



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:20 am BST

PDB ID : 5KQ5  
Title : AMPK bound to allosteric activator  
Authors : Calabrese, M.F.; Kurumbail, R.G.  
Deposited on : 2016-07-05  
Resolution : 3.41 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](mailto: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.

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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

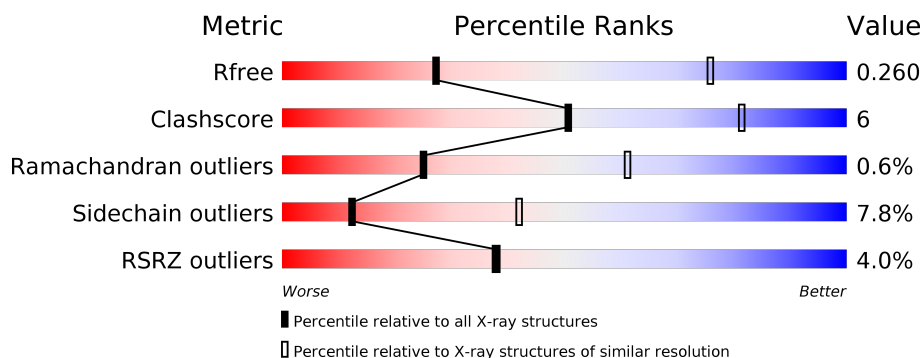
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>12%</div> <div>•</div> <div>28%</div> </div> </div>
2	B	204	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>18%</div> <div>•</div> <div>22%</div> </div> </div>
3	C	330	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>•</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6230 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
1	A	363	Total	C	N	O	P	S	0	0	0
			2832	1820	483	511	1	17			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P54645
A	?	-	ILE	deletion	UNP P54645
A	?	-	THR	deletion	UNP P54645
A	?	-	GLU	deletion	UNP P54645
A	?	-	ALA	deletion	UNP P54645
A	?	-	LYS	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	GLY	deletion	UNP P54645
A	?	-	THR	deletion	UNP P54645
A	?	-	ALA	deletion	UNP P54645
A	?	-	THR	deletion	UNP P54645
A	?	-	PRO	deletion	UNP P54645
A	?	-	GLN	deletion	UNP P54645
A	?	-	ARG	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	GLY	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	ILE	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	ASN	deletion	UNP P54645
A	?	-	TYR	deletion	UNP P54645
A	?	-	ARG	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	CYS	deletion	UNP P54645
A	?	-	GLN	deletion	UNP P54645
A	?	-	ARG	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	ASP	deletion	UNP P54645
A	?	-	ALA	deletion	UNP P54645
A	?	-	GLU	deletion	UNP P54645
A	?	-	ALA	deletion	UNP P54645
A	?	-	GLN	deletion	UNP P54645
A	?	-	GLY	deletion	UNP P54645
A	?	-	LYS	deletion	UNP P54645
A	?	-	PRO	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	GLU	deletion	UNP P54645
A	?	-	VAL	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	LEU	deletion	UNP P54645
A	?	-	THR	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	?	-	VAL	deletion	UNP P54645
A	?	-	THR	deletion	UNP P54645
A	?	-	SER	deletion	UNP P54645
A	517	ALA	LEU	linker	UNP P54645
A	518	SER	ASP	linker	UNP P54645
A	519	GLY	SER	linker	UNP P54645
A	520	GLY	SER	linker	UNP P54645
A	522	GLY	VAL	linker	UNP P54645
A	523	GLY	ASP	linker	UNP P54645
A	524	SER	VAL	linker	UNP P54645

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1227	799	207	218	3			

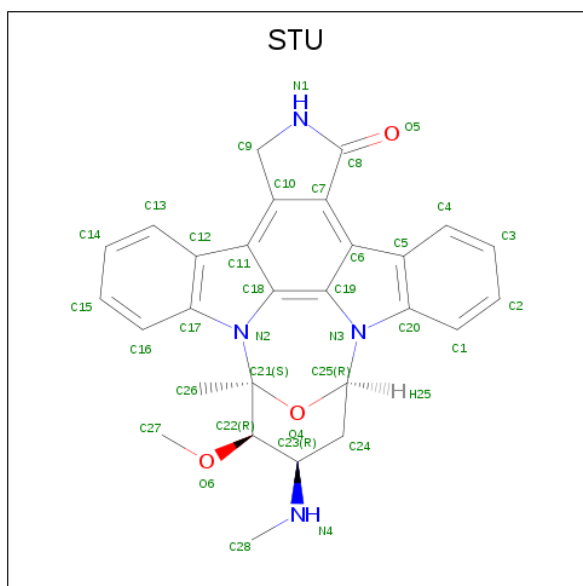
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	initiating methionine	UNP P80386
B	108	ASP	SER	engineered mutation	UNP P80386

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

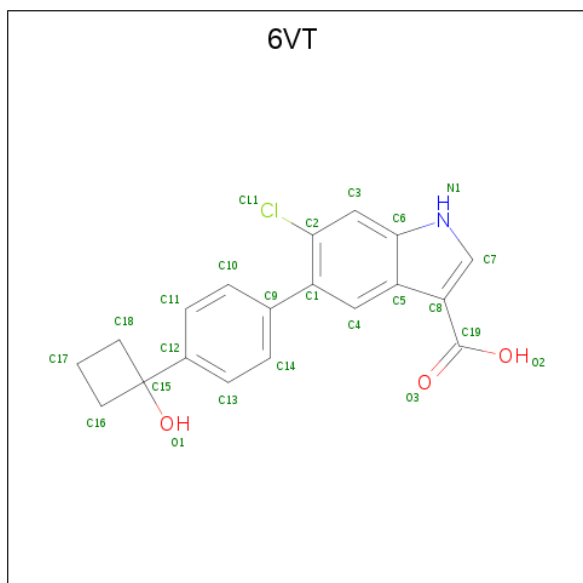
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2030	1316	339	369	6			

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



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

- Molecule 5 is 6-chloranyl-5-[4-(1-oxidanylcyclobutyl)phenyl]-1 {H}-indole-3-carboxylic acid (three-letter code: 6VT) (formula:  $C_{19}H_{16}ClNO_3$ ).

