Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:13 am BST

PDB ID	:	6E4T
Title	:	Structure of AMPK bound to activator
Authors	:	Calabrese, M.F.; Kurumbail, R.G.
Deposited on	:	2018-07-18
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

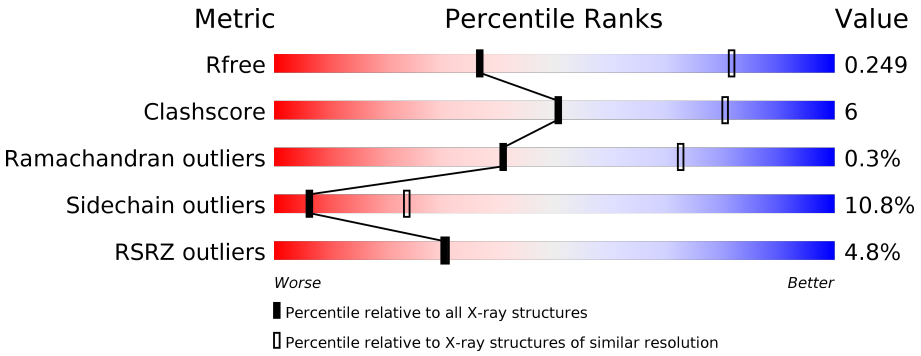
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	503	3% 57% 14% • 28%
2	B	204	2% 59% 17% • 22%
3	C	330	6% 69% 14% • 15%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6369 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	362	Total	C	N	O	P	S	0	0	0
			2880	1848	492	521	1	18			

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
2	B	159	Total	C	N	O	P	S	0	0	0
			1208	783	201	221	1	2			

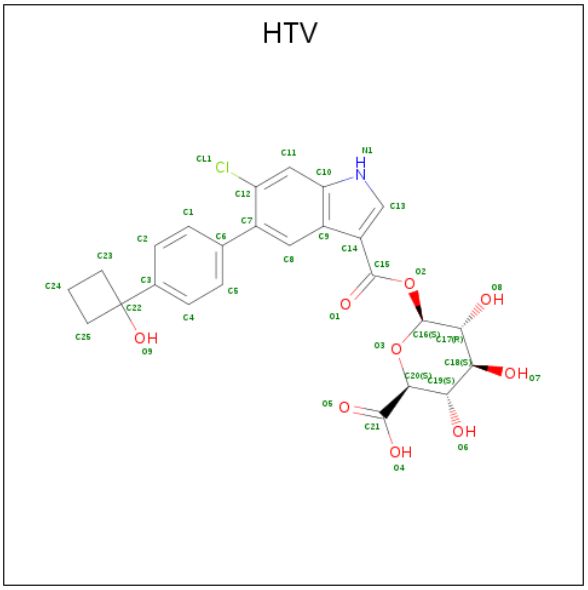
There is a discrepancy between the modelled and reference sequences:

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.

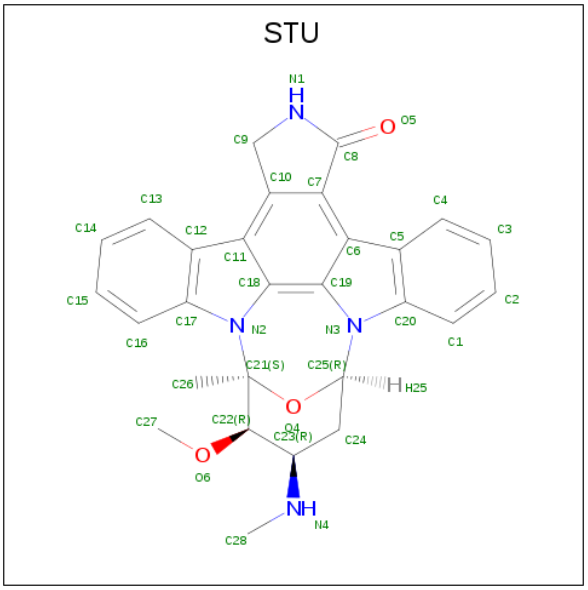
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2127	1379	350	392	6			

- Molecule 4 is 1-O-{6-chloro-5-[4-(1-hydroxycyclobutyl)phenyl]-1H-indole-3-carbonyl}-beta-D-glucopyranuronic acid (three-letter code: HTV) (formula: $C_{25}H_{24}ClNO_9$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			36	25	1	1	9		

- Molecule 5 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).

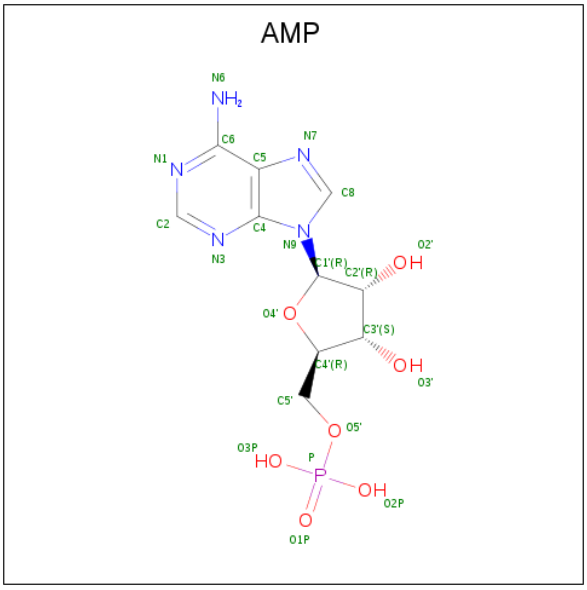


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			35	28	4	3		

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

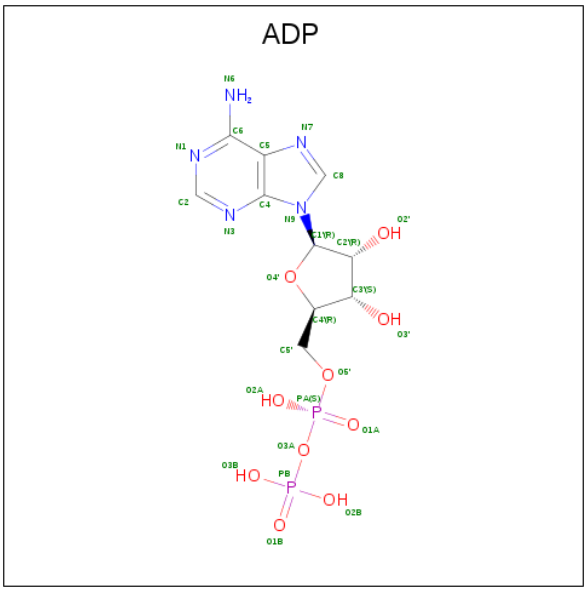
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	4	Total Cl 4 4	0	0

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



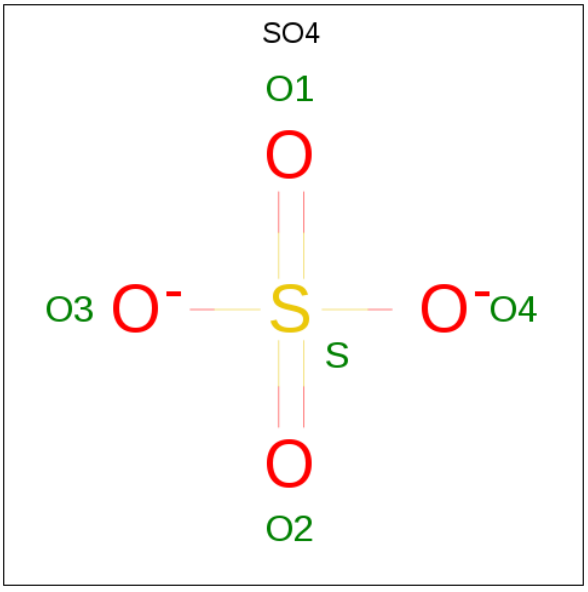
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N O P 23 10 5 7 1	0	0
7	C	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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_4S).



