Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 11:05 pm BST

PDB ID	:	4YED
Title	:	TcdA (CsdL)
Authors	:	Kim, S.; Park, S.Y.
Deposited on	:	2015-02-24
Resolution	:	1.90 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 following versions of software and data (see references (i)) were used in the production of this report:

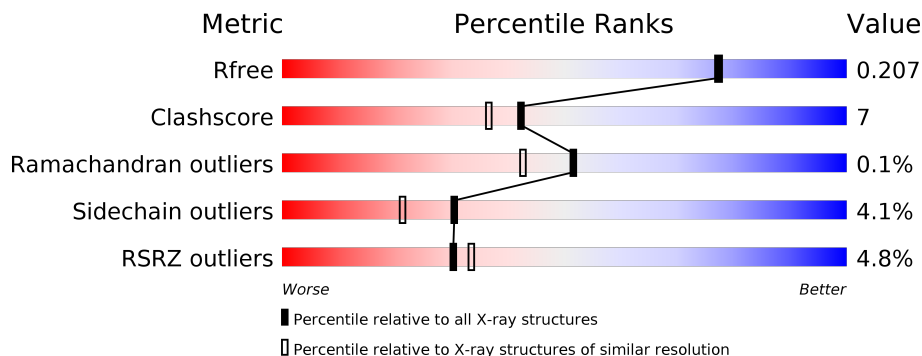|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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	Percentile Ranks	Value
Rfree		0.207
Clashscore		7
Ramachandran outliers		0.1%
Sidechain outliers		4.1%
RSRZ outliers		4.8%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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% 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	271	2% 82% 7% · 10%
1	B	271	7% 79% 14% · 6%
1	C	271	4% 83% 7% · 7%
1	D	271	4% 81% 11% · 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8220 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 tRNA threonylcarbamoyladenosine dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	Se	0	0	0
			1840	1158	329	342	5	6			
1	B	254	Total	C	N	O	S	Se	0	0	0
			1900	1193	339	355	6	7			
1	C	252	Total	C	N	O	S	Se	0	0	0
			1885	1184	336	352	6	7			
1	D	255	Total	C	N	O	S	Se	0	0	0
			1906	1197	340	356	6	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q46927
A	-1	SER	-	expression tag	UNP Q46927
A	0	HIS	-	expression tag	UNP Q46927
B	-2	GLY	-	expression tag	UNP Q46927
B	-1	SER	-	expression tag	UNP Q46927
B	0	HIS	-	expression tag	UNP Q46927
C	-2	GLY	-	expression tag	UNP Q46927
C	-1	SER	-	expression tag	UNP Q46927
C	0	HIS	-	expression tag	UNP Q46927
D	-2	GLY	-	expression tag	UNP Q46927
D	-1	SER	-	expression tag	UNP Q46927
D	0	HIS	-	expression tag	UNP Q46927

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).
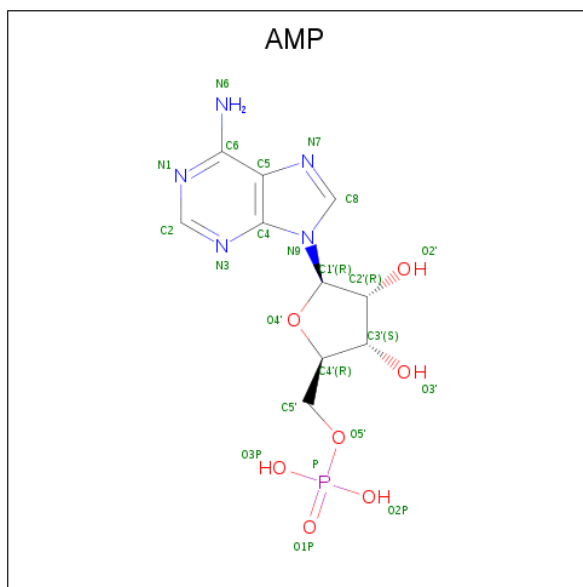
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	171	Total 171	O 171	0	0
4	B	125	Total 125	O 125	0	0
4	C	132	Total 132	O 132	0	0
4	D	145	Total 145	O 145	0	0

# 3 Residue-property plots ⓘ

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.
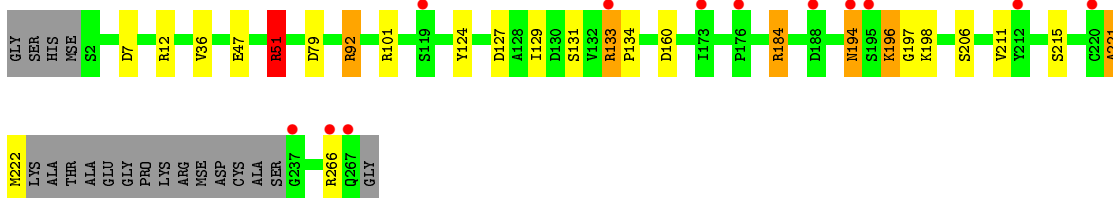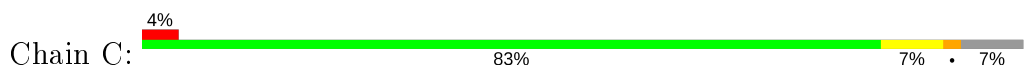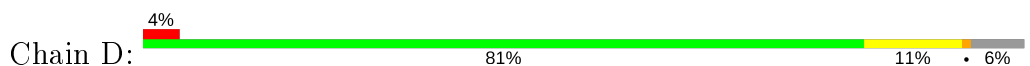
- Molecule 1: tRNA threonylcarbamoyladenosine dehydratase
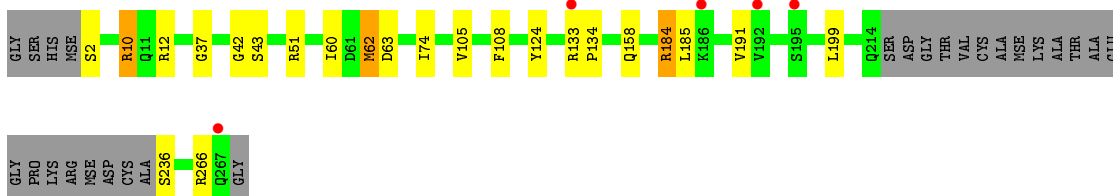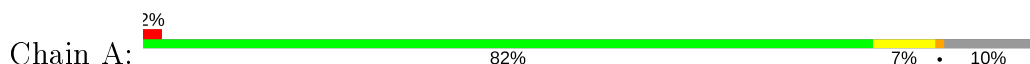
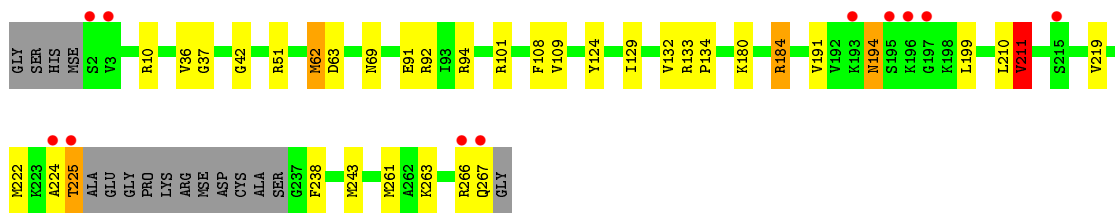- Molecule 1: tRNA threonylcarbamoyladenosine dehydratase
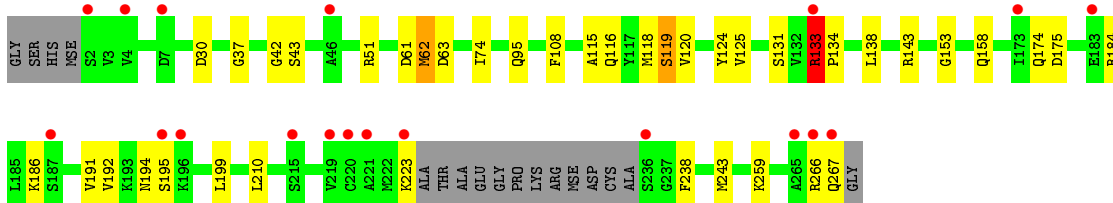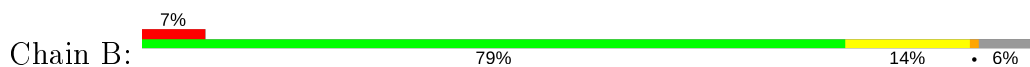
- Molecule 1: tRNA threonylcarbamoyladenosine dehydratase

