> <div>%</div> <div>88% 10% .</div> </div>
1	D	290	<div> <div>%</div> <div>86% 12% .</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9198 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	B	284	Total	C	N	O	S	0	0	0
			2234	1429	386	406	13			
1	A	284	Total	C	N	O	S	0	0	0
			2243	1436	387	407	13			
1	C	284	Total	C	N	O	S	0	0	0
			2251	1439	386	413	13			
1	D	284	Total	C	N	O	S	0	0	0
			2240	1432	385	410	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P04818
B	?	-	LEU	deletion	UNP P04818
B	?	-	PRO	deletion	UNP P04818
B	?	-	ARG	deletion	UNP P04818
B	?	-	ARG	deletion	UNP P04818
B	?	-	PRO	deletion	UNP P04818
B	?	-	LEU	deletion	UNP P04818
B	?	-	PRO	deletion	UNP P04818
B	?	-	PRO	deletion	UNP P04818
B	?	-	ALA	deletion	UNP P04818
B	?	-	ALA	deletion	UNP P04818
B	?	-	GLN	deletion	UNP P04818
B	?	-	GLU	deletion	UNP P04818
B	?	-	ARG	deletion	UNP P04818
B	?	-	ASP	deletion	UNP P04818
B	?	-	ALA	deletion	UNP P04818
B	?	-	GLU	deletion	UNP P04818
B	?	-	PRO	deletion	UNP P04818
B	?	-	ARG	deletion	UNP P04818
B	?	-	PRO	deletion	UNP P04818
B	?	-	PRO	deletion	UNP P04818

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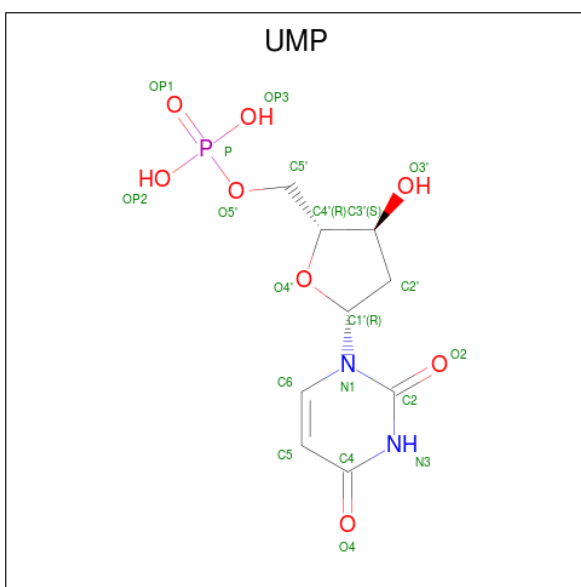
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	HIS	deletion	UNP P04818
B	?	-	GLY	deletion	UNP P04818
A	?	-	GLU	deletion	UNP P04818
A	?	-	LEU	deletion	UNP P04818
A	?	-	PRO	deletion	UNP P04818
A	?	-	ARG	deletion	UNP P04818
A	?	-	ARG	deletion	UNP P04818
A	?	-	PRO	deletion	UNP P04818
A	?	-	LEU	deletion	UNP P04818
A	?	-	PRO	deletion	UNP P04818
A	?	-	PRO	deletion	UNP P04818
A	?	-	ALA	deletion	UNP P04818
A	?	-	ALA	deletion	UNP P04818
A	?	-	GLN	deletion	UNP P04818
A	?	-	GLU	deletion	UNP P04818
A	?	-	ARG	deletion	UNP P04818
A	?	-	ASP	deletion	UNP P04818
A	?	-	ALA	deletion	UNP P04818
A	?	-	GLU	deletion	UNP P04818
A	?	-	PRO	deletion	UNP P04818
A	?	-	ARG	deletion	UNP P04818
A	?	-	PRO	deletion	UNP P04818
A	?	-	PRO	deletion	UNP P04818
A	?	-	HIS	deletion	UNP P04818
A	?	-	GLY	deletion	UNP P04818
C	?	-	GLU	deletion	UNP P04818
C	?	-	LEU	deletion	UNP P04818
C	?	-	PRO	deletion	UNP P04818
C	?	-	ARG	deletion	UNP P04818
C	?	-	ARG	deletion	UNP P04818
C	?	-	PRO	deletion	UNP P04818
C	?	-	LEU	deletion	UNP P04818
C	?	-	PRO	deletion	UNP P04818
C	?	-	PRO	deletion	UNP P04818
C	?	-	ALA	deletion	UNP P04818
C	?	-	ALA	deletion	UNP P04818
C	?	-	GLN	deletion	UNP P04818
C	?	-	GLU	deletion	UNP P04818
C	?	-	ARG	deletion	UNP P04818
C	?	-	ASP	deletion	UNP P04818
C	?	-	ALA	deletion	UNP P04818
C	?	-	GLU	deletion	UNP P04818

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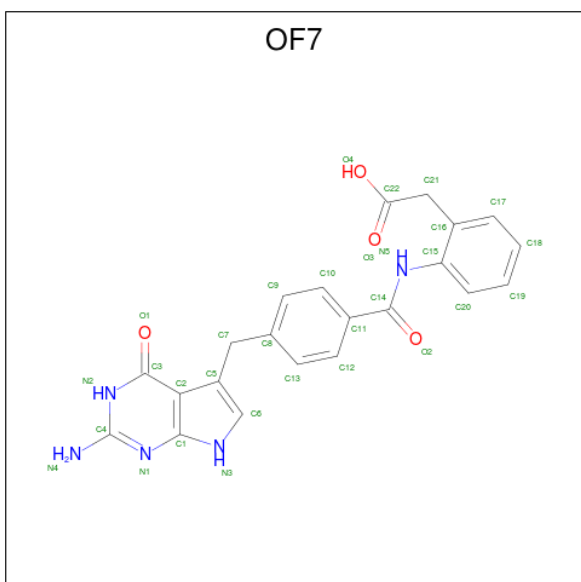
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PRO	deletion	UNP P04818
C	?	-	ARG	deletion	UNP P04818
C	?	-	PRO	deletion	UNP P04818
C	?	-	PRO	deletion	UNP P04818
C	?	-	HIS	deletion	UNP P04818
C	?	-	GLY	deletion	UNP P04818
D	?	-	GLU	deletion	UNP P04818
D	?	-	LEU	deletion	UNP P04818
D	?	-	PRO	deletion	UNP P04818
D	?	-	ARG	deletion	UNP P04818
D	?	-	ARG	deletion	UNP P04818
D	?	-	PRO	deletion	UNP P04818
D	?	-	LEU	deletion	UNP P04818
D	?	-	PRO	deletion	UNP P04818
D	?	-	PRO	deletion	UNP P04818
D	?	-	ALA	deletion	UNP P04818
D	?	-	ALA	deletion	UNP P04818
D	?	-	GLN	deletion	UNP P04818
D	?	-	GLU	deletion	UNP P04818
D	?	-	ARG	deletion	UNP P04818
D	?	-	ASP	deletion	UNP P04818
D	?	-	ALA	deletion	UNP P04818
D	?	-	GLU	deletion	UNP P04818
D	?	-	PRO	deletion	UNP P04818
D	?	-	ARG	deletion	UNP P04818
D	?	-	PRO	deletion	UNP P04818
D	?	-	PRO	deletion	UNP P04818
D	?	-	HIS	deletion	UNP P04818
D	?	-	GLY	deletion	UNP P04818

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



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

- Molecule 3 is [2-({4-[(2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl]benzene-1-carbonyl}amino)phenyl]acetic acid (three-letter code: OF7) (formula: C₂₂H₁₉N₅O₄) (labeled as "Ligand of Interest" by author).



