



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2019 – 09:45 AM EDT

PDB ID : 6PF3
Title : Crystal structure of human thymidylate synthase Delta (7-29) in complex with dUMP and 2-(4-((2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl)benzamido)-4-chlorobenzoic acid
Authors : Czyzyk, D.J.; Valhondo, M.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2019-06-21
Resolution : 2.39 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

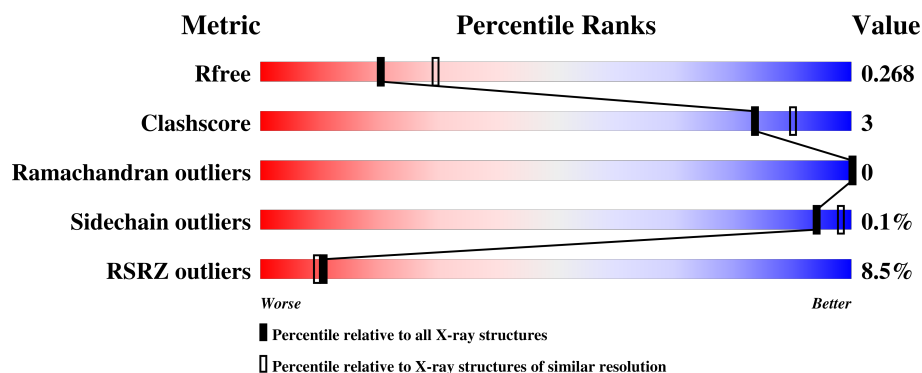
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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>6%</div> <div> <div></div> <div>91%</div> <div>7% •</div> </div> </div>
1	B	290	<div> <div>8%</div> <div> <div></div> <div>91%</div> <div>7% •</div> </div> </div>
1	C	290	<div> <div>9%</div> <div> <div></div> <div>90%</div> <div>8% •</div> </div> </div>
1	D	290	<div> <div>11%</div> <div> <div></div> <div>93%</div> <div>5% •</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9080 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	285	Total	C	N	O	S	0	0	0
			2199	1408	382	396	13			
1	B	285	Total	C	N	O	S	0	0	0
			2208	1415	384	396	13			
1	C	285	Total	C	N	O	S	0	0	0
			2215	1412	389	401	13			
1	D	285	Total	C	N	O	S	0	0	0
			2212	1416	388	396	12			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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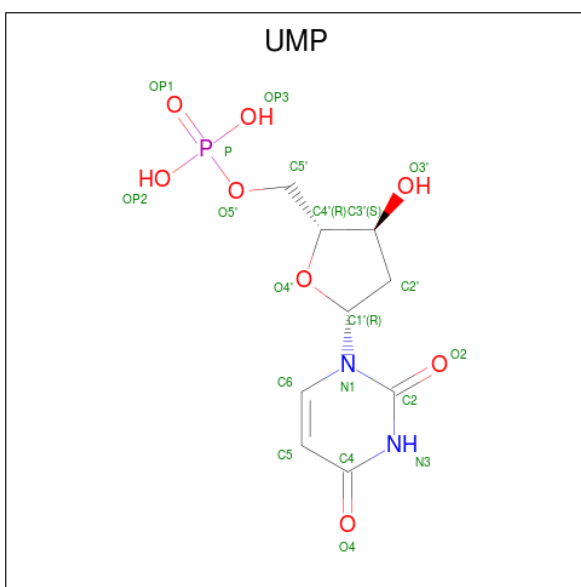
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P04818
A	?	-	GLY	deletion	UNP P04818
B	?	-	GLU	deletion	UNP P04818
B	?	-	LEU	deletion	UNP P04818
B	?	-	PRO	deletion	UNP P04818
B	?	-	ARG	deletion	UNP P04818
B	?	-	ARG	deletion	UNP P04818
B	?	-	PRO	deletion	UNP P04818
B	?	-	LEU	deletion	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
B	?	-	HIS	deletion	UNP P04818
B	?	-	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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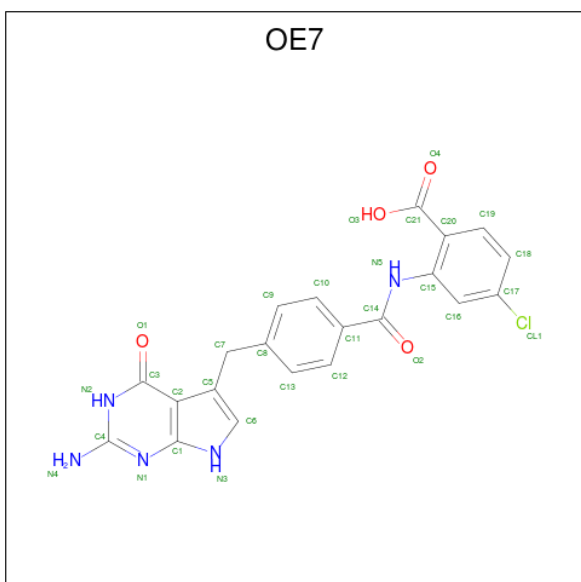
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PRO	deletion	UNP P04818
C	?	-	ARG	deletion	UNP P04818
C	?	-	PRO	deletion	UNP P04818
C	?	-	PRO	deletion	UNP P04818
C	?	-	HIS	deletion	UNP P04818
C	?	-	GLY	deletion	UNP P04818
D	?	-	GLU	deletion	UNP P04818
D	?	-	LEU	deletion	UNP P04818
D	?	-	PRO	deletion	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: C₉H₁₃N₂O₈P).



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		

- 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)-4-chlorobenzoic acid (three-letter code: OE7) (formula: $C_{21}H_{16}ClN_5O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 21	Cl 1	N 5	O 4	0	0
3	B	1	Total 31	C 21	Cl 1	N 5	O 4	0	0
3	C	1	Total 31	C 21	Cl 1	N 5	O 4	0	0
3	D	1	Total 31	C 21	Cl 1	N 5	O 4	0	0

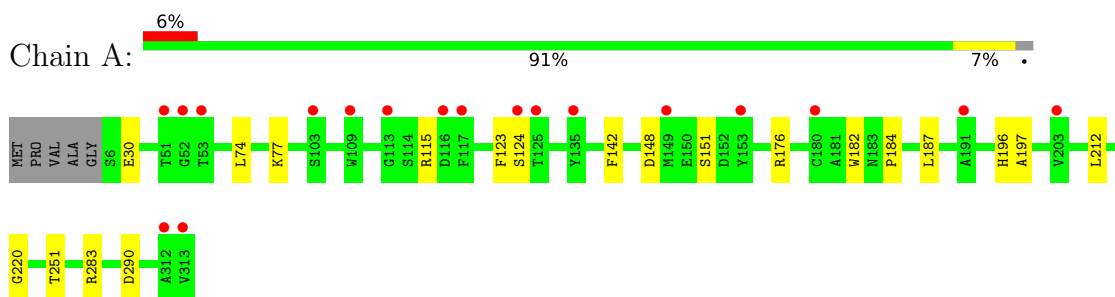
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total 11	O 11	0	0
4	B	10	Total 10	O 10	0	0
4	C	12	Total 12	O 12	0	0
4	D	9	Total 9	O 9	0	0

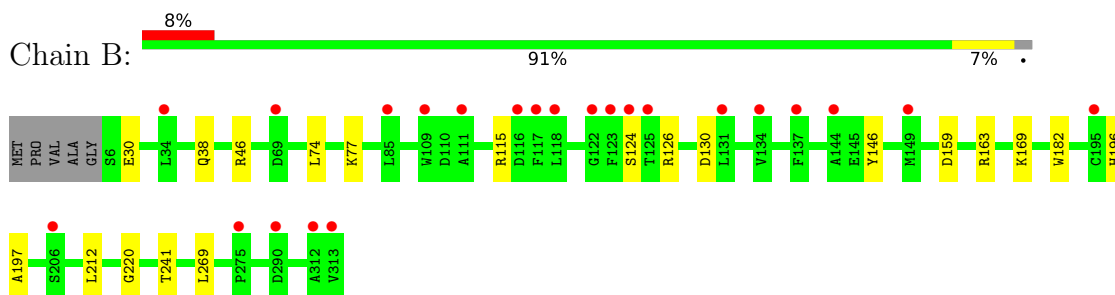
3 Residue-property plots [i](#)

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.

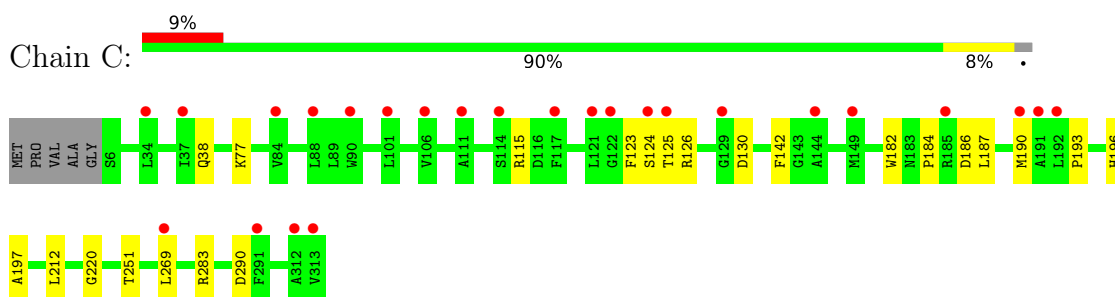
• Molecule 1: Thymidylate synthase



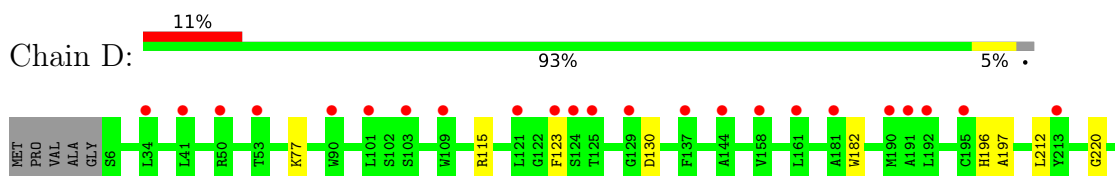
• Molecule 1: Thymidylate synthase

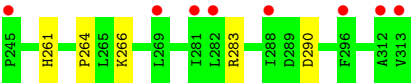


• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.14Å 89.32Å 163.48Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	44.66 – 2.39 44.66 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.66-2.39) 98.7 (44.66-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.257 , 0.289 0.258 , 0.268	Depositor DCC
R_{free} test set	2515 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.477 for k,h,-l 0.477 for -k,-h,-l 0.477 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9080	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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: OE7, 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	0.25	0/2256	0.41	0/3068
1	B	0.25	0/2265	0.41	0/3081
1	C	0.25	0/2270	0.41	0/3085
1	D	0.24	0/2269	0.40	0/3085
All	All	0.24	0/9060	0.41	0/12319

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	2199	0	2079	14	0
1	B	2208	0	2102	12	0
1	C	2215	0	2115	16	0
1	D	2212	0	2108	7	0
2	A	20	0	11	0	0
2	B	20	0	11	0	0
2	C	20	0	11	0	0
2	D	20	0	11	0	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	1	0
4	A	11	0	0	0	0
4	B	10	0	0	0	0
4	C	12	0	0	0	0
4	D	9	0	0	1	0
All	All	9080	0	8448	45	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 3.

All (45) 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:196:HIS:HB2	1:D:212:LEU:HD11	1.74	0.69
1:B:196:HIS:HB2	1:B:212:LEU:HD11	1.75	0.69
1:C:196:HIS:HB2	1:C:212:LEU:HD11	1.77	0.67
1:A:196:HIS:HB2	1:A:212:LEU:HD11	1.79	0.65
1:C:115:ARG:HH22	1:C:124:SER:HA	1.62	0.65
1:A:115:ARG:HH22	1:A:124:SER:HA	1.62	0.65
1:B:115:ARG:HH22	1:B:124:SER:HA	1.64	0.61
1:C:283:ARG:NH2	1:C:290:ASP:O	2.39	0.56
1:A:182:TRP:HB2	1:A:197:ALA:HB1	1.89	0.54
1:A:77:LYS:NZ	1:A:220:GLY:O	2.43	0.52
1:D:77:LYS:NZ	1:D:220:GLY:O	2.42	0.52
1:D:283:ARG:NH2	1:D:290:ASP:O	2.42	0.51
1:C:38:GLN:HG2	1:C:269:LEU:HD21	1.93	0.51
1:A:142:PHE:CE1	1:C:184:PRO:HD2	2.45	0.51
1:A:184:PRO:HD2	1:C:142:PHE:CE1	2.46	0.50
1:B:38:GLN:HG2	1:B:269:LEU:HD21	1.94	0.50
1:A:283:ARG:NH2	1:A:290:ASP:O	2.45	0.49
1:A:251:THR:HG21	1:C:251:THR:HG21	1.94	0.49
1:A:176:ARG:HD2	1:C:193:PRO:HG2	1.95	0.49
1:B:77:LYS:NZ	1:B:220:GLY:O	2.45	0.49
1:C:182:TRP:HB2	1:C:197:ALA:HB1	1.96	0.48
1:B:30:GLU:HG3	1:B:74:LEU:HD22	1.97	0.47
1:C:77:LYS:NZ	1:C:220:GLY:O	2.48	0.46
1:A:115:ARG:NH2	1:A:123:PHE:O	2.49	0.45
1:B:182:TRP:HB2	1:B:197:ALA:HB1	1.99	0.45
1:D:266:LYS:NZ	4:D:705:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ARG:NH2	1:C:123:PHE:O	2.50	0.44
1:A:184:PRO:HA	1:A:187:LEU:HG	2.00	0.44
1:A:115:ARG:HA	1:A:115:ARG:HE	1.83	0.43
1:B:159:ASP:H	1:B:163:ARG:HH12	1.66	0.43
1:D:182:TRP:HB2	1:D:197:ALA:HB1	2.01	0.43
1:B:169:LYS:HG3	1:B:241:THR:HG22	2.01	0.43
1:B:46:ARG:HD2	1:B:46:ARG:HA	1.86	0.42
1:C:125:THR:HG23	3:D:601:OE7:C18	2.49	0.42
1:B:126:ARG:HD3	1:B:130:ASP:O	2.21	0.41
1:C:186:ASP:O	1:C:190:MET:HG3	2.20	0.41
1:C:126:ARG:HD3	1:C:130:ASP:O	2.21	0.41
1:C:184:PRO:HA	1:C:187:LEU:HG	2.03	0.41
1:B:159:ASP:H	1:B:163:ARG:NH1	2.19	0.41
1:B:130:ASP:OD1	1:B:146:TYR:OH	2.34	0.41
1:A:30:GLU:HG3	1:A:74:LEU:HD22	2.03	0.41
1:A:148:ASP:OD1	1:A:151:SER:OG	2.36	0.41
1:D:261:HIS:C	1:D:264:PRO:HD2	2.41	0.40
1:C:115:ARG:HA	1:C:115:ARG:HE	1.87	0.40
1:D:115:ARG:NH2	1:D:123:PHE:O	2.51	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	283/290 (98%)	270 (95%)	13 (5%)	0	100	100
1	B	283/290 (98%)	270 (95%)	13 (5%)	0	100	100
1	C	283/290 (98%)	269 (95%)	14 (5%)	0	100	100
1	D	283/290 (98%)	269 (95%)	14 (5%)	0	100	100
All	All	1132/1160 (98%)	1078 (95%)	54 (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	222/252 (88%)	222 (100%)	0	100	100
1	B	225/252 (89%)	225 (100%)	0	100	100
1	C	227/252 (90%)	227 (100%)	0	100	100
1	D	225/252 (89%)	224 (100%)	1 (0%)	92	97
All	All	899/1008 (89%)	898 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	130	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 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	1.70	3 (17%)	22,31,31	1.63	4 (18%)
3	OE7	A	601	-	31,34,34	1.53	4 (12%)	35,49,49	2.25	6 (17%)
2	UMP	B	600	-	17,21,21	1.52	2 (11%)	22,31,31	1.52	2 (9%)
3	OE7	B	601	-	31,34,34	1.54	4 (12%)	35,49,49	2.25	6 (17%)
2	UMP	C	600	-	17,21,21	1.51	2 (11%)	22,31,31	1.56	3 (13%)
3	OE7	C	601	-	31,34,34	1.52	4 (12%)	35,49,49	2.24	6 (17%)
2	UMP	D	600	-	17,21,21	1.71	3 (17%)	22,31,31	1.62	4 (18%)
3	OE7	D	601	-	31,34,34	1.53	4 (12%)	35,49,49	2.25	6 (17%)

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	-	-	2/6/22/22	0/2/2/2
3	OE7	A	601	-	-	0/12/16/16	0/4/4/4
2	UMP	B	600	-	-	4/6/22/22	0/2/2/2
3	OE7	B	601	-	-	0/12/16/16	0/4/4/4
2	UMP	C	600	-	-	2/6/22/22	0/2/2/2
3	OE7	C	601	-	-	0/12/16/16	0/4/4/4
2	UMP	D	600	-	-	4/6/22/22	0/2/2/2
3	OE7	D	601	-	-	0/12/16/16	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	OE7	C20-C21	4.31	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	OE7	C20-C21	4.28	1.51	1.47
3	A	601	OE7	C20-C21	4.27	1.51	1.47
2	B	600	UMP	C4-N3	4.21	1.40	1.33
3	D	601	OE7	C20-C21	4.21	1.51	1.47
2	C	600	UMP	C4-N3	4.16	1.40	1.33
2	A	600	UMP	C4-N3	4.12	1.40	1.33
2	D	600	UMP	C4-N3	4.11	1.40	1.33
2	A	600	UMP	P-OP1	3.63	1.62	1.50
2	D	600	UMP	P-OP1	3.61	1.62	1.50
3	B	601	OE7	C4-N2	3.21	1.41	1.35
3	D	601	OE7	C4-N2	3.18	1.41	1.35
3	C	601	OE7	C4-N2	3.13	1.40	1.35
3	A	601	OE7	C4-N2	3.11	1.40	1.35
2	D	600	UMP	C6-N1	2.68	1.39	1.35
2	C	600	UMP	C6-N1	2.58	1.39	1.35
2	B	600	UMP	C6-N1	2.58	1.39	1.35
2	A	600	UMP	C6-N1	2.55	1.39	1.35
3	D	601	OE7	C4-N4	2.26	1.38	1.33
3	B	601	OE7	C4-N4	2.24	1.38	1.33
3	A	601	OE7	C4-N4	2.22	1.38	1.33
3	C	601	OE7	C4-N4	2.21	1.38	1.33
3	D	601	OE7	C2-C1	-2.10	1.37	1.43
3	C	601	OE7	C2-C1	-2.08	1.37	1.43
3	A	601	OE7	C2-C1	-2.08	1.37	1.43
3	B	601	OE7	C2-C1	-2.07	1.37	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	OE7	C2-C3-N2	-9.77	115.35	124.08
3	A	601	OE7	C2-C3-N2	-9.77	115.35	124.08
3	D	601	OE7	C2-C3-N2	-9.75	115.37	124.08
3	C	601	OE7	C2-C3-N2	-9.64	115.46	124.08
3	B	601	OE7	C3-N2-C4	4.56	122.56	116.06
3	A	601	OE7	C3-N2-C4	4.55	122.53	116.06
3	D	601	OE7	C3-N2-C4	4.52	122.50	116.06
3	C	601	OE7	C3-N2-C4	4.48	122.44	116.06
2	D	600	UMP	C5-C4-N3	-3.97	114.39	123.28
2	B	600	UMP	C5-C4-N3	-3.94	114.46	123.28
2	A	600	UMP	C5-C4-N3	-3.93	114.47	123.28
3	C	601	OE7	N4-C4-N1	3.90	124.21	117.77
3	A	601	OE7	N4-C4-N1	3.88	124.18	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	UMP	C5'-C4'-N3	-3.88	114.59	123.28
3	D	601	OE7	N4'-C4'-N1	3.85	124.13	117.77
3	B	601	OE7	N4'-C4'-N1	3.82	124.08	117.77
3	C	601	OE7	N4'-C4'-N2	-3.78	111.33	117.25
3	A	601	OE7	N4'-C4'-N2	-3.76	111.36	117.25
3	D	601	OE7	N4'-C4'-N2	-3.67	111.51	117.25
3	B	601	OE7	N4'-C4'-N2	-3.65	111.54	117.25
2	C	600	UMP	O5'-P-OP1	3.63	116.65	106.47
2	A	600	UMP	OP2-P-O5'	3.61	116.33	106.73
2	D	600	UMP	OP2-P-O5'	3.59	116.30	106.73
3	D	601	OE7	C3'-C2'-C1	3.54	117.01	115.04
2	B	600	UMP	O5'-P-OP1	3.38	115.95	106.47
3	C	601	OE7	C3'-C2'-C1	3.32	116.89	115.04
3	A	601	OE7	C3'-C2'-C1	3.31	116.89	115.04
3	B	601	OE7	C3'-C2'-C1	3.25	116.85	115.04
2	A	600	UMP	OP3-P-OP2	2.51	117.31	107.57
2	D	600	UMP	OP3-P-OP2	2.48	117.20	107.57
2	A	600	UMP	OP3-P-OP1	-2.19	101.88	110.53
2	D	600	UMP	OP3-P-OP1	-2.18	101.93	110.53
2	C	600	UMP	P-O5'-C5'	2.17	124.26	118.30
3	D	601	OE7	N1'-C4'-N2	-2.14	124.36	127.25
3	B	601	OE7	N1'-C4'-N2	-2.12	124.38	127.25
3	A	601	OE7	N1'-C4'-N2	-2.06	124.46	127.25
3	C	601	OE7	N1'-C4'-N2	-2.06	124.46	127.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

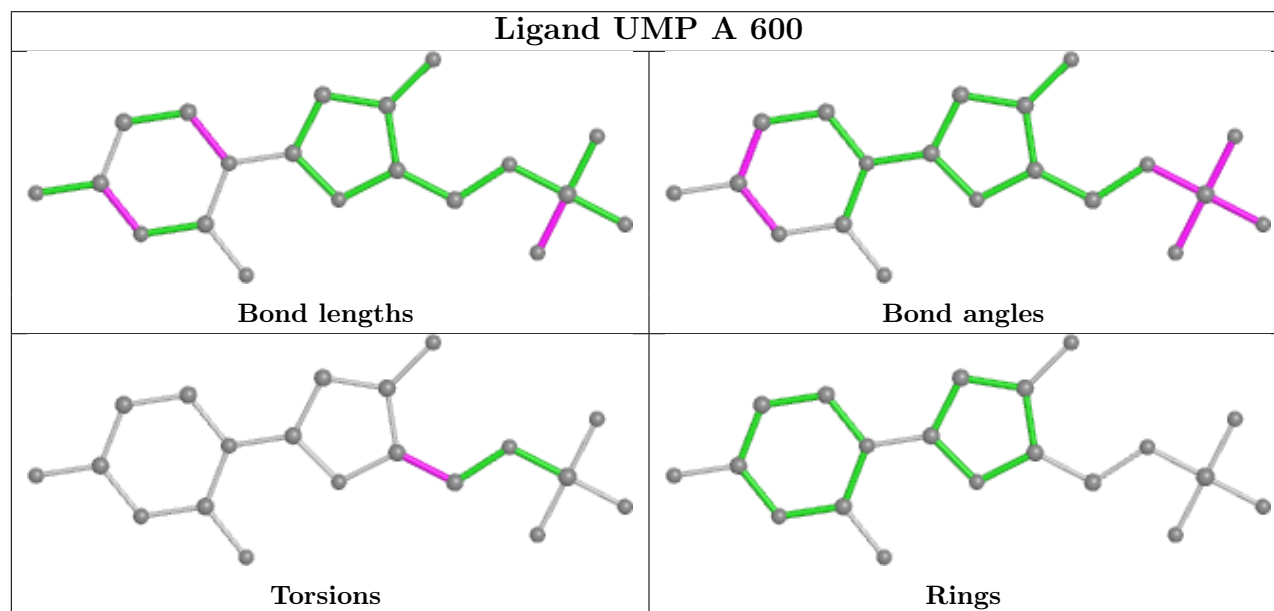
Mol	Chain	Res	Type	Atoms
2	D	600	UMP	C5'-O5'-P-OP3
2	C	600	UMP	C5'-O5'-P-OP3
2	D	600	UMP	C3'-C4'-C5'-O5'
2	D	600	UMP	O4'-C4'-C5'-O5'
2	A	600	UMP	O4'-C4'-C5'-O5'
2	B	600	UMP	O4'-C4'-C5'-O5'
2	A	600	UMP	C3'-C4'-C5'-O5'
2	B	600	UMP	C3'-C4'-C5'-O5'
2	B	600	UMP	C5'-O5'-P-OP1
2	D	600	UMP	C4'-C5'-O5'-P
2	C	600	UMP	O4'-C4'-C5'-O5'
2	B	600	UMP	C5'-O5'-P-OP2

There are no ring outliers.

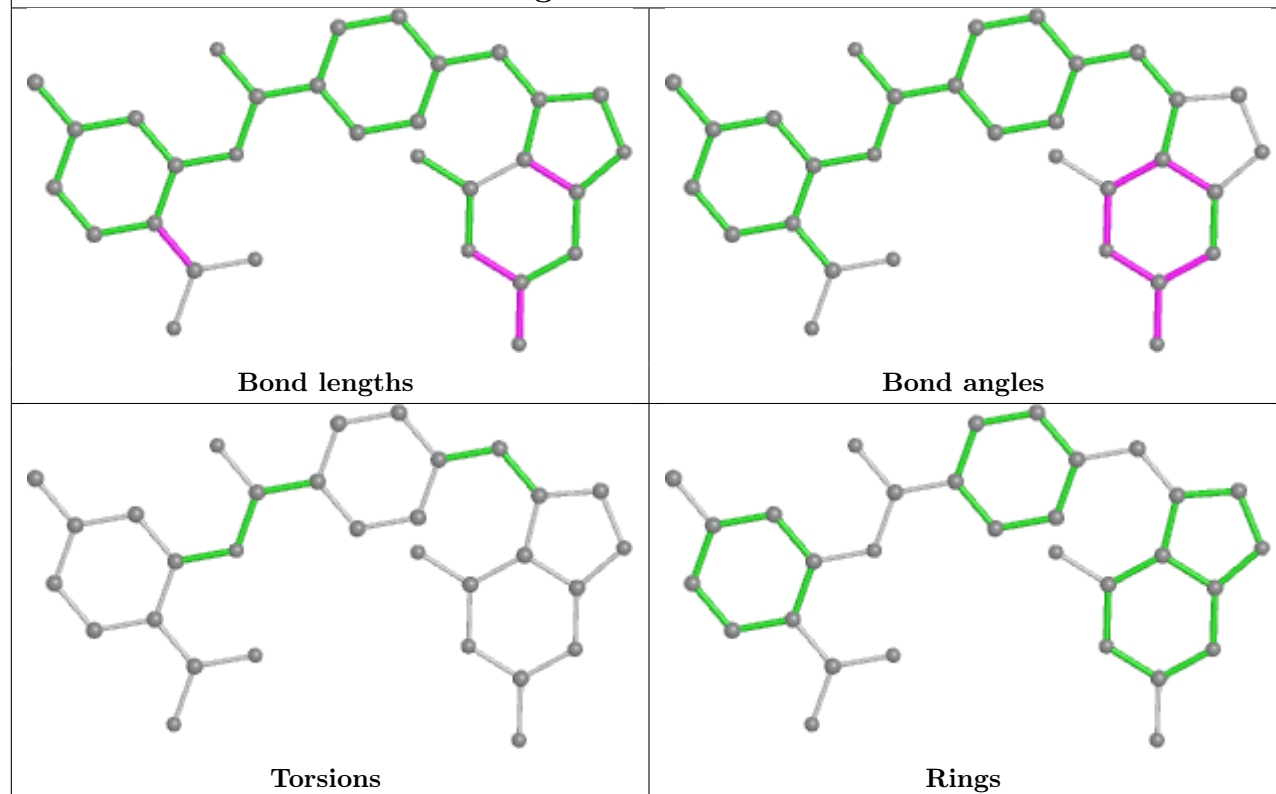
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	OE7	1	0

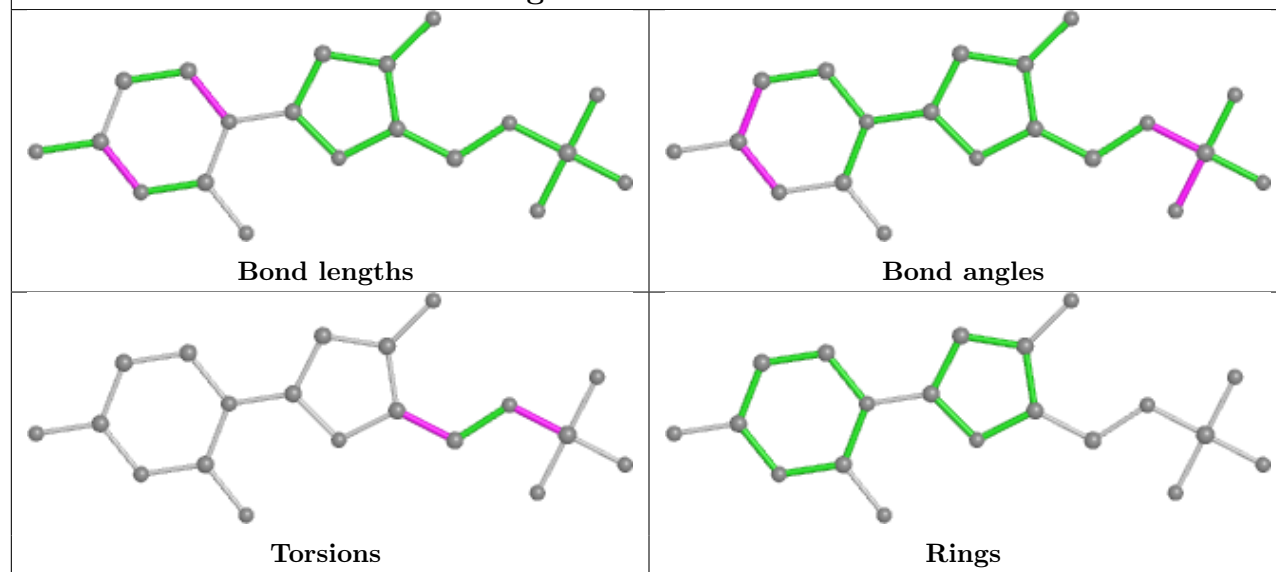
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



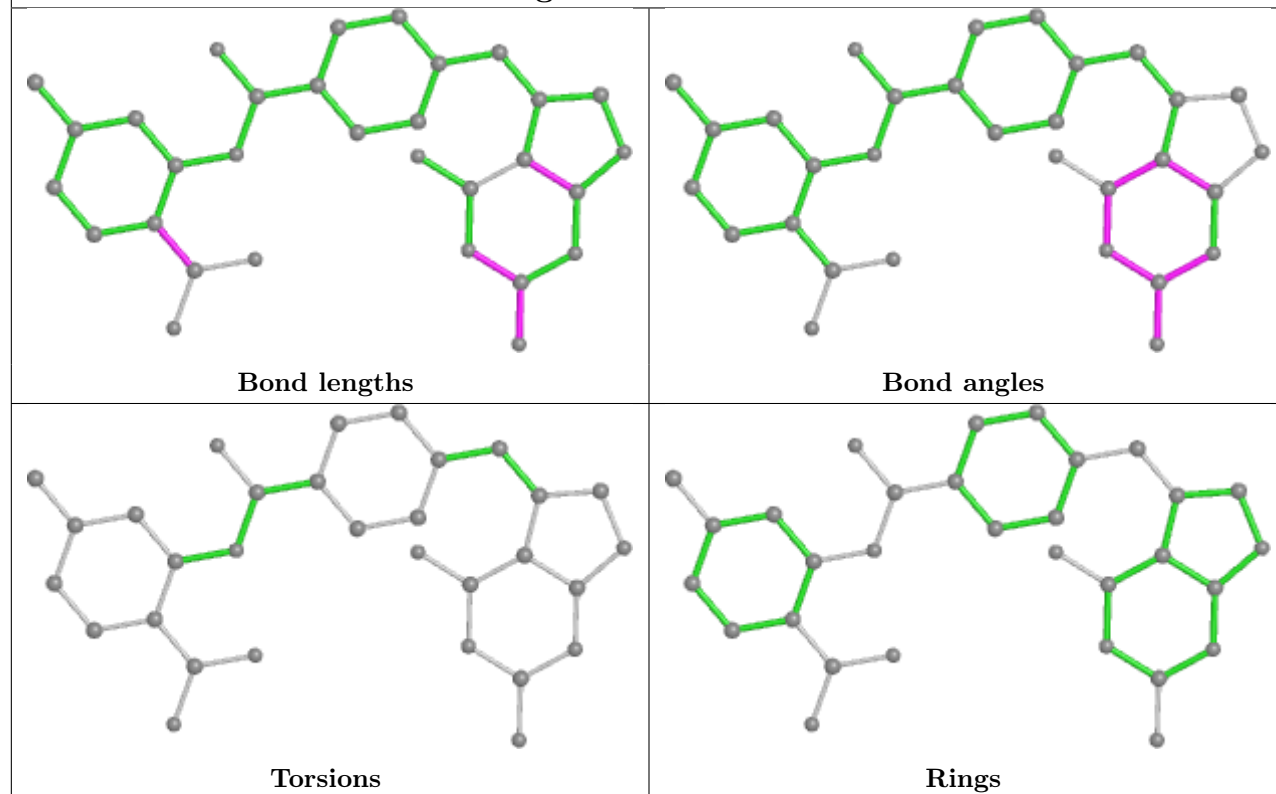
Ligand OE7 A 601



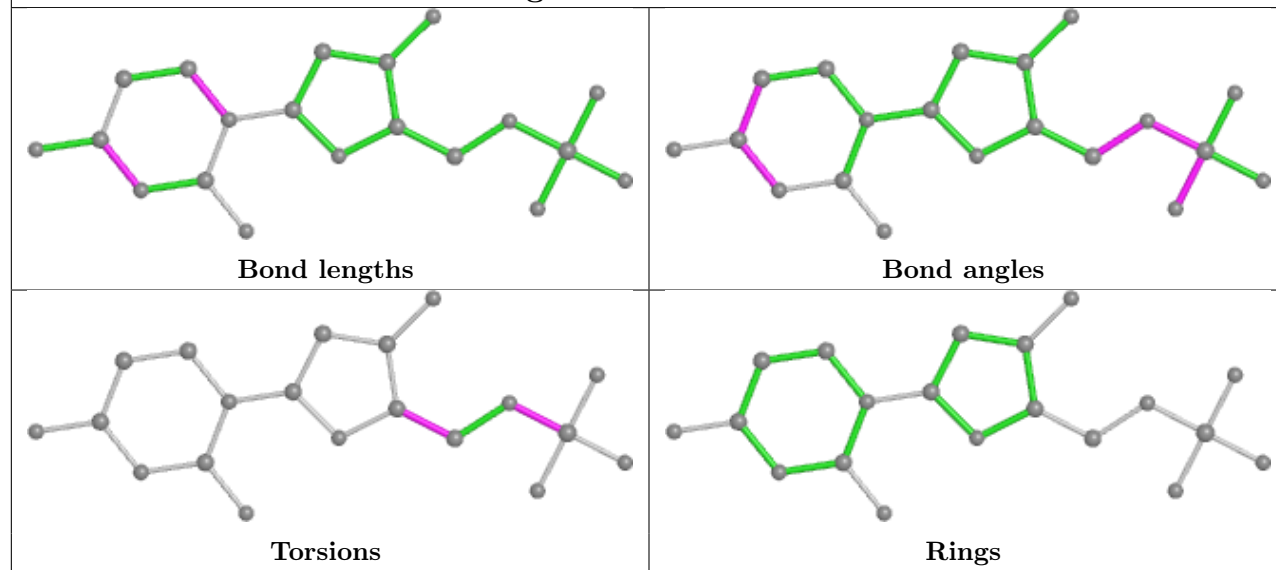
Ligand UMP B 600



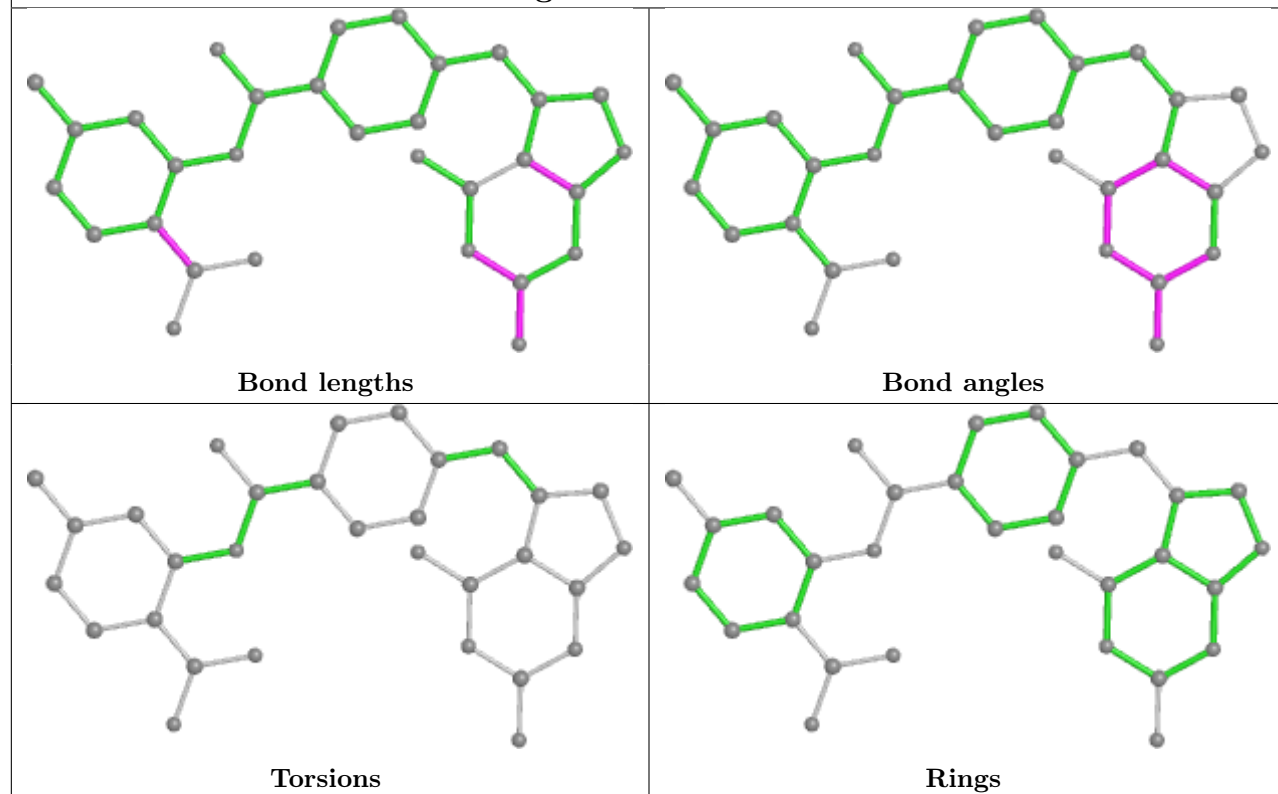
Ligand OE7 B 601



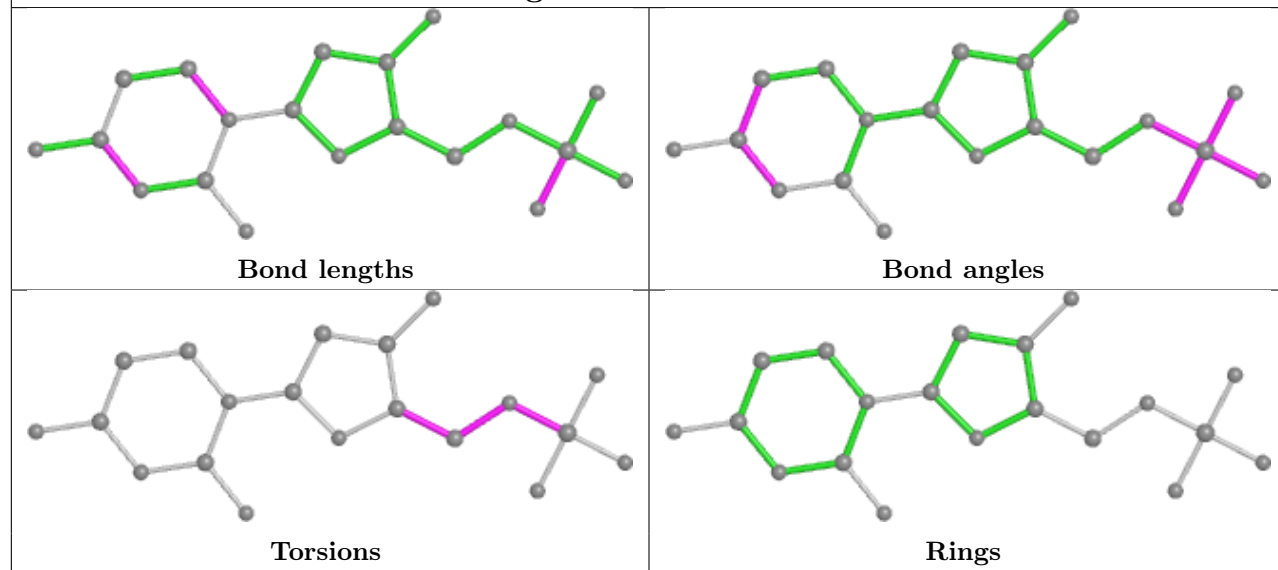
Ligand UMP C 600

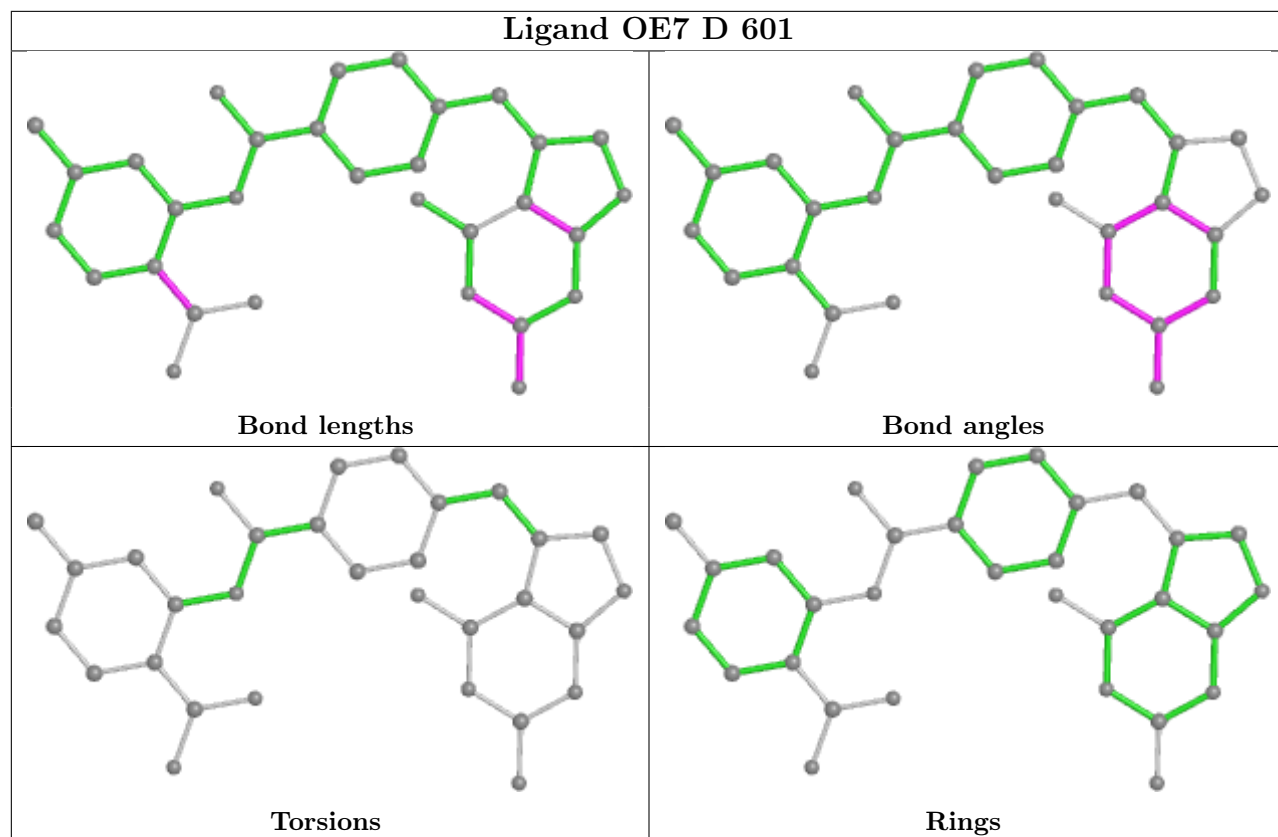


Ligand OE7 C 601



Ligand UMP D 600





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	285/290 (98%)	0.78	18 (6%)	20 18	42, 62, 78, 87	0
1	B	285/290 (98%)	0.68	23 (8%)	12 10	44, 62, 79, 87	0
1	C	285/290 (98%)	0.77	25 (8%)	10 9	42, 61, 80, 87	0
1	D	285/290 (98%)	0.81	31 (10%)	5 5	43, 62, 81, 87	0
All	All	1140/1160 (98%)	0.76	97 (8%)	11 9	42, 62, 81, 87	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	SER	5.6
1	C	121	LEU	5.4
1	C	144	ALA	5.1
1	C	192	LEU	5.0
1	A	124	SER	5.0
1	A	125	THR	4.2
1	B	122	GLY	4.1
1	A	117	PHE	4.1
1	D	281	ILE	3.9
1	D	121	LEU	3.8
1	C	129	GLY	3.8
1	B	123	PHE	3.7
1	C	313	VAL	3.6
1	C	125	THR	3.4
1	A	149	MET	3.4
1	D	53	THR	3.4
1	A	53	THR	3.4
1	D	190	MET	3.4
1	A	312	ALA	3.3
1	A	313	VAL	3.3
1	D	192	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	125	THR	3.2
1	C	191	ALA	3.2
1	D	41	LEU	3.1
1	B	85	LEU	3.1
1	B	313	VAL	3.0
1	B	131	LEU	3.0
1	D	101	LEU	3.0
1	D	123	PHE	3.0
1	D	313	VAL	3.0
1	B	290	ASP	3.0
1	D	158	VAL	3.0
1	C	106	VAL	3.0
1	D	109	TRP	2.9
1	A	103	SER	2.9
1	C	101	LEU	2.8
1	C	124	SER	2.8
1	C	88	LEU	2.8
1	A	116	ASP	2.7
1	D	129	GLY	2.7
1	B	109	TRP	2.7
1	D	296	PHE	2.7
1	A	113	GLY	2.7
1	D	137	PHE	2.7
1	A	52	GLY	2.7
1	D	288	ILE	2.7
1	C	117	PHE	2.7
1	A	191	ALA	2.6
1	A	135	TYR	2.6
1	D	282	LEU	2.6
1	B	206	SER	2.6
1	B	275	PRO	2.6
1	C	114	SER	2.5
1	B	111	ALA	2.5
1	D	124	SER	2.5
1	D	50	ARG	2.5
1	D	191	ALA	2.5
1	C	149	MET	2.5
1	D	103	SER	2.5
1	B	137	PHE	2.4
1	B	125	THR	2.4
1	C	90	TRP	2.4
1	D	90	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	144	ALA	2.4
1	B	312	ALA	2.4
1	C	37	ILE	2.4
1	D	312	ALA	2.4
1	B	117	PHE	2.4
1	A	109	TRP	2.3
1	D	144	ALA	2.3
1	A	153	TYR	2.3
1	D	34	LEU	2.3
1	B	134	VAL	2.3
1	B	69	ASP	2.2
1	A	51	THR	2.2
1	C	111	ALA	2.2
1	A	180	CYS	2.2
1	C	190	MET	2.2
1	D	245	PRO	2.2
1	A	203	VAL	2.2
1	B	195	CYS	2.2
1	B	118	LEU	2.2
1	D	181	ALA	2.1
1	C	269	LEU	2.1
1	B	149	MET	2.1
1	C	312	ALA	2.1
1	B	34	LEU	2.1
1	C	34	LEU	2.1
1	D	161	LEU	2.1
1	D	269	LEU	2.1
1	B	116	ASP	2.1
1	C	185	ARG	2.1
1	C	84	VAL	2.1
1	C	122	GLY	2.1
1	C	291	PHE	2.1
1	D	195	CYS	2.0
1	D	213	TYR	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](#)

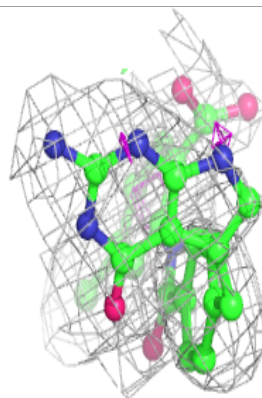
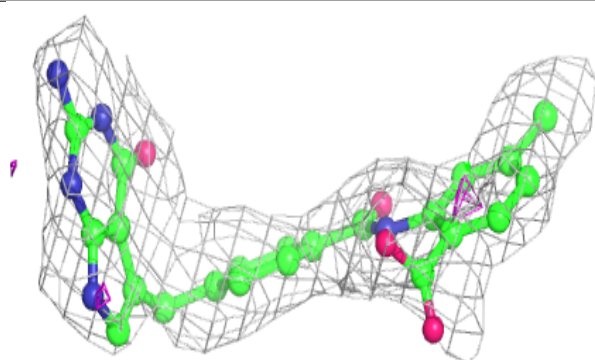
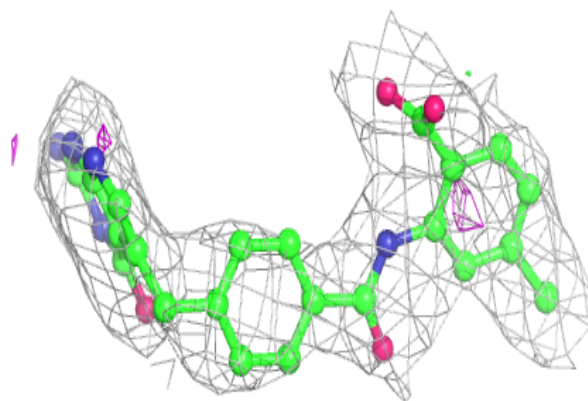
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	OE7	D	601	31/31	0.79	0.23	63,66,75,79	0
3	OE7	A	601	31/31	0.81	0.21	62,66,75,80	0
3	OE7	B	601	31/31	0.82	0.21	62,65,76,81	0
3	OE7	C	601	31/31	0.83	0.26	62,66,76,83	0
2	UMP	A	600	20/20	0.91	0.18	54,58,62,62	0
2	UMP	B	600	20/20	0.91	0.17	55,58,62,63	0
2	UMP	C	600	20/20	0.92	0.17	54,58,63,64	0
2	UMP	D	600	20/20	0.93	0.14	55,59,62,63	0

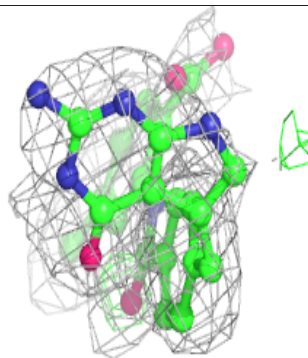
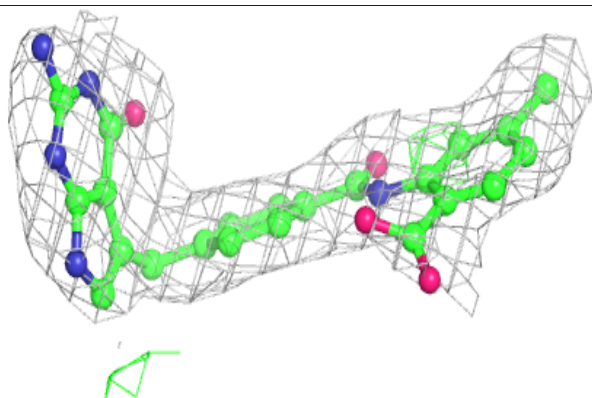
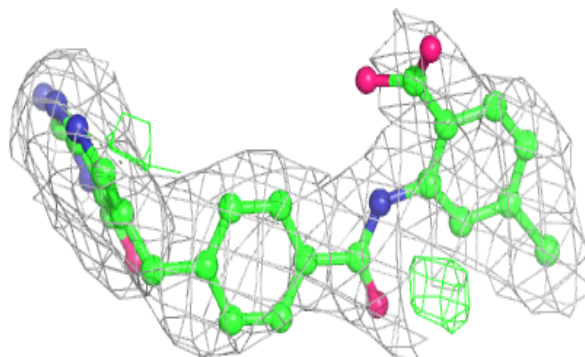
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OE7 D 601:

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

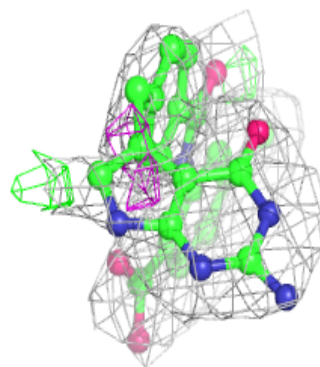
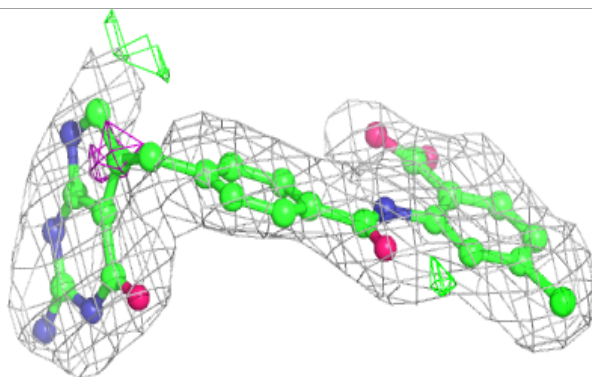
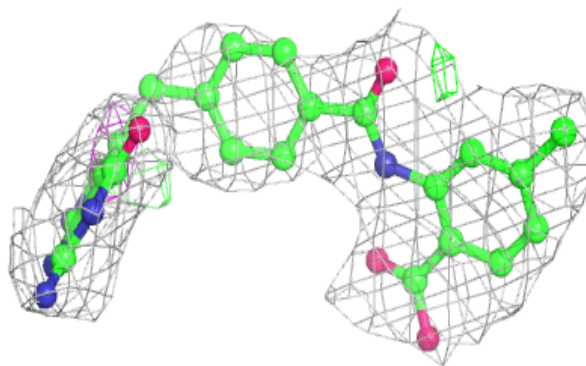
**Electron density around OE7 A 601:**

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

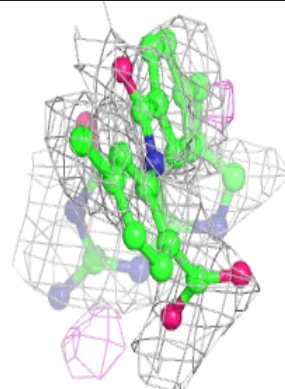
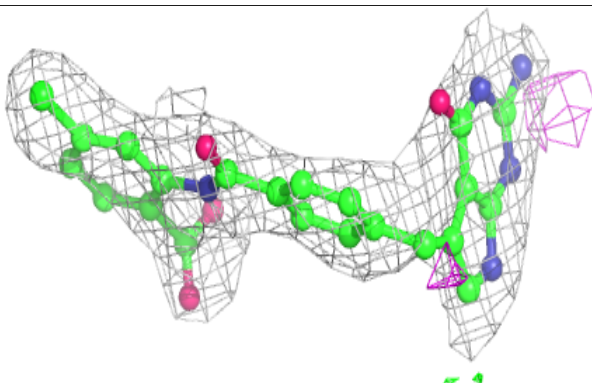
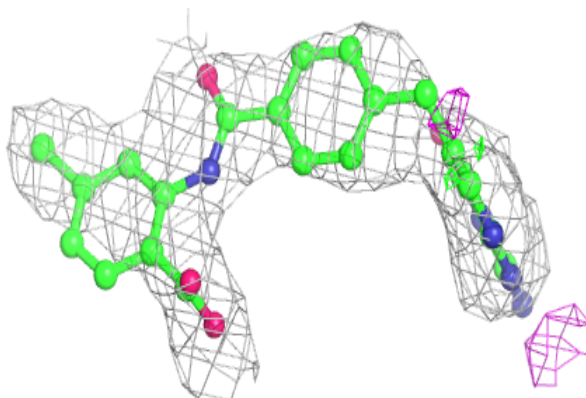


Electron density around OE7 B 601:

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

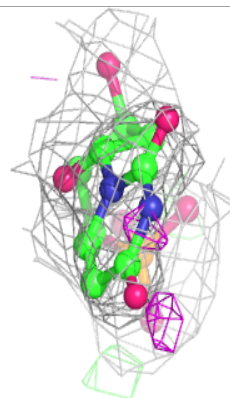
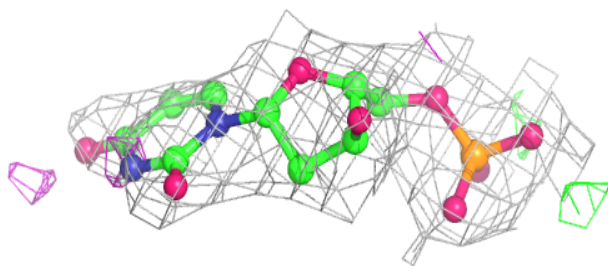
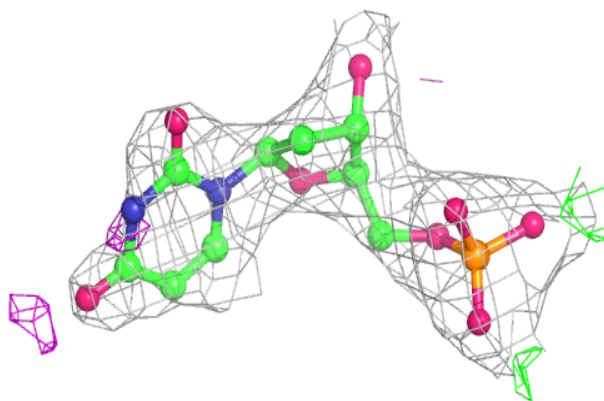
**Electron density around OE7 C 601:**

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

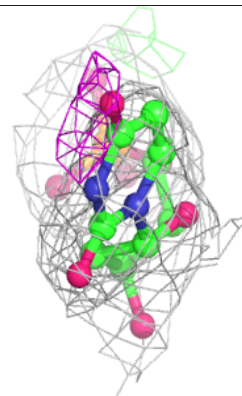
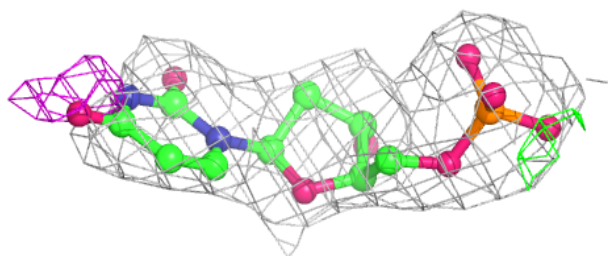
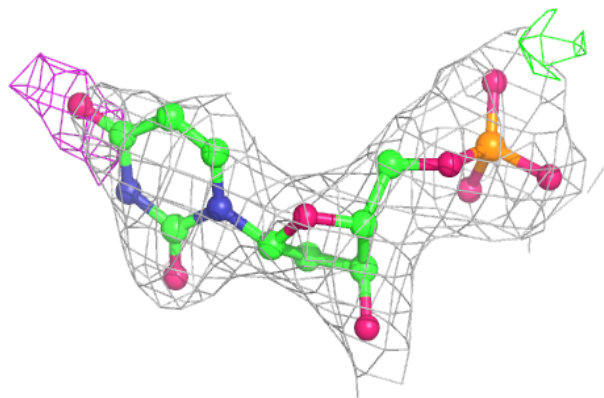


Electron density around UMP A 600:

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

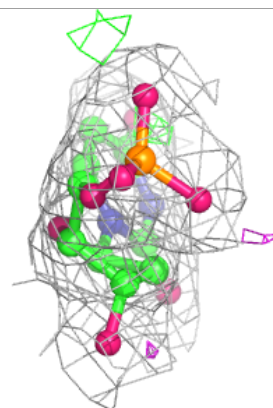
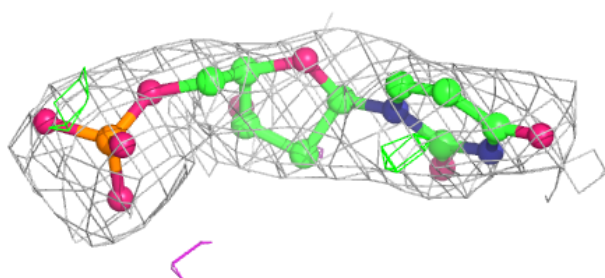
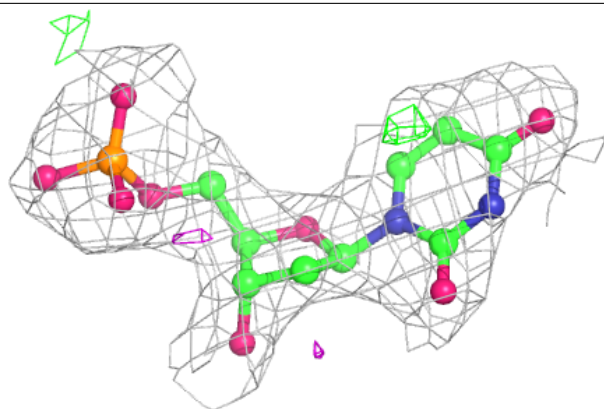
**Electron density around UMP B 600:**

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

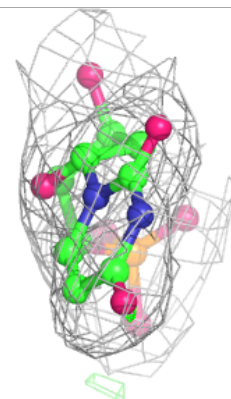
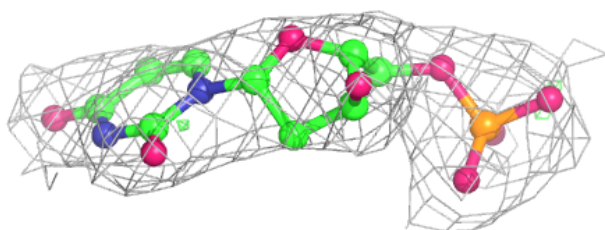
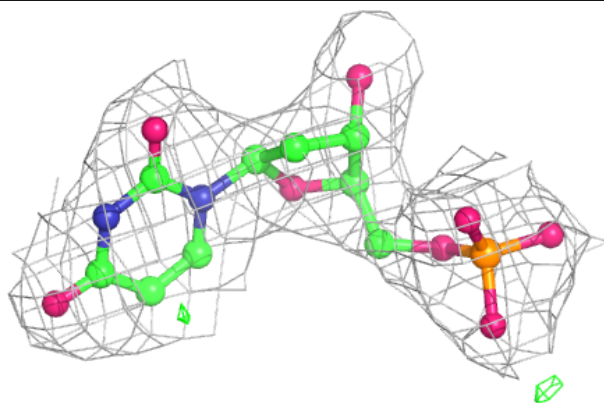


Electron density around UMP C 600:

$2mF_o-DF_c$ (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.