- Molecule 1: tRNA threonylcarbamoyladenosine dehydratase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.56Å　97.12Å　83.34Å 90.00°　111.65°　90.00°	Depositor
Resolution (Å)	32.77 − 1.90 32.77 − 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.77-1.90) 99.7 (32.77-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.159　,　0.200 0.173　,　0.207	Depositor DCC
R_{free} test set	3841 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8220	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, AMP

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	0.92	0/1860	1.03	8/2508 (0.3%)
1	B	0.86	1/1919 (0.1%)	1.18	7/2585 (0.3%)
1	C	0.84	2/1904 (0.1%)	1.17	8/2566 (0.3%)
1	D	0.85	0/1925	0.93	6/2594 (0.2%)
All	All	0.87	3/7608 (0.0%)	1.08	29/10253 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	ARG	CD-NE	6.58	1.57	1.46
1	B	51	ARG	CD-NE	-6.55	1.35	1.46
1	C	51	ARG	CD-NE	-5.76	1.36	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ARG	NE-CZ-NH2	-28.96	105.82	120.30
1	B	51	ARG	NE-CZ-NH1	23.74	132.17	120.30
1	C	92	ARG	NE-CZ-NH1	-21.30	109.65	120.30
1	C	51	ARG	NE-CZ-NH2	-20.85	109.88	120.30
1	C	92	ARG	NE-CZ-NH2	16.62	128.61	120.30
1	C	51	ARG	CD-NE-CZ	12.22	140.70	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	NE-CZ-NH1	-11.64	114.48	120.30
1	A	10	ARG	NE-CZ-NH2	-10.57	115.01	120.30
1	C	92	ARG	CD-NE-CZ	-9.88	109.77	123.60
1	B	51	ARG	CD-NE-CZ	9.43	136.80	123.60
1	A	266	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	10	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	266	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	C	12	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	B	51	ARG	CG-CD-NE	-6.04	99.11	111.80
1	B	133	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	160	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	12	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	10	ARG	CG-CD-NE	-5.42	100.42	111.80
1	A	51	ARG	CD-NE-CZ	5.38	131.13	123.60
1	B	30	ASP	CB-CG-OD1	5.36	123.13	118.30
1	C	79	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	94	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	D	92	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	61	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	211	VAL	CG1-CB-CG2	5.08	119.02	110.90
1	A	51	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	D	261	MSE	CG-SE-CE	5.02	109.95	98.90
1	D	51	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	51	ARG	Sidechain