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

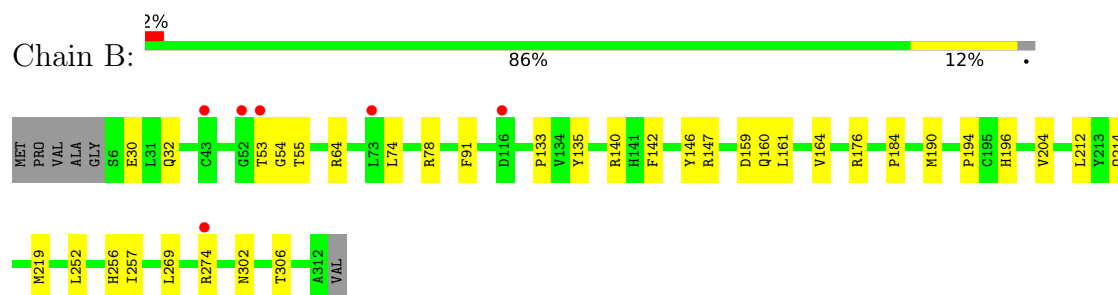
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	O	0	0
			6	6		
4	A	10	Total	O	0	0
			10	10		
4	C	6	Total	O	0	0
			6	6		
4	D	4	Total	O	0	0
			4	4		

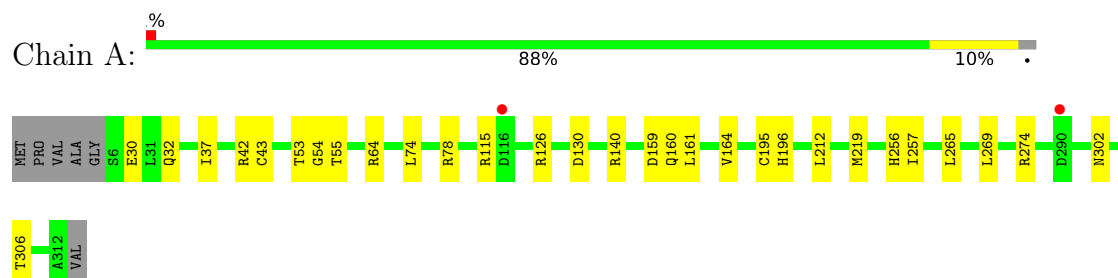
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

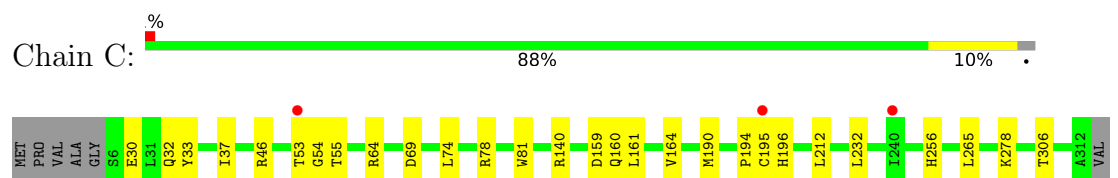
• Molecule 1: Thymidylate synthase



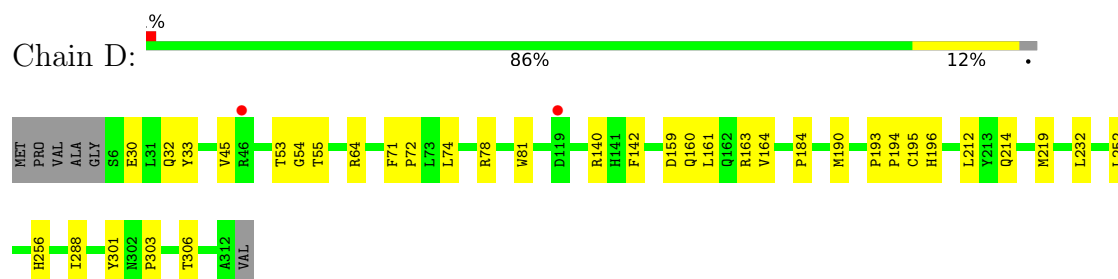
• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase



• Molecule 1: 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	92.19Å 96.44Å 135.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.55 – 2.85 47.55 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.55-2.85) 98.4 (47.55-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: 000)	Depositor
R, R_{free}	0.239 , 0.254 0.240 , 0.254	Depositor DCC
R_{free} test set	1416 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.953	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 12.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9198	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 48.29 % 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 8.7823e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UMP, OF7

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	0.27	0/2300	0.45	0/3120
1	B	0.26	0/2291	0.44	0/3111
1	C	0.27	0/2308	0.47	0/3130
1	D	0.28	0/2297	0.46	0/3118
All	All	0.27	0/9196	0.46	0/12479

