



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 10:01 pm BST

PDB ID : 5T5T
Title : AMPK bound to allosteric activator
Authors : Calabrese, M.F.; Kurumbail, R.G.
Deposited on : 2016-08-31
Resolution : 3.46 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

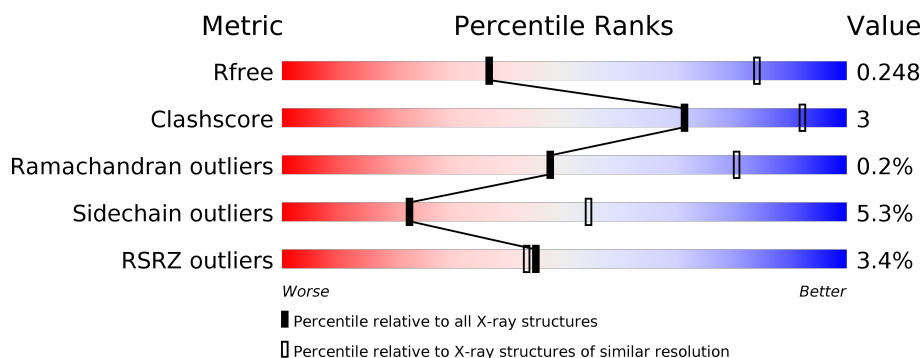
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>9%</div> <div>27%</div> </div> </div>
2	B	204	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>12%</div> <div>20%</div> </div> </div>
3	C	330	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6322 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	369	Total	C	N	O	P	S	0	0	0
			2827	1807	485	517	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	163	Total	C	N	O	S	0	0	0
			1233	802	208	221	2			

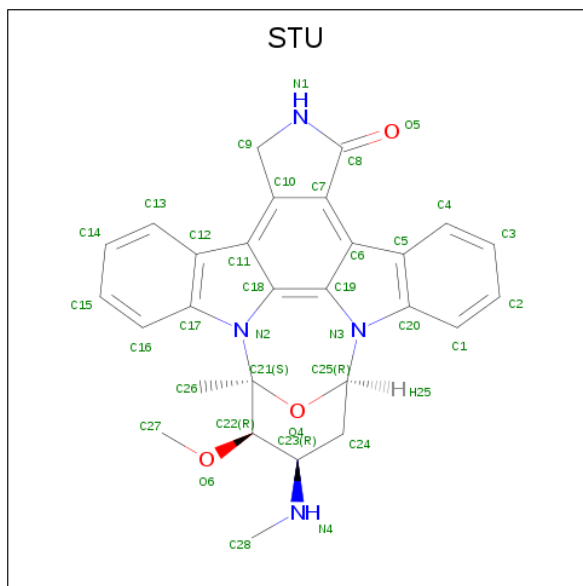
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	initiating methionine	UNP P80386
B	108	ASP	SER	engineered mutation	UNP P80386
B	109	HIS	GLN	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	293	Total	C	N	O	S	0	0	0
			2117	1369	356	386	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

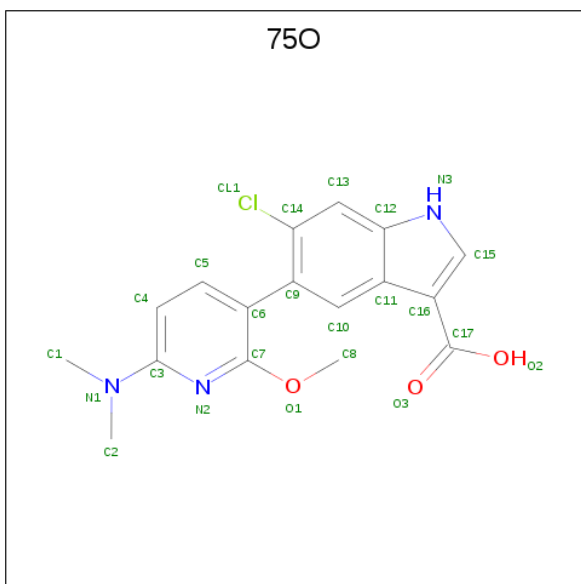
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total	0	0
			3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



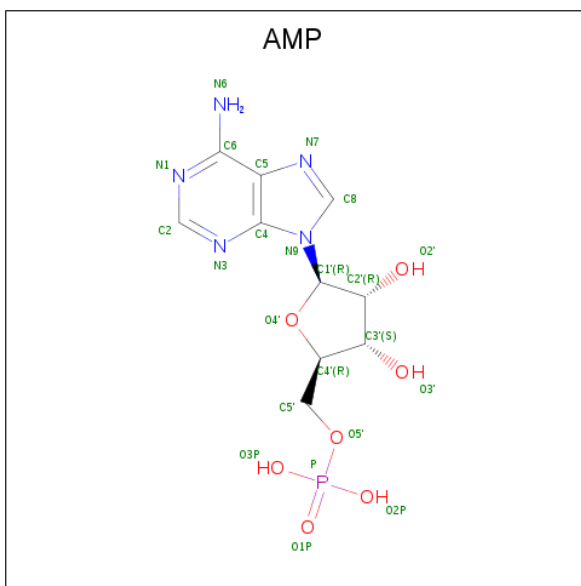
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 6-chloro-5-[6-(dimethylamino)-2-methoxypyridin-3-yl]-1H-indole-3-carboxylic acid (three-letter code: 75O) (formula: C₁₇H₁₆ClN₃O₃).