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	1840	0	1878	11	0
1	B	1900	0	1938	42	0
1	C	1885	0	1920	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1906	0	1945	38	0
2	A	23	0	12	2	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	5	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	171	0	0	3	0
4	B	125	0	0	4	0
4	C	132	0	0	3	0
4	D	145	0	0	4	0
All	All	8220	0	7761	106	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 7.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:VAL:CG2	1:D:222:MSE:HE3	1.41	1.47
1:C:194:ASN:ND2	1:C:198:LYS:H	1.28	1.28
1:B:120:VAL:HG23	1:D:222:MSE:CE	1.72	1.17
1:B:120:VAL:CG2	1:D:222:MSE:CE	2.29	1.10
1:C:194:ASN:ND2	1:C:198:LYS:N	2.05	1.03
1:B:120:VAL:HG21	1:D:222:MSE:HE3	1.45	0.98
1:B:118:MSE:CE	1:B:138:LEU:HD11	1.93	0.98
1:C:194:ASN:HD21	1:C:198:LYS:N	1.61	0.94
1:B:118:MSE:HE3	1:B:138:LEU:CD1	2.00	0.92
1:B:118:MSE:CE	1:B:138:LEU:CD1	2.48	0.92
1:B:120:VAL:HG23	1:D:222:MSE:HE3	0.87	0.85
1:B:62:MSE:HE2	1:B:108:PHE:CD2	2.12	0.83
1:D:62:MSE:HE3	1:D:108:PHE:CE2	2.13	0.83
1:C:221:ALA:O	1:C:222:MSE:HG2	1.79	0.82
1:B:62:MSE:CE	1:B:108:PHE:CD2	2.62	0.82
1:B:118:MSE:HE3	1:B:138:LEU:HD11	1.61	0.76
1:D:108:PHE:HB3	2:D:301:AMP:N6	2.02	0.75
1:D:211:VAL:HG13	1:D:219:VAL:HG13	1.69	0.74
1:B:116:GLN:HE22	1:D:225:THR:N	1.84	0.74
1:D:62:MSE:CE	1:D:108:PHE:CD2	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ASN:HD21	1:C:198:LYS:H	0.76	0.71
1:B:95:GLN:HG2	4:B:412:HOH:O	1.90	0.70
1:D:211:VAL:HG13	1:D:219:VAL:CG1	2.24	0.67
1:C:101:ARG:NH1	4:C:403:HOH:O	2.28	0.66
1:D:62:MSE:HE3	1:D:108:PHE:CD2	2.30	0.66
1:D:263:LYS:O	1:D:267:GLN:HG3	1.95	0.66
1:A:158:GLN:OE1	4:A:401:HOH:O	2.13	0.65
1:B:116:GLN:NE2	1:D:225:THR:N	2.44	0.65
1:B:116:GLN:HE22	1:D:225:THR:H	1.44	0.65
1:D:101:ARG:NH1	4:D:402:HOH:O	2.19	0.65
1:B:267:GLN:OE1	1:B:267:GLN:HA	1.96	0.64
1:D:194:ASN:HD22	1:D:194:ASN:C	2.02	0.64
1:B:158:GLN:OE1	4:B:401:HOH:O	2.15	0.64
2:A:301:AMP:O1P	4:A:402:HOH:O	2.15	0.63
1:B:120:VAL:HG21	1:D:222:MSE:CE	2.11	0.62
1:B:118:MSE:HE3	1:B:138:LEU:HD12	1.82	0.61
2:D:301:AMP:O2P	4:D:401:HOH:O	2.16	0.60
1:C:47:GLU:OE1	1:C:92:ARG:NH1	2.30	0.60
1:C:194:ASN:OD1	1:C:196:LYS:HB2	2.03	0.59
1:B:62:MSE:CE	1:B:108:PHE:CE2	2.86	0.58
1:D:210:LEU:HD23	1:D:238:PHE:CZ	2.39	0.58
1:A:10:ARG:NH2	4:A:403:HOH:O	2.24	0.58
1:B:62:MSE:HE3	1:B:108:PHE:CE2	2.39	0.58
1:B:118:MSE:HE1	1:B:138:LEU:HD11	1.83	0.57
1:C:221:ALA:C	1:C:222:MSE:HG2	2.25	0.57
1:B:116:GLN:NE2	1:D:225:THR:H	2.02	0.56
1:D:224:ALA:O	1:D:225:THR:HB	2.05	0.55
1:A:191:VAL:HG12	1:A:199:LEU:HD22	1.90	0.54
1:D:224:ALA:O	1:D:225:THR:CB	2.56	0.54
1:D:91:GLU:HG3	4:D:435:HOH:O	2.08	0.54
1:B:62:MSE:HE2	1:B:108:PHE:CG	2.43	0.53
1:C:133:ARG:HB2	1:C:134:PRO:HD3	1.91	0.53
1:A:185:LEU:HB3	1:A:191:VAL:HB	1.89	0.52
1:C:194:ASN:HD22	1:C:194:ASN:N	2.08	0.52
1:C:194:ASN:ND2	1:C:197:GLY:N	2.59	0.51
1:D:109:VAL:O	1:D:134:PRO:HB3	2.11	0.51
1:A:37:GLY:O	1:A:42:GLY:HA3	2.11	0.51
1:B:118:MSE:HE1	1:B:125:VAL:HG11	1.92	0.51
1:B:133:ARG:HH11	1:B:133:ARG:CG	2.22	0.51
1:C:133:ARG:HG2	1:C:184:ARG:NH2	2.26	0.50
1:B:266:ARG:O	1:B:267:GLN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ASN:HD22	1:C:194:ASN:H	1.61	0.49
1:C:92:ARG:HH11	1:C:92:ARG:HG2	1.79	0.48
1:B:259:LYS:HE3	4:B:447:HOH:O	2.13	0.48
1:D:132:VAL:HG21	1:D:180:LYS:HD2	1.96	0.47
1:C:92:ARG:HH11	1:C:92:ARG:CG	2.15	0.47
1:B:210:LEU:HD23	1:B:238:PHE:CZ	2.49	0.47
1:A:134:PRO:CB	2:A:301:AMP:N6	2.77	0.47
1:C:194:ASN:HD21	1:C:197:GLY:N	2.14	0.46
1:C:92:ARG:NH1	1:C:92:ARG:CG	2.72	0.46
1:C:36:VAL:CG1	1:C:129:ILE:HD11	2.47	0.45
1:A:60:ILE:HG12	1:A:105:VAL:HB	1.98	0.45
1:C:36:VAL:HG11	1:C:129:ILE:HD11	1.96	0.45
1:A:236:SER:O	1:A:236:SER:OG	2.31	0.45
1:C:92:ARG:HD2	4:C:440:HOH:O	2.17	0.45
1:D:108:PHE:HB3	2:D:301:AMP:C6	2.52	0.45
1:D:243:MSE:SE	1:D:243:MSE:H	2.49	0.45
1:B:186:LYS:HD2	1:B:192:VAL:HG12	1.99	0.44
1:C:206:SER:O	4:C:401:HOH:O	2.21	0.44
1:B:143:ARG:CZ	1:B:191:VAL:HG13	2.48	0.44
1:D:191:VAL:HG12	1:D:199:LEU:HD22	2.00	0.43
1:D:36:VAL:HG11	1:D:129:ILE:HD11	2.01	0.43
1:B:115:ALA:O	1:B:119:SER:HB3	2.18	0.43
1:B:37:GLY:O	1:B:42:GLY:HA3	2.18	0.43
1:B:118:MSE:HE2	1:B:138:LEU:CD1	2.41	0.43
1:C:92:ARG:NH1	1:C:92:ARG:HG2	2.33	0.43
1:B:153:GLY:HA3	1:B:175:ASP:OD2	2.19	0.43
1:D:62:MSE:HE2	1:D:108:PHE:CD2	2.52	0.42
1:D:210:LEU:HD23	1:D:238:PHE:CE1	2.54	0.42
1:D:134:PRO:CB	2:D:301:AMP:N6	2.82	0.42
1:C:131:SER:O	1:C:134:PRO:HD2	2.19	0.42
1:A:133:ARG:HG2	1:A:184:ARG:NH2	2.35	0.42
1:B:210:LEU:HD21	4:B:474:HOH:O	2.20	0.42
1:B:191:VAL:HG12	1:B:199:LEU:HD22	2.02	0.42
1:D:63:ASP:OD2	2:D:301:AMP:O2'	2.31	0.42
1:B:243:MSE:SE	1:B:243:MSE:H	2.53	0.42
1:D:224:ALA:O	1:D:225:THR:HG22	2.19	0.42
1:B:133:ARG:N	1:B:134:PRO:HD2	2.34	0.42
1:D:133:ARG:HG2	1:D:184:ARG:NH2	2.35	0.41
1:B:43:SER:HB2	1:B:74:ILE:HG22	2.02	0.41
1:D:37:GLY:O	1:D:42:GLY:HA3	2.20	0.41
1:A:62:MSE:HE3	1:A:108:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:SER:HB2	1:A:74:ILE:HG22	2.03	0.41
1:D:69:ASN:ND2	4:D:404:HOH:O	2.42	0.41
1:B:120:VAL:HG21	1:D:222:MSE:SE	2.71	0.41
1:B:174:GLN:HE22	1:B:223:LYS:HB3	1.85	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	241/271 (89%)	236 (98%)	5 (2%)	0	100	100
1	B	250/271 (92%)	244 (98%)	6 (2%)	0	100	100
1	C	248/271 (92%)	242 (98%)	5 (2%)	1 (0%)	34	24
1	D	251/271 (93%)	243 (97%)	8 (3%)	0	100	100
All	All	990/1084 (91%)	965 (98%)	24 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	221	ALA