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	2243	0	2168	20	0
1	B	2234	0	2146	22	0
1	C	2251	0	2175	17	0
1	D	2240	0	2153	23	0
2	A	20	0	11	1	0
2	B	20	0	11	0	0
2	C	20	0	11	1	0
2	D	20	0	11	1	0
3	A	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	0	0	0
3	C	31	0	0	0	0
3	D	31	0	0	0	0
4	A	10	0	0	0	0
4	B	6	0	0	1	0
4	C	6	0	0	0	0
4	D	4	0	0	0	0
All	All	9198	0	8686	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ARG:HB3	1:D:306:THR:HG22	1.69	0.74
1:C:196:HIS:HB2	1:C:212:LEU:HD11	1.69	0.74
1:A:196:HIS:HB2	1:A:212:LEU:HD11	1.74	0.70
1:B:196:HIS:HB2	1:B:212:LEU:HD11	1.74	0.69
1:B:78:ARG:HB3	1:B:306:THR:HG22	1.73	0.69
1:D:196:HIS:HB2	1:D:212:LEU:HD11	1.74	0.68
1:C:78:ARG:HB3	1:C:306:THR:HG22	1.78	0.64
1:A:78:ARG:HB3	1:A:306:THR:HG22	1.82	0.62
1:D:32:GLN:NE2	1:D:64:ARG:O	2.34	0.60
1:D:140:ARG:NH1	1:D:159:ASP:OD1	2.35	0.59
1:B:53:THR:HG22	1:B:54:GLY:H	1.68	0.58
1:B:204:VAL:HG21	1:D:45:VAL:HG21	1.85	0.58
1:B:140:ARG:NH1	1:B:159:ASP:OD1	2.37	0.57
1:C:140:ARG:NH1	1:C:159:ASP:OD1	2.37	0.57
1:D:53:THR:HG22	1:D:54:GLY:H	1.70	0.57
1:A:53:THR:HG22	1:A:54:GLY:H	1.70	0.56
1:C:53:THR:HG22	1:C:54:GLY:H	1.69	0.56
1:B:147:ARG:NH1	4:B:701:HOH:O	2.38	0.56
1:B:53:THR:HG22	1:B:54:GLY:N	2.21	0.55
1:B:176:ARG:HD3	1:D:193:PRO:HG2	1.89	0.55
1:A:30:GLU:HG3	1:A:74:LEU:HD22	1.88	0.54
1:A:53:THR:HG22	1:A:54:GLY:N	2.23	0.53
1:B:142:PHE:CE1	1:D:184:PRO:HD2	2.44	0.53
1:D:159:ASP:H	1:D:163:ARG:HH12	1.57	0.52
1:C:37:ILE:HD13	1:C:265:LEU:HD22	1.91	0.52
1:A:32:GLN:NE2	1:A:64:ARG:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLN:NE2	1:B:64:ARG:O	2.43	0.52
1:D:30:GLU:HG3	1:D:74:LEU:HD22	1.91	0.51
1:C:53:THR:HG22	1:C:54:GLY:N	2.25	0.51
1:D:161:LEU:HD21	1:D:288:ILE:HD13	1.92	0.51
1:D:53:THR:HG22	1:D:54:GLY:N	2.25	0.50
1:D:140:ARG:HH11	1:D:161:LEU:HB3	1.76	0.50
1:D:55:THR:HB	1:D:256:HIS:HB2	1.93	0.50
1:A:140:ARG:HH11	1:A:161:LEU:HB3	1.77	0.50
1:C:32:GLN:NE2	1:C:64:ARG:O	2.45	0.49
1:A:160:GLN:O	1:A:164:VAL:HG13	2.13	0.49
1:A:140:ARG:NH1	1:A:159:ASP:OD1	2.46	0.49
1:D:190:MET:SD	1:D:194:PRO:HD3	2.53	0.48
1:B:30:GLU:HG3	1:B:74:LEU:HD22	1.95	0.47
1:C:33:TYR:CZ	1:C:37:ILE:HD11	2.48	0.47
1:C:55:THR:HB	1:C:256:HIS:HB2	1.96	0.47
1:C:195:CYS:SG	2:C:600:UMP:C6	3.08	0.47
1:D:160:GLN:O	1:D:164:VAL:HG13	2.15	0.46
1:C:140:ARG:HH11	1:C:161:LEU:HB3	1.80	0.46
1:A:140:ARG:NH1	1:A:161:LEU:HB3	2.30	0.46
1:D:214:GLN:HB3	1:D:252:LEU:HD23	1.96	0.46
1:C:46:ARG:NH1	1:C:55:THR:O	2.49	0.45
1:B:55:THR:HB	1:B:256:HIS:HB2	1.98	0.45
1:A:115:ARG:NH2	1:A:126:ARG:O	2.31	0.45
1:B:184:PRO:HD2	1:D:142:PHE:CE1	2.51	0.44
1:B:214:GLN:HB3	1:B:252:LEU:HD23	1.98	0.44
1:B:190:MET:SD	1:B:194:PRO:HD3	2.57	0.44
1:D:195:CYS:SG	2:D:600:UMP:C6	3.11	0.43
1:A:55:THR:HB	1:A:256:HIS:HB2	2.00	0.43
1:D:81:TRP:HH2	1:D:232:LEU:HD13	1.83	0.43
1:B:91:PHE:CE1	1:B:135:TYR:HB2	2.53	0.43
1:C:160:GLN:O	1:C:164:VAL:HG13	2.19	0.43
1:B:160:GLN:O	1:B:164:VAL:HG13	2.18	0.43
1:B:274:ARG:NH1	1:B:302:ASN:O	2.47	0.43
1:C:81:TRP:HH2	1:C:232:LEU:HD13	1.84	0.42
1:A:42:ARG:HG3	1:A:43:CYS:SG	2.59	0.42
1:B:140:ARG:HH11	1:B:161:LEU:HB3	1.85	0.42
1:A:219:MET:HB2	1:A:257:ILE:HG12	2.02	0.42
1:A:195:CYS:SG	2:A:600:UMP:C6	3.13	0.41
1:D:33:TYR:OH	1:D:219:MET:O	2.30	0.41
1:A:126:ARG:HD3	1:A:130:ASP:O	2.20	0.41
1:B:133:PRO:HG3	1:B:146:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASP:OD2	1:C:278:LYS:NZ	2.46	0.41
1:A:269:LEU:HD12	1:A:269:LEU:HA	1.85	0.41
1:C:30:GLU:HG3	1:C:74:LEU:HD22	2.02	0.41
1:D:301:TYR:CE2	1:D:303:PRO:HG3	2.56	0.41
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.86	0.41
1:D:71:PHE:HA	1:D:72:PRO:HD3	1.93	0.41
1:A:161:LEU:O	1:A:164:VAL:HG22	2.21	0.40
1:C:190:MET:SD	1:C:194:PRO:HD3	2.61	0.40
1:B:219:MET:HB2	1:B:257:ILE:HG12	2.02	0.40
1:A:37:ILE:HD12	1:A:265:LEU:HD13	2.03	0.40
1:A:274:ARG:HD2	1:A:302:ASN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/290 (97%)	269 (95%)	13 (5%)	0	100	100
1	B	282/290 (97%)	268 (95%)	14 (5%)	0	100	100
1	C	282/290 (97%)	268 (95%)	14 (5%)	0	100	100
1	D	282/290 (97%)	268 (95%)	14 (5%)	0	100	100
All	All	1128/1160 (97%)	1073 (95%)	55 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/252 (93%)	235 (100%)	0	100	100
1	B	233/252 (92%)	233 (100%)	0	100	100
1	C	238/252 (94%)	238 (100%)	0	100	100
1	D	235/252 (93%)	235 (100%)	0	100	100
All	All	941/1008 (93%)	941 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	196	HIS
1	C	211	GLN
1	D	196	HIS
1	D	250	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	A	600	-	17,21,21	1.50	2 (11%)	22,31,31	1.42	2 (9%)
3	OF7	A	601	-	30,34,34	1.32	3 (10%)	35,48,48	2.20	7 (20%)
2	UMP	B	600	-	17,21,21	1.69	3 (17%)	22,31,31	1.54	2 (9%)
3	OF7	B	601	-	30,34,34	1.28	3 (10%)	35,48,48	2.29	7 (20%)
2	UMP	C	600	-	17,21,21	1.70	3 (17%)	22,31,31	1.49	2 (9%)
3	OF7	C	601	-	30,34,34	1.32	4 (13%)	35,48,48	2.25	6 (17%)
2	UMP	D	600	-	17,21,21	1.69	3 (17%)	22,31,31	1.55	3 (13%)
3	OF7	D	601	-	30,34,34	1.32	4 (13%)	35,48,48	2.33	7 (20%)