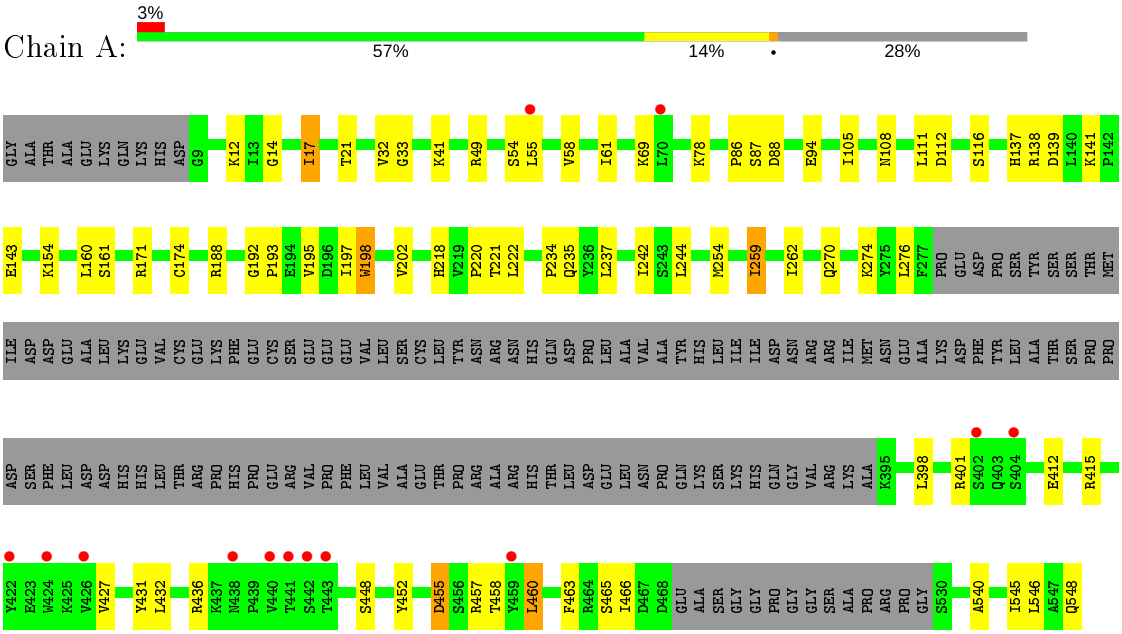
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	O	S		0	0
			5	4	1			

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.

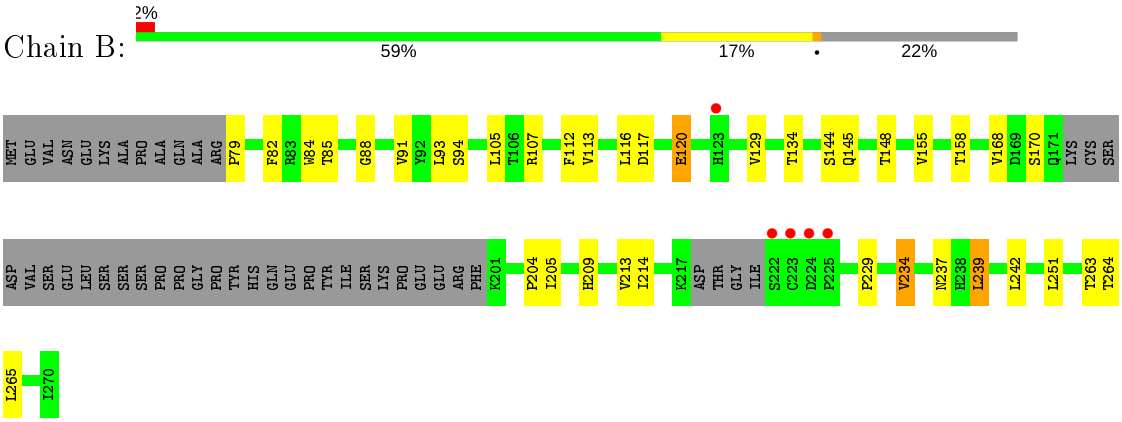
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1

Chain A:



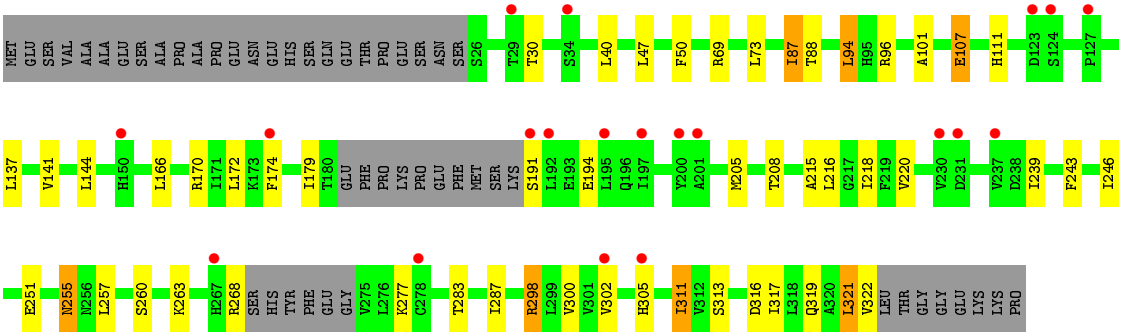
- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

Chain B:



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

Chain C:


MET GLU SER VAL ALA ALA GLU SER ALA PRO ALA PRO GLU ASN GLU HIS SER GLN GLU THR PRO GLU SER ASN SER S26 T29 T30 S34 L40 L47 F50 R69 L73 I87 T88 L94 H95 R96 A101 E107 H111 D123 S124 P127
L137 V141 L144 H150 L166 R170 I171 L172 K173 F174 I179 T180 GLU PHE PRO LYS PRO GLU PHE MET SER LYS S191 L192 E193 E194 L195 Q196 I197 Y200 A201 M205 T208 A215 L216 G217 I218 F219 V220 V230 D231 V237 D238 I239 F243 I246
E251 N255 N256 L257 S260 K263 H267 R268 SER HIS TYR PHE GLU GLY V275 L276 K277 C278 T283 I287 R298 L299 V300 V301 V302 H305 I311 V312 S313 D316 I317 L318 Q319 A320 L321 V322 LEU THR GLY GLY GLU LYS LYS PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.61Å 123.61Å 402.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.01 – 3.40 30.01 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.01-3.40) 99.9 (30.01-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.39Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.216 , 0.245 0.217 , 0.249	Depositor DCC
R_{free} test set	1318 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	88.4	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 101.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6369	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.53	0/2933	0.77	1/3968 (0.0%)
2	B	0.54	0/1231	0.77	0/1689
3	C	0.50	0/2167	0.72	0/2967
All	All	0.52	0/6331	0.75	1/8624 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	GLY	N-CA-C	-5.45	99.48	113.10