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	192/201 (96%)	187 (97%)	5 (3%)	46	39
1	B	199/201 (99%)	190 (96%)	9 (4%)	27	18
1	C	197/201 (98%)	186 (94%)	11 (6%)	21	11
1	D	199/201 (99%)	192 (96%)	7 (4%)	36	27
All	All	787/804 (98%)	755 (96%)	32 (4%)	30	21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	62	MSE
1	A	63	ASP
1	A	124	TYR
1	A	184	ARG
1	B	62	MSE
1	B	63	ASP
1	B	119	SER
1	B	124	TYR
1	B	131	SER
1	B	133	ARG
1	B	184	ARG
1	B	194	ASN
1	B	195	SER
1	C	7	ASP
1	C	51	ARG
1	C	124	TYR
1	C	127	ASP
1	C	133	ARG
1	C	184	ARG
1	C	194	ASN
1	C	196	LYS
1	C	211	VAL
1	C	215	SER
1	C	266	ARG
1	D	62	MSE
1	D	124	TYR
1	D	184	ARG
1	D	194	ASN
1	D	211	VAL
1	D	225	THR
1	D	266	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	116	GLN
1	C	194	ASN
1	C	214	GLN
1	D	194	ASN
1	D	214	GLN

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 (i)

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	AMP	C	301	-	22,25,25	1.22	3 (13%)	25,38,38	1.70	6 (24%)
2	AMP	A	301	-	22,25,25	1.83	5 (22%)	25,38,38	1.44	4 (16%)
3	GOL	A	302	-	5,5,5	1.12	0	5,5,5	0.92	0
3	GOL	C	302	-	5,5,5	1.18	0	5,5,5	1.02	0
3	GOL	D	302	-	5,5,5	1.39	0	5,5,5	1.05	0
2	AMP	D	301	-	22,25,25	1.74	5 (22%)	25,38,38	1.67	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	B	302	-	5,5,5	1.36	0	5,5,5	0.91	0
2	AMP	B	301	-	22,25,25	1.51	3 (13%)	25,38,38	1.68	5 (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	AMP	C	301	-	-	1/6/26/26	0/3/3/3
2	AMP	A	301	-	-	3/6/26/26	0/3/3/3
3	GOL	A	302	-	-	1/4/4/4	-
3	GOL	C	302	-	-	0/4/4/4	-
3	GOL	D	302	-	-	0/4/4/4	-
2	AMP	D	301	-	-	2/6/26/26	0/3/3/3
3	GOL	B	302	-	-	1/4/4/4	-
2	AMP	B	301	-	-	4/6/26/26	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	AMP	O4'-C1'	4.61	1.47	1.41
2	B	301	AMP	C4-N3	4.29	1.41	1.35
2	A	301	AMP	C2-N1	4.14	1.41	1.33
2	A	301	AMP	C5-C4	3.85	1.51	1.40
2	D	301	AMP	C5-C4	3.45	1.50	1.40
2	A	301	AMP	C4-N3	3.43	1.40	1.35
2	D	301	AMP	C4-N3	3.24	1.40	1.35
2	C	301	AMP	O4'-C1'	3.12	1.45	1.41
2	A	301	AMP	O4'-C1'	3.07	1.45	1.41
2	B	301	AMP	C5-C4	3.05	1.49	1.40
2	D	301	AMP	C2-N1	2.68	1.38	1.33
2	C	301	AMP	C5-C4	2.62	1.47	1.40
2	C	301	AMP	C2-N1	2.48	1.38	1.33
2	B	301	AMP	C2-N3	2.21	1.35	1.32
2	D	301	AMP	C2-N3	2.17	1.35	1.32
2	A	301	AMP	C2-N3	2.12	1.35	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	AMP	N3-C2-N1	-4.02	122.39	128.68
2	D	301	AMP	N3-C2-N1	-3.65	122.97	128.68
2	C	301	AMP	O2P-P-O5'	3.52	116.10	106.73
2	D	301	AMP	O3P-P-O5'	-3.52	97.37	106.73
2	B	301	AMP	N3-C2-N1	-3.42	123.33	128.68
2	B	301	AMP	C5-C6-N6	-3.37	115.24	120.35
2	B	301	AMP	O3P-P-O2P	3.16	119.72	107.64
2	B	301	AMP	N6-C6-N1	3.05	124.90	118.57
2	A	301	AMP	C5-C6-N6	-2.98	115.83	120.35
2	A	301	AMP	N3-C2-N1	-2.96	124.05	128.68
2	C	301	AMP	O5'-P-O1P	-2.91	98.31	106.47
2	B	301	AMP	O3P-P-O5'	-2.89	99.04	106.73
2	C	301	AMP	O3P-P-O2P	2.85	118.54	107.64
2	C	301	AMP	C2-N1-C6	2.75	123.46	118.75
2	D	301	AMP	O4'-C4'-C3'	2.60	110.26	105.11
2	A	301	AMP	N6-C6-N1	2.47	123.69	118.57
2	D	301	AMP	O3'-C3'-C4'	2.43	118.08	111.05
2	D	301	AMP	O5'-P-O1P	2.41	113.23	106.47
2	D	301	AMP	N6-C6-N1	2.38	123.52	118.57
2	A	301	AMP	O3P-P-O5'	-2.21	100.84	106.73
2	D	301	AMP	C5-C6-N6	-2.12	117.12	120.35
2	C	301	AMP	C1'-N9-C4	-2.08	122.99	126.64

There are no chirality outliers.