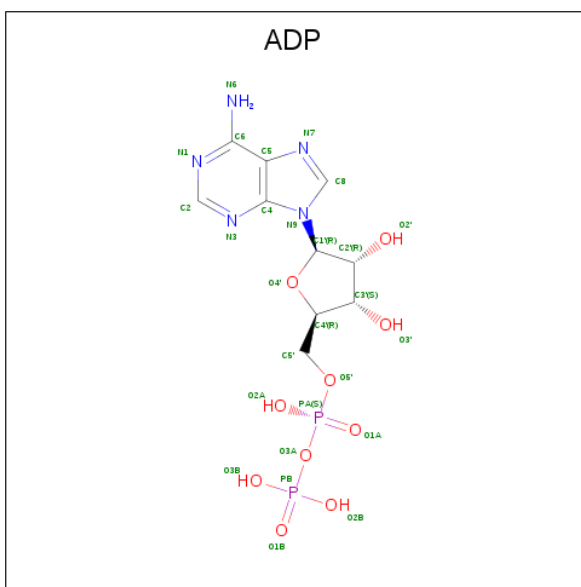
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Cl	N	O	0	0
			24	17	1	3	3		

- Molecule 8 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

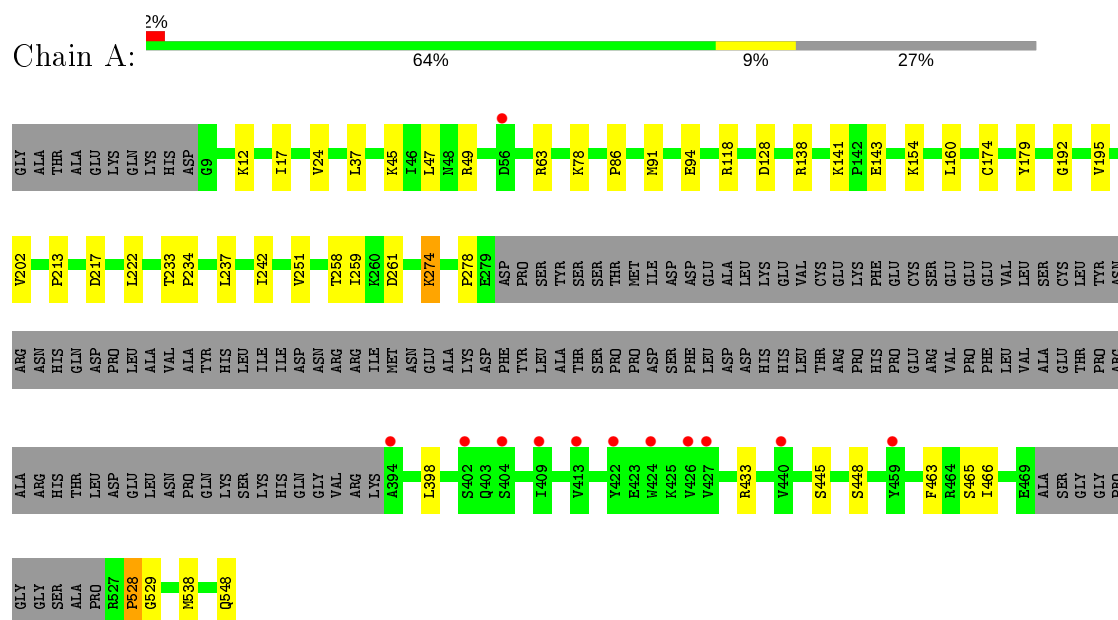


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

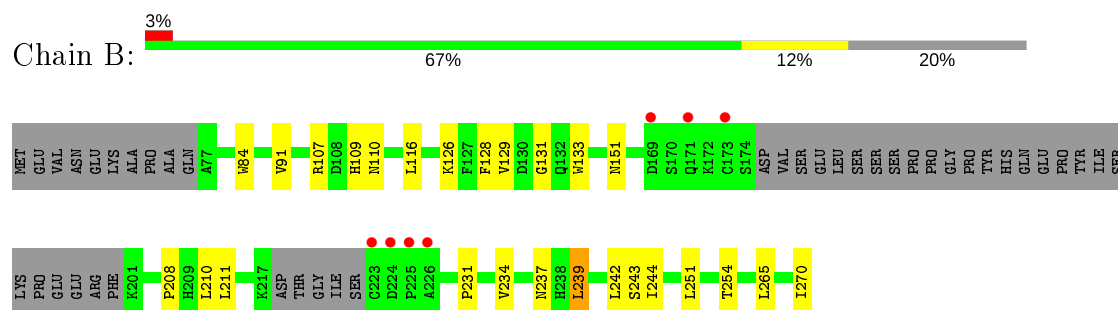
3 Residue-property plots

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.

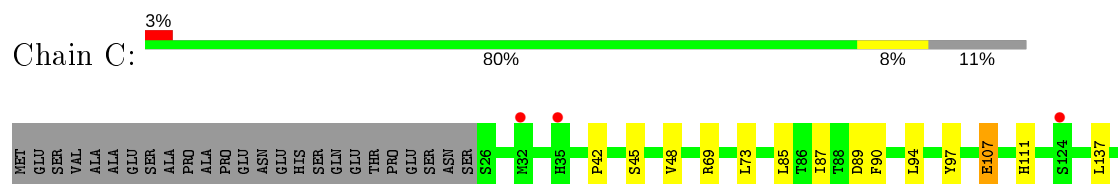
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1

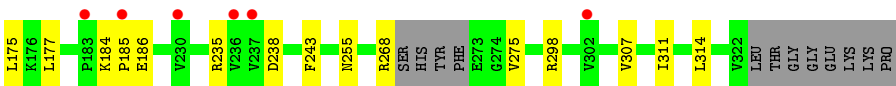


- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



- 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, α , β , γ	125.04Å 125.04Å 403.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.93 – 3.46 40.93 – 3.46	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.93-3.46) 99.9 (40.93-3.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.48Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.7	Depositor
R, R_{free}	0.211 , 0.231 0.230 , 0.248	Depositor DCC
R_{free} test set	1246 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	100.4	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 90.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6322	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CL, TPO, STU, SO4, AMP, 75O

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	0.39	0/2881	0.61	0/3919
2	B	0.37	0/1268	0.59	0/1742
3	C	0.40	0/2160	0.57	0/2970
All	All	0.39	0/6309	0.60	0/8631

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

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	2827	0	2667	22	0
2	B	1233	0	1168	13	0
3	C	2117	0	1967	10	0
4	A	35	0	26	1	0
5	A	3	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
7	B	24	0	0	0	0
8	C	46	0	24	1	0
9	C	27	0	12	0	0
All	All	6322	0	5864	42	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 3.