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	A	600	-	-	1/6/22/22	0/2/2/2
3	OF7	A	601	-	-	0/14/16/16	0/4/4/4
2	UMP	B	600	-	-	1/6/22/22	0/2/2/2
3	OF7	B	601	-	-	0/14/16/16	0/4/4/4
2	UMP	C	600	-	-	1/6/22/22	0/2/2/2
3	OF7	C	601	-	-	3/14/16/16	0/4/4/4
2	UMP	D	600	-	-	1/6/22/22	0/2/2/2
3	OF7	D	601	-	-	2/14/16/16	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	UMP	C4-N3	4.10	1.40	1.33
2	C	600	UMP	C4-N3	4.06	1.40	1.33
2	B	600	UMP	C4-N3	3.98	1.40	1.33
2	D	600	UMP	C4-N3	3.94	1.39	1.33
2	C	600	UMP	P-OP1	3.69	1.62	1.50
2	B	600	UMP	P-OP1	3.61	1.62	1.50
2	D	600	UMP	P-OP1	3.60	1.62	1.50
3	A	601	OF7	C4-N2	3.25	1.41	1.35
3	B	601	OF7	C4-N2	3.18	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	OF7	C4-N2	3.16	1.41	1.35
3	C	601	OF7	C4-N2	2.98	1.40	1.35
2	B	600	UMP	C6-N1	2.62	1.39	1.35
2	D	600	UMP	C6-N1	2.62	1.39	1.35
2	A	600	UMP	C6-N1	2.52	1.39	1.35
2	C	600	UMP	C6-N1	2.43	1.39	1.35
3	D	601	OF7	C15-C16	2.40	1.43	1.40
3	C	601	OF7	C2-C1	-2.32	1.36	1.43
3	A	601	OF7	C4-N4	2.27	1.38	1.33
3	C	601	OF7	C15-C16	2.20	1.43	1.40
3	D	601	OF7	C2-C1	-2.19	1.37	1.43
3	B	601	OF7	C4-N4	2.19	1.38	1.33
3	C	601	OF7	C4-N4	2.16	1.38	1.33
3	B	601	OF7	C2-C1	-2.15	1.37	1.43
3	A	601	OF7	C2-C1	-2.12	1.37	1.43
3	D	601	OF7	C4-N4	2.10	1.38	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	OF7	C2-C3-N2	-9.92	115.21	124.08
3	D	601	OF7	C2-C3-N2	-9.84	115.29	124.08
3	C	601	OF7	C2-C3-N2	-9.71	115.41	124.08
3	A	601	OF7	C2-C3-N2	-9.63	115.47	124.08
3	B	601	OF7	C3-N2-C4	4.65	122.69	116.06
3	A	601	OF7	C3-N2-C4	4.65	122.68	116.06
3	C	601	OF7	C3-N2-C4	4.62	122.64	116.06
3	D	601	OF7	C3-N2-C4	4.56	122.55	116.06
2	C	600	UMP	C5-C4-N3	-4.01	114.29	123.28
2	D	600	UMP	C5-C4-N3	-3.86	114.63	123.28
2	A	600	UMP	C5-C4-N3	-3.85	114.64	123.28
2	B	600	UMP	C5-C4-N3	-3.82	114.72	123.28
2	B	600	UMP	OP2-P-O5'	3.75	116.70	106.73
3	C	601	OF7	N4-C4-N1	3.71	123.90	117.77
3	D	601	OF7	N4-C4-N1	3.70	123.88	117.77
3	B	601	OF7	N4-C4-N1	3.68	123.84	117.77
3	A	601	OF7	N4-C4-N1	3.66	123.82	117.77
2	D	600	UMP	OP2-P-O5'	3.60	116.31	106.73
3	D	601	OF7	C3-C2-C1	3.54	117.01	115.04
3	B	601	OF7	C3-C2-C1	3.54	117.01	115.04
3	D	601	OF7	N4-C4-N2	-3.51	111.76	117.25
3	B	601	OF7	N4-C4-N2	-3.36	112.00	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	OF7	N4-C4-N2	-3.33	112.03	117.25
2	C	600	UMP	OP2-P-O5'	3.27	115.45	106.73
3	C	601	OF7	C3-C2-C1	3.18	116.81	115.04
3	A	601	OF7	N4-C4-N2	-3.16	112.31	117.25
2	A	600	UMP	O5'-P-OP1	3.04	115.01	106.47
3	A	601	OF7	C3-C2-C1	3.02	116.72	115.04
3	A	601	OF7	N1-C4-N2	-2.50	123.87	127.25
3	C	601	OF7	N1-C4-N2	-2.35	124.07	127.25
3	D	601	OF7	C21-C16-C17	-2.33	116.59	120.45
3	B	601	OF7	N1-C4-N2	-2.28	124.16	127.25
2	D	600	UMP	OP3-P-OP2	2.14	115.90	107.57
3	D	601	OF7	N1-C4-N2	-2.13	124.37	127.25
3	B	601	OF7	C15-N5-C14	2.07	132.63	126.95
3	A	601	OF7	C22-C21-C16	-2.03	110.00	114.71

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	OF7	C17-C16-C21-C22
2	D	600	UMP	O4'-C4'-C5'-O5'
2	A	600	UMP	O4'-C4'-C5'-O5'
2	B	600	UMP	O4'-C4'-C5'-O5'
2	C	600	UMP	O4'-C4'-C5'-O5'
3	C	601	OF7	C20-C15-N5-C14
3	D	601	OF7	C20-C15-N5-C14
3	C	601	OF7	C16-C15-N5-C14
3	D	601	OF7	C16-C15-N5-C14

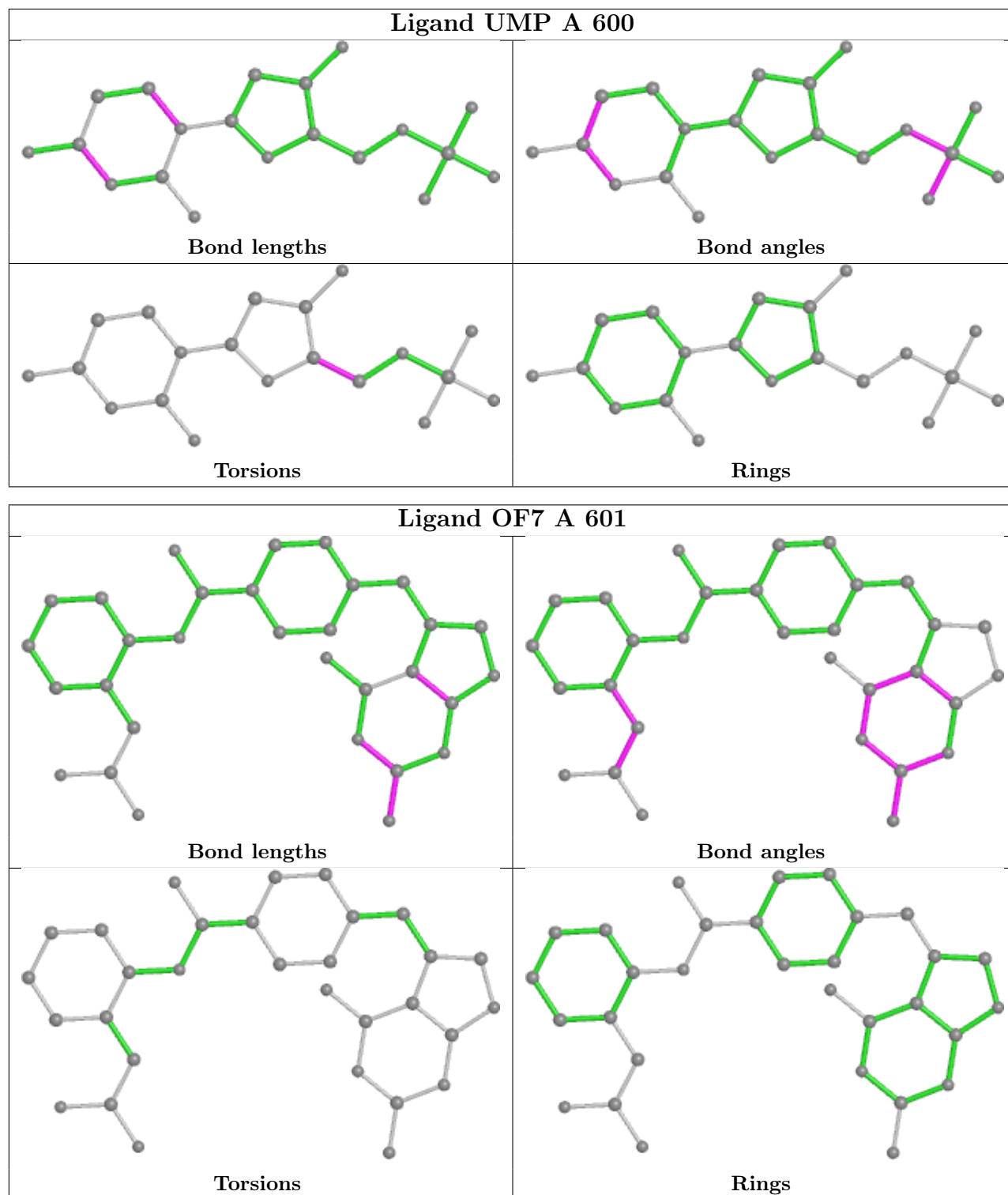
There are no ring outliers.