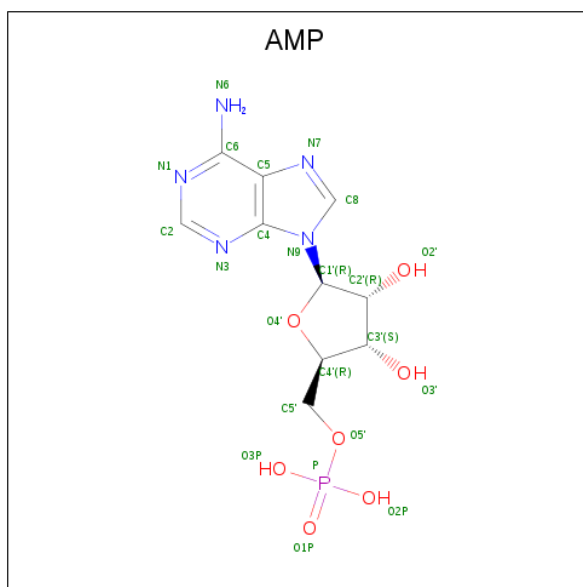


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			24	19	1	1	3		

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

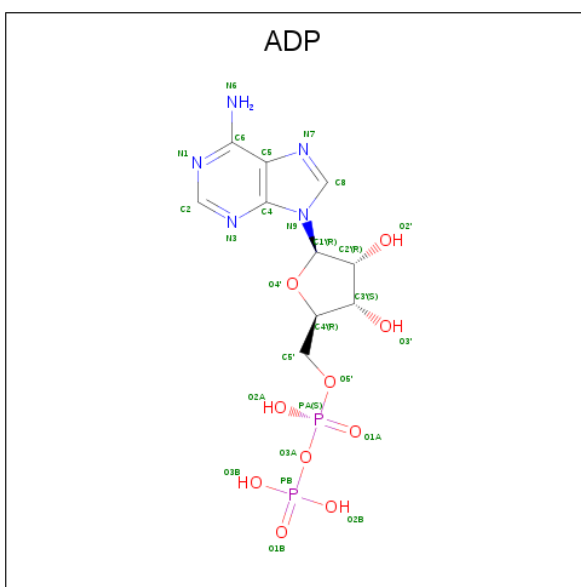
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Cl	0	0
			4	4		

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



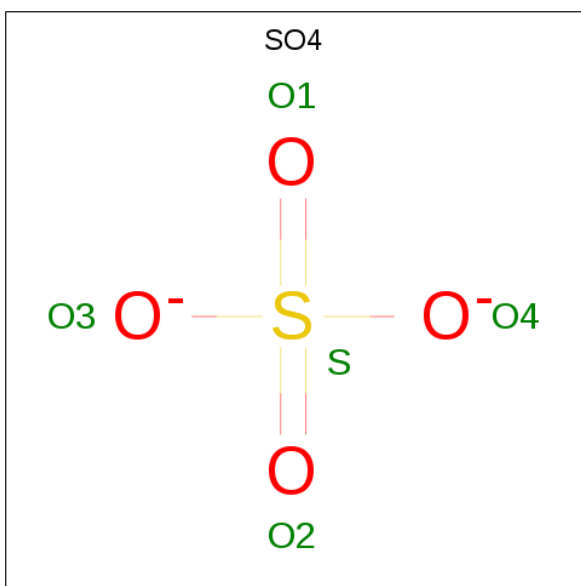
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

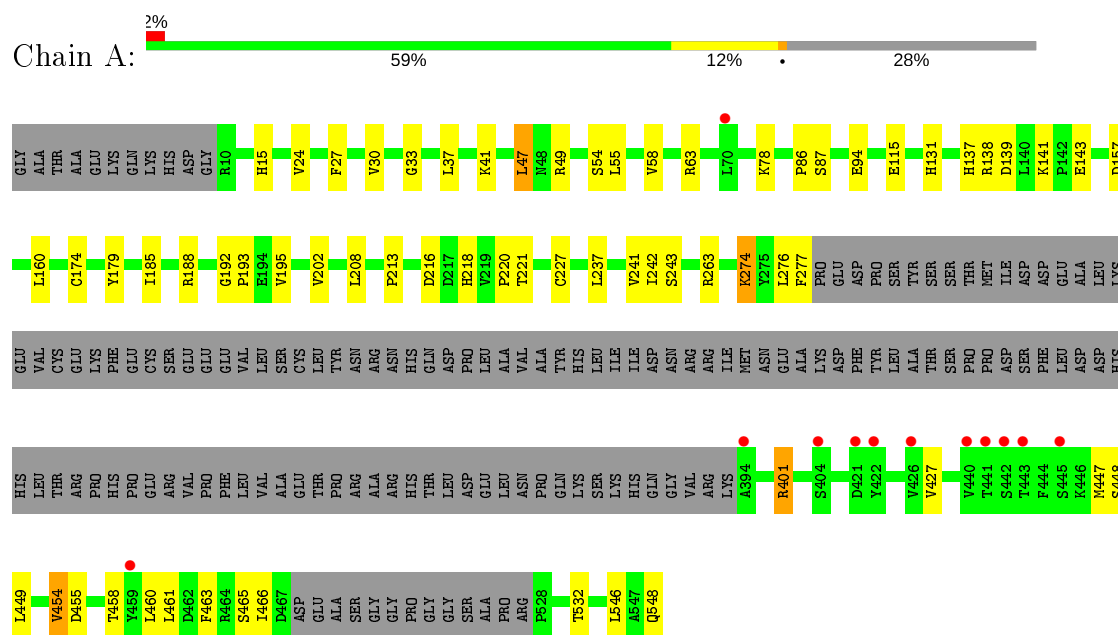


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	O	S	0	0
			5	4	1		

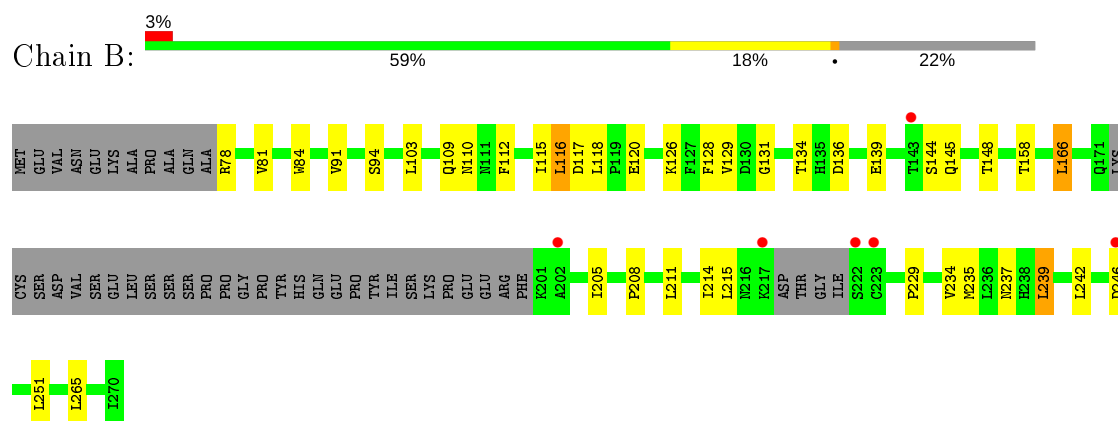
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

