Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 05:00 AM EST

PDB ID	:	2DLC
Title	:	Crystal structure of the ternary complex of yeast tyrosyl-tRNA synthetase
Authors	:	Tsunoda, M.; Kusakabe, Y.; Tanaka, N.; Nakamura, K.T.
Deposited on	:	2006-04-18
Resolution	:	2.40 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 (i) 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 (1)) were used in the production of this report:

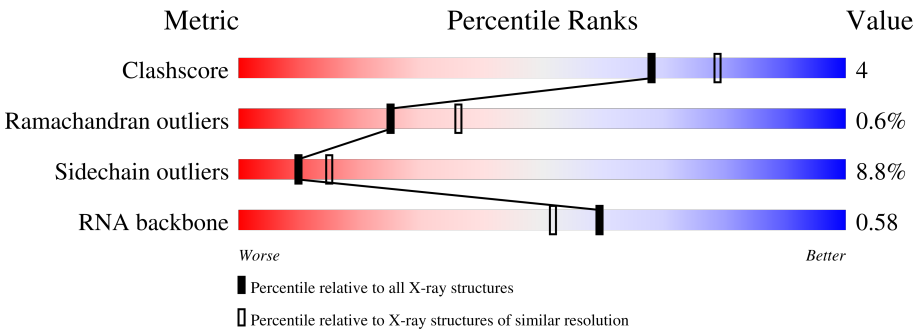
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	Y	76	66% 21% 11% •
2	X	394	71% 14% • 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4263 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 RNA chain called T-RNA (76-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	Y	74	1472	650	265	484	73	0	0	1

- Molecule 2 is a protein called Tyrosyl-tRNA synthetase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	X	339	2698	1746	444	497	11	0	0	0

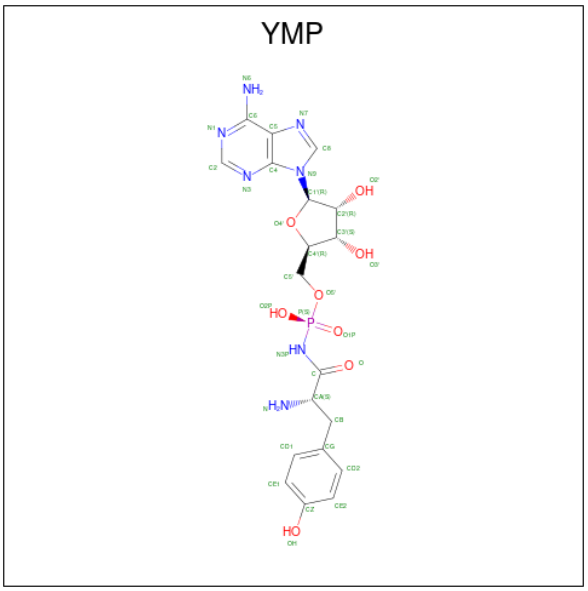
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	initiating methionine	UNP P36421

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	X	1	1	1	0	0

- Molecule 4 is O-(ADENOSINE-5'-O-YL)-N-(L-TYROSYL)PHOSPHORAMIDATE (three-letter code: YMP) (formula: $C_{19}H_{24}N_7O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	X	1	35	19	7	8	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	Y	7	7	7	0	0
			Total	O		
5	X	50	50	50	0	0

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. 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. 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.

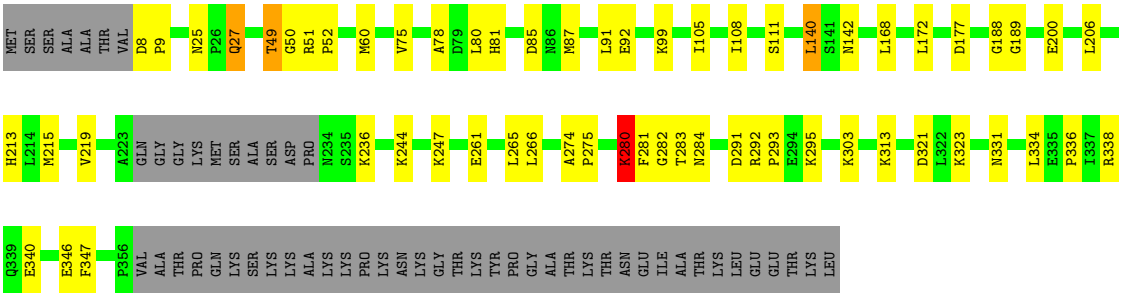
Note EDS was not executed.