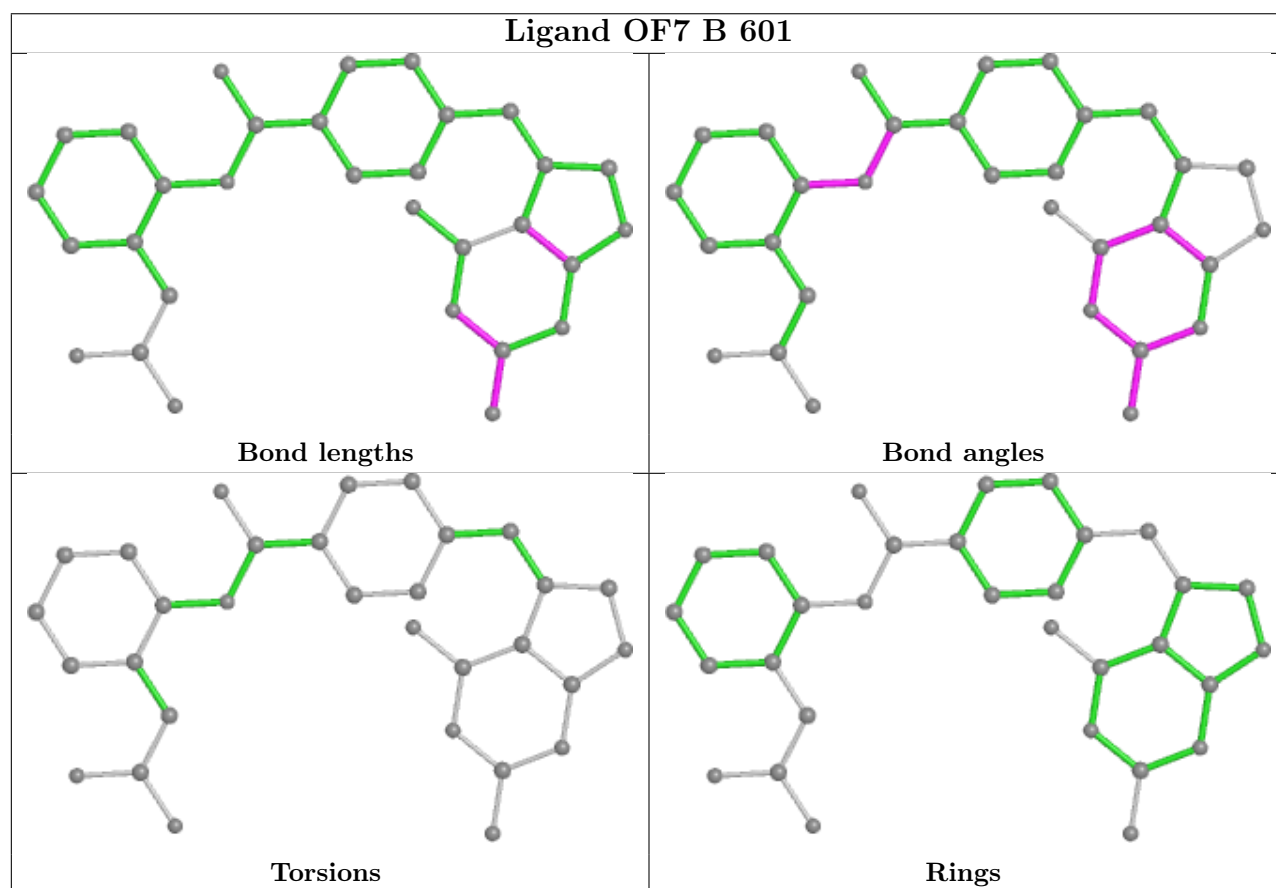
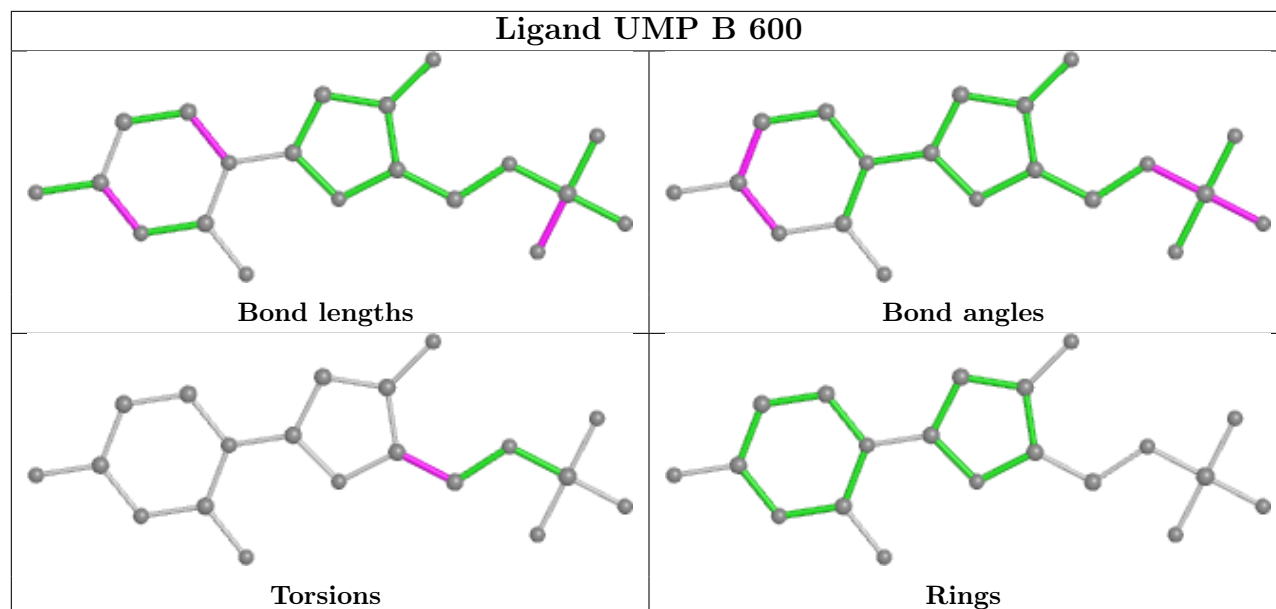
3 monomers are involved in 3 short contacts:

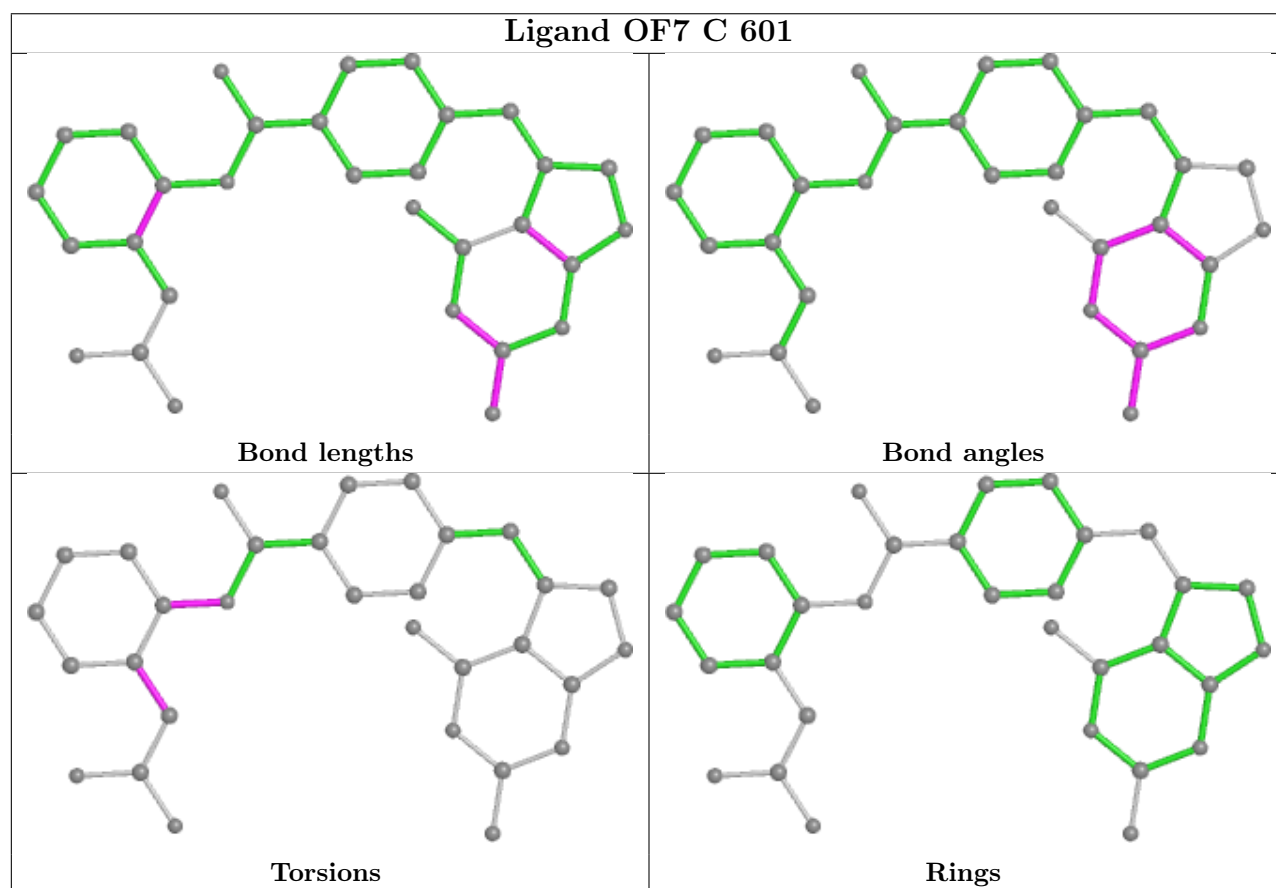
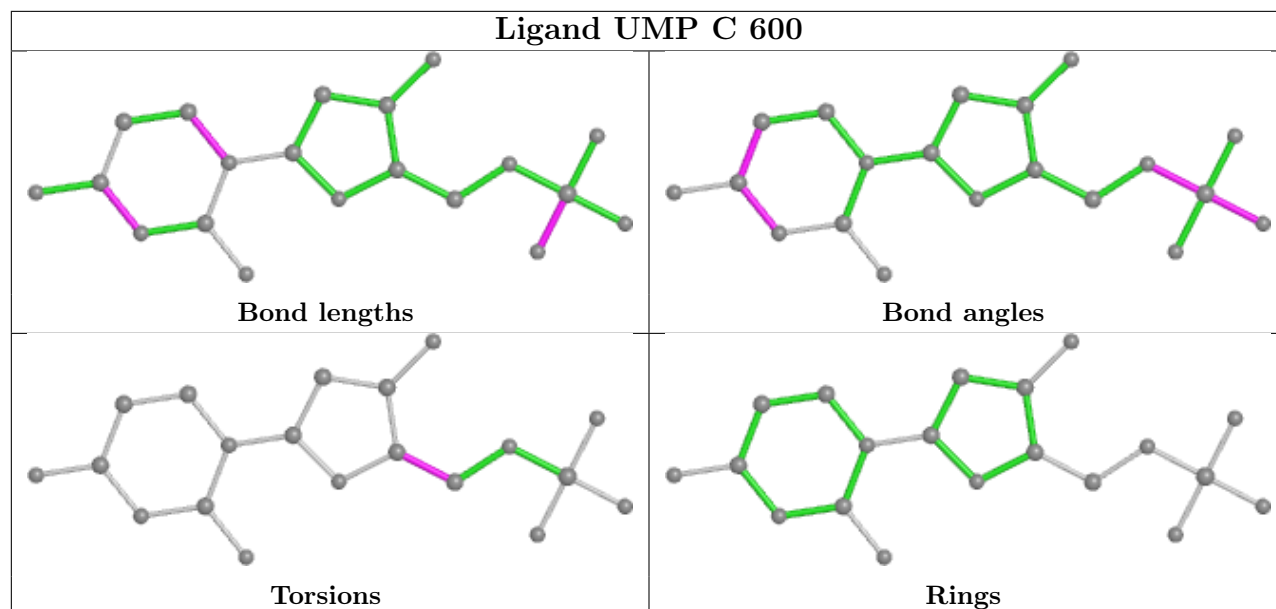
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	UMP	1	0
2	C	600	UMP	1	0
2	D	600	UMP	1	0

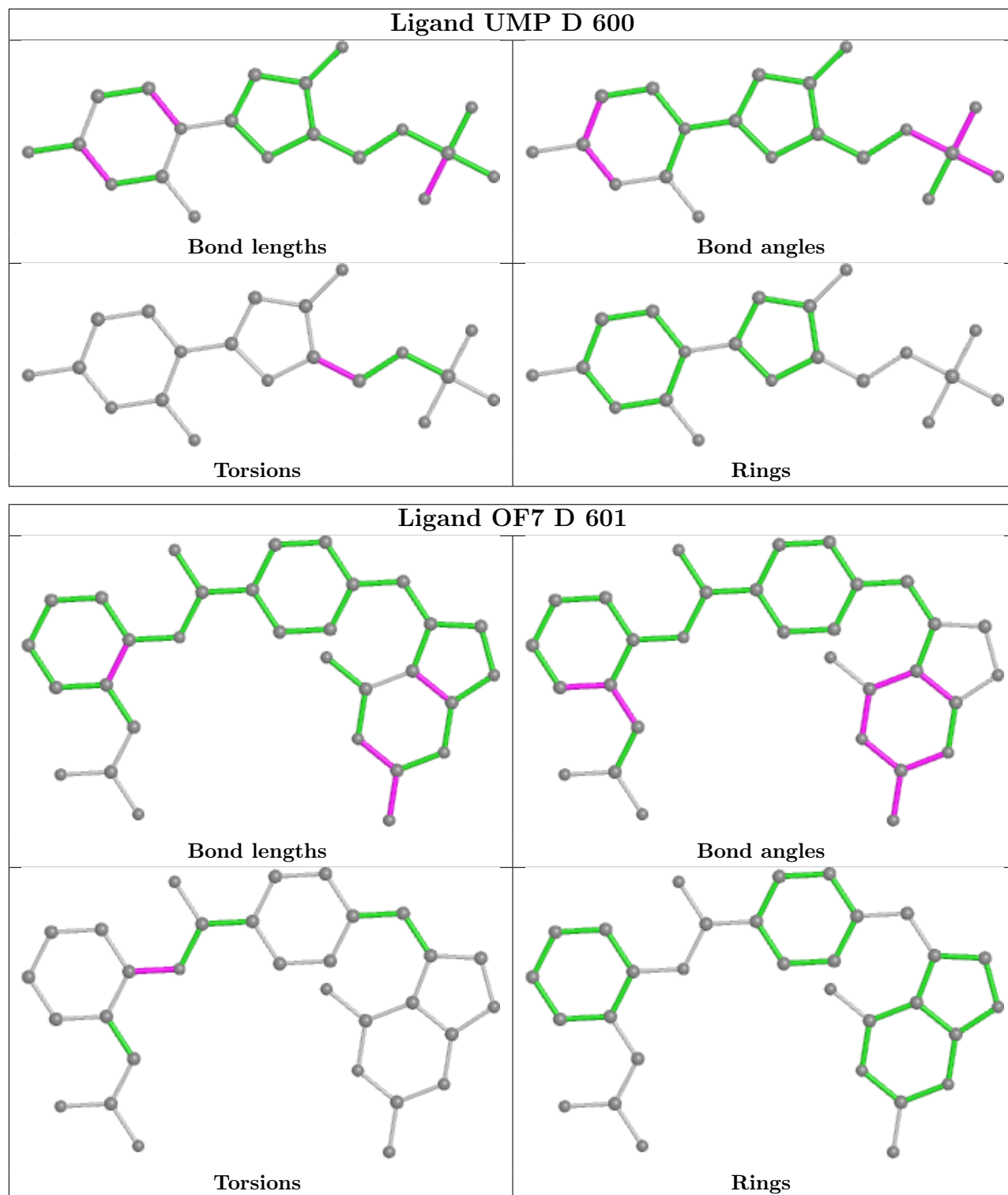
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	284/290 (97%)	0.29	2 (0%) 87 87	27, 34, 44, 52	0
1	B	284/290 (97%)	0.52	6 (2%) 63 60	30, 38, 54, 60	0
1	C	284/290 (97%)	0.40	3 (1%) 80 79	27, 33, 42, 50	0
1	D	284/290 (97%)	0.44	2 (0%) 87 87	29, 38, 48, 60	0
All	All	1136/1160 (97%)	0.41	13 (1%) 80 79	27, 36, 47, 60	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	GLY	3.5
1	B	116	ASP	3.1
1	A	290	ASP	3.1
1	A	116	ASP	2.6
1	D	46	ARG	2.6
1	D	119	ASP	2.6
1	C	240	ILE	2.4
1	B	43	CYS	2.3
1	B	274	ARG	2.3
1	C	53	THR	2.2
1	B	53	THR	2.0
1	C	195	CYS	2.0
1	B	73	LEU	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