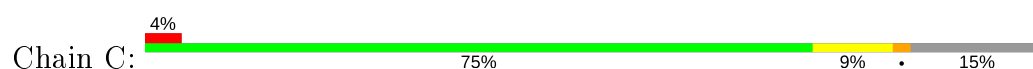
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1



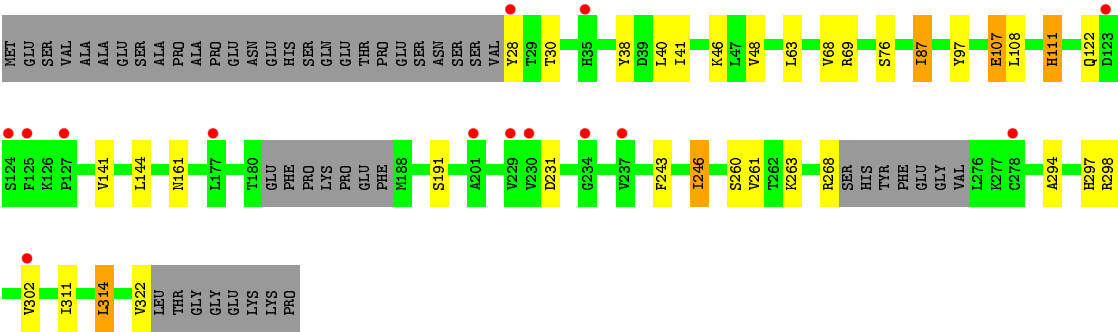
- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.50 Å   124.50 Å   402.25 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	29.90 – 3.41 29.82 – 3.41	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.90-3.41) 96.5 (29.82-3.41)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 3.39 Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, $R_{free}$	0.221   ,   0.259 0.223   ,   0.260	Depositor DCC
$R_{free}$ test set	1248 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.4	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 102.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 6VT, STU, 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	0.44	0/2886	0.69	0/3917
2	B	0.43	0/1261	0.66	0/1727
3	C	0.44	0/2069	0.65	0/2844
All	All	0.44	0/6216	0.67	0/8488

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	2832	0	2747	35	0
2	B	1227	0	1190	21	0
3	C	2030	0	1900	18	0
4	A	35	0	26	5	0
5	A	24	0	0	1	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	6230	0	5899	69	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 6.

All (69) 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:H16	4:A:601:STU:H261	1.52	0.90
3:C:69:ARG:HD2	3:C:243:PHE:HD1	1.54	0.72
1:A:532:THR:H	3:C:161:ASN:HD21	1.39	0.71
1:A:455:ASP:HB2	1:A:458:THR:H	1.58	0.68
1:A:274:LYS:HD3	1:A:274:LYS:H	1.59	0.68
3:C:243:PHE:HB3	7:C:402:AMP:H5'1	1.75	0.67
2:B:208:PRO:HA	2:B:211:LEU:HD12	1.78	0.65
1:A:49:ARG:HH21	1:A:86:PRO:HA	1.61	0.65
1:A:185:ILE:HD11	1:A:227:CYS:SG	2.38	0.63
2:B:214:ILE:HB	2:B:229:PRO:HD2	1.82	0.62
2:B:116:LEU:HD12	2:B:118:LEU:HD21	1.83	0.61
3:C:97:TYR:CG	3:C:107:GLU:HG3	2.36	0.60
1:A:448:SER:HB3	1:A:466:ILE:HD11	1.84	0.60
1:A:141:LYS:HG3	1:A:143:GLU:HB2	1.84	0.59
1:A:237:LEU:HB3	1:A:242:ILE:HD11	1.85	0.58
3:C:97:TYR:CD1	3:C:107:GLU:HG3	2.37	0.58
1:A:218:HIS:HD2	1:A:221:THR:H	1.51	0.57
3:C:69:ARG:HD2	3:C:243:PHE:CD1	2.37	0.56
1:A:188:ARG:HG2	2:B:205:ILE:HD13	1.88	0.56
3:C:63:LEU:HD23	3:C:68:VAL:HG13	1.88	0.54
3:C:69:ARG:HG2	3:C:87:ILE:HD11	1.90	0.54
1:A:532:THR:H	3:C:161:ASN:ND2	2.03	0.53
2:B:81:VAL:HG22	2:B:115:ILE:HG12	1.91	0.52
4:A:601:STU:C16	4:A:601:STU:H261	2.24	0.52
1:A:27:PHE:O	1:A:47:LEU:HD23	2.11	0.51
1:A:179:TYR:HD1	1:A:202:VAL:CG2	2.24	0.51
1:A:463:PHE:HB2	2:B:239:LEU:HB3	1.92	0.50
1:A:274:LYS:CD	1:A:274:LYS:H	2.24	0.49
4:A:601:STU:C26	4:A:601:STU:C16	2.89	0.48
1:A:179:TYR:HD1	1:A:202:VAL:HG23	1.79	0.47
1:A:58:VAL:HG23	2:B:166:LEU:HD12	1.95	0.47
3:C:243:PHE:CB	7:C:402:AMP:H5'1	2.41	0.47
3:C:243:PHE:O	3:C:246:ILE:HG13	2.14	0.47
2:B:265:LEU:HD12	3:C:48:VAL:HG22	1.97	0.47
2:B:128:PHE:CZ	2:B:131:GLY:HA2	2.49	0.47
3:C:107:GLU:O	3:C:111:HIS:HB2	2.15	0.47
5:A:602:6VT:CL1	5:A:602:6VT:C14	3.00	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD13	1:A:174:CYS:HB2	1.97	0.46
3:C:260:SER:H	3:C:263:LYS:HD2	1.81	0.46
1:A:465:SER:HB3	2:B:237:ASN:HB3	1.98	0.46
1:A:87:SER:OG	2:B:81:VAL:HB	2.16	0.45
3:C:141:VAL:HA	3:C:144:LEU:HD12	1.98	0.45
2:B:109:GLN:HB3	2:B:110:ASN:H	1.66	0.45
1:A:263:ARG:HD3	1:A:277:PHE:CD1	2.52	0.45
2:B:84:TRP:HB3	2:B:112:PHE:HB2	1.98	0.45
1:A:78:LYS:H	1:A:94:GLU:HG2	1.82	0.45
2:B:265:LEU:HD11	3:C:46:LYS:HD2	1.99	0.45
1:A:137:HIS:HE1	1:A:139:ASP:O	2.00	0.44
2:B:145:GLN:H	2:B:145:GLN:CD	2.20	0.44
3:C:297:HIS:HA	3:C:314:LEU:HD22	1.98	0.44
1:A:179:TYR:CD1	1:A:202:VAL:CG2	3.01	0.44
2:B:144:SER:HB3	2:B:148:THR:H	1.83	0.44
1:A:401:ARG:O	1:A:548:GLN:HB3	2.18	0.44
2:B:136:ASP:HB3	2:B:139:GLU:HB2	1.99	0.44
2:B:91:VAL:HG22	2:B:129:VAL:HG13	2.00	0.43
1:A:208:LEU:HD11	1:A:241:VAL:HG21	2.00	0.43
1:A:401:ARG:HH22	1:A:454:VAL:HG11	1.84	0.43
2:B:239:LEU:HD11	2:B:251:LEU:HD22	2.00	0.42
1:A:192:GLY:O	1:A:195:VAL:HG22	2.19	0.42
2:B:78:ARG:O	2:B:117:ASP:HA	2.19	0.42
1:A:202:VAL:HG12	1:A:213:PRO:HG2	2.02	0.42
1:A:449:LEU:HD23	1:A:461:LEU:HD11	2.01	0.41
1:A:131:HIS:CE1	1:A:193:PRO:HA	2.55	0.41
1:A:218:HIS:CD2	1:A:220:PRO:HD2	2.55	0.41
3:C:38:TYR:HA	3:C:41:ILE:HD12	2.03	0.41
1:A:143:GLU:HB3	4:A:601:STU:H281	2.02	0.41
1:A:33:GLY:O	1:A:41:LYS:HA	2.21	0.40
2:B:84:TRP:CE2	2:B:129:VAL:HG21	2.56	0.40
1:A:30:VAL:HG21	4:A:601:STU:C17	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/503 (71%)	329 (92%)	26 (7%)	1 (0%)	41	74
2	B	154/204 (76%)	142 (92%)	11 (7%)	1 (1%)	25	61
3	C	275/330 (83%)	257 (94%)	15 (6%)	3 (1%)	14	49
All	All	785/1037 (76%)	728 (93%)	52 (7%)	5 (1%)	25	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	294	ALA
2	B	120	GLU
3	C	231	ASP
3	C	122	GLN
1	A	427	VAL