All (42) 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)
3:C:97:TYR:HB3	3:C:107:GLU:HG3	1.75	0.69
4:A:601:STU:H16	4:A:601:STU:H261	1.79	0.65
1:A:12:LYS:HG2	1:A:17:ILE:HG22	1.79	0.65
1:A:160:LEU:HD13	1:A:174:CYS:HB2	1.80	0.62
1:A:202:VAL:HG12	1:A:213:PRO:HG2	1.85	0.57
3:C:238:ASP:HA	3:C:275:VAL:HG11	1.88	0.54
1:A:141:LYS:HG3	1:A:143:GLU:HB2	1.89	0.54
1:A:192:GLY:O	1:A:195:VAL:HG22	2.07	0.53
3:C:73:LEU:HD21	3:C:85:LEU:HB2	1.90	0.52
2:B:208:PRO:HA	2:B:211:LEU:HD12	1.91	0.52
1:A:445:SER:HB2	1:A:538:MET:HE3	1.92	0.52
1:A:179:TYR:HA	1:A:202:VAL:HG21	1.91	0.51
3:C:42:PRO:HG2	3:C:45:SER:HB3	1.91	0.50
1:A:463:PHE:HB2	2:B:239:LEU:HB3	1.94	0.50
1:A:78:LYS:H	1:A:94:GLU:HG2	1.76	0.49
2:B:128:PHE:CZ	2:B:131:GLY:HA2	2.49	0.47
2:B:91:VAL:HG22	2:B:129:VAL:HG13	1.96	0.47
1:A:179:TYR:HD1	1:A:202:VAL:HG23	1.79	0.47
3:C:243:PHE:HB3	8:C:402:AMP:H5'1	1.97	0.47
3:C:90:PHE:O	3:C:94:LEU:HB2	2.16	0.46
2:B:265:LEU:HD12	3:C:48:VAL:HG22	1.98	0.46
2:B:244:ILE:HG21	2:B:270:ILE:HD11	1.98	0.46
2:B:231:PRO:HG3	2:B:254:THR:HG21	1.99	0.45
3:C:69:ARG:HD2	3:C:243:PHE:HD1	1.82	0.45
1:A:49:ARG:HH21	1:A:86:PRO:HA	1.81	0.45
1:A:233:THR:HG21	1:A:242:ILE:HG23	1.99	0.44
1:A:237:LEU:HB3	1:A:242:ILE:HD11	2.00	0.44
2:B:84:TRP:CZ2	2:B:129:VAL:HG21	2.53	0.44
1:A:128:ASP:HB2	1:A:259:ILE:HG21	2.00	0.43
1:A:465:SER:HB3	2:B:237:ASN:HB3	2.01	0.42
1:A:274:LYS:HD3	1:A:274:LYS:H	1.84	0.42
1:A:448:SER:HB3	1:A:466:ILE:HD11	2.01	0.42
1:A:45:LYS:HB3	1:A:91:MET:HB2	2.01	0.42
1:A:398:LEU:HD22	2:B:210:LEU:HB3	2.02	0.42
2:B:239:LEU:HD11	2:B:251:LEU:HD22	2.02	0.42
3:C:235:ARG:HA	3:C:307:VAL:HA	2.03	0.41
2:B:109:HIS:CD2	2:B:110:ASN:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PRO:HD2	1:A:237:LEU:HD22	2.03	0.41
2:B:126:LYS:HE3	2:B:133:TRP:HB3	2.03	0.41
1:A:258:THR:H	1:A:261:ASP:HB2	1.85	0.40
1:A:528:PRO:HB2	1:A:529:GLY:H	1.72	0.40
3:C:184:LYS:HA	3:C:185:PRO:HD3	1.99	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	362/503 (72%)	346 (96%)	14 (4%)	2 (1%)	25	62
2	B	157/204 (77%)	147 (94%)	10 (6%)	0	100	100
3	C	289/330 (88%)	279 (96%)	10 (4%)	0	100	100
All	All	808/1037 (78%)	772 (96%)	34 (4%)	2 (0%)	47	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	PRO
1	A	278	PRO

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	290/448 (65%)	277 (96%)	13 (4%)	27	60
2	B	128/185 (69%)	121 (94%)	7 (6%)	21	53
3	C	206/299 (69%)	193 (94%)	13 (6%)	18	50
All	All	624/932 (67%)	591 (95%)	33 (5%)	22	54

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	37	LEU
1	A	47	LEU
1	A	63	ARG
1	A	118	ARG
1	A	138	ARG
1	A	154	LYS
1	A	217	ASP
1	A	222	LEU
1	A	251	VAL
1	A	274	LYS
1	A	433	ARG
1	A	548	GLN
2	B	107	ARG
2	B	116	LEU
2	B	151	ASN
2	B	234	VAL
2	B	239	LEU
2	B	242	LEU
2	B	243	SER
3	C	87	ILE
3	C	89	ASP
3	C	107	GLU
3	C	111	HIS
3	C	137	LEU
3	C	175	LEU
3	C	177	LEU
3	C	186	GLU
3	C	255	ASN
3	C	268	ARG
3	C	298	ARG
3	C	311	ILE
3	C	314	LEU

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	111	ASN

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	1.19	1 (12%)	10,14,16	1.33	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
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	-2.90	1.53	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TPO	P-OG1-CB	-2.87	114.54	123.21

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, 3 are monoatomic - leaving 7 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	$\# Z > 2$
9	ADP	C	403	-	24,29,29	0.63	0	29,45,45	0.89	1 (3%)
7	75O	B	4000	-	23,26,26	0.83	0	27,38,38	0.73	1 (3%)
8	AMP	C	401	-	22,25,25	0.53	0	25,38,38	1.26	2 (8%)
8	AMP	C	402	-	22,25,25	0.67	0	25,38,38	1.18	3 (12%)
6	SO4	C	404	-	4,4,4	0.16	0	6,6,6	0.08	0
6	SO4	A	605	-	4,4,4	0.15	0	6,6,6	0.07	0
4	STU	A	601	-	30,42,42	1.30	1 (3%)	31,68,68	0.81	3 (9%)

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
9	ADP	C	403	-	-	2/12/32/32	0/3/3/3
7	75O	B	4000	-	-	0/10/14/14	0/3/3/3
8	AMP	C	401	-	-	3/6/26/26	0/3/3/3
8	AMP	C	402	-	-	3/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	STU	A	601	-	-	2/4/42/42	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	STU	C8-N1	5.69	1.39	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	401	AMP	P-O5'-C5'	5.16	132.51	118.30
8	C	402	AMP	P-O5'-C5'	4.05	129.45	118.30
8	C	402	AMP	C5-C6-N6	2.28	123.81	120.35
9	C	403	ADP	C5-C6-N6	2.24	123.75	120.35
7	B	4000	75O	N2-C3-N1	-2.24	115.68	116.91
8	C	401	AMP	C5-C6-N6	2.23	123.75	120.35
4	A	601	STU	C16-C17-N2	-2.22	129.60	132.29
8	C	402	AMP	O2P-P-O5'	2.18	112.55	106.73
4	A	601	STU	C7-C10-C11	-2.02	119.70	122.42
4	A	601	STU	C1-C20-N3	-2.01	129.85	132.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