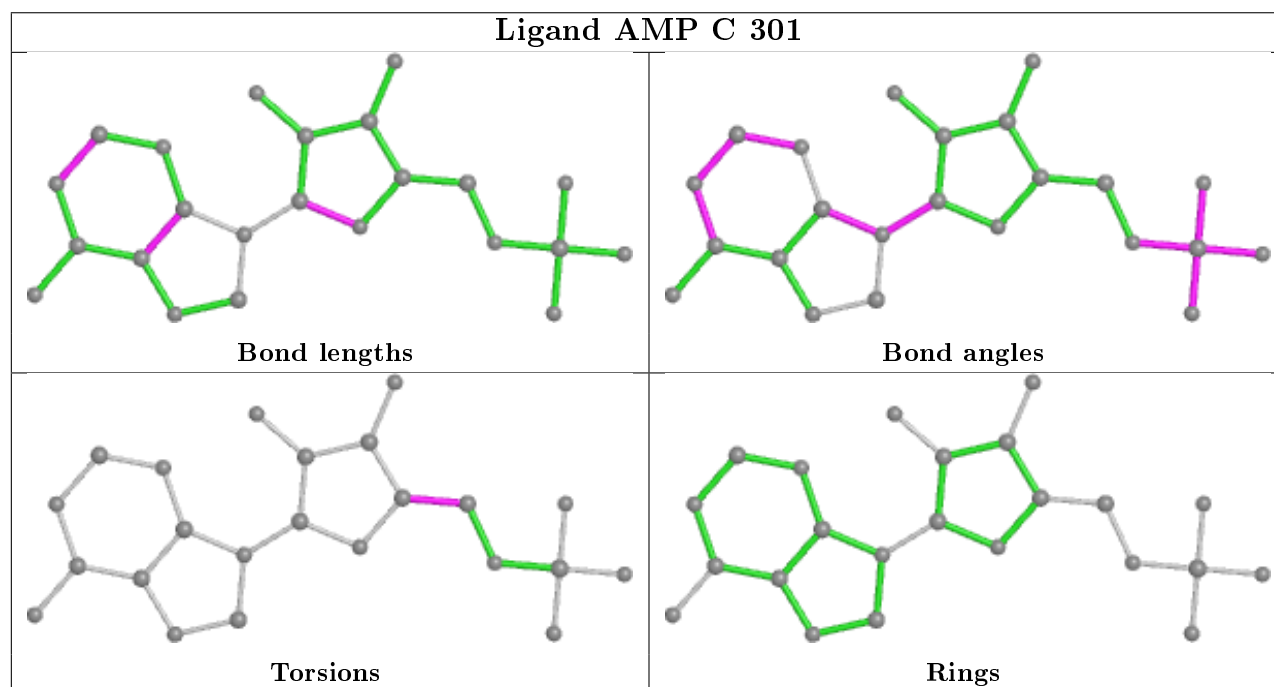All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	AMP	O4'-C4'-C5'-O5'
2	B	301	AMP	C5'-O5'-P-O1P
2	B	301	AMP	C5'-O5'-P-O2P
2	D	301	AMP	C3'-C4'-C5'-O5'
3	A	302	GOL	C1-C2-C3-O3
2	A	301	AMP	O4'-C4'-C5'-O5'
2	B	301	AMP	C5'-O5'-P-O3P
2	A	301	AMP	C5'-O5'-P-O1P
2	C	301	AMP	O4'-C4'-C5'-O5'
2	B	301	AMP	O4'-C4'-C5'-O5'
2	A	301	AMP	C3'-C4'-C5'-O5'
3	B	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	AMP	2	0
2	D	301	AMP	5	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 AMP C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP B 301