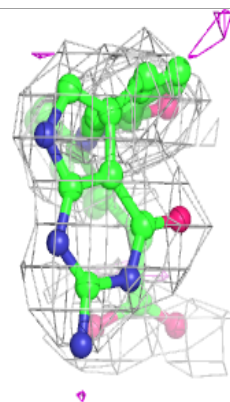
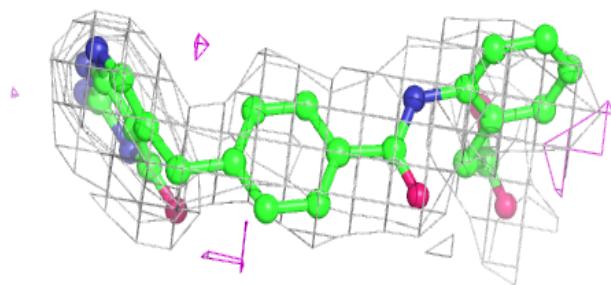
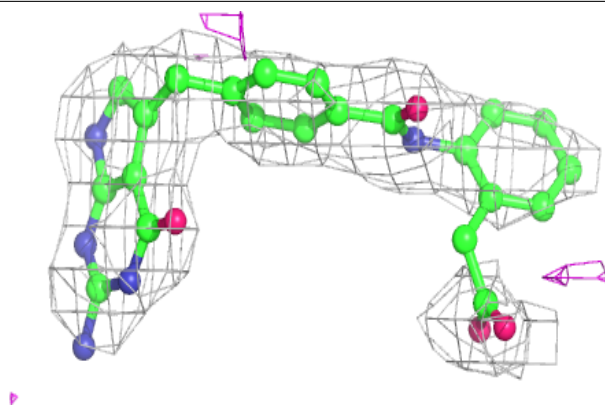
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	OF7	C	601	31/31	0.84	0.29	29,31,40,44	0
3	OF7	D	601	31/31	0.86	0.26	33,35,41,44	0
3	OF7	B	601	31/31	0.87	0.23	37,39,46,47	0
3	OF7	A	601	31/31	0.87	0.24	32,34,36,44	0
2	UMP	A	600	20/20	0.90	0.23	31,32,34,34	0
2	UMP	B	600	20/20	0.90	0.19	35,37,40,41	0
2	UMP	C	600	20/20	0.91	0.21	28,29,31,31	0
2	UMP	D	600	20/20	0.93	0.22	32,34,34,35	0

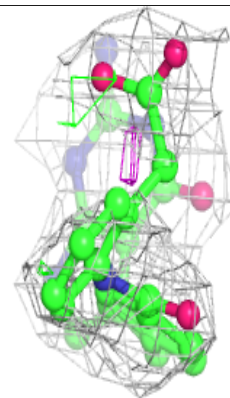
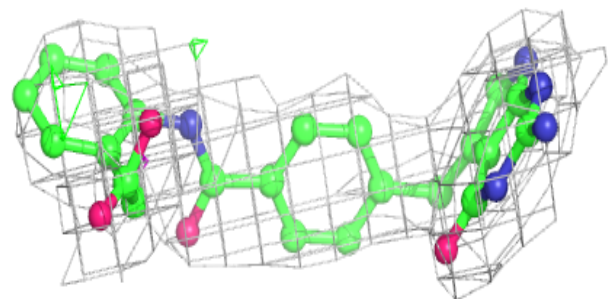
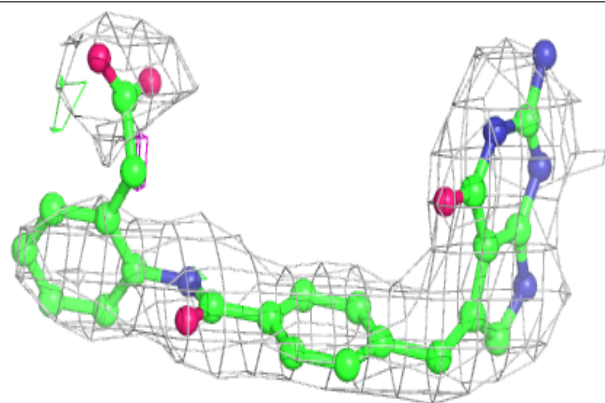
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OF7 C 601:

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

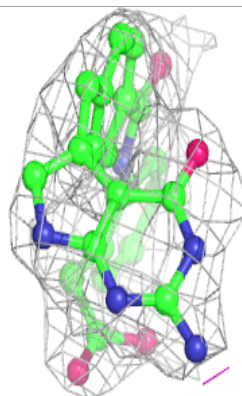
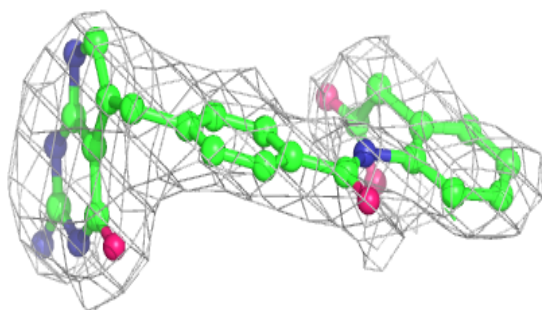
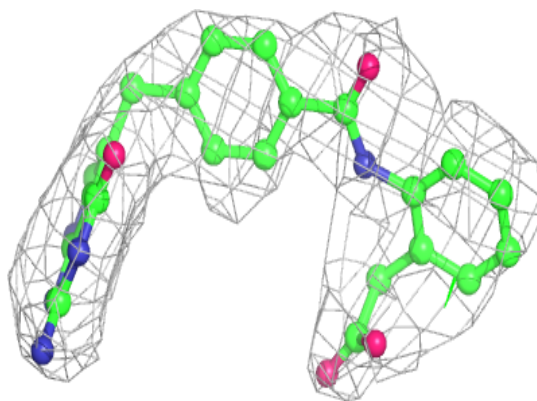
**Electron density around OF7 D 601:**

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

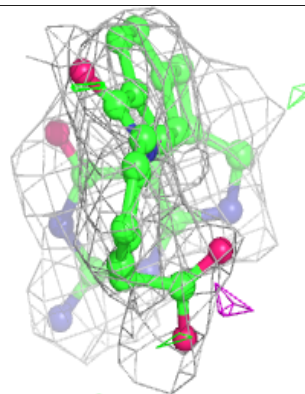
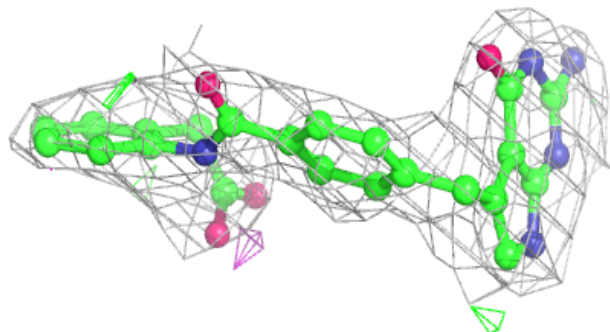
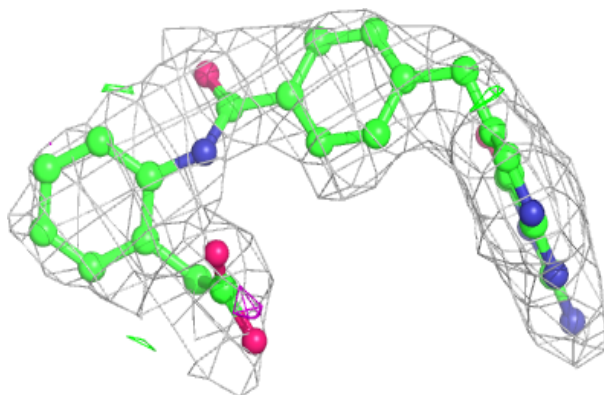


Electron density around OF7 B 601:

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

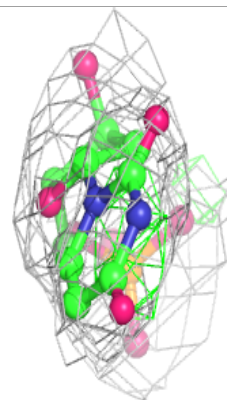
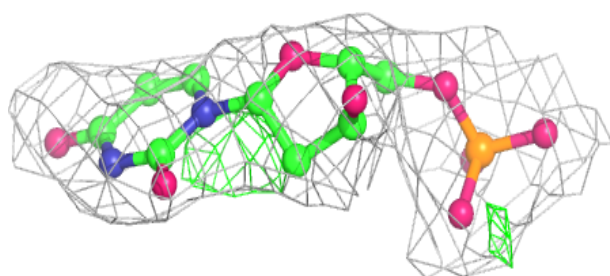
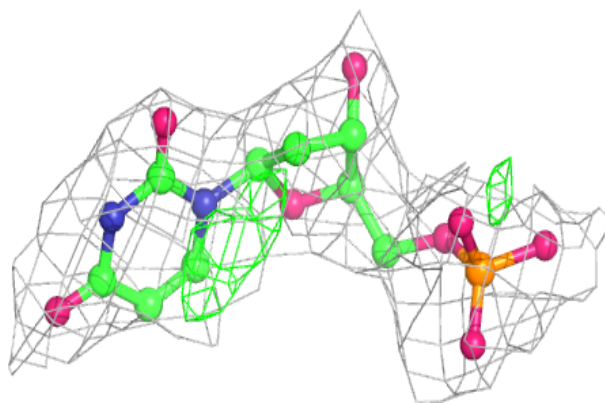
**Electron density around OF7 A 601:**

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

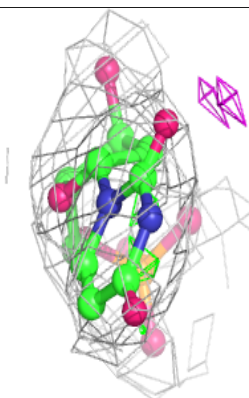
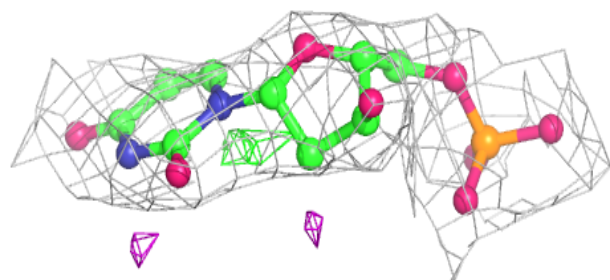
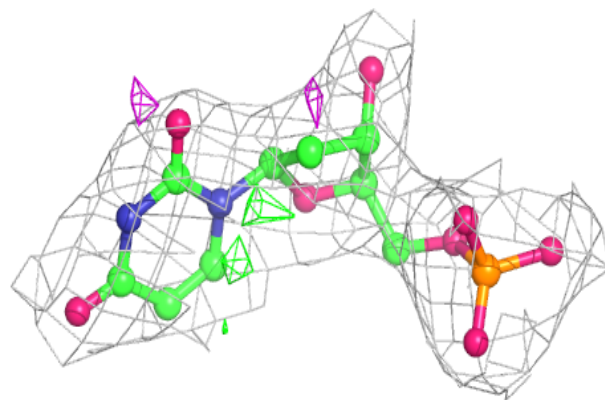


Electron density around UMP A 600:

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

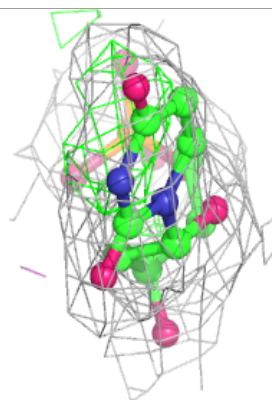
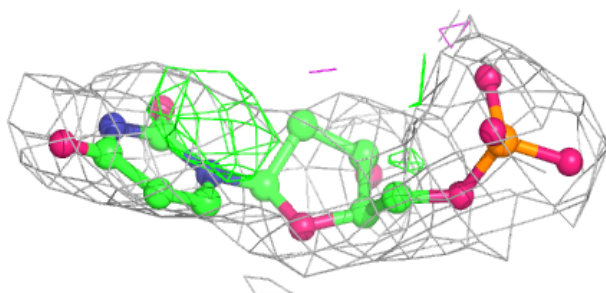
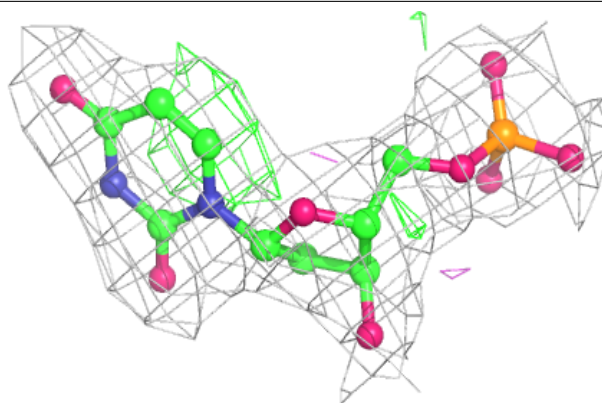
**Electron density around UMP B 600:**

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

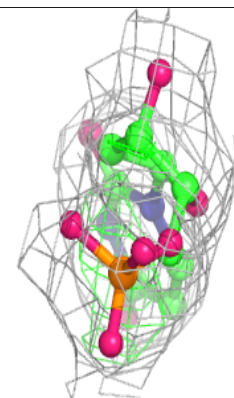
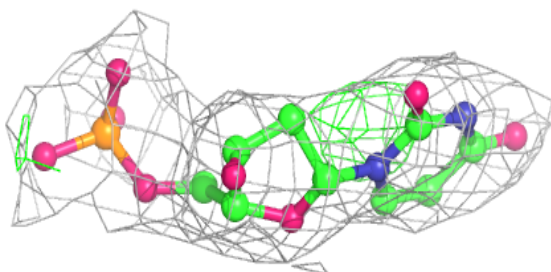
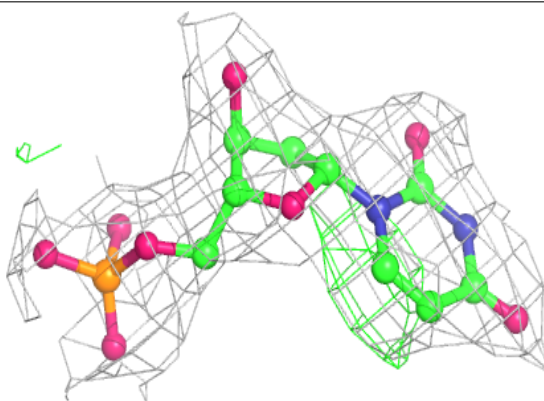


Electron density around UMP C 600:

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

**Electron density around UMP D 600:**

$2mF_o-DF_c$ (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.