### 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	
1	A	299/448 (67%)	280 (94%)	19 (6%)	17	50
2	B	131/185 (71%)	118 (90%)	13 (10%)	8	32
3	C	198/299 (66%)	181 (91%)	17 (9%)	10	38
All	All	628/932 (67%)	579 (92%)	49 (8%)	12	42

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	24	VAL
1	A	37	LEU
1	A	47	LEU

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Mol	Chain	Res	Type
1	A	54	SER
1	A	55	LEU
1	A	63	ARG
1	A	115	GLU
1	A	138	ARG
1	A	157	ASP
1	A	216	ASP
1	A	243	SER
1	A	274	LYS
1	A	276	LEU
1	A	401	ARG
1	A	447	MET
1	A	454	VAL
1	A	460	LEU
1	A	546	LEU
2	B	94	SER
2	B	103	LEU
2	B	116	LEU
2	B	126	LYS
2	B	134	THR
2	B	158	THR
2	B	166	LEU
2	B	215	LEU
2	B	234	VAL
2	B	235	MET
2	B	239	LEU
2	B	242	LEU
2	B	246	ASP
3	C	28	TYR
3	C	30	THR
3	C	40	LEU
3	C	76	SER
3	C	87	ILE
3	C	107	GLU
3	C	108	LEU
3	C	111	HIS
3	C	191	SER
3	C	246	ILE
3	C	261	VAL
3	C	268	ARG
3	C	298	ARG
3	C	302	VAL

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Mol	Chain	Res	Type
3	C	311	ILE
3	C	314	LEU
3	C	322	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	548	GLN
3	C	161	ASN
3	C	221	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TPO	A	172	1	8,10,11	1.08	1 (12%)	10,14,16	1.48	2 (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
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	-2.50	1.54	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TPO	P-OG1-CB	-2.72	115.00	123.21
1	A	172	TPO	O3P-P-O1P	-2.18	102.14	110.68

There are no chirality outliers.

There are no torsion outliers.

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	$\# Z  > 2$
8	ADP	C	403	-	24,29,29	0.71	0	29,45,45	0.90	1 (3%)
7	AMP	C	401	-	22,25,25	0.57	0	25,38,38	1.12	2 (8%)
7	AMP	C	402	-	22,25,25	0.66	0	25,38,38	1.22	3 (12%)
5	6VT	A	602	-	22,27,27	0.80	0	26,41,41	0.51	0
9	SO4	C	404	-	4,4,4	0.14	0	6,6,6	0.15	0
4	STU	A	601	-	30,42,42	2.52	10 (33%)	31,68,68	2.45	13 (41%)

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
5	6VT	A	602	-	-	0/10/22/22	0/4/4/4
8	ADP	C	403	-	-	3/12/32/32	0/3/3/3
4	STU	A	601	-	-	1/4/42/42	-
7	AMP	C	402	-	-	2/6/26/26	0/3/3/3
7	AMP	C	401	-	-	0/6/26/26	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	STU	C9-C10	-5.96	1.46	1.50
4	A	601	STU	C12-C17	4.61	1.49	1.41
4	A	601	STU	C5-C20	4.51	1.48	1.41
4	A	601	STU	C10-C11	4.35	1.49	1.42
4	A	601	STU	C11-C18	4.16	1.47	1.42
4	A	601	STU	C9-N1	3.91	1.49	1.45
4	A	601	STU	C7-C6	3.66	1.49	1.43
4	A	601	STU	C6-C19	3.20	1.46	1.42
4	A	601	STU	C19-C18	3.15	1.49	1.42
4	A	601	STU	O5-C8	2.79	1.29	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C7-C8-N1	5.51	111.94	106.37
4	A	601	STU	C9-N1-C8	-5.09	108.96	113.85
4	A	601	STU	O5-C8-C7	-4.43	124.06	129.32
4	A	601	STU	C7-C10-C11	-4.29	116.64	122.42
7	C	401	AMP	P-O5'-C5'	4.22	129.93	118.30
7	C	402	AMP	P-O5'-C5'	4.09	129.56	118.30
4	A	601	STU	C16-C17-N2	3.34	136.33	132.29
4	A	601	STU	C4-C5-C20	3.32	123.60	119.39
4	A	601	STU	C10-C9-N1	3.01	104.82	101.76
4	A	601	STU	C1-C20-C5	-2.73	116.80	120.73
4	A	601	STU	C13-C12-C17	2.63	122.72	119.39
4	A	601	STU	C3-C4-C5	-2.58	116.52	120.86
4	A	601	STU	C14-C13-C12	-2.43	116.78	120.86
4	A	601	STU	C26-C21-C22	-2.35	108.07	112.64
7	C	402	AMP	C5-C6-N6	2.27	123.80	120.35
7	C	402	AMP	O2P-P-O5'	2.25	112.72	106.73
7	C	401	AMP	C5-C6-N6	2.25	123.77	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	403	ADP	C5-C6-N6	2.22	123.72	120.35
4	A	601	STU	C16-C17-C12	-2.02	117.81	120.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