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	2880	0	2842	32	0
2	B	1208	0	1142	19	0
3	C	2127	0	2080	19	0
4	A	36	0	0	0	0
5	A	35	0	26	7	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	46	0	24	1	0
8	C	27	0	12	0	0
9	C	5	0	0	0	0
All	All	6369	0	6126	71	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 (71) 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)
5:A:602:STU:H283	5:A:602:STU:H272	1.27	1.08
5:A:602:STU:H261	5:A:602:STU:H16	1.51	0.90
5:A:602:STU:C28	5:A:602:STU:H272	2.02	0.90
5:A:602:STU:H283	5:A:602:STU:C27	2.05	0.85
1:A:218:HIS:HD2	1:A:221:THR:H	1.27	0.82
1:A:455:ASP:HB2	1:A:458:THR:HG22	1.62	0.79
2:B:79:PRO:HA	2:B:117:ASP:HA	1.79	0.65
1:A:160:LEU:HD13	1:A:174:CYS:HB3	1.79	0.64
3:C:40:LEU:HD12	3:C:137:LEU:HD11	1.82	0.62
3:C:260:SER:H	3:C:263:LYS:HD2	1.64	0.61
3:C:40:LEU:HD21	3:C:174:PHE:HB2	1.82	0.61
1:A:401:ARG:O	1:A:548:GLN:HB3	2.02	0.59
1:A:465:SER:HB3	2:B:237:ASN:HB3	1.85	0.58
3:C:243:PHE:O	3:C:246:ILE:HG13	2.03	0.58
1:A:455:ASP:HB3	1:A:457:ARG:H	1.70	0.57
2:B:144:SER:HB3	2:B:148:THR:H	1.70	0.56
1:A:192:GLY:O	1:A:195:VAL:HG22	2.06	0.55
1:A:141:LYS:HG3	1:A:143:GLU:HB2	1.89	0.54
1:A:412:GLU:HG2	1:A:415:ARG:HE	1.72	0.54
3:C:40:LEU:HD22	3:C:170:ARG:HG3	1.88	0.54
5:A:602:STU:H261	5:A:602:STU:C16	2.23	0.54
1:A:234:PRO:HD2	1:A:237:LEU:HD22	1.90	0.54
1:A:237:LEU:HB3	1:A:242:ILE:HD11	1.89	0.53
1:A:78:LYS:H	1:A:94:GLU:HG2	1.73	0.53
1:A:49:ARG:HH21	1:A:86:PRO:HA	1.73	0.53
1:A:448:SER:HB3	1:A:466:ILE:HD11	1.90	0.53
3:C:69:ARG:HG2	3:C:87:ILE:HD11	1.92	0.52
1:A:218:HIS:CD2	1:A:220:PRO:HD2	2.45	0.51
1:A:463:PHE:HB2	2:B:239:LEU:HB3	1.93	0.51
2:B:214:ILE:HB	2:B:229:PRO:HD2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:VAL:HG22	2:B:129:VAL:HG13	1.93	0.50
5:A:602:STU:C16	5:A:602:STU:C26	2.89	0.49
1:A:12:LYS:HG2	1:A:17:ILE:HG22	1.94	0.49
2:B:93:LEU:HB2	2:B:105:LEU:HD21	1.95	0.49
3:C:107:GLU:HG2	3:C:107:GLU:H	1.39	0.48
3:C:317:ILE:O	3:C:321:LEU:HD12	2.13	0.48
1:A:139:ASP:HB2	1:A:160:LEU:HD12	1.93	0.48
1:A:540:ALA:HB2	2:B:251:LEU:HD11	1.96	0.47
3:C:300:VAL:HA	3:C:311:ILE:HG13	1.97	0.47
3:C:298:ARG:HH11	7:C:401:AMP:H8	1.63	0.47
2:B:213:VAL:HG22	2:B:214:ILE:H	1.79	0.47
3:C:298:ARG:HB2	3:C:313:SER:HA	1.96	0.46
3:C:216:LEU:O	3:C:220:VAL:HG23	2.15	0.46
1:A:193:PRO:O	1:A:197:ILE:HG12	2.15	0.46
3:C:101:ALA:HA	3:C:255:ASN:O	2.16	0.46
1:A:198:TRP:O	1:A:202:VAL:HG23	2.16	0.46
3:C:191:SER:HA	3:C:283:THR:HA	1.98	0.46
1:A:218:HIS:CD2	1:A:221:THR:HG23	2.52	0.45
1:A:138:ARG:O	1:A:139:ASP:HB3	2.17	0.45
1:A:188:ARG:HB3	2:B:205:ILE:HD11	1.98	0.45
3:C:137:LEU:O	3:C:141:VAL:HG23	2.17	0.45
2:B:88:GLY:O	2:B:112:PHE:HZ	2.00	0.44
3:C:215:ALA:HA	3:C:218:ILE:HD12	1.99	0.44
3:C:94:LEU:HG	3:C:257:LEU:HD11	1.99	0.44
1:A:137:HIS:HE1	1:A:139:ASP:O	2.01	0.43
3:C:50:PHE:HB2	3:C:73:LEU:HD23	2.01	0.43
2:B:84:TRP:HB3	2:B:112:PHE:HB2	2.00	0.43
2:B:107:ARG:HB2	2:B:112:PHE:CE2	2.53	0.43
1:A:244:LEU:HD11	1:A:262:ILE:HG23	2.01	0.42
1:A:143:GLU:O	5:A:602:STU:H281	2.19	0.42
2:B:82:PHE:O	2:B:113:VAL:HA	2.19	0.42
2:B:145:GLN:H	2:B:145:GLN:CD	2.23	0.41
1:A:398:LEU:HD23	1:A:460:LEU:HD21	2.02	0.41
2:B:107:ARG:HD3	2:B:112:PHE:CZ	2.55	0.41
3:C:141:VAL:HA	3:C:144:LEU:HD12	2.02	0.41
2:B:120:GLU:HA	2:B:155:VAL:HG13	2.02	0.41
2:B:209:HIS:HB3	2:B:234:VAL:HG11	2.02	0.41
1:A:105:ILE:O	1:A:108:ASN:O	2.38	0.41
1:A:259:ILE:HG13	1:A:259:ILE:H	1.64	0.41
1:A:33:GLY:O	1:A:41:LYS:HA	2.22	0.40
1:A:452:TYR:HA	2:B:204:PRO:O	2.21	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	355/503 (71%)	326 (92%)	28 (8%)	1 (0%)	41 72
2	B	152/204 (74%)	138 (91%)	13 (9%)	1 (1%)	22 55
3	C	275/330 (83%)	258 (94%)	17 (6%)	0	100 100
All	All	782/1037 (75%)	722 (92%)	58 (7%)	2 (0%)	41 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	120	GLU
1	A	427	VAL

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	312/448 (70%)	281 (90%)	31 (10%)	8 27
2	B	126/184 (68%)	113 (90%)	13 (10%)	7 26
3	C	226/299 (76%)	198 (88%)	28 (12%)	4 17
All	All	664/931 (71%)	592 (89%)	72 (11%)	6 24

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	21	THR
1	A	32	VAL
1	A	54	SER
1	A	55	LEU
1	A	58	VAL
1	A	61	ILE
1	A	69	LYS
1	A	87	SER
1	A	88	ASP
1	A	111	LEU
1	A	112	ASP
1	A	116	SER
1	A	154	LYS
1	A	161	SER
1	A	171	ARG
1	A	198	TRP
1	A	222	LEU
1	A	235	GLN
1	A	254	MET
1	A	259	ILE
1	A	270	GLN
1	A	274	LYS
1	A	276	LEU
1	A	431	TYR
1	A	432	LEU
1	A	436	ARG
1	A	455	ASP
1	A	460	LEU
1	A	545	ILE
1	A	546	LEU
2	B	85	THR
2	B	94	SER
2	B	116	LEU
2	B	134	THR
2	B	158	THR
2	B	168	VAL
2	B	170	SER
2	B	234	VAL
2	B	239	LEU
2	B	242	LEU
2	B	263	THR
2	B	264	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	265	LEU
3	C	30	THR
3	C	47	LEU
3	C	87	ILE
3	C	88	THR
3	C	94	LEU
3	C	96	ARG
3	C	107	GLU
3	C	111	HIS
3	C	166	LEU
3	C	172	LEU
3	C	179	ILE
3	C	194	GLU
3	C	205	MET
3	C	208	THR
3	C	239	ILE
3	C	251	GLU
3	C	255	ASN
3	C	268	ARG
3	C	277	LYS
3	C	287	ILE
3	C	298	ARG
3	C	302	VAL
3	C	305	HIS
3	C	311	ILE
3	C	316	ASP
3	C	319	GLN
3	C	321	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	428	ASN
1	A	548	GLN
3	C	35	HIS

