



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:22 am BST

PDB ID : 6E4U
Title : Structure of AMPK bound to activator
Authors : Calabrese, M.F.; Kurumbail, R.G.
Deposited on : 2018-07-18
Resolution : 3.27 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 : 1.8.5 (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

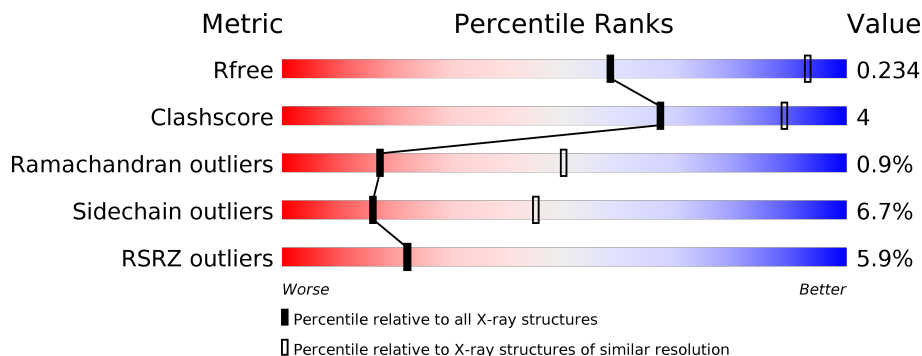
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 $\leq 5\%$. 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	503	<p>3% 62% 10% • 27%</p>
2	B	204	<p>2% 60% 17% • 21%</p>
3	C	330	<p>8% 77% 8% 14%</p>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6340 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 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	366	2884	1849	494	522	1	18	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P54645
A	517	ALA	-	linker	UNP P54645
A	518	SER	-	linker	UNP P54645
A	519	GLY	-	linker	UNP P54645
A	520	GLY	-	linker	UNP P54645
A	521	PRO	-	linker	UNP P54645
A	522	GLY	-	linker	UNP P54645
A	523	GLY	-	linker	UNP P54645
A	524	SER	-	linker	UNP P54645

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	161	1242	805	208	226	1	2	0	0	0

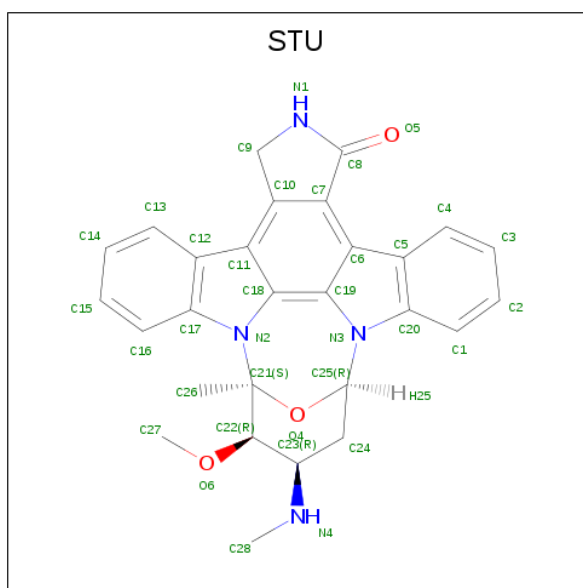
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	initiating methionine	UNP P80386

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

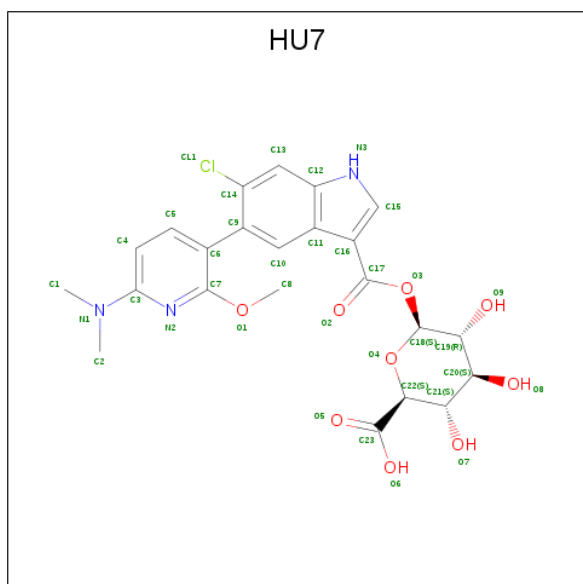
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	283	2061	1329	350	377	5	0	0	0

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	35	28	4	3	0	0

- Molecule 5 is 1-O-{6-chloro-5-[6-(dimethylamino)-2-methoxypyridin-3-yl]-1H-indole-3-carbonyl}-beta-D-glucopyranuronic acid (three-letter code: HU7) (formula: $C_{23}H_{24}ClN_3O_9$).

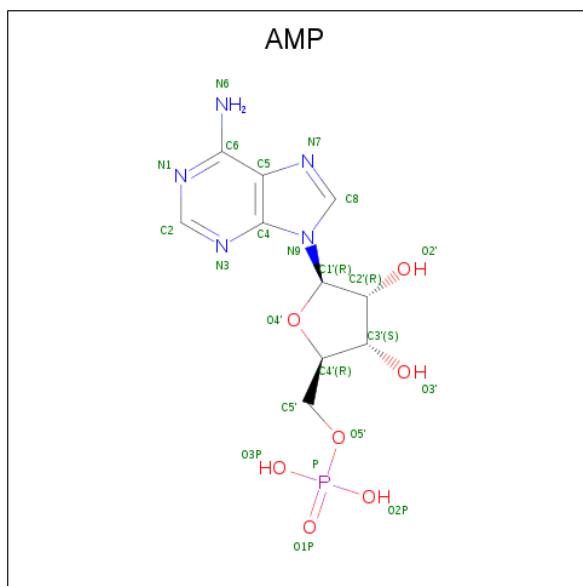


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	A	1	36	23	1	3	9	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