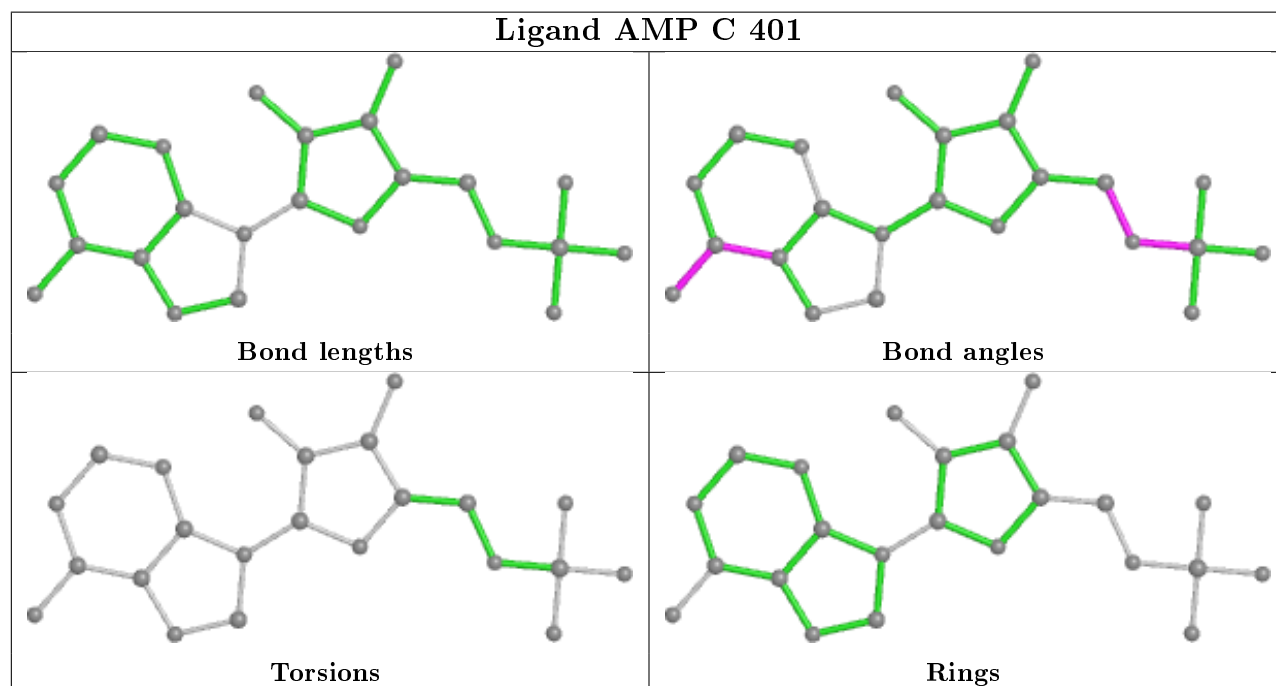
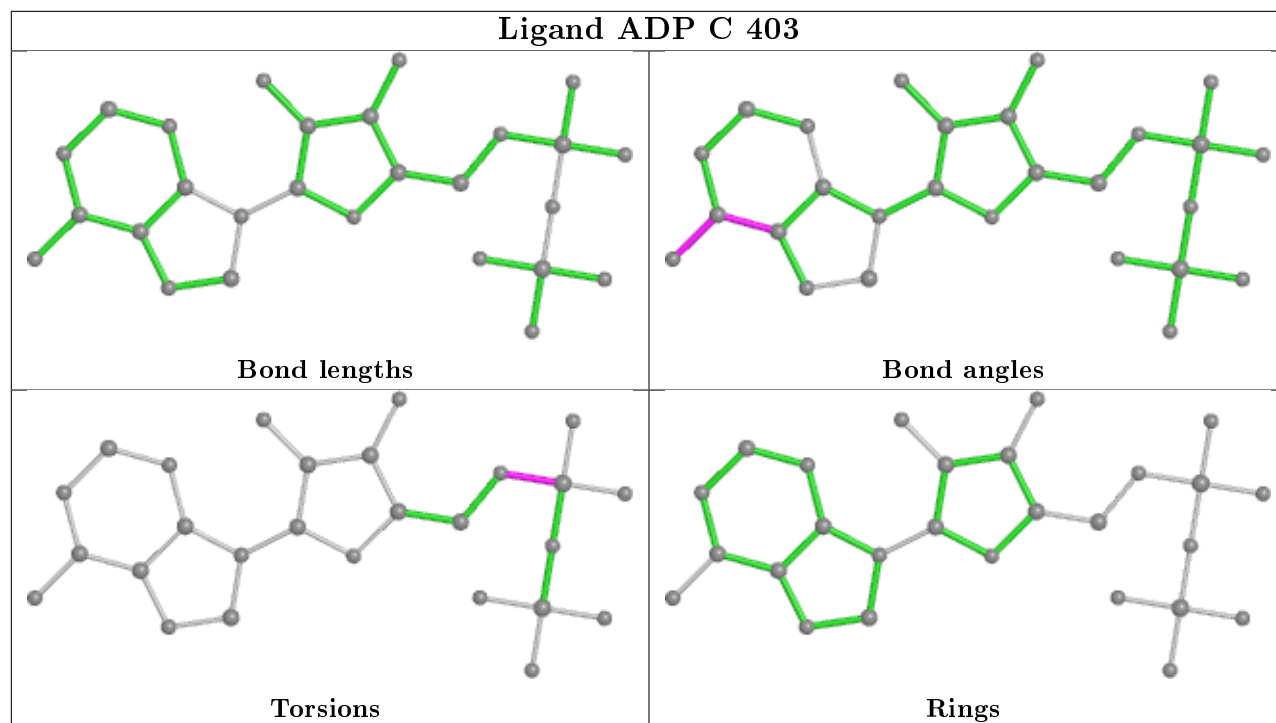
Mol	Chain	Res	Type	Atoms
8	C	403	ADP	C5'-O5'-PA-O1A
8	C	403	ADP	C5'-O5'-PA-O2A
7	C	402	AMP	C5'-O5'-P-O3P
8	C	403	ADP	C5'-O5'-PA-O3A
7	C	402	AMP	C5'-O5'-P-O2P
4	A	601	STU	C24-C23-N4-C28