5.3.3 RNA

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	$\#\|Z\| > 2$
1	TPO	A	172	1	8,10,11	1.56	1 (12%)	10,14,16	2.05	3 (30%)
2	SEP	B	108	2	8,9,10	1.39	1 (12%)	8,12,14	3.96	3 (37%)

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	-	1/9/11/13	-
2	SEP	B	108	2	-	5/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TPO	P-OG1	-4.10	1.51	1.59
2	B	108	SEP	CB-CA	2.13	1.58	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	108	SEP	OG-CB-CA	9.39	117.28	108.14
2	B	108	SEP	O3P-P-OG	4.66	119.13	106.73
1	A	172	TPO	O3P-P-O2P	3.70	121.78	107.64
1	A	172	TPO	P-OG1-CB	-3.24	113.42	123.21
2	B	108	SEP	O3P-P-O2P	-2.94	96.38	107.64
1	A	172	TPO	O3P-P-O1P	-2.75	99.92	110.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	172	TPO	O-C-CA-CB
2	B	108	SEP	N-CA-CB-OG
2	B	108	SEP	CB-OG-P-O2P
2	B	108	SEP	CB-OG-P-O3P
2	B	108	SEP	CA-CB-OG-P
2	B	108	SEP	CB-OG-P-O1P

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 11 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
7	AMP	C	402	-	22,25,25	0.61	0	25,38,38	1.29	2 (8%)
9	SO4	C	404	-	4,4,4	0.16	0	6,6,6	0.16	0
7	AMP	C	401	-	22,25,25	0.63	0	25,38,38	1.40	3 (12%)
5	STU	A	602	-	30,42,42	2.51	10 (33%)	31,68,68	2.43	12 (38%)
8	ADP	C	403	-	24,29,29	0.68	0	29,45,45	0.94	1 (3%)
4	HTV	A	601	-	34,40,40	1.39	7 (20%)	47,61,61	1.72	4 (8%)

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	401	-	-	1/6/26/26	0/3/3/3
7	AMP	C	402	-	-	3/6/26/26	0/3/3/3
5	STU	A	602	-	-	1/4/42/42	-
8	ADP	C	403	-	-	3/12/32/32	0/3/3/3
4	HTV	A	601	-	-	0/18/50/50	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	STU	C9-C10	-5.99	1.45	1.50
5	A	602	STU	C5-C20	4.60	1.49	1.41
5	A	602	STU	C12-C17	4.50	1.48	1.41
5	A	602	STU	C10-C11	4.35	1.49	1.42
5	A	602	STU	C11-C18	4.25	1.48	1.42
4	A	601	HTV	C14-C15	-3.98	1.42	1.50
5	A	602	STU	C9-N1	3.82	1.49	1.45
5	A	602	STU	C7-C6	3.60	1.49	1.43
5	A	602	STU	C6-C19	3.22	1.46	1.42
5	A	602	STU	C19-C18	3.12	1.49	1.42
5	A	602	STU	O5-C8	2.74	1.28	1.23
4	A	601	HTV	C4-C3	2.65	1.43	1.39
4	A	601	HTV	C12-CL1	-2.58	1.67	1.73
4	A	601	HTV	C7-C12	2.44	1.44	1.39
4	A	601	HTV	C14-C9	-2.32	1.40	1.42
4	A	601	HTV	C11-C10	-2.24	1.38	1.41
4	A	601	HTV	O2-C15	2.05	1.38	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	HTV	C11-C12-C7	6.40	126.44	121.92
4	A	601	HTV	C11-C12-CL1	-6.10	113.14	119.20
5	A	602	STU	C7-C8-N1	5.44	111.88	106.37
7	C	402	AMP	P-O5'-C5'	5.39	133.15	118.30
4	A	601	HTV	C12-C11-C10	-5.09	114.74	119.70
5	A	602	STU	C9-N1-C8	-5.00	109.05	113.85
5	A	602	STU	O5-C8-C7	-4.46	124.02	129.32
5	A	602	STU	C7-C10-C11	-4.32	116.60	122.42
7	C	401	AMP	O2P-P-O5'	4.05	117.50	106.73
7	C	401	AMP	P-O5'-C5'	3.62	128.25	118.30
5	A	602	STU	C4-C5-C20	3.30	123.56	119.39
5	A	602	STU	C16-C17-N2	3.28	136.25	132.29
5	A	602	STU	C10-C9-N1	3.01	104.82	101.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	602	STU	C1-C20-C5	-2.75	116.77	120.73
5	A	602	STU	C13-C12-C17	2.67	122.77	119.39
4	A	601	HTV	C8-C9-C10	2.63	121.85	118.26
5	A	602	STU	C3-C4-C5	-2.58	116.53	120.86
5	A	602	STU	C14-C13-C12	-2.49	116.68	120.86
5	A	602	STU	C26-C21-C22	-2.35	108.07	112.64
7	C	401	AMP	C5-C6-N6	2.31	123.87	120.35
7	C	402	AMP	C5-C6-N6	2.23	123.74	120.35
8	C	403	ADP	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

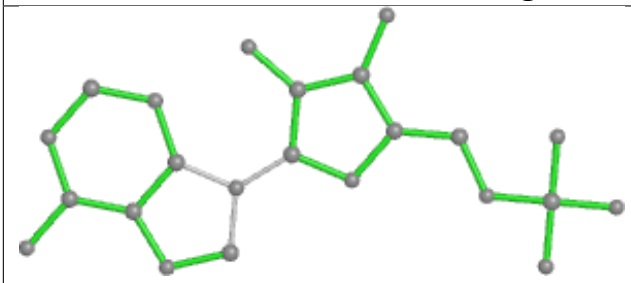
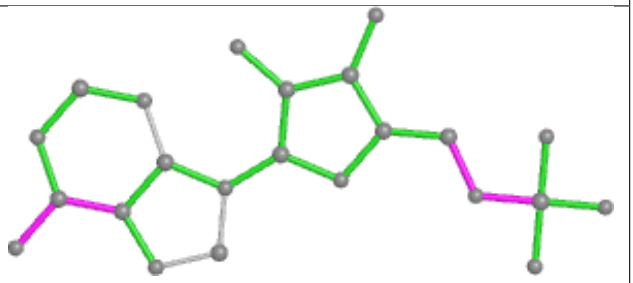
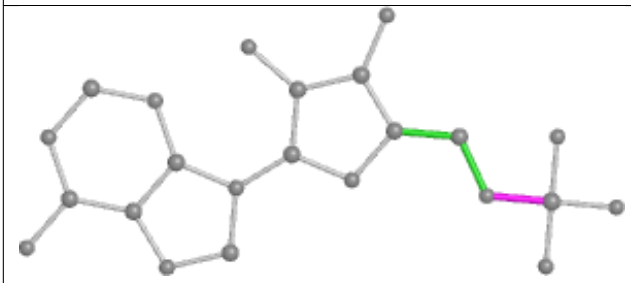
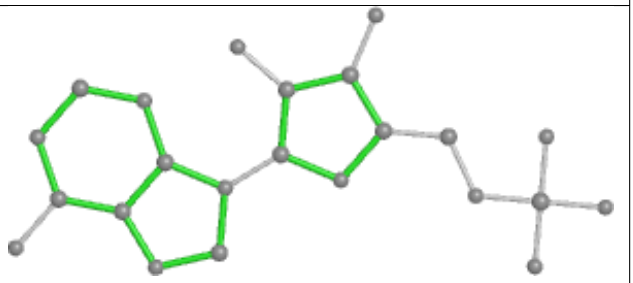
Mol	Chain	Res	Type	Atoms
7	C	402	AMP	C5'-O5'-P-O2P
7	C	402	AMP	C5'-O5'-P-O3P
5	A	602	STU	C22-C23-N4-C28
8	C	403	ADP	C5'-O5'-PA-O1A
8	C	403	ADP	C5'-O5'-PA-O2A
7	C	402	AMP	C5'-O5'-P-O1P
7	C	401	AMP	C5'-O5'-P-O2P
8	C	403	ADP	C5'-O5'-PA-O3A