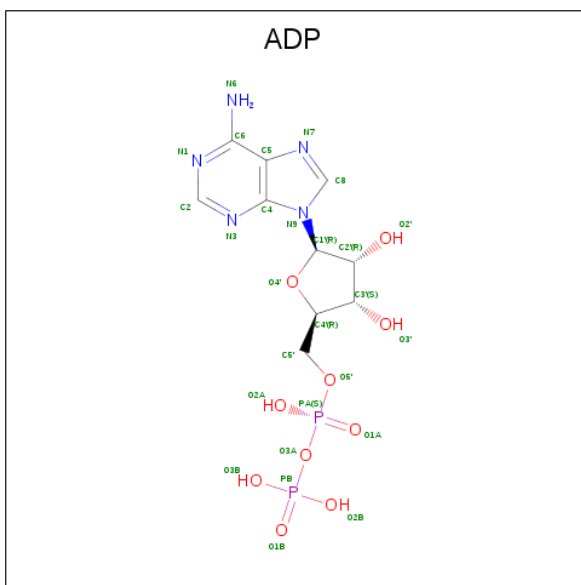
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total Cl 4 4	0	0

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



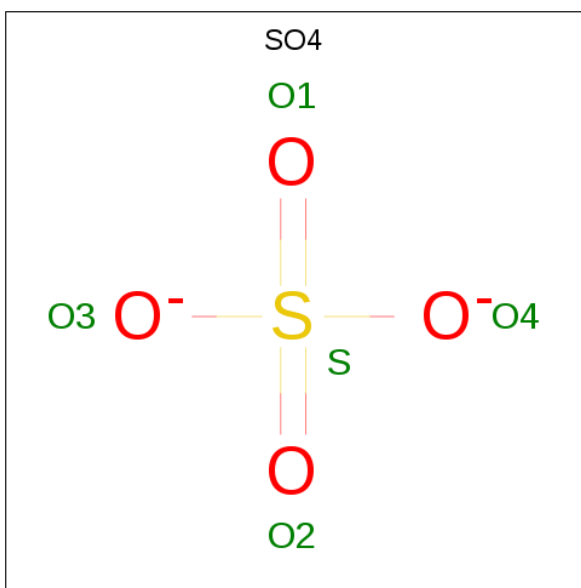
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N O P 23 10 5 7 1	0	0
7	C	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

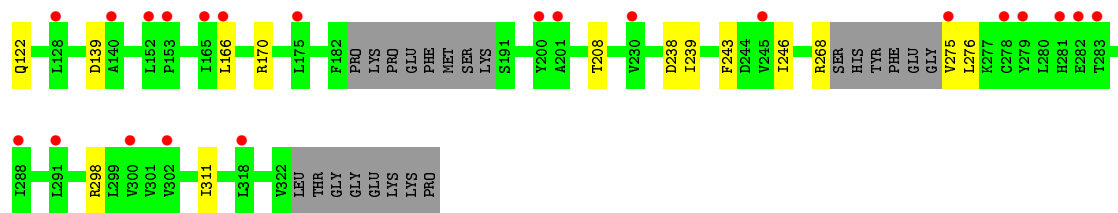


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
8	C	1	27	10	5	10	2	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O S		
9	C	1	5	4 1	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.50Å 124.50Å 402.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	107.82 – 3.27 104.15 – 3.35	Depositor EDS
% Data completeness (in resolution range)	92.9 (107.82-3.27) 99.9 (104.15-3.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 3.33Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.212 , 0.231 0.211 , 0.234	Depositor DCC
R_{free} test set	1369 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	81.1	Xtrriage
Anisotropy	0.563	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6340	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: ADP, CL, TPO, SEP, STU, HU7, SO4, 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	0.40	0/2939	0.65	0/3982
2	B	0.37	0/1265	0.63	0/1730
3	C	0.41	0/2099	0.60	0/2880
All	All	0.40	0/6303	0.63	0/8592

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	2884	0	2812	21	0
2	B	1242	0	1202	13	0
3	C	2061	0	1938	11	0
4	A	35	0	26	6	0
5	A	36	0	0	0	0
6	A	4	0	0	0	0
7	C	46	0	24	2	0
8	C	27	0	12	0	0
9	C	5	0	0	0	0
All	All	6340	0	6014	48	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 (48) 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)
4:A:601:STU:H272	4:A:601:STU:H283	1.27	1.09
4:A:601:STU:H16	4:A:601:STU:H261	1.51	0.91
4:A:601:STU:C28	4:A:601:STU:H272	2.02	0.90
4:A:601:STU:C27	4:A:601:STU:H283	2.05	0.85
1:A:455:ASP:HB2	1:A:458:THR:HG22	1.76	0.66
1:A:78:LYS:H	1:A:94:GLU:HG2	1.69	0.57
3:C:243:PHE:O	3:C:246:ILE:HG13	2.05	0.57
1:A:412:GLU:HA	1:A:415:ARG:HE	1.69	0.56
2:B:214:ILE:HB	2:B:229:PRO:HD2	1.89	0.55
1:A:234:PRO:HD2	1:A:237:LEU:HD22	1.89	0.54
3:C:97:TYR:CG	3:C:107:GLU:HG3	2.42	0.54
1:A:273:PRO:HD2	1:A:276:LEU:HD12	1.91	0.52
3:C:73:LEU:HD21	3:C:85:LEU:HB2	1.90	0.52
3:C:107:GLU:O	3:C:111:HIS:HB2	2.10	0.52
4:A:601:STU:C16	4:A:601:STU:H261	2.23	0.52
1:A:401:ARG:O	1:A:548:GLN:HB3	2.09	0.51
3:C:238:ASP:HA	3:C:275:VAL:HG21	1.93	0.51
1:A:218:HIS:HD2	1:A:221:THR:H	1.57	0.51
4:A:601:STU:C16	4:A:601:STU:C26	2.89	0.49
1:A:540:ALA:HB2	2:B:251:LEU:HD11	1.94	0.49
2:B:208:PRO:HA	2:B:211:LEU:HD12	1.96	0.48
2:B:81:VAL:HG22	2:B:115:ILE:HG12	1.95	0.48
3:C:276:LEU:H	7:C:402:AMP:H2	1.62	0.47
1:A:192:GLY:O	1:A:195:VAL:HG22	2.15	0.47
2:B:120:GLU:HA	2:B:155:VAL:HB	1.96	0.47
2:B:213:VAL:HG22	2:B:215:LEU:H	1.80	0.46
1:A:463:PHE:HB2	2:B:239:LEU:HB3	1.97	0.46
1:A:10:ARG:HG3	1:A:12:LYS:HE3	1.96	0.46
1:A:185:ILE:HD11	1:A:227:CYS:SG	2.56	0.46
2:B:231:PRO:HG3	2:B:254:THR:HG21	1.99	0.45
3:C:40:LEU:HD22	3:C:170:ARG:HG3	1.98	0.45
2:B:233:HIS:HA	2:B:236:LEU:HD12	1.98	0.45
3:C:243:PHE:HB3	7:C:402:AMP:H5'1	2.00	0.44
1:A:188:ARG:HG2	2:B:205:ILE:HD13	1.99	0.44
1:A:244:LEU:HD11	1:A:262:ILE:HG23	1.99	0.44
3:C:75:ASP:HB3	3:C:78:LYS:HB2	1.99	0.43
2:B:107:ARG:HD2	2:B:109:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:VAL:HG22	2:B:129:VAL:HG13	2.01	0.42
1:A:127:VAL:HG22	1:A:140:LEU:HD21	2.00	0.42
2:B:84:TRP:HB3	2:B:112:PHE:HB2	2.02	0.42
1:A:545:ILE:HG13	1:A:545:ILE:H	1.76	0.42
3:C:87:ILE:HG23	3:C:246:ILE:HG23	2.02	0.41
1:A:202:VAL:HG13	1:A:213:PRO:HD2	2.01	0.41
1:A:141:LYS:HG3	1:A:143:GLU:HB2	2.03	0.40
1:A:428:ASN:H	1:A:431:TYR:HB3	1.85	0.40
1:A:173:SER:HA	1:A:184:VAL:HG13	2.02	0.40
1:A:453:GLN:HG3	1:A:459:TYR:CE2	2.57	0.40
3:C:73:LEU:HD22	3:C:113:ILE:HG21	2.02	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	359/503 (71%)	345 (96%)	12 (3%)	2 (1%)	25 58
2	B	154/204 (76%)	141 (92%)	9 (6%)	4 (3%)	5 28
3	C	277/330 (84%)	265 (96%)	11 (4%)	1 (0%)	34 67
All	All	790/1037 (76%)	751 (95%)	32 (4%)	7 (1%)	17 50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
3	C	122	GLN
2	B	120	GLU
2	B	162	VAL
2	B	170	SER
1	A	427	VAL