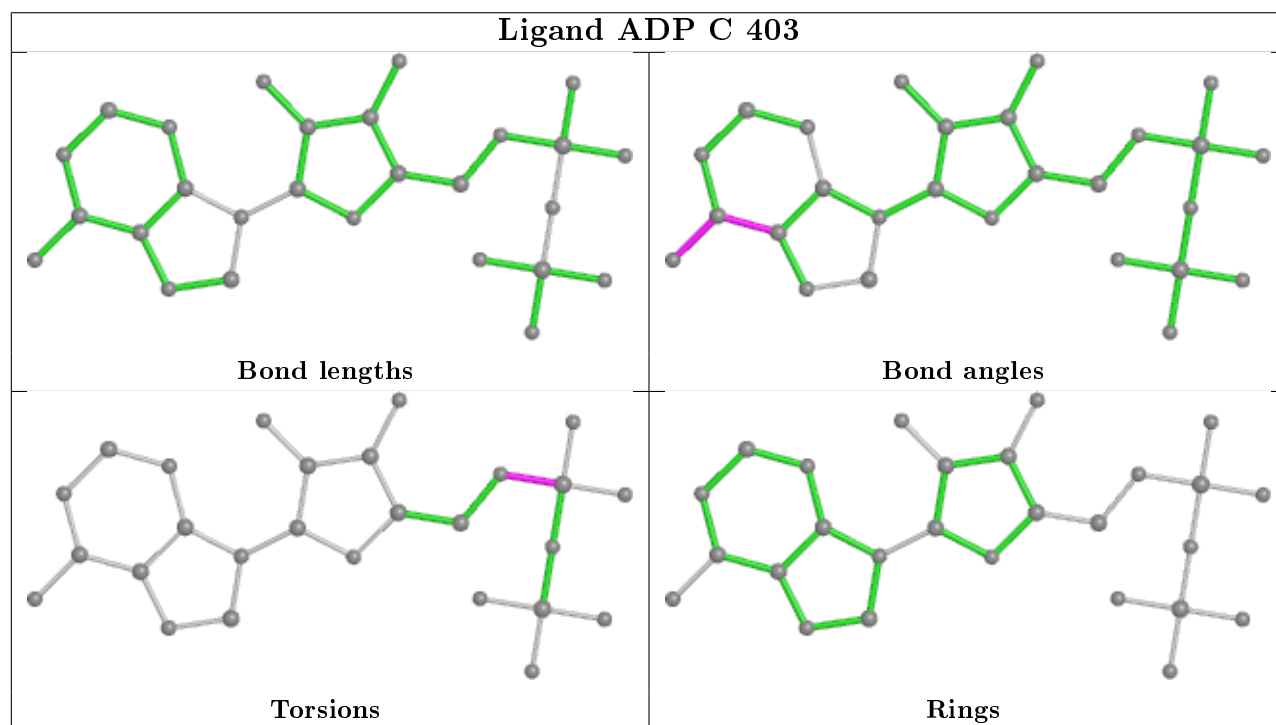
Mol	Chain	Res	Type	Atoms
8	C	401	AMP	C5'-O5'-P-O2P
8	C	401	AMP	C5'-O5'-P-O3P
8	C	402	AMP	C5'-O5'-P-O1P
8	C	402	AMP	C5'-O5'-P-O2P
8	C	402	AMP	C5'-O5'-P-O3P
4	A	601	STU	C22-C23-N4-C28
4	A	601	STU	C24-C23-N4-C28
8	C	401	AMP	C5'-O5'-P-O1P
9	C	403	ADP	C5'-O5'-PA-O3A
9	C	403	ADP	C5'-O5'-PA-O1A