- Molecule 1: T-RNA (76-MER)

Chain Y:

- Molecule 2: Tyrosyl-tRNA synthetase, cytoplasmic

Chain X:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	63.85Å 63.85Å 330.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40	Depositor
% Data completeness (in resolution range)	99.3 (40.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.245 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4263	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

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: OMG, MG, 6IA, YMP, 1MA, 2MG, M2G, 5MU, PSU, 5MC

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	Y	0.63	0/1408	1.08	3/2186 (0.1%)
2	X	0.37	0/2757	0.66	4/3728 (0.1%)
All	All	0.47	0/4165	0.84	7/5914 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	528	A	O4'-C1'-N9	7.36	114.09	108.20
2	X	177	ASP	CB-CG-OD2	6.32	123.99	118.30
2	X	85	ASP	CB-CG-OD2	6.18	123.86	118.30
2	X	291	ASP	CB-CG-OD2	5.82	123.54	118.30
1	Y	575	C	P-O3'-C3'	5.57	126.38	119.70
2	X	321	ASP	CB-CG-OD2	5.34	123.11	118.30
1	Y	530	G	O4'-C1'-N9	5.11	112.29	108.20

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	Y	1472	0	734	4	0
2	X	2698	0	2734	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	1	0	0	0	0
4	X	35	0	22	2	0
5	X	50	0	0	2	0
5	Y	7	0	0	0	0
All	All	4263	0	3490	29	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 (29) 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)
2:X:49:THR:CG2	2:X:50:GLY:H	1.73	1.00
2:X:49:THR:HG22	2:X:50:GLY:H	1.31	0.92
2:X:340:GLU:HG3	5:X:815:HOH:O	1.81	0.80
2:X:49:THR:CG2	2:X:50:GLY:N	2.44	0.76
2:X:49:THR:HG22	2:X:50:GLY:N	2.07	0.67
2:X:49:THR:HG23	2:X:50:GLY:H	1.60	0.66
2:X:140:LEU:HB3	2:X:172:LEU:HD13	1.82	0.61
2:X:274:ALA:HB3	2:X:275:PRO:HD3	1.84	0.59
2:X:188:GLY:O	2:X:215:MET:HA	2.03	0.57
2:X:280:LYS:HB3	5:X:850:HOH:O	2.05	0.57
2:X:331:ASN:HD22	2:X:338:ARG:HH12	1.58	0.52
2:X:49:THR:HG23	2:X:50:GLY:N	2.23	0.51
2:X:189:GLY:HA3	4:X:601:YMP:O2'	2.14	0.47
2:X:78:ALA:HB1	2:X:81:HIS:HB2	1.97	0.46
2:X:111:SER:HB2	2:X:336:PRO:HG2	1.98	0.46
1:Y:528:A:H61	1:Y:542:U:H3	1.63	0.45
2:X:60:MET:HG3	2:X:108:ILE:HG21	1.99	0.44
2:X:8:ASP:HA	2:X:9:PRO:HD3	1.86	0.43
1:Y:553:G:H3'	1:Y:554:5MU:H71	2.00	0.43
2:X:292:ARG:HA	2:X:293:PRO:HD3	1.93	0.43
1:Y:536:A:H2'	1:Y:537:6IA:O4'	2.18	0.42
2:X:51:ARG:HA	2:X:52:PRO:HD3	1.94	0.42
2:X:81:HIS:CE1	4:X:601:YMP:HE2	2.55	0.42
1:Y:509:A:N3	1:Y:545:G:H2'	2.35	0.41
2:X:25:ASN:HA	2:X:27:GLN:HE22	1.85	0.41
2:X:265:LEU:HD11	2:X:323:LYS:HE2	2.01	0.41
2:X:200:GLU:HG3	2:X:213:HIS:CE1	2.55	0.41
2:X:282:GLY:C	2:X:284:ASN:H	2.22	0.41
2:X:105:ILE:HA	2:X:108:ILE:HD12	2.03	0.41

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
2	X	335/394 (85%)	325 (97%)	8 (2%)	2 (1%)	25 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	91	LEU
2	X	280	LYS

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
2	X	296/340 (87%)	270 (91%)	26 (9%)	10 15

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	27	GLN
2	X	49	THR
2	X	75	VAL
2	X	80	LEU
2	X	87	MET
2	X	92	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	X	99	LYS
2	X	140	LEU
2	X	142	ASN
2	X	168	LEU
2	X	206	LEU
2	X	219	VAL
2	X	236	LYS
2	X	244	LYS
2	X	247	LYS
2	X	261	GLU
2	X	266	LEU
2	X	280	LYS
2	X	281	PHE
2	X	283	THR
2	X	295	LYS
2	X	303	LYS
2	X	313	LYS
2	X	334	LEU
2	X	346	GLU
2	X	347	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	X	21	GLN
2	X	25	ASN
2	X	216	ASN
2	X	245	GLN
2	X	251	ASN
2	X	331	ASN
2	X	343	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Y	61/76 (80%)	10 (16%)	1 (1%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Y	509	A
1	Y	513	A
1	Y	522	A
1	Y	539	PSU
1	Y	540	C
1	Y	541	U
1	Y	548	5MC
1	Y	553	G
1	Y	574	C
1	Y	576	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	Y	575	C