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Mol	Chain	Res	Type
2	B	244	ILE

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	308/448 (69%)	292 (95%)	16 (5%)	23 54
2	B	132/184 (72%)	117 (89%)	15 (11%)	5 23
3	C	202/299 (68%)	190 (94%)	12 (6%)	19 50
All	All	642/931 (69%)	599 (93%)	43 (7%)	16 45

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	32	VAL
1	A	50	GLN
1	A	55	LEU
1	A	63	ARG
1	A	87	SER
1	A	138	ARG
1	A	154	LYS
1	A	185	ILE
1	A	274	LYS
1	A	400	ILE
1	A	431	TYR
1	A	460	LEU
1	A	538	MET
1	A	545	ILE
1	A	546	LEU
2	B	94	SER
2	B	109	GLN
2	B	110	ASN
2	B	113	VAL
2	B	116	LEU

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Mol	Chain	Res	Type
2	B	134	THR
2	B	144	SER
2	B	148	THR
2	B	153	ILE
2	B	171	GLN
2	B	215	LEU
2	B	230	GLU
2	B	234	VAL
2	B	239	LEU
2	B	265	LEU
3	C	68	VAL
3	C	69	ARG
3	C	84	MET
3	C	103	VAL
3	C	111	HIS
3	C	139	ASP
3	C	166	LEU
3	C	208	THR
3	C	239	ILE
3	C	268	ARG
3	C	298	ARG
3	C	311	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
2	B	216	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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
2	SEP	B	108	2	8,9,10	0.85	0	8,12,14	4.25	3 (37%)
1	TPO	A	172	1	8,10,11	1.13	1 (12%)	10,14,16	1.34	1 (10%)

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	SEP	B	108	2	-	5/5/8/10	-
1	TPO	A	172	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TPO	P-OG1	-2.73	1.54	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	SEP	OG-CB-CA	11.20	119.04	108.14
2	B	108	SEP	O2P-P-OG	2.79	114.16	106.73
1	A	172	TPO	P-OG1-CB	-2.48	115.71	123.21
2	B	108	SEP	O3P-P-O1P	-2.19	102.09	110.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	108	SEP	N-CA-CB-OG
2	B	108	SEP	CB-OG-P-O1P
2	B	108	SEP	CB-OG-P-O2P
2	B	108	SEP	CB-OG-P-O3P
2	B	108	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
5	HU7	A	602	-	35,39,39	1.11	2 (5%)	48,58,58	0.69	1 (2%)
7	AMP	C	401	-	22,25,25	0.58	0	25,38,38	1.21	2 (8%)
8	ADP	C	403	-	24,29,29	0.71	0	29,45,45	0.88	1 (3%)
4	STU	A	601	-	30,42,42	2.52	10 (33%)	31,68,68	2.42	13 (41%)
9	SO4	C	404	-	4,4,4	0.11	0	6,6,6	0.10	0
7	AMP	C	402	-	22,25,25	0.65	0	25,38,38	1.24	3 (12%)