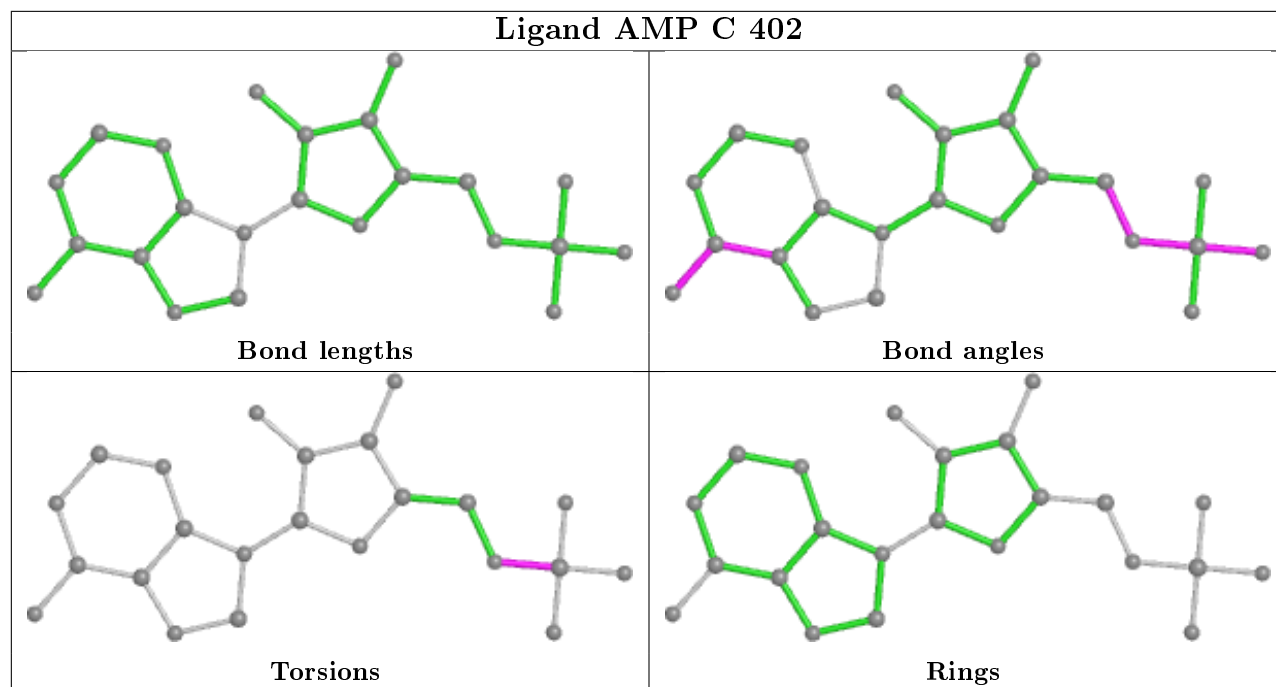
There are no ring outliers.

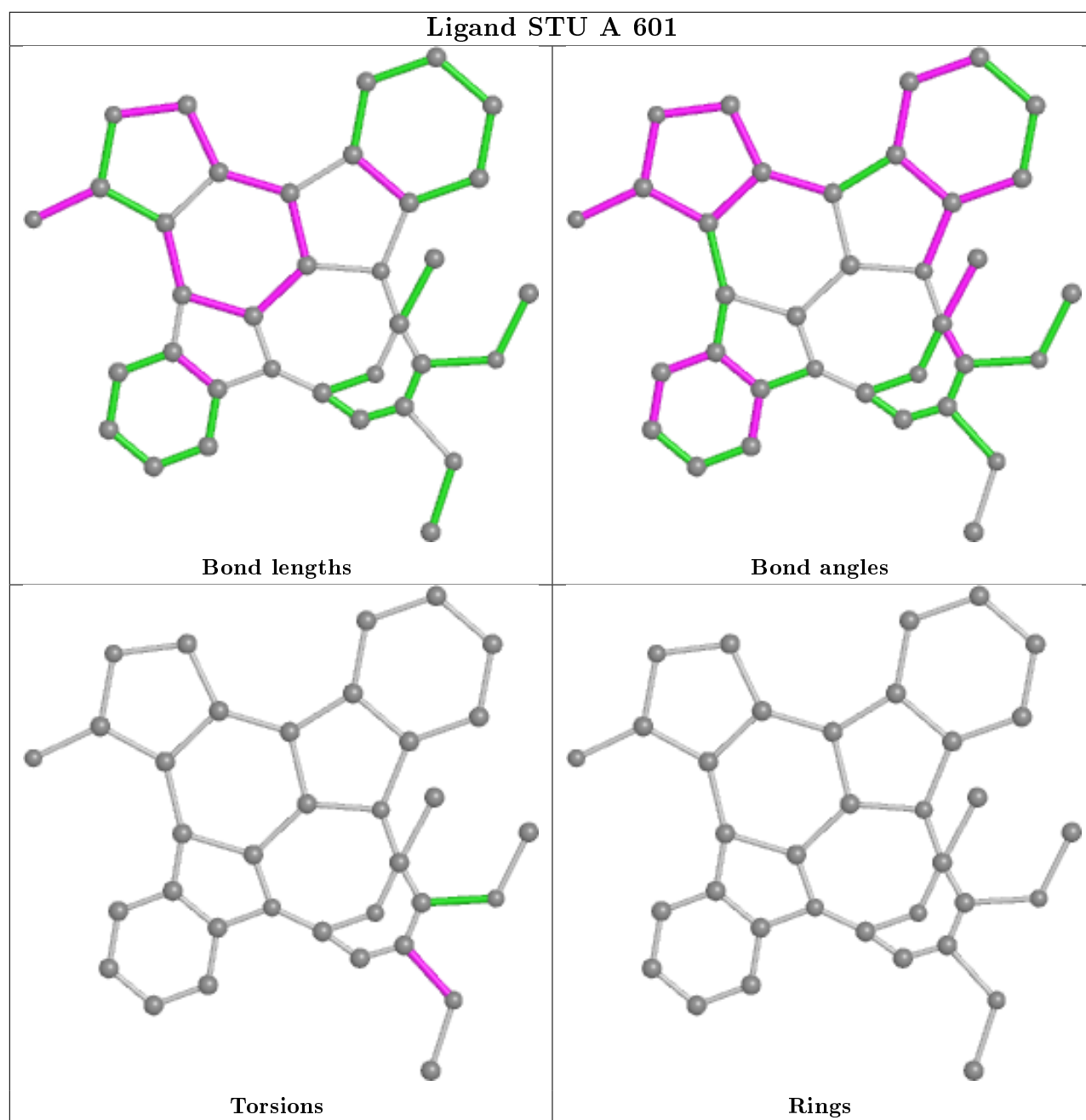
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	402	AMP	2	0
5	A	602	6VT	1	0
4	A	601	STU	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	362/503 (71%)	-0.06	12 (3%)	46	46	64, 93, 163, 188	0
2	B	160/204 (78%)	0.11	6 (3%)	40	40	72, 103, 144, 178	0
3	C	281/330 (85%)	0.16	14 (4%)	28	29	86, 138, 192, 198	0
All	All	803/1037 (77%)	0.05	32 (3%)	38	38	64, 108, 184, 198	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	302	VAL	4.5
1	A	422	TYR	4.4
2	B	222	SER	4.4
3	C	123	ASP	3.9
3	C	230	VAL	3.7
3	C	201	ALA	3.7
1	A	442	SER	3.0
3	C	278	CYS	3.0
1	A	441	THR	3.0
3	C	124	SER	2.9
1	A	440	VAL	2.8
1	A	443	THR	2.7
3	C	125	PHE	2.5
2	B	217	LYS	2.5
3	C	237	VAL	2.4
1	A	394	ALA	2.4
2	B	246	ASP	2.3
2	B	202	ALA	2.3
3	C	28	TYR	2.3
3	C	234	GLY	2.3
1	A	459	TYR	2.3
3	C	127	PRO	2.3
1	A	445	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	143	THR	2.2
1	A	70	LEU	2.2
1	A	426	VAL	2.1
2	B	223	CYS	2.1
3	C	229	VAL	2.1
1	A	404	SER	2.1
1	A	421	ASP	2.1
3	C	177	LEU	2.0
3	C	35	HIS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TPO	A	172	11/12	0.96	0.12	99,102,106,107	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	CL	A	606	1/1	0.63	0.15	115,115,115,115	0
7	AMP	C	402	23/23	0.68	0.31	168,180,198,200	0
7	AMP	C	401	23/23	0.82	0.31	153,172,179,182	0
8	ADP	C	403	27/27	0.86	0.28	182,189,194,194	0
6	CL	A	603	1/1	0.89	0.15	64,64,64,64	0
5	6VT	A	602	24/24	0.93	0.26	57,64,72,73	0
6	CL	A	605	1/1	0.94	0.14	90,90,90,90	0
9	SO4	C	404	5/5	0.94	0.34	158,159,159,159	0

