Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:35 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

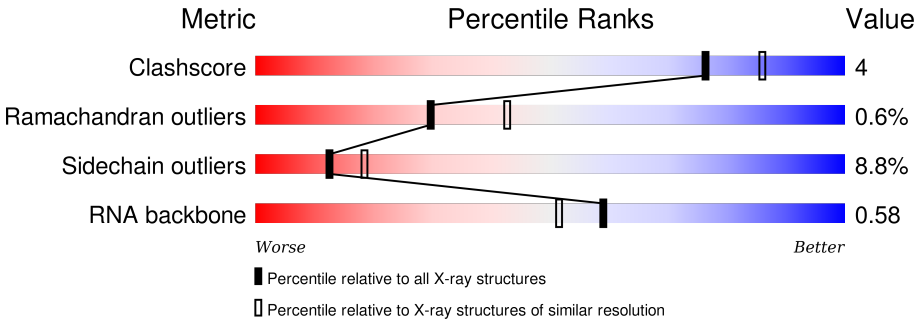
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RNA backbone	2183	1073 (2.90-1.90)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	Y	76	74% 18% 5% ·
2	X	394	71% 14% · 14%

2 Entry composition

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
1	Y	74	Total	C	N	O	P	0	0	1
			1472	650	265	484	73			

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

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

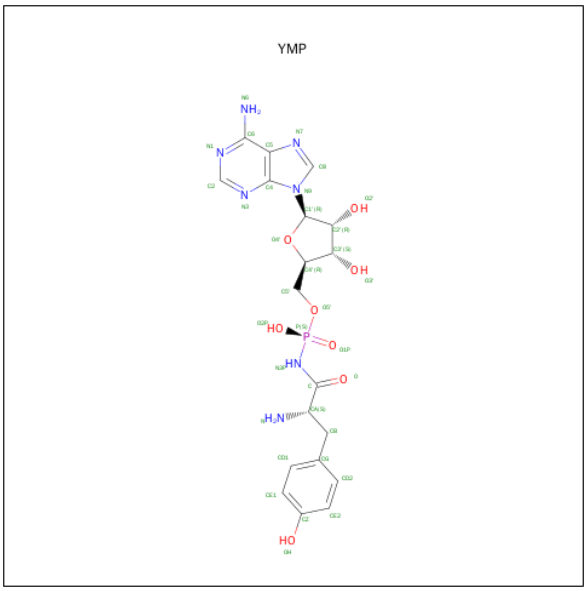
There is a discrepancy between the modelled and reference sequences:

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
3	X	1	Total	Mg	0	0
			1	1		

- 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
4	X	1	Total	C	N	O	P	0	0
			35	19	7	8	1		

- Molecule 5 is water.

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

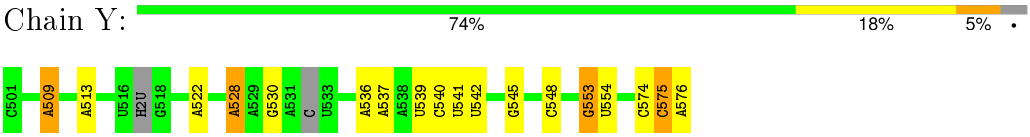
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

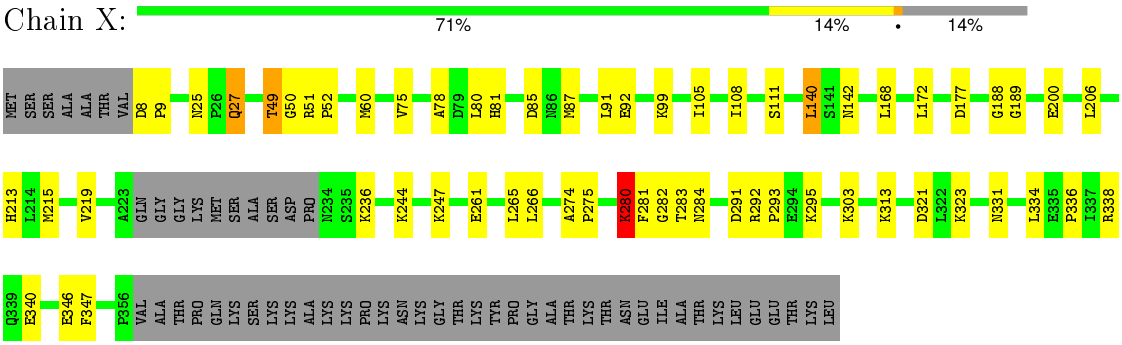
- Molecule 1: T-RNA (76-MER)

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 will therefore be 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, YMP, MG, 6IA, OMG, 2MG, 5MC, 1MA, M2G, PSU

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

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

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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

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
2	X	335/394 (85%)	325 (97%)	8 (2%)	2 (1%)	30 43

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	X	296/340 (87%)	270 (91%)	26 (9%)	12 18

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

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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