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
7	AMP	C	402	-	-	0/6/26/26	0/3/3/3
7	AMP	C	401	-	-	3/6/26/26	0/3/3/3
5	HU7	A	602	-	-	4/18/42/42	0/4/4/4
8	ADP	C	403	-	-	2/12/32/32	0/3/3/3
4	STU	A	601	-	-	1/4/42/42	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	STU	C9-C10	-5.92	1.46	1.50
5	A	602	HU7	C3-N1	4.82	1.43	1.35
4	A	601	STU	C5-C20	4.57	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	STU	C12-C17	4.55	1.48	1.41
4	A	601	STU	C10-C11	4.35	1.49	1.42
4	A	601	STU	C11-C18	4.23	1.48	1.42
4	A	601	STU	C9-N1	3.96	1.49	1.45
4	A	601	STU	C7-C6	3.63	1.49	1.43
4	A	601	STU	C6-C19	3.19	1.46	1.42
4	A	601	STU	C19-C18	3.11	1.49	1.42
4	A	601	STU	O5-C8	2.76	1.28	1.23
5	A	602	HU7	C16-C11	2.43	1.44	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C7-C8-N1	5.43	111.86	106.37
4	A	601	STU	C9-N1-C8	-5.01	109.04	113.85
7	C	401	AMP	P-O5'-C5'	4.76	131.40	118.30
4	A	601	STU	O5-C8-C7	-4.41	124.08	129.32
7	C	402	AMP	P-O5'-C5'	4.41	130.44	118.30
4	A	601	STU	C7-C10-C11	-4.30	116.63	122.42
4	A	601	STU	C4-C5-C20	3.32	123.58	119.39
4	A	601	STU	C16-C17-N2	3.26	136.24	132.29
4	A	601	STU	C10-C9-N1	2.94	104.75	101.76
4	A	601	STU	C1-C20-C5	-2.77	116.73	120.73
4	A	601	STU	C13-C12-C17	2.68	122.78	119.39
5	A	602	HU7	N2-C3-N1	-2.57	115.50	116.91
4	A	601	STU	C3-C4-C5	-2.55	116.58	120.86
4	A	601	STU	C14-C13-C12	-2.49	116.68	120.86
7	C	402	AMP	O2P-P-O5'	2.41	113.14	106.73
4	A	601	STU	C26-C21-C22	-2.36	108.05	112.64
7	C	402	AMP	C5-C6-N6	2.28	123.82	120.35
8	C	403	ADP	C5-C6-N6	2.26	123.78	120.35
7	C	401	AMP	C5-C6-N6	2.23	123.74	120.35
4	A	601	STU	C16-C17-C12	-2.01	117.84	120.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	HU7	C4-C3-N1-C2
5	A	602	HU7	N2-C3-N1-C2
7	C	401	AMP	C5'-O5'-P-O2P
4	A	601	STU	C22-C23-N4-C28

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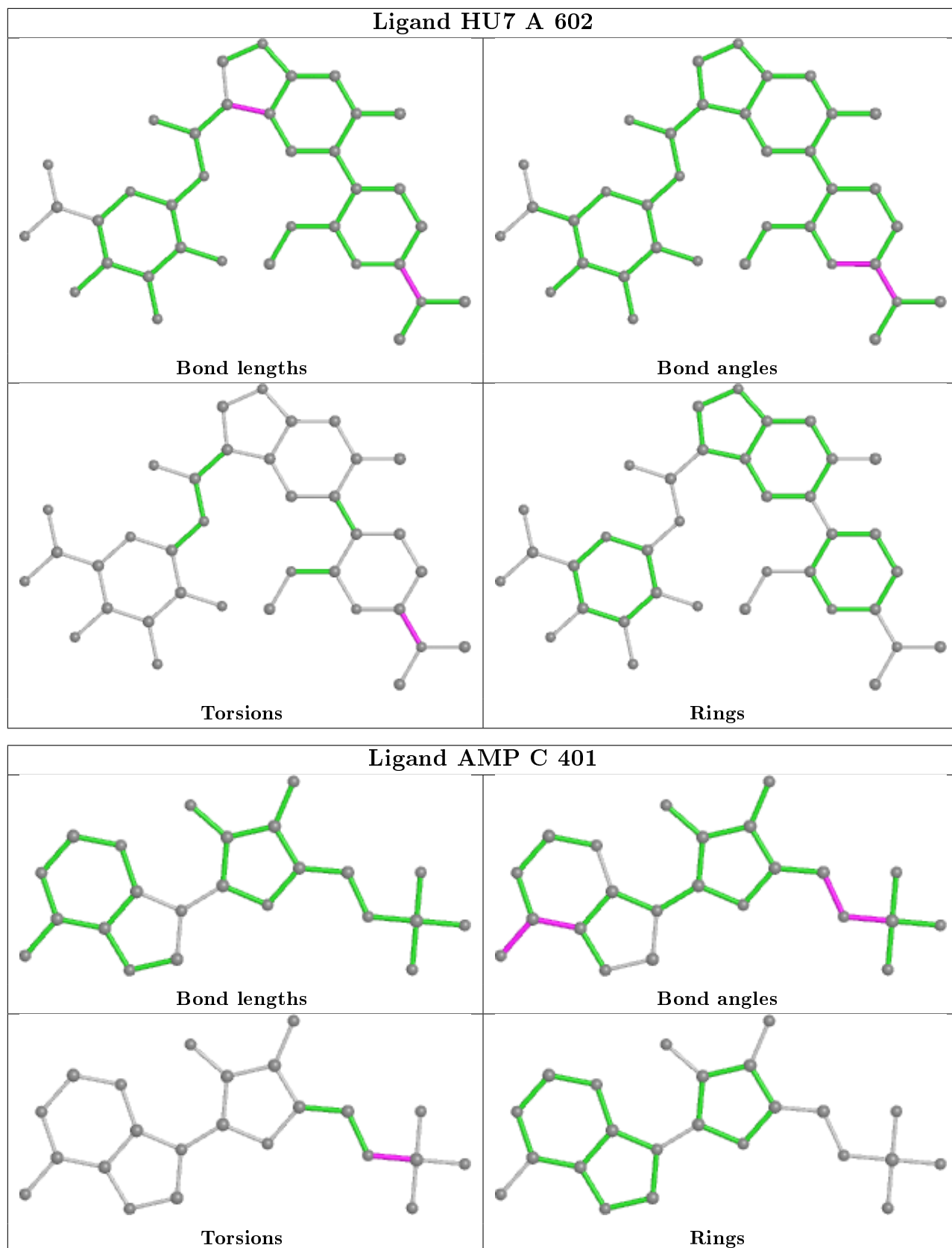
Mol	Chain	Res	Type	Atoms
5	A	602	HU7	N2-C3-N1-C1
5	A	602	HU7	C4-C3-N1-C1
7	C	401	AMP	C5'-O5'-P-O1P
8	C	403	ADP	C5'-O5'-PA-O3A
8	C	403	ADP	C5'-O5'-PA-O1A
7	C	401	AMP	C5'-O5'-P-O3P