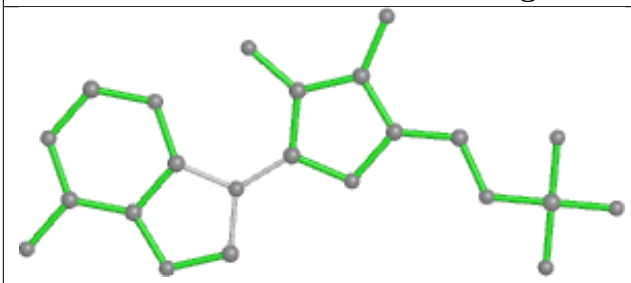
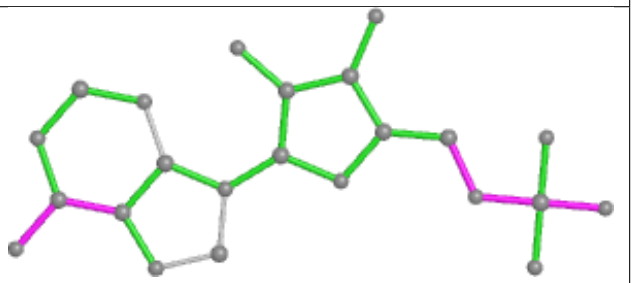
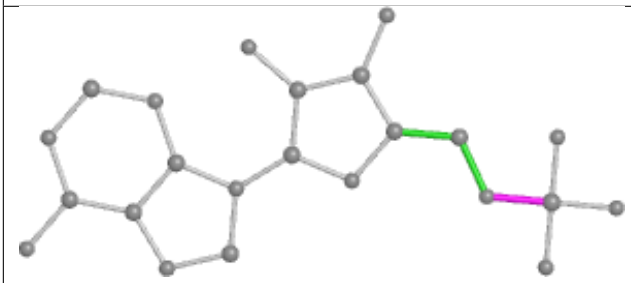
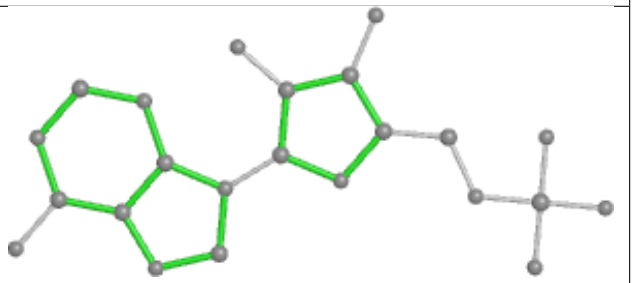
There are no ring outliers.

2 monomers are involved in 8 short contacts:

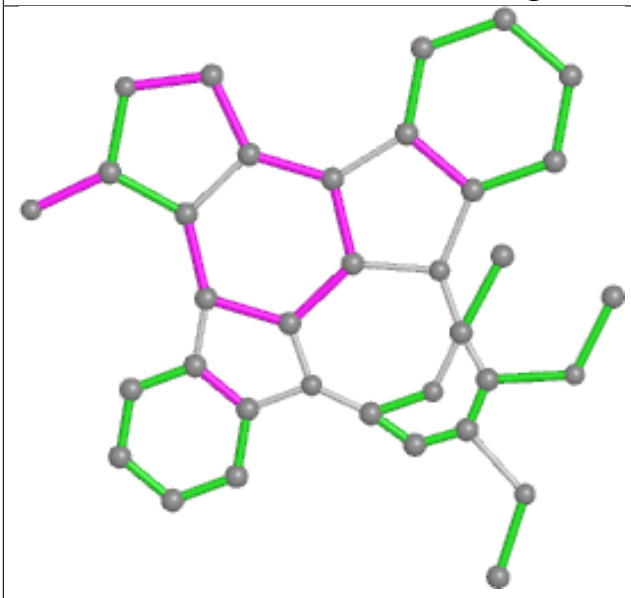
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	AMP	1	0
5	A	602	STU	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

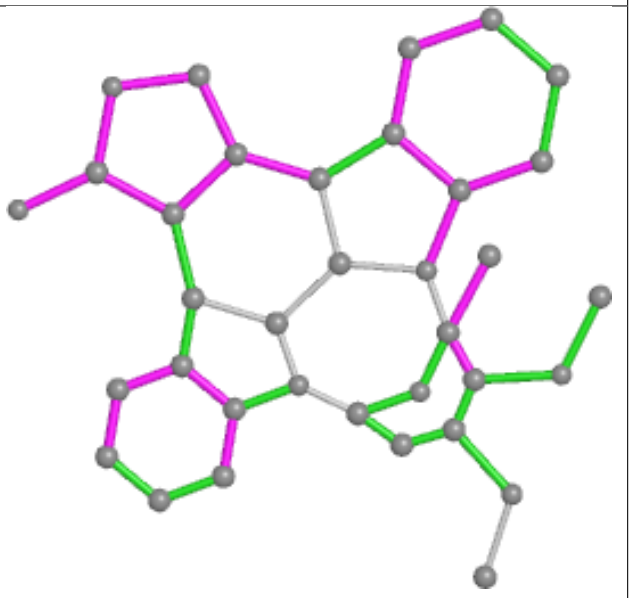
Ligand AMP C 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