Bond lengths

Bond angles

Torsions

Rings
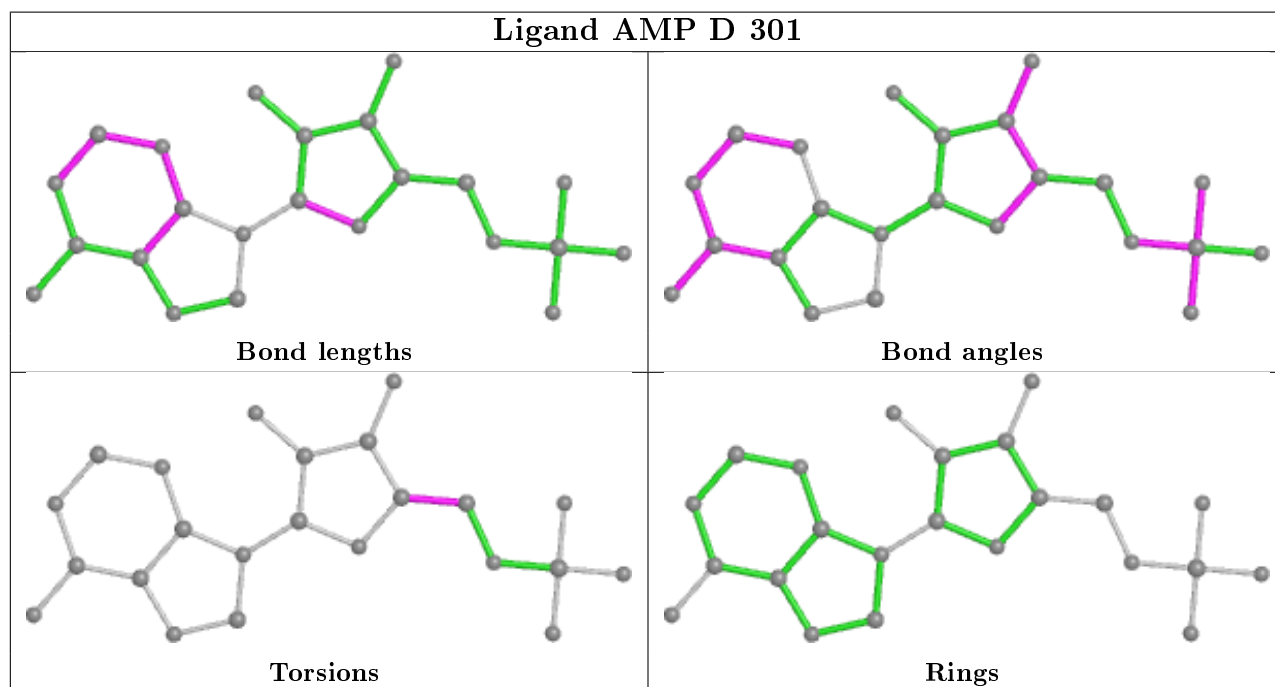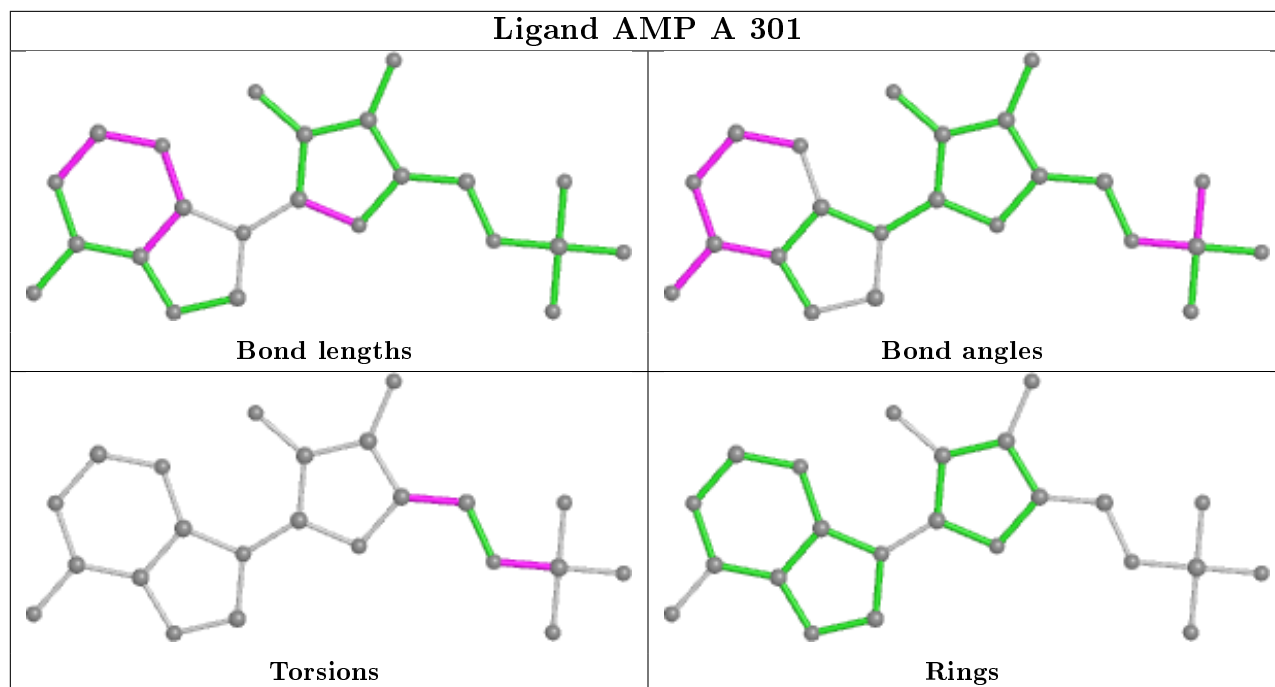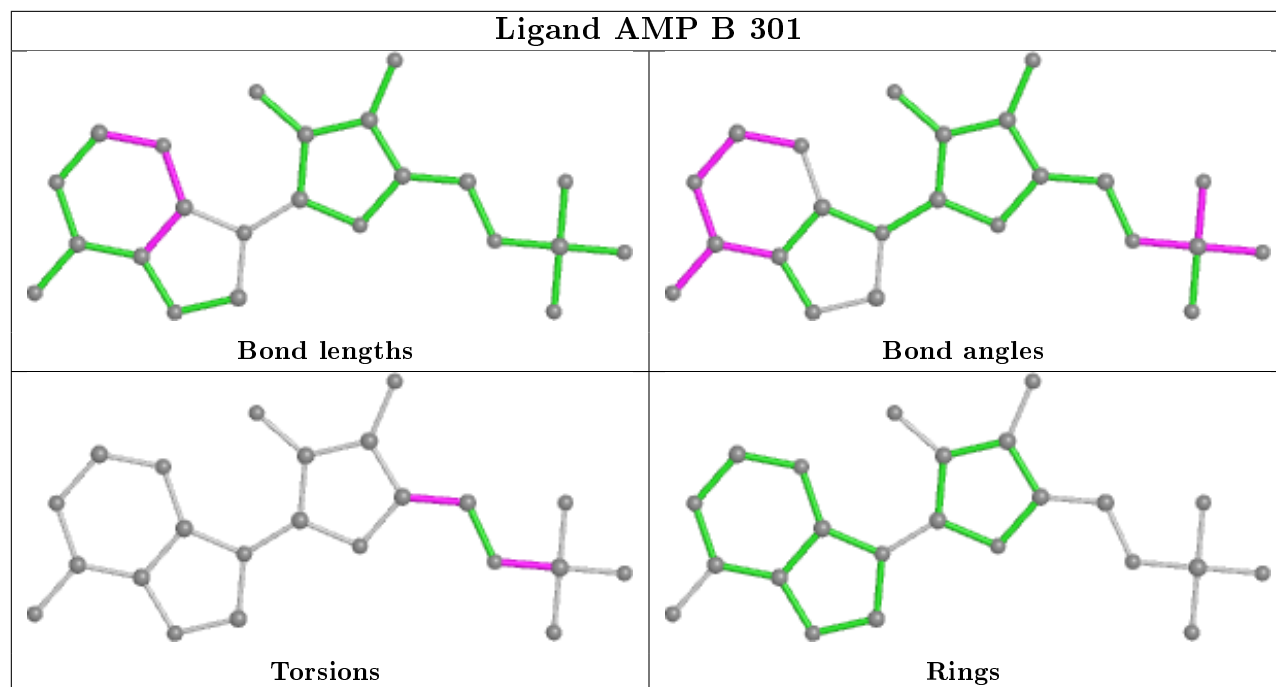
5.7 Other polymers (i)

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)