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

10 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	M2G	Y	526	1	18,25,28	1.08	2 (11%)	19,37,43	0.63	0
1	5MC	Y	548	1	18,22,23	0.34	0	26,32,35	0.98	1 (3%)
1	1MA	Y	558	1	16,25,26	1.44	3 (18%)	18,37,40	6.33	4 (22%)
1	5MU	Y	554	1	19,22,23	0.51	0	28,32,35	1.30	2 (7%)
1	OMG	Y	518	1	18,25,27	1.07	2 (11%)	19,37,41	0.84	1 (5%)
1	6IA	Y	537	1	18,24,30	0.60	0	18,35,44	0.77	1 (5%)
1	PSU	Y	539	1	9,12,22	0.91	0	10,16,33	1.31	2 (20%)
1	2MG	Y	510	1	18,25,27	1.03	2 (11%)	19,37,41	0.60	0
1	PSU	Y	555	1	18,21,22	1.21	1 (5%)	22,30,33	1.69	4 (18%)
1	PSU	Y	535	1	18,21,22	1.24	1 (5%)	22,30,33	1.71	4 (18%)

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
1	M2G	Y	526	1	-	0/3/25/30	0/3/3/3
1	5MC	Y	548	1	-	2/7/25/26	0/2/2/2
1	1MA	Y	558	1	-	0/3/25/26	0/3/3/3
1	5MU	Y	554	1	-	0/7/25/26	0/2/2/2
1	OMG	Y	518	1	-	0/3/25/28	0/3/3/3
1	6IA	Y	537	1	-	0/3/25/32	0/3/3/3
1	PSU	Y	539	1	-	2/3/18/26	0/1/1/2
1	2MG	Y	510	1	-	0/3/25/28	0/3/3/3
1	PSU	Y	555	1	-	2/7/25/26	0/2/2/2
1	PSU	Y	535	1	-	0/7/25/26	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	558	1MA	C2-N3	4.15	1.34	1.29
1	Y	555	PSU	C6-C5	4.07	1.40	1.35
1	Y	535	PSU	C6-C5	3.92	1.39	1.35
1	Y	558	1MA	C6-N6	2.66	1.34	1.27
1	Y	526	M2G	C5-C6	-2.54	1.42	1.47
1	Y	526	M2G	C8-N7	-2.51	1.30	1.35
1	Y	518	OMG	C8-N7	-2.50	1.30	1.35
1	Y	518	OMG	C5-C6	-2.46	1.42	1.47
1	Y	510	2MG	C8-N7	-2.43	1.30	1.35
1	Y	510	2MG	C5-C6	-2.33	1.42	1.47
1	Y	558	1MA	C8-N7	-2.05	1.31	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	558	1MA	CM1-N1-C6	21.29	152.52	120.27
1	Y	558	1MA	CM1-N1-C2	-15.91	87.06	120.55
1	Y	535	PSU	C4-N3-C2	-4.51	119.84	126.34
1	Y	555	PSU	C4-N3-C2	-4.38	120.02	126.34
1	Y	554	5MU	C5M-C5-C4	4.34	123.54	118.77
1	Y	535	PSU	N1-C2-N3	4.32	120.03	115.13
1	Y	555	PSU	N1-C2-N3	4.27	119.97	115.13
1	Y	554	5MU	C5M-C5-C6	-4.09	117.39	122.85
1	Y	548	5MC	CM5-C5-C6	-3.96	117.56	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	535	PSU	O2-C2-N1	-2.67	119.85	122.79
1	Y	555	PSU	O2-C2-N1	-2.59	119.94	122.79
1	Y	558	1MA	C5-C6-N1	2.57	117.73	113.90
1	Y	539	PSU	O4'-C4'-C3'	2.52	106.94	104.70
1	Y	537	6IA	C5-C6-N6	2.37	123.96	120.35
1	Y	539	PSU	C1'-C2'-C3'	2.35	105.21	101.63
1	Y	558	1MA	N1-C2-N3	2.20	128.58	126.02
1	Y	518	OMG	O4'-C1'-C2'	-2.20	103.72	106.93
1	Y	535	PSU	C6-N1-C2	-2.13	120.51	122.68
1	Y	555	PSU	C6-N1-C2	-2.10	120.54	122.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Y	539	PSU	C3'-C4'-C5'-O5'
1	Y	548	5MC	O4'-C4'-C5'-O5'
1	Y	548	5MC	C3'-C4'-C5'-O5'
1	Y	539	PSU	O4'-C4'-C5'-O5'
1	Y	555	PSU	C3'-C4'-C5'-O5'
1	Y	555	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Y	554	5MU	1	0
1	Y	537	6IA	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	YMP	X	601	3	34,38,38	2.12	5 (14%)	38,56,56	2.40	8 (21%)