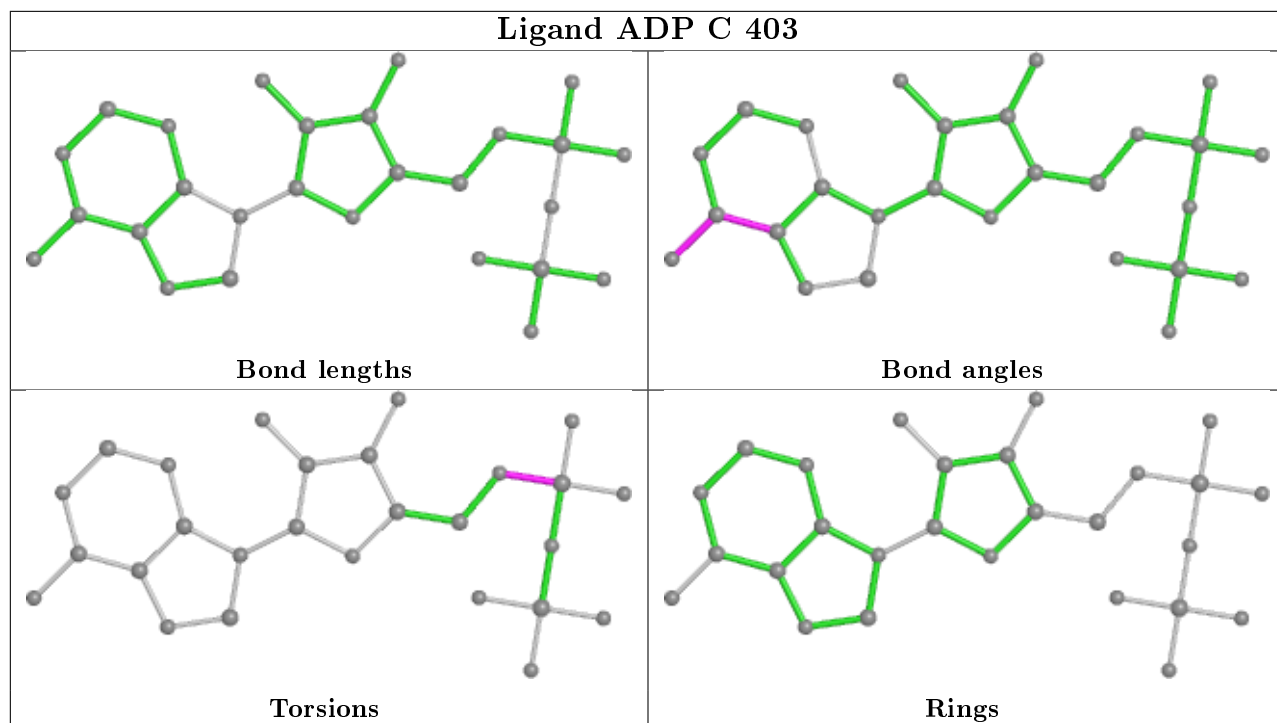
There are no ring outliers.

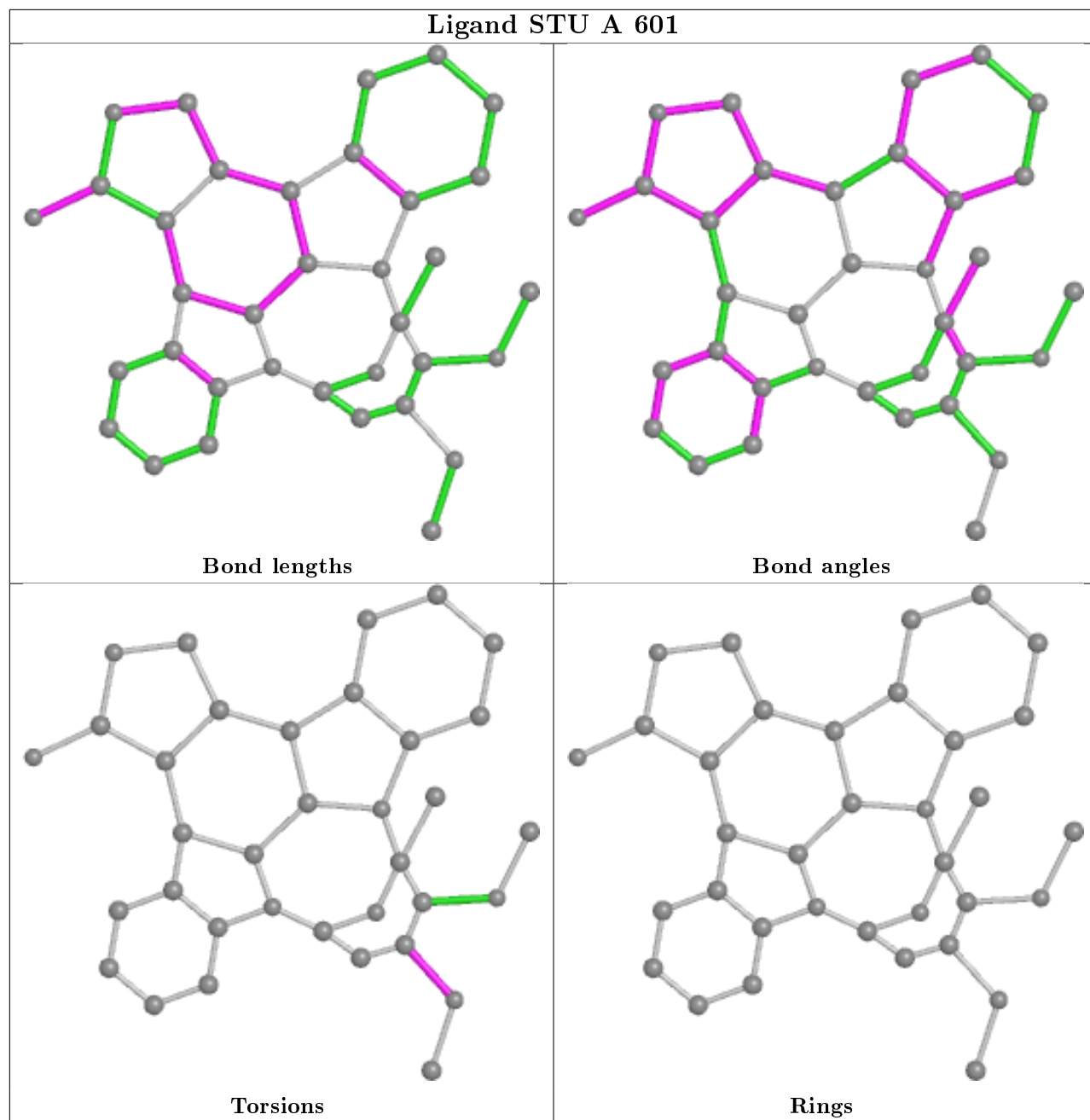
2 monomers are involved in 8 short contacts:

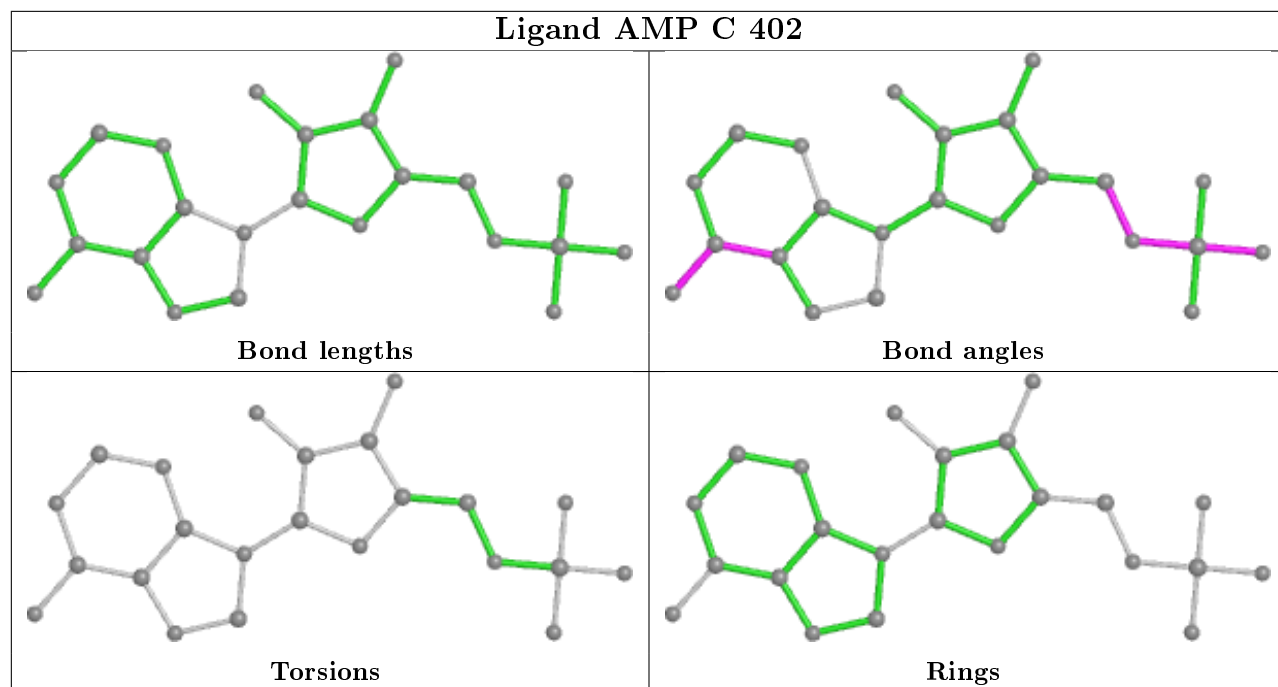
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	STU	6	0
7	C	402	AMP	2	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [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	365/503 (72%)	0.68	17 (4%) 31 29	45, 73, 154, 175	0
2	B	160/204 (78%)	0.68	5 (3%) 49 48	53, 88, 125, 141	0
3	C	283/330 (85%)	0.69	26 (9%) 9 9	72, 128, 183, 193	0
All	All	808/1037 (77%)	0.68	48 (5%) 22 22	45, 92, 176, 193	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	422	TYR	4.4
3	C	300	VAL	4.3
3	C	318	LEU	4.1
3	C	278	CYS	3.7
3	C	166	LEU	3.3
3	C	201	ALA	2.8
3	C	128	LEU	2.8
3	C	140	ALA	2.8
3	C	230	VAL	2.7
1	A	449	LEU	2.6
1	A	413	VAL	2.6
2	B	214	ILE	2.6
1	A	434	VAL	2.6
1	A	13	ILE	2.6
1	A	461	LEU	2.6
3	C	282	GLU	2.5
3	C	81	PHE	2.5
1	A	459	TYR	2.4
2	B	265	LEU	2.4
3	C	279	TYR	2.4
3	C	153	PRO	2.3
1	A	447	MET	2.3
1	A	410	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	543	ILE	2.3
3	C	302	VAL	2.3
3	C	200	TYR	2.3
1	A	463	PHE	2.3
3	C	275	VAL	2.3
1	A	409	ILE	2.2
1	A	460	LEU	2.2
3	C	175	LEU	2.2
3	C	281	HIS	2.2
3	C	165	ILE	2.1
1	A	70	LEU	2.1
1	A	424	TRP	2.1
2	B	250	VAL	2.1
3	C	283	THR	2.1
3	C	63	LEU	2.1
1	A	417	ILE	2.1
3	C	245	VAL	2.1
3	C	152	LEU	2.1
2	B	252	SER	2.1
2	B	91	VAL	2.0
3	C	93	ILE	2.0
3	C	288	ILE	2.0
3	C	291	LEU	2.0
1	A	33	GLY	2.0
3	C	82	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	SEP	B	108	10/11	0.87	0.21	73,78,83,84	0
1	TPO	A	172	11/12	0.95	0.23	75,78,80,81	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