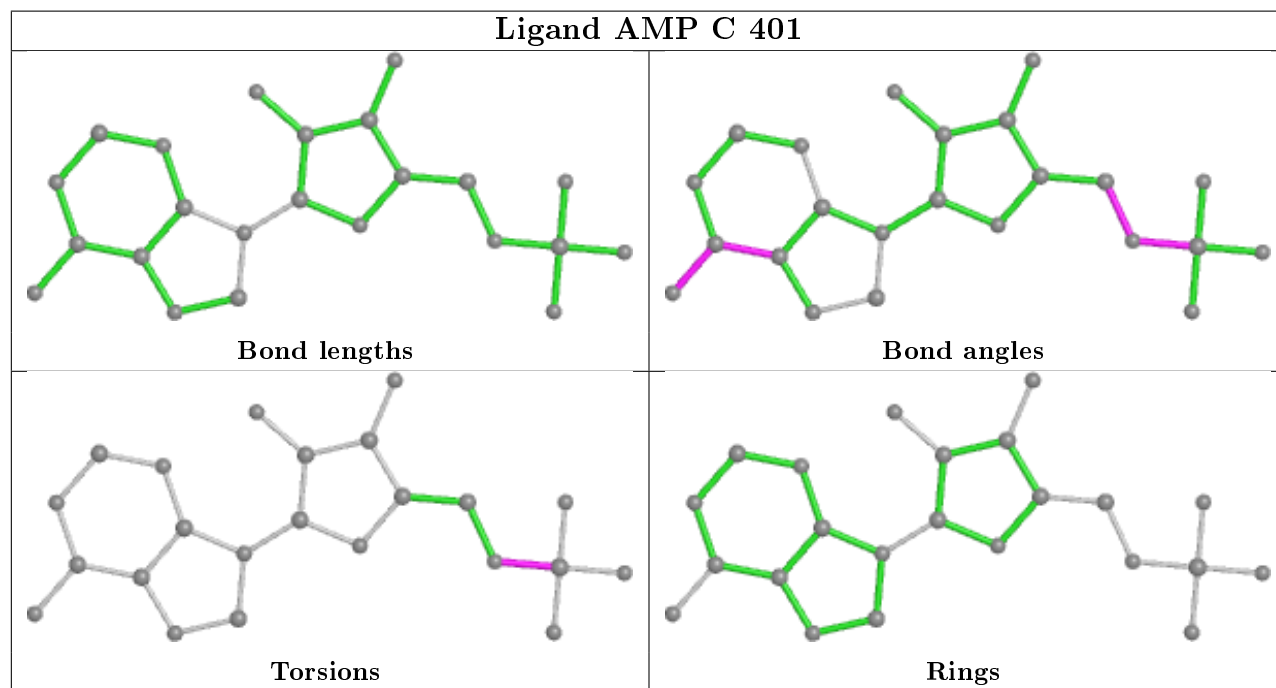
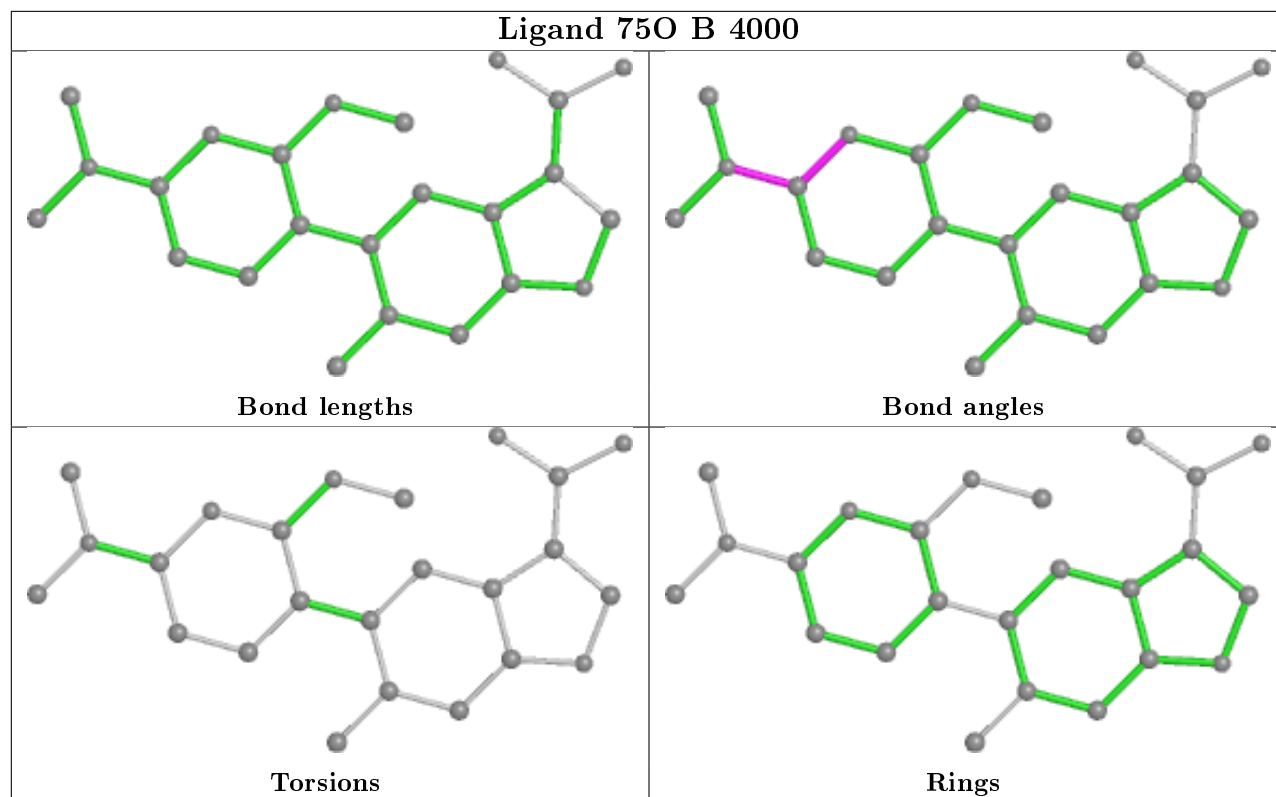
There are no ring outliers.

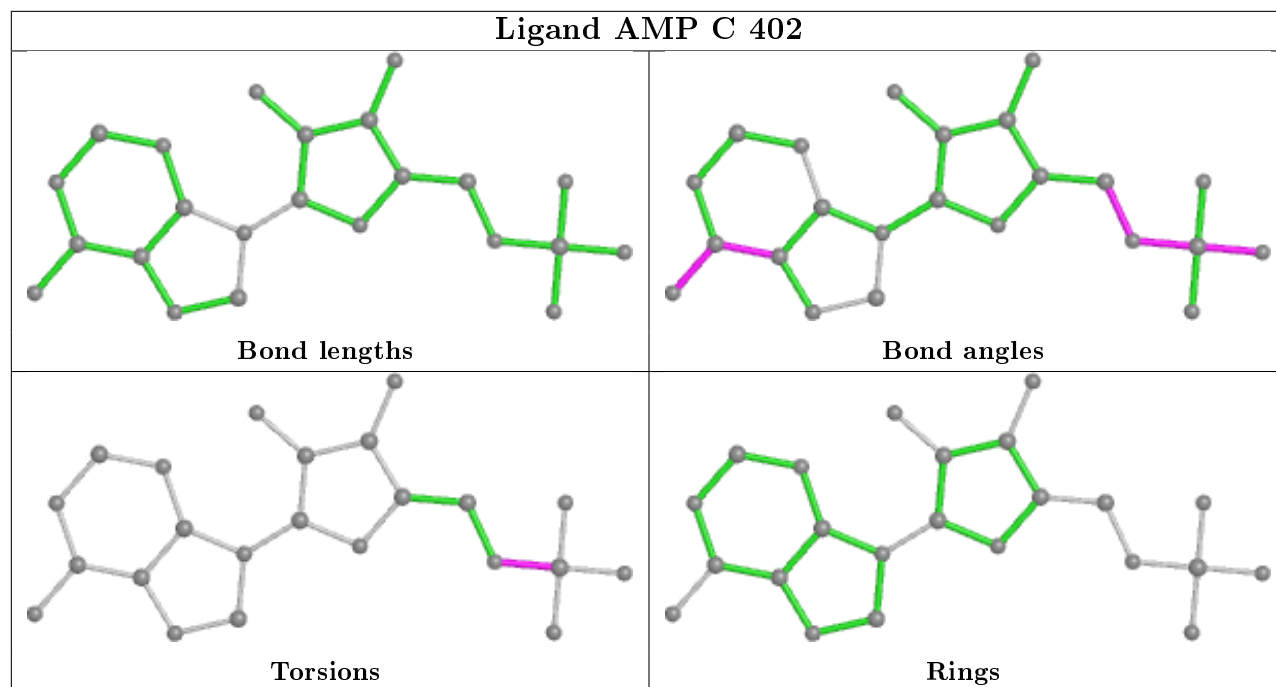
2 monomers are involved in 2 short contacts:

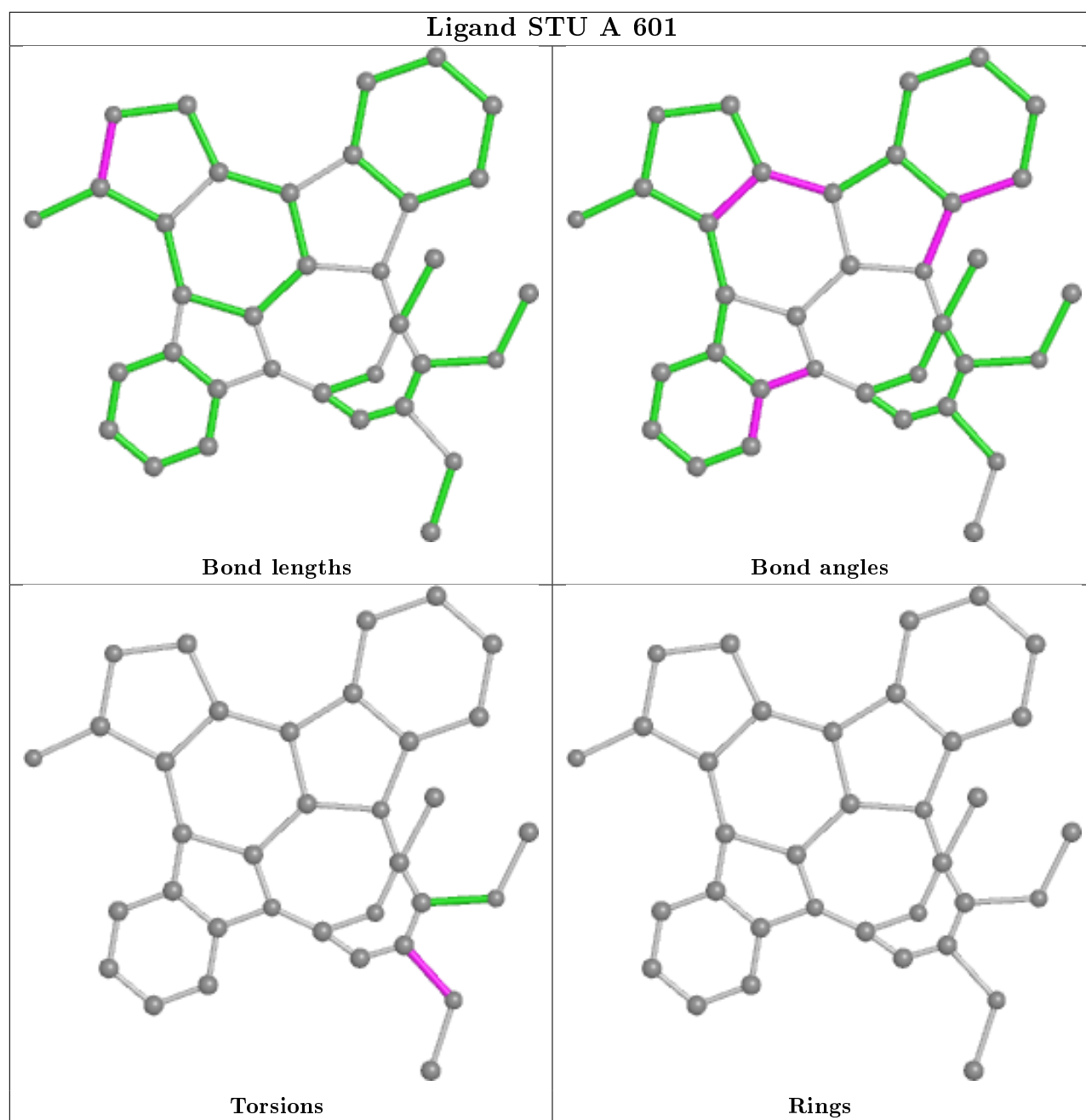
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	402	AMP	1	0
4	A	601	STU	1	0

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	368/503 (73%)	0.12	12 (3%) 46 44	63, 99, 177, 186	0
2	B	163/204 (79%)	0.22	7 (4%) 35 34	88, 121, 161, 197	0
3	C	293/330 (88%)	0.19	9 (3%) 49 47	100, 145, 193, 211	0
All	All	824/1037 (79%)	0.16	28 (3%) 45 43	63, 121, 183, 211	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	ALA	5.5
2	B	223	CYS	4.1
2	B	225	PRO	3.7
1	A	459	TYR	3.4
3	C	183	PRO	3.3
3	C	230	VAL	3.3
1	A	402	SER	3.3
1	A	424	TRP	2.9
1	A	426	VAL	2.9
1	A	56	ASP	2.8
2	B	173	CYS	2.8
2	B	171	GLN	2.7
2	B	224	ASP	2.6
2	B	226	ALA	2.6
3	C	35	HIS	2.6
3	C	185	PRO	2.6
3	C	236	VAL	2.5
1	A	409	ILE	2.5
1	A	404	SER	2.4
1	A	413	VAL	2.3
2	B	169	ASP	2.2
3	C	32	MET	2.2
1	A	427	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	124	SER	2.2
1	A	440	VAL	2.2
3	C	302	VAL	2.0
1	A	422	TYR	2.0
3	C	237	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
1	TPO	A	172	11/12	0.96	0.18	101,104,105,108	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