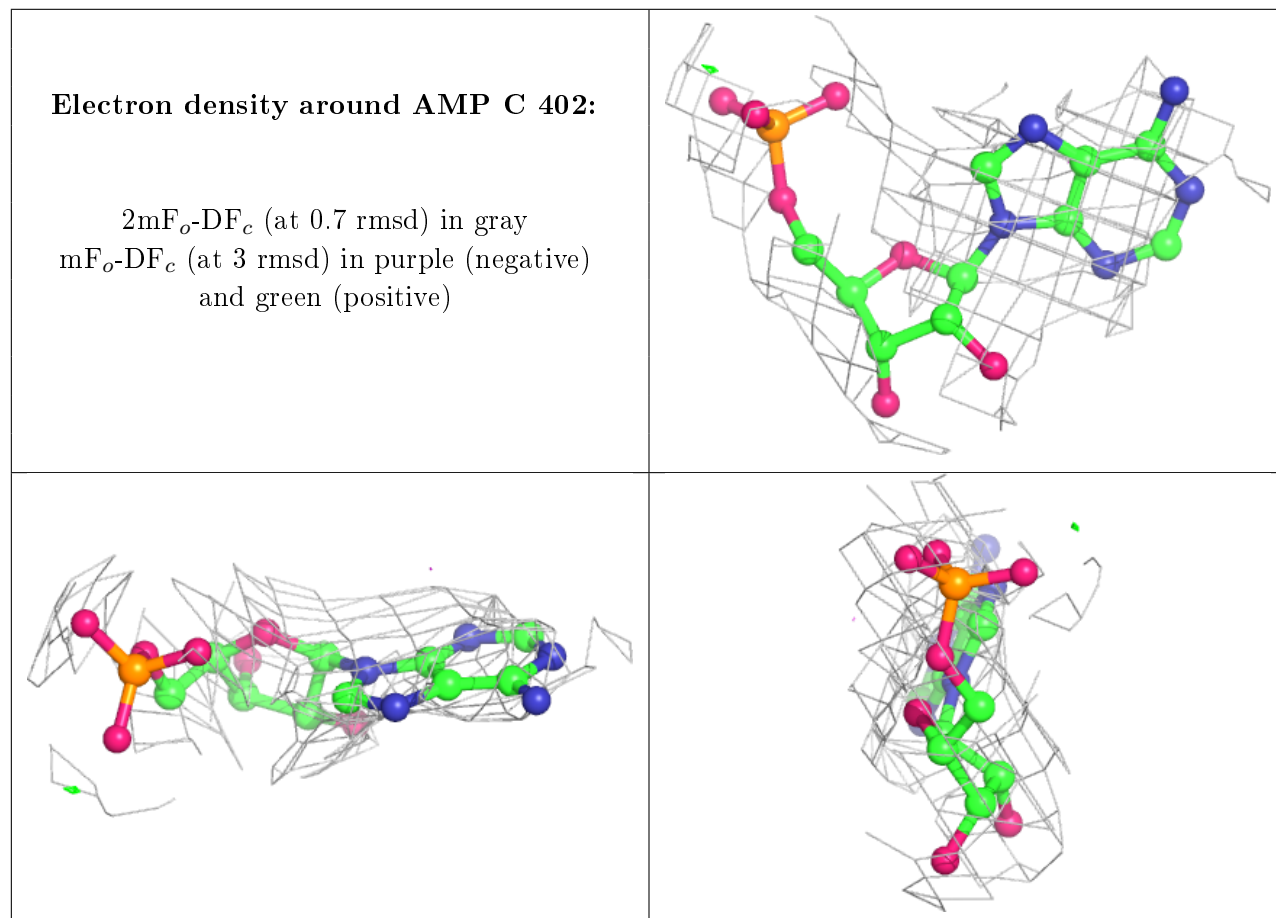
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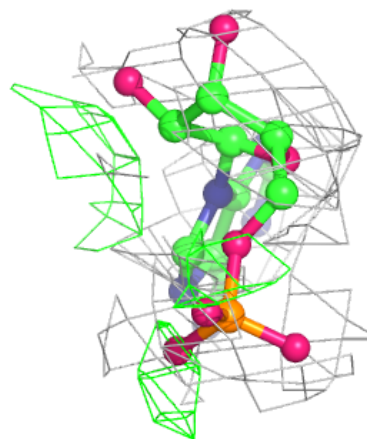
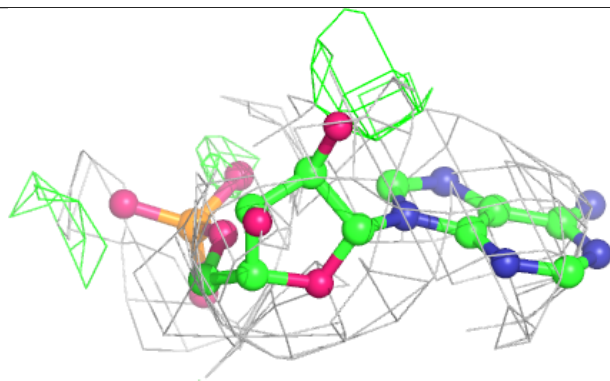
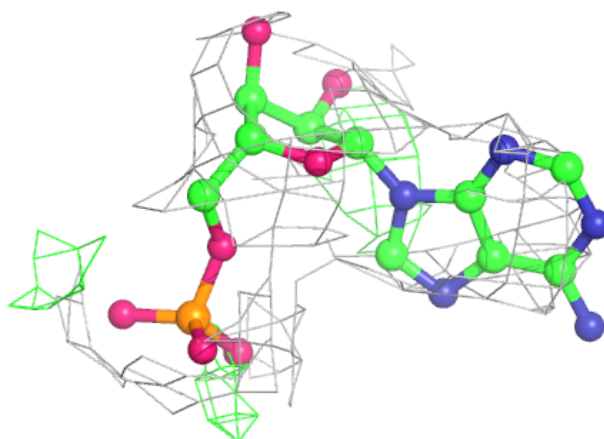
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	STU	A	601	35/35	0.97	0.20	66,70,73,74	0
6	CL	A	604	1/1	0.98	0.19	69,69,69,69	0