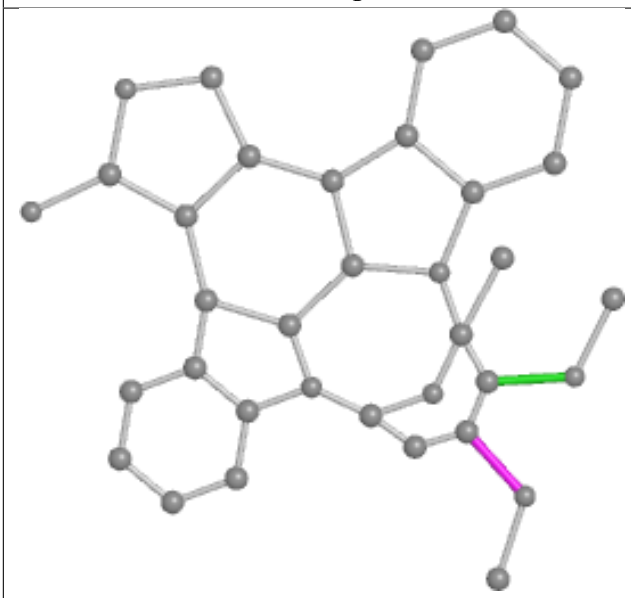
Ligand STU A 602



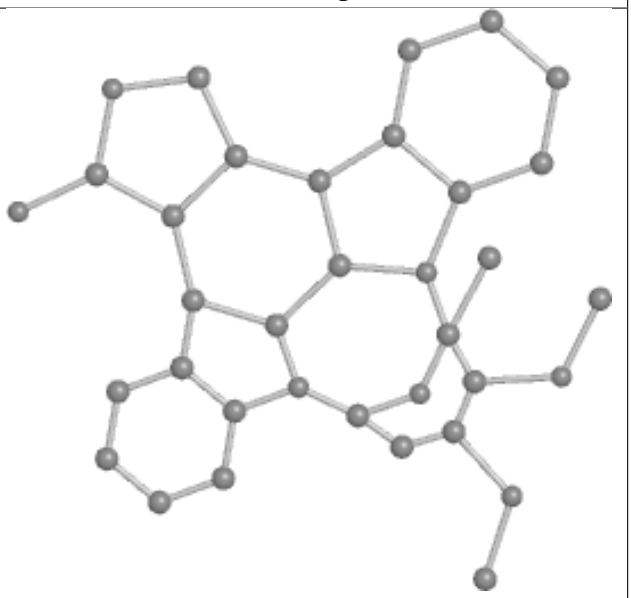
Bond lengths



Bond angles

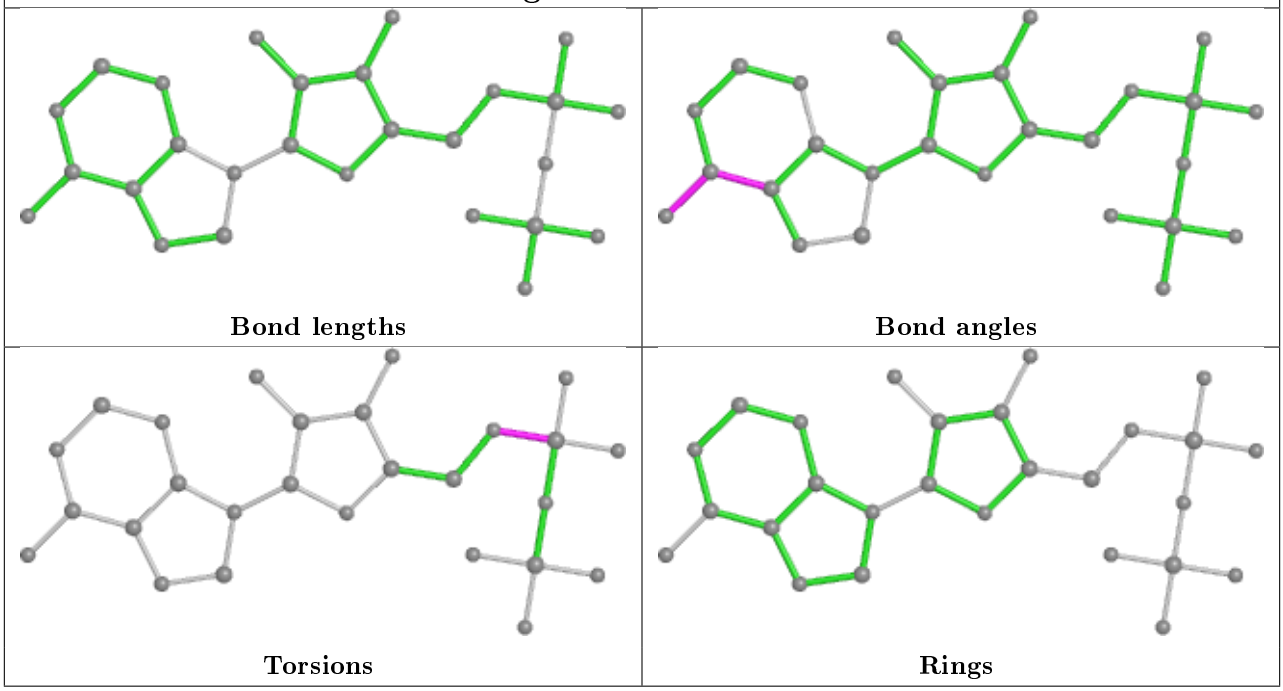


Torsions

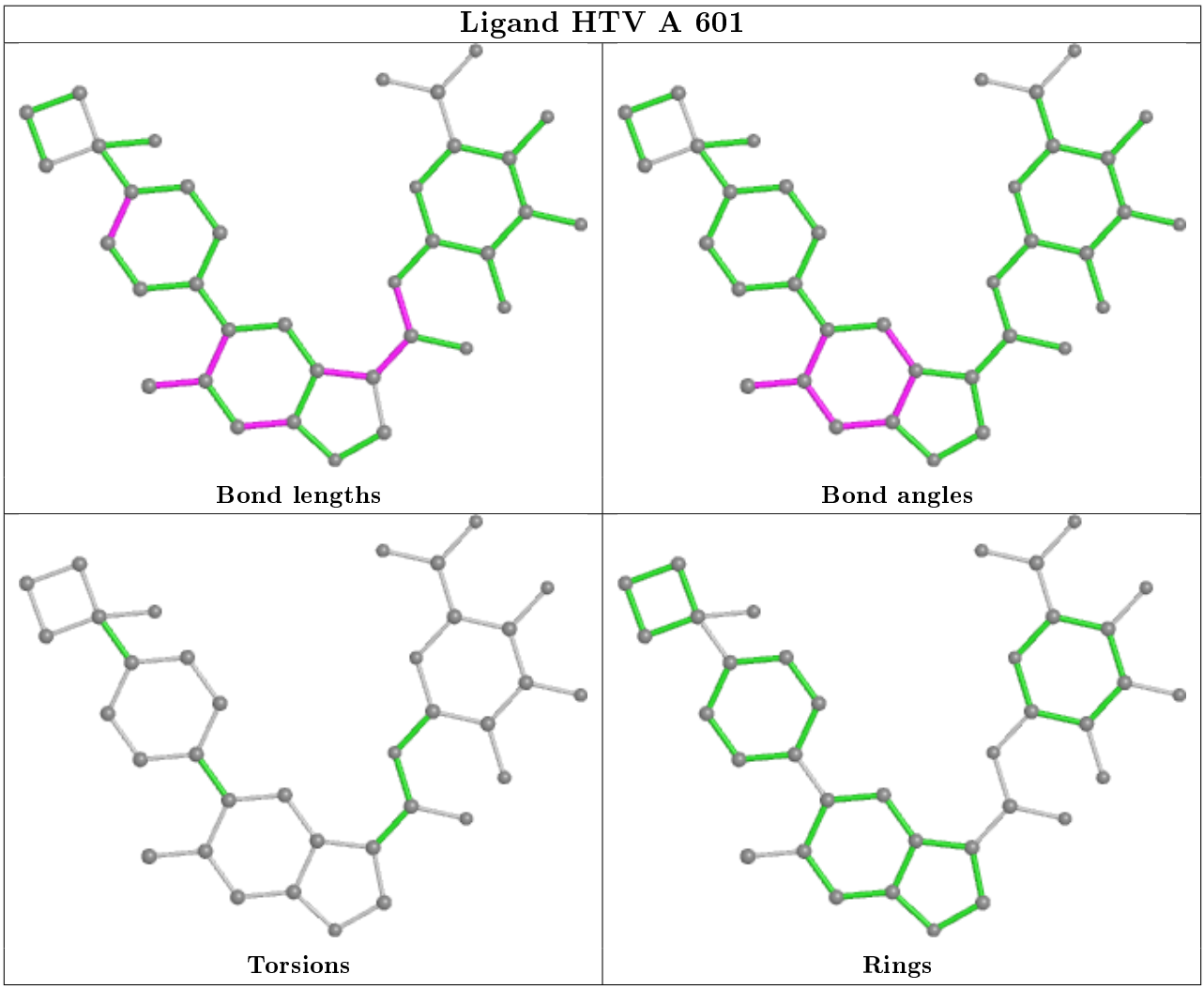


Rings

Ligand ADP C 403



Ligand HTV A 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	361/503 (71%)	-0.05	13 (3%)	42	42	56, 89, 174, 196	0
2	B	158/204 (77%)	0.13	5 (3%)	47	46	71, 103, 140, 162	0
3	C	281/330 (85%)	0.25	20 (7%)	16	18	83, 139, 188, 205	0
All	All	800/1037 (77%)	0.09	38 (4%)	30	31	56, 107, 181, 205	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	222	SER	5.8
3	C	201	ALA	4.2
1	A	441	THR	4.1
2	B	223	CYS	3.6
3	C	230	VAL	3.6
3	C	127	PRO	3.5
1	A	422	TYR	3.5
3	C	197	ILE	3.2
1	A	55	LEU	3.2
3	C	123	ASP	3.1
1	A	459	TYR	3.0
3	C	174	PHE	3.0
3	C	195	LEU	3.0
1	A	440	VAL	3.0
3	C	200	TYR	2.9
1	A	442	SER	2.8
1	A	426	VAL	2.8
3	C	191	SER	2.8
2	B	225	PRO	2.7
3	C	267	HIS	2.7
1	A	443	THR	2.6
3	C	29	THR	2.6
3	C	305	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	34	SER	2.4
3	C	192	LEU	2.4
2	B	224	ASP	2.3
1	A	424	TRP	2.3
1	A	402	SER	2.3
3	C	150	HIS	2.3
2	B	123	HIS	2.3
3	C	302	VAL	2.3
3	C	237	VAL	2.2
1	A	70	LEU	2.2
1	A	438	ASN	2.2
1	A	404	SER	2.1
3	C	231	ASP	2.1
3	C	124	SER	2.1
3	C	278	CYS	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^{th} 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	0.93	0.13	98,105,107,109	0
1	TPO	A	172	11/12	0.96	0.13	91,92,98,101	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^{th} 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	0.49	0.15	117,117,117,117	0

Continued on next page...