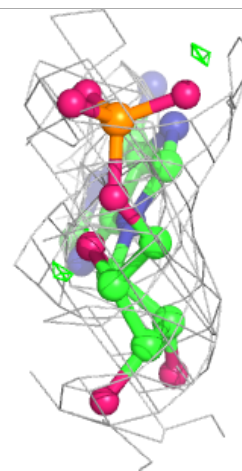
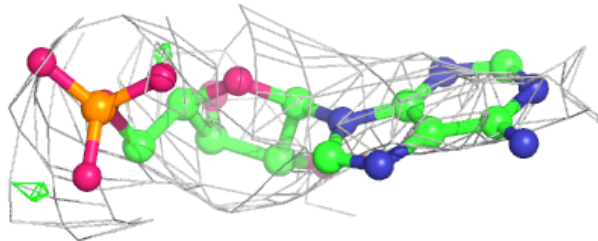
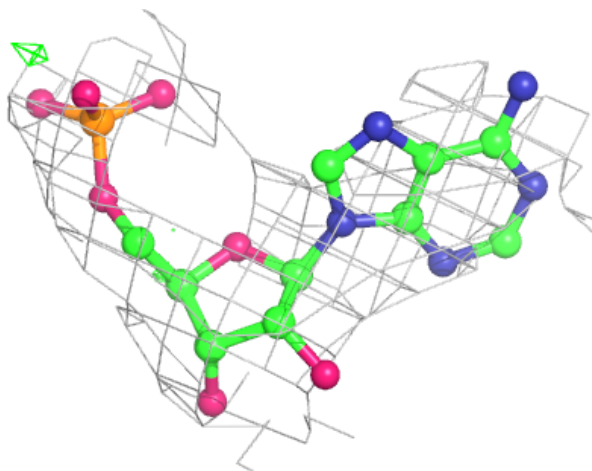
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CL	A	606	1/1	0.40	0.17	113,113,113,113	0
7	AMP	C	402	23/23	0.78	0.38	169,180,196,198	0
6	CL	A	605	1/1	0.87	0.24	88,88,88,88	0
8	ADP	C	403	27/27	0.89	0.48	165,175,187,190	0
6	CL	A	603	1/1	0.90	0.27	61,61,61,61	0
7	AMP	C	401	23/23	0.91	0.25	143,162,168,173	0
5	HU7	A	602	36/36	0.93	0.31	53,70,102,103	0
9	SO4	C	404	5/5	0.94	0.20	157,158,158,158	0
6	CL	A	604	1/1	0.97	0.20	54,54,54,54	0
4	STU	A	601	35/35	0.97	0.40	49,51,55,57	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.

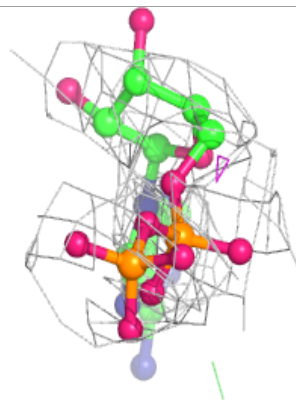
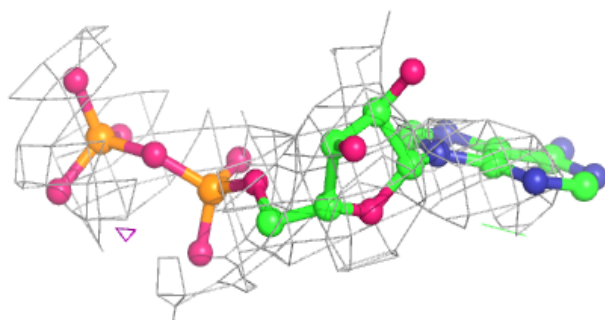
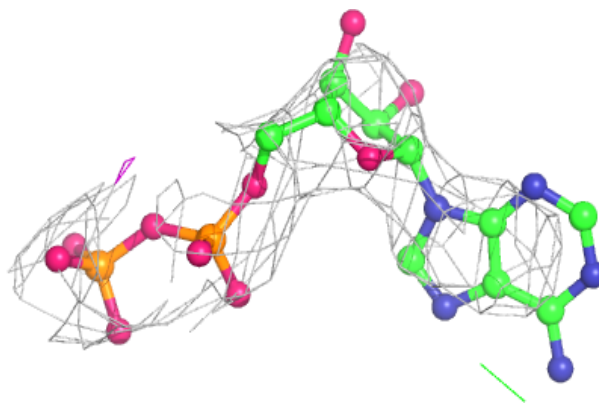
Electron density around AMP C 402:

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

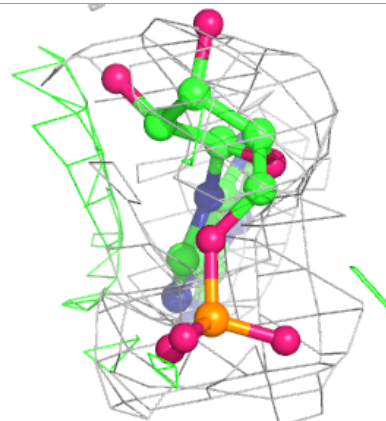
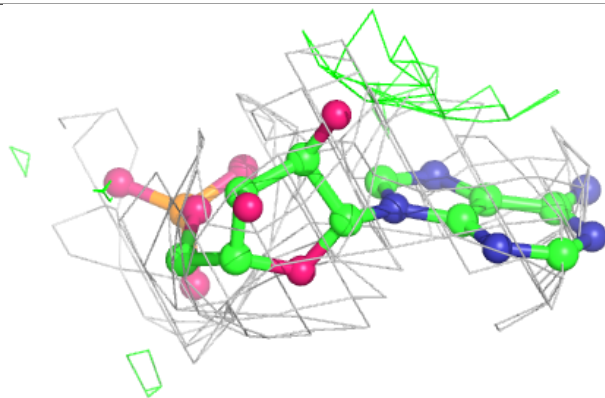
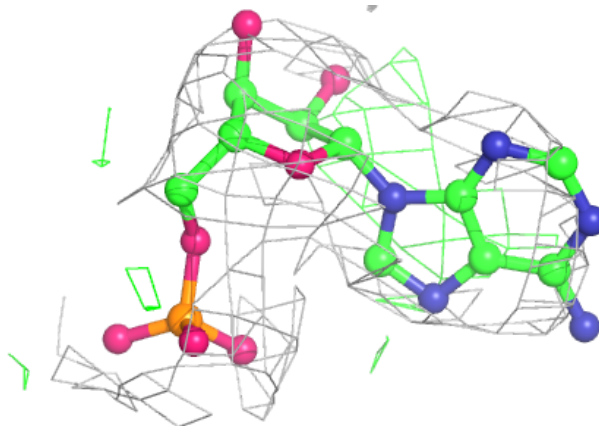