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	239/271 (88%)	-0.16	5 (2%)	63	66	14, 22, 45, 76	0
1	B	247/271 (91%)	0.31	19 (7%)	13	15	14, 26, 60, 93	0
1	C	245/271 (90%)	0.07	12 (4%)	29	33	16, 27, 56, 71	0
1	D	248/271 (91%)	-0.01	11 (4%)	34	37	17, 26, 47, 78	0
All	All	979/1084 (90%)	0.06	47 (4%)	30	33	14, 25, 53, 93	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	LYS	7.0
1	D	195	SER	6.6
1	B	195	SER	5.9
1	D	225	THR	5.4
1	B	236	SER	5.1
1	B	267	GLN	5.1
1	A	195	SER	4.8
1	D	2	SER	4.7
1	D	267	GLN	4.5
1	D	266	ARG	4.0
1	B	266	ARG	4.0
1	B	221	ALA	3.7
1	A	267	GLN	3.7
1	D	215	SER	3.5
1	B	2	SER	3.2
1	A	192	VAL	3.1
1	C	267	GLN	3.1
1	D	196	LYS	3.1
1	B	173	ILE	2.9
1	C	173	ILE	2.9
1	C	212	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	133	ARG	2.7
1	C	266	ARG	2.7
1	B	265	ALA	2.6
1	C	195	SER	2.6
1	B	196	LYS	2.6
1	B	4	VAL	2.6
1	B	220	CYS	2.6
1	B	183	GLU	2.5
1	B	46	ALA	2.5
1	C	176	PRO	2.4
1	B	133	ARG	2.4
1	C	237	GLY	2.3
1	C	119	SER	2.3
1	C	188	ASP	2.3
1	B	219	VAL	2.3
1	B	215	SER	2.3
1	D	193	LYS	2.3
1	A	133	ARG	2.2
1	D	224	ALA	2.2
1	C	194	ASN	2.2
1	B	7	ASP	2.1
1	B	187	SER	2.1
1	A	186	LYS	2.1
1	C	220	CYS	2.1
1	D	197	GLY	2.1
1	D	3	VAL	2.0

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

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(Å^2)	Q<0.9
3	GOL	D	302	6/6	0.74	0.18	30,36,40,42	0
2	AMP	D	301	23/23	0.80	0.27	33,53,61,64	0
2	AMP	A	301	23/23	0.85	0.22	29,46,52,55	0
3	GOL	C	302	6/6	0.85	0.12	31,39,41,41	0
3	GOL	B	302	6/6	0.89	0.13	24,29,33,35	0
3	GOL	A	302	6/6	0.93	0.11	23,29,32,38	0
2	AMP	B	301	23/23	0.94	0.11	27,34,39,41	0
2	AMP	C	301	23/23	0.96	0.07	25,31,36,43	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.
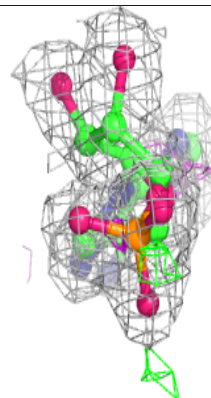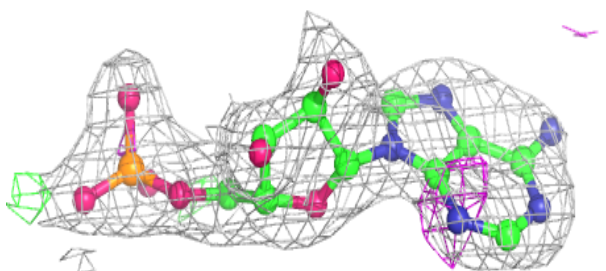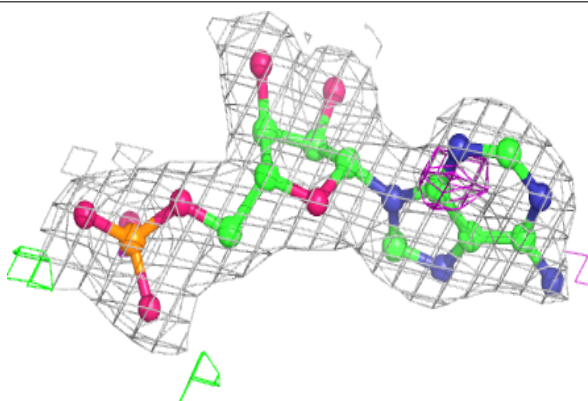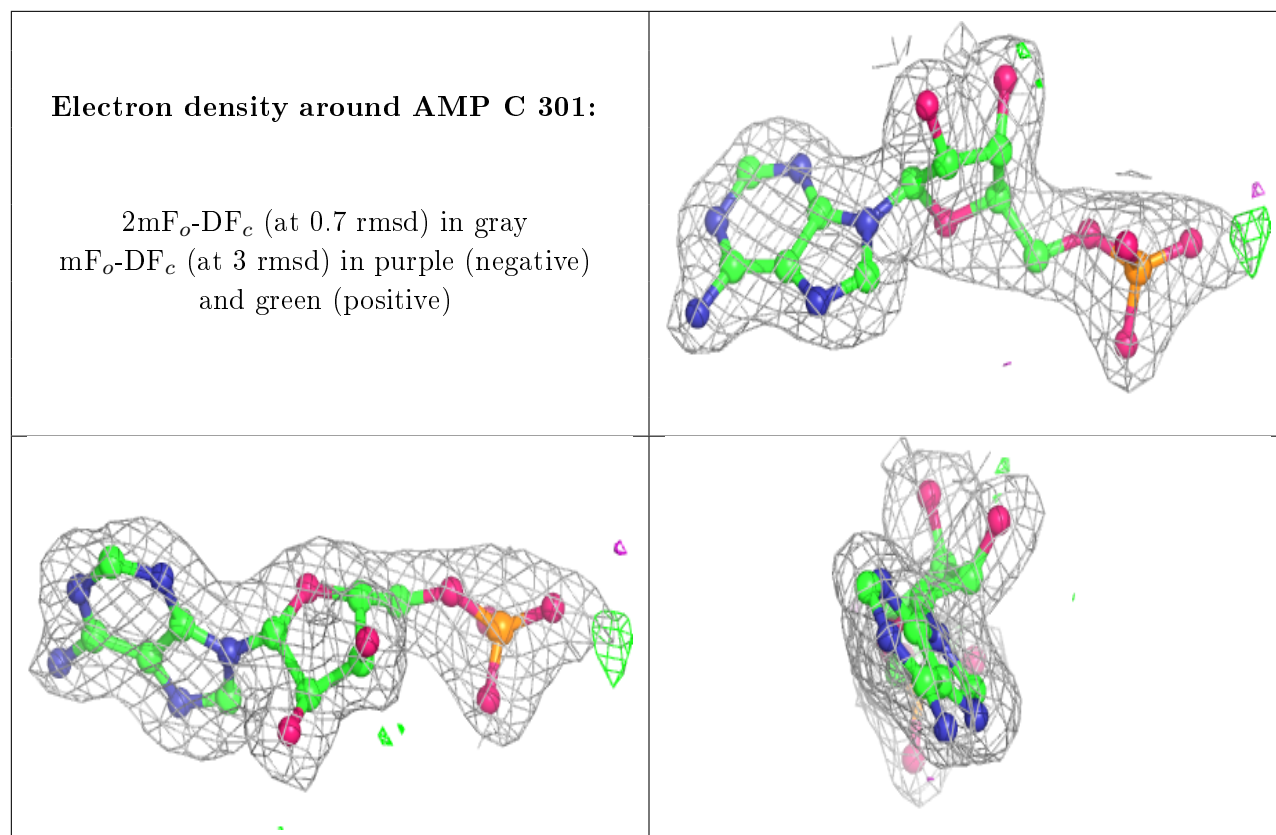