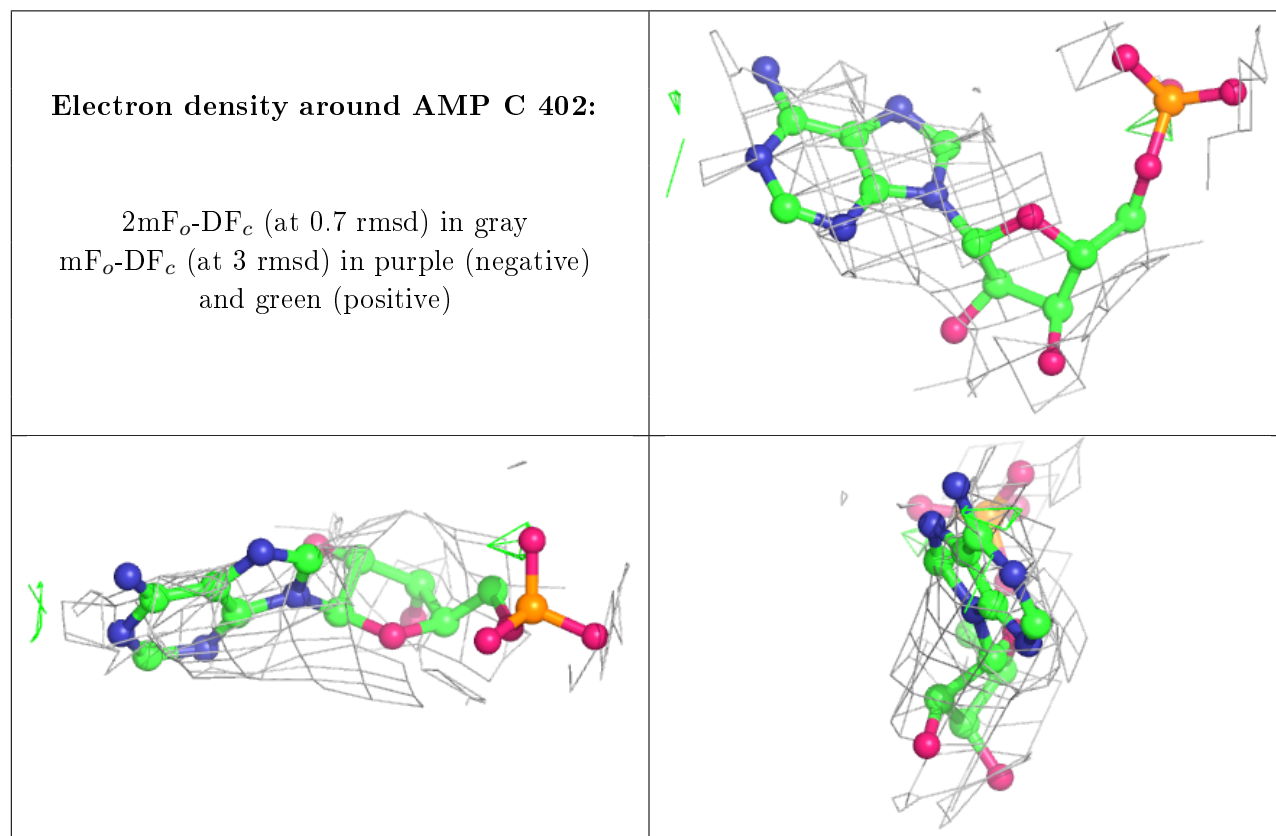
6.4 Ligands [i](#)

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, 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
5	CL	A	602	1/1	0.65	0.20	77,77,77,77	0
8	AMP	C	402	23/23	0.66	0.36	195,203,207,207	0
6	SO4	A	605	5/5	0.70	0.21	210,210,211,211	0
9	ADP	C	403	27/27	0.82	0.29	193,199,206,209	0
8	AMP	C	401	23/23	0.82	0.25	148,156,163,169	0
5	CL	A	604	1/1	0.84	0.38	121,121,121,121	0
6	SO4	C	404	5/5	0.93	0.44	165,166,166,166	0
5	CL	A	603	1/1	0.94	0.25	79,79,79,79	0
7	75O	B	4000	24/24	0.94	0.25	77,85,89,91	0
4	STU	A	601	35/35	0.98	0.27	65,68,71,72	0

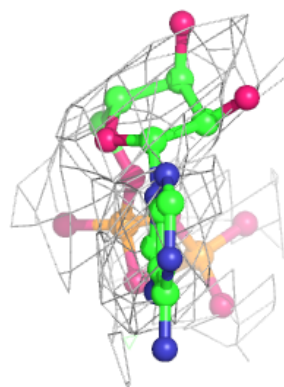
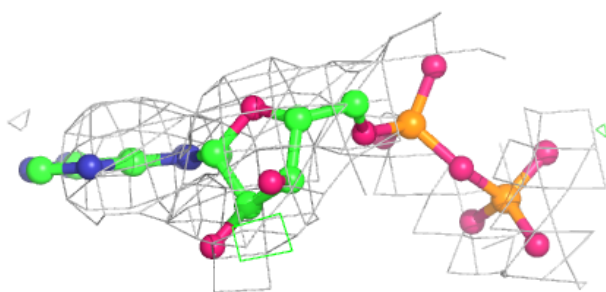
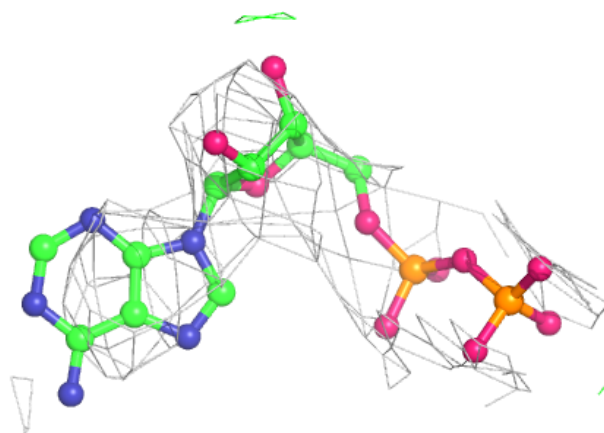
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