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.

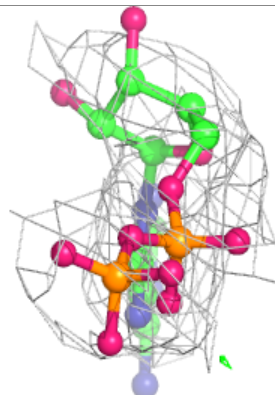
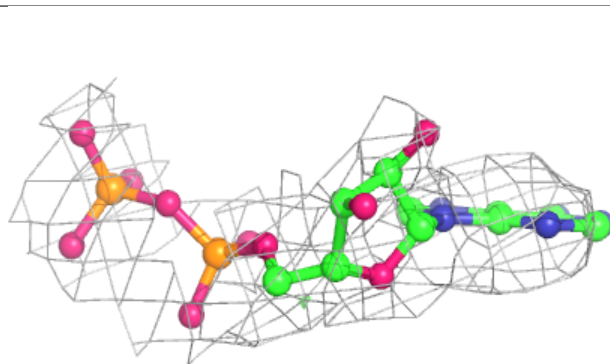
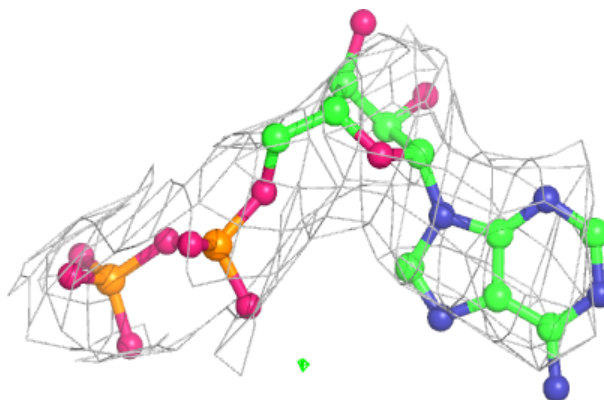


**Electron density around AMP C 401:**

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

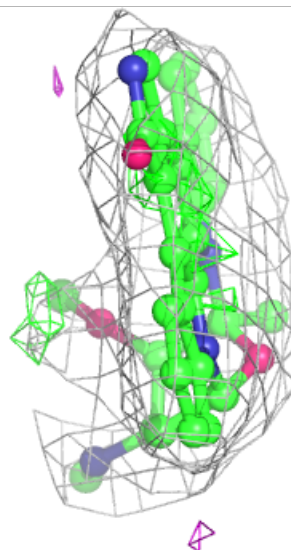
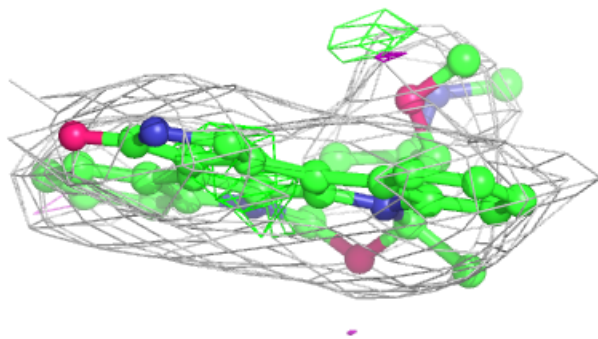
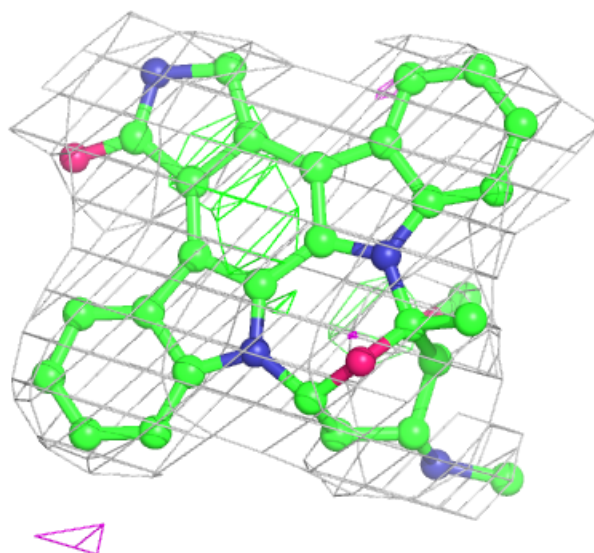
**Electron density around ADP C 403:**

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



**Electron density around STU A 601:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.