Some 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	2MG	Y	510	1	16,25,27	1.25	1 (6%)	19,37,41	2.50	3 (15%)
1	OMG	Y	518	1	16,25,27	1.22	2 (12%)	19,37,41	2.56	3 (15%)
1	M2G	Y	526	1	16,25,28	1.25	2 (12%)	19,37,43	2.59	3 (15%)
1	PSU	Y	535	1	13,21,22	1.23	1 (7%)	18,30,33	3.64	5 (27%)
1	6IA	Y	537	1	15,24,30	0.58	0	16,35,44	0.56	0
1	PSU	Y	539	1	8,12,22	0.77	0	12,16,33	1.06	1 (8%)
1	5MC	Y	548	1	13,22,23	0.91	1 (7%)	15,32,35	0.48	0
1	5MU	Y	554	1	12,22,23	1.46	3 (25%)	14,32,35	4.59	3 (21%)
1	PSU	Y	555	1	13,21,22	1.11	1 (7%)	18,30,33	3.71	5 (27%)
1	1MA	Y	558	1	14,25,26	1.05	1 (7%)	15,37,40	1.05	1 (6%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	554	5MU	C6-C5	-2.07	1.34	1.40
1	Y	548	5MC	C6-C5	-2.03	1.34	1.40
1	Y	526	M2G	C8-N7	-2.02	1.30	1.34
1	Y	518	OMG	C8-N7	-2.01	1.30	1.34
1	Y	554	5MU	C6-N1	2.82	1.39	1.35
1	Y	558	1MA	C6-N6	2.83	1.34	1.29
1	Y	535	PSU	C4-N3	3.04	1.38	1.33
1	Y	555	PSU	C4-N3	3.09	1.38	1.33
1	Y	554	5MU	C4-N3	3.28	1.39	1.33
1	Y	518	OMG	C6-N1	3.83	1.40	1.33
1	Y	526	M2G	C6-N1	3.92	1.40	1.33
1	Y	510	2MG	C6-N1	3.95	1.40	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	555	PSU	N1-C2-N3	-13.11	119.97	128.33
1	Y	535	PSU	N1-C2-N3	-13.02	120.03	128.33
1	Y	554	5MU	C5-C4-N3	-9.45	114.61	125.14
1	Y	526	M2G	C5-C6-N1	-8.40	112.11	123.59
1	Y	518	OMG	C5-C6-N1	-8.34	112.19	123.59
1	Y	510	2MG	C5-C6-N1	-8.24	112.32	123.59
1	Y	555	PSU	C5-C1'-C2'	-4.24	107.98	115.52
1	Y	535	PSU	C5-C1'-C2'	-3.84	108.70	115.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	558	1MA	C2-N3-C4	-3.43	111.09	116.40
1	Y	526	M2G	N3-C2-N1	-2.51	123.62	127.44
1	Y	535	PSU	C5-C6-N1	-2.47	120.91	124.39
1	Y	518	OMG	N3-C2-N1	-2.47	123.68	127.44
1	Y	510	2MG	N3-C2-N1	-2.43	123.74	127.44
1	Y	555	PSU	C5-C6-N1	-2.41	120.98	124.39
1	Y	539	PSU	C1'-C2'-C3'	2.22	105.21	101.64
1	Y	554	5MU	C5M-C5-C4	2.71	123.54	120.05
1	Y	535	PSU	C6-N1-C2	3.13	120.51	115.47
1	Y	555	PSU	C6-N1-C2	3.15	120.54	115.47
1	Y	535	PSU	C4-N3-C2	5.31	119.84	115.25
1	Y	555	PSU	C4-N3-C2	5.53	120.02	115.25
1	Y	510	2MG	C6-N1-C2	6.13	124.45	115.94
1	Y	518	OMG	C6-N1-C2	6.25	124.62	115.94
1	Y	526	M2G	C6-N1-C2	6.29	124.68	115.94
1	Y	554	5MU	C4-N3-C2	13.92	127.28	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	32,38,38	2.12	5 (15%)	37,56,56	4.12	9 (24%)

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	-	0/17/39/39	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	P-O2P	-2.10	1.50	1.56
4	X	601	YMP	P-N3P	2.26	1.68	1.64
4	X	601	YMP	P-O1P	3.61	1.50	1.46
4	X	601	YMP	C2-N1	6.66	1.46	1.33
4	X	601	YMP	C2-N3	7.62	1.45	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	601	YMP	N3-C2-N1	-22.67	111.54	128.89
4	X	601	YMP	C4-C5-N7	-3.82	105.96	109.48
4	X	601	YMP	C2'-C1'-N9	-2.85	109.93	114.29
4	X	601	YMP	C1'-N9-C4	-2.18	123.66	126.94
4	X	601	YMP	O3'-C3'-C4'	-2.06	104.87	111.05
4	X	601	YMP	O5'-P-O1P	-2.04	104.85	113.31
4	X	601	YMP	O2P-P-O1P	3.38	117.05	110.00
4	X	601	YMP	O4'-C1'-N9	4.84	118.22	108.10
4	X	601	YMP	C2-N1-C6	4.97	127.66	118.77

There are no chirality outliers.

There are no torsion outliers.

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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.