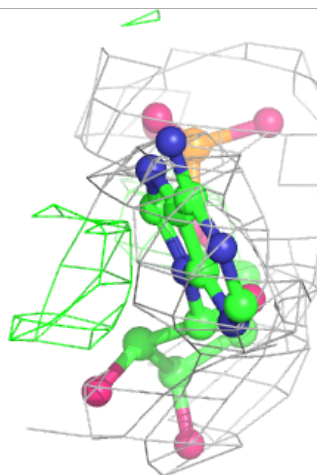
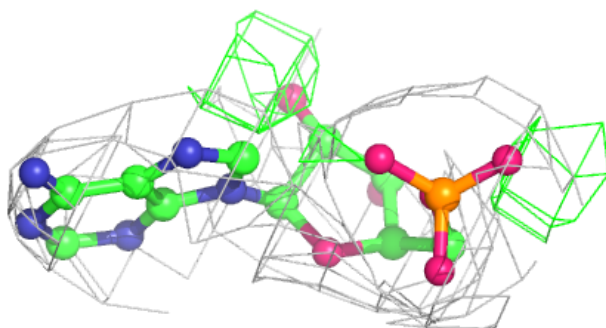
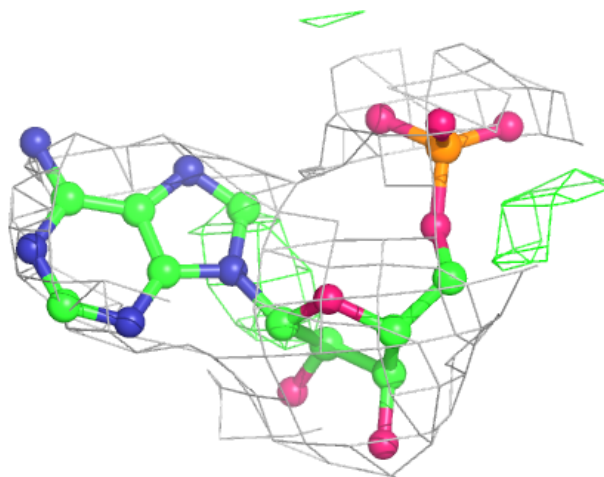
Electron density around ADP C 403:

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



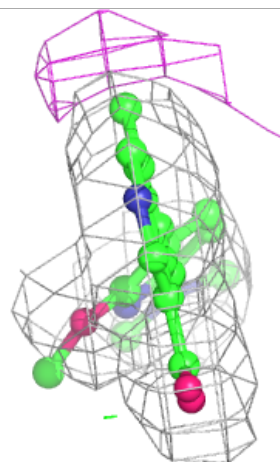
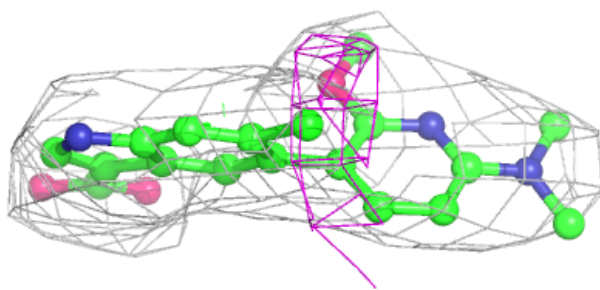
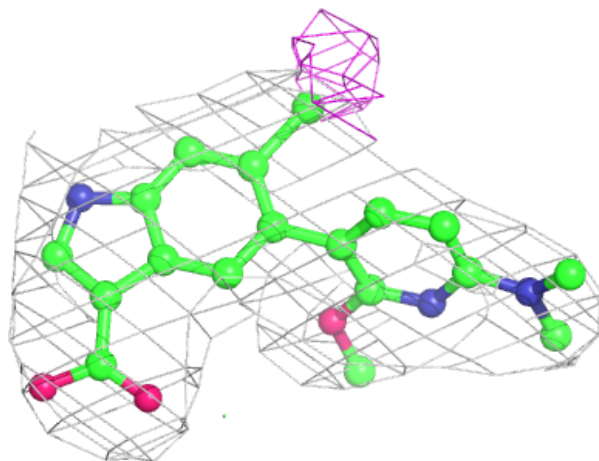
Electron density around AMP C 401:

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



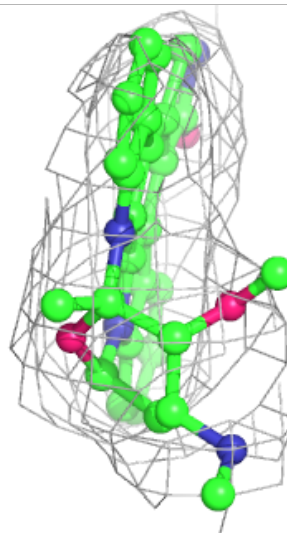
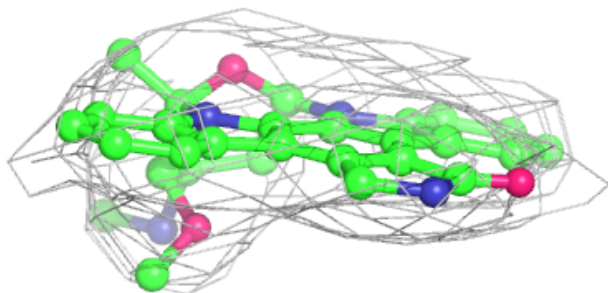
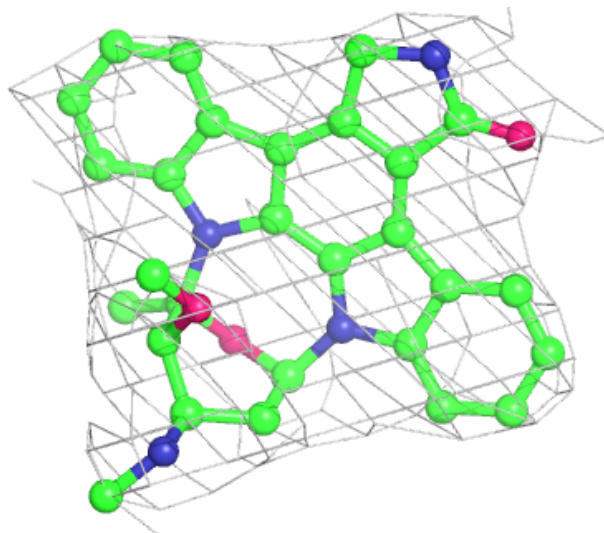
Electron density around 75O B 4000:

$2mF_o-DF_c$ (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.