Electron density around AMP D 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
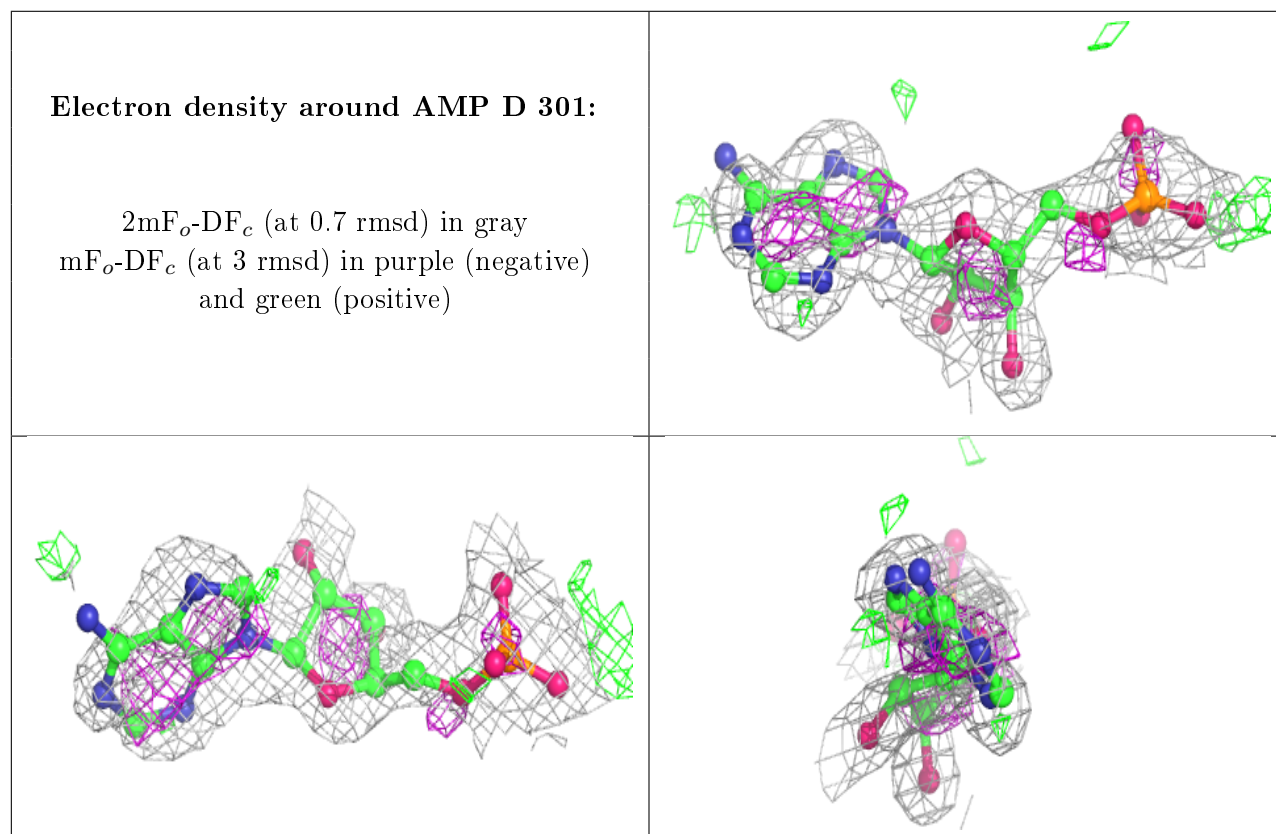
Electron density around AMP A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
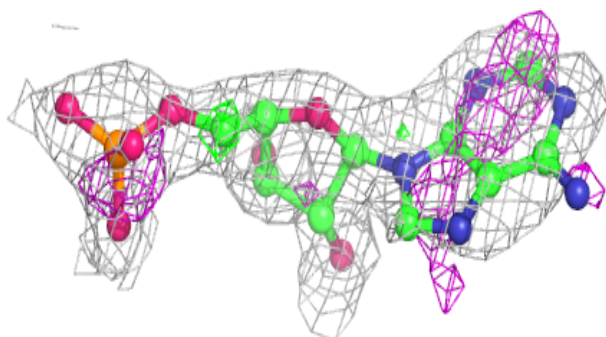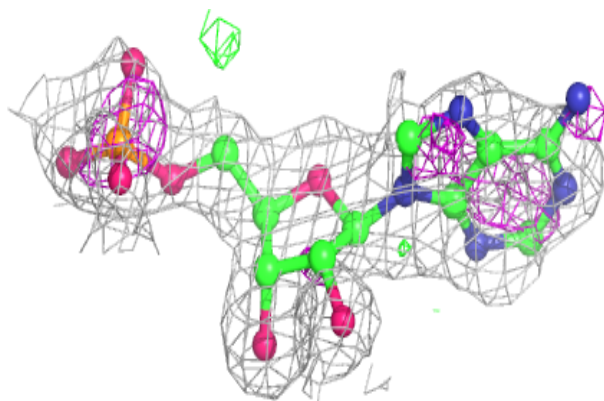
Electron density around AMP B 301:

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

Electron density around AMP C 301:

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

6.5 Other polymers (i)

There are no such residues in this entry.