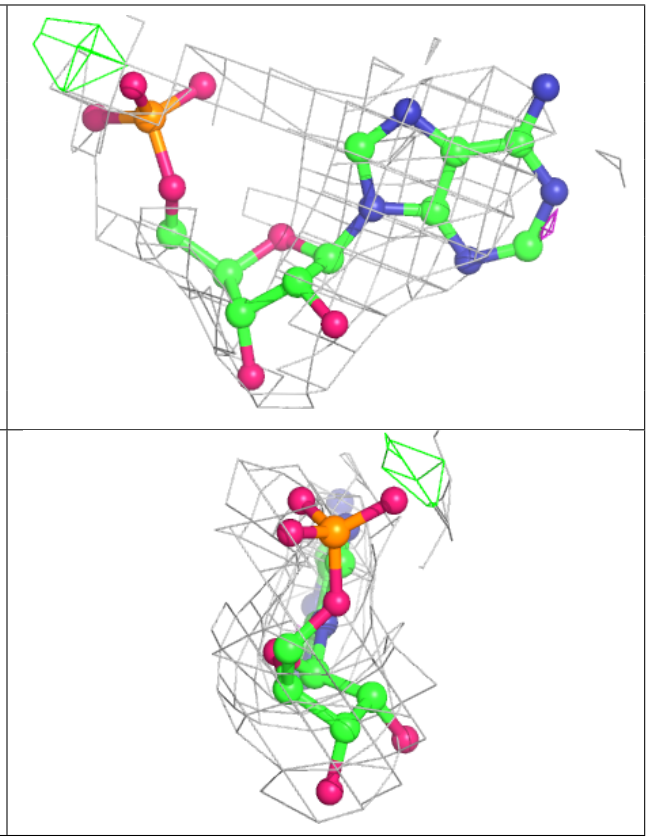
Continued from previous page...

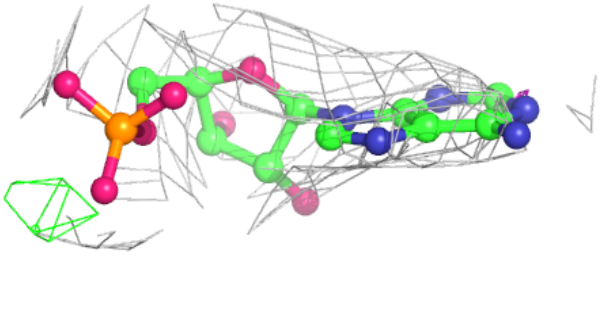
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	AMP	C	401	23/23	0.76	0.30	159,172,185,187	0
8	ADP	C	403	27/27	0.81	0.31	183,193,200,202	0
6	CL	B	301	1/1	0.82	0.32	97,97,97,97	0
7	AMP	C	402	23/23	0.86	0.29	148,165,171,176	0
4	HTV	A	601	36/36	0.90	0.25	82,96,144,145	0
6	CL	A	603	1/1	0.91	0.17	65,65,65,65	0
6	CL	A	605	1/1	0.92	0.18	85,85,85,85	0
9	SO4	C	404	5/5	0.94	0.38	154,155,156,156	0
5	STU	A	602	35/35	0.96	0.22	63,68,72,75	0
6	CL	A	604	1/1	0.98	0.19	57,57,57,57	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 401:

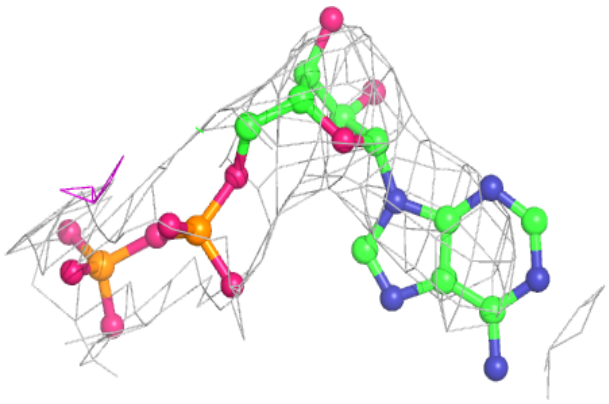
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

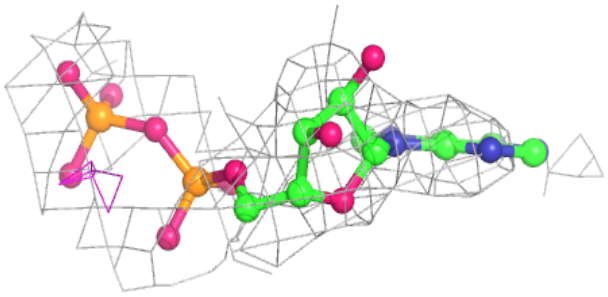


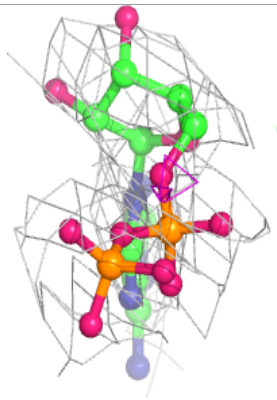


Electron density around ADP C 403:

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

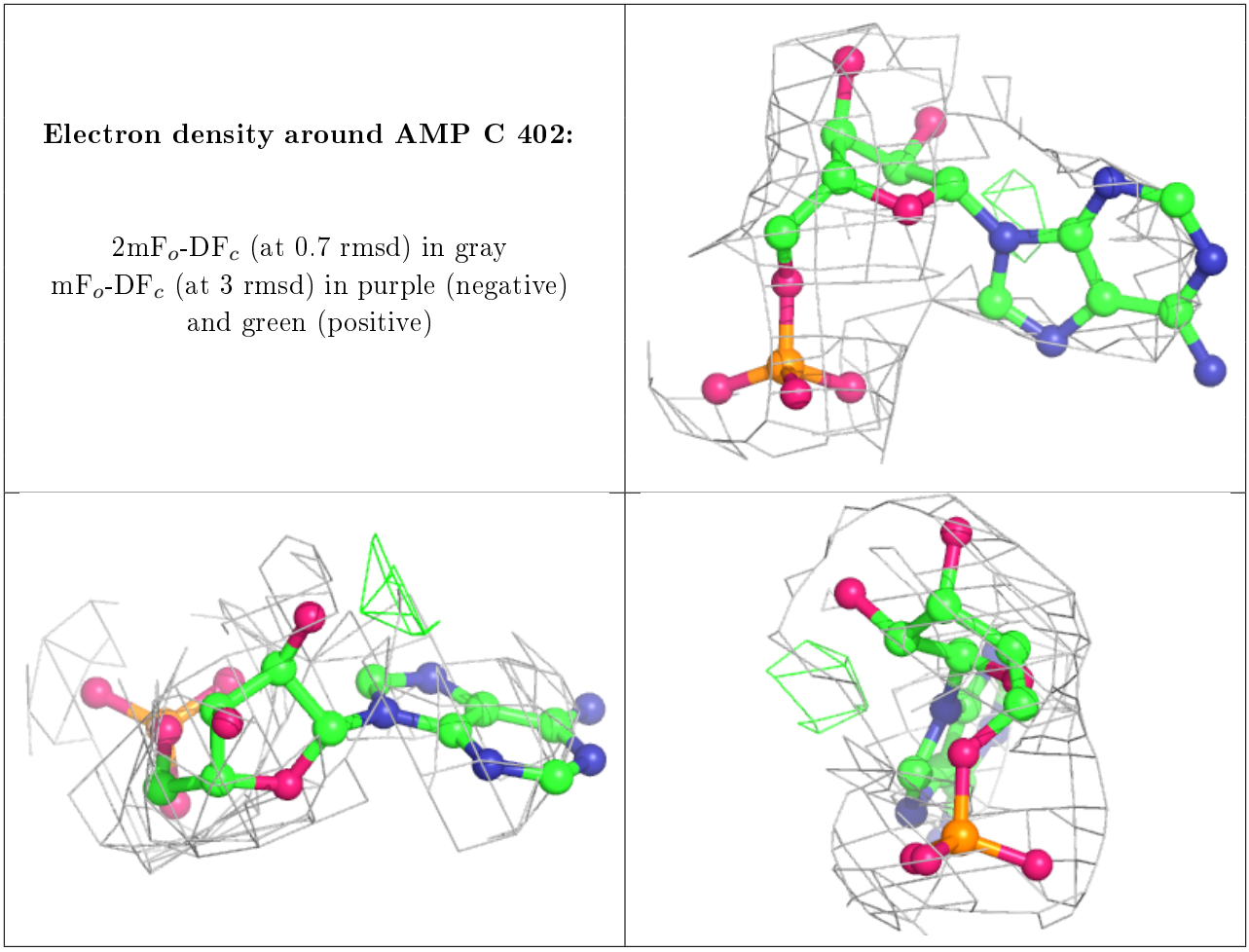






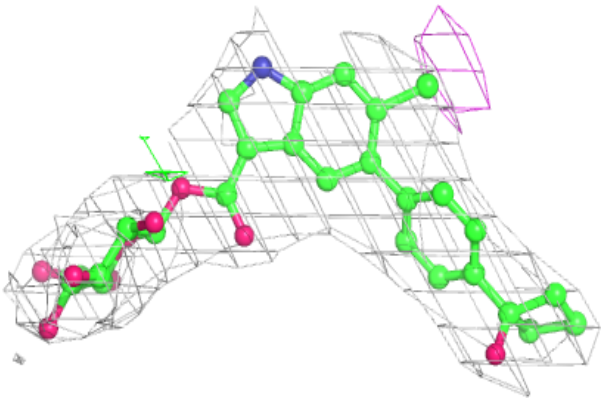
Electron density around AMP C 402:

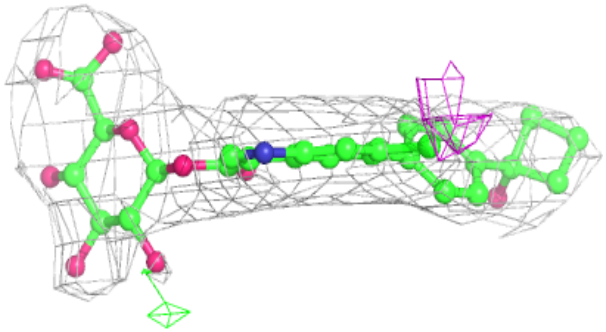
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

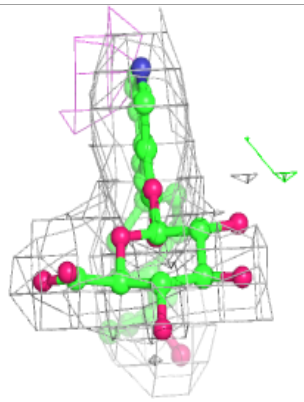


Electron density around HTV A 601:

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

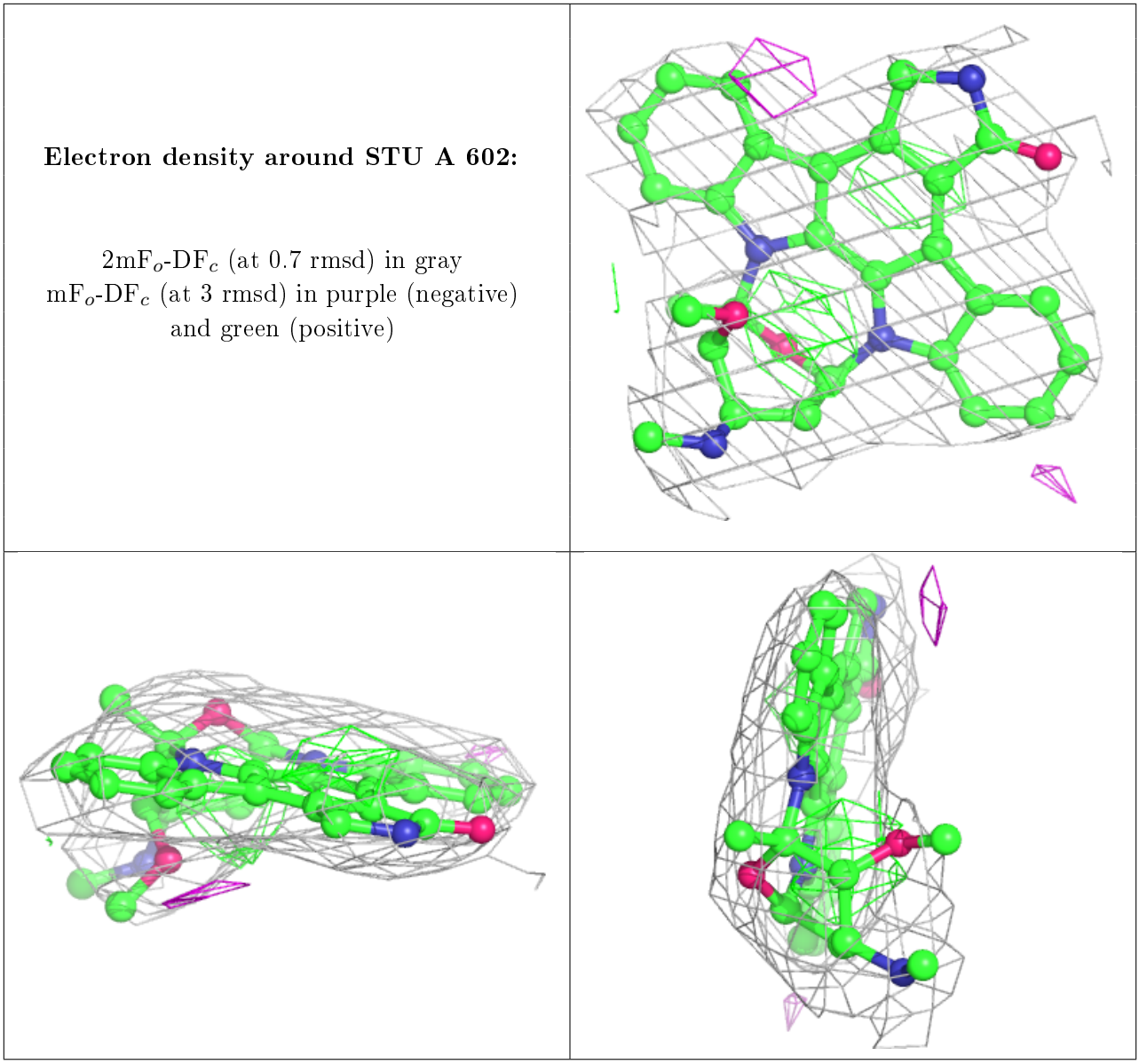






Electron density around STU A 602:

$2mF_o$-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

There are no such residues in this entry.