Electron density around ADP C 403:

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

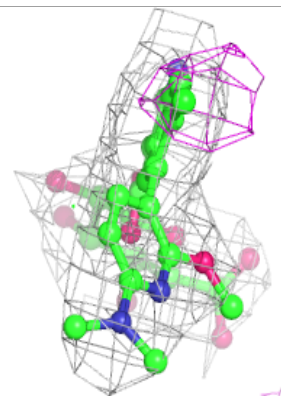
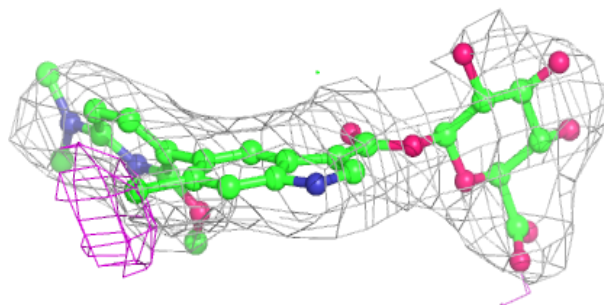
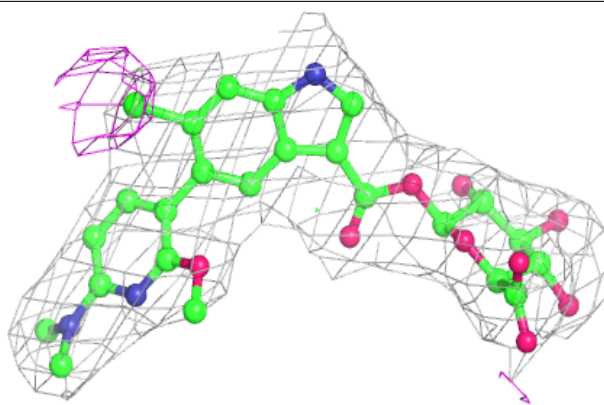
**Electron density around AMP C 401:**

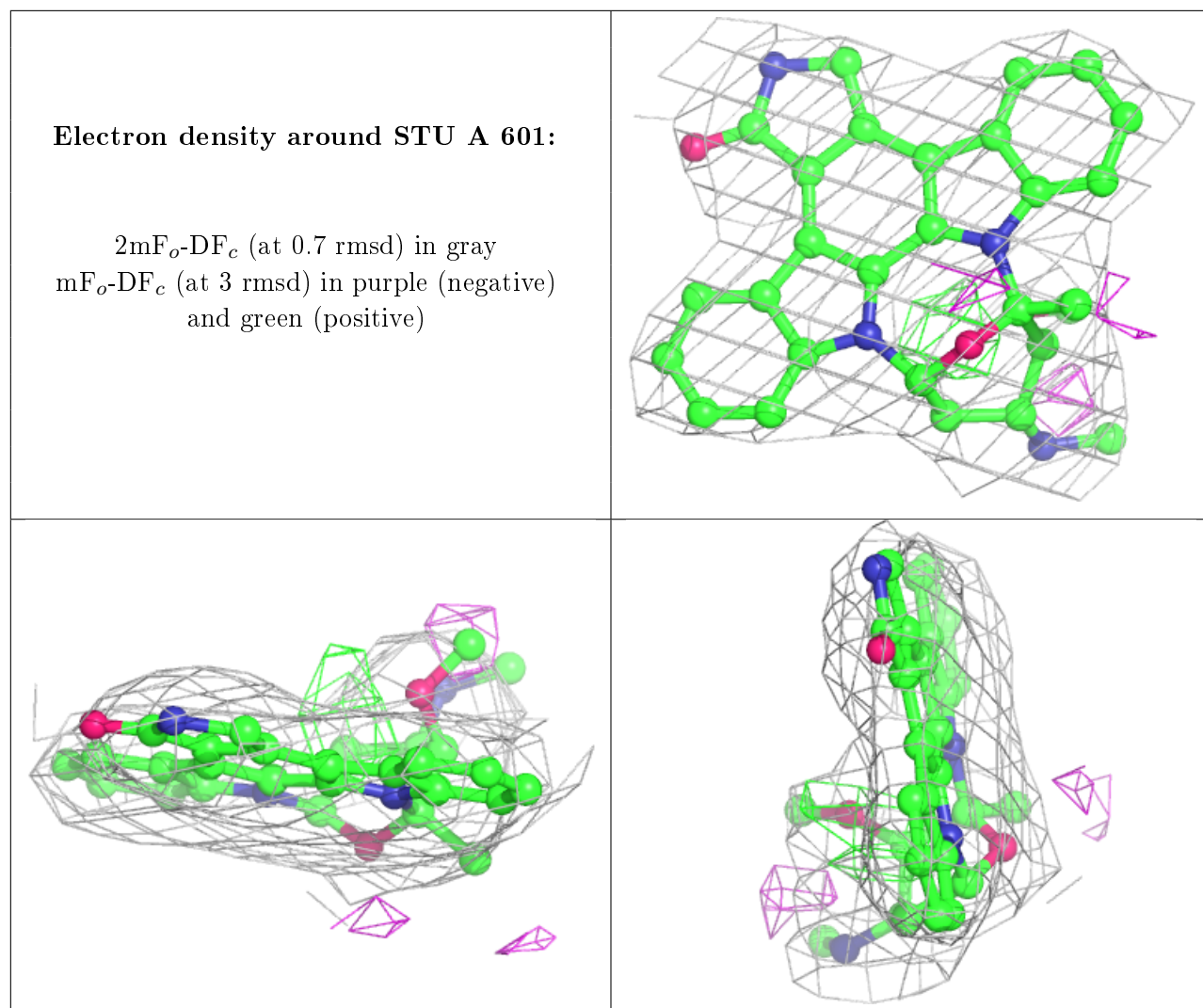
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HU7 A 602:

$2mF_o-DF_c$ (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.