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	YMP	X	601	3	-	6/17/39/39	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	601	YMP	C2-N3	8.40	1.45	1.32
4	X	601	YMP	C2-N1	6.80	1.46	1.33
4	X	601	YMP	P-O1P	2.57	1.50	1.46
4	X	601	YMP	P-N3P	2.40	1.68	1.63
4	X	601	YMP	P-O2P	-2.20	1.50	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	601	YMP	N3-C2-N1	-10.97	111.54	128.68
4	X	601	YMP	C2-N1-C6	5.21	127.66	118.75
4	X	601	YMP	O2P-P-O1P	3.40	117.05	109.92
4	X	601	YMP	C4-C5-N7	-3.30	105.96	109.40
4	X	601	YMP	C3'-C2'-C1'	3.11	105.66	100.98
4	X	601	YMP	O5'-P-O1P	-2.44	104.85	114.24
4	X	601	YMP	O3'-C3'-C4'	-2.14	104.87	111.05
4	X	601	YMP	O4'-C4'-C3'	2.03	109.14	105.11

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	601	YMP	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	X	601	YMP	N3P-C-CA-CB
4	X	601	YMP	C-N3P-P-O5'
4	X	601	YMP	O-C-CA-N
4	X	601	YMP	C-N3P-P-O1P
4	X	601	YMP	N3P-C-CA-N

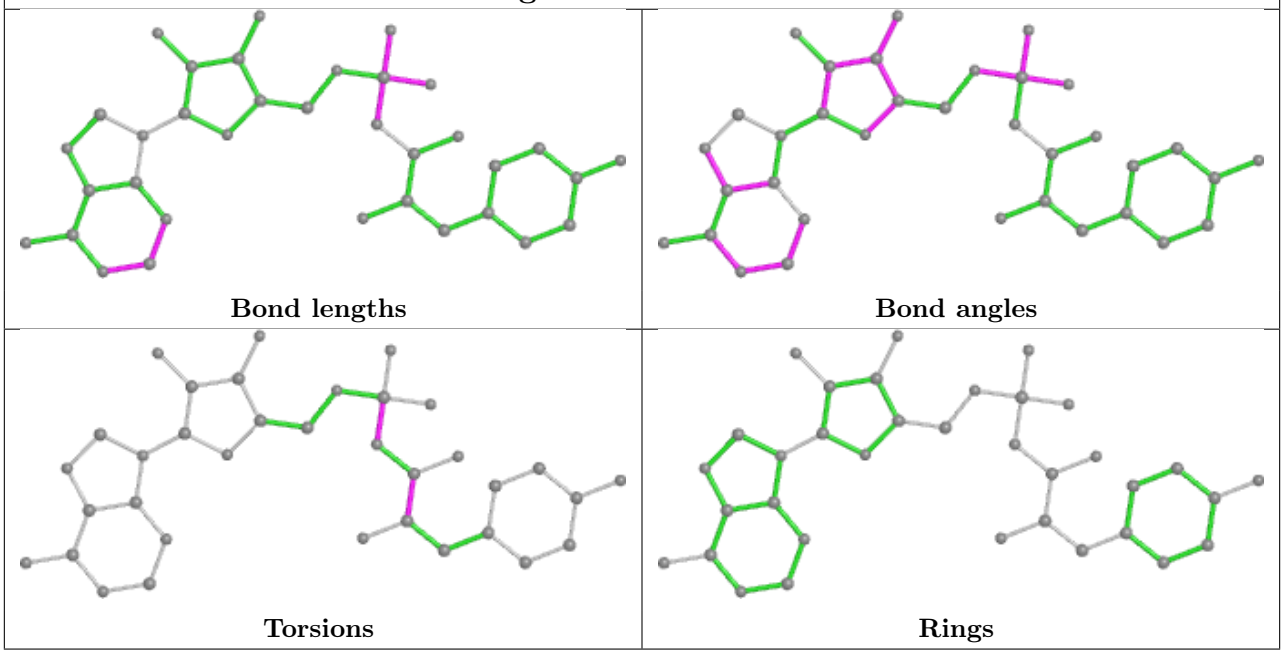
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	601	YMP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